



Full wwPDB EM Validation Report ⓘ

Dec 16, 2024 – 04:31 PM EST

PDB ID : 7UA1
EMDB ID : EMD-26412
Title : Structure of PKA phosphorylated human RyR2-R2474S in the closed state in the presence of ARM210
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2022-03-11
Resolution : 2.99 Å(reported)
Based on initial model : 7U9X

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

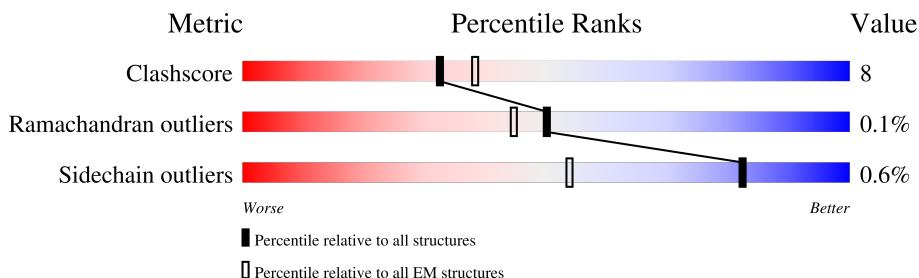
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4967	<div> <div>6%</div> <div>67%</div> <div>18%</div> <div>15%</div> </div>
1	B	4967	<div> <div>6%</div> <div>67%</div> <div>18%</div> <div>15%</div> </div>
1	C	4967	<div> <div>6%</div> <div>67%</div> <div>18%</div> <div>15%</div> </div>
1	D	4967	<div> <div>6%</div> <div>67%</div> <div>18%</div> <div>15%</div> </div>
2	E	108	<div> <div>78%</div> <div>21%</div> <div>.</div> </div>
2	F	108	<div> <div>78%</div> <div>21%</div> <div>.</div> </div>
2	G	108	<div> <div>78%</div> <div>21%</div> <div>.</div> </div>
2	H	108	<div> <div>78%</div> <div>21%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ATP	A	5003	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 138680 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4224	Total	C	N	O	S	2	0
			33766	21513	5742	6281	230		
1	B	4224	Total	C	N	O	S	2	0
			33766	21513	5742	6281	230		
1	C	4224	Total	C	N	O	S	2	0
			33766	21513	5742	6281	230		
1	D	4224	Total	C	N	O	S	2	0
			33766	21513	5742	6281	230		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2474	SER	ARG	variant	UNP Q92736
B	2474	SER	ARG	variant	UNP Q92736
C	2474	SER	ARG	variant	UNP Q92736
D	2474	SER	ARG	variant	UNP Q92736

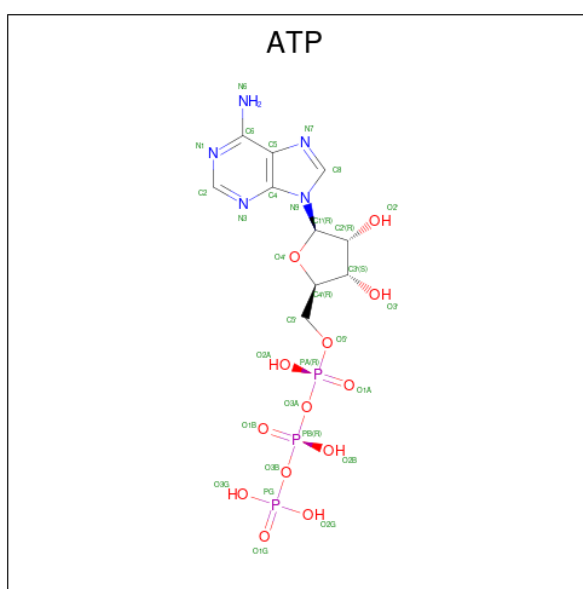
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	G	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	

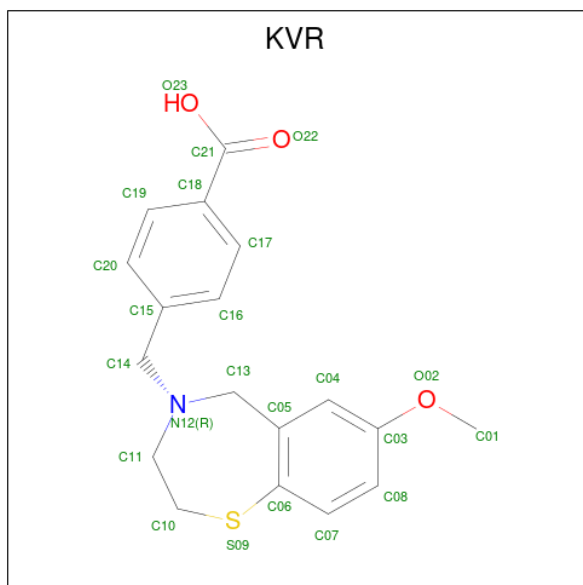
- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					AltConf
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is 4-[(7-methoxy-2,3-dihydro-1,4-benzothiazepin-4(5H)-yl)methyl]benzoic acid (three-letter code: KVR) (formula: C₁₈H₁₉NO₃S).

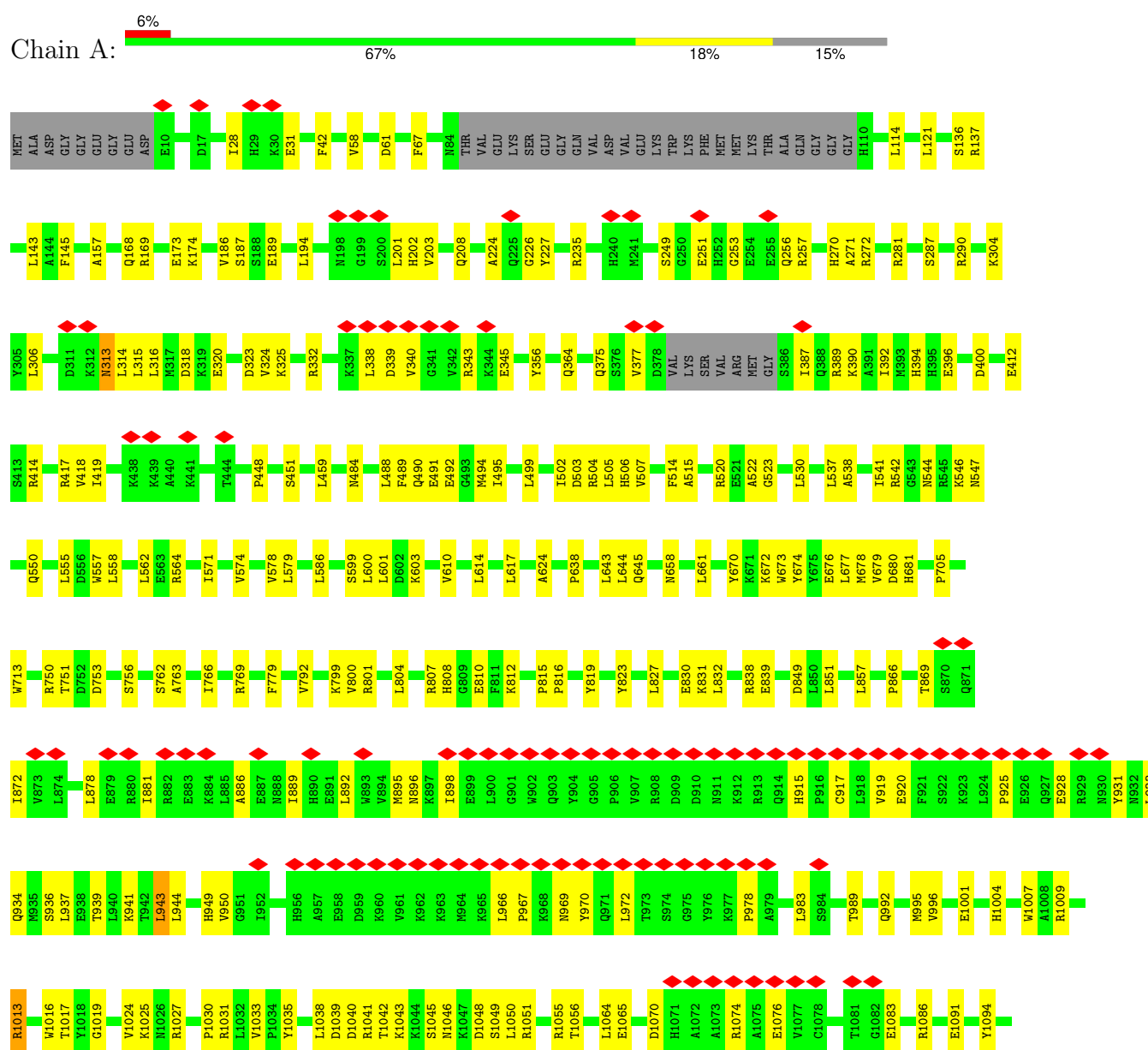


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	S	0
			23	18	1	3	1	
5	B	1	Total	C	N	O	S	0
			23	18	1	3	1	
5	C	1	Total	C	N	O	S	0
			23	18	1	3	1	
5	D	1	Total	C	N	O	S	0
			23	18	1	3	1	

3 Residue-property plots

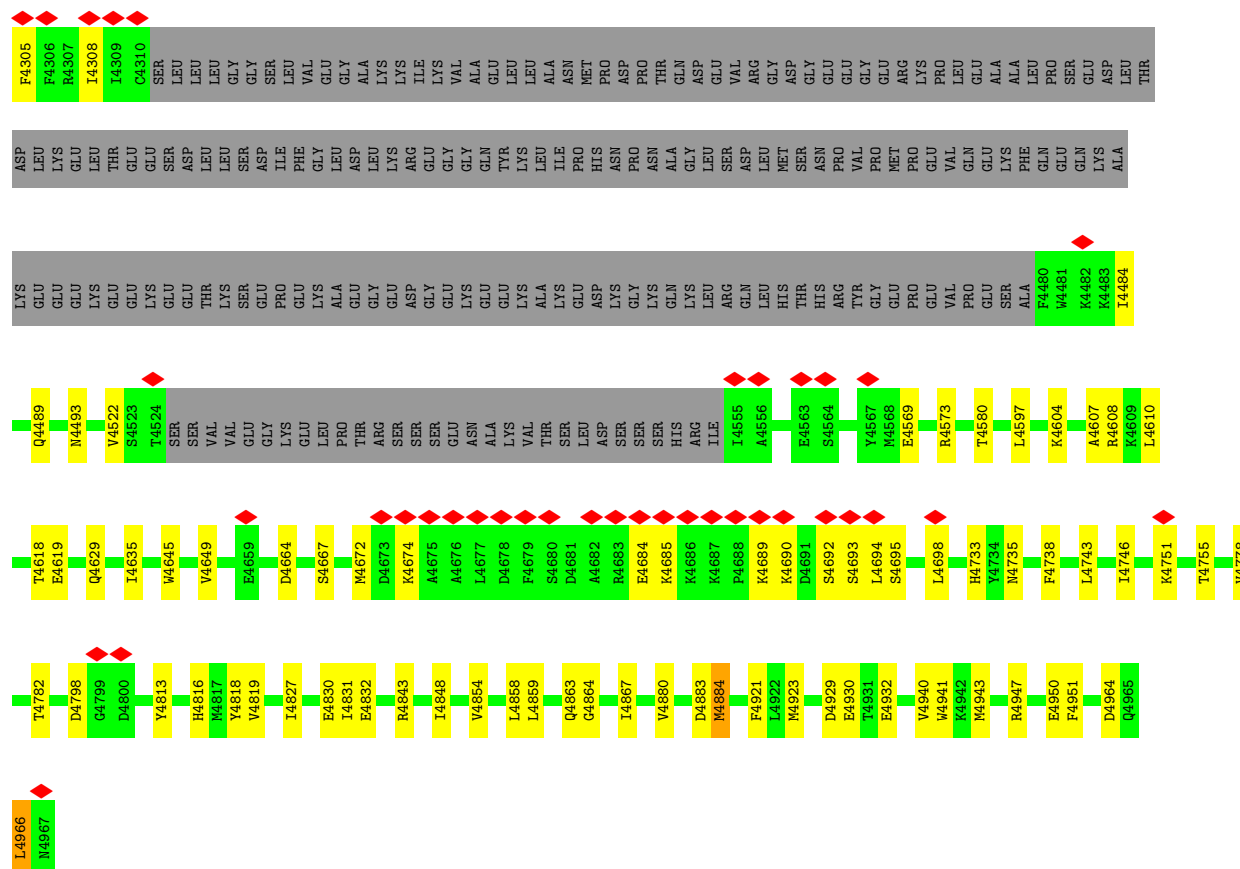
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Ryanodine receptor 2

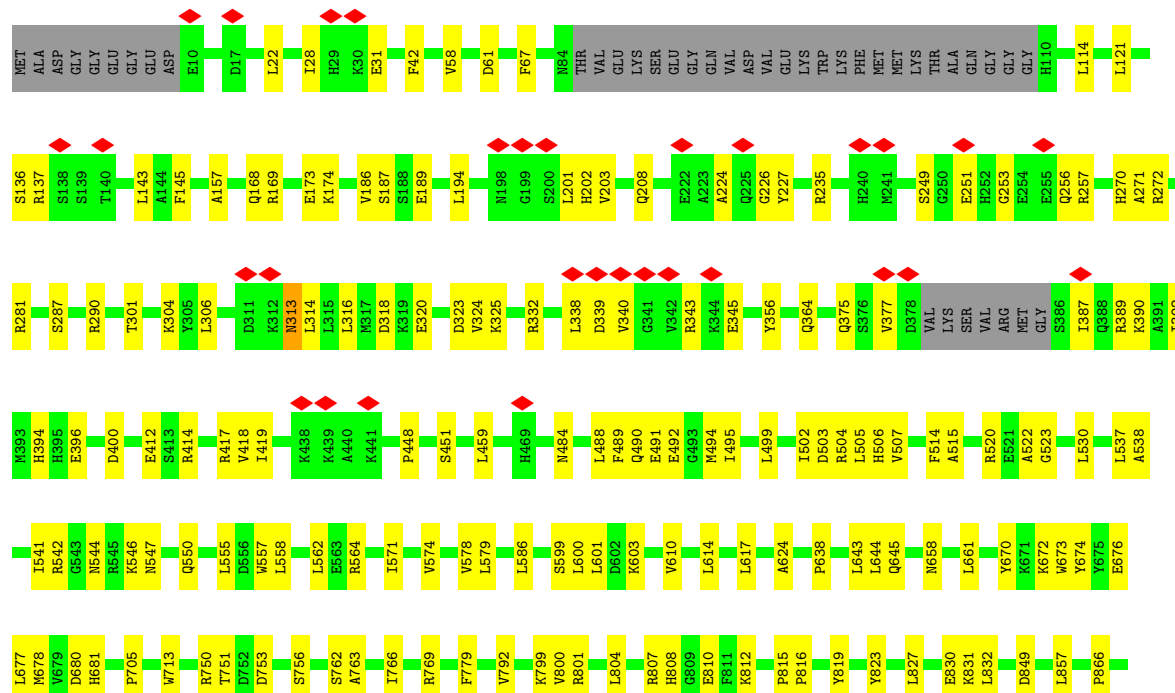






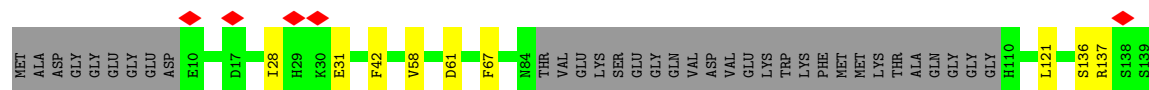


• Molecule 1: Ryanodine receptor 2







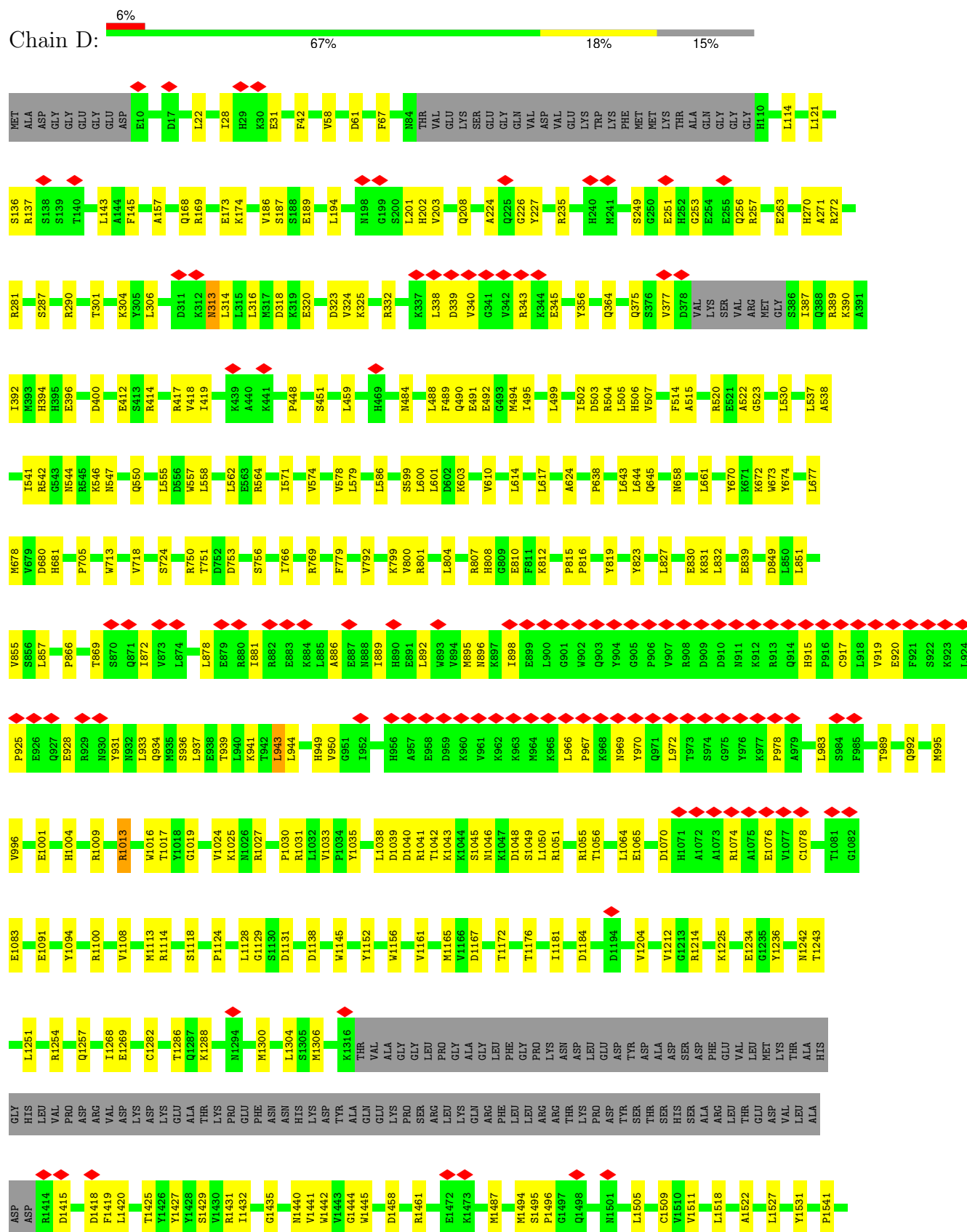






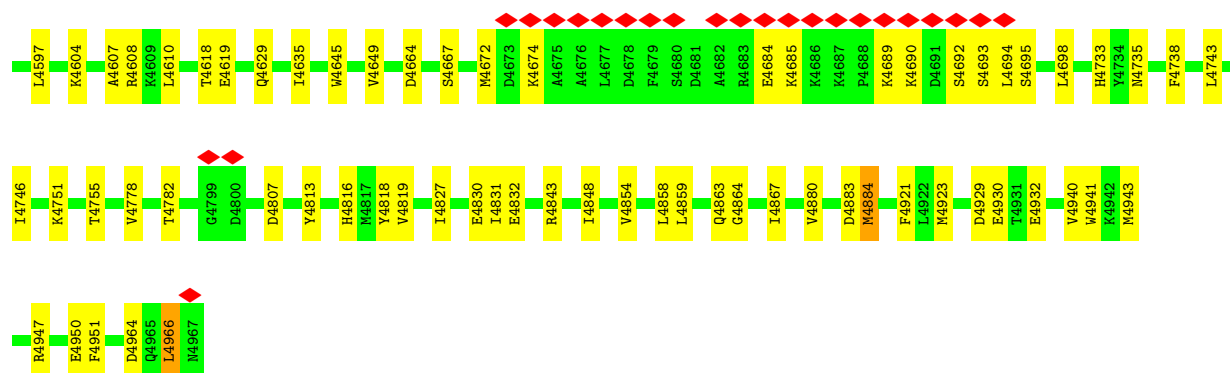


● Molecule 1: Ryanodine receptor 2





[illegible]



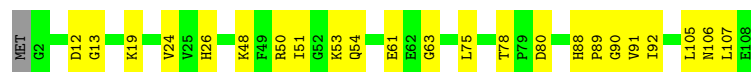
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 78% 21%



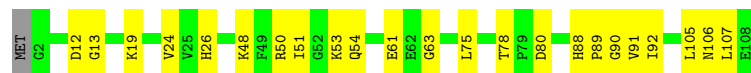
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 78% 21%



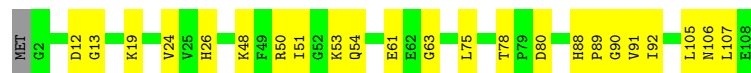
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G: 78% 21%



