



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2024 – 07:58 AM EST

PDB ID : 6BYU
Title : X-ray crystal structure of Escherichia coli RNA polymerase (RpoB-H526Y) and ppApp complex
Authors : Murakami, K.S.; Molodtsov, V.
Deposited on : 2017-12-21
Resolution : 3.60 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

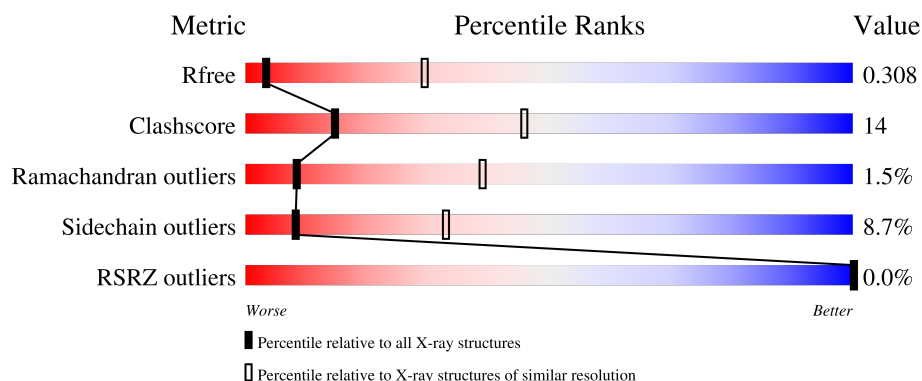
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1563 (3.70-3.50)
Clashscore	180529	1665 (3.70-3.50)
Ramachandran outliers	177936	1641 (3.70-3.50)
Sidechain outliers	177891	1640 (3.70-3.50)
RSRZ outliers	164620	1562 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	
1	B	329	
1	G	329	
1	H	329	
2	C	1342	

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Mol	Chain	Length	Quality of chain
2	I	1342	<div><div></div><div>64%</div><div>32%</div><div></div><div>.</div></div>
3	D	1407	<div><div></div><div>52%</div><div>26%</div><div>5%</div><div>17%</div></div>
3	J	1407	<div><div></div><div>52%</div><div>26%</div><div>.</div><div>18%</div></div>
4	E	91	<div><div></div><div>66%</div><div>30%</div><div>.</div><div>.</div></div>
4	K	91	<div><div>%</div><div></div><div>47%</div><div>38%</div><div>.</div><div>13%</div></div>
5	F	613	<div><div></div><div>51%</div><div>23%</div><div>.</div><div>24%</div></div>
5	L	613	<div><div></div><div>57%</div><div>17%</div><div>.</div><div>23%</div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 54996 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1768	1102	312	348	6			
1	B	217	Total	C	N	O	S	0	0	0
			1672	1044	295	327	6			
1	G	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	H	217	Total	C	N	O	S	0	0	0
			1667	1041	293	327	6			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10561	6626	1837	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10557	6624	1836	2054	43			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	526	TYR	HIS	engineered mutation	UNP P0A8V2
I	526	TYR	HIS	engineered mutation	UNP P0A8V2

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1163	Total	C	N	O	S	0	0	0
			9063	5696	1622	1699	46			
3	J	1155	Total	C	N	O	S	0	0	0
			8998	5656	1612	1684	46			

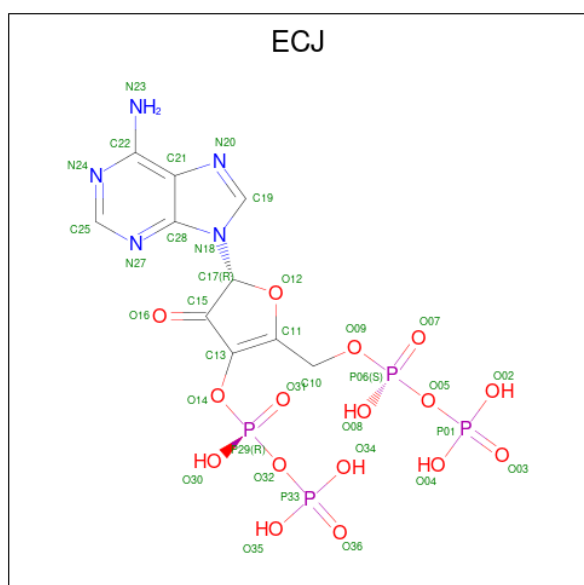
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total 685	C 418	N 126	O 140	S 1	0	0	0
4	K	79	Total 627	C 382	N 118	O 126	S 1	0	0	0

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	467	Total 3796	C 2379	N 677	O 717	S 23	0	0	0
5	L	469	Total 3796	C 2379	N 677	O 717	S 23	0	0	0

- Molecule 6 is (5R)-5-(6-amino-9H-purin-9-yl)-2-([[(S)-hydroxy(phosphonooxy)phosphoryl]oxy)methyl)-4-oxo-4,5-dihydrofuran-3-yl trihydrogen diphosphate (three-letter code: ECJ) (formula: C₁₀H₁₃N₅O₁₆P₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total 35	C 10	N 5	O 16	P 4	0	0
6	J	1	Total 35	C 10	N 5	O 16	P 4	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total 1	Mg 1	0	0
7	J	1	Total 1	Mg 1	0	0

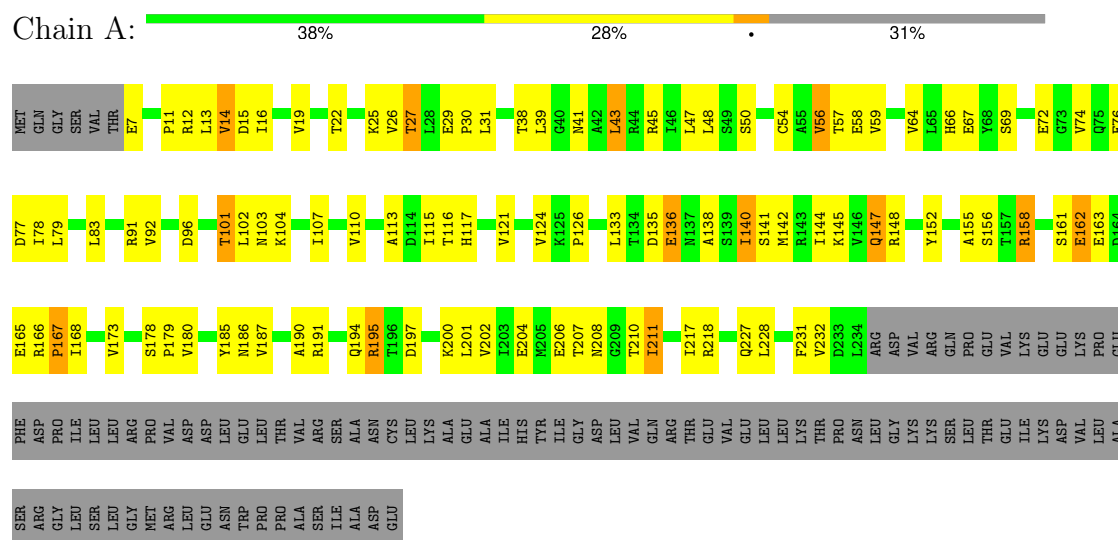
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total 2	Zn 2	0	0
8	J	2	Total 2	Zn 2	0	0

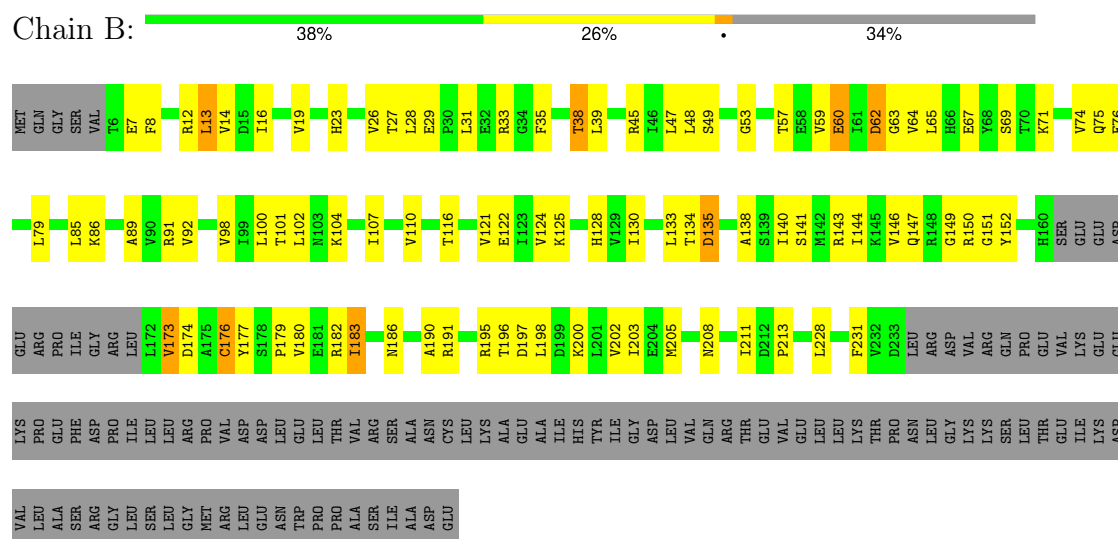
3 Residue-property plots

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: DNA-directed RNA polymerase subunit alpha