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 78% 21%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113172	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.040	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.13	Depositor
Map size (\AA)	425.984, 425.984, 425.984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KVR, ATP, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/34506	0.49	5/46608 (0.0%)
1	B	0.25	0/34506	0.49	5/46608 (0.0%)
1	C	0.25	0/34506	0.49	5/46608 (0.0%)
1	D	0.25	0/34506	0.49	5/46608 (0.0%)
2	E	0.29	0/834	0.55	0/1123
2	F	0.29	0/834	0.55	0/1123
2	G	0.29	0/834	0.55	0/1123
2	H	0.29	0/834	0.55	0/1123
All	All	0.26	0/141360	0.49	20/190924 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1957	LEU	CA-CB-CG	7.92	133.51	115.30
1	D	1957	LEU	CA-CB-CG	7.91	133.49	115.30
1	C	1957	LEU	CA-CB-CG	7.90	133.47	115.30
1	A	1957	LEU	CA-CB-CG	7.89	133.46	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1960	ARG	CG-CD-NE	-6.99	97.11	111.80
1	B	1960	ARG	CG-CD-NE	-6.99	97.12	111.80
1	D	1960	ARG	CG-CD-NE	-6.99	97.13	111.80
1	C	1960	ARG	CG-CD-NE	-6.99	97.13	111.80
1	B	1960	ARG	CA-CB-CG	6.86	128.50	113.40
1	A	1960	ARG	CA-CB-CG	6.86	128.50	113.40
1	D	1960	ARG	CA-CB-CG	6.86	128.49	113.40
1	C	1960	ARG	CA-CB-CG	6.84	128.46	113.40
1	A	3281	LEU	CA-CB-CG	6.49	130.23	115.30
1	C	3281	LEU	CA-CB-CG	6.48	130.19	115.30
1	D	3281	LEU	CA-CB-CG	6.48	130.19	115.30
1	B	3281	LEU	CA-CB-CG	6.47	130.19	115.30
1	B	943	LEU	CA-CB-CG	5.99	129.07	115.30
1	C	943	LEU	CA-CB-CG	5.99	129.07	115.30
1	A	943	LEU	CA-CB-CG	5.97	129.03	115.30
1	D	943	LEU	CA-CB-CG	5.97	129.03	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3187	LYS	Peptide
1	B	3187	LYS	Peptide
1	C	3187	LYS	Peptide
1	D	3187	LYS	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33766	0	33444	581	0
1	B	33766	0	33444	571	0
1	C	33766	0	33444	571	0
1	D	33766	0	33444	574	0
2	E	818	0	821	12	0
2	F	818	0	821	12	0
2	G	818	0	821	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	818	0	821	12	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	62	0	24	9	0
4	B	62	0	24	0	0
4	C	62	0	24	0	0
4	D	62	0	24	0	0
5	A	23	0	0	3	0
5	B	23	0	0	0	0
5	C	23	0	0	0	0
5	D	23	0	0	0	0
All	All	138680	0	137156	2298	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (2298) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:931:TYR:HD2	4:A:5003:ATP:N6	0.96	1.44
1:A:931:TYR:CD2	4:A:5003:ATP:N6	1.86	1.41
4:A:5003:ATP:H5'1	5:A:5004:KVR:C19	1.97	0.95
1:C:3149:GLU:HA	1:C:3152:ARG:HG2	1.52	0.92
1:A:3149:GLU:HA	1:A:3152:ARG:HG2	1.52	0.91
1:B:3149:GLU:HA	1:B:3152:ARG:HG2	1.52	0.91
1:D:3149:GLU:HA	1:D:3152:ARG:HG2	1.52	0.90
1:A:931:TYR:HD2	4:A:5003:ATP:HN62	0.93	0.89
1:A:928:GLU:OE2	4:A:5003:ATP:C2	2.24	0.86
1:C:1957:LEU:O	1:C:1960:ARG:NH1	2.11	0.84
1:D:1960:ARG:H	1:D:1960:ARG:HD3	1.43	0.84
1:A:1960:ARG:HD3	1:A:1960:ARG:H	1.43	0.83
1:C:1960:ARG:HD3	1:C:1960:ARG:H	1.43	0.83
1:A:1957:LEU:O	1:A:1960:ARG:NH1	2.11	0.83
1:B:1960:ARG:H	1:B:1960:ARG:HD3	1.43	0.83
1:B:1957:LEU:O	1:B:1960:ARG:NH1	2.11	0.83
1:D:1957:LEU:O	1:D:1960:ARG:NH1	2.11	0.83
1:D:3314:LEU:O	1:D:3318:HIS:HB3	1.82	0.80
1:A:3189:SER:HA	1:A:3192:ARG:HG2	1.64	0.80
1:C:3314:LEU:O	1:C:3318:HIS:HB3	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3314:LEU:O	1:B:3318:HIS:HB3	1.82	0.80
1:D:3189:SER:HA	1:D:3192:ARG:HG2	1.64	0.79
1:B:3189:SER:HA	1:B:3192:ARG:HG2	1.64	0.79
1:B:3227:ARG:HE	1:B:3228:TYR:H	1.30	0.79
1:A:3227:ARG:HE	1:A:3228:TYR:H	1.30	0.79
1:A:3314:LEU:O	1:A:3318:HIS:HB3	1.82	0.79
1:D:3227:ARG:HE	1:D:3228:TYR:H	1.30	0.79
1:C:2592:LEU:HD22	1:C:2606:PRO:HB3	1.64	0.78
1:C:3189:SER:HA	1:C:3192:ARG:HG2	1.64	0.78
1:A:2592:LEU:HD22	1:A:2606:PRO:HB3	1.64	0.78
1:C:1957:LEU:HG	1:C:1960:ARG:HH12	1.49	0.78
1:B:2592:LEU:HD22	1:B:2606:PRO:HB3	1.64	0.78
1:D:1957:LEU:HG	1:D:1960:ARG:HH12	1.49	0.78
1:B:3281:LEU:HA	1:B:3284:ILE:HG12	1.66	0.78
1:C:3281:LEU:HA	1:C:3284:ILE:HG12	1.66	0.77
1:D:2592:LEU:HD22	1:D:2606:PRO:HB3	1.64	0.77
1:D:3281:LEU:HA	1:D:3284:ILE:HG12	1.66	0.77
1:B:1957:LEU:HG	1:B:1960:ARG:HH12	1.49	0.77
1:A:3281:LEU:HA	1:A:3284:ILE:HG12	1.66	0.77
1:C:3227:ARG:HE	1:C:3228:TYR:H	1.30	0.77
1:A:1957:LEU:HG	1:A:1960:ARG:HH12	1.49	0.76
1:C:4269:LYS:HA	1:C:4272:LYS:HE3	1.68	0.75
1:B:4269:LYS:HA	1:B:4272:LYS:HE3	1.68	0.75
1:A:4269:LYS:HA	1:A:4272:LYS:HE3	1.69	0.75
1:D:4269:LYS:HA	1:D:4272:LYS:HE3	1.68	0.74
2:F:91:VAL:HG23	2:F:92:ILE:HD12	1.70	0.73
1:A:2418:ARG:HD2	1:B:189:GLU:HG2	1.69	0.73
2:G:91:VAL:HG23	2:G:92:ILE:HD12	1.70	0.73
1:D:3227:ARG:HB3	1:D:3230:GLN:HG2	1.71	0.73
1:A:3828:LYS:O	1:A:3831:GLN:NE2	2.22	0.72
2:E:91:VAL:HG23	2:E:92:ILE:HD12	1.70	0.72
1:C:3227:ARG:HB3	1:C:3230:GLN:HG2	1.71	0.72
1:C:1795:LEU:HD23	1:C:1842:ILE:HD11	1.72	0.72
1:D:1795:LEU:HD23	1:D:1842:ILE:HD11	1.72	0.72
1:C:3828:LYS:O	1:C:3831:GLN:NE2	2.23	0.72
1:D:3828:LYS:O	1:D:3831:GLN:NE2	2.22	0.72
2:H:91:VAL:HG23	2:H:92:ILE:HD12	1.70	0.72
1:A:3227:ARG:HB3	1:A:3230:GLN:HG2	1.71	0.72
1:B:3828:LYS:O	1:B:3831:GLN:NE2	2.22	0.72
1:B:1795:LEU:HD23	1:B:1842:ILE:HD11	1.72	0.72
1:B:3227:ARG:HB3	1:B:3230:GLN:HG2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1766:PRO:HG3	1:C:1780:PRO:HB3	1.72	0.71
1:D:1766:PRO:HG3	1:D:1780:PRO:HB3	1.72	0.71
1:A:1795:LEU:HD23	1:A:1842:ILE:HD11	1.72	0.71
1:D:3228:TYR:HB2	1:D:3287:ASN:HD21	1.56	0.71
1:A:1766:PRO:HG3	1:A:1780:PRO:HB3	1.72	0.71
1:A:3228:TYR:HB2	1:A:3287:ASN:HD21	1.56	0.71
1:C:2418:ARG:HD2	1:D:189:GLU:HG2	1.73	0.71
1:C:3228:TYR:HB2	1:C:3287:ASN:HD21	1.56	0.71
1:A:3119:GLU:OE2	1:A:3248:ARG:NH2	2.24	0.70
1:D:502:ILE:HG23	1:D:506:HIS:CE1	2.26	0.70
1:A:502:ILE:HG23	1:A:506:HIS:CE1	2.26	0.70
1:B:1766:PRO:HG3	1:B:1780:PRO:HB3	1.72	0.70
1:B:3119:GLU:OE2	1:B:3248:ARG:NH2	2.24	0.70
1:C:502:ILE:HG23	1:C:506:HIS:CE1	2.26	0.70
1:D:3119:GLU:OE2	1:D:3248:ARG:NH2	2.24	0.70
1:B:2418:ARG:HD2	1:C:189:GLU:HG2	1.73	0.70
1:B:502:ILE:HG23	1:B:506:HIS:CE1	2.26	0.69
1:B:3228:TYR:HB2	1:B:3287:ASN:HD21	1.56	0.69
1:C:3119:GLU:OE2	1:C:3248:ARG:NH2	2.24	0.69
1:D:3205:CYS:HB3	1:D:3208:ILE:HB	1.75	0.69
1:A:323:ASP:O	1:A:325:LYS:N	2.25	0.69
1:B:3205:CYS:HB3	1:B:3208:ILE:HB	1.75	0.69
1:C:939:THR:O	1:C:943:LEU:HD12	1.93	0.69
1:A:939:THR:O	1:A:943:LEU:HD12	1.93	0.69
1:C:2868:HIS:HB3	1:C:2871:LEU:HD23	1.74	0.69
1:D:644:LEU:HD13	1:D:1630:LEU:HD21	1.75	0.69
1:D:3200:ASN:HB3	1:D:3203:ASP:HB2	1.75	0.69
1:A:2868:HIS:HB3	1:A:2871:LEU:HD23	1.74	0.69
1:C:644:LEU:HD13	1:C:1630:LEU:HD21	1.75	0.69
1:C:3205:CYS:HB3	1:C:3208:ILE:HB	1.75	0.69
1:C:2684:ASN:ND2	1:C:2913:ASP:OD2	2.26	0.69
1:A:189:GLU:HG2	1:D:2418:ARG:HD2	1.74	0.69
1:A:644:LEU:HD13	1:A:1630:LEU:HD21	1.75	0.69
1:A:2684:ASN:ND2	1:A:2913:ASP:OD2	2.26	0.69
1:B:2684:ASN:ND2	1:B:2913:ASP:OD2	2.26	0.69
1:A:3200:ASN:HB3	1:A:3203:ASP:HB2	1.75	0.68
1:D:2868:HIS:HB3	1:D:2871:LEU:HD23	1.74	0.68
1:B:939:THR:O	1:B:943:LEU:HD12	1.93	0.68
1:B:3200:ASN:HB3	1:B:3203:ASP:HB2	1.75	0.68
1:A:3205:CYS:HB3	1:A:3208:ILE:HB	1.75	0.68
1:B:644:LEU:HD13	1:B:1630:LEU:HD21	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2868:HIS:HB3	1:B:2871:LEU:HD23	1.74	0.68
1:C:2418:ARG:NH1	1:D:186:VAL:O	2.27	0.68
1:C:3832:ASP:HB3	1:C:3835:PHE:HB3	1.75	0.68
1:C:4782:THR:HG21	1:C:4813:TYR:HA	1.76	0.68
1:D:2684:ASN:ND2	1:D:2913:ASP:OD2	2.26	0.68
1:C:1129:GLY:HA3	1:C:1145:TRP:HB3	1.76	0.68
1:A:4782:THR:HG21	1:A:4813:TYR:HA	1.76	0.68
1:C:3200:ASN:HB3	1:C:3203:ASP:HB2	1.75	0.68
1:D:4782:THR:HG21	1:D:4813:TYR:HA	1.76	0.68
1:B:1129:GLY:HA3	1:B:1145:TRP:HB3	1.76	0.68
1:B:2173:GLU:HA	1:B:2176:VAL:HG22	1.76	0.68
1:B:3832:ASP:HB3	1:B:3835:PHE:HB3	1.75	0.68
1:B:4782:THR:HG21	1:B:4813:TYR:HA	1.76	0.67
1:D:939:THR:O	1:D:943:LEU:HD12	1.93	0.67
1:A:186:VAL:O	1:D:2418:ARG:NH1	2.28	0.67
1:B:3312:PRO:HA	1:B:3315:LEU:HD23	1.76	0.67
1:D:1129:GLY:HA3	1:D:1145:TRP:HB3	1.76	0.67
1:D:3832:ASP:HB3	1:D:3835:PHE:HB3	1.75	0.67
1:B:168:GLN:HG3	1:B:169:ARG:HD2	1.77	0.67
1:A:168:GLN:HG3	1:A:169:ARG:HD2	1.77	0.67
1:C:2405:GLU:OE1	1:C:2407:HIS:ND1	2.25	0.67
1:D:2173:GLU:HA	1:D:2176:VAL:HG22	1.75	0.67
1:D:323:ASP:O	1:D:325:LYS:N	2.25	0.67
1:A:889:ILE:HG21	1:A:936:SER:HB3	1.76	0.67
1:B:889:ILE:HG21	1:B:936:SER:HB3	1.76	0.67
1:A:1496:PRO:HA	1:D:2798:MET:HG2	1.77	0.66
1:D:1440:ASN:HB3	1:D:1546:GLN:HB3	1.78	0.66
1:A:1129:GLY:HA3	1:A:1145:TRP:HB3	1.76	0.66
1:A:2405:GLU:OE1	1:A:2407:HIS:ND1	2.25	0.66
1:C:1440:ASN:HB3	1:C:1546:GLN:HB3	1.78	0.66
1:C:2173:GLU:HA	1:C:2176:VAL:HG22	1.75	0.66
1:A:2860:LEU:HD11	1:A:2867:ASN:HA	1.78	0.66
1:A:1100:ARG:NH1	1:A:1234:GLU:O	2.29	0.66
1:C:892:LEU:HD11	1:C:1056:THR:HG21	1.78	0.66
1:A:2173:GLU:HA	1:A:2176:VAL:HG22	1.75	0.66
1:A:3312:PRO:HA	1:A:3315:LEU:HD23	1.76	0.66
1:B:2860:LEU:HD11	1:B:2867:ASN:HA	1.78	0.66
1:D:168:GLN:HG3	1:D:169:ARG:HD2	1.77	0.66
1:D:3312:PRO:HA	1:D:3315:LEU:HD23	1.77	0.66
1:C:168:GLN:HG3	1:C:169:ARG:HD2	1.77	0.66
1:C:989:THR:HB	1:C:992:GLN:OE1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1100:ARG:NH1	1:C:1234:GLU:O	2.29	0.66
1:A:3832:ASP:HB3	1:A:3835:PHE:HB3	1.75	0.66
1:C:889:ILE:HG21	1:C:936:SER:HB3	1.76	0.66
1:C:3312:PRO:HA	1:C:3315:LEU:HD23	1.76	0.66
1:D:892:LEU:HD11	1:D:1056:THR:HG21	1.78	0.66
1:A:972:LEU:HG	1:A:978:PRO:HG3	1.78	0.66
1:C:1685:LEU:HB3	1:C:1706:LEU:HD12	1.78	0.66
1:C:4689:LYS:NZ	1:C:4694:LEU:O	2.29	0.66
1:B:2418:ARG:NH1	1:C:186:VAL:O	2.29	0.66
1:B:4689:LYS:NZ	1:B:4694:LEU:O	2.29	0.66
1:A:2418:ARG:NH1	1:B:186:VAL:O	2.28	0.65
1:B:1685:LEU:HB3	1:B:1706:LEU:HD12	1.78	0.65
1:A:989:THR:HB	1:A:992:GLN:OE1	1.95	0.65
1:D:2726:GLU:OE2	1:D:2761:LYS:NZ	2.30	0.65
1:B:1048:ASP:HA	1:B:1051:ARG:HG2	1.79	0.65
1:B:1100:ARG:NH1	1:B:1234:GLU:O	2.29	0.65
1:C:323:ASP:O	1:C:325:LYS:N	2.25	0.65
1:D:989:THR:HB	1:D:992:GLN:OE1	1.95	0.65
1:A:4689:LYS:NZ	1:A:4694:LEU:O	2.29	0.65
1:B:989:THR:HB	1:B:992:GLN:OE1	1.95	0.65
1:B:972:LEU:HG	1:B:978:PRO:HG3	1.78	0.65
1:B:1440:ASN:HB3	1:B:1546:GLN:HB3	1.77	0.65
1:B:4123:GLU:OE2	1:B:4127:ASN:ND2	2.30	0.65
1:D:889:ILE:HG21	1:D:936:SER:HB3	1.76	0.65
1:D:1100:ARG:NH1	1:D:1234:GLU:O	2.29	0.65
1:D:1685:LEU:HB3	1:D:1706:LEU:HD12	1.78	0.65
1:D:4689:LYS:NZ	1:D:4694:LEU:O	2.29	0.65
1:A:1048:ASP:HA	1:A:1051:ARG:HG2	1.79	0.65
1:D:1048:ASP:HA	1:D:1051:ARG:HG2	1.79	0.65
1:A:892:LEU:HD11	1:A:1056:THR:HG21	1.78	0.65
1:A:4883:ASP:O	1:A:4884:MET:HG2	1.96	0.65
1:C:2726:GLU:OE2	1:C:2761:LYS:NZ	2.30	0.65
1:A:4123:GLU:OE2	1:A:4127:ASN:ND2	2.30	0.65
1:B:677:LEU:HD22	1:B:792:VAL:HG11	1.79	0.65
1:C:4883:ASP:O	1:C:4884:MET:HG2	1.97	0.65
1:A:1685:LEU:HB3	1:A:1706:LEU:HD12	1.78	0.65
1:A:1440:ASN:HB3	1:A:1546:GLN:HB3	1.78	0.64
1:B:4883:ASP:O	1:B:4884:MET:HG2	1.97	0.64
1:C:972:LEU:HG	1:C:978:PRO:HG3	1.78	0.64
1:D:4123:GLU:OE2	1:D:4127:ASN:ND2	2.30	0.64
1:B:323:ASP:O	1:B:325:LYS:N	2.25	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2726:GLU:OE2	1:A:2761:LYS:NZ	2.30	0.64
1:D:677:LEU:HD22	1:D:792:VAL:HG11	1.79	0.64
1:D:972:LEU:HG	1:D:978:PRO:HG3	1.78	0.64
1:D:2860:LEU:HD11	1:D:2867:ASN:HA	1.78	0.64
1:C:2860:LEU:HD11	1:C:2867:ASN:HA	1.78	0.64
1:B:892:LEU:HD11	1:B:1056:THR:HG21	1.78	0.64
1:C:1048:ASP:HA	1:C:1051:ARG:HG2	1.79	0.64
1:D:4883:ASP:O	1:D:4884:MET:HG2	1.97	0.64
1:A:677:LEU:HD22	1:A:792:VAL:HG11	1.79	0.64
1:A:1269:GLU:HB2	1:A:1288:LYS:HG3	1.80	0.64
1:D:1269:GLU:HB2	1:D:1288:LYS:HG3	1.80	0.64
2:F:78:THR:OG1	2:F:80:ASP:OD1	2.15	0.64
1:B:2726:GLU:OE2	1:B:2761:LYS:NZ	2.30	0.64
1:C:677:LEU:HD22	1:C:792:VAL:HG11	1.79	0.64
1:C:4123:GLU:OE2	1:C:4127:ASN:ND2	2.30	0.64
1:B:1269:GLU:HB2	1:B:1288:LYS:HG3	1.80	0.63
1:D:3846:LEU:HB3	1:D:3854:PHE:CE2	2.34	0.63
1:C:2748:SER:HB2	1:C:2753:VAL:HB	1.81	0.63
1:B:599:SER:OG	1:B:603:LYS:NZ	2.32	0.63
1:B:3149:GLU:HA	1:B:3152:ARG:CG	2.28	0.63
1:A:3846:LEU:HB3	1:A:3854:PHE:CE2	2.34	0.63
1:D:3148:VAL:HG12	1:D:3152:ARG:HD2	1.81	0.63
1:C:599:SER:OG	1:C:603:LYS:NZ	2.32	0.63
1:D:2748:SER:HB2	1:D:2753:VAL:HB	1.81	0.63
1:A:249:SER:H	1:A:272:ARG:HH21	1.47	0.63
1:A:599:SER:OG	1:A:603:LYS:NZ	2.32	0.63
1:B:2748:SER:HB2	1:B:2753:VAL:HB	1.81	0.63
1:D:2405:GLU:OE1	1:D:2407:HIS:ND1	2.25	0.63
1:B:3153:SER:O	1:B:3156:GLY:N	2.32	0.62
1:C:1269:GLU:HB2	1:C:1288:LYS:HG3	1.80	0.62
1:C:3148:VAL:HG12	1:C:3152:ARG:HD2	1.81	0.62
1:C:3153:SER:O	1:C:3156:GLY:N	2.32	0.62
1:C:3846:LEU:HB3	1:C:3854:PHE:CE2	2.34	0.62
1:D:1286:THR:HG23	1:D:1551:ASN:HA	1.81	0.62
1:D:3152:ARG:HH21	1:D:3237:VAL:HG21	1.65	0.62
1:D:3153:SER:O	1:D:3156:GLY:N	2.32	0.62
1:A:1962:THR:O	1:A:1966:ARG:HG2	1.99	0.62
2:G:78:THR:OG1	2:G:80:ASP:OD1	2.15	0.62
1:B:3148:VAL:HG12	1:B:3152:ARG:HD2	1.81	0.62
1:D:599:SER:OG	1:D:603:LYS:NZ	2.32	0.62
1:D:1541:PRO:HG2	1:D:1566:LEU:HD21	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2996:ALA:O	1:D:3001:LYS:NZ	2.33	0.62
1:A:1541:PRO:HG2	1:A:1566:LEU:HD21	1.82	0.62
1:A:2748:SER:HB2	1:A:2753:VAL:HB	1.81	0.62
1:A:3149:GLU:HA	1:A:3152:ARG:CG	2.28	0.62
1:B:2405:GLU:OE1	1:B:2407:HIS:ND1	2.25	0.62
1:B:2653:SER:O	1:B:2958:GLN:NE2	2.33	0.62
1:C:1962:THR:O	1:C:1966:ARG:HG2	1.99	0.62
1:C:2996:ALA:O	1:C:3001:LYS:NZ	2.33	0.62
1:D:3697:LYS:HA	1:D:3700:HIS:CD2	2.35	0.62
1:A:3148:VAL:HG12	1:A:3152:ARG:HD2	1.81	0.62
1:B:249:SER:H	1:B:272:ARG:HH21	1.47	0.62
1:B:3846:LEU:HB3	1:B:3854:PHE:CE2	2.34	0.62
1:C:3697:LYS:HA	1:C:3700:HIS:CD2	2.34	0.62
1:A:281:ARG:NH2	1:A:287:SER:OG	2.33	0.62
1:A:3152:ARG:HH21	1:A:3237:VAL:HG21	1.65	0.62
1:A:3701:ASP:OD2	1:A:3727:GLN:NE2	2.33	0.62
1:C:3050:LEU:HB3	1:C:3053:VAL:HG23	1.82	0.62
1:D:1494:MET:O	1:D:1496:PRO:HD2	2.00	0.62
1:A:2996:ALA:O	1:A:3001:LYS:NZ	2.33	0.62
2:H:78:THR:OG1	2:H:80:ASP:OD1	2.15	0.62
1:B:2721:ILE:HD11	1:B:2779:LEU:HD12	1.82	0.62
1:B:2996:ALA:O	1:B:3001:LYS:NZ	2.33	0.62
1:B:3050:LEU:HB3	1:B:3053:VAL:HG23	1.82	0.62
1:C:3149:GLU:HA	1:C:3152:ARG:CG	2.28	0.62
1:D:249:SER:H	1:D:272:ARG:HH21	1.47	0.62
1:A:2721:ILE:HD11	1:A:2779:LEU:HD12	1.82	0.62
1:A:3153:SER:O	1:A:3156:GLY:N	2.32	0.62
1:C:2238:THR:HG22	1:C:2240:LEU:H	1.65	0.62
1:C:2721:ILE:HD11	1:C:2779:LEU:HD12	1.82	0.62
1:D:281:ARG:NH2	1:D:287:SER:OG	2.33	0.62
1:D:1962:THR:O	1:D:1966:ARG:HG2	1.99	0.62
1:A:1286:THR:HG23	1:A:1551:ASN:HA	1.81	0.61
1:A:1494:MET:O	1:A:1496:PRO:HD2	2.00	0.61
1:B:1494:MET:O	1:B:1496:PRO:HD2	2.00	0.61
1:B:2238:THR:HG22	1:B:2240:LEU:H	1.65	0.61
1:B:3701:ASP:OD2	1:B:3727:GLN:NE2	2.33	0.61
1:C:281:ARG:NH2	1:C:287:SER:OG	2.33	0.61
1:D:2721:ILE:HD11	1:D:2779:LEU:HD12	1.82	0.61
1:A:2653:SER:O	1:A:2958:GLN:NE2	2.33	0.61
1:A:4859:LEU:O	1:A:4863:GLN:HG2	2.01	0.61
1:B:4667:SER:OG	1:B:4672:MET:O	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2072:GLU:O	1:D:3660:ARG:NH1	2.33	0.61
1:D:4187:GLU:OE2	1:D:4947:ARG:NH2	2.33	0.61
1:A:3697:LYS:HA	1:A:3700:HIS:CD2	2.35	0.61
1:B:281:ARG:NH2	1:B:287:SER:OG	2.33	0.61
1:B:1286:THR:HG23	1:B:1551:ASN:HA	1.81	0.61
1:C:3701:ASP:OD2	1:C:3727:GLN:NE2	2.33	0.61
1:C:3152:ARG:HH21	1:C:3237:VAL:HG21	1.65	0.61
1:A:2072:GLU:O	1:A:3660:ARG:NH1	2.33	0.61
2:E:106:ASN:OD1	2:E:107:LEU:N	2.33	0.61
1:C:249:SER:H	1:C:272:ARG:HH21	1.47	0.61
1:C:1176:THR:HG22	1:C:1181:ILE:HA	1.83	0.61
1:D:3149:GLU:HA	1:D:3152:ARG:CG	2.27	0.61
1:A:4667:SER:OG	1:A:4672:MET:O	2.18	0.61
1:B:1962:THR:O	1:B:1966:ARG:HG2	1.99	0.61
1:B:2072:GLU:O	1:B:3660:ARG:NH1	2.33	0.61
1:B:3697:LYS:HA	1:B:3700:HIS:CD2	2.34	0.61
1:D:2653:SER:O	1:D:2958:GLN:NE2	2.33	0.61
2:G:106:ASN:OD1	2:G:107:LEU:N	2.33	0.61
1:B:1176:THR:HG22	1:B:1181:ILE:HA	1.83	0.61
1:C:1494:MET:O	1:C:1496:PRO:HD2	2.00	0.61
1:C:2072:GLU:O	1:C:3660:ARG:NH1	2.33	0.61
1:C:2653:SER:O	1:C:2958:GLN:NE2	2.33	0.61
1:D:4859:LEU:O	1:D:4863:GLN:HG2	2.01	0.61
2:E:78:THR:OG1	2:E:80:ASP:OD1	2.15	0.61
1:B:2788:ARG:HE	1:B:2906:GLY:HA3	1.66	0.61
1:B:4187:GLU:OE2	1:B:4947:ARG:NH2	2.33	0.61
1:D:1176:THR:HG22	1:D:1181:ILE:HA	1.83	0.61
1:D:2788:ARG:HE	1:D:2906:GLY:HA3	1.66	0.61
1:D:4667:SER:OG	1:D:4672:MET:O	2.18	0.61
1:B:3152:ARG:HH21	1:B:3237:VAL:HG21	1.65	0.61
1:D:3050:LEU:HB3	1:D:3053:VAL:HG23	1.82	0.61
1:B:1541:PRO:HG2	1:B:1566:LEU:HD21	1.82	0.61
1:C:1541:PRO:HG2	1:C:1566:LEU:HD21	1.82	0.61
1:C:4569:GLU:OE2	1:C:4573:ARG:NH1	2.34	0.61
1:C:4667:SER:OG	1:C:4672:MET:O	2.18	0.61
1:C:2788:ARG:HE	1:C:2906:GLY:HA3	1.66	0.60
1:C:3840:PHE:HA	1:C:3843:LEU:HD12	1.83	0.60
1:A:3050:LEU:HB3	1:A:3053:VAL:HG23	1.82	0.60
1:B:4569:GLU:OE2	1:B:4573:ARG:NH1	2.34	0.60
1:C:1286:THR:HG23	1:C:1551:ASN:HA	1.81	0.60
1:D:1418:ASP:OD1	1:D:1419:PHE:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:106:ASN:OD1	2:F:107:LEU:N	2.33	0.60
1:A:2238:THR:HG22	1:A:2240:LEU:H	1.65	0.60
1:B:3840:PHE:HA	1:B:3843:LEU:HD12	1.83	0.60
1:B:4859:LEU:O	1:B:4863:GLN:HG2	2.01	0.60
1:C:3192:ARG:HH11	1:C:3192:ARG:HG3	1.65	0.60
1:D:4569:GLU:OE2	1:D:4573:ARG:NH1	2.34	0.60
1:A:2212:LYS:NZ	1:A:2216:ASP:OD1	2.33	0.60
1:C:4489:GLN:NE2	1:C:4493:ASN:OD1	2.33	0.60
1:D:2238:THR:HG22	1:D:2240:LEU:H	1.65	0.60
1:D:3840:PHE:HA	1:D:3843:LEU:HD12	1.83	0.60
1:A:1418:ASP:OD1	1:A:1419:PHE:N	2.34	0.60
2:H:26:HIS:CD2	2:H:105:LEU:HD11	2.37	0.60
1:B:1685:LEU:O	1:B:1689:ILE:HG12	2.02	0.60
1:C:2798:MET:HG2	1:D:1496:PRO:HA	1.82	0.60
1:D:2697:SER:O	1:D:2698:GLU:HG3	2.02	0.60
1:D:3192:ARG:HG3	1:D:3192:ARG:HH11	1.65	0.60
1:A:1176:THR:HG22	1:A:1181:ILE:HA	1.83	0.60
1:A:1685:LEU:O	1:A:1689:ILE:HG12	2.02	0.60
1:D:1721:MET:HE2	1:D:1758:ARG:HA	1.84	0.60
1:A:4177:VAL:HG11	1:A:4880:VAL:HA	1.84	0.60
2:E:63:GLY:HA3	2:E:75:LEU:HD13	1.84	0.60
1:B:2798:MET:HG2	1:C:1496:PRO:HA	1.82	0.60
1:B:3192:ARG:HH11	1:B:3192:ARG:HG3	1.66	0.60
1:B:4832:GLU:O	1:B:4843:ARG:NH2	2.21	0.60
1:C:1685:LEU:O	1:C:1689:ILE:HG12	2.02	0.60
2:H:106:ASN:OD1	2:H:107:LEU:N	2.33	0.60
1:B:2697:SER:O	1:B:2698:GLU:HG3	2.02	0.60
1:A:1007:TRP:HE1	4:A:5003:ATP:PG	2.25	0.60
1:A:2697:SER:O	1:A:2698:GLU:HG3	2.02	0.60
1:C:2697:SER:O	1:C:2698:GLU:HG3	2.02	0.60
1:A:2798:MET:HG2	1:B:1496:PRO:HA	1.84	0.59
1:A:3192:ARG:HH11	1:A:3192:ARG:HG3	1.66	0.59
1:A:4569:GLU:OE2	1:A:4573:ARG:NH1	2.34	0.59
1:C:4859:LEU:O	1:C:4863:GLN:HG2	2.01	0.59
1:D:515:ALA:HB2	1:D:523:GLY:HA3	1.83	0.59
1:A:2580:LEU:O	1:A:2616:ARG:NH2	2.35	0.59
2:G:26:HIS:CD2	2:G:105:LEU:HD11	2.37	0.59
1:C:4832:GLU:O	1:C:4843:ARG:NH2	2.21	0.59
1:D:1685:LEU:O	1:D:1689:ILE:HG12	2.02	0.59
1:D:3701:ASP:OD2	1:D:3727:GLN:NE2	2.33	0.59
1:A:419:ILE:HG21	1:A:492:GLU:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4187:GLU:OE2	1:A:4947:ARG:NH2	2.33	0.59
2:F:26:HIS:CD2	2:F:105:LEU:HD11	2.37	0.59
1:C:3171:LEU:HD11	1:C:3241:MET:HE1	1.83	0.59
1:A:1721:MET:HE2	1:A:1758:ARG:HA	1.83	0.59
1:C:502:ILE:HG23	1:C:506:HIS:HE1	1.67	0.59
1:D:2590:ARG:NH2	1:D:2875:ASP:OD2	2.33	0.59
1:D:4177:VAL:HG11	1:D:4880:VAL:HA	1.84	0.59
1:B:541:ILE:HD11	1:B:574:VAL:HG13	1.84	0.59
1:C:1418:ASP:OD1	1:C:1419:PHE:N	2.34	0.59
1:C:1721:MET:HE2	1:C:1758:ARG:HA	1.85	0.59
1:A:2788:ARG:HE	1:A:2906:GLY:HA3	1.66	0.59
1:A:3840:PHE:HA	1:A:3843:LEU:HD12	1.83	0.59
1:B:3674:THR:O	1:B:3679:LYS:NZ	2.36	0.59
2:E:26:HIS:CD2	2:E:105:LEU:HD11	2.37	0.59
1:B:515:ALA:HB2	1:B:523:GLY:HA3	1.83	0.59
1:B:1418:ASP:OD1	1:B:1419:PHE:N	2.34	0.59
1:C:2590:ARG:NH2	1:C:2875:ASP:OD2	2.33	0.59
1:D:1013:ARG:HG2	1:D:1013:ARG:HH11	1.66	0.59
1:D:3695:MET:HB3	1:D:3731:LEU:HD11	1.85	0.59
1:A:1242:ASN:HB3	1:A:1807:ARG:HG3	1.85	0.59
1:B:1844:GLN:NE2	1:B:1853:GLU:OE1	2.35	0.59
1:B:4177:VAL:HG11	1:B:4880:VAL:HA	1.84	0.59
1:C:515:ALA:HB2	1:C:523:GLY:HA3	1.83	0.59
1:D:1844:GLN:NE2	1:D:1853:GLU:OE1	2.35	0.59
1:C:4187:GLU:OE2	1:C:4947:ARG:NH2	2.33	0.59
1:D:502:ILE:HG23	1:D:506:HIS:HE1	1.67	0.59
1:A:515:ALA:HB2	1:A:523:GLY:HA3	1.83	0.59
1:C:1242:ASN:HB3	1:C:1807:ARG:HG3	1.85	0.59
1:D:419:ILE:HG21	1:D:492:GLU:HG3	1.85	0.59
1:D:1242:ASN:HB3	1:D:1807:ARG:HG3	1.85	0.59
1:B:1721:MET:HE2	1:B:1758:ARG:HA	1.85	0.58
1:C:1844:GLN:NE2	1:C:1853:GLU:OE1	2.35	0.58
1:C:2580:LEU:O	1:C:2616:ARG:NH2	2.35	0.58
1:A:1013:ARG:HG2	1:A:1013:ARG:HH11	1.66	0.58
2:H:63:GLY:HA3	2:H:75:LEU:HD13	1.84	0.58
1:B:2580:LEU:O	1:B:2616:ARG:NH2	2.36	0.58
1:B:419:ILE:HG21	1:B:492:GLU:HG3	1.85	0.58
1:B:1013:ARG:HG2	1:B:1013:ARG:HH11	1.66	0.58
1:C:3695:MET:HB3	1:C:3731:LEU:HD11	1.85	0.58
1:A:1844:GLN:NE2	1:A:1853:GLU:OE1	2.35	0.58
2:F:63:GLY:HA3	2:F:75:LEU:HD13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:63:GLY:HA3	2:G:75:LEU:HD13	1.84	0.58
1:B:502:ILE:HG23	1:B:506:HIS:HE1	1.67	0.58
1:C:541:ILE:HD11	1:C:574:VAL:HG13	1.85	0.58
1:A:502:ILE:HG23	1:A:506:HIS:HE1	1.67	0.58
1:A:983:LEU:O	1:A:1055:ARG:NH1	2.37	0.58
1:A:3674:THR:O	1:A:3679:LYS:NZ	2.36	0.58
1:C:4177:VAL:HG11	1:C:4880:VAL:HA	1.84	0.58
1:D:2580:LEU:O	1:D:2616:ARG:NH2	2.35	0.58
1:B:983:LEU:O	1:B:1055:ARG:NH1	2.37	0.58
1:D:681:HIS:HA	1:D:751:THR:HG22	1.85	0.58
1:C:681:HIS:HA	1:C:751:THR:HG22	1.85	0.58
1:C:2442:MET:HE1	1:C:2498:ALA:HB1	1.84	0.58
1:D:3674:THR:O	1:D:3679:LYS:NZ	2.36	0.58
1:A:541:ILE:HD11	1:A:574:VAL:HG13	1.84	0.58
1:C:983:LEU:O	1:C:1055:ARG:NH1	2.37	0.58
1:D:1957:LEU:CG	1:D:1960:ARG:HH12	2.17	0.58
1:D:983:LEU:O	1:D:1055:ARG:NH1	2.37	0.58
1:A:3695:MET:HB3	1:A:3731:LEU:HD11	1.85	0.58
1:B:249:SER:HB3	1:B:272:ARG:HE	1.69	0.58
1:D:3171:LEU:HD11	1:D:3241:MET:HE1	1.85	0.58
1:A:249:SER:HB3	1:A:272:ARG:HE	1.69	0.57
4:A:5003:ATP:H5'1	5:A:5004:KVR:C18	2.34	0.57
1:B:1242:ASN:HB3	1:B:1807:ARG:HG3	1.85	0.57
1:B:2212:LYS:NZ	1:B:2216:ASP:OD1	2.33	0.57
1:D:249:SER:HB3	1:D:272:ARG:HE	1.69	0.57
1:D:3259:GLU:O	1:D:3260:ARG:HD3	2.04	0.57
1:C:1013:ARG:HG2	1:C:1013:ARG:HH11	1.66	0.57
1:C:2212:LYS:NZ	1:C:2216:ASP:OD1	2.33	0.57
1:D:2333:PRO:HA	1:D:2336:ARG:HE	1.69	0.57
1:A:3171:LEU:HD11	1:A:3241:MET:HE1	1.86	0.57
1:B:3259:GLU:O	1:B:3260:ARG:HD3	2.04	0.57
1:C:332:ARG:NH1	1:C:364:GLN:OE1	2.35	0.57
1:C:2333:PRO:HA	1:C:2336:ARG:HE	1.70	0.57
1:A:3259:GLU:O	1:A:3260:ARG:HD3	2.04	0.57
1:B:681:HIS:HA	1:B:751:THR:HG22	1.85	0.57
1:B:3695:MET:HB3	1:B:3731:LEU:HD11	1.85	0.57
1:C:419:ILE:HG21	1:C:492:GLU:HG3	1.84	0.57
1:D:2706:VAL:HG21	1:D:2785:TRP:NE1	2.20	0.57
1:A:680:ASP:OD1	1:A:801:ARG:NH2	2.38	0.57
1:A:2176:VAL:HG12	1:A:2220:TYR:CE2	2.40	0.57
1:A:2706:VAL:HG21	1:A:2785:TRP:NE1	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3259:GLU:O	1:C:3260:ARG:HD3	2.04	0.57
1:A:2333:PRO:HA	1:A:2336:ARG:HE	1.69	0.57
1:A:3043:ARG:NH2	1:A:3116:GLN:O	2.38	0.57
1:B:680:ASP:OD1	1:B:801:ARG:NH2	2.38	0.57
1:B:3043:ARG:NH2	1:B:3116:GLN:O	2.38	0.57
1:C:680:ASP:OD1	1:C:801:ARG:NH2	2.38	0.57
1:C:2995:HIS:HE2	1:D:1070:ASP:HB3	1.69	0.57
1:A:670:TYR:HD1	1:A:1017:THR:HG21	1.70	0.57
1:A:681:HIS:HA	1:A:751:THR:HG22	1.85	0.57
1:B:2590:ARG:NH2	1:B:2875:ASP:OD2	2.33	0.57
1:B:2979:ARG:HG3	1:B:3039:THR:HG22	1.87	0.57
1:B:3152:ARG:HH22	1:B:3233:HIS:HB2	1.69	0.57
1:C:249:SER:HB3	1:C:272:ARG:HE	1.69	0.57
1:B:1793:GLN:NE2	1:B:1797:GLU:OE2	2.38	0.57
1:D:541:ILE:HD11	1:D:574:VAL:HG13	1.84	0.57
1:D:1716:THR:O	1:D:1720:MET:HG3	2.05	0.57
1:D:3152:ARG:HH22	1:D:3233:HIS:HB2	1.69	0.57
1:A:1957:LEU:CG	1:A:1960:ARG:HH12	2.17	0.57
1:A:2833:LEU:HB3	1:A:2837:LEU:HB3	1.87	0.57
1:B:1957:LEU:CG	1:B:1960:ARG:HH12	2.17	0.57
1:B:2202:TYR:O	1:B:2206:ILE:HG12	2.05	0.57
1:C:1793:GLN:NE2	1:C:1797:GLU:OE2	2.38	0.57
1:A:1716:THR:O	1:A:1720:MET:HG3	2.05	0.56
1:B:601:LEU:HG	1:B:610:VAL:HG11	1.87	0.56
1:B:2833:LEU:HB3	1:B:2837:LEU:HB3	1.87	0.56
1:D:4489:GLN:NE2	1:D:4493:ASN:OD1	2.33	0.56
1:A:2590:ARG:NH2	1:A:2875:ASP:OD2	2.33	0.56
1:A:2979:ARG:HG3	1:A:3039:THR:HG22	1.87	0.56
1:A:3152:ARG:HH22	1:A:3233:HIS:HB2	1.69	0.56
1:B:1941:ARG:NH2	1:B:3609:TYR:O	2.38	0.56
1:B:2593:VAL:HG12	1:B:2644:LEU:HG	1.88	0.56
1:C:2593:VAL:HG12	1:C:2644:LEU:HG	1.87	0.56
1:C:3152:ARG:HH22	1:C:3233:HIS:HB2	1.69	0.56
1:D:3043:ARG:NH2	1:D:3116:GLN:O	2.38	0.56
1:B:2176:VAL:HG12	1:B:2220:TYR:CE2	2.40	0.56
1:C:866:PRO:HG3	1:C:1009:ARG:HD3	1.88	0.56
1:C:1716:THR:O	1:C:1720:MET:HG3	2.05	0.56
1:C:1941:ARG:NH2	1:C:3609:TYR:O	2.38	0.56
1:C:2176:VAL:HG12	1:C:2220:TYR:CE2	2.40	0.56
1:D:670:TYR:HD1	1:D:1017:THR:HG21	1.70	0.56
1:D:866:PRO:HG3	1:D:1009:ARG:HD3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1793:GLN:NE2	1:D:1797:GLU:OE2	2.38	0.56
1:D:1941:ARG:NH2	1:D:3609:TYR:O	2.38	0.56
1:A:143:LEU:HD22	1:D:2426:LEU:HD23	1.88	0.56
1:B:304:LYS:HB2	1:B:316:LEU:HD23	1.87	0.56
1:B:2706:VAL:HG21	1:B:2785:TRP:NE1	2.20	0.56
1:B:3171:LEU:HD11	1:B:3241:MET:HE1	1.86	0.56
1:D:2176:VAL:HG12	1:D:2220:TYR:CE2	2.40	0.56
1:D:2589:LEU:O	1:D:2593:VAL:HG13	2.06	0.56
1:A:332:ARG:NH1	1:A:364:GLN:OE1	2.36	0.56
1:A:950:VAL:HG22	1:A:1064:LEU:HD13	1.88	0.56
1:A:4489:GLN:NE2	1:A:4493:ASN:OD1	2.33	0.56
2:F:90:GLY:HA2	1:B:638:PRO:HD3	1.86	0.56
1:C:2979:ARG:HG3	1:C:3039:THR:HG22	1.87	0.56
1:D:680:ASP:OD1	1:D:801:ARG:NH2	2.38	0.56
1:B:808:HIS:CG	1:B:832:LEU:HD23	2.41	0.56
1:B:3271:GLU:HA	1:B:3274:ASN:HD21	1.70	0.56
1:B:4489:GLN:NE2	1:B:4493:ASN:OD1	2.33	0.56
1:C:827:LEU:HB2	1:C:830:GLU:HB2	1.88	0.56
1:C:2202:TYR:O	1:C:2206:ILE:HG12	2.05	0.56
1:C:2277:CYS:SG	1:C:2280:LEU:HD23	2.46	0.56
1:C:2589:LEU:O	1:C:2593:VAL:HG13	2.06	0.56
1:C:3043:ARG:NH2	1:C:3116:GLN:O	2.38	0.56
1:D:2277:CYS:SG	1:D:2280:LEU:HD23	2.46	0.56
1:B:670:TYR:HD1	1:B:1017:THR:HG21	1.70	0.56
1:B:1716:THR:O	1:B:1720:MET:HG3	2.05	0.56
1:C:2706:VAL:HG21	1:C:2785:TRP:NE1	2.20	0.56
1:C:3661:VAL:HG23	1:C:3666:GLN:HG2	1.88	0.56
1:D:601:LEU:HG	1:D:610:VAL:HG11	1.87	0.56
1:D:2212:LYS:NZ	1:D:2216:ASP:OD1	2.33	0.56
1:D:2979:ARG:HG3	1:D:3039:THR:HG22	1.87	0.56
1:A:3278:GLY:HA2	1:A:3281:LEU:HD23	1.88	0.56
1:C:2779:LEU:HD23	1:C:2782:MET:HE3	1.87	0.56
1:D:2593:VAL:HG12	1:D:2644:LEU:HG	1.87	0.56
1:A:808:HIS:CG	1:A:832:LEU:HD23	2.41	0.56
1:A:866:PRO:HG3	1:A:1009:ARG:HD3	1.88	0.56
1:A:2593:VAL:HG12	1:A:2644:LEU:HG	1.88	0.56
1:B:3661:VAL:HG23	1:B:3666:GLN:HG2	1.87	0.56
1:C:601:LEU:HG	1:C:610:VAL:HG11	1.87	0.56
1:C:3271:GLU:HA	1:C:3274:ASN:HD21	1.70	0.56
1:C:4604:LYS:HD2	1:C:4608:ARG:HH21	1.71	0.56
1:D:304:LYS:HB2	1:D:316:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:808:HIS:CG	1:D:832:LEU:HD23	2.41	0.56
1:B:827:LEU:HB2	1:B:830:GLU:HB2	1.88	0.56
1:B:3134:LEU:HB2	1:B:3162:PHE:CE2	2.41	0.56
1:D:827:LEU:HB2	1:D:830:GLU:HB2	1.88	0.56
1:D:4832:GLU:O	1:D:4843:ARG:NH2	2.21	0.56
1:B:1974:ASN:OD1	1:B:1975:MET:N	2.39	0.55
1:B:2333:PRO:HA	1:B:2336:ARG:HE	1.69	0.55
1:C:304:LYS:HB2	1:C:316:LEU:HD23	1.87	0.55
1:C:950:VAL:HG22	1:C:1064:LEU:HD13	1.87	0.55
1:C:2833:LEU:HB3	1:C:2837:LEU:HB3	1.87	0.55
1:D:4604:LYS:HD2	1:D:4608:ARG:HH21	1.71	0.55
1:A:304:LYS:HB2	1:A:316:LEU:HD23	1.87	0.55
1:A:1511:VAL:HG22	1:A:1518:LEU:HG	1.89	0.55
1:A:1793:GLN:NE2	1:A:1797:GLU:OE2	2.38	0.55
1:B:332:ARG:NH1	1:B:364:GLN:OE1	2.35	0.55
1:B:3116:GLN:OE1	1:B:3116:GLN:N	2.40	0.55
1:B:4854:VAL:HA	1:B:4858:LEU:HD12	1.88	0.55
1:A:562:LEU:HB3	1:A:600:LEU:HD13	1.89	0.55
1:A:1941:ARG:NH2	1:A:3609:TYR:O	2.38	0.55
1:A:2202:TYR:O	1:A:2206:ILE:HG12	2.05	0.55
1:B:866:PRO:HG3	1:B:1009:ARG:HD3	1.88	0.55
1:B:2779:LEU:HD23	1:B:2782:MET:HE3	1.87	0.55
1:C:808:HIS:CG	1:C:832:LEU:HD23	2.41	0.55
1:C:1974:ASN:OD1	1:C:1975:MET:N	2.39	0.55
1:C:3278:GLY:HA2	1:C:3281:LEU:HD23	1.88	0.55
1:D:2202:TYR:O	1:D:2206:ILE:HG12	2.05	0.55
1:D:2833:LEU:HB3	1:D:2837:LEU:HB3	1.87	0.55
1:A:3134:LEU:HB2	1:A:3162:PHE:CE2	2.41	0.55
1:A:3271:GLU:HA	1:A:3274:ASN:ND2	2.22	0.55
1:B:950:VAL:HG22	1:B:1064:LEU:HD13	1.87	0.55
1:D:950:VAL:HG22	1:D:1064:LEU:HD13	1.87	0.55
1:D:1511:VAL:HG22	1:D:1518:LEU:HG	1.89	0.55
1:D:3271:GLU:HA	1:D:3274:ASN:ND2	2.22	0.55
1:A:1974:ASN:OD1	1:A:1975:MET:N	2.39	0.55
1:C:3674:THR:O	1:C:3679:LYS:NZ	2.36	0.55
1:D:3661:VAL:HG23	1:D:3666:GLN:HG2	1.87	0.55
1:A:506:HIS:HB3	1:A:564:ARG:NH1	2.22	0.55
1:A:601:LEU:HG	1:A:610:VAL:HG11	1.87	0.55
1:A:3074:ASN:OD1	1:A:3075:LEU:N	2.40	0.55
1:A:3271:GLU:HA	1:A:3274:ASN:HD21	1.70	0.55
1:B:2589:LEU:O	1:B:2593:VAL:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:670:TYR:HD1	1:C:1017:THR:HG21	1.70	0.55
1:C:4854:VAL:HA	1:C:4858:LEU:HD12	1.88	0.55
1:D:562:LEU:HB3	1:D:600:LEU:HD13	1.89	0.55
1:D:1257:GLN:HG3	1:D:1595:LEU:HD11	1.88	0.55
1:D:2442:MET:HE1	1:D:2498:ALA:HB1	1.89	0.55
1:A:827:LEU:HB2	1:A:830:GLU:HB2	1.88	0.55
1:A:1070:ASP:HB3	1:D:2995:HIS:HE2	1.71	0.55
1:B:4604:LYS:HD2	1:B:4608:ARG:HH21	1.71	0.55
1:C:562:LEU:HB3	1:C:600:LEU:HD13	1.89	0.55
1:C:3134:LEU:HB2	1:C:3162:PHE:CE2	2.41	0.55
1:D:1974:ASN:OD1	1:D:1975:MET:N	2.39	0.55
1:B:4580:THR:OG1	1:B:4733:HIS:NE2	2.26	0.55
1:C:1957:LEU:CG	1:C:1960:ARG:HH12	2.17	0.55
1:D:3134:LEU:HB2	1:D:3162:PHE:CE2	2.41	0.55
1:B:3074:ASN:OD1	1:B:3075:LEU:N	2.40	0.55
1:C:506:HIS:HB3	1:C:564:ARG:NH1	2.22	0.55
1:C:3838:ASP:OD1	1:C:3839:LEU:N	2.40	0.55
1:D:4854:VAL:HA	1:D:4858:LEU:HD12	1.88	0.55
1:A:2277:CYS:SG	1:A:2280:LEU:HD23	2.46	0.55
1:A:3116:GLN:OE1	1:A:3116:GLN:N	2.40	0.55
1:C:1511:VAL:HG22	1:C:1518:LEU:HG	1.89	0.55
1:C:2765:GLU:HA	1:C:2768:LYS:HG2	1.89	0.55
1:D:506:HIS:HB3	1:D:564:ARG:NH1	2.22	0.55
1:D:3072:MET:HE3	1:D:3136:SER:HA	1.89	0.55
1:D:3271:GLU:HA	1:D:3274:ASN:HD21	1.70	0.55
1:D:3278:GLY:HA2	1:D:3281:LEU:HD23	1.88	0.55
1:A:3176:ASP:O	1:A:3185:ASN:ND2	2.31	0.54
1:A:3661:VAL:HG23	1:A:3666:GLN:HG2	1.87	0.54
1:B:506:HIS:HB3	1:B:564:ARG:NH1	2.22	0.54
1:B:2277:CYS:SG	1:B:2280:LEU:HD23	2.46	0.54
1:B:3072:MET:HE3	1:B:3136:SER:HA	1.89	0.54
1:B:3271:GLU:HA	1:B:3274:ASN:ND2	2.22	0.54
1:C:1257:GLN:HG3	1:C:1595:LEU:HD11	1.88	0.54
1:C:2426:LEU:HD23	1:D:143:LEU:HD22	1.88	0.54
1:C:3271:GLU:HA	1:C:3274:ASN:ND2	2.22	0.54
1:D:3116:GLN:OE1	1:D:3116:GLN:N	2.40	0.54
1:A:2765:GLU:HA	1:A:2768:LYS:HG2	1.89	0.54
1:A:3838:ASP:OD1	1:A:3839:LEU:N	2.40	0.54
1:C:3074:ASN:OD1	1:C:3075:LEU:N	2.40	0.54
1:D:1039:ASP:OD1	1:D:1042:THR:OG1	2.25	0.54
1:D:3074:ASN:OD1	1:D:3075:LEU:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3838:ASP:OD1	1:D:3839:LEU:N	2.40	0.54
1:A:3729:ALA:HA	1:A:3732:HIS:CD2	2.43	0.54
1:A:4604:LYS:HD2	1:A:4608:ARG:HH21	1.71	0.54
1:A:4854:VAL:HA	1:A:4858:LEU:HD12	1.88	0.54
1:B:1511:VAL:HG22	1:B:1518:LEU:HG	1.89	0.54
1:B:3278:GLY:HA2	1:B:3281:LEU:HD23	1.88	0.54
1:C:3116:GLN:N	1:C:3116:GLN:OE1	2.40	0.54
1:D:3729:ALA:HA	1:D:3732:HIS:CD2	2.43	0.54
1:A:42:PHE:HZ	1:A:459:LEU:HG	1.73	0.54
1:A:1257:GLN:HG3	1:A:1595:LEU:HD11	1.88	0.54
1:A:2589:LEU:O	1:A:2593:VAL:HG13	2.06	0.54
1:A:3072:MET:HE3	1:A:3136:SER:HA	1.89	0.54
1:B:562:LEU:HB3	1:B:600:LEU:HD13	1.89	0.54
1:C:3729:ALA:HA	1:C:3732:HIS:CD2	2.43	0.54
1:A:2779:LEU:HD23	1:A:2782:MET:HE3	1.89	0.54
1:B:2833:LEU:HD22	1:B:2837:LEU:HD23	1.89	0.54
1:B:3838:ASP:OD1	1:B:3839:LEU:N	2.40	0.54
1:A:1024:VAL:HG23	1:A:1025:LYS:HD3	1.90	0.54
1:A:1031:ARG:NH2	1:A:1046:ASN:OD1	2.41	0.54
1:A:1898:LEU:HD13	1:A:1902:VAL:HG12	1.90	0.54
1:A:4580:THR:OG1	1:A:4733:HIS:NE2	2.26	0.54
1:B:42:PHE:HZ	1:B:459:LEU:HG	1.73	0.54
1:B:253:GLY:O	1:B:257:ARG:HG3	2.08	0.54
1:B:1024:VAL:HG23	1:B:1025:LYS:HD3	1.90	0.54
1:D:2833:LEU:HD22	1:D:2837:LEU:HD23	1.89	0.54
1:B:2593:VAL:HG11	1:B:2640:LEU:HD12	1.90	0.54
1:D:253:GLY:O	1:D:257:ARG:HG3	2.08	0.54
1:D:4107:GLU:OE2	1:D:4147:ARG:NH1	2.41	0.54
1:D:4580:THR:OG1	1:D:4733:HIS:NE2	2.26	0.54
1:A:1980:LYS:HZ1	1:A:3632:GLU:HG2	1.73	0.53
1:A:2833:LEU:HD22	1:A:2837:LEU:HD23	1.89	0.53
1:A:4618:THR:OG1	1:A:4619:GLU:OE1	2.26	0.53
1:D:1024:VAL:HG23	1:D:1025:LYS:HD3	1.90	0.53
1:D:4618:THR:OG1	1:D:4619:GLU:OE1	2.26	0.53
1:A:4107:GLU:OE2	1:A:4147:ARG:NH1	2.41	0.53
1:B:1124:PRO:HD2	1:B:1594:VAL:HG23	1.91	0.53
1:B:2995:HIS:HE2	1:C:1070:ASP:HB3	1.73	0.53
1:C:1124:PRO:HD2	1:C:1594:VAL:HG23	1.91	0.53
1:C:1980:LYS:HZ1	1:C:3632:GLU:HG2	1.74	0.53
1:D:1635:GLU:OE1	1:D:1637:ARG:NH1	2.41	0.53
1:D:2765:GLU:HA	1:D:2768:LYS:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1124:PRO:HD2	1:A:1594:VAL:HG23	1.91	0.53
1:A:4832:GLU:O	1:A:4843:ARG:NH2	2.21	0.53
1:C:4107:GLU:OE2	1:C:4147:ARG:NH1	2.41	0.53
1:A:2995:HIS:HE2	1:B:1070:ASP:HB3	1.74	0.53
1:C:919:VAL:HG22	1:C:920:GLU:H	1.74	0.53
1:C:2593:VAL:HG11	1:C:2640:LEU:HD12	1.90	0.53
1:C:2706:VAL:HG21	1:C:2785:TRP:HE1	1.74	0.53
1:D:1031:ARG:NH2	1:D:1046:ASN:OD1	2.41	0.53
1:B:1898:LEU:HD13	1:B:1902:VAL:HG12	1.90	0.53
1:B:3729:ALA:HA	1:B:3732:HIS:CD2	2.43	0.53
1:D:3803:LEU:HB2	1:D:3884:SER:HB2	1.91	0.53
1:A:3803:LEU:HB2	1:A:3884:SER:HB2	1.91	0.53
1:B:919:VAL:HG22	1:B:920:GLU:H	1.74	0.53
1:B:2706:VAL:HG21	1:B:2785:TRP:HE1	1.74	0.53
1:B:3074:ASN:O	1:B:3078:GLY:HA3	2.08	0.53
1:C:3074:ASN:O	1:C:3078:GLY:HA3	2.08	0.53
1:C:3803:LEU:HB2	1:C:3884:SER:HB2	1.91	0.53
1:D:42:PHE:HZ	1:D:459:LEU:HG	1.73	0.53
1:A:643:LEU:O	1:A:645:GLN:NE2	2.42	0.53
1:B:1257:GLN:HG3	1:B:1595:LEU:HD11	1.88	0.53
1:B:2426:LEU:HD23	1:C:143:LEU:HD22	1.90	0.53
1:B:3803:LEU:HB2	1:B:3884:SER:HB2	1.91	0.53
1:C:1024:VAL:HG23	1:C:1025:LYS:HD3	1.90	0.53
1:C:3072:MET:HE3	1:C:3136:SER:HA	1.91	0.53
1:C:4618:THR:OG1	1:C:4619:GLU:OE1	2.26	0.53
1:D:919:VAL:HG22	1:D:920:GLU:H	1.74	0.53
1:D:1980:LYS:HZ1	1:D:3632:GLU:HG2	1.74	0.53
1:A:2706:VAL:HG21	1:A:2785:TRP:HE1	1.74	0.53
1:A:3179:ASN:O	1:A:3185:ASN:ND2	2.42	0.53
1:B:643:LEU:O	1:B:645:GLN:NE2	2.42	0.53
1:D:3074:ASN:O	1:D:3078:GLY:HA3	2.08	0.53
1:A:3074:ASN:O	1:A:3078:GLY:HA3	2.08	0.53
1:B:1013:ARG:HG2	1:B:1013:ARG:NH1	2.24	0.53
1:B:4107:GLU:OE2	1:B:4147:ARG:NH1	2.41	0.53
1:D:332:ARG:NH1	1:D:364:GLN:OE1	2.36	0.53
1:A:4819:VAL:HG12	1:A:4830:GLU:HG3	1.90	0.53
1:B:2102:LEU:O	1:B:2105:THR:HG22	2.09	0.53
1:B:4819:VAL:HG12	1:B:4830:GLU:HG3	1.90	0.53
1:C:42:PHE:HZ	1:C:459:LEU:HG	1.73	0.53
1:C:2833:LEU:HD22	1:C:2837:LEU:HD23	1.89	0.53
1:D:1124:PRO:HD2	1:D:1594:VAL:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2706:VAL:HG21	1:D:2785:TRP:HE1	1.74	0.53
1:A:1891:GLU:HB3	1:A:1895:GLN:HG3	1.91	0.52
1:A:2593:VAL:HG11	1:A:2640:LEU:HD12	1.90	0.52
1:A:3700:HIS:CE1	1:A:3702:GLU:HG2	2.44	0.52
1:B:3176:ASP:O	1:B:3185:ASN:ND2	2.31	0.52
1:B:4618:THR:OG1	1:B:4619:GLU:OE1	2.26	0.52
1:C:520:ARG:O	1:C:523:GLY:N	2.43	0.52
1:C:3677:THR:HB	1:C:3679:LYS:HZ2	1.74	0.52
1:D:3317:THR:H	1:D:3320:LEU:HD23	1.75	0.52
1:D:3700:HIS:CE1	1:D:3702:GLU:HG2	2.44	0.52
1:D:4607:ALA:HB1	1:D:4649:VAL:HG21	1.91	0.52
1:A:253:GLY:O	1:A:257:ARG:HG3	2.08	0.52
1:C:1031:ARG:NH2	1:C:1046:ASN:OD1	2.41	0.52
1:D:643:LEU:O	1:D:645:GLN:NE2	2.42	0.52
1:D:1891:GLU:HB3	1:D:1895:GLN:HG3	1.92	0.52
1:D:1898:LEU:HD13	1:D:1902:VAL:HG12	1.90	0.52
1:D:2717:LEU:O	1:D:2721:ILE:HG12	2.10	0.52
1:A:919:VAL:HG22	1:A:920:GLU:H	1.74	0.52
1:A:4607:ALA:HB1	1:A:4649:VAL:HG21	1.91	0.52
1:C:1039:ASP:OD1	1:C:1042:THR:OG1	2.25	0.52
1:A:202:HIS:HD2	1:A:203:VAL:N	2.08	0.52
1:A:1091:GLU:HB3	1:A:1094:TYR:HD2	1.75	0.52
1:B:3166:PHE:CE1	1:B:3168:VAL:HB	2.45	0.52
1:C:253:GLY:O	1:C:257:ARG:HG3	2.08	0.52
1:C:643:LEU:O	1:C:645:GLN:NE2	2.42	0.52
1:C:1891:GLU:HB3	1:C:1895:GLN:HG3	1.91	0.52
1:C:2717:LEU:O	1:C:2721:ILE:HG12	2.10	0.52
1:A:3317:THR:H	1:A:3320:LEU:HD23	1.75	0.52
1:A:4011:GLU:HG2	1:A:4121:LEU:HD22	1.92	0.52
1:B:520:ARG:O	1:B:523:GLY:N	2.42	0.52
1:B:1980:LYS:HZ1	1:B:3632:GLU:HG2	1.73	0.52
1:B:2241:ASP:OD2	1:B:2297:ARG:NH2	2.38	0.52
1:B:2717:LEU:O	1:B:2721:ILE:HG12	2.10	0.52
1:B:3740:VAL:HG13	1:B:3758:THR:HG22	1.92	0.52
1:C:1013:ARG:HG2	1:C:1013:ARG:NH1	2.24	0.52
1:C:1635:GLU:OE1	1:C:1637:ARG:NH1	2.41	0.52
1:C:1898:LEU:HD13	1:C:1902:VAL:HG12	1.90	0.52
1:C:3317:THR:H	1:C:3320:LEU:HD23	1.75	0.52
1:C:4011:GLU:HG2	1:C:4121:LEU:HD22	1.92	0.52
1:D:2593:VAL:HG11	1:D:2640:LEU:HD12	1.90	0.52
1:A:3166:PHE:CE1	1:A:3168:VAL:HB	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:PHE:CE2	1:B:522:ALA:HB1	2.45	0.52
1:B:1031:ARG:NH2	1:B:1046:ASN:OD1	2.41	0.52
1:B:3700:HIS:CE1	1:B:3702:GLU:HG2	2.44	0.52
1:C:202:HIS:HD2	1:C:203:VAL:N	2.08	0.52
1:C:514:PHE:CE2	1:C:522:ALA:HB1	2.45	0.52
1:C:4827:ILE:O	1:C:4831:ILE:HG12	2.10	0.52
1:D:520:ARG:O	1:D:523:GLY:N	2.43	0.52
1:D:4011:GLU:HG2	1:D:4121:LEU:HD22	1.92	0.52
1:A:514:PHE:CE2	1:A:522:ALA:HB1	2.45	0.52
1:A:3740:VAL:HG13	1:A:3758:THR:HG22	1.92	0.52
1:B:2765:GLU:HA	1:B:2768:LYS:HG2	1.89	0.52
1:C:2102:LEU:O	1:C:2105:THR:HG22	2.09	0.52
1:D:1114:ARG:NH1	1:D:1128:LEU:O	2.43	0.52
1:D:2102:LEU:O	1:D:2105:THR:HG22	2.09	0.52