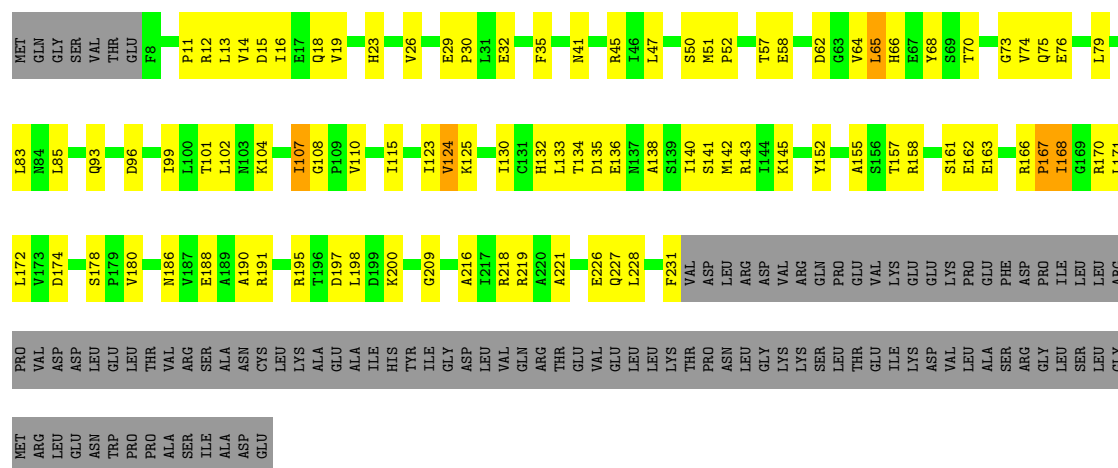


• Molecule 1: DNA-directed RNA polymerase subunit alpha

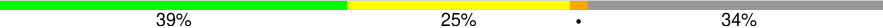


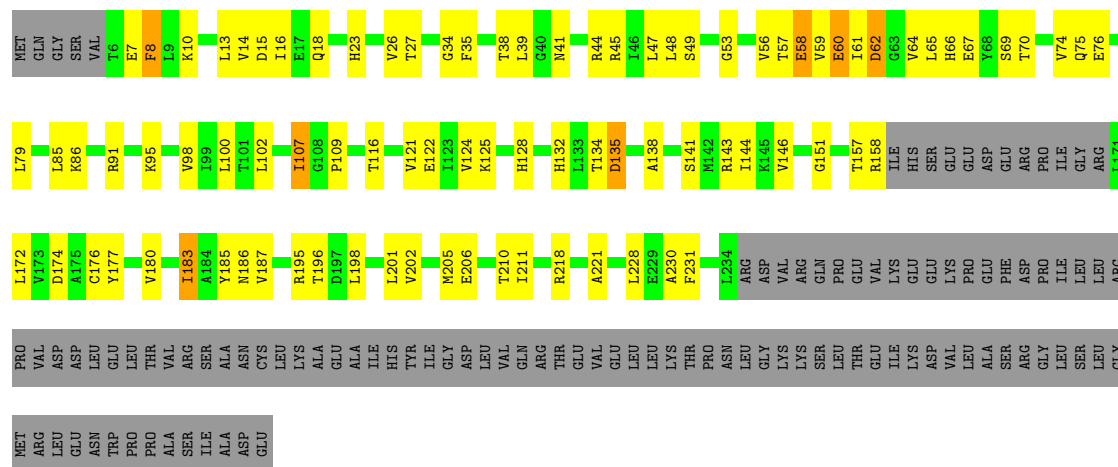
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain G:  40% 27% 32%



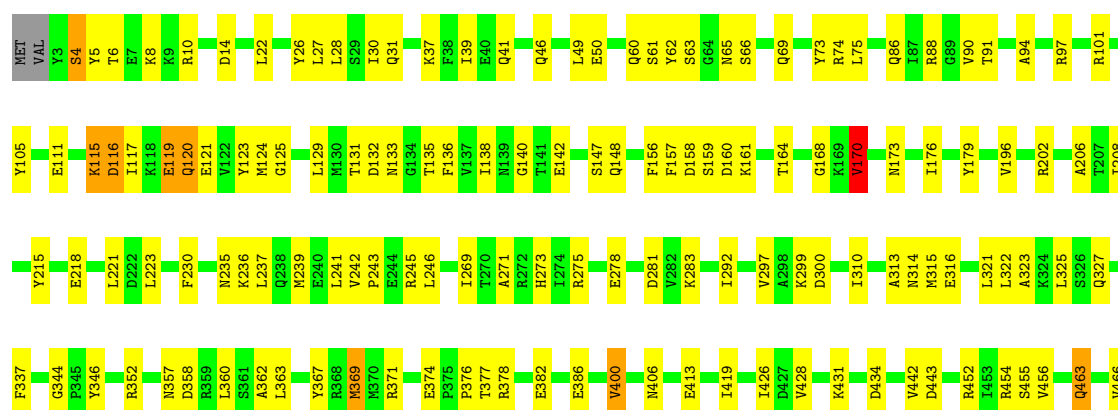
• Molecule 1: DNA-directed RNA polymerase subunit alpha