1:B:1039:ASP:OD1	1:B:1042:THR:OG1	2.25	0.52
1:B:4011:GLU:HG2	1:B:4121:LEU:HD22	1.92	0.52
1:C:313:ASN:HD21	1:C:390:LYS:NZ	2.07	0.52
1:A:313:ASN:HD21	1:A:390:LYS:NZ	2.07	0.52
1:A:520:ARG:O	1:A:523:GLY:N	2.42	0.52
1:A:1013:ARG:HG2	1:A:1013:ARG:NH1	2.24	0.52
1:A:1635:GLU:OE1	1:A:1637:ARG:NH1	2.41	0.52
1:A:2102:LEU:O	1:A:2105:THR:HG22	2.09	0.52
1:A:3215:MET:O	1:A:3219:VAL:HG23	2.10	0.52
1:B:202:HIS:HD2	1:B:203:VAL:N	2.08	0.52
1:B:313:ASN:HD21	1:B:390:LYS:NZ	2.07	0.52
1:B:2442:MET:HE1	1:B:2498:ALA:HB1	1.91	0.52
1:C:3166:PHE:CE1	1:C:3168:VAL:HB	2.45	0.52
1:C:3700:HIS:CE1	1:C:3702:GLU:HG2	2.44	0.52
1:C:4819:VAL:HG12	1:C:4830:GLU:HG3	1.91	0.52
1:D:235:ARG:NH2	1:D:412:GLU:OE2	2.25	0.52
1:D:1091:GLU:HB3	1:D:1094:TYR:HD2	1.75	0.52
1:A:2717:LEU:O	1:A:2721:ILE:HG12	2.09	0.52
1:B:1091:GLU:HB3	1:B:1094:TYR:HD2	1.75	0.52
1:B:3043:ARG:NE	1:B:3120:ASP:OD2	2.43	0.52
1:A:1114:ARG:NH1	1:A:1128:LEU:O	2.43	0.51
1:B:1891:GLU:HB3	1:B:1895:GLN:HG3	1.92	0.51
1:C:67:PHE:HB3	1:C:121:LEU:HD22	1.91	0.51
1:C:4607:ALA:HB1	1:C:4649:VAL:HG21	1.91	0.51
1:D:202:HIS:HD2	1:D:203:VAL:N	2.08	0.51
1:D:3166:PHE:CE1	1:D:3168:VAL:HB	2.45	0.51
1:A:1825:PHE:CE1	1:A:1842:ILE:HG12	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3215:MET:O	1:B:3219:VAL:HG23	2.10	0.51
1:B:4778:VAL:O	1:B:4782:THR:HG23	2.10	0.51
1:C:1004:HIS:NE2	1:C:1033:VAL:O	2.42	0.51
1:D:849:ASP:OD1	1:D:1214:ARG:NE	2.43	0.51
1:D:3215:MET:O	1:D:3219:VAL:HG23	2.10	0.51
1:D:4819:VAL:HG12	1:D:4830:GLU:HG3	1.90	0.51
1:D:4827:ILE:O	1:D:4831:ILE:HG12	2.10	0.51
1:B:2914:THR:N	1:B:2915:PRO:HD2	2.26	0.51
1:B:3179:ASN:O	1:B:3185:ASN:ND2	2.42	0.51
1:C:1091:GLU:HB3	1:C:1094:TYR:HD2	1.75	0.51
1:C:1304:LEU:HB3	1:C:1586:LEU:HD11	1.92	0.51
1:C:3740:VAL:HG13	1:C:3758:THR:HG22	1.92	0.51
1:C:4695:SER:HA	1:C:4698:LEU:HD12	1.93	0.51
1:D:67:PHE:HB3	1:D:121:LEU:HD22	1.91	0.51
1:D:1013:ARG:HG2	1:D:1013:ARG:NH1	2.24	0.51
1:A:67:PHE:HB3	1:A:121:LEU:HD22	1.91	0.51
1:A:4827:ILE:O	1:A:4831:ILE:HG12	2.10	0.51
1:D:4778:VAL:O	1:D:4782:THR:HG23	2.10	0.51
1:B:1304:LEU:HB3	1:B:1586:LEU:HD11	1.92	0.51
1:B:3317:THR:H	1:B:3320:LEU:HD23	1.75	0.51
1:B:4827:ILE:O	1:B:4831:ILE:HG12	2.10	0.51
1:D:313:ASN:HD21	1:D:390:LYS:NZ	2.07	0.51
1:D:1825:PHE:CE1	1:D:1842:ILE:HG12	2.46	0.51
1:D:3740:VAL:HG13	1:D:3758:THR:HG22	1.92	0.51
1:B:678:MET:SD	1:B:812:LYS:NZ	2.84	0.51
1:A:2426:LEU:HD23	1:B:143:LEU:HD22	1.91	0.51
1:B:4695:SER:HA	1:B:4698:LEU:HD12	1.93	0.51
1:C:1825:PHE:CE1	1:C:1842:ILE:HG12	2.46	0.51
1:D:4695:SER:HA	1:D:4698:LEU:HD12	1.93	0.51
1:A:2442:MET:HE1	1:A:2498:ALA:HB1	1.93	0.51
1:A:4778:VAL:O	1:A:4782:THR:HG23	2.10	0.51
1:B:3976:LYS:HB2	1:B:4094:ILE:HG12	1.93	0.51
1:A:235:ARG:NH2	1:A:412:GLU:OE2	2.25	0.51
1:B:235:ARG:NH2	1:B:412:GLU:OE2	2.25	0.51
1:B:969:ASN:OD1	1:B:970:TYR:N	2.44	0.51
1:B:1825:PHE:CE1	1:B:1842:ILE:HG12	2.46	0.51
1:C:801:ARG:HA	1:C:1617:TRP:O	2.11	0.51
1:C:969:ASN:OD1	1:C:970:TYR:N	2.44	0.51
1:D:514:PHE:CE2	1:D:522:ALA:HB1	2.45	0.51
1:A:1304:LEU:HB3	1:A:1586:LEU:HD11	1.92	0.51
1:A:1435:GLY:HA2	1:D:2831:VAL:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1161:VAL:HG21	1:C:1225:LYS:HD2	1.93	0.51
1:C:3976:LYS:HB2	1:C:4094:ILE:HG12	1.93	0.51
1:D:2937:HIS:HA	1:D:3014:LEU:HD21	1.93	0.51
1:A:1039:ASP:OD1	1:A:1042:THR:OG1	2.25	0.50
1:B:67:PHE:HB3	1:B:121:LEU:HD22	1.91	0.50
1:B:1635:GLU:OE1	1:B:1637:ARG:NH1	2.41	0.50
1:B:3250:TRP:CZ3	1:B:3309:LYS:HB3	2.46	0.50
1:B:4607:ALA:HB1	1:B:4649:VAL:HG21	1.91	0.50
1:C:3215:MET:O	1:C:3219:VAL:HG23	2.10	0.50
1:D:713:TRP:HZ2	1:D:1251:LEU:HD21	1.76	0.50
1:A:3901:GLN:OE1	1:A:3904:ARG:NH2	2.45	0.50
1:B:2599:LEU:HB3	1:B:2661:LEU:HD21	1.94	0.50
1:B:4831:ILE:HB	1:B:4843:ARG:HH22	1.76	0.50
1:C:3043:ARG:NE	1:C:3120:ASP:OD2	2.43	0.50
1:C:3250:TRP:CZ3	1:C:3309:LYS:HB3	2.46	0.50
1:A:4831:ILE:HB	1:A:4843:ARG:HH22	1.77	0.50
1:B:801:ARG:HA	1:B:1617:TRP:O	2.11	0.50
1:B:2937:HIS:HA	1:B:3014:LEU:HD21	1.93	0.50
1:C:849:ASP:OD1	1:C:1214:ARG:NE	2.43	0.50
1:D:801:ARG:HA	1:D:1617:TRP:O	2.11	0.50
1:D:1304:LEU:HB3	1:D:1586:LEU:HD11	1.92	0.50
1:A:1431:ARG:HA	1:A:1505:LEU:O	2.12	0.50
1:C:713:TRP:HZ2	1:C:1251:LEU:HD21	1.76	0.50
1:C:1431:ARG:HA	1:C:1505:LEU:O	2.12	0.50
1:C:2937:HIS:HA	1:C:3014:LEU:HD21	1.93	0.50
1:C:3179:ASN:O	1:C:3185:ASN:ND2	2.42	0.50
1:C:3901:GLN:OE1	1:C:3904:ARG:NH2	2.45	0.50
1:D:925:PRO:HB2	1:D:928:GLU:HB3	1.94	0.50
1:D:1718:ARG:NH1	1:D:1758:ARG:HD3	2.27	0.50
1:D:4042:VAL:HB	1:D:4077:THR:HB	1.93	0.50
1:A:849:ASP:OD1	1:A:1214:ARG:NE	2.43	0.50
1:A:992:GLN:HA	1:A:995:MET:HE2	1.94	0.50
1:A:2914:THR:N	1:A:2915:PRO:HD2	2.26	0.50
1:B:925:PRO:HB2	1:B:928:GLU:HB3	1.94	0.50
1:C:1074:ARG:NH2	1:C:1076:GLU:OE1	2.43	0.50
1:D:1161:VAL:HG21	1:D:1225:LYS:HD2	1.93	0.50
1:D:3793:LEU:HD21	1:D:3843:LEU:HD21	1.94	0.50
1:D:4048:PHE:CE2	1:D:4052:MET:HE3	2.46	0.50
1:A:3250:TRP:CZ3	1:A:3309:LYS:HB3	2.46	0.50
1:B:713:TRP:HZ2	1:B:1251:LEU:HD21	1.77	0.50
1:B:3793:LEU:HD21	1:B:3843:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3901:GLN:OE1	1:B:3904:ARG:NH2	2.45	0.50
1:C:677:LEU:HD11	1:C:800:VAL:HB	1.94	0.50
1:C:3176:ASP:O	1:C:3185:ASN:ND2	2.31	0.50
1:C:4580:THR:OG1	1:C:4733:HIS:NE2	2.26	0.50
1:C:4831:ILE:HB	1:C:4843:ARG:HH22	1.76	0.50
1:D:1074:ARG:NH2	1:D:1076:GLU:OE1	2.43	0.50
1:D:1083:GLU:OE1	1:D:1254:ARG:NH1	2.45	0.50
1:D:1429:SER:OG	1:D:1556:GLU:HB2	2.12	0.50
1:A:678:MET:SD	1:A:812:LYS:NZ	2.84	0.50
1:A:1718:ARG:NH1	1:A:1758:ARG:HD3	2.27	0.50
1:A:2599:LEU:HB3	1:A:2661:LEU:HD21	1.94	0.50
1:A:4199:GLU:HG2	1:A:4597:LEU:HD13	1.94	0.50
1:A:4695:SER:HA	1:A:4698:LEU:HD12	1.93	0.50
1:B:1431:ARG:HA	1:B:1505:LEU:O	2.12	0.50
1:B:1718:ARG:NH1	1:B:1758:ARG:HD3	2.27	0.50
1:B:2442:MET:CE	1:B:2498:ALA:HB1	2.42	0.50
1:C:925:PRO:HB2	1:C:928:GLU:HB3	1.94	0.50
1:A:1083:GLU:OE1	1:A:1254:ARG:NH1	2.45	0.50
1:A:2874:TYR:CZ	1:A:2882:LYS:HD2	2.47	0.50
1:B:674:TYR:OH	1:B:676:GLU:OE2	2.26	0.50
1:C:810:GLU:HG2	1:C:1614:ARG:HA	1.94	0.50
1:C:1718:ARG:NH1	1:C:1758:ARG:HD3	2.27	0.50
1:C:2914:THR:N	1:C:2915:PRO:HD2	2.26	0.50
1:C:4118:PHE:HA	1:C:4121:LEU:HD12	1.94	0.50
1:D:3901:GLN:OE1	1:D:3904:ARG:NH2	2.45	0.50
1:A:387:ILE:HG22	1:A:389:ARG:HG3	1.94	0.50
1:B:1004:HIS:NE2	1:B:1033:VAL:O	2.42	0.50
1:B:1415:ASP:OD2	1:B:1559:ARG:NH2	2.43	0.50
1:C:235:ARG:NH2	1:C:412:GLU:OE2	2.25	0.50
1:C:992:GLN:HA	1:C:995:MET:HE2	1.94	0.50
1:C:1083:GLU:OE1	1:C:1254:ARG:NH1	2.45	0.50
1:D:3179:ASN:O	1:D:3185:ASN:ND2	2.42	0.50
1:A:713:TRP:HZ2	1:A:1251:LEU:HD21	1.76	0.49
1:A:925:PRO:HB2	1:A:928:GLU:HB3	1.94	0.49
1:A:3303:SER:O	1:A:3306:ILE:HG22	2.12	0.49
1:A:4929:ASP:HB3	1:A:4932:GLU:HG2	1.94	0.49
1:B:4042:VAL:HB	1:B:4077:THR:HB	1.93	0.49
1:C:2599:LEU:HB3	1:C:2661:LEU:HD21	1.94	0.49
1:A:969:ASN:OD1	1:A:970:TYR:N	2.44	0.49
1:A:2937:HIS:HA	1:A:3014:LEU:HD21	1.93	0.49
1:B:1429:SER:OG	1:B:1556:GLU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2480:VAL:HG23	1:B:2483:PHE:HB3	1.94	0.49
1:C:1114:ARG:NH1	1:C:1128:LEU:O	2.43	0.49
1:C:2279:MET:SD	1:C:2280:LEU:HD22	2.52	0.49
1:C:3325:LYS:HA	1:C:3328:LYS:HG2	1.94	0.49
1:C:4778:VAL:O	1:C:4782:THR:HG23	2.11	0.49
1:D:992:GLN:HA	1:D:995:MET:HE2	1.94	0.49
1:D:2279:MET:SD	1:D:2280:LEU:HD22	2.52	0.49
1:D:3176:ASP:O	1:D:3185:ASN:ND2	2.31	0.49
1:D:3250:TRP:CZ3	1:D:3309:LYS:HB3	2.46	0.49
1:D:4199:GLU:HG2	1:D:4597:LEU:HD13	1.94	0.49
1:A:1981:ASP:N	1:A:1981:ASP:OD1	2.45	0.49
1:B:2556:SER:HB3	1:B:2569:ILE:HG21	1.93	0.49
1:B:4118:PHE:HA	1:B:4121:LEU:HD12	1.94	0.49
1:C:1167:ASP:HB3	1:C:1172:THR:HG22	1.94	0.49
1:D:3976:LYS:HB2	1:D:4094:ILE:HG12	1.93	0.49
1:A:2279:MET:SD	1:A:2280:LEU:HD22	2.52	0.49
1:B:677:LEU:HD11	1:B:800:VAL:HB	1.94	0.49
1:D:387:ILE:HG22	1:D:389:ARG:HG3	1.94	0.49
1:D:969:ASN:OD1	1:D:970:TYR:N	2.44	0.49
1:D:1981:ASP:N	1:D:1981:ASP:OD1	2.45	0.49
1:D:4831:ILE:HB	1:D:4843:ARG:HH22	1.76	0.49
1:A:801:ARG:HA	1:A:1617:TRP:O	2.11	0.49
1:A:1074:ARG:NH2	1:A:1076:GLU:OE1	2.43	0.49
1:A:2442:MET:CE	1:A:2498:ALA:HB1	2.42	0.49
1:A:2556:SER:HB3	1:A:2569:ILE:HG21	1.93	0.49
1:A:4049:HIS:ND1	1:A:4067:LEU:HD11	2.28	0.49
1:B:1161:VAL:HG21	1:B:1225:LYS:HD2	1.93	0.49
1:B:2279:MET:SD	1:B:2280:LEU:HD22	2.52	0.49
1:C:1429:SER:OG	1:C:1556:GLU:HB2	2.12	0.49
1:D:2914:THR:N	1:D:2915:PRO:HD2	2.26	0.49
1:A:3976:LYS:HB2	1:A:4094:ILE:HG12	1.93	0.49
1:B:558:LEU:HG	1:B:571:ILE:HG23	1.95	0.49
1:B:810:GLU:HG2	1:B:1614:ARG:HA	1.94	0.49
1:B:849:ASP:OD1	1:B:1214:ARG:NE	2.43	0.49
1:B:2406:MET:O	1:B:2410:HIS:ND1	2.46	0.49
1:B:2496:LEU:HD23	1:B:2520:LEU:HD13	1.95	0.49
1:B:3152:ARG:HH12	1:B:3233:HIS:HB3	1.78	0.49
1:C:2157:GLN:O	1:C:3615:ARG:NH2	2.46	0.49
1:C:2556:SER:HB3	1:C:2569:ILE:HG21	1.93	0.49
1:C:4049:HIS:ND1	1:C:4067:LEU:HD11	2.28	0.49
1:C:4818:TYR:HA	1:D:4848:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2480:VAL:HG23	1:D:2483:PHE:HB3	1.95	0.49
1:D:2556:SER:HB3	1:D:2569:ILE:HG21	1.93	0.49
1:D:3235:MET:O	1:D:3299:LEU:HD12	2.13	0.49
1:A:1118:SER:HB3	1:A:1204:VAL:HG11	1.94	0.49
1:A:1429:SER:OG	1:A:1556:GLU:HB2	2.12	0.49
1:A:2480:VAL:HG23	1:A:2483:PHE:HB3	1.94	0.49
1:B:4275:THR:HG22	1:B:4278:ASP:H	1.78	0.49
1:C:387:ILE:HG22	1:C:389:ARG:HG3	1.94	0.49
1:C:1114:ARG:HG2	1:C:1138:ASP:HB2	1.95	0.49
1:C:2874:TYR:CZ	1:C:2882:LYS:HD2	2.47	0.49
1:C:3793:LEU:HD21	1:C:3843:LEU:HD21	1.94	0.49
1:C:4042:VAL:HB	1:C:4077:THR:HB	1.93	0.49
1:D:2157:GLN:O	1:D:3615:ARG:NH2	2.46	0.49
1:D:2442:MET:CE	1:D:2498:ALA:HB1	2.42	0.49
1:D:2599:LEU:HB3	1:D:2661:LEU:HD21	1.94	0.49
1:D:4049:HIS:ND1	1:D:4067:LEU:HD11	2.28	0.49
1:A:1689:ILE:HG23	1:A:1703:TYR:CZ	2.48	0.49
1:A:2157:GLN:O	1:A:3615:ARG:NH2	2.46	0.49
1:A:4118:PHE:HA	1:A:4121:LEU:HD12	1.94	0.49
1:B:1083:GLU:OE1	1:B:1254:ARG:NH1	2.45	0.49
1:B:1167:ASP:HB3	1:B:1172:THR:HG22	1.94	0.49
1:B:3227:ARG:HG3	1:B:3229:THR:H	1.78	0.49
1:B:3303:SER:O	1:B:3306:ILE:HG22	2.12	0.49
1:B:4049:HIS:ND1	1:B:4067:LEU:HD11	2.28	0.49
1:C:490:GLN:HG2	1:C:495:ILE:HD13	1.95	0.49
1:C:756:SER:OG	1:C:769:ARG:HB2	2.13	0.49
1:C:886:ALA:HB1	1:C:933:LEU:HD11	1.95	0.49
1:C:2442:MET:CE	1:C:2498:ALA:HB1	2.42	0.49
1:C:3303:SER:O	1:C:3306:ILE:HG22	2.12	0.49
1:C:4199:GLU:HG2	1:C:4597:LEU:HD13	1.94	0.49
1:D:810:GLU:HG2	1:D:1614:ARG:HA	1.94	0.49
1:D:2874:TYR:CZ	1:D:2882:LYS:HD2	2.47	0.49
1:D:3152:ARG:HH12	1:D:3233:HIS:HB3	1.78	0.49
1:D:3303:SER:O	1:D:3306:ILE:HG22	2.12	0.49
1:A:1161:VAL:HG21	1:A:1225:LYS:HD2	1.93	0.49
1:A:4042:VAL:HB	1:A:4077:THR:HB	1.93	0.49
1:A:4275:THR:HG22	1:A:4278:ASP:H	1.78	0.49
1:B:1689:ILE:HG23	1:B:1703:TYR:CZ	2.48	0.49
1:C:558:LEU:HG	1:C:571:ILE:HG23	1.95	0.49
1:D:1118:SER:HB3	1:D:1204:VAL:HG11	1.94	0.49
1:D:4943:MET:HE2	1:D:4951:PHE:HD1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:SER:OG	1:A:769:ARG:HB2	2.13	0.49
1:A:886:ALA:HB1	1:A:933:LEU:HD11	1.95	0.49
1:A:3325:LYS:HA	1:A:3328:LYS:HG2	1.94	0.49
1:A:3793:LEU:HD21	1:A:3843:LEU:HD21	1.94	0.49
1:B:387:ILE:HG22	1:B:389:ARG:HG3	1.94	0.49
1:B:799:LYS:HG2	1:B:1618:LEU:HD11	1.95	0.49
1:C:1689:ILE:HG23	1:C:1703:TYR:CZ	2.48	0.49
1:C:2406:MET:O	1:C:2410:HIS:ND1	2.46	0.49
1:C:2496:LEU:HD23	1:C:2520:LEU:HD13	1.95	0.49
1:D:677:LEU:HD11	1:D:800:VAL:HB	1.94	0.49
1:D:799:LYS:HG2	1:D:1618:LEU:HD11	1.95	0.49
1:D:1167:ASP:HB3	1:D:1172:THR:HG22	1.94	0.49
1:D:2406:MET:O	1:D:2410:HIS:ND1	2.46	0.49
1:D:4118:PHE:HA	1:D:4121:LEU:HD12	1.94	0.49
1:A:558:LEU:HG	1:A:571:ILE:HG23	1.95	0.48
1:A:677:LEU:HD11	1:A:800:VAL:HB	1.94	0.48
1:A:799:LYS:HG2	1:A:1618:LEU:HD11	1.95	0.48
1:A:3227:ARG:HG3	1:A:3229:THR:H	1.78	0.48
1:B:28:ILE:O	1:B:31:GLU:HG3	2.13	0.48
1:B:756:SER:OG	1:B:769:ARG:HB2	2.13	0.48
1:B:1114:ARG:HG2	1:B:1138:ASP:HB2	1.95	0.48
1:B:3325:LYS:HA	1:B:3328:LYS:HG2	1.94	0.48
1:B:4199:GLU:HG2	1:B:4597:LEU:HD13	1.94	0.48
1:C:3235:MET:O	1:C:3299:LEU:HD12	2.13	0.48
1:D:226:GLY:HA2	1:D:356:TYR:HD2	1.78	0.48
1:D:756:SER:OG	1:D:769:ARG:HB2	2.13	0.48
1:D:1114:ARG:HG2	1:D:1138:ASP:HB2	1.95	0.48
1:D:4929:ASP:HB3	1:D:4932:GLU:HG2	1.94	0.48
1:A:2406:MET:O	1:A:2410:HIS:ND1	2.46	0.48
1:A:4831:ILE:HD12	1:A:4843:ARG:NH1	2.28	0.48
1:B:490:GLN:HG2	1:B:495:ILE:HD13	1.95	0.48
1:B:3025:ASP:O	1:B:3029:ILE:HD12	2.13	0.48
1:B:4831:ILE:HD12	1:B:4843:ARG:NH1	2.28	0.48
1:C:1981:ASP:OD1	1:C:1981:ASP:N	2.45	0.48
1:C:4048:PHE:CE2	1:C:4052:MET:HE3	2.48	0.48
1:D:28:ILE:O	1:D:31:GLU:HG3	2.13	0.48
1:D:1415:ASP:OD2	1:D:1559:ARG:NH2	2.43	0.48
1:D:1431:ARG:HA	1:D:1505:LEU:O	2.12	0.48
1:D:4831:ILE:HD12	1:D:4843:ARG:NH1	2.28	0.48
1:B:2549:LEU:HD13	1:B:2588:LEU:HD22	1.95	0.48
1:C:1945:ASN:O	1:C:1949:GLN:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3025:ASP:O	1:D:3029:ILE:HD12	2.14	0.48
1:A:338:LEU:HG	1:A:340:VAL:HG13	1.96	0.48
1:A:1167:ASP:HB3	1:A:1172:THR:HG22	1.94	0.48
1:A:1945:ASN:O	1:A:1949:GLN:HG2	2.13	0.48
1:A:2588:LEU:O	1:A:2592:LEU:HG	2.14	0.48
1:A:3068:LEU:O	1:A:3071:THR:OG1	2.28	0.48
1:A:3310:VAL:HG21	1:A:3314:LEU:HD23	1.95	0.48
1:B:1243:THR:HG22	1:B:1808:ASP:HB2	1.96	0.48
1:B:2874:TYR:CZ	1:B:2882:LYS:HD2	2.47	0.48
1:B:3855:GLN:NE2	1:B:3922:GLU:O	2.46	0.48
1:C:28:ILE:O	1:C:31:GLU:HG3	2.13	0.48
1:C:799:LYS:HG2	1:C:1618:LEU:HD11	1.95	0.48
1:C:1108:VAL:HB	1:C:1212:VAL:HB	1.96	0.48
1:C:2482:ASP:OD1	1:C:2483:PHE:N	2.47	0.48
1:D:2588:LEU:O	1:D:2592:LEU:HG	2.14	0.48
1:D:3325:LYS:HA	1:D:3328:LYS:HG2	1.94	0.48
1:A:28:ILE:O	1:A:31:GLU:HG3	2.13	0.48
1:A:1004:HIS:NE2	1:A:1033:VAL:O	2.42	0.48
1:A:1243:THR:HG22	1:A:1808:ASP:HB2	1.96	0.48
1:A:3677:THR:HB	1:A:3679:LYS:HZ2	1.78	0.48
1:C:226:GLY:HA2	1:C:356:TYR:HD2	1.78	0.48
1:C:4831:ILE:HD12	1:C:4843:ARG:NH1	2.28	0.48
1:A:1415:ASP:OD2	1:A:1559:ARG:NH2	2.43	0.48
1:A:2719:TYR:CZ	1:A:2723:LYS:HD2	2.49	0.48
1:B:61:ASP:OD2	1:B:417:ARG:NH2	2.42	0.48
1:B:506:HIS:HB3	1:B:564:ARG:HH12	1.79	0.48
1:B:886:ALA:HB1	1:B:933:LEU:HD11	1.95	0.48
1:B:3310:VAL:HG21	1:B:3314:LEU:HD23	1.95	0.48
1:B:4943:MET:HE2	1:B:4951:PHE:HD1	1.78	0.48
1:C:658:ASN:ND2	1:C:831:LYS:O	2.34	0.48
1:C:1243:THR:HG22	1:C:1808:ASP:HB2	1.96	0.48
1:D:579:LEU:HD22	1:D:586:LEU:HD23	1.96	0.48
1:D:1945:ASN:O	1:D:1949:GLN:HG2	2.13	0.48
1:D:2788:ARG:NE	1:D:2906:GLY:HA3	2.28	0.48
1:A:194:LEU:HD11	1:A:201:LEU:HB3	1.96	0.48
1:A:810:GLU:HG2	1:A:1614:ARG:HA	1.94	0.48
1:A:3235:MET:O	1:A:3299:LEU:HD12	2.13	0.48
1:A:3855:GLN:NE2	1:A:3922:GLU:O	2.46	0.48
1:B:579:LEU:HD22	1:B:586:LEU:HD23	1.96	0.48
1:B:1108:VAL:HB	1:B:1212:VAL:HB	1.96	0.48
1:C:678:MET:SD	1:C:812:LYS:NZ	2.84	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2480:VAL:HG23	1:C:2483:PHE:HB3	1.94	0.48
1:C:2719:TYR:CZ	1:C:2723:LYS:HD2	2.49	0.48
1:C:3939:ARG:HH12	1:D:173:GLU:HG2	1.77	0.48
1:C:4275:THR:HG22	1:C:4278:ASP:H	1.78	0.48
1:D:558:LEU:HG	1:D:571:ILE:HG23	1.95	0.48
1:D:1689:ILE:HG23	1:D:1703:TYR:CZ	2.48	0.48
1:D:2779:LEU:HD23	1:D:2782:MET:HE3	1.94	0.48
1:D:3855:GLN:NE2	1:D:3922:GLU:O	2.46	0.48
1:D:4275:THR:HG22	1:D:4278:ASP:H	1.78	0.48
1:A:2549:LEU:HD13	1:A:2588:LEU:HD22	1.95	0.48
1:A:4156:SER:HB3	1:A:4923:MET:HE1	1.96	0.48
2:G:90:GLY:HA2	1:C:638:PRO:HD3	1.96	0.48
2:H:24:VAL:HG22	2:H:48:LYS:HG2	1.96	0.48
1:B:271:ALA:HB2	1:B:488:LEU:HD12	1.96	0.48
1:B:489:PHE:CD2	1:B:494:MET:HG3	2.49	0.48
1:B:1074:ARG:NH2	1:B:1076:GLU:OE1	2.43	0.48
1:B:2062:ILE:O	1:B:2066:MET:HG2	2.14	0.48
1:B:2157:GLN:O	1:B:3615:ARG:NH2	2.46	0.48
1:C:489:PHE:CD2	1:C:494:MET:HG3	2.49	0.48
1:C:1016:TRP:CD2	1:C:1027:ARG:HG2	2.49	0.48
1:C:3152:ARG:HH12	1:C:3233:HIS:HB3	1.78	0.48
1:C:3939:ARG:NH1	1:D:173:GLU:HG2	2.29	0.48
1:C:4929:ASP:HB3	1:C:4932:GLU:HG2	1.94	0.48
1:D:1016:TRP:CD2	1:D:1027:ARG:HG2	2.49	0.48
1:D:1243:THR:HG22	1:D:1808:ASP:HB2	1.96	0.48
1:D:1896:MET:HB2	1:D:1896:MET:HE3	1.69	0.48
1:D:3043:ARG:NE	1:D:3120:ASP:OD2	2.43	0.48
1:A:271:ALA:HB2	1:A:488:LEU:HD12	1.96	0.48
1:A:490:GLN:HG2	1:A:495:ILE:HD13	1.95	0.48
1:A:1114:ARG:HG2	1:A:1138:ASP:HB2	1.95	0.48
1:A:3939:ARG:HH12	1:B:173:GLU:HG2	1.79	0.48
1:C:3068:LEU:O	1:C:3071:THR:OG1	2.28	0.48
1:D:2756:LEU:O	1:D:2758:LYS:HG2	2.14	0.48
1:A:281:ARG:NH1	1:A:345:GLU:OE2	2.44	0.48
1:B:1118:SER:HB3	1:B:1204:VAL:HG11	1.94	0.48
1:B:2588:LEU:O	1:B:2592:LEU:HG	2.14	0.48
1:A:579:LEU:HD22	1:A:586:LEU:HD23	1.96	0.47
1:A:2756:LEU:O	1:A:2758:LYS:HG2	2.14	0.47
1:A:3152:ARG:HH12	1:A:3233:HIS:HB3	1.78	0.47
1:A:4079:ASP:O	1:A:4082:GLU:HG3	2.14	0.47
1:B:194:LEU:HD11	1:B:201:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1945:ASN:O	1:B:1949:GLN:HG2	2.13	0.47
1:C:579:LEU:HD22	1:C:586:LEU:HD23	1.96	0.47
1:C:1118:SER:HB3	1:C:1204:VAL:HG11	1.94	0.47
1:C:1718:ARG:HD2	1:C:1830:ILE:O	2.14	0.47
1:C:2290:TRP:CZ2	1:C:2388:ILE:HG12	2.49	0.47
1:C:2588:LEU:O	1:C:2592:LEU:HG	2.14	0.47
1:D:506:HIS:HB3	1:D:564:ARG:HH12	1.79	0.47
1:D:624:ALA:HB2	1:D:1667:LEU:HD12	1.96	0.47
1:D:1431:ARG:NH1	1:D:1556:GLU:OE2	2.47	0.47
1:D:2062:ILE:O	1:D:2066:MET:HG2	2.14	0.47
1:D:2290:TRP:CZ2	1:D:2388:ILE:HG12	2.49	0.47
1:D:2496:LEU:HD23	1:D:2520:LEU:HD13	1.95	0.47
1:D:4079:ASP:O	1:D:4082:GLU:HG3	2.14	0.47
1:A:226:GLY:HA2	1:A:356:TYR:HD2	1.78	0.47
1:A:3102:LEU:HB2	1:A:3103:PRO:HD3	1.96	0.47
1:B:624:ALA:HB2	1:B:1667:LEU:HD12	1.96	0.47
1:B:1114:ARG:NH1	1:B:1128:LEU:O	2.43	0.47
1:B:1431:ARG:NH1	1:B:1556:GLU:OE2	2.47	0.47
1:B:2719:TYR:CZ	1:B:2723:LYS:HD2	2.49	0.47
1:B:3137:LEU:HB3	1:B:3159:LEU:HD12	1.96	0.47
1:B:4079:ASP:O	1:B:4082:GLU:HG3	2.14	0.47
1:C:281:ARG:NH1	1:C:345:GLU:OE2	2.44	0.47
1:C:2937:HIS:O	1:C:2941:LEU:HG	2.14	0.47
1:C:3025:ASP:O	1:C:3029:ILE:HD12	2.13	0.47
1:D:886:ALA:HB1	1:D:933:LEU:HD11	1.95	0.47
1:D:2753:VAL:O	1:D:2753:VAL:HG12	2.14	0.47
1:D:3122:ILE:HG22	1:D:3127:GLN:HG3	1.97	0.47
1:A:537:LEU:O	1:A:541:ILE:HG12	2.15	0.47
1:A:2482:ASP:OD1	1:A:2483:PHE:N	2.47	0.47
1:A:2496:LEU:HD23	1:A:2520:LEU:HD13	1.95	0.47
1:A:4818:TYR:HA	1:B:4848:ILE:HD11	1.95	0.47
1:A:4943:MET:HE1	1:A:4951:PHE:HD1	1.79	0.47
2:E:24:VAL:HG22	2:E:48:LYS:HG2	1.96	0.47
2:G:24:VAL:HG22	2:G:48:LYS:HG2	1.96	0.47
1:B:226:GLY:HA2	1:B:356:TYR:HD2	1.78	0.47
1:B:1718:ARG:HD2	1:B:1830:ILE:O	2.14	0.47
1:B:4929:ASP:HB3	1:B:4932:GLU:HG2	1.94	0.47
1:C:506:HIS:HB3	1:C:564:ARG:HH12	1.79	0.47
1:C:1431:ARG:NH1	1:C:1556:GLU:OE2	2.47	0.47
1:C:4079:ASP:O	1:C:4082:GLU:HG3	2.14	0.47
1:C:4684:GLU:HG2	1:C:4685:LYS:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:LEU:HG	1:D:340:VAL:HG13	1.96	0.47
1:D:489:PHE:CD2	1:D:494:MET:HG3	2.49	0.47
1:D:678:MET:SD	1:D:812:LYS:NZ	2.84	0.47
1:D:1718:ARG:HD2	1:D:1830:ILE:O	2.14	0.47
1:D:4156:SER:HB3	1:D:4923:MET:HE1	1.96	0.47
1:A:2062:ILE:O	1:A:2066:MET:HG2	2.14	0.47
1:A:2290:TRP:CZ2	1:A:2388:ILE:HG12	2.49	0.47
1:B:1016:TRP:CD2	1:B:1027:ARG:HG2	2.49	0.47
1:B:3235:MET:O	1:B:3299:LEU:HD12	2.13	0.47
1:D:490:GLN:HG2	1:D:495:ILE:HD13	1.95	0.47
1:D:1004:HIS:NE2	1:D:1033:VAL:O	2.42	0.47
1:D:2482:ASP:OD1	1:D:2483:PHE:N	2.47	0.47
1:D:3124:GLU:HG2	1:D:3125:ASP:H	1.80	0.47
1:D:3227:ARG:HG3	1:D:3229:THR:H	1.78	0.47
1:A:61:ASP:OD2	1:A:417:ARG:NH2	2.42	0.47
1:A:304:LYS:NZ	1:A:318:ASP:OD1	2.45	0.47
1:A:489:PHE:CD2	1:A:494:MET:HG3	2.49	0.47
1:A:2241:ASP:OD2	1:A:2297:ARG:NH2	2.38	0.47
1:A:2753:VAL:HG12	1:A:2753:VAL:O	2.14	0.47
1:A:2842:GLU:OE2	1:A:2886:ARG:NE	2.48	0.47
1:A:3025:ASP:O	1:A:3029:ILE:HD12	2.14	0.47
1:B:338:LEU:HG	1:B:340:VAL:HG13	1.96	0.47
1:C:2062:ILE:O	1:C:2066:MET:HG2	2.14	0.47
1:C:2549:LEU:HD13	1:C:2588:LEU:HD22	1.96	0.47
1:C:2788:ARG:NE	1:C:2906:GLY:HA3	2.28	0.47
1:D:2241:ASP:OD2	1:D:2297:ARG:NH2	2.38	0.47
1:D:2719:TYR:CZ	1:D:2723:LYS:HD2	2.49	0.47
1:A:674:TYR:OH	1:A:676:GLU:OE2	2.26	0.47
1:A:3043:ARG:NE	1:A:3120:ASP:OD2	2.43	0.47
2:H:90:GLY:HA2	1:D:638:PRO:HD3	1.95	0.47
1:B:2756:LEU:O	1:B:2758:LYS:HG2	2.14	0.47
1:B:3691:TYR:O	1:B:3695:MET:HG3	2.14	0.47
1:B:4684:GLU:HG2	1:B:4685:LYS:H	1.79	0.47
1:C:2841:ALA:HB2	1:C:2893:LEU:HD12	1.96	0.47
1:C:3227:ARG:HG3	1:C:3229:THR:H	1.78	0.47
1:D:766:ILE:HB	1:D:779:PHE:HB2	1.97	0.47
1:D:2842:GLU:OE2	1:D:2886:ARG:NE	2.48	0.47
1:A:934:GLN:HA	1:A:937:LEU:HG	1.95	0.47
1:A:1016:TRP:CD2	1:A:1027:ARG:HG2	2.49	0.47
1:A:1431:ARG:NH1	1:A:1556:GLU:OE2	2.47	0.47
1:A:4092:LYS:HA	1:A:4129:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:51:ILE:HD12	2:F:61:GLU:OE1	2.14	0.47
1:B:281:ARG:NH1	1:B:345:GLU:OE2	2.44	0.47
1:B:537:LEU:O	1:B:541:ILE:HG12	2.15	0.47
1:B:934:GLN:HA	1:B:937:LEU:HG	1.95	0.47
1:B:2156:TYR:HE1	1:B:2202:TYR:HE2	1.63	0.47
1:B:2413:LYS:HZ2	1:B:2416:ALA:N	2.13	0.47
1:B:2841:ALA:HB2	1:B:2893:LEU:HD12	1.97	0.47
1:B:2842:GLU:OE2	1:B:2886:ARG:NE	2.48	0.47
1:B:2945:GLY:O	1:B:2948:ARG:NH1	2.48	0.47
1:B:3046:MET:HA	1:B:3054:LYS:HE2	1.97	0.47
1:C:271:ALA:HB2	1:C:488:LEU:HD12	1.96	0.47
1:C:624:ALA:HB2	1:C:1667:LEU:HD12	1.96	0.47
1:C:934:GLN:HA	1:C:937:LEU:HG	1.95	0.47
1:C:1019:GLY:O	1:C:1030:PRO:HA	2.14	0.47
1:C:2756:LEU:O	1:C:2758:LYS:HG2	2.14	0.47
1:C:3122:ILE:HG22	1:C:3127:GLN:HG3	1.97	0.47
1:C:3124:GLU:HG2	1:C:3125:ASP:H	1.79	0.47
1:C:3691:TYR:O	1:C:3695:MET:HG3	2.14	0.47
1:C:4867:ILE:HG12	1:D:4864:GLY:HA2	1.97	0.47
1:D:61:ASP:OD2	1:D:417:ARG:NH2	2.42	0.47
1:D:934:GLN:HA	1:D:937:LEU:HG	1.95	0.47
1:D:2549:LEU:HD13	1:D:2588:LEU:HD22	1.96	0.47
1:D:2937:HIS:O	1:D:2941:LEU:HG	2.14	0.47
1:D:2945:GLY:O	1:D:2948:ARG:NH1	2.48	0.47
1:D:3102:LEU:HB2	1:D:3103:PRO:HD3	1.97	0.47
1:D:3310:VAL:HG21	1:D:3314:LEU:HD23	1.95	0.47
1:A:506:HIS:HB3	1:A:564:ARG:HH12	1.79	0.47
1:A:1019:GLY:O	1:A:1030:PRO:HA	2.14	0.47
1:A:1108:VAL:HB	1:A:1212:VAL:HB	1.96	0.47
1:A:1718:ARG:HD2	1:A:1830:ILE:O	2.14	0.47
1:A:2788:ARG:NE	1:A:2906:GLY:HA3	2.28	0.47
1:A:2945:GLY:O	1:A:2948:ARG:NH1	2.48	0.47
1:B:1019:GLY:O	1:B:1030:PRO:HA	2.14	0.47
1:B:2937:HIS:O	1:B:2941:LEU:HG	2.14	0.47
1:B:3285:TYR:HA	1:B:3288:LEU:HD23	1.97	0.47
1:C:338:LEU:HG	1:C:340:VAL:HG13	1.96	0.47
1:C:2241:ASP:OD2	1:C:2297:ARG:NH2	2.38	0.47
1:C:3046:MET:HA	1:C:3054:LYS:HE2	1.97	0.47
1:C:3278:GLY:HA2	1:C:3281:LEU:CD2	2.44	0.47
1:A:3278:GLY:HA2	1:A:3281:LEU:CD2	2.44	0.47
1:A:3691:TYR:O	1:A:3695:MET:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2290:TRP:CZ2	1:B:2388:ILE:HG12	2.49	0.47
1:B:3122:ILE:HG22	1:B:3127:GLN:HG3	1.97	0.47
1:B:4048:PHE:CE2	1:B:4052:MET:HE3	2.50	0.47
1:B:4690:LYS:O	1:B:4693:SER:OG	2.33	0.47
1:C:304:LYS:NZ	1:C:318:ASP:OD1	2.45	0.47
1:C:2842:GLU:OE2	1:C:2886:ARG:NE	2.48	0.47
1:C:3855:GLN:NE2	1:C:3922:GLU:O	2.46	0.47
1:C:3872:ILE:HA	1:C:3875:VAL:HG12	1.97	0.47
1:C:4196:THR:O	1:C:4200:MET:HG3	2.15	0.47
1:A:878:LEU:HA	1:A:881:ILE:HG22	1.97	0.47
1:A:1929:SER:HG	1:A:3620:PHE:HD2	1.63	0.47
1:A:2156:TYR:HE1	1:A:2202:TYR:HE2	1.63	0.47
1:B:2753:VAL:O	1:B:2753:VAL:HG12	2.14	0.47
1:C:2753:VAL:O	1:C:2753:VAL:HG12	2.14	0.47
1:C:3310:VAL:HG21	1:C:3314:LEU:HD23	1.95	0.47
1:C:4943:MET:HE2	1:C:4951:PHE:HD1	1.80	0.47
1:D:537:LEU:O	1:D:541:ILE:HG12	2.15	0.47
1:D:1019:GLY:O	1:D:1030:PRO:HA	2.14	0.47
1:D:1108:VAL:HB	1:D:1212:VAL:HB	1.96	0.47
1:D:3958:LEU:HD22	1:D:3964:GLN:HG3	1.97	0.47
1:A:766:ILE:HB	1:A:779:PHE:HB2	1.97	0.46
1:A:2937:HIS:O	1:A:2941:LEU:HG	2.14	0.46
1:A:4684:GLU:HG2	1:A:4685:LYS:H	1.79	0.46
2:F:24:VAL:HG22	2:F:48:LYS:HG2	1.96	0.46
2:H:51:ILE:HD12	2:H:61:GLU:OE1	2.14	0.46
1:B:766:ILE:HB	1:B:779:PHE:HB2	1.97	0.46
1:B:878:LEU:HA	1:B:881:ILE:HG22	1.97	0.46
1:B:992:GLN:HA	1:B:995:MET:HE2	1.96	0.46
1:B:3102:LEU:HB2	1:B:3103:PRO:HD3	1.97	0.46
1:B:3227:ARG:HH12	1:B:3290:ILE:HG21	1.81	0.46
1:B:4092:LYS:HA	1:B:4129:PHE:CZ	2.50	0.46
1:C:3285:TYR:HA	1:C:3288:LEU:HD23	1.97	0.46
1:D:136:SER:HB2	1:D:145:PHE:HA	1.97	0.46
1:D:2413:LYS:HZ2	1:D:2415:GLU:HB3	1.78	0.46
1:D:3046:MET:HA	1:D:3054:LYS:HE2	1.97	0.46
1:D:3137:LEU:HB3	1:D:3159:LEU:HD12	1.96	0.46
1:D:3778:LEU:HD13	1:D:3854:PHE:HD1	1.81	0.46
1:D:4684:GLU:HG2	1:D:4685:LYS:H	1.79	0.46
1:A:1690:GLU:HG3	1:A:1790:LYS:HD2	1.97	0.46
1:A:3046:MET:HA	1:A:3054:LYS:HE2	1.97	0.46
1:A:3227:ARG:HH12	1:A:3290:ILE:HG21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:51:ILE:HD12	2:E:61:GLU:OE1	2.14	0.46
1:B:137:ARG:HD3	1:B:202:HIS:HE1	1.80	0.46
1:B:3778:LEU:HD13	1:B:3854:PHE:HD1	1.81	0.46
1:D:137:ARG:HD3	1:D:202:HIS:HE1	1.80	0.46
1:D:271:ALA:HB2	1:D:488:LEU:HD12	1.96	0.46
1:D:281:ARG:NH1	1:D:345:GLU:OE2	2.44	0.46
1:D:3285:TYR:HA	1:D:3288:LEU:HD23	1.97	0.46
1:C:194:LEU:HD11	1:C:201:LEU:HB3	1.96	0.46
1:C:2178:VAL:HG21	1:C:2192:MET:CE	2.45	0.46
1:C:2945:GLY:O	1:C:2948:ARG:NH1	2.48	0.46
1:C:4156:SER:HB3	1:C:4923:MET:HE1	1.95	0.46
1:D:194:LEU:HD11	1:D:201:LEU:HB3	1.96	0.46
1:D:304:LYS:NZ	1:D:318:ASP:OD1	2.45	0.46
1:D:3691:TYR:O	1:D:3695:MET:HG3	2.14	0.46
1:A:3251:GLU:O	1:A:3257:ASN:ND2	2.48	0.46
1:A:4048:PHE:CE2	1:A:4052:MET:HE3	2.50	0.46
1:A:4196:THR:O	1:A:4200:MET:HG3	2.15	0.46
2:G:51:ILE:HD12	2:G:61:GLU:OE1	2.14	0.46
1:B:136:SER:HB2	1:B:145:PHE:HA	1.97	0.46
1:B:3124:GLU:HG2	1:B:3125:ASP:H	1.80	0.46
1:B:3278:GLY:HA2	1:B:3281:LEU:CD2	2.44	0.46
1:C:137:ARG:HD3	1:C:202:HIS:HE1	1.80	0.46
1:C:3137:LEU:HB3	1:C:3159:LEU:HD12	1.96	0.46
1:C:3778:LEU:HD13	1:C:3854:PHE:HD1	1.80	0.46
1:C:3958:LEU:HD22	1:C:3964:GLN:HG3	1.98	0.46
1:A:2178:VAL:HG21	1:A:2192:MET:CE	2.45	0.46
1:B:3872:ILE:HA	1:B:3875:VAL:HG12	1.97	0.46
1:C:3152:ARG:HH21	1:C:3237:VAL:CG2	2.28	0.46
1:D:658:ASN:ND2	1:D:831:LYS:O	2.34	0.46
1:D:949:HIS:CE1	1:D:1065:GLU:HB3	2.50	0.46
1:A:3108:LEU:O	1:A:3112:ILE:HG12	2.16	0.46
1:A:3939:ARG:NH1	1:B:173:GLU:HG2	2.31	0.46
1:B:2788:ARG:NE	1:B:2906:GLY:HA3	2.28	0.46
1:B:4196:THR:O	1:B:4200:MET:HG3	2.15	0.46
1:C:537:LEU:O	1:C:541:ILE:HG12	2.15	0.46
1:C:4092:LYS:HA	1:C:4129:PHE:CZ	2.50	0.46
1:D:3278:GLY:HA2	1:D:3281:LEU:CD2	2.44	0.46
1:A:1518:LEU:HB2	1:A:1531:TYR:HB2	1.97	0.46
1:A:2841:ALA:HB2	1:A:2893:LEU:HD12	1.97	0.46
1:A:3137:LEU:HB3	1:A:3159:LEU:HD12	1.96	0.46
1:A:3285:TYR:HA	1:A:3288:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3778:LEU:HD13	1:A:3854:PHE:HD1	1.80	0.46
1:B:555:LEU:HD21	1:B:578:VAL:HG11	1.98	0.46
1:B:2413:LYS:HD2	1:B:2416:ALA:H	1.81	0.46
1:B:3152:ARG:HH21	1:B:3237:VAL:CG2	2.28	0.46
1:B:3939:ARG:HH12	1:C:173:GLU:HG2	1.80	0.46
1:C:878:LEU:HA	1:C:881:ILE:HG22	1.97	0.46
1:C:3108:LEU:O	1:C:3112:ILE:HG12	2.16	0.46
1:D:2136:LYS:HD3	1:D:2136:LYS:HA	1.76	0.46
1:D:2178:VAL:HG21	1:D:2192:MET:CE	2.45	0.46
1:A:624:ALA:HB2	1:A:1667:LEU:HD12	1.96	0.46
1:A:2937:HIS:O	1:A:2940:ILE:HG22	2.16	0.46
1:A:3122:ILE:HG22	1:A:3127:GLN:HG3	1.97	0.46
1:A:3872:ILE:HA	1:A:3875:VAL:HG12	1.97	0.46
1:A:4867:ILE:HG12	1:B:4864:GLY:HA2	1.97	0.46
2:H:88:HIS:HD2	2:H:89:PRO:HD2	1.80	0.46
1:B:1690:GLU:HG3	1:B:1790:LYS:HD2	1.97	0.46
1:B:3939:ARG:NH1	1:C:173:GLU:HG2	2.31	0.46
1:B:3958:LEU:HD22	1:B:3964:GLN:HG3	1.98	0.46
1:C:503:ASP:O	1:C:507:VAL:HG13	2.16	0.46
1:C:2156:TYR:HE1	1:C:2202:TYR:HE2	1.63	0.46
1:D:3227:ARG:HH12	1:D:3290:ILE:HG21	1.81	0.46
1:D:3872:ILE:HA	1:D:3875:VAL:HG12	1.97	0.46
1:D:4092:LYS:HA	1:D:4129:PHE:CZ	2.50	0.46
1:A:2754:GLN:N	1:A:2755:PRO:HD2	2.31	0.46
1:B:2178:VAL:HG21	1:B:2192:MET:CE	2.45	0.46
1:C:555:LEU:HD21	1:C:578:VAL:HG11	1.98	0.46
1:C:2754:GLN:N	1:C:2755:PRO:HD2	2.31	0.46
1:C:3102:LEU:HB2	1:C:3103:PRO:HD3	1.96	0.46
1:A:2413:LYS:HD2	1:A:2416:ALA:H	1.81	0.46
2:E:88:HIS:HD2	2:E:89:PRO:HD2	1.80	0.46
2:H:88:HIS:CD2	2:H:89:PRO:HD2	2.51	0.46
1:B:448:PRO:HB2	1:B:451:SER:HB2	1.98	0.46
1:B:2754:GLN:N	1:B:2755:PRO:HD2	2.31	0.46
1:B:2937:HIS:O	1:B:2940:ILE:HG22	2.16	0.46
1:B:4091:ALA:C	1:B:4093:ASP:H	2.20	0.46
1:C:136:SER:HB2	1:C:145:PHE:HA	1.97	0.46
1:C:3227:ARG:HH12	1:C:3290:ILE:HG21	1.81	0.46
1:D:448:PRO:HB2	1:D:451:SER:HB2	1.98	0.46
1:D:1788:LYS:NZ	1:D:1833:ILE:O	2.48	0.46
1:D:2841:ALA:HB2	1:D:2893:LEU:HD12	1.97	0.46
1:D:2937:HIS:O	1:D:2940:ILE:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3152:ARG:HH21	1:D:3237:VAL:CG2	2.28	0.46
1:D:4196:THR:O	1:D:4200:MET:HG3	2.15	0.46
1:A:3293:GLY:H	1:A:3296:MET:HE1	1.81	0.45
1:A:3784:LYS:HA	1:A:3784:LYS:HD3	1.79	0.45
1:B:4964:ASP:OD1	1:B:4964:ASP:N	2.49	0.45
1:C:766:ILE:HB	1:C:779:PHE:HB2	1.97	0.45
1:D:2754:GLN:N	1:D:2755:PRO:HD2	2.31	0.45
1:A:173:GLU:HG2	1:D:3939:ARG:HH12	1.80	0.45
1:A:503:ASP:O	1:A:507:VAL:HG13	2.16	0.45
1:A:2252:GLU:HG2	1:A:2253:LEU:N	2.32	0.45
1:A:3958:LEU:HD22	1:A:3964:GLN:HG3	1.98	0.45
2:E:88:HIS:CD2	2:E:89:PRO:HD2	2.51	0.45
1:B:949:HIS:CE1	1:B:1065:GLU:HB3	2.50	0.45
1:B:3108:LEU:O	1:B:3112:ILE:HG12	2.16	0.45
1:C:949:HIS:CE1	1:C:1065:GLU:HB3	2.50	0.45
1:C:2252:GLU:HG2	1:C:2253:LEU:N	2.32	0.45
1:D:1518:LEU:HB2	1:D:1531:TYR:HB2	1.98	0.45
1:D:4690:LYS:HE3	1:D:4692:SER:HB2	1.98	0.45
1:A:949:HIS:CE1	1:A:1065:GLU:HB3	2.50	0.45
1:A:3124:GLU:HG2	1:A:3125:ASP:H	1.80	0.45
1:A:3325:LYS:HD3	1:A:3328:LYS:HD3	1.97	0.45
2:G:88:HIS:HD2	2:G:89:PRO:HD2	1.80	0.45
1:B:306:LEU:HD11	1:B:314:LEU:HD22	1.99	0.45
1:B:503:ASP:O	1:B:507:VAL:HG13	2.16	0.45
1:B:505:LEU:HD13	1:B:530:LEU:HG	1.98	0.45
1:C:1001:GLU:OE1	1:C:1035:TYR:HB3	2.17	0.45
1:C:2937:HIS:O	1:C:2940:ILE:HG22	2.16	0.45
1:C:4091:ALA:C	1:C:4093:ASP:H	2.20	0.45
1:D:2156:TYR:HE1	1:D:2202:TYR:HE2	1.63	0.45
1:D:2413:LYS:HD2	1:D:2416:ALA:H	1.81	0.45
1:A:3986:LEU:HD12	1:A:4101:LEU:HD12	1.99	0.45
1:A:4690:LYS:O	1:A:4693:SER:OG	2.33	0.45
2:F:88:HIS:CD2	2:F:89:PRO:HD2	2.51	0.45
1:B:1518:LEU:HB2	1:B:1531:TYR:HB2	1.97	0.45
1:C:1415:ASP:OD2	1:C:1559:ARG:NH2	2.43	0.45
1:C:1690:GLU:HG3	1:C:1790:LYS:HD2	1.97	0.45
1:A:3152:ARG:HH21	1:A:3237:VAL:CG2	2.28	0.45
1:A:3164:GLY:O	1:A:3248:ARG:HG3	2.17	0.45
2:H:12:ASP:OD1	2:H:13:GLY:N	2.50	0.45
1:B:3986:LEU:HD12	1:B:4101:LEU:HD12	1.99	0.45
1:B:4156:SER:HB3	1:B:4923:MET:HE1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1518:LEU:HB2	1:C:1531:TYR:HB2	1.97	0.45
1:C:4690:LYS:HE3	1:C:4692:SER:HB2	1.99	0.45
1:C:4964:ASP:N	1:C:4964:ASP:OD1	2.49	0.45
1:D:1911:GLN:OE1	1:D:2090:ARG:NH1	2.37	0.45
1:A:555:LEU:HD21	1:A:578:VAL:HG11	1.98	0.45
1:A:2136:LYS:HD3	1:A:2136:LYS:HA	1.76	0.45
1:A:2413:LYS:HZ2	1:A:2415:GLU:HB3	1.82	0.45
1:B:270:HIS:CD2	1:B:491:GLU:HG3	2.52	0.45
1:B:1425:THR:HG22	1:B:1563:VAL:HG13	1.98	0.45
1:B:3325:LYS:HD3	1:B:3328:LYS:HD3	1.97	0.45
1:C:61:ASP:OD2	1:C:417:ARG:NH2	2.42	0.45
1:D:1690:GLU:HG3	1:D:1790:LYS:HD2	1.97	0.45
1:D:1732:GLU:HB3	1:D:1753:LEU:HD21	1.99	0.45
1:D:2570:GLU:HG2	1:D:2605:MET:HG3	1.99	0.45
1:D:3325:LYS:HD3	1:D:3328:LYS:HD3	1.97	0.45
1:A:136:SER:HB2	1:A:145:PHE:HA	1.97	0.45
1:A:137:ARG:HD3	1:A:202:HIS:HE1	1.80	0.45
1:A:504:ARG:O	1:A:507:VAL:HG22	2.17	0.45
1:A:892:LEU:HA	1:A:895:MET:HG2	1.99	0.45
1:A:4110:PRO:HG3	1:A:4966:LEU:HD12	1.99	0.45
1:B:1732:GLU:HB3	1:B:1753:LEU:HD21	1.99	0.45
1:B:3012:GLY:O	1:B:3016:ARG:HG3	2.17	0.45
1:B:3653:GLU:OE1	1:B:3660:ARG:NH2	2.50	0.45
1:C:2570:GLU:HG2	1:C:2605:MET:HG3	1.99	0.45
1:C:4690:LYS:O	1:C:4693:SER:OG	2.33	0.45
1:D:504:ARG:O	1:D:507:VAL:HG22	2.17	0.45
1:D:3108:LEU:O	1:D:3112:ILE:HG12	2.16	0.45
1:D:3164:GLY:O	1:D:3248:ARG:HG3	2.17	0.45
1:D:4305:PHE:HA	1:D:4308:ILE:HG12	1.99	0.45
1:A:1445:TRP:HE1	1:A:1509:CYS:HB3	1.82	0.45
1:A:3012:GLY:O	1:A:3016:ARG:HG3	2.17	0.45
1:B:400:ASP:N	1:B:400:ASP:OD1	2.50	0.45
1:B:2570:GLU:HG2	1:B:2605:MET:HG3	1.99	0.45
1:B:3164:GLY:O	1:B:3248:ARG:HG3	2.17	0.45
1:D:270:HIS:CD2	1:D:491:GLU:HG3	2.52	0.45
1:D:555:LEU:HD21	1:D:578:VAL:HG11	1.98	0.45
1:D:878:LEU:HA	1:D:881:ILE:HG22	1.97	0.45
1:D:1001:GLU:OE1	1:D:1035:TYR:HB3	2.17	0.45
1:D:1268:ILE:HD11	1:D:1300:MET:HE2	1.98	0.45
1:D:2252:GLU:HG2	1:D:2253:LEU:N	2.31	0.45
1:D:4091:ALA:C	1:D:4093:ASP:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:LEU:HD13	1:A:530:LEU:HG	1.98	0.45
1:A:4245:LEU:HD21	1:B:4629:GLN:HB3	1.99	0.45
1:B:892:LEU:HA	1:B:895:MET:HG2	1.99	0.45
1:B:1788:LYS:NZ	1:B:1833:ILE:O	2.48	0.45
1:B:1929:SER:HG	1:B:3620:PHE:HD2	1.63	0.45
1:B:2831:VAL:HG22	1:C:1435:GLY:HA2	1.99	0.45
1:C:2154:VAL:HA	1:C:2157:GLN:HG2	1.99	0.45
1:C:3892:TYR:OH	1:C:3899:ASP:OD1	2.25	0.45
1:C:4305:PHE:HA	1:C:4308:ILE:HG12	1.99	0.45
1:C:4943:MET:HE2	1:C:4951:PHE:H	1.82	0.45
1:D:3653:GLU:OE1	1:D:3660:ARG:NH2	2.50	0.45
1:A:1415:ASP:N	1:A:1415:ASP:OD1	2.50	0.45
1:A:2154:VAL:HA	1:A:2157:GLN:HG2	1.99	0.45
1:A:2344:LEU:HD22	1:A:2434:GLY:HA3	1.99	0.45
1:A:2570:GLU:HG2	1:A:2605:MET:HG3	1.99	0.45
1:A:3321:PRO:HA	1:A:3324:GLU:HG3	1.99	0.45
2:G:12:ASP:OD1	2:G:13:GLY:N	2.50	0.45
1:B:304:LYS:NZ	1:B:318:ASP:OD1	2.45	0.45
1:B:2344:LEU:HD22	1:B:2434:GLY:HA3	1.99	0.45
1:B:2482:ASP:OD1	1:B:2483:PHE:N	2.47	0.45
1:C:306:LEU:HD11	1:C:314:LEU:HD22	1.98	0.45
1:C:705:PRO:HG3	1:C:857:LEU:HB2	1.99	0.45
1:C:892:LEU:HA	1:C:895:MET:HG2	1.99	0.45
1:C:1131:ASP:N	1:C:1131:ASP:OD1	2.50	0.45
1:C:1960:ARG:HD3	1:C:1960:ARG:N	2.23	0.45
1:C:3012:GLY:O	1:C:3016:ARG:HG3	2.17	0.45
1:C:3653:GLU:OE1	1:C:3660:ARG:NH2	2.50	0.45
1:D:202:HIS:CD2	1:D:203:VAL:N	2.85	0.45
1:D:503:ASP:O	1:D:507:VAL:HG13	2.16	0.45
1:D:1445:TRP:HE1	1:D:1509:CYS:HB3	1.82	0.45
1:D:2087:LEU:O	1:D:2091:GLN:HG2	2.17	0.45
1:D:2344:LEU:HD22	1:D:2434:GLY:HA3	1.99	0.45
1:A:202:HIS:CD2	1:A:203:VAL:N	2.85	0.44
1:A:375:GLN:HG3	1:A:377:VAL:HG12	1.99	0.44
1:A:448:PRO:HB2	1:A:451:SER:HB2	1.98	0.44
1:A:1960:ARG:HD3	1:A:1960:ARG:N	2.23	0.44
1:A:3653:GLU:OE1	1:A:3660:ARG:NH2	2.50	0.44
2:F:12:ASP:OD1	2:F:13:GLY:N	2.50	0.44
2:F:88:HIS:HD2	2:F:89:PRO:HD2	1.80	0.44
1:B:504:ARG:O	1:B:507:VAL:HG22	2.17	0.44
1:B:1001:GLU:OE1	1:B:1035:TYR:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1445:TRP:HE1	1:B:1509:CYS:HB3	1.82	0.44
1:B:1981:ASP:OD1	1:B:1981:ASP:N	2.45	0.44
1:B:2252:GLU:HG2	1:B:2253:LEU:N	2.31	0.44
1:B:3219:VAL:HG12	1:B:3220:GLU:OE1	2.17	0.44
1:C:400:ASP:OD1	1:C:400:ASP:N	2.50	0.44
1:C:4110:PRO:HG3	1:C:4966:LEU:HD12	1.99	0.44
1:D:2436:ILE:HG22	1:D:2491:GLY:HA3	1.98	0.44
1:D:3012:GLY:O	1:D:3016:ARG:HG3	2.17	0.44
1:D:3986:LEU:HD12	1:D:4101:LEU:HD12	1.99	0.44
1:A:750:ARG:HG2	1:A:753:ASP:OD2	2.17	0.44
1:A:1001:GLU:OE1	1:A:1035:TYR:HB3	2.17	0.44
1:A:1100:ARG:HB3	1:A:1236:TYR:CD1	2.53	0.44
1:A:3198:PRO:CG	1:A:3204:VAL:HA	2.47	0.44
2:G:88:HIS:CD2	2:G:89:PRO:HD2	2.51	0.44
1:B:705:PRO:HG3	1:B:857:LEU:HB2	1.99	0.44
1:B:1113:MET:HB2	1:B:1156:TRP:HZ2	1.82	0.44
1:B:3124:GLU:CG	1:B:3125:ASP:H	2.31	0.44
1:C:505:LEU:HD13	1:C:530:LEU:HG	1.98	0.44
1:C:750:ARG:HG2	1:C:753:ASP:OD2	2.17	0.44
1:C:1415:ASP:OD1	1:C:1415:ASP:N	2.50	0.44
1:D:400:ASP:OD1	1:D:400:ASP:N	2.50	0.44
1:D:1425:THR:HG22	1:D:1563:VAL:HG13	1.98	0.44
1:A:1425:THR:HG22	1:A:1563:VAL:HG13	1.98	0.44
1:A:3124:GLU:CG	1:A:3125:ASP:H	2.31	0.44
1:A:4091:ALA:C	1:A:4093:ASP:H	2.20	0.44
1:B:2154:VAL:HA	1:B:2157:GLN:HG2	1.99	0.44
1:B:4818:TYR:HA	1:C:4848:ILE:HD11	1.98	0.44
1:C:504:ARG:O	1:C:507:VAL:HG22	2.17	0.44
1:C:1896:MET:HB2	1:C:1896:MET:HE3	1.70	0.44
1:C:3050:LEU:HG	1:C:3052:SER:H	1.83	0.44
1:C:3325:LYS:HD3	1:C:3328:LYS:HD3	1.97	0.44
1:D:1960:ARG:HD3	1:D:1960:ARG:N	2.23	0.44
1:D:3124:GLU:CG	1:D:3125:ASP:H	2.31	0.44
1:D:4690:LYS:O	1:D:4693:SER:OG	2.33	0.44
1:A:173:GLU:HG2	1:D:3939:ARG:NH1	2.32	0.44
1:A:915:HIS:NE2	1:A:917:CYS:HB2	2.32	0.44
1:B:1038:LEU:HB3	1:B:1043:LYS:HE2	1.99	0.44
1:B:1696:GLY:HA3	1:B:1816:PHE:CD2	2.53	0.44
1:B:2436:ILE:HG22	1:B:2491:GLY:HA3	1.98	0.44
1:B:3140:LEU:HD12	1:B:3155:LEU:HD11	2.00	0.44
1:C:1113:MET:HB2	1:C:1156:TRP:HZ2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4522:VAL:HG12	1:D:4807:ASP:O	2.18	0.44
1:D:313:ASN:ND2	1:D:392:ILE:HG22	2.33	0.44
1:D:4610:LEU:HD11	1:D:4635:ILE:HG22	2.00	0.44
1:A:270:HIS:CD2	1:A:491:GLU:HG3	2.52	0.44
1:A:306:LEU:HD11	1:A:314:LEU:HD22	1.98	0.44
1:A:2087:LEU:O	1:A:2091:GLN:HG2	2.17	0.44
1:A:3219:VAL:HG12	1:A:3220:GLU:OE1	2.18	0.44
1:B:4110:PRO:HG3	1:B:4966:LEU:HD12	1.99	0.44
1:C:1973:ILE:HG13	1:C:3619:LEU:HB3	2.00	0.44
1:C:2344:LEU:HD22	1:C:2434:GLY:HA3	1.99	0.44
1:C:2413:LYS:HD2	1:C:2416:ALA:H	1.81	0.44
1:C:3219:VAL:HG12	1:C:3220:GLU:OE1	2.18	0.44
1:C:3321:PRO:HA	1:C:3324:GLU:HG3	1.99	0.44
1:D:253:GLY:HA3	1:D:256:GLN:NE2	2.33	0.44
1:D:1100:ARG:HB3	1:D:1236:TYR:CD1	2.53	0.44
1:D:2185:LYS:HD2	1:D:2186:GLU:O	2.18	0.44
1:D:3650:GLU:HB2	1:D:3651:PRO:HD3	2.00	0.44
1:A:658:ASN:ND2	1:A:831:LYS:O	2.34	0.44
1:A:996:VAL:HG13	1:A:1050:LEU:CD1	2.48	0.44
1:A:1031:ARG:HG3	1:A:1038:LEU:HD11	2.00	0.44
1:A:1911:GLN:OE1	1:A:2090:ARG:NH1	2.37	0.44
1:A:2436:ILE:HG22	1:A:2491:GLY:HA3	1.98	0.44
1:A:4027:THR:HA	1:A:4032:PHE:CD2	2.53	0.44
1:A:4203:ALA:HA	1:A:4206:ILE:HG12	2.00	0.44
1:A:4305:PHE:HA	1:A:4308:ILE:HG12	1.99	0.44
1:A:4964:ASP:N	1:A:4964:ASP:OD1	2.49	0.44
1:B:1031:ARG:HG3	1:B:1038:LEU:HD11	2.00	0.44
1:B:3187:LYS:O	1:B:3191:GLU:HB2	2.18	0.44
1:B:4690:LYS:HE3	1:B:4692:SER:HB2	1.98	0.44
1:C:58:VAL:HG22	1:C:320:GLU:HA	2.00	0.44
1:C:1425:THR:HG22	1:C:1563:VAL:HG13	1.98	0.44
1:C:2087:LEU:O	1:C:2091:GLN:HG2	2.17	0.44
1:C:3164:GLY:O	1:C:3248:ARG:HG3	2.17	0.44
1:D:1038:LEU:HB3	1:D:1043:LYS:HE2	1.99	0.44
1:D:4110:PRO:HG3	1:D:4966:LEU:HD12	1.99	0.44
1:A:1988:CYS:O	1:A:1993:ARG:NE	2.44	0.44
1:A:4848:ILE:HD11	1:D:4818:TYR:HA	2.00	0.44
1:B:375:GLN:HG3	1:B:377:VAL:HG12	1.99	0.44
1:B:750:ARG:HG2	1:B:753:ASP:OD2	2.17	0.44
1:B:3050:LEU:HG	1:B:3052:SER:H	1.83	0.44
1:B:4305:PHE:HA	1:B:4308:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:HIS:CD2	1:C:491:GLU:HG3	2.52	0.44
1:C:2436:ILE:HG22	1:C:2491:GLY:HA3	1.98	0.44
1:C:3069:GLU:O	1:C:3072:MET:HB2	2.18	0.44
1:C:3251:GLU:O	1:C:3257:ASN:ND2	2.48	0.44
1:C:4021:LEU:HD23	1:C:4088:HIS:CD2	2.53	0.44
1:C:4203:ALA:HA	1:C:4206:ILE:HG12	2.00	0.44
1:D:996:VAL:HG13	1:D:1050:LEU:CD1	2.48	0.44
1:D:2624:PRO:HD2	1:D:2992:SER:HB2	2.00	0.44
1:D:3198:PRO:CG	1:D:3204:VAL:HA	2.47	0.44
1:D:3312:PRO:O	1:D:3315:LEU:HB2	2.18	0.44
1:A:804:LEU:O	1:A:823:TYR:HD1	2.01	0.44
1:A:1732:GLU:HB3	1:A:1753:LEU:HD21	1.99	0.44
1:A:3140:LEU:HD12	1:A:3155:LEU:HD11	2.00	0.44
1:A:4026:LEU:HD12	1:A:4055:HIS:CG	2.53	0.44
1:A:4690:LYS:HE3	1:A:4692:SER:HB2	1.99	0.44
2:E:12:ASP:OD1	2:E:13:GLY:N	2.50	0.44
2:H:50:ARG:NH1	2:H:53:LYS:HG3	2.33	0.44
1:B:1131:ASP:OD1	1:B:1131:ASP:N	2.50	0.44
1:B:1415:ASP:N	1:B:1415:ASP:OD1	2.50	0.44
1:B:3198:PRO:CG	1:B:3204:VAL:HA	2.47	0.44
1:C:804:LEU:O	1:C:823:TYR:HD1	2.01	0.44
1:C:869:THR:O	1:C:872:ILE:HG12	2.18	0.44
1:C:996:VAL:HG13	1:C:1050:LEU:CD1	2.48	0.44
1:C:1414:ARG:NE	1:C:1415:ASP:OD1	2.50	0.44
1:C:2185:LYS:HD2	1:C:2186:GLU:O	2.18	0.44
1:C:4610:LEU:HD11	1:C:4635:ILE:HG22	2.00	0.44
1:D:58:VAL:HG22	1:D:320:GLU:HA	2.00	0.44
1:D:306:LEU:HD11	1:D:314:LEU:HD22	1.99	0.44
1:D:892:LEU:HA	1:D:895:MET:HG2	1.99	0.44
1:D:1040:ASP:OD1	1:D:1041:ARG:N	2.51	0.44
1:D:1131:ASP:OD1	1:D:1131:ASP:N	2.50	0.44
1:D:1549:SER:OG	1:D:1551:ASN:O	2.33	0.44
1:D:1979:PHE:CZ	1:D:1996:LEU:HD23	2.53	0.44
1:D:2115:ASP:HB2	1:D:2152:ASN:OD1	2.18	0.44
1:D:2172:MET:O	1:D:2176:VAL:HG13	2.18	0.44
1:A:1896:MET:HB2	1:A:1896:MET:HE3	1.70	0.44
1:A:1979:PHE:CZ	1:A:1996:LEU:HD23	2.53	0.44
1:A:3050:LEU:HG	1:A:3052:SER:H	1.83	0.44
1:A:3312:PRO:O	1:A:3315:LEU:HB2	2.18	0.44
1:A:4921:PHE:HE2	1:A:4940:VAL:HG11	1.83	0.44
2:E:50:ARG:NH1	2:E:53:LYS:HG3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:VAL:HG22	1:B:320:GLU:HA	2.00	0.44
1:B:1979:PHE:CZ	1:B:1996:LEU:HD23	2.53	0.44
1:B:2590:ARG:O	1:B:2593:VAL:HG22	2.18	0.44
1:B:2624:PRO:HD2	1:B:2992:SER:HB2	2.00	0.44
1:B:2760:TYR:HA	1:B:2763:LEU:HD23	2.00	0.44
1:B:3319:PHE:N	1:B:3319:PHE:CD1	2.86	0.44
1:B:4203:ALA:HA	1:B:4206:ILE:HG12	2.00	0.44
1:C:202:HIS:CD2	1:C:203:VAL:N	2.85	0.44
1:C:375:GLN:HG3	1:C:377:VAL:HG12	1.99	0.44
1:C:931:TYR:HA	1:C:934:GLN:HG3	2.00	0.44
1:C:1445:TRP:HE1	1:C:1509:CYS:HB3	1.82	0.44
1:D:505:LEU:HD13	1:D:530:LEU:HG	1.98	0.44
1:D:895:MET:HA	1:D:898:ILE:HG22	1.99	0.44
1:D:915:HIS:NE2	1:D:917:CYS:HB2	2.32	0.44
1:D:4021:LEU:HD23	1:D:4088:HIS:CD2	2.53	0.44
1:D:4026:LEU:HD12	1:D:4055:HIS:CG	2.53	0.44
1:D:4203:ALA:HA	1:D:4206:ILE:HG12	2.00	0.44
1:D:4248:LEU:HG	1:D:4297:PHE:CE1	2.53	0.44
1:A:1040:ASP:OD1	1:A:1041:ARG:N	2.51	0.43
1:A:3137:LEU:HD13	1:A:3159:LEU:HA	2.00	0.43
1:B:2172:MET:O	1:B:2176:VAL:HG13	2.18	0.43
1:B:4027:THR:HA	1:B:4032:PHE:CD2	2.53	0.43
1:B:4921:PHE:HE2	1:B:4940:VAL:HG11	1.83	0.43
1:C:249:SER:N	1:C:272:ARG:HH21	2.15	0.43
1:C:313:ASN:ND2	1:C:392:ILE:HG22	2.33	0.43
1:C:448:PRO:HB2	1:C:451:SER:HB2	1.98	0.43
1:C:1038:LEU:HB3	1:C:1043:LYS:HE2	1.99	0.43
1:C:1911:GLN:OE1	1:C:2090:ARG:NH1	2.37	0.43
1:C:2172:MET:O	1:C:2176:VAL:HG13	2.18	0.43
1:C:2277:CYS:HB3	1:C:2280:LEU:HB2	2.00	0.43
1:C:2413:LYS:HZ2	1:C:2416:ALA:N	2.15	0.43
1:D:375:GLN:HG3	1:D:377:VAL:HG12	1.99	0.43
1:D:750:ARG:HG2	1:D:753:ASP:OD2	2.17	0.43
1:D:931:TYR:HA	1:D:934:GLN:HG3	2.00	0.43
1:D:3137:LEU:HD13	1:D:3159:LEU:HA	2.00	0.43
1:D:3319:PHE:CD1	1:D:3319:PHE:N	2.86	0.43
1:D:4921:PHE:HE2	1:D:4940:VAL:HG11	1.83	0.43
1:A:1038:LEU:HB3	1:A:1043:LYS:HE2	1.99	0.43
1:A:1113:MET:HB2	1:A:1156:TRP:HZ2	1.82	0.43
1:A:2277:CYS:HB3	1:A:2280:LEU:HB2	2.00	0.43
1:A:3069:GLU:O	1:A:3072:MET:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3187:LYS:O	1:A:3191:GLU:HB2	2.18	0.43
1:B:313:ASN:ND2	1:B:392:ILE:HG22	2.33	0.43
1:B:996:VAL:HG13	1:B:1050:LEU:CD1	2.48	0.43
1:B:3246:MET:HA	1:B:3268:LEU:HD13	2.01	0.43
1:B:3803:LEU:HD23	1:B:3830:LEU:HB2	2.00	0.43
1:B:4026:LEU:HD12	1:B:4055:HIS:CG	2.53	0.43
1:C:895:MET:HA	1:C:898:ILE:HG22	1.99	0.43
1:C:915:HIS:NE2	1:C:917:CYS:HB2	2.32	0.43
1:C:2590:ARG:O	1:C:2593:VAL:HG22	2.18	0.43
1:C:2624:PRO:HD2	1:C:2992:SER:HB2	2.00	0.43
1:C:3187:LYS:O	1:C:3191:GLU:HB2	2.18	0.43
1:C:3198:PRO:CG	1:C:3204:VAL:HA	2.47	0.43
1:C:3803:LEU:HD23	1:C:3830:LEU:HB2	2.00	0.43
1:C:3986:LEU:HD12	1:C:4101:LEU:HD12	1.99	0.43
1:C:4027:THR:HA	1:C:4032:PHE:CD2	2.53	0.43
1:D:2154:VAL:HA	1:D:2157:GLN:HG2	1.99	0.43
1:D:2427:ILE:O	1:D:2476:TYR:OH	2.29	0.43
1:D:4027:THR:HA	1:D:4032:PHE:CD2	2.53	0.43
1:A:58:VAL:HG22	1:A:320:GLU:HA	2.00	0.43
1:A:253:GLY:HA3	1:A:256:GLN:NE2	2.33	0.43
1:A:313:ASN:ND2	1:A:392:ILE:HG22	2.33	0.43
1:A:400:ASP:OD1	1:A:400:ASP:N	2.50	0.43
1:A:2624:PRO:HD2	1:A:2992:SER:HB2	2.00	0.43
1:A:3237:VAL:C	1:A:3240:PRO:HD2	2.38	0.43
1:A:3650:GLU:HB2	1:A:3651:PRO:HD3	2.00	0.43
1:A:4248:LEU:HG	1:A:4297:PHE:CE1	2.53	0.43
1:B:253:GLY:HA3	1:B:256:GLN:NE2	2.33	0.43
1:B:915:HIS:NE2	1:B:917:CYS:HB2	2.32	0.43
1:B:3321:PRO:HA	1:B:3324:GLU:HG3	1.99	0.43
1:B:3730:ARG:O	1:B:3734:ARG:NH1	2.50	0.43
1:C:3246:MET:HA	1:C:3268:LEU:HD13	2.01	0.43
1:D:1113:MET:HB2	1:D:1156:TRP:HZ2	1.82	0.43
1:D:2760:TYR:HA	1:D:2763:LEU:HD23	2.00	0.43
1:D:3050:LEU:HG	1:D:3052:SER:H	1.83	0.43
1:D:3069:GLU:O	1:D:3072:MET:HB2	2.18	0.43
1:D:3237:VAL:C	1:D:3240:PRO:HD2	2.38	0.43
1:A:2115:ASP:HB2	1:A:2152:ASN:OD1	2.18	0.43
1:A:2590:ARG:O	1:A:2593:VAL:HG22	2.18	0.43
1:A:4021:LEU:HD23	1:A:4088:HIS:CD2	2.53	0.43
1:A:4943:MET:HE1	1:A:4951:PHE:H	1.83	0.43
1:B:804:LEU:O	1:B:823:TYR:HD1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:807:ARG:O	1:B:1613:GLU:HA	2.18	0.43
1:B:895:MET:HA	1:B:898:ILE:HG22	1.99	0.43
1:B:1040:ASP:OD1	1:B:1041:ARG:N	2.51	0.43
1:B:2087:LEU:O	1:B:2091:GLN:HG2	2.17	0.43
1:B:2596:VAL:HG22	1:B:2606:PRO:HB2	2.00	0.43
1:B:3036:LEU:HD23	1:B:3036:LEU:HA	1.90	0.43
1:B:3069:GLU:O	1:B:3072:MET:HB2	2.18	0.43
1:B:3312:PRO:O	1:B:3315:LEU:HB2	2.18	0.43
1:C:394:HIS:NE2	1:C:396:GLU:HG3	2.33	0.43
1:C:1729:MET:HE1	1:C:3617:VAL:HG21	1.99	0.43
1:C:2760:TYR:HA	1:C:2763:LEU:HD23	2.00	0.43
1:C:3137:LEU:HD13	1:C:3159:LEU:HA	2.00	0.43
1:C:3293:GLY:H	1:C:3296:MET:HE1	1.82	0.43
1:C:3319:PHE:N	1:C:3319:PHE:CD1	2.86	0.43
1:C:3650:GLU:HB2	1:C:3651:PRO:HD3	2.00	0.43
1:C:4245:LEU:HD21	1:D:4629:GLN:HB3	1.99	0.43
1:D:157:ALA:HA	1:D:187:SER:HB3	2.00	0.43
1:D:249:SER:N	1:D:272:ARG:HH21	2.15	0.43
1:D:804:LEU:O	1:D:823:TYR:HD1	2.01	0.43
1:A:157:ALA:HA	1:A:187:SER:HB3	2.00	0.43
1:A:249:SER:N	1:A:272:ARG:HH21	2.15	0.43
1:A:869:THR:O	1:A:872:ILE:HG12	2.18	0.43
1:A:3169:ALA:HB1	1:A:3245:TYR:OH	2.19	0.43
1:A:4206:ILE:HA	1:A:4493:ASN:ND2	2.34	0.43
1:B:271:ALA:O	1:B:301:THR:OG1	2.36	0.43
1:B:394:HIS:NE2	1:B:396:GLU:HG3	2.34	0.43
1:B:4610:LEU:HD11	1:B:4635:ILE:HG22	2.00	0.43
1:C:807:ARG:O	1:C:1613:GLU:HA	2.18	0.43
1:C:1040:ASP:OD1	1:C:1041:ARG:N	2.51	0.43
1:C:1979:PHE:CZ	1:C:1996:LEU:HD23	2.53	0.43
1:D:290:ARG:HH11	1:D:343:ARG:HH11	1.67	0.43
1:D:674:TYR:CD2	1:D:815:PRO:HB3	2.54	0.43
1:D:1696:GLY:HA3	1:D:1816:PHE:CD2	2.53	0.43
1:D:3169:ALA:HB1	1:D:3245:TYR:OH	2.19	0.43
1:D:3187:LYS:O	1:D:3191:GLU:HB2	2.18	0.43
1:D:3219:VAL:HG12	1:D:3220:GLU:OE1	2.18	0.43
1:A:674:TYR:CD2	1:A:815:PRO:HB3	2.54	0.43
1:A:895:MET:HA	1:A:898:ILE:HG22	1.99	0.43
1:A:1696:GLY:HA3	1:A:1816:PHE:CD2	2.53	0.43
1:A:2303:ARG:HG2	1:A:2401:ARG:HD2	2.00	0.43
2:G:50:ARG:NH1	2:G:53:LYS:HG3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ALA:HA	1:B:187:SER:HB3	2.00	0.43
1:B:869:THR:O	1:B:872:ILE:HG12	2.18	0.43
1:B:1100:ARG:HB3	1:B:1236:TYR:CD1	2.53	0.43
1:B:2115:ASP:HB2	1:B:2152:ASN:OD1	2.18	0.43
1:B:2277:CYS:HB3	1:B:2280:LEU:HB2	2.00	0.43
1:B:4206:ILE:HA	1:B:4493:ASN:ND2	2.34	0.43
1:C:253:GLY:HA3	1:C:256:GLN:NE2	2.33	0.43
1:C:2115:ASP:HB2	1:C:2152:ASN:OD1	2.18	0.43
1:C:4248:LEU:HG	1:C:4297:PHE:CE1	2.53	0.43
1:C:4271:VAL:HG23	1:C:4275:THR:HB	2.01	0.43
1:D:2277:CYS:HB3	1:D:2280:LEU:HB2	2.00	0.43
1:D:2590:ARG:O	1:D:2593:VAL:HG22	2.18	0.43
1:D:2596:VAL:HG22	1:D:2606:PRO:HB2	2.00	0.43
1:D:3140:LEU:HD12	1:D:3155:LEU:HD11	2.00	0.43
1:D:3321:PRO:HA	1:D:3324:GLU:HG3	1.99	0.43
1:D:3730:ARG:O	1:D:3734:ARG:NH1	2.50	0.43
1:D:4271:VAL:HG23	1:D:4275:THR:HB	2.01	0.43
1:D:4782:THR:HG22	1:D:4816:HIS:ND1	2.34	0.43
1:A:1973:ILE:HG13	1:A:3619:LEU:HB3	2.00	0.43
1:A:2185:LYS:HD2	1:A:2186:GLU:O	2.18	0.43
1:A:3121:LEU:HD23	1:A:3126:VAL:HG11	2.01	0.43
1:B:202:HIS:CD2	1:B:203:VAL:N	2.85	0.43
1:B:1549:SER:OG	1:B:1551:ASN:O	2.33	0.43
1:B:2185:LYS:HD2	1:B:2186:GLU:O	2.18	0.43
1:B:3237:VAL:C	1:B:3240:PRO:HD2	2.38	0.43
1:B:3305:PRO:O	1:B:3309:LYS:HG2	2.19	0.43
1:B:4021:LEU:HD23	1:B:4088:HIS:CD2	2.53	0.43
1:C:1100:ARG:HB3	1:C:1236:TYR:CD1	2.53	0.43
1:C:2596:VAL:HG22	1:C:2606:PRO:HB2	2.00	0.43
1:C:3124:GLU:CG	1:C:3125:ASP:H	2.31	0.43
1:C:3169:ALA:HB1	1:C:3245:TYR:OH	2.19	0.43
1:C:3305:PRO:O	1:C:3309:LYS:HG2	2.19	0.43
1:C:4026:LEU:HD12	1:C:4055:HIS:CG	2.53	0.43
1:D:251:GLU:HG3	1:D:256:GLN:HG3	2.01	0.43
1:D:4194:GLU:HG2	1:D:4645:TRP:HZ3	1.83	0.43
1:A:1045:SER:HA	1:A:1048:ASP:OD2	2.19	0.43
1:A:1131:ASP:N	1:A:1131:ASP:OD1	2.50	0.43
1:B:3637:GLU:HG2	1:B:3694:ILE:HA	2.01	0.43
1:C:538:ALA:O	1:C:542:ARG:HB2	2.19	0.43
1:C:1696:GLY:HA3	1:C:1816:PHE:CD2	2.53	0.43
1:D:224:ALA:HB3	1:D:227:TYR:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:HIS:NE2	1:D:396:GLU:HG3	2.33	0.43
1:D:1282:CYS:SG	1:D:1556:GLU:HG2	2.59	0.43
1:D:3246:MET:HA	1:D:3268:LEU:HD13	2.00	0.43
1:D:4943:MET:HE2	1:D:4951:PHE:H	1.84	0.43
1:A:394:HIS:NE2	1:A:396:GLU:HG3	2.33	0.43
1:A:538:ALA:O	1:A:542:ARG:HB2	2.19	0.43
1:A:807:ARG:O	1:A:1613:GLU:HA	2.18	0.43
1:B:224:ALA:HB3	1:B:227:TYR:HD2	1.84	0.43
1:B:1045:SER:HA	1:B:1048:ASP:OD2	2.19	0.43
1:B:1165:MET:HB3	1:B:1236:TYR:CE1	2.54	0.43
1:B:3137:LEU:HD13	1:B:3159:LEU:HA	2.00	0.43
1:B:3169:ALA:HB1	1:B:3245:TYR:OH	2.18	0.43
1:B:3251:GLU:O	1:B:3257:ASN:ND2	2.48	0.43
1:C:271:ALA:O	1:C:301:THR:OG1	2.36	0.43
1:C:1031:ARG:HG3	1:C:1038:LEU:HD11	2.00	0.43
1:C:1282:CYS:SG	1:C:1556:GLU:HG2	2.59	0.43
1:C:3237:VAL:C	1:C:3240:PRO:HD2	2.38	0.43
1:C:4194:GLU:HG2	1:C:4645:TRP:HZ3	1.83	0.43
1:D:271:ALA:O	1:D:301:THR:OG1	2.36	0.43
1:D:869:THR:O	1:D:872:ILE:HG12	2.18	0.43
1:A:705:PRO:HG3	1:A:857:LEU:HB2	1.99	0.43
1:A:1282:CYS:SG	1:A:1556:GLU:HG2	2.59	0.43
1:A:1501:ASN:HB3	1:D:2826:ILE:HD13	2.01	0.43
1:A:3803:LEU:HD23	1:A:3830:LEU:HB2	2.00	0.43
1:B:1432:ILE:HG12	1:B:1441:VAL:HG11	2.01	0.43
1:B:1943:ARG:NH2	1:B:1964:GLU:OE2	2.48	0.43
1:B:2849:HIS:CE1	1:B:2877:LEU:HD11	2.54	0.43
1:B:4271:VAL:HG23	1:B:4275:THR:HB	2.01	0.43
1:B:4867:ILE:HG12	1:C:4864:GLY:HA2	2.01	0.43
1:B:4943:MET:HE1	1:B:4950:GLU:HB3	2.01	0.43
1:C:224:ALA:HB3	1:C:227:TYR:HD2	1.84	0.43
1:C:2791:ARG:HE	1:C:2796:ASP:HB3	1.84	0.43
1:C:3140:LEU:HD12	1:C:3155:LEU:HD11	2.00	0.43
1:D:672:LYS:HB3	1:D:819:TYR:CD2	2.54	0.43
1:D:1045:SER:HA	1:D:1048:ASP:OD2	2.19	0.43
1:D:1442:TRP:HB2	1:D:1544:PHE:HB2	2.01	0.43
1:D:2849:HIS:CE1	1:D:2877:LEU:HD11	2.54	0.43
1:A:290:ARG:HH11	1:A:343:ARG:HH11	1.67	0.42
1:A:4782:THR:HG22	1:A:4816:HIS:ND1	2.34	0.42
1:A:4831:ILE:HD12	1:A:4843:ARG:HH12	1.84	0.42
1:B:1973:ILE:HG13	1:B:3619:LEU:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3121:LEU:HD23	1:B:3126:VAL:HG11	2.01	0.42
1:B:3125:ASP:HA	1:B:3128:VAL:HG12	2.01	0.42
1:B:4248:LEU:HG	1:B:4297:PHE:CE1	2.53	0.42
1:C:1649:GLU:HG2	1:C:1650:LEU:N	2.34	0.42
1:C:1732:GLU:HB3	1:C:1753:LEU:HD21	1.99	0.42
1:C:3324:GLU:OE2	1:C:3325:LYS:HE3	2.19	0.42
1:C:4206:ILE:HA	1:C:4493:ASN:ND2	2.34	0.42
1:D:705:PRO:HG3	1:D:857:LEU:HB2	1.99	0.42
1:D:1415:ASP:OD1	1:D:1415:ASP:N	2.50	0.42
1:A:224:ALA:HB3	1:A:227:TYR:HD2	1.84	0.42
1:A:1432:ILE:HG12	1:A:1441:VAL:HG11	2.01	0.42
1:A:2172:MET:O	1:A:2176:VAL:HG13	2.18	0.42
1:A:2596:VAL:HG22	1:A:2606:PRO:HB2	1.99	0.42
1:A:3730:ARG:O	1:A:3734:ARG:NH1	2.50	0.42
1:A:4083:PHE:O	1:A:4086:ARG:HG2	2.19	0.42
1:A:4267:GLN:O	1:A:4271:VAL:HG12	2.19	0.42
1:A:4610:LEU:HD11	1:A:4635:ILE:HG22	2.00	0.42
1:A:4943:MET:HE3	1:A:4950:GLU:HB3	2.01	0.42
1:B:1282:CYS:SG	1:B:1556:GLU:HG2	2.59	0.42
1:B:2251:ASN:O	1:B:2255:LEU:HG	2.19	0.42
1:C:290:ARG:HH11	1:C:343:ARG:HH11	1.67	0.42
1:C:672:LYS:HB3	1:C:819:TYR:CD2	2.54	0.42
1:C:966:LEU:HD23	1:C:967:PRO:O	2.20	0.42
1:C:1165:MET:HB3	1:C:1236:TYR:CE1	2.54	0.42
1:C:3730:ARG:O	1:C:3734:ARG:NH1	2.50	0.42
1:D:2303:ARG:HG2	1:D:2401:ARG:HD2	2.01	0.42
1:D:3068:LEU:O	1:D:3071:THR:OG1	2.28	0.42
1:D:3803:LEU:HD23	1:D:3830:LEU:HB2	2.01	0.42
1:D:4943:MET:HE1	1:D:4950:GLU:HB3	2.01	0.42
1:A:931:TYR:HA	1:A:934:GLN:HG3	2.00	0.42
1:A:2760:TYR:HA	1:A:2763:LEU:HD23	2.00	0.42
1:A:2914:THR:O	1:A:2915:PRO:C	2.58	0.42
2:F:50:ARG:NH1	2:F:53:LYS:HG3	2.33	0.42
1:B:931:TYR:HA	1:B:934:GLN:HG3	2.00	0.42
1:B:1748:LEU:O	1:B:1751:ILE:HG12	2.19	0.42
1:B:4782:THR:HG22	1:B:4816:HIS:ND1	2.34	0.42
1:C:674:TYR:CE1	1:C:756:SER:HB2	2.54	0.42
1:C:983:LEU:HD23	1:C:983:LEU:H	1.84	0.42
1:C:1038:LEU:HD23	1:C:1043:LYS:HB3	2.02	0.42
1:C:3315:LEU:HD13	1:C:3319:PHE:CD2	2.55	0.42
1:C:4743:LEU:O	1:C:4746:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4930:GLU:OE1	1:C:4941:TRP:NE1	2.52	0.42
1:D:966:LEU:HD23	1:D:967:PRO:O	2.20	0.42
1:D:983:LEU:HD23	1:D:983:LEU:H	1.84	0.42
1:D:1973:ILE:HG13	1:D:3619:LEU:HB3	2.00	0.42
1:D:2140:LYS:HG2	1:D:2144:ARG:HH21	1.84	0.42
1:D:2791:ARG:HE	1:D:2796:ASP:HB3	1.84	0.42
1:D:3305:PRO:O	1:D:3309:LYS:HG2	2.19	0.42
1:A:966:LEU:HD23	1:A:967:PRO:O	2.20	0.42
1:A:1748:LEU:O	1:A:1751:ILE:HG12	2.19	0.42
1:A:1894:LEU:HD23	1:A:1894:LEU:HA	1.88	0.42
1:A:2427:ILE:O	1:A:2476:TYR:OH	2.29	0.42
1:A:3305:PRO:O	1:A:3309:LYS:HG2	2.19	0.42
1:A:3315:LEU:HD13	1:A:3319:PHE:CD2	2.55	0.42
1:A:3637:GLU:HG2	1:A:3694:ILE:HA	2.01	0.42
1:A:4007:SER:HA	1:A:4118:PHE:HZ	1.84	0.42
1:A:4930:GLU:OE1	1:A:4941:TRP:NE1	2.52	0.42
1:B:3324:GLU:OE2	1:B:3325:LYS:HE3	2.19	0.42
1:B:4194:GLU:HG2	1:B:4645:TRP:HZ3	1.83	0.42
1:B:4743:LEU:O	1:B:4746:ILE:HG12	2.19	0.42
1:C:2585:MET:O	1:C:2589:LEU:HG	2.20	0.42
1:C:4782:THR:HG22	1:C:4816:HIS:ND1	2.34	0.42
1:D:1957:LEU:HG	1:D:1960:ARG:NH1	2.27	0.42
1:D:2424:ARG:HE	1:D:2424:ARG:HB2	1.54	0.42
1:D:4083:PHE:O	1:D:4086:ARG:HG2	2.19	0.42
1:A:2440:PHE:CZ	1:A:2465:LYS:HD3	2.55	0.42
1:A:4271:VAL:HG23	1:A:4275:THR:HB	2.01	0.42
1:B:208:GLN:OE1	1:B:208:GLN:N	2.53	0.42
1:B:251:GLU:HG3	1:B:256:GLN:HG3	2.01	0.42
1:B:538:ALA:O	1:B:542:ARG:HB2	2.19	0.42
1:B:1306:MET:HB2	1:B:1570:LEU:HD22	2.02	0.42
1:B:1522:ALA:HB2	1:B:1527:LEU:HD21	2.02	0.42
1:C:674:TYR:CD2	1:C:815:PRO:HB3	2.54	0.42
1:C:896:ASN:HD21	1:C:1049:SER:CB	2.33	0.42
1:C:3121:LEU:HD23	1:C:3126:VAL:HG11	2.01	0.42
1:D:1031:ARG:HG3	1:D:1038:LEU:HD11	2.00	0.42
1:D:4267:GLN:O	1:D:4271:VAL:HG12	2.19	0.42
1:A:1165:MET:HB3	1:A:1236:TYR:CE1	2.54	0.42
1:A:1442:TRP:HB2	1:A:1544:PHE:HB2	2.01	0.42
1:A:1649:GLU:HG2	1:A:1650:LEU:N	2.34	0.42
1:A:2666:LEU:HD21	1:A:2969:PRO:HB2	2.02	0.42
1:A:3319:PHE:CD1	1:A:3319:PHE:N	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:966:LEU:HD23	1:B:967:PRO:O	2.20	0.42
1:B:1911:GLN:OE1	1:B:2090:ARG:NH1	2.37	0.42
1:B:3650:GLU:HB2	1:B:3651:PRO:HD3	2.00	0.42
1:C:966:LEU:HA	1:C:967:PRO:HD3	1.93	0.42
1:C:2178:VAL:HG21	1:C:2192:MET:HE2	2.02	0.42
1:C:2641:SER:HB2	1:C:2676:LEU:HD21	2.01	0.42
1:C:3312:PRO:O	1:C:3315:LEU:HB2	2.18	0.42
1:C:4921:PHE:HE2	1:C:4940:VAL:HG11	1.83	0.42
1:D:338:LEU:HD12	1:D:338:LEU:HA	1.91	0.42
1:D:674:TYR:CE1	1:D:756:SER:HB2	2.54	0.42
1:D:807:ARG:O	1:D:1613:GLU:HA	2.18	0.42
1:D:1748:LEU:O	1:D:1751:ILE:HG12	2.19	0.42
1:D:2251:ASN:O	1:D:2255:LEU:HG	2.19	0.42
1:D:3315:LEU:HD13	1:D:3319:PHE:CD2	2.55	0.42
1:D:4206:ILE:HA	1:D:4493:ASN:ND2	2.34	0.42
1:D:4743:LEU:O	1:D:4746:ILE:HG12	2.19	0.42
1:A:896:ASN:HD21	1:A:1049:SER:CB	2.33	0.42
1:A:2791:ARG:HE	1:A:2796:ASP:HB3	1.84	0.42
1:A:3125:ASP:HA	1:A:3128:VAL:HG12	2.01	0.42
1:A:3246:MET:HA	1:A:3268:LEU:HD13	2.01	0.42
1:A:4135:ARG:HG2	1:A:4149:TYR:CD1	2.55	0.42
1:B:1649:GLU:HG2	1:B:1650:LEU:N	2.34	0.42
1:B:2585:MET:O	1:B:2589:LEU:HG	2.20	0.42
1:B:2914:THR:O	1:B:2915:PRO:C	2.58	0.42
1:B:3068:LEU:O	1:B:3071:THR:OG1	2.28	0.42
1:B:3315:LEU:HD13	1:B:3319:PHE:CD2	2.55	0.42
1:B:4267:GLN:O	1:B:4271:VAL:HG12	2.19	0.42
1:B:4930:GLU:OE1	1:B:4941:TRP:NE1	2.52	0.42
1:C:208:GLN:OE1	1:C:208:GLN:N	2.53	0.42
1:C:4083:PHE:O	1:C:4086:ARG:HG2	2.19	0.42
1:D:1943:ARG:NH2	1:D:1964:GLU:OE2	2.48	0.42
1:D:2585:MET:O	1:D:2589:LEU:HG	2.20	0.42
1:D:4735:ASN:HB3	1:D:4738:PHE:CD2	2.55	0.42
1:A:638:PRO:HD3	2:E:90:GLY:HA2	2.01	0.42
1:A:1306:MET:HB2	1:A:1570:LEU:HD22	2.02	0.42
1:A:2849:HIS:CE1	1:A:2877:LEU:HD11	2.54	0.42
1:A:3324:GLU:OE2	1:A:3325:LYS:HE3	2.19	0.42
4:A:5003:ATP:H5'1	5:A:5004:KVR:C20	2.49	0.42
1:B:249:SER:N	1:B:272:ARG:HH21	2.15	0.42
1:B:896:ASN:HD21	1:B:1049:SER:CB	2.33	0.42
1:B:1458:ASP:OD1	1:B:1461:ARG:NE	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2136:LYS:HD3	1:B:2136:LYS:HA	1.77	0.42
1:B:2440:PHE:CZ	1:B:2465:LYS:HD3	2.55	0.42
1:B:4943:MET:HE2	1:B:4951:PHE:H	1.84	0.42
1:C:157:ALA:HA	1:C:187:SER:HB3	2.00	0.42
1:C:411:GLU:OE2	1:C:485:ARG:NE	2.35	0.42
1:C:546:LYS:O	1:C:550:GLN:HG2	2.20	0.42
1:C:1432:ILE:HG12	1:C:1441:VAL:HG11	2.01	0.42
1:C:2640:LEU:HA	1:C:2643:LYS:HZ3	1.85	0.42
1:D:414:ARG:O	1:D:418:VAL:HG23	2.20	0.42
1:D:941:LYS:HA	1:D:944:LEU:HG	2.01	0.42
1:D:1649:GLU:HG2	1:D:1650:LEU:N	2.35	0.42
1:D:1711:LEU:HB3	1:D:1831:MET:SD	2.60	0.42
1:D:4930:GLU:OE1	1:D:4941:TRP:NE1	2.52	0.42
1:A:414:ARG:O	1:A:418:VAL:HG23	2.20	0.42
1:A:546:LYS:O	1:A:550:GLN:HG2	2.20	0.42
1:A:672:LYS:HB3	1:A:819:TYR:CD2	2.54	0.42
1:A:816:PRO:HB2	1:A:819:TYR:CD1	2.55	0.42
1:A:1414:ARG:NE	1:A:1415:ASP:OD1	2.50	0.42
1:A:1788:LYS:NZ	1:A:1833:ILE:O	2.48	0.42
1:A:2641:SER:HB2	1:A:2676:LEU:HD21	2.01	0.42
1:A:4073:ASP:OD1	1:A:4074:GLU:N	2.53	0.42
1:A:4194:GLU:HG2	1:A:4645:TRP:HZ3	1.83	0.42
1:B:290:ARG:HH11	1:B:343:ARG:HH11	1.67	0.42
1:B:672:LYS:HB3	1:B:819:TYR:CD2	2.54	0.42
1:B:674:TYR:CD2	1:B:815:PRO:HB3	2.54	0.42
1:B:674:TYR:CE1	1:B:756:SER:HB2	2.54	0.42
1:B:983:LEU:HD23	1:B:983:LEU:H	1.84	0.42
1:B:1442:TRP:HB2	1:B:1544:PHE:HB2	2.01	0.42
1:B:1711:LEU:HB3	1:B:1831:MET:SD	2.60	0.42
1:B:1988:CYS:O	1:B:1993:ARG:NE	2.44	0.42
1:B:2140:LYS:HG2	1:B:2144:ARG:HH21	1.84	0.42
1:B:4735:ASN:HB3	1:B:4738:PHE:CD2	2.55	0.42
1:C:941:LYS:HA	1:C:944:LEU:HG	2.01	0.42
1:C:1152:TYR:HD1	1:C:1184:ASP:HB3	1.84	0.42
1:C:2140:LYS:HG2	1:C:2144:ARG:HH21	1.84	0.42
1:C:2222:LEU:HD23	1:C:2222:LEU:HA	1.89	0.42
1:C:2303:ARG:HG2	1:C:2401:ARG:HD2	2.00	0.42
1:C:2440:PHE:CZ	1:C:2465:LYS:HD3	2.55	0.42
1:C:2914:THR:O	1:C:2915:PRO:C	2.58	0.42
1:D:332:ARG:HH22	1:D:339:ASP:H	1.68	0.42
1:D:1420:LEU:HG	1:D:1564:MET:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1427:TYR:HB2	1:D:1563:VAL:HG11	2.01	0.42
1:D:2532:ALA:HA	1:D:2535:PHE:HD2	1.84	0.42
1:D:3324:GLU:OE2	1:D:3325:LYS:HE3	2.19	0.42
1:A:332:ARG:HH22	1:A:339:ASP:H	1.68	0.42
1:A:674:TYR:CE1	1:A:756:SER:HB2	2.54	0.42
1:A:2178:VAL:HG21	1:A:2192:MET:HE2	2.02	0.42
1:A:4735:ASN:HB3	1:A:4738:PHE:CD2	2.55	0.42
1:B:546:LYS:O	1:B:550:GLN:HG2	2.20	0.42
1:B:2666:LEU:HD21	1:B:2969:PRO:HB2	2.02	0.42
1:C:1458:ASP:OD1	1:C:1461:ARG:NE	2.45	0.42
1:C:1522:ALA:HB2	1:C:1527:LEU:HD21	2.02	0.42
1:C:1711:LEU:HB3	1:C:1831:MET:SD	2.60	0.42
1:C:2251:ASN:O	1:C:2255:LEU:HG	2.19	0.42
1:C:2596:VAL:HG21	1:C:2610:LEU:HD11	2.02	0.42
1:C:2849:HIS:CE1	1:C:2877:LEU:HD11	2.54	0.42
1:C:3138:TYR:CG	1:C:3208:ILE:HG12	2.55	0.42
1:C:4040:LYS:HG3	1:C:4042:VAL:HG13	2.02	0.42
1:C:4267:GLN:O	1:C:4271:VAL:HG12	2.19	0.42
1:C:4943:MET:HE1	1:C:4950:GLU:HB3	2.02	0.42
1:D:538:ALA:O	1:D:542:ARG:HB2	2.19	0.42
1:D:661:LEU:HD22	1:D:673:TRP:CE2	2.55	0.42
1:D:1165:MET:HB3	1:D:1236:TYR:CE1	2.54	0.42
1:D:1432:ILE:HG12	1:D:1441:VAL:HG11	2.01	0.42
1:D:2582:PRO:HG3	1:D:2617:CYS:SG	2.60	0.42
1:D:2666:LEU:HD21	1:D:2969:PRO:HB2	2.02	0.42
1:D:3121:LEU:HD23	1:D:3126:VAL:HG11	2.01	0.42
1:D:3251:GLU:HA	1:D:3256:ASN:HD22	1.85	0.42
1:D:3677:THR:HB	1:D:3679:LYS:HZ2	1.85	0.42
1:D:4073:ASP:OD1	1:D:4074:GLU:N	2.53	0.42
1:A:1268:ILE:HD11	1:A:1300:MET:HE2	2.02	0.41
1:A:2251:ASN:O	1:A:2255:LEU:HG	2.19	0.41
1:A:2532:ALA:HA	1:A:2535:PHE:HD2	1.84	0.41
1:B:816:PRO:HB2	1:B:819:TYR:CD1	2.55	0.41
1:B:1038:LEU:HD23	1:B:1043:LYS:HB3	2.02	0.41
1:B:1218:GLY:HA3	1:B:1238:PRO:HB3	2.02	0.41
1:B:2791:ARG:HE	1:B:2796:ASP:HB3	1.84	0.41
1:B:4007:SER:HA	1:B:4118:PHE:HZ	1.85	0.41
1:B:4073:ASP:OD1	1:B:4074:GLU:N	2.53	0.41
1:B:4083:PHE:O	1:B:4086:ARG:HG2	2.19	0.41
1:B:4135:ARG:HG2	1:B:4149:TYR:CD1	2.55	0.41
1:C:332:ARG:HH22	1:C:339:ASP:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1943:ARG:NH2	1:C:1964:GLU:OE2	2.48	0.41
1:C:3637:GLU:HG2	1:C:3694:ILE:HA	2.01	0.41
1:C:4735:ASN:HB3	1:C:4738:PHE:CD2	2.55	0.41
1:D:208:GLN:N	1:D:208:GLN:OE1	2.53	0.41
1:D:263:GLU:OE1	1:D:272:ARG:NH1	2.47	0.41
1:D:614:LEU:HA	1:D:617:LEU:HD12	2.02	0.41
1:D:896:ASN:HD21	1:D:1049:SER:CB	2.33	0.41
1:D:1805:HIS:ND1	1:D:1805:HIS:N	2.68	0.41
1:D:2914:THR:O	1:D:2915:PRO:C	2.58	0.41
1:D:4831:ILE:HD12	1:D:4843:ARG:HH12	1.84	0.41
1:A:544:ASN:HB3	1:A:547:ASN:HB2	2.03	0.41
1:A:1935:LYS:HE2	1:A:1935:LYS:HB3	1.90	0.41
1:A:2585:MET:O	1:A:2589:LEU:HG	2.20	0.41
1:B:2596:VAL:HG21	1:B:2610:LEU:HD11	2.02	0.41
1:C:251:GLU:HG3	1:C:256:GLN:HG3	2.01	0.41
1:C:816:PRO:HB2	1:C:819:TYR:CD1	2.55	0.41
1:C:1427:TYR:HB2	1:C:1563:VAL:HG11	2.01	0.41
1:C:2272:CYS:HB3	1:C:2291:ASN:HB3	2.02	0.41
1:C:3251:GLU:HA	1:C:3256:ASN:HD22	1.85	0.41
1:D:3138:TYR:CG	1:D:3208:ILE:HG12	2.55	0.41
1:D:4664:ASP:HA	1:D:4674:LYS:HD3	2.02	0.41
1:A:941:LYS:HA	1:A:944:LEU:HG	2.01	0.41
1:A:983:LEU:HD23	1:A:983:LEU:H	1.84	0.41
1:A:1522:ALA:HB2	1:A:1527:LEU:HD21	2.02	0.41
1:A:2541:HIS:O	1:A:2545:ILE:HG12	2.20	0.41
1:A:4743:LEU:O	1:A:4746:ILE:HG12	2.19	0.41
1:B:332:ARG:HH22	1:B:339:ASP:H	1.68	0.41
1:B:1152:TYR:HD1	1:B:1184:ASP:HB3	1.84	0.41
1:B:3787:VAL:HG11	1:B:3866:THR:HB	2.02	0.41
1:C:1748:LEU:O	1:C:1751:ILE:HG12	2.19	0.41
1:C:2135:GLY:H	1:C:2138:GLU:HB2	1.86	0.41
1:C:2582:PRO:HG3	1:C:2617:CYS:SG	2.60	0.41
1:C:3125:ASP:HA	1:C:3128:VAL:HG12	2.02	0.41
1:C:3277:LEU:HA	1:C:3280:ILE:HD12	2.02	0.41
1:C:4073:ASP:OD1	1:C:4074:GLU:N	2.53	0.41
1:C:4664:ASP:HA	1:C:4674:LYS:HD3	2.03	0.41
1:C:4751:LYS:O	1:C:4755:THR:HG23	2.21	0.41
1:D:2440:PHE:CZ	1:D:2465:LYS:HD3	2.55	0.41
1:D:2714:PRO:HD3	1:D:2783:LEU:HD11	2.03	0.41
1:D:2833:LEU:HD21	1:D:2894:LYS:HG3	2.03	0.41
1:A:614:LEU:HA	1:A:617:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1711:LEU:HB3	1:A:1831:MET:SD	2.60	0.41
1:A:4629:GLN:HB3	1:D:4245:LEU:HD21	2.02	0.41
1:B:2303:ARG:HG2	1:B:2401:ARG:HD2	2.00	0.41
1:B:2641:SER:HB2	1:B:2676:LEU:HD21	2.01	0.41
1:B:2833:LEU:HD21	1:B:2894:LYS:HG3	2.03	0.41
1:B:3293:GLY:H	1:B:3296:MET:HE1	1.85	0.41
1:B:4831:ILE:HD12	1:B:4843:ARG:HH12	1.84	0.41
1:C:315:LEU:HD12	1:C:315:LEU:HA	1.93	0.41
1:C:674:TYR:OH	1:C:676:GLU:OE2	2.26	0.41
1:C:1442:TRP:HB2	1:C:1544:PHE:HB2	2.01	0.41
1:C:2948:ARG:HD3	1:C:2948:ARG:H	1.86	0.41
1:C:4831:ILE:HD12	1:C:4843:ARG:HH12	1.84	0.41
1:D:1038:LEU:HD23	1:D:1043:LYS:HB3	2.02	0.41
1:D:2948:ARG:H	1:D:2948:ARG:HD3	1.86	0.41
1:D:3145:SER:O	1:D:3148:VAL:N	2.51	0.41
1:D:3637:GLU:HG2	1:D:3694:ILE:HA	2.01	0.41
1:D:3743:THR:HB	1:D:3758:THR:HG21	2.02	0.41
1:D:3784:LYS:HA	1:D:3784:LYS:HD3	1.79	0.41
1:D:4040:LYS:HG3	1:D:4042:VAL:HG13	2.02	0.41
1:D:4751:LYS:O	1:D:4755:THR:HG23	2.21	0.41
1:A:42:PHE:CZ	1:A:459:LEU:HG	2.55	0.41
1:A:251:GLU:HG3	1:A:256:GLN:HG3	2.01	0.41
1:A:1152:TYR:HD1	1:A:1184:ASP:HB3	1.85	0.41
1:A:1199:ASP:OD1	1:A:1199:ASP:N	2.50	0.41
1:A:2596:VAL:HG21	1:A:2610:LEU:HD11	2.02	0.41
1:B:1444:GLY:HA3	1:B:1487:MET:HG2	2.02	0.41
1:B:2741:TRP:O	1:B:2757:MET:HE3	2.21	0.41
1:B:3896:ASP:OD1	1:B:3897:VAL:N	2.54	0.41
1:C:661:LEU:HD22	1:C:673:TRP:CE2	2.55	0.41
1:C:2532:ALA:HA	1:C:2535:PHE:HD2	1.84	0.41
1:C:4135:ARG:HG2	1:C:4149:TYR:CD1	2.55	0.41
1:D:925:PRO:HB2	1:D:928:GLU:CB	2.51	0.41
1:D:1306:MET:HB2	1:D:1570:LEU:HD22	2.02	0.41
1:D:1935:LYS:HB3	1:D:1935:LYS:HE2	1.90	0.41
1:D:2641:SER:HB2	1:D:2676:LEU:HD21	2.01	0.41
1:A:661:LEU:HD22	1:A:673:TRP:CE2	2.55	0.41
1:A:1444:GLY:HA3	1:A:1487:MET:HG2	2.02	0.41
1:A:3124:GLU:HG2	1:A:3125:ASP:N	2.36	0.41
1:A:3743:THR:HB	1:A:3758:THR:HG21	2.02	0.41
1:A:3763:ILE:HD11	1:A:3838:ASP:O	2.21	0.41
1:B:42:PHE:CZ	1:B:459:LEU:HG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1086:ARG:HG3	1:B:1252:SER:OG	2.21	0.41
1:B:2532:ALA:HA	1:B:2535:PHE:HD2	1.84	0.41
1:B:3124:GLU:HG2	1:B:3125:ASP:N	2.36	0.41
1:B:3138:TYR:CG	1:B:3208:ILE:HG12	2.55	0.41
1:B:4245:LEU:HD21	1:C:4629:GLN:HB3	2.01	0.41
1:C:2392:TYR:O	1:C:2396:ILE:HG12	2.21	0.41
1:C:3960:GLN:HA	1:C:4069:CYS:HA	2.03	0.41
1:D:499:LEU:HD22	1:D:557:TRP:CZ3	2.56	0.41
1:D:3125:ASP:HA	1:D:3128:VAL:HG12	2.02	0.41
1:A:1218:GLY:HA3	1:A:1238:PRO:HB3	2.03	0.41
1:A:2140:LYS:HG2	1:A:2144:ARG:HH21	1.84	0.41
1:A:2714:PRO:HD3	1:A:2783:LEU:HD11	2.03	0.41
1:A:2833:LEU:HD21	1:A:2894:LYS:HG3	2.03	0.41
1:A:4046:ARG:HH12	1:A:4076:GLU:HG2	1.86	0.41
1:A:4522:VAL:HG12	1:B:4807:ASP:O	2.20	0.41
1:B:941:LYS:HA	1:B:944:LEU:HG	2.01	0.41
1:B:2135:GLY:H	1:B:2138:GLU:HB2	1.86	0.41
1:B:2787:TRP:CD1	1:B:2905:ARG:HA	2.56	0.41
1:B:4664:ASP:HA	1:B:4674:LYS:HD3	2.03	0.41
1:B:4751:LYS:O	1:B:4755:THR:HG23	2.21	0.41
1:C:1045:SER:HA	1:C:1048:ASP:OD2	2.19	0.41
1:D:816:PRO:HB2	1:D:819:TYR:CD1	2.55	0.41
1:D:3054:LYS:O	1:D:3058:ARG:HG3	2.21	0.41
1:D:4135:ARG:HG2	1:D:4149:TYR:CD1	2.55	0.41
1:A:208:GLN:N	1:A:208:GLN:OE1	2.53	0.41
1:A:925:PRO:HB2	1:A:928:GLU:CB	2.51	0.41
1:A:3054:LYS:O	1:A:3058:ARG:HG3	2.21	0.41
1:B:414:ARG:O	1:B:418:VAL:HG23	2.20	0.41
1:B:661:LEU:HD22	1:B:673:TRP:CE2	2.55	0.41
1:B:4040:LYS:HG3	1:B:4042:VAL:HG13	2.02	0.41
1:C:1937:GLN:NE2	1:C:3608:LEU:O	2.54	0.41
1:C:2831:VAL:HG22	1:D:1435:GLY:HA2	2.03	0.41
1:C:3896:ASP:OD1	1:C:3897:VAL:N	2.54	0.41
1:D:22:LEU:HD23	1:D:22:LEU:HA	1.95	0.41
1:D:2596:VAL:HG21	1:D:2610:LEU:HD11	2.02	0.41
1:A:499:LEU:HD22	1:A:557:TRP:CZ3	2.56	0.41
1:A:677:LEU:HD12	1:A:801:ARG:O	2.21	0.41
1:A:839:GLU:HB3	1:A:851:LEU:HD12	2.03	0.41
1:A:1086:ARG:HG3	1:A:1252:SER:OG	2.21	0.41
1:A:1427:TYR:HB2	1:A:1563:VAL:HG11	2.01	0.41
1:A:1697:LEU:HD23	1:A:1697:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2280:LEU:HD11	1:A:2382:ILE:HG13	2.02	0.41
1:A:2434:GLY:O	1:A:2438:ILE:HG13	2.20	0.41
1:A:2582:PRO:HG3	1:A:2617:CYS:SG	2.60	0.41
1:A:3178:HIS:CD2	1:A:3263:MET:HA	2.56	0.41
1:A:3277:LEU:HA	1:A:3280:ILE:HD12	2.02	0.41
1:A:3787:VAL:HG11	1:A:3866:THR:HB	2.02	0.41
1:B:544:ASN:HB3	1:B:547:ASN:HB2	2.03	0.41
1:B:658:ASN:ND2	1:B:831:LYS:O	2.34	0.41
1:B:872:ILE:HD12	1:B:941:LYS:NZ	2.36	0.41
1:B:941:LYS:O	1:B:944:LEU:HG	2.21	0.41
1:B:1805:HIS:ND1	1:B:1805:HIS:N	2.68	0.41
1:B:2178:VAL:HG21	1:B:2192:MET:HE2	2.03	0.41
1:B:2290:TRP:HZ3	1:B:2391:PHE:CD1	2.39	0.41
1:B:2392:TYR:O	1:B:2396:ILE:HG12	2.21	0.41
1:B:2434:GLY:O	1:B:2438:ILE:HG13	2.20	0.41
1:B:2582:PRO:HG3	1:B:2617:CYS:SG	2.60	0.41
1:B:2640:LEU:HA	1:B:2643:LYS:HZ3	1.86	0.41
1:B:4046:ARG:HH12	1:B:4076:GLU:HG2	1.86	0.41
1:B:4721:TYR:OH	1:B:4745:ASP:OD1	2.32	0.41
1:C:414:ARG:O	1:C:418:VAL:HG23	2.20	0.41
1:C:484:ASN:O	1:C:488:LEU:HD23	2.21	0.41
1:C:499:LEU:HD22	1:C:557:TRP:CZ3	2.56	0.41
1:C:872:ILE:HD12	1:C:941:LYS:NZ	2.36	0.41
1:C:1086:ARG:HG3	1:C:1252:SER:OG	2.21	0.41
1:C:1218:GLY:HA3	1:C:1238:PRO:HB3	2.02	0.41
1:C:1306:MET:HB2	1:C:1570:LEU:HD22	2.02	0.41
1:C:1444:GLY:HA3	1:C:1487:MET:HG2	2.02	0.41
1:C:1788:LYS:NZ	1:C:1833:ILE:O	2.48	0.41
1:C:2666:LEU:HD21	1:C:2969:PRO:HB2	2.02	0.41
1:C:2833:LEU:HD21	1:C:2894:LYS:HG3	2.03	0.41
1:C:2913:ASP:C	1:C:2915:PRO:HD2	2.42	0.41
1:C:3787:VAL:HG11	1:C:3866:THR:HB	2.02	0.41
1:D:114:LEU:HD11	1:D:174:LYS:HG2	2.03	0.41
1:D:546:LYS:O	1:D:550:GLN:HG2	2.20	0.41
1:D:1444:GLY:HA3	1:D:1487:MET:HG2	2.02	0.41
1:D:1458:ASP:OD1	1:D:1461:ARG:NE	2.45	0.41
1:D:2272:CYS:HB3	1:D:2291:ASN:HB3	2.02	0.41
1:D:2280:LEU:HD11	1:D:2382:ILE:HG13	2.02	0.41
1:D:2541:HIS:O	1:D:2545:ILE:HG12	2.20	0.41
1:D:2913:ASP:C	1:D:2915:PRO:HD2	2.42	0.41
1:D:3036:LEU:O	1:D:3040:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3251:GLU:O	1:D:3257:ASN:ND2	2.48	0.41
1:D:3960:GLN:HA	1:D:4069:CYS:HA	2.03	0.41
1:D:4007:SER:HA	1:D:4118:PHE:HZ	1.85	0.41
1:D:4046:ARG:HH12	1:D:4076:GLU:HG2	1.86	0.41
1:A:762:SER:OG	1:A:763:ALA:N	2.54	0.41
1:A:1038:LEU:HD23	1:A:1043:LYS:HB3	2.02	0.41
1:A:1805:HIS:ND1	1:A:1805:HIS:N	2.68	0.41
1:A:2135:GLY:H	1:A:2138:GLU:HB2	1.86	0.41
1:A:2640:LEU:HA	1:A:2643:LYS:HZ3	1.86	0.41
1:A:4040:LYS:HG3	1:A:4042:VAL:HG13	2.02	0.41
1:A:4664:ASP:HA	1:A:4674:LYS:HD3	2.03	0.41
1:B:1121:GLY:O	1:B:1123:GLN:NE2	2.53	0.41
1:B:2272:CYS:HB3	1:B:2291:ASN:HB3	2.02	0.41
1:B:3763:ILE:HD11	1:B:3838:ASP:O	2.21	0.41
1:B:4522:VAL:HG12	1:C:4807:ASP:O	2.21	0.41
1:C:2714:PRO:HD3	1:C:2783:LEU:HD11	2.03	0.41
1:C:2998:ASN:O	1:C:3002:GLU:HG3	2.21	0.41
1:C:3124:GLU:HG2	1:C:3125:ASP:N	2.36	0.41
1:C:3192:ARG:N	1:C:3192:ARG:HD3	2.36	0.41
1:C:4113:THR:O	1:C:4117:THR:HG23	2.21	0.41
1:D:544:ASN:HB3	1:D:547:ASN:HB2	2.03	0.41
1:D:2392:TYR:O	1:D:2396:ILE:HG12	2.21	0.41
1:D:3787:VAL:HG11	1:D:3866:THR:HB	2.02	0.41
1:A:315:LEU:HD12	1:A:315:LEU:HA	1.93	0.40
1:A:1458:ASP:OD1	1:A:1461:ARG:NE	2.46	0.40
1:A:2272:CYS:HB3	1:A:2291:ASN:HB3	2.02	0.40
1:A:2290:TRP:HZ3	1:A:2391:PHE:CD1	2.39	0.40
1:A:3138:TYR:CG	1:A:3208:ILE:HG12	2.55	0.40
1:A:3192:ARG:HD3	1:A:3192:ARG:N	2.36	0.40
1:A:3896:ASP:OD1	1:A:3897:VAL:N	2.54	0.40
1:B:2280:LEU:HD11	1:B:2382:ILE:HG13	2.02	0.40
1:B:3178:HIS:CD2	1:B:3263:MET:HA	2.56	0.40
1:C:925:PRO:HB2	1:C:928:GLU:CB	2.51	0.40
1:C:2208:ARG:NH2	1:C:2252:GLU:OE1	2.55	0.40
1:C:2265:VAL:HG21	1:C:2301:PHE:CE2	2.56	0.40
1:C:2541:HIS:O	1:C:2545:ILE:HG12	2.20	0.40
1:C:3743:THR:HB	1:C:3758:THR:HG21	2.02	0.40
1:C:4007:SER:HA	1:C:4118:PHE:HZ	1.85	0.40
1:C:4625:ASP:OD1	1:C:4625:ASP:N	2.46	0.40
1:D:202:HIS:HD2	1:D:203:VAL:H	1.68	0.40
1:D:484:ASN:O	1:D:488:LEU:HD23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1152:TYR:HD1	1:D:1184:ASP:HB3	1.84	0.40
1:D:1729:MET:HE1	1:D:3617:VAL:HG21	2.02	0.40
1:D:3124:GLU:HG2	1:D:3125:ASP:N	2.36	0.40
1:D:3821:THR:HG23	1:D:3821:THR:O	2.21	0.40
1:D:4964:ASP:OD1	1:D:4964:ASP:N	2.49	0.40
1:A:3171:LEU:HB3	1:A:3211:LEU:HB2	2.03	0.40
1:A:3211:LEU:O	1:A:3215:MET:HG2	2.21	0.40
1:A:4155:SER:O	1:A:4159:GLN:HG2	2.22	0.40
1:A:4751:LYS:O	1:A:4755:THR:HG23	2.21	0.40
1:B:22:LEU:HD23	1:B:22:LEU:HA	1.95	0.40
1:B:677:LEU:HD12	1:B:801:ARG:O	2.21	0.40
1:B:1310:CYS:HA	1:B:1513:ALA:HB1	2.03	0.40
1:B:1427:TYR:HB2	1:B:1563:VAL:HG11	2.01	0.40
1:B:2714:PRO:HD3	1:B:2783:LEU:HD11	2.03	0.40
1:B:2724:TYR:OH	1:B:2891:ASP:OD2	2.35	0.40
1:B:3036:LEU:O	1:B:3040:LEU:HG	2.21	0.40
1:B:3171:LEU:HB3	1:B:3211:LEU:HB2	2.03	0.40
1:B:3192:ARG:HD3	1:B:3192:ARG:H	1.87	0.40
1:B:3211:LEU:O	1:B:3215:MET:HG2	2.21	0.40
1:B:3277:LEU:HA	1:B:3280:ILE:HD12	2.02	0.40
1:B:3960:GLN:HA	1:B:4069:CYS:HA	2.03	0.40
1:B:4520:TYR:HE1	1:B:4561:LEU:HG	1.86	0.40
1:C:514:PHE:HD2	1:C:526:TRP:HB2	1.87	0.40
1:C:2290:TRP:HZ3	1:C:2391:PHE:CD1	2.39	0.40
1:C:2787:TRP:CD1	1:C:2905:ARG:HA	2.56	0.40
1:D:2055:SER:HB3	1:D:2060:GLN:HB2	2.03	0.40
1:D:2333:PRO:O	1:D:2336:ARG:HG2	2.21	0.40
1:D:2434:GLY:O	1:D:2438:ILE:HG13	2.20	0.40
1:D:3001:LYS:HD2	1:D:3041:ASP:HB3	2.03	0.40
1:A:114:LEU:HD11	1:A:174:LYS:HG2	2.03	0.40
1:A:2392:TYR:O	1:A:2396:ILE:HG12	2.21	0.40
1:A:2497:ARG:HG2	1:A:2551:THR:HG21	2.04	0.40
1:A:2948:ARG:H	1:A:2948:ARG:HD3	1.86	0.40
1:A:4864:GLY:HA2	1:D:4867:ILE:HG12	2.02	0.40
4:A:5003:ATP:O3G	4:A:5003:ATP:H3'	2.21	0.40
1:B:484:ASN:O	1:B:488:LEU:HD23	2.21	0.40
1:B:2333:PRO:O	1:B:2336:ARG:HG2	2.21	0.40
1:C:227:TYR:HA	1:C:354:ILE:O	2.21	0.40
1:C:614:LEU:HA	1:C:617:LEU:HD12	2.02	0.40
1:C:677:LEU:HD12	1:C:801:ARG:O	2.21	0.40
1:C:718:VAL:HG13	1:C:724:SER:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2280:LEU:HD11	1:C:2382:ILE:HG13	2.02	0.40
1:C:2434:GLY:O	1:C:2438:ILE:HG13	2.20	0.40
1:C:3036:LEU:O	1:C:3040:LEU:HG	2.21	0.40
1:C:3171:LEU:HB3	1:C:3211:LEU:HB2	2.03	0.40
1:C:3192:ARG:HH11	1:C:3192:ARG:CG	2.34	0.40
1:C:4520:TYR:HE1	1:C:4561:LEU:HG	1.86	0.40
1:C:4795:LYS:HA	1:C:4795:LYS:HD2	1.91	0.40
1:C:4798:ASP:N	1:C:4798:ASP:OD1	2.55	0.40
1:D:718:VAL:HG13	1:D:724:SER:HB2	2.03	0.40
1:D:839:GLU:HB3	1:D:851:LEU:HD12	2.03	0.40
1:D:2208:ARG:NH2	1:D:2252:GLU:OE1	2.54	0.40
1:D:2998:ASN:O	1:D:3002:GLU:HG3	2.21	0.40
1:D:3763:ILE:HD11	1:D:3838:ASP:O	2.21	0.40
1:D:3966:GLU:HG2	1:D:3967:LEU:N	2.37	0.40
1:D:4484:ILE:H	1:D:4484:ILE:HD12	1.87	0.40
1:A:679:VAL:HG22	1:A:800:VAL:HG12	2.04	0.40
1:A:838:ARG:HA	1:A:838:ARG:HD3	1.87	0.40
1:A:2055:SER:HB3	1:A:2060:GLN:HB2	2.04	0.40
1:A:2265:VAL:HG21	1:A:2301:PHE:CE2	2.56	0.40
1:A:2333:PRO:O	1:A:2336:ARG:HG2	2.21	0.40
1:A:2787:TRP:CD1	1:A:2905:ARG:HA	2.56	0.40
1:A:4484:ILE:HD12	1:A:4484:ILE:H	1.87	0.40
1:B:114:LEU:HD11	1:B:174:LYS:HG2	2.03	0.40
1:B:614:LEU:HA	1:B:617:LEU:HD12	2.02	0.40
1:B:1729:MET:HE1	1:B:3617:VAL:HG21	2.02	0.40
1:B:2070:ALA:O	1:B:3666:GLN:NE2	2.55	0.40
1:B:2541:HIS:O	1:B:2545:ILE:HG12	2.20	0.40
1:B:3821:THR:O	1:B:3821:THR:HG23	2.21	0.40
1:B:4484:ILE:HD12	1:B:4484:ILE:H	1.86	0.40
1:C:3763:ILE:HD11	1:C:3838:ASP:O	2.20	0.40
1:D:815:PRO:HA	1:D:816:PRO:HD3	1.97	0.40
1:D:1522:ALA:HB2	1:D:1527:LEU:HD21	2.02	0.40
1:D:2290:TRP:HZ3	1:D:2391:PHE:CD1	2.39	0.40
1:D:2456:MET:HB3	1:D:2461:CYS:SG	2.62	0.40
1:D:3293:GLY:H	1:D:3296:MET:HE1	1.87	0.40
1:D:3896:ASP:OD1	1:D:3897:VAL:N	2.54	0.40
1:D:4155:SER:O	1:D:4159:GLN:HG2	2.22	0.40
1:A:137:ARG:HD3	1:A:202:HIS:CE1	2.56	0.40
1:A:484:ASN:O	1:A:488:LEU:HD23	2.21	0.40
1:A:2070:ALA:O	1:A:3666:GLN:NE2	2.55	0.40
1:A:2322:ARG:O	1:A:2326:ARG:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2413:LYS:HZ2	1:A:2416:ALA:N	2.20	0.40
1:A:3848:GLU:HA	1:A:3922:GLU:OE2	2.22	0.40
1:A:3966:GLU:HG2	1:A:3967:LEU:N	2.37	0.40
1:A:4798:ASP:OD1	1:A:4798:ASP:N	2.55	0.40
1:B:499:LEU:HD22	1:B:557:TRP:CZ3	2.56	0.40
1:B:762:SER:OG	1:B:763:ALA:N	2.54	0.40
1:B:1937:GLN:NE2	1:B:3608:LEU:O	2.54	0.40
1:B:2244:ALA:O	1:B:2248:MET:HB2	2.21	0.40
1:B:2265:VAL:HG21	1:B:2301:PHE:CE2	2.56	0.40
1:B:2913:ASP:C	1:B:2915:PRO:HD2	2.42	0.40
1:B:2948:ARG:HD3	1:B:2948:ARG:H	1.86	0.40
1:B:3743:THR:HB	1:B:3758:THR:HG21	2.02	0.40
1:B:3784:LYS:HA	1:B:3784:LYS:HD3	1.79	0.40
1:C:718:VAL:HG23	1:C:793:SER:HB3	2.04	0.40
1:C:762:SER:OG	1:C:763:ALA:N	2.54	0.40
1:C:1805:HIS:ND1	1:C:1805:HIS:N	2.68	0.40
1:C:2244:ALA:O	1:C:2248:MET:HB2	2.21	0.40
1:D:677:LEU:HD12	1:D:801:ARG:O	2.21	0.40
1:D:855:VAL:HG23	1:D:1078:CYS:HB2	2.04	0.40
1:D:2640:LEU:HA	1:D:2643:LYS:HZ3	1.86	0.40
1:D:2787:TRP:CD1	1:D:2905:ARG:HA	2.56	0.40
1:D:3211:LEU:O	1:D:3215:MET:HG2	2.21	0.40
1:D:4113:THR:O	1:D:4117:THR:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4198/4967 (84%)	4053 (96%)	140 (3%)	5 (0%)	48	81
1	B	4198/4967 (84%)	4053 (96%)	140 (3%)	5 (0%)	48	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	4198/4967 (84%)	4053 (96%)	140 (3%)	5 (0%)	48	81
1	D	4198/4967 (84%)	4053 (96%)	140 (3%)	5 (0%)	48	81
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
All	All	17212/20300 (85%)	16620 (97%)	572 (3%)	20 (0%)	50	81