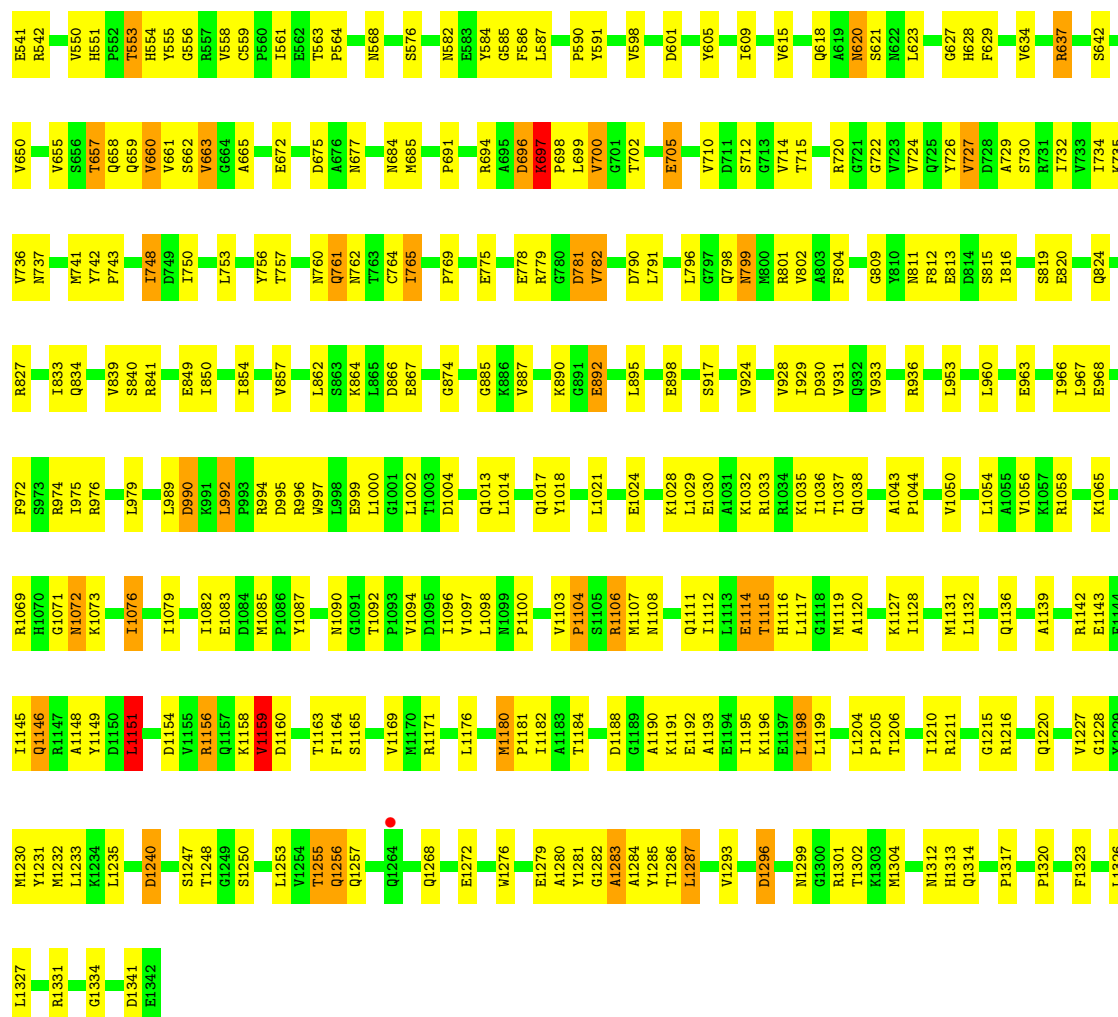
Chain H:  39% 25% 34%



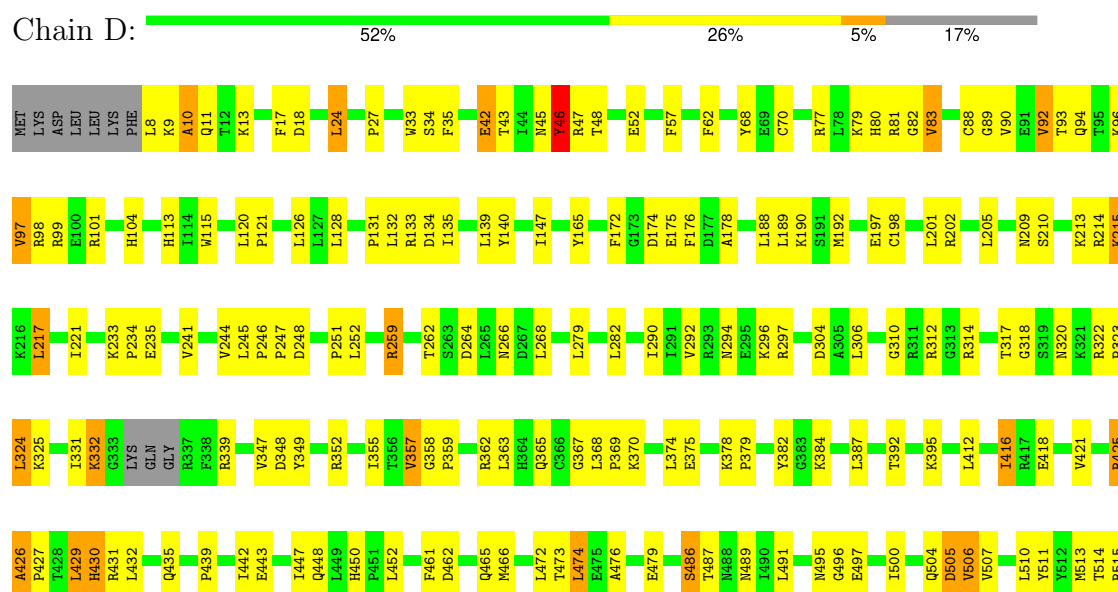
• Molecule 2: DNA-directed RNA polymerase subunit beta