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1495	SER
1	A	2915	PRO
1	A	4884	MET
1	B	1495	SER
1	B	2915	PRO
1	B	4884	MET
1	C	1495	SER
1	C	2915	PRO
1	C	4884	MET
1	D	1495	SER
1	D	2915	PRO
1	D	4884	MET
1	A	324	VAL
1	B	324	VAL
1	C	324	VAL
1	D	324	VAL
1	A	313	ASN
1	B	313	ASN
1	C	313	ASN
1	D	313	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3708/4358 (85%)	3689 (100%)	19 (0%)	86	94
1	B	3708/4358 (85%)	3689 (100%)	19 (0%)	86	94
1	C	3708/4358 (85%)	3689 (100%)	19 (0%)	86	94
1	D	3708/4358 (85%)	3689 (100%)	19 (0%)	86	94
2	E	88/89 (99%)	86 (98%)	2 (2%)	45	75
2	F	88/89 (99%)	86 (98%)	2 (2%)	45	75
2	G	88/89 (99%)	86 (98%)	2 (2%)	45	75
2	H	88/89 (99%)	86 (98%)	2 (2%)	45	75
All	All	15184/17788 (85%)	15100 (99%)	84 (1%)	82	93

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1013	ARG
1	A	1805	HIS
1	A	1939	ASN
1	A	1960	ARG
1	A	2185	LYS
1	A	2788	ARG
1	A	2884	LYS
1	A	2948	ARG
1	A	3018	ARG
1	A	3187	LYS
1	A	3192	ARG
1	A	3220	GLU
1	A	3248	ARG
1	A	3260	ARG
1	A	3298	ARG
1	A	3319	PHE
1	A	3327	LYS
1	A	3904	ARG
1	A	4966	LEU
2	E	19	LYS
2	E	54	GLN
2	F	19	LYS
2	F	54	GLN
2	G	19	LYS
2	G	54	GLN
2	H	19	LYS
2	H	54	GLN

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Mol	Chain	Res	Type
1	B	1013	ARG
1	B	1805	HIS
1	B	1939	ASN
1	B	1960	ARG
1	B	2185	LYS
1	B	2788	ARG
1	B	2884	LYS
1	B	2948	ARG
1	B	3018	ARG
1	B	3187	LYS
1	B	3192	ARG
1	B	3220	GLU
1	B	3248	ARG
1	B	3260	ARG
1	B	3298	ARG
1	B	3319	PHE
1	B	3327	LYS
1	B	3904	ARG
1	B	4966	LEU
1	C	1013	ARG
1	C	1805	HIS
1	C	1939	ASN
1	C	1960	ARG
1	C	2185	LYS
1	C	2788	ARG
1	C	2884	LYS
1	C	2948	ARG
1	C	3018	ARG
1	C	3187	LYS
1	C	3192	ARG
1	C	3220	GLU
1	C	3248	ARG
1	C	3260	ARG
1	C	3298	ARG
1	C	3319	PHE
1	C	3327	LYS
1	C	3904	ARG
1	C	4966	LEU
1	D	1013	ARG
1	D	1805	HIS
1	D	1939	ASN
1	D	1960	ARG

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Mol	Chain	Res	Type
1	D	2185	LYS
1	D	2788	ARG
1	D	2884	LYS
1	D	2948	ARG
1	D	3018	ARG
1	D	3187	LYS
1	D	3192	ARG
1	D	3220	GLU
1	D	3248	ARG
1	D	3260	ARG
1	D	3298	ARG
1	D	3319	PHE
1	D	3327	LYS
1	D	3904	ARG
1	D	4966	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	HIS
1	A	313	ASN
1	A	3256	ASN
1	B	202	HIS
1	B	313	ASN
1	B	1939	ASN
1	B	3256	ASN
1	C	150	GLN
1	C	202	HIS
1	C	313	ASN
1	D	202	HIS
1	D	313	ASN
1	D	3274	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	A	5002	-	28,33,33	0.63	0	34,52,52	0.90	2 (5%)
4	ATP	D	5003	-	28,33,33	0.63	0	34,52,52	0.58	1 (2%)
4	ATP	B	5002	-	28,33,33	0.62	0	34,52,52	0.90	2 (5%)
4	ATP	C	5003	-	28,33,33	0.63	0	34,52,52	0.58	1 (2%)
5	KVR	C	5004	-	24,25,25	1.63	3 (12%)	31,34,34	2.07	5 (16%)
5	KVR	A	5004	-	24,25,25	0.51	0	31,34,34	0.97	2 (6%)
4	ATP	B	5003	-	28,33,33	0.63	0	34,52,52	0.58	1 (2%)
5	KVR	B	5004	-	24,25,25	1.63	3 (12%)	31,34,34	2.07	5 (16%)
5	KVR	D	5004	-	24,25,25	1.65	3 (12%)	31,34,34	2.07	5 (16%)
4	ATP	C	5002	-	28,33,33	0.63	0	34,52,52	0.90	2 (5%)
4	ATP	A	5003	-	28,33,33	0.90	0	34,52,52	1.20	4 (11%)
4	ATP	D	5002	-	28,33,33	0.63	0	34,52,52	0.90	2 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	5002	-	-	8/18/38/38	0/3/3/3
4	ATP	D	5003	-	-	8/18/38/38	0/3/3/3
4	ATP	B	5002	-	-	8/18/38/38	0/3/3/3
4	ATP	C	5003	-	-	8/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	KVR	C	5004	-	-	6/10/20/20	0/2/3/3
5	KVR	A	5004	-	-	8/10/20/20	0/2/3/3
4	ATP	B	5003	-	-	8/18/38/38	0/3/3/3
5	KVR	B	5004	-	-	6/10/20/20	0/2/3/3
5	KVR	D	5004	-	-	6/10/20/20	0/2/3/3
4	ATP	C	5002	-	-	8/18/38/38	0/3/3/3
4	ATP	A	5003	-	-	5/18/38/38	0/3/3/3
4	ATP	D	5002	-	-	9/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	5004	KVR	C06-S09	6.15	1.83	1.77
5	D	5004	KVR	C06-S09	6.15	1.83	1.77
5	C	5004	KVR	C06-S09	6.11	1.83	1.77
5	D	5004	KVR	C13-N12	-2.66	1.45	1.47
5	B	5004	KVR	C13-N12	-2.56	1.45	1.47
5	C	5004	KVR	C13-N12	-2.56	1.45	1.47
5	D	5004	KVR	C13-C05	2.43	1.55	1.51
5	B	5004	KVR	C13-C05	2.35	1.54	1.51
5	C	5004	KVR	C13-C05	2.35	1.54	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	5004	KVR	C10-S09-C06	8.54	114.81	102.71
5	B	5004	KVR	C10-S09-C06	8.52	114.78	102.71
5	D	5004	KVR	C10-S09-C06	8.51	114.77	102.71
5	C	5004	KVR	C14-N12-C11	4.44	118.32	111.09
5	B	5004	KVR	C14-N12-C11	4.43	118.30	111.09
5	D	5004	KVR	C14-N12-C11	4.43	118.30	111.09
4	C	5002	ATP	C4'-O4'-C1'	-3.93	106.33	109.92
4	B	5002	ATP	C4'-O4'-C1'	-3.93	106.33	109.92
4	D	5002	ATP	C4'-O4'-C1'	-3.92	106.33	109.92
4	A	5002	ATP	C4'-O4'-C1'	-3.89	106.36	109.92
4	A	5003	ATP	N3-C2-N1	-3.72	123.63	128.67
5	A	5004	KVR	C11-C10-S09	-3.45	110.22	114.26
5	D	5004	KVR	C05-C13-N12	-3.25	106.64	114.35
5	B	5004	KVR	C05-C13-N12	-3.25	106.64	114.35
5	C	5004	KVR	C05-C13-N12	-3.25	106.64	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	5004	KVR	C14-N12-C13	2.81	117.23	112.72
5	B	5004	KVR	C14-N12-C13	2.80	117.22	112.72
5	C	5004	KVR	C14-N12-C13	2.77	117.18	112.72
4	A	5002	ATP	C5-C6-N6	2.32	123.84	120.31
4	B	5003	ATP	C5-C6-N6	2.32	123.84	120.31
4	C	5002	ATP	C5-C6-N6	2.31	123.83	120.31
4	D	5003	ATP	C5-C6-N6	2.30	123.82	120.31
4	D	5002	ATP	C5-C6-N6	2.29	123.80	120.31
4	C	5003	ATP	C5-C6-N6	2.28	123.79	120.31
4	B	5002	ATP	C5-C6-N6	2.27	123.77	120.31
5	A	5004	KVR	C14-N12-C11	2.14	114.57	111.09
4	A	5003	ATP	O4'-C1'-N9	2.13	111.57	108.75
5	D	5004	KVR	O23-C21-C18	2.09	120.19	114.84
5	B	5004	KVR	O23-C21-C18	2.08	120.17	114.84
5	C	5004	KVR	O23-C21-C18	2.06	120.12	114.84
4	A	5003	ATP	C4-C5-N7	-2.02	107.20	109.34
4	A	5003	ATP	O3G-PG-O2G	2.02	115.37	107.80