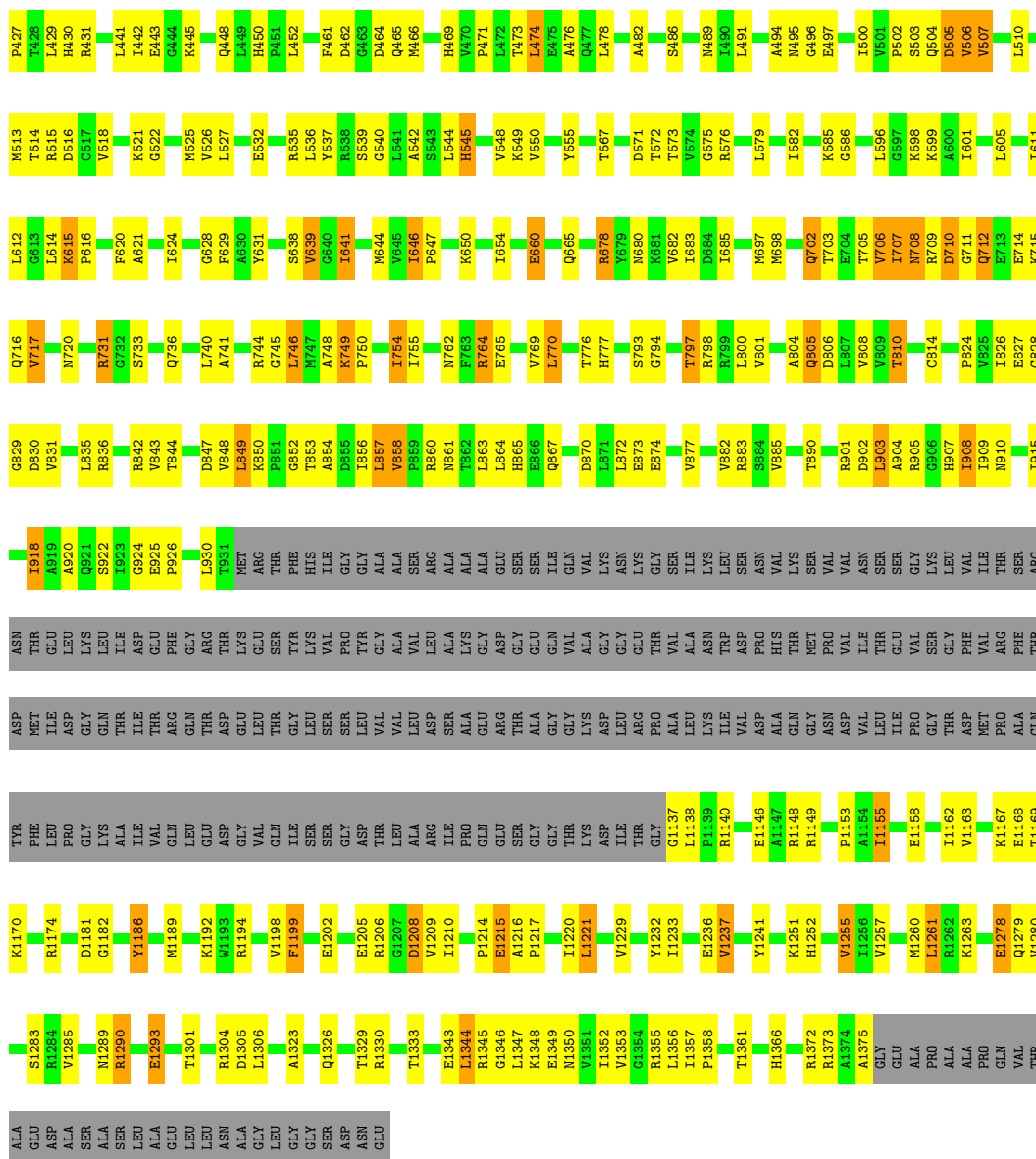
Chain C:  64% 31%





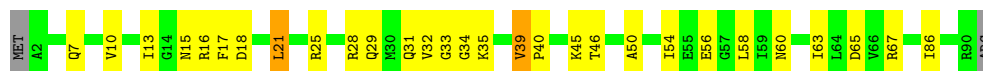
- Molecule 3: DNA-directed RNA polymerase subunit beta'





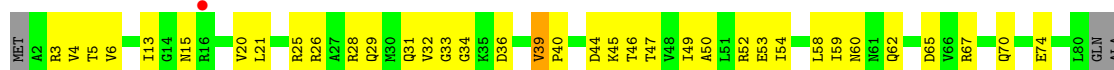
• Molecule 4: DNA-directed RNA polymerase subunit omega

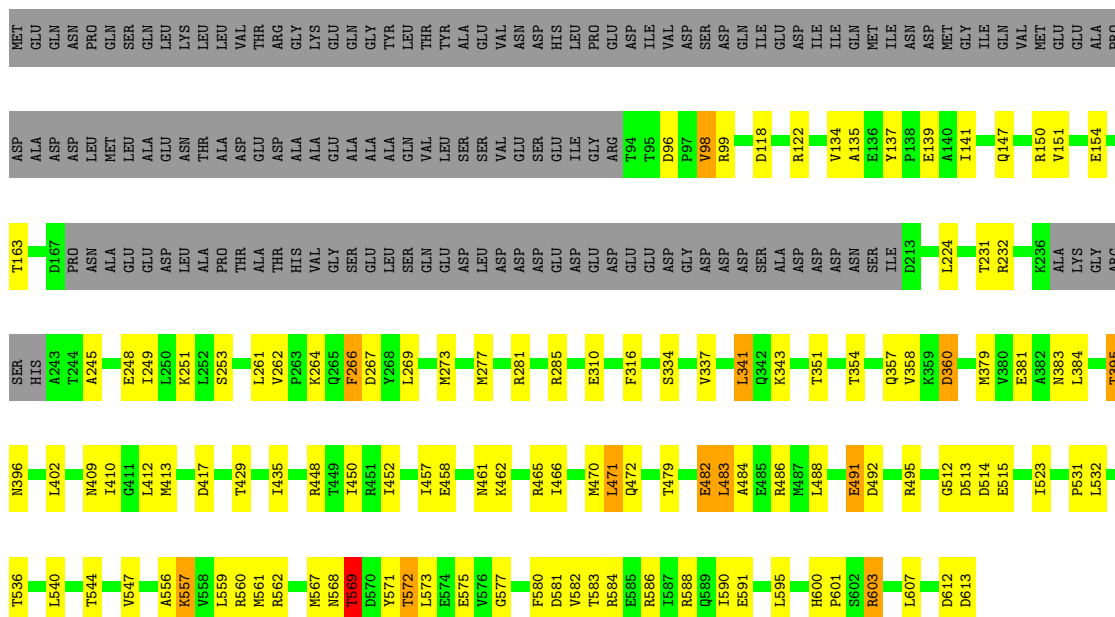
Chain E: 66% 30% ..



• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K: 47% 38% 13%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	186.25Å 203.66Å 308.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.60 30.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-3.60) 98.3 (30.00-3.60)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 3.56Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.244 , 0.311 0.245 , 0.308	Depositor DCC
R_{free} test set	133657 reflections (1.48%)	wwPDB-VP
Wilson B-factor (Å ²)	119.5	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 121.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	54996	wwPDB-VP
Average B, all atoms (Å ²)	153.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.30	0/1790	0.57	0/2426
1	B	0.27	0/1692	0.54	1/2293 (0.0%)
1	G	0.27	0/1751	0.56	0/2373
1	H	0.27	0/1686	0.55	1/2285 (0.0%)
2	C	0.26	0/10730	0.50	0/14479
2	I	0.26	0/10726	0.49	0/14474
3	D	0.26	0/9201	0.49	0/12420
3	J	0.26	0/9137	0.49	0/12337
4	E	0.26	0/687	0.48	0/928
4	K	0.23	0/629	0.47	0/847
5	F	0.25	0/3847	0.45	0/5171
5	L	0.25	0/3846	0.44	0/5171
All	All	0.26	0/55722	0.50	2/75204 (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
2	C	0	1
2	I	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	13	LEU	CA-CB-CG	5.80	128.64	115.30
1	B	13	LEU	CA-CB-CG	5.48	127.90	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1159	VAL	Peptide
2	I	1159	VAL	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	1768	0	1793	74	0
1	B	1672	0	1694	64	0
1	G	1730	0	1756	73	0
1	H	1667	0	1689	60	0
2	C	10561	0	10555	305	0
2	I	10557	0	10549	301	0
3	D	9063	0	9234	291	0
3	J	8998	0	9154	287	0
4	E	685	0	684	18	0
4	K	627	0	634	19	0
5	F	3796	0	3858	96	1
5	L	3796	0	3848	71	1
6	C	35	0	0	0	0
6	J	35	0	0	1	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
All	All	54996	0	55448	1510	1

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 14.