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	C5'-O5'-PA-O1A
4	A	5002	ATP	C5'-O5'-PA-O3A
4	A	5002	ATP	O4'-C4'-C5'-O5'
4	A	5002	ATP	C3'-C4'-C5'-O5'
4	A	5003	ATP	C5'-O5'-PA-O1A
4	A	5003	ATP	C5'-O5'-PA-O2A
4	A	5003	ATP	C5'-O5'-PA-O3A
4	B	5002	ATP	C5'-O5'-PA-O1A
4	B	5002	ATP	C5'-O5'-PA-O3A
4	B	5002	ATP	O4'-C4'-C5'-O5'
4	B	5002	ATP	C3'-C4'-C5'-O5'
4	B	5003	ATP	C5'-O5'-PA-O1A
4	B	5003	ATP	C5'-O5'-PA-O2A
4	C	5002	ATP	C5'-O5'-PA-O1A
4	C	5002	ATP	C5'-O5'-PA-O3A
4	C	5002	ATP	O4'-C4'-C5'-O5'
4	C	5002	ATP	C3'-C4'-C5'-O5'
4	C	5003	ATP	C5'-O5'-PA-O1A
4	C	5003	ATP	C5'-O5'-PA-O2A
4	D	5002	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	D	5002	ATP	C5'-O5'-PA-O3A
4	D	5002	ATP	O4'-C4'-C5'-O5'
4	D	5002	ATP	C3'-C4'-C5'-O5'
4	D	5003	ATP	C5'-O5'-PA-O1A
4	D	5003	ATP	C5'-O5'-PA-O2A
5	A	5004	KVR	C15-C14-N12-C11
5	A	5004	KVR	C15-C14-N12-C13
5	A	5004	KVR	C19-C18-C21-O23
5	B	5004	KVR	C17-C18-C21-O23
5	B	5004	KVR	C19-C18-C21-O22
5	C	5004	KVR	C17-C18-C21-O23
5	C	5004	KVR	C19-C18-C21-O22
5	D	5004	KVR	C17-C18-C21-O23
5	D	5004	KVR	C19-C18-C21-O22
5	A	5004	KVR	C17-C18-C21-O22
5	A	5004	KVR	C17-C18-C21-O23
5	B	5004	KVR	C19-C18-C21-O23
5	C	5004	KVR	C19-C18-C21-O23
5	D	5004	KVR	C19-C18-C21-O23
5	A	5004	KVR	C19-C18-C21-O22
5	B	5004	KVR	C17-C18-C21-O22
5	C	5004	KVR	C17-C18-C21-O22
5	D	5004	KVR	C17-C18-C21-O22
5	A	5004	KVR	C04-C03-O02-C01
5	A	5004	KVR	C08-C03-O02-C01
5	C	5004	KVR	C08-C03-O02-C01
5	B	5004	KVR	C04-C03-O02-C01
5	B	5004	KVR	C08-C03-O02-C01
5	C	5004	KVR	C04-C03-O02-C01
5	D	5004	KVR	C04-C03-O02-C01
5	D	5004	KVR	C08-C03-O02-C01
4	A	5003	ATP	O4'-C4'-C5'-O5'
4	A	5003	ATP	C3'-C4'-C5'-O5'
4	B	5003	ATP	C3'-C4'-C5'-O5'
4	C	5003	ATP	C3'-C4'-C5'-O5'
4	D	5003	ATP	C3'-C4'-C5'-O5'
4	B	5003	ATP	O4'-C4'-C5'-O5'
4	C	5003	ATP	O4'-C4'-C5'-O5'
4	D	5003	ATP	O4'-C4'-C5'-O5'
4	B	5003	ATP	C4'-C5'-O5'-PA
4	C	5003	ATP	C4'-C5'-O5'-PA
4	D	5003	ATP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	PB-O3B-PG-O1G
4	B	5002	ATP	PB-O3B-PG-O1G
4	C	5002	ATP	PB-O3B-PG-O1G
4	D	5002	ATP	PB-O3B-PG-O1G
4	A	5002	ATP	C5'-O5'-PA-O2A
4	B	5002	ATP	C5'-O5'-PA-O2A
4	B	5003	ATP	C5'-O5'-PA-O3A
4	C	5002	ATP	C5'-O5'-PA-O2A
4	C	5003	ATP	C5'-O5'-PA-O3A
4	D	5002	ATP	C5'-O5'-PA-O2A
4	D	5003	ATP	C5'-O5'-PA-O3A
4	A	5002	ATP	PA-O3A-PB-O1B
4	B	5002	ATP	PA-O3A-PB-O1B
4	C	5002	ATP	PA-O3A-PB-O1B
4	D	5002	ATP	PA-O3A-PB-O1B
4	D	5002	ATP	PB-O3B-PG-O3G
4	A	5002	ATP	PA-O3A-PB-O3B
4	B	5002	ATP	PA-O3A-PB-O3B
4	C	5002	ATP	PA-O3A-PB-O3B
4	D	5002	ATP	PA-O3A-PB-O3B
4	B	5003	ATP	PA-O3A-PB-O2B
4	B	5003	ATP	PB-O3A-PA-O2A
4	C	5003	ATP	PA-O3A-PB-O2B
4	C	5003	ATP	PB-O3A-PA-O2A
4	D	5003	ATP	PA-O3A-PB-O2B
4	D	5003	ATP	PB-O3A-PA-O2A

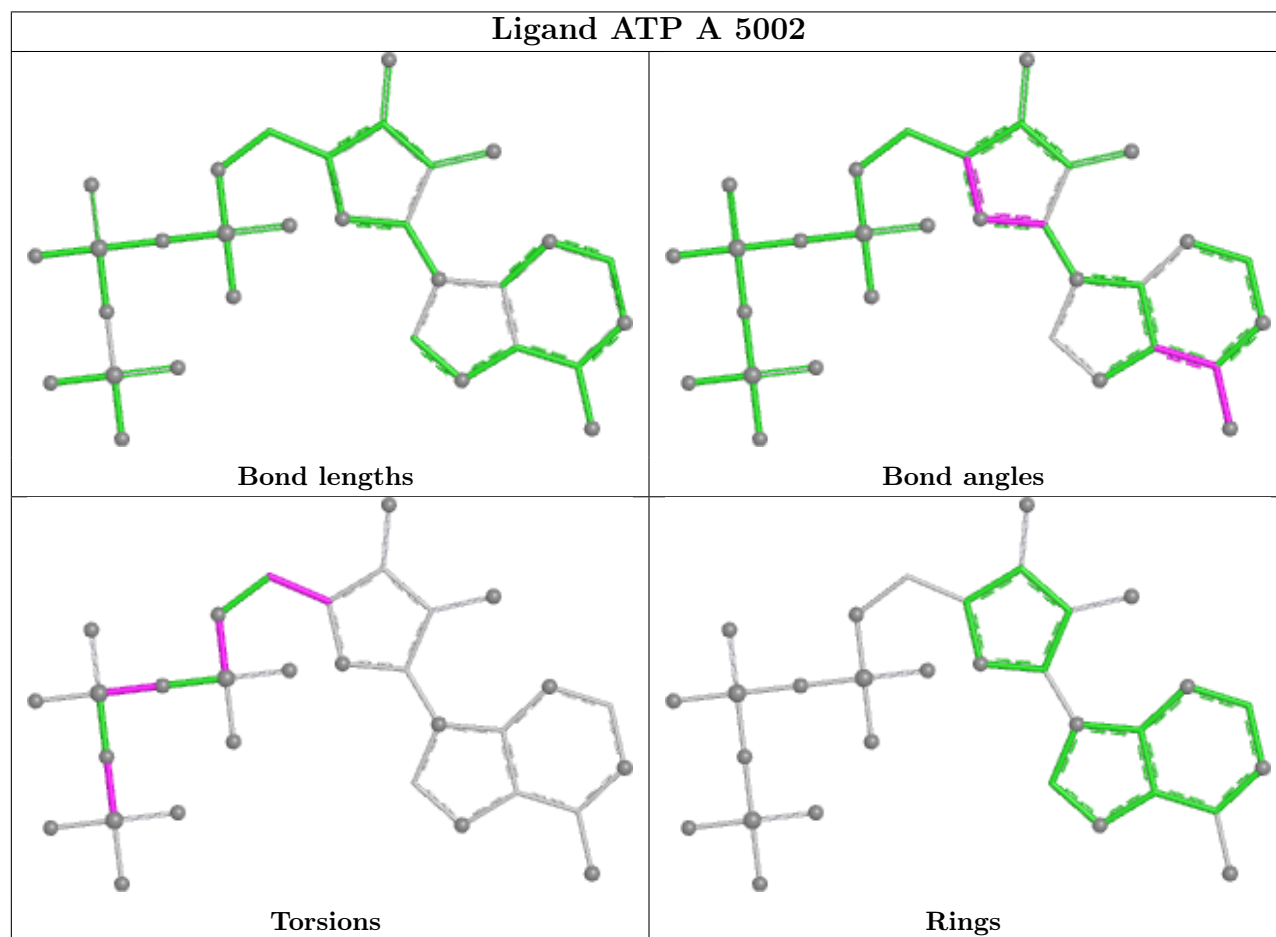
There are no ring outliers.

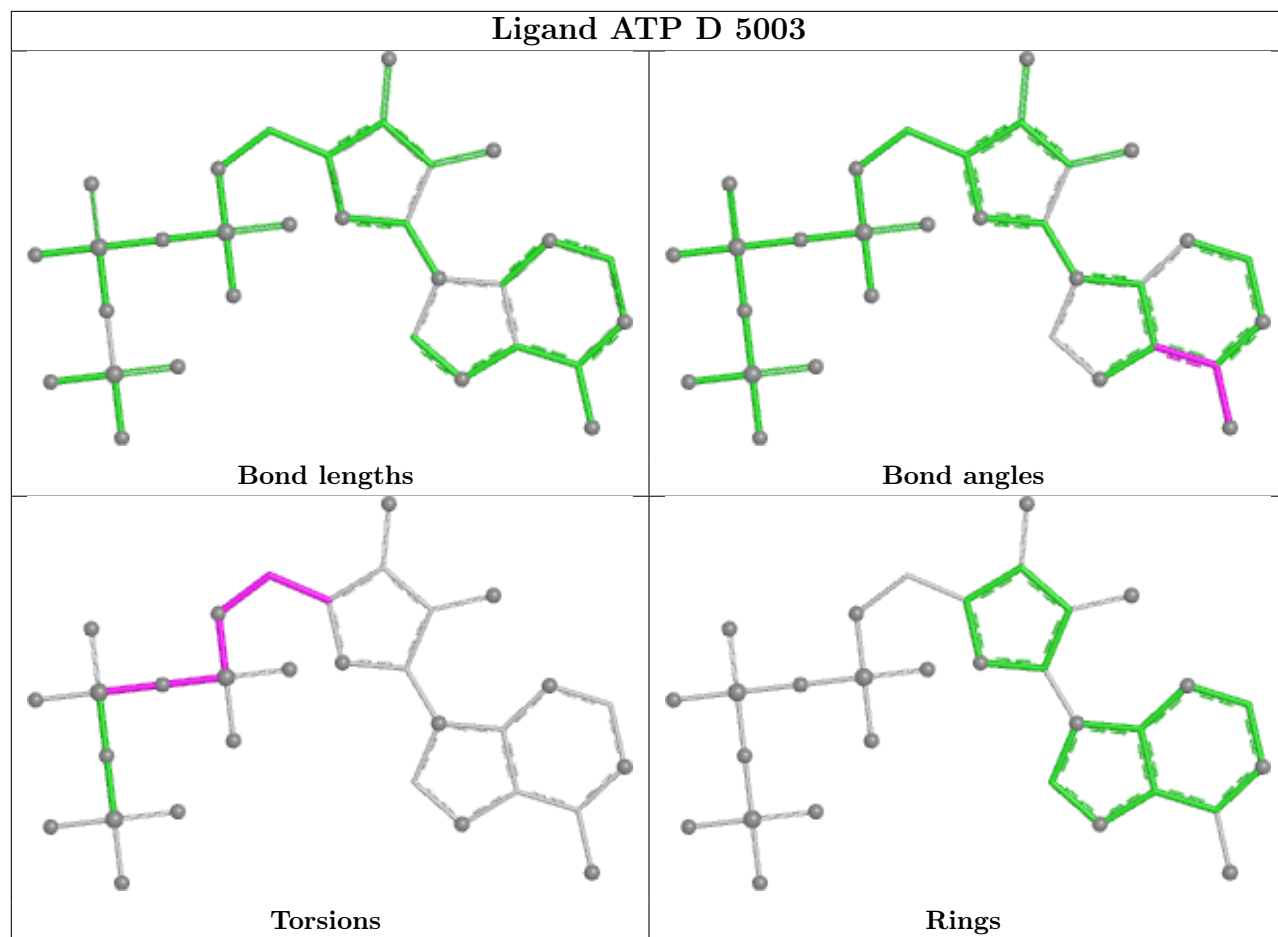
2 monomers are involved in 9 short contacts:

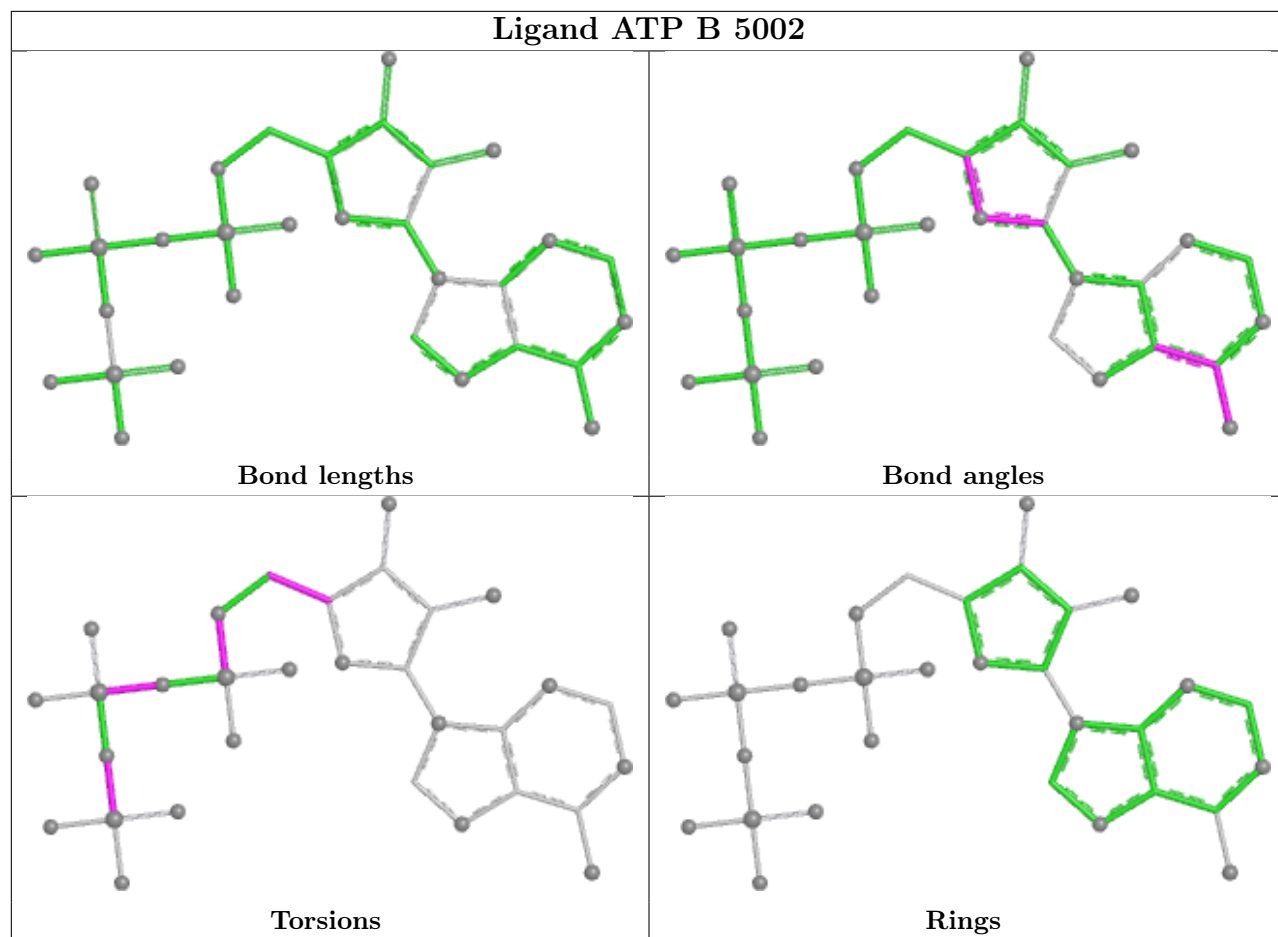
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	5004	KVR	3	0
4	A	5003	ATP	9	0

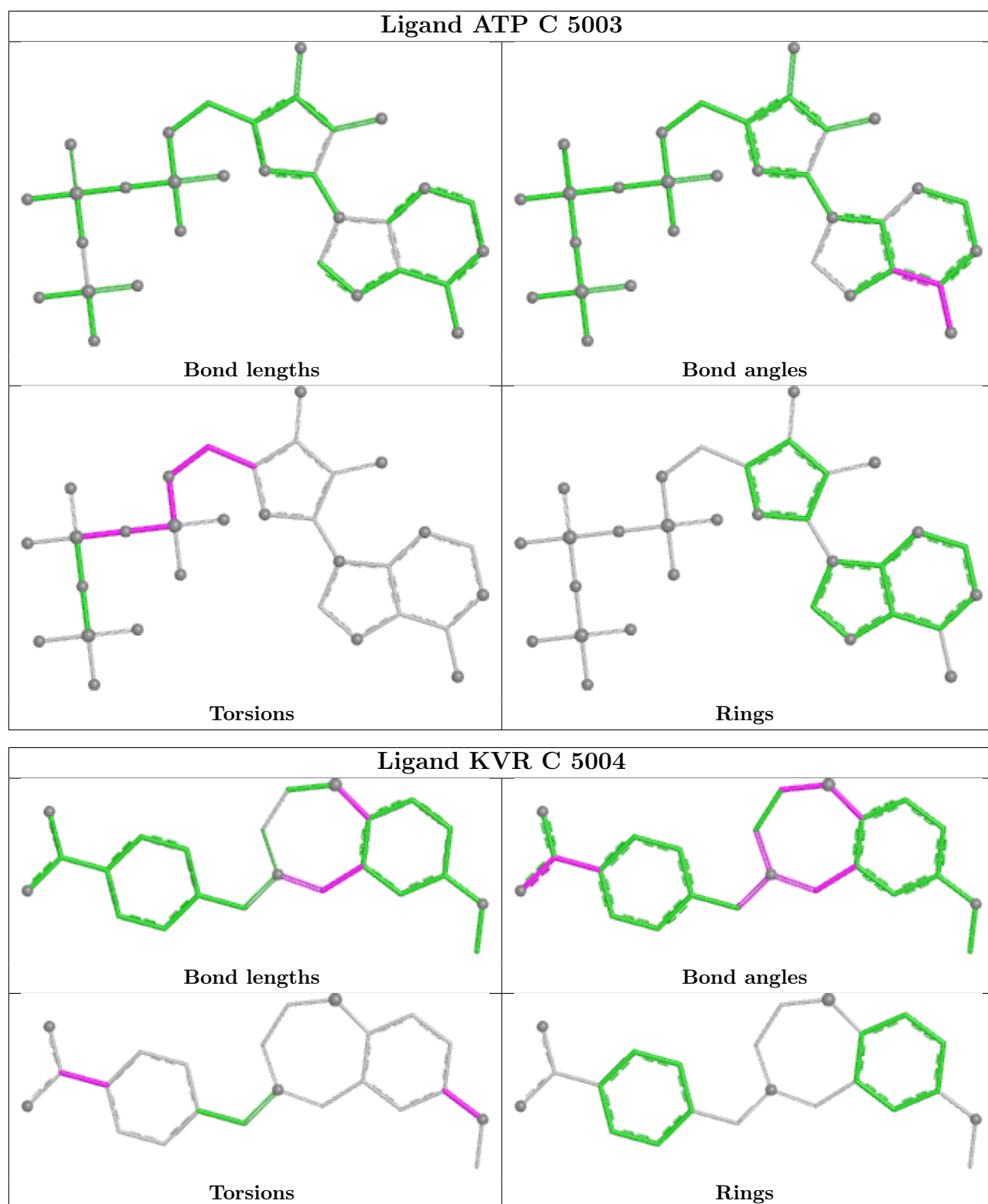
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

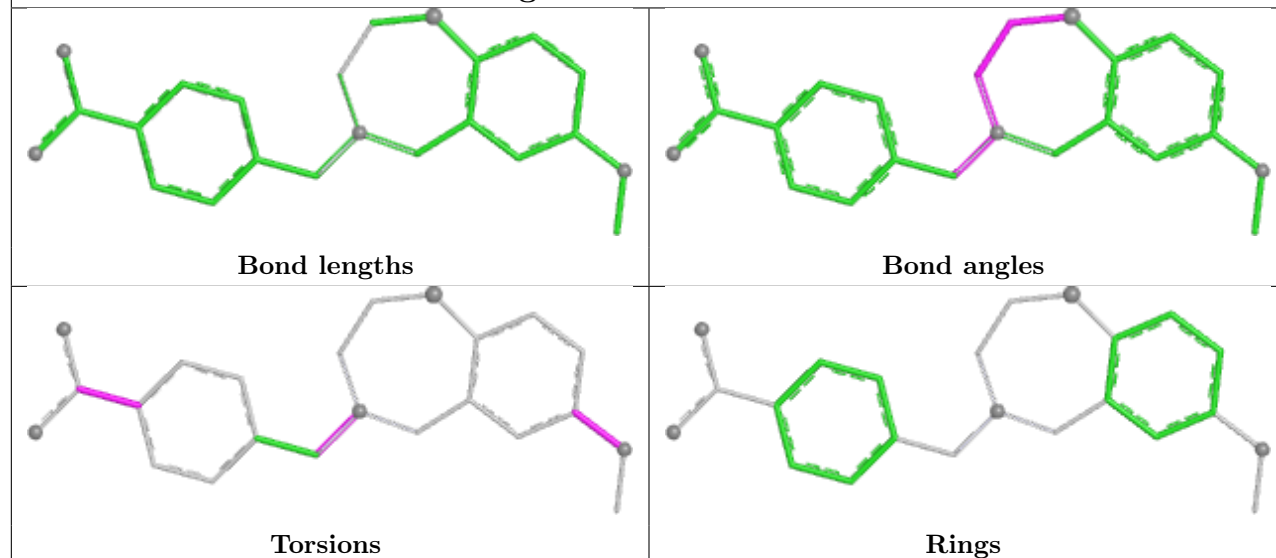




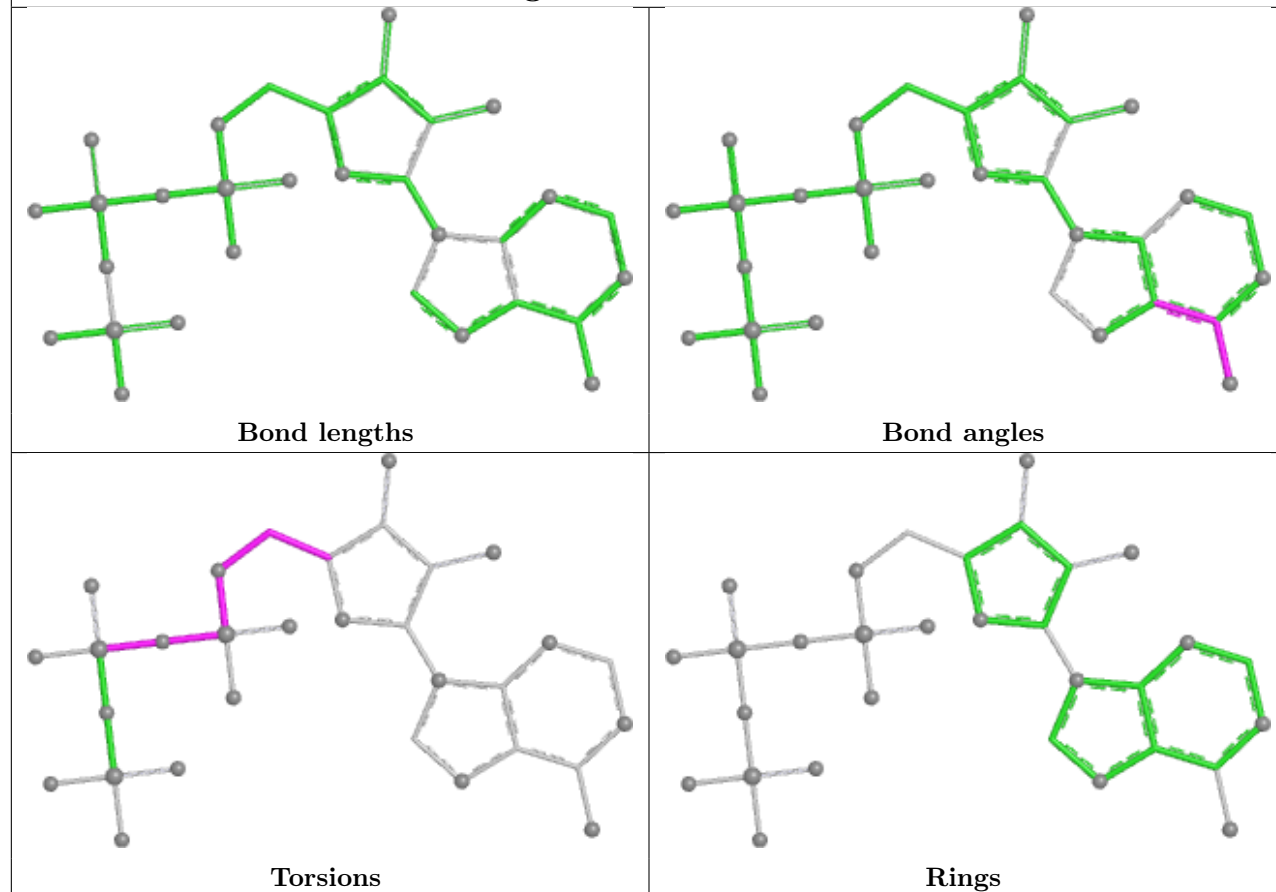


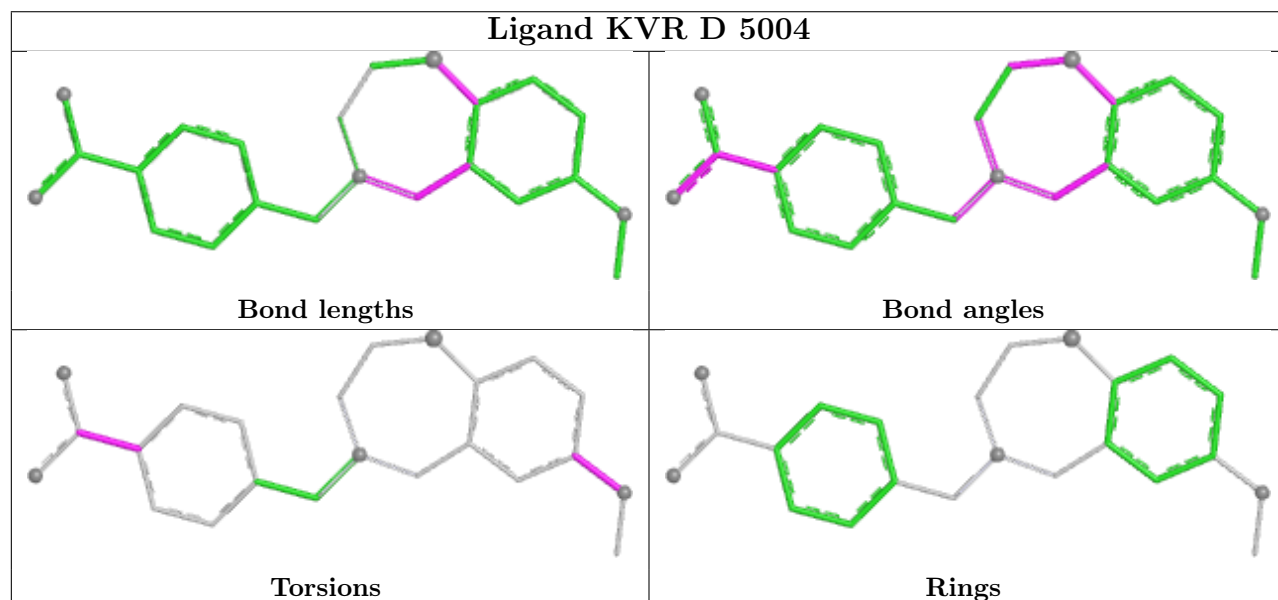
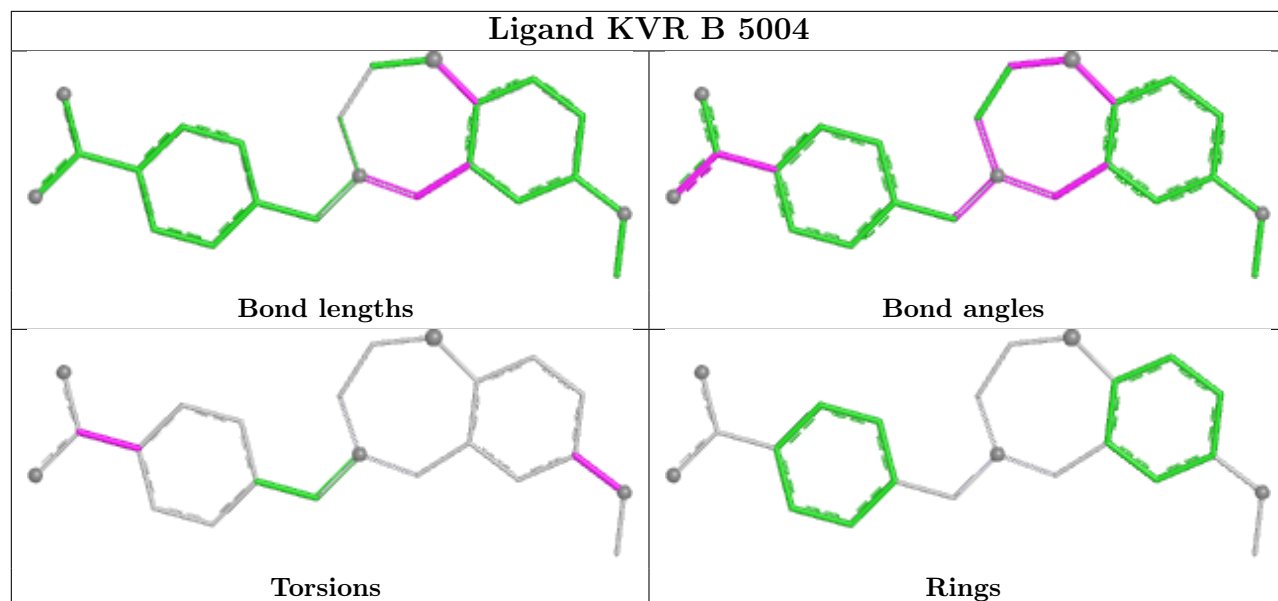


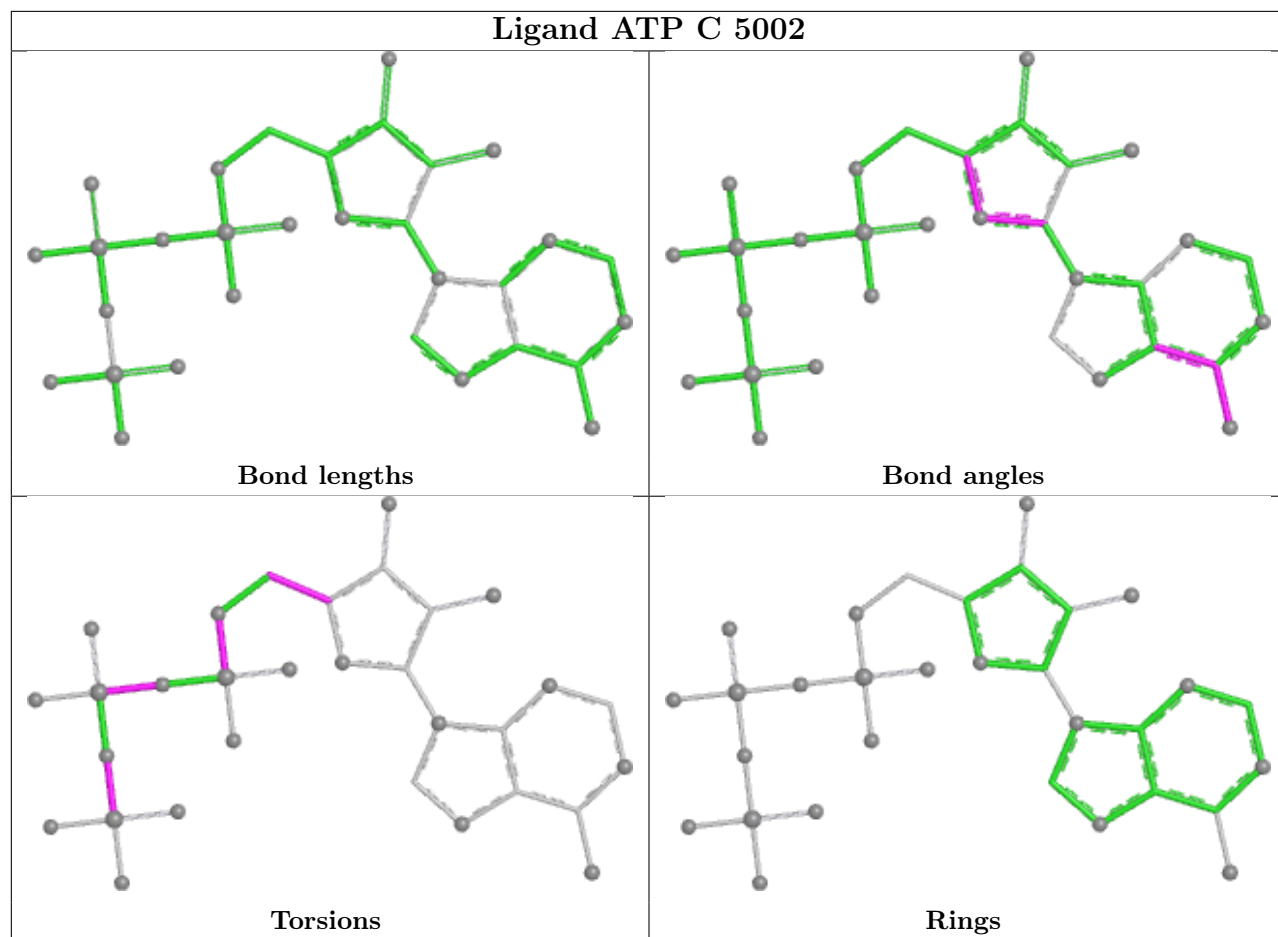
Ligand KVR A 5004

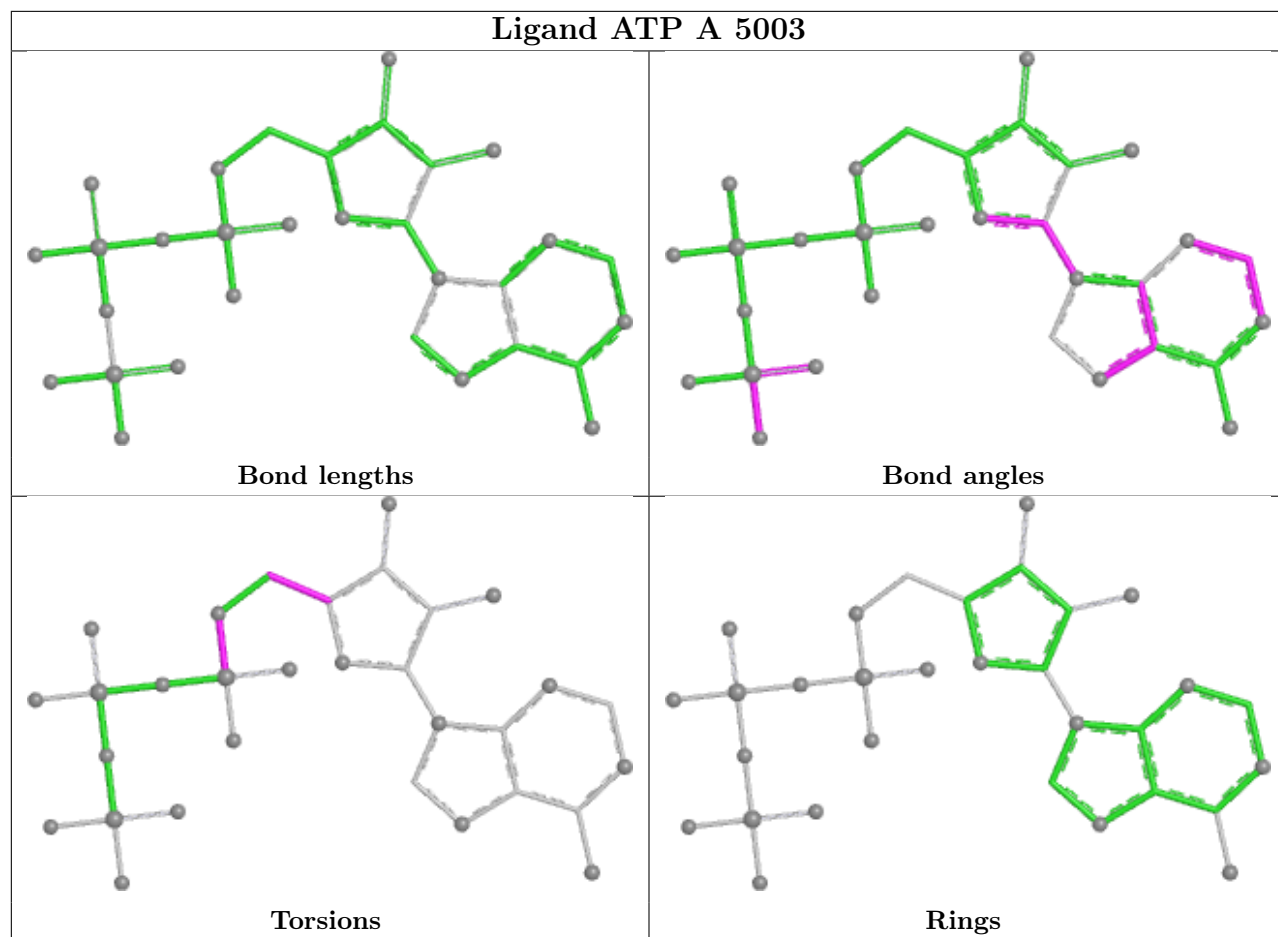


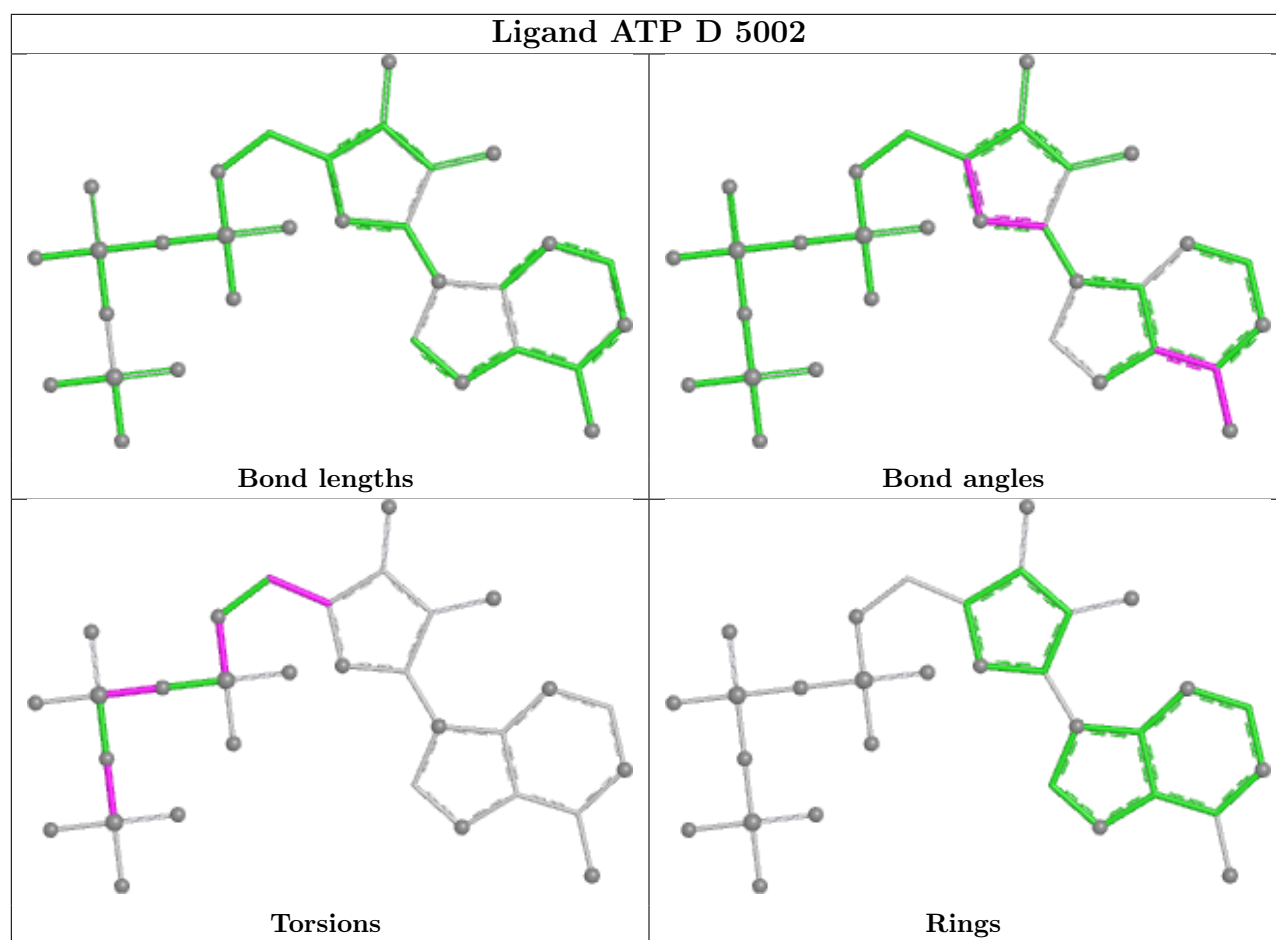
Ligand ATP B 5003











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

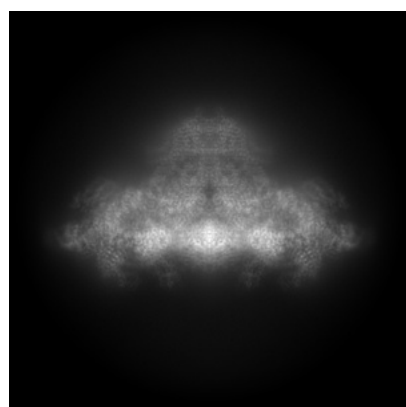
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26412. These allow visual inspection of the internal detail of the map and identification of artifacts.

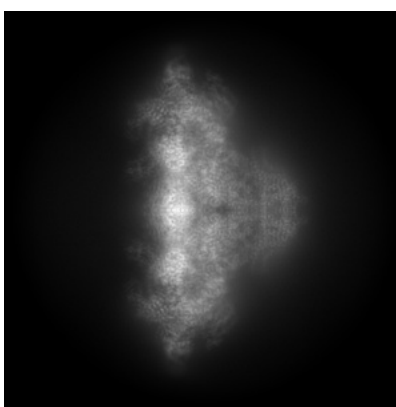
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

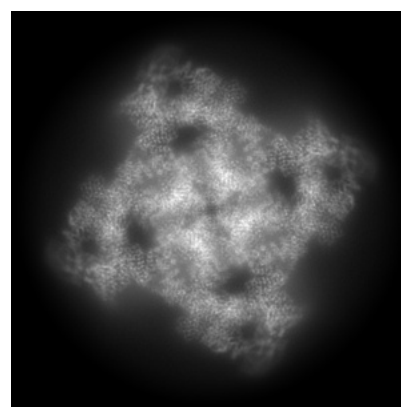
6.1.1 Primary map



X



Y

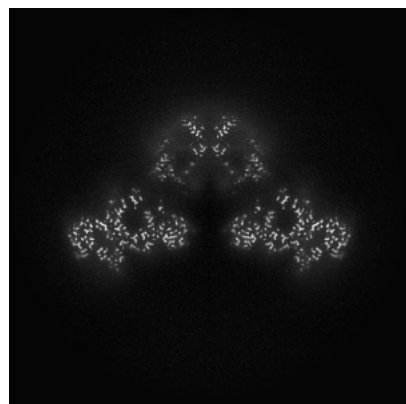


Z

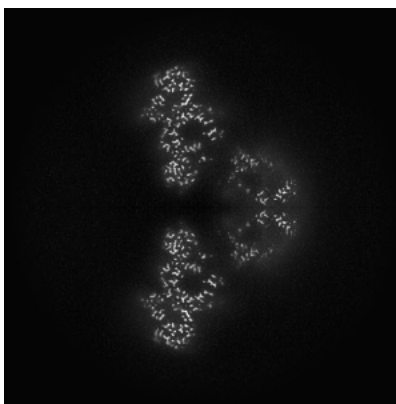
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

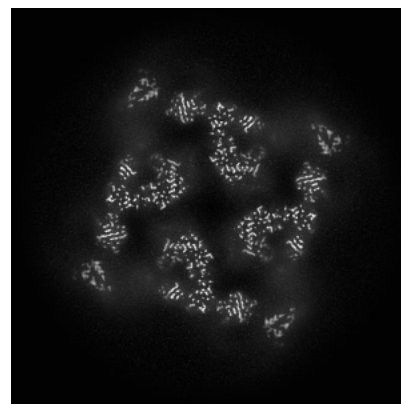
6.2.1 Primary map



X Index: 256



Y Index: 256

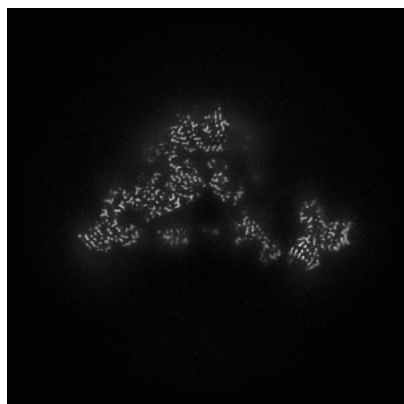


Z Index: 256

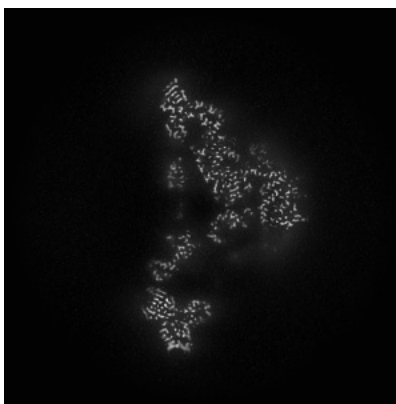
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

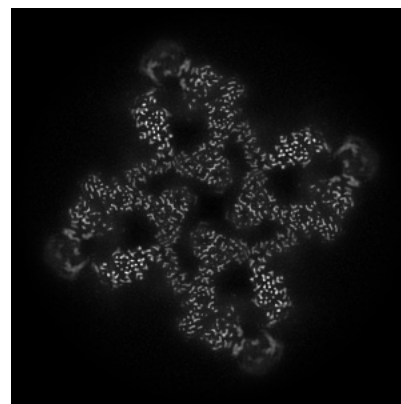
6.3.1 Primary map



X Index: 237



Y Index: 238

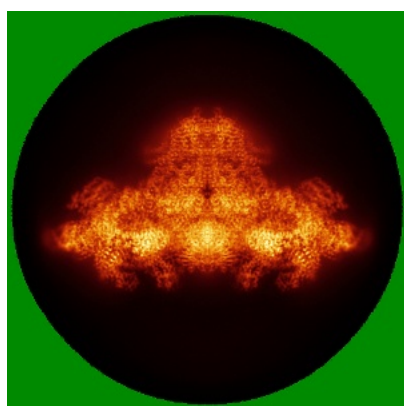


Z Index: 223

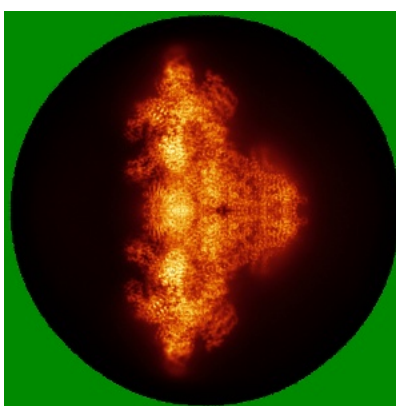
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

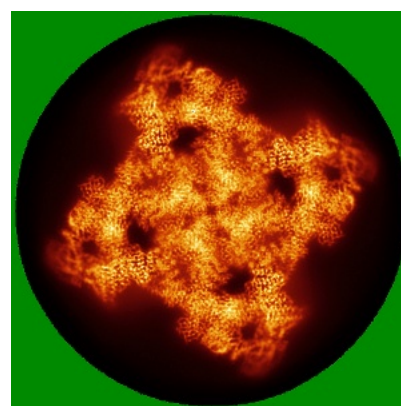
6.4.1 Primary map



X



Y

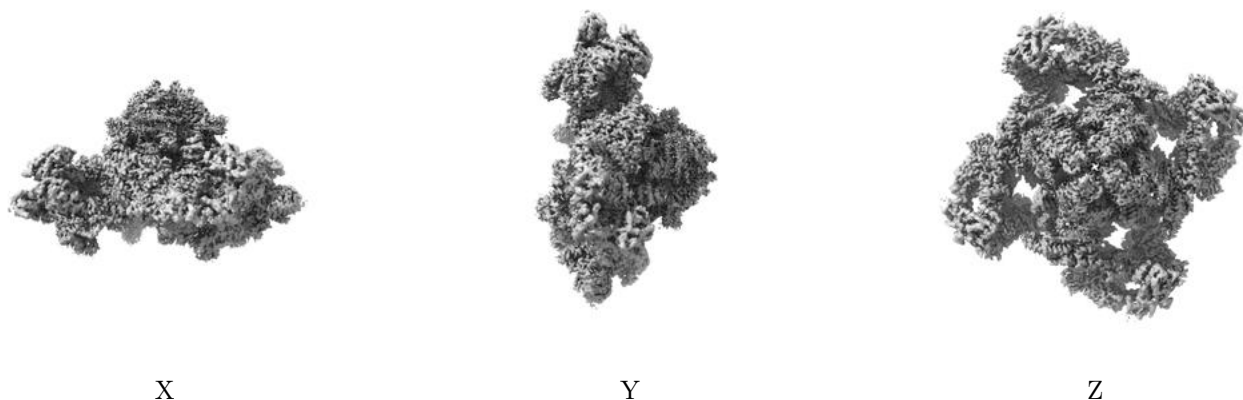


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

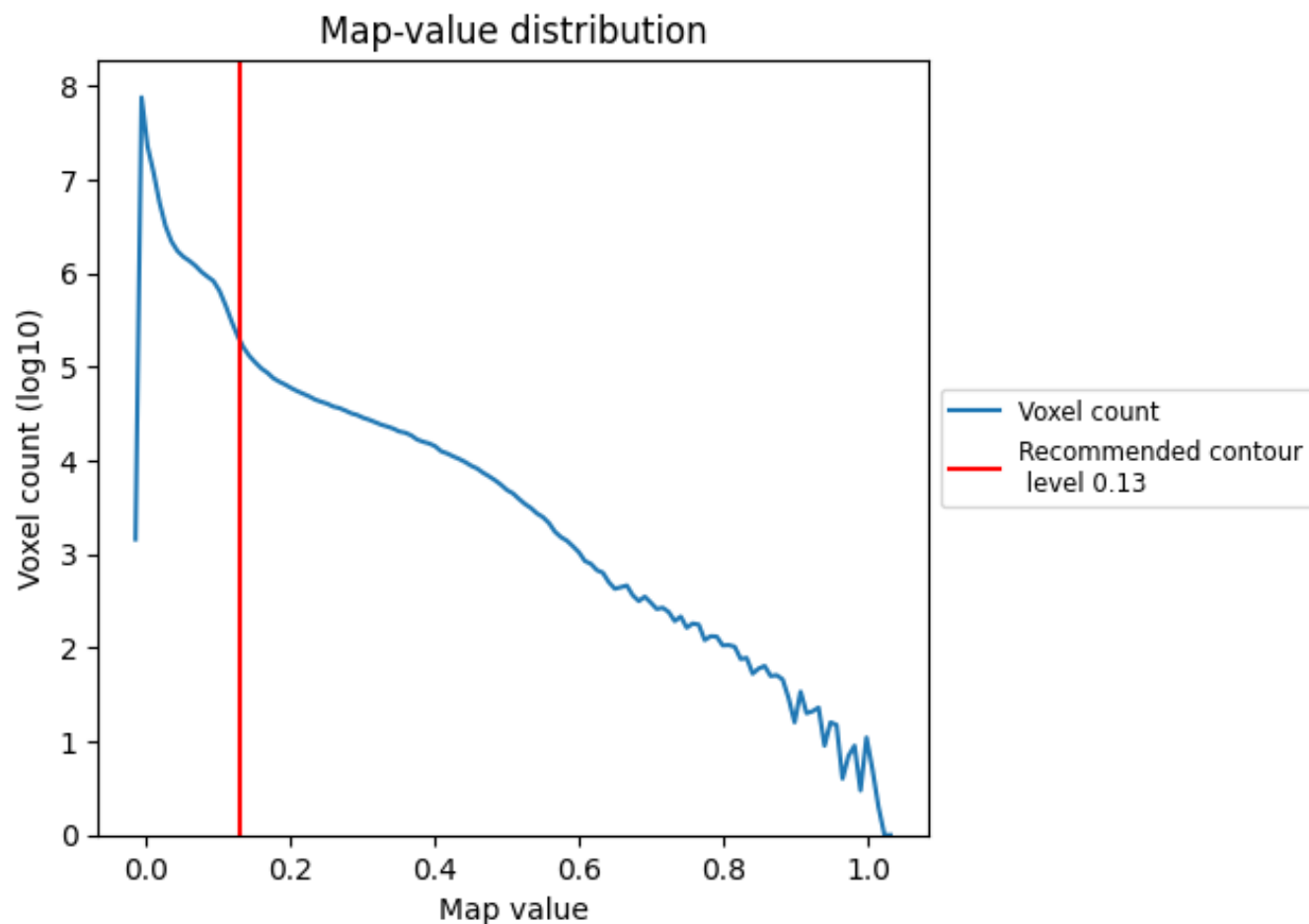
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

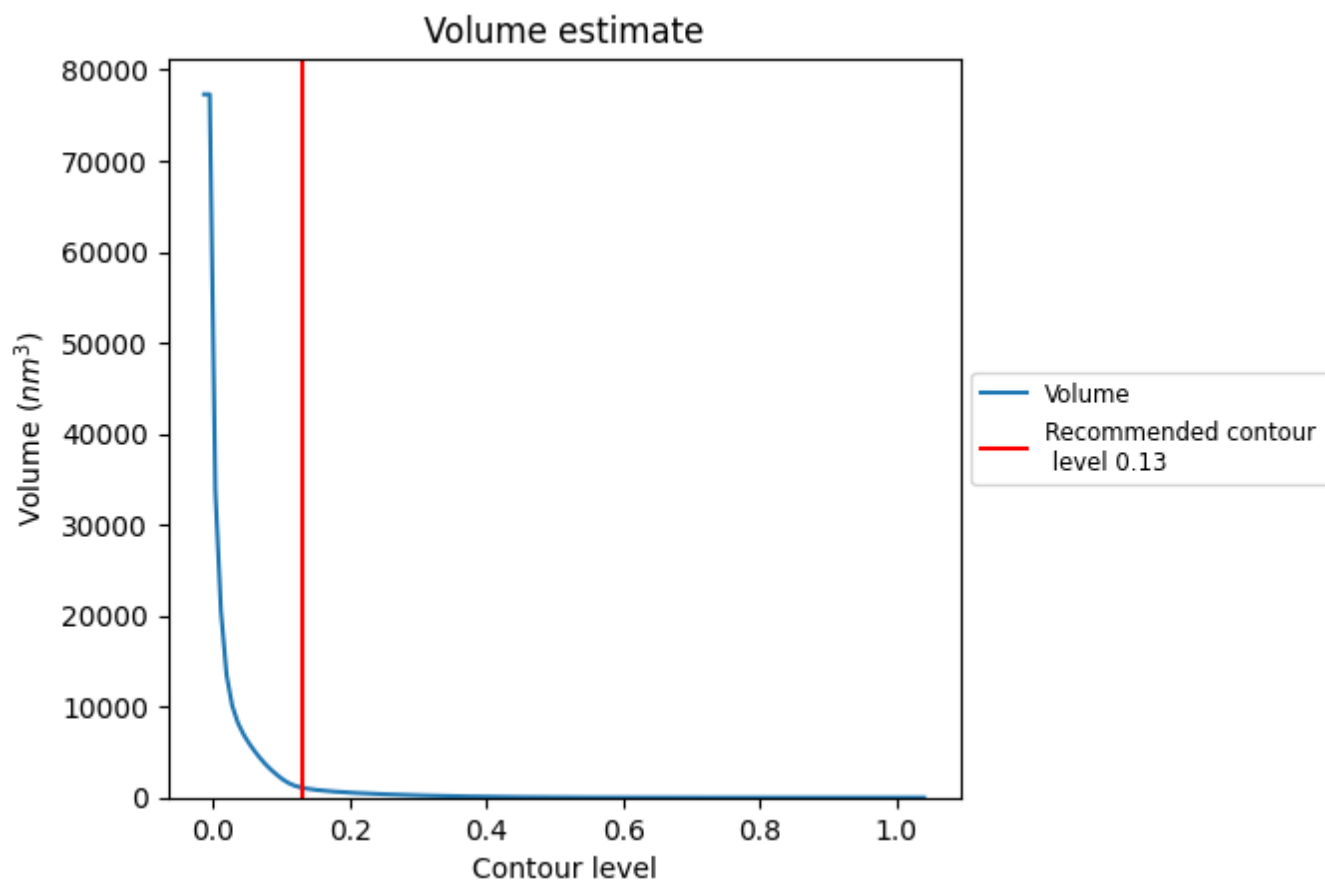
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

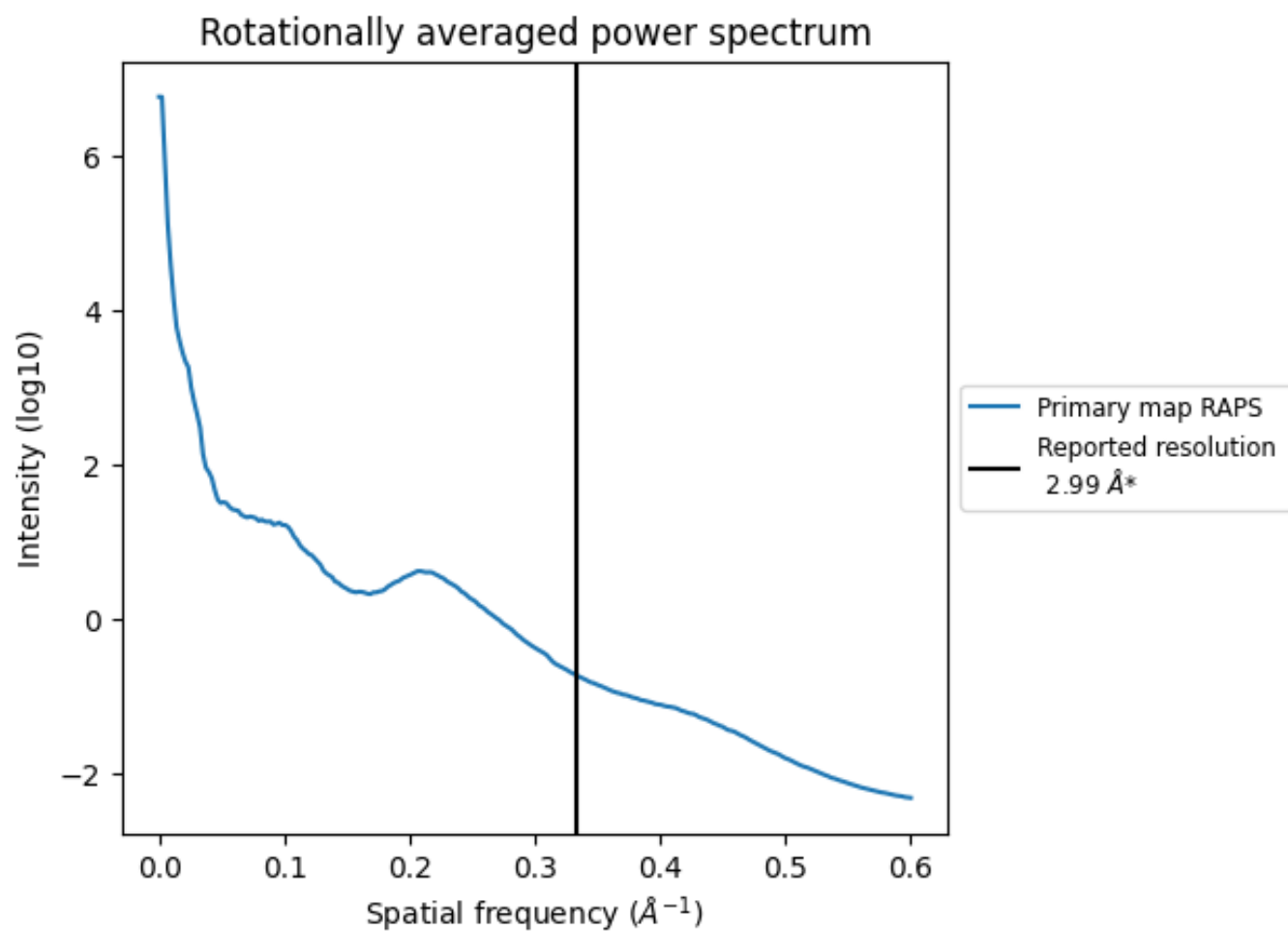
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1081 nm³; this corresponds to an approximate mass of 977 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.334 Å⁻¹

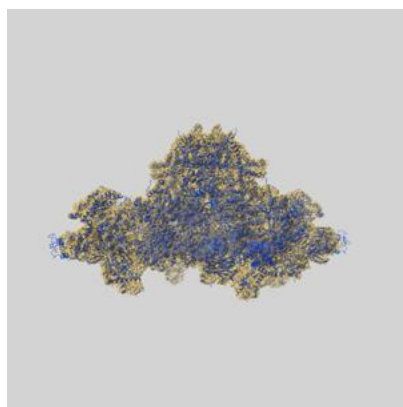
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

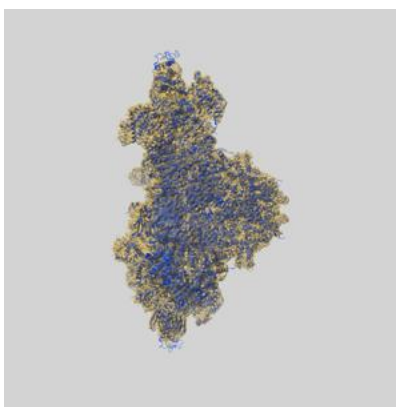
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26412 and PDB model 7UA1. Per-residue inclusion information can be found in section [3](#) on page [7](#).

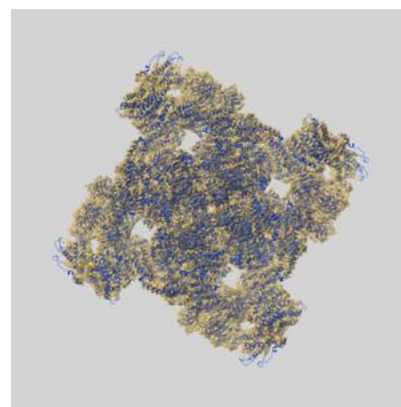
9.1 Map-model overlay [i](#)



X



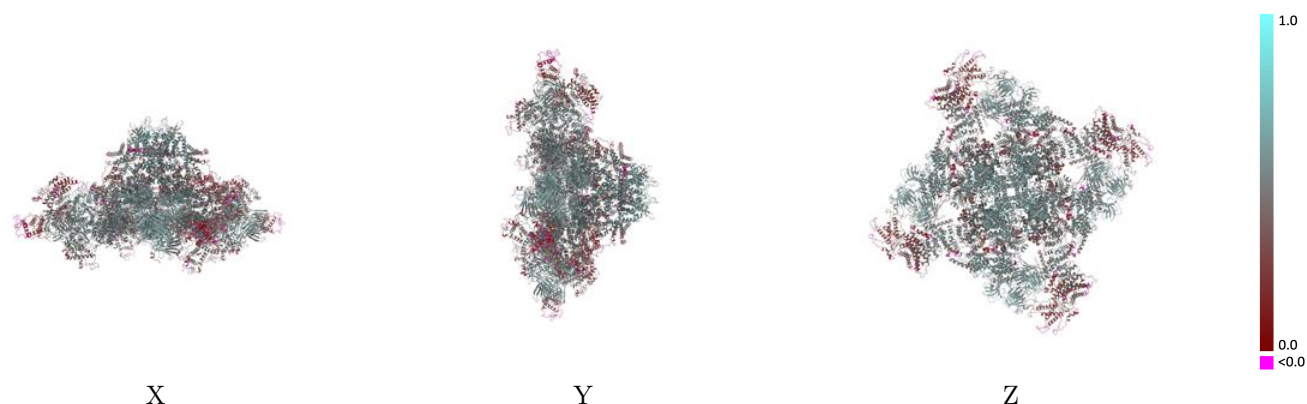
Y



Z

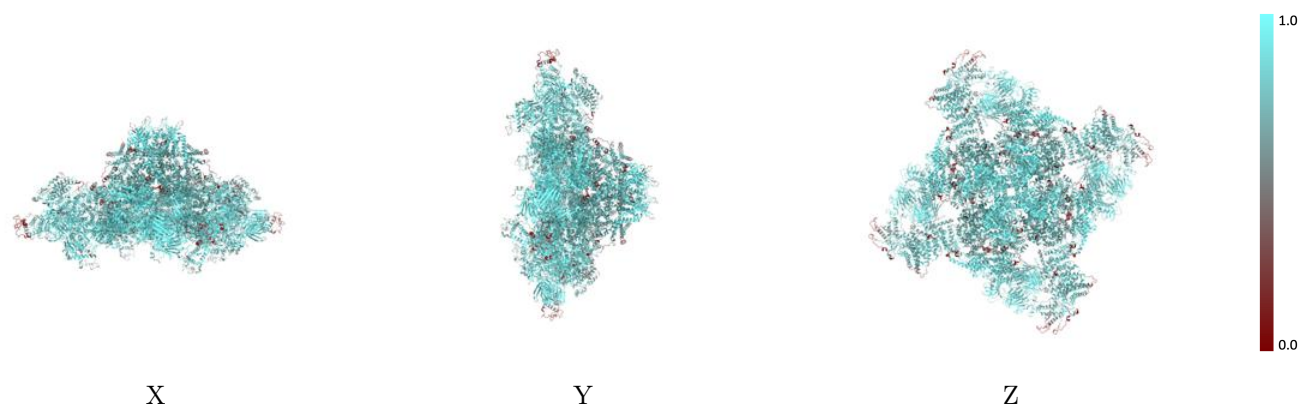
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



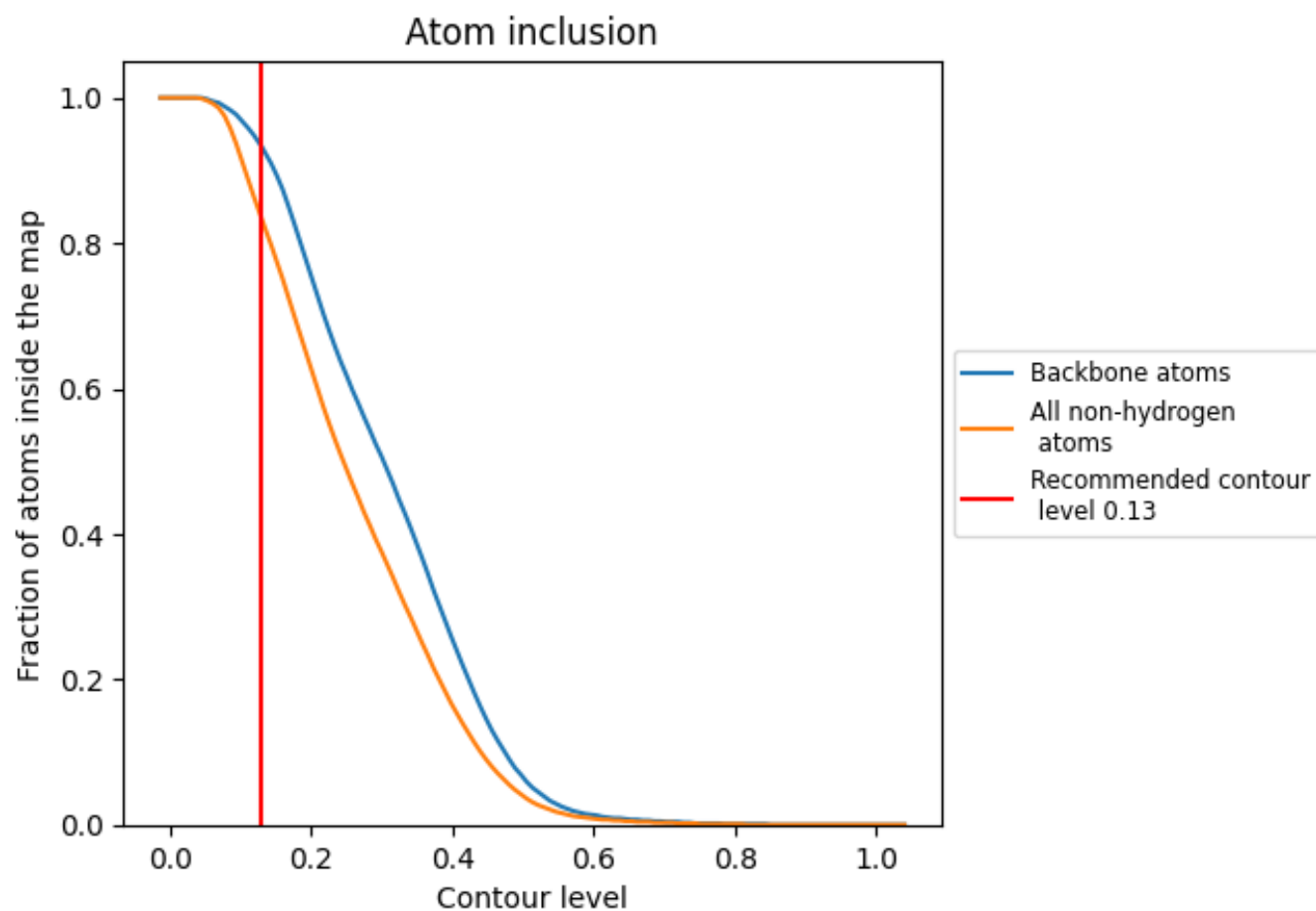
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).

9.4 Atom inclusion ⓘ



At the recommended contour level, 93% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8320	<div></div> 0.4650
A	<div></div> 0.8310	<div></div> 0.4660
B	<div></div> 0.8280	<div></div> 0.4580
C	<div></div> 0.8300	<div></div> 0.4630
D	<div></div> 0.8310	<div></div> 0.4660
E	<div></div> 0.9300	<div></div> 0.5600
F	<div></div> 0.9240	<div></div> 0.5540
G	<div></div> 0.9280	<div></div> 0.5570
H	<div></div> 0.9330	<div></div> 0.5720