All (1510) 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:G:45:ARG:HG2	1:H:38:THR:HB	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.51	0.92
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.53	0.91
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.54	0.88
3:D:418:GLU:HG3	4:E:45:LYS:H	1.42	0.85
1:A:135:ASP:HB3	1:A:138:ALA:HB2	1.59	0.82
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.60	0.82
3:J:1158:GLU:O	3:J:1206:ARG:NH1	2.14	0.81
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.61	0.81
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.45	0.81
3:D:527:LEU:HB2	3:D:550:VAL:HG12	1.63	0.80
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.14	0.79
1:B:16:ILE:HG23	1:B:26:VAL:HG22	1.66	0.78
1:A:57:THR:HG22	1:A:58:GLU:HG3	1.64	0.78
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.64	0.78
5:L:580:PHE:O	5:L:582:VAL:N	2.17	0.77
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.67	0.77
4:K:32:VAL:O	4:K:34:GLY:N	2.15	0.77
2:C:4:SER:OG	2:C:5:TYR:N	2.18	0.77
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.65	0.77
2:I:1313:HIS:HB2	3:J:474:LEU:HD22	1.66	0.76
1:H:64:VAL:HG12	1:H:66:HIS:H	1.49	0.76
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.67	0.76
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.51	0.75
3:D:495:ASN:O	3:D:497:GLU:N	2.19	0.75
2:C:720:ARG:HH21	2:C:741:MET:HA	1.51	0.74
2:C:1149:TYR:HB3	2:C:1159:VAL:HG21	1.69	0.74
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.69	0.74
3:J:452:LEU:HB3	3:J:500:ILE:HG23	1.70	0.74
5:F:470:MET:SD	5:F:486:ARG:NH1	2.61	0.74
5:L:571:TYR:HD1	5:L:575:GLU:HG2	1.53	0.74
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.69	0.74
1:H:48:LEU:HD22	3:J:539:SER:HB3	1.69	0.73
4:E:32:VAL:O	4:E:34:GLY:N	2.21	0.73
4:K:49:ILE:HA	4:K:52:ARG:HD3	1.71	0.73
3:J:1198:VAL:HB	3:J:1210:ILE:HG23	1.69	0.73
3:D:1280:VAL:HG21	3:D:1304:ARG:NE	2.04	0.72
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.22	0.72
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.23	0.72
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.69	0.72
3:D:646:ILE:HD11	3:D:764:ARG:HD2	1.70	0.72
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.72	0.72
1:H:195:ARG:HB3	1:H:198:LEU:HD21	1.72	0.71
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.70	0.71
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.72	0.71
3:J:97:VAL:HG12	3:J:101:ARG:HG3	1.73	0.71
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.55	0.71
2:C:1142:ARG:HH22	2:C:1165:SER:HA	1.55	0.71
1:B:60:GLU:OE2	1:B:143:ARG:NH1	2.23	0.71
2:C:452:ARG:NH1	2:C:584:TYR:O	2.24	0.71
1:H:60:GLU:OE2	1:H:143:ARG:NH1	2.24	0.71
3:D:854:ALA:HB2	3:J:1372:ARG:HG3	1.71	0.70
1:G:45:ARG:HH21	2:I:1216:ARG:HA	1.54	0.70
5:F:166:VAL:HB	5:F:258:GLN:HE21	1.57	0.70
1:G:64:VAL:HG12	1:G:66:HIS:H	1.56	0.70
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.72	0.70
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.72	0.70
3:J:495:ASN:O	3:J:497:GLU:N	2.23	0.70
2:C:131:THR:HG23	2:C:133:ASN:H	1.56	0.70
1:H:124:VAL:HG21	1:H:210:THR:HA	1.73	0.70
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.25	0.70
1:B:196:THR:HG23	3:D:443:GLU:HG3	1.74	0.70
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.55	0.70
1:B:100:LEU:HD21	1:B:121:VAL:HG11	1.72	0.70
2:C:142:GLU:HB2	2:C:760:ASN:HD21	1.57	0.69
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.72	0.69
3:J:848:VAL:HB	3:J:858:VAL:HG13	1.73	0.69
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.72	0.69
3:D:905:ARG:HH21	3:D:907:HIS:HB2	1.57	0.69
5:L:379:MET:O	5:L:383:ASN:ND2	2.24	0.69
2:C:124:MET:HB3	2:C:493:ILE:HD11	1.75	0.69
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.07	0.69
2:I:23:ASP:OD1	2:I:23:ASP:N	2.25	0.69
1:A:102:LEU:HB3	1:A:142:MET:HG2	1.74	0.69
5:L:470:MET:SD	5:L:486:ARG:NH1	2.65	0.69
2:C:1282:GLY:O	2:C:1284:ALA:N	2.25	0.69
1:G:166:ARG:O	1:G:168:ILE:N	2.26	0.68
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.74	0.68
3:D:310:GLY:HA2	3:D:314:ARG:HD2	1.75	0.68
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.57	0.68
3:J:844:THR:OG1	3:J:860:ARG:O	2.09	0.68
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLN:HB3	1:B:39:LEU:HD11	1.76	0.68
2:C:685:MET:HE1	2:C:1071:GLY:HA2	1.76	0.68
2:C:864:LYS:NZ	2:C:881:ASP:OD2	2.26	0.68
1:H:14:VAL:HG13	1:H:15:ASP:H	1.58	0.68
3:J:521:LYS:NZ	3:J:540:GLY:O	2.27	0.68
3:D:57:PHE:HB3	3:D:98:ARG:HH22	1.58	0.68
2:I:86:GLN:HA	2:I:140:GLY:HA2	1.76	0.68
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.76	0.67
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.76	0.67
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.27	0.67
3:J:905:ARG:HH21	3:J:907:HIS:HB2	1.59	0.67
2:C:1120:ALA:HB2	2:C:1199:LEU:HG	1.77	0.67
1:A:158:ARG:NH2	1:A:173:VAL:O	2.28	0.67
3:J:473:THR:HG23	3:J:476:ALA:H	1.59	0.67
2:C:97:ARG:HB3	2:C:121:GLU:HB3	1.75	0.67
1:H:196:THR:HG23	3:J:443:GLU:HG3	1.76	0.67
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.60	0.67
3:J:128:LEU:HA	3:J:192:MET:HE1	1.76	0.67
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.76	0.67
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.28	0.67
2:I:142:GLU:HB2	2:I:760:ASN:HD21	1.60	0.67
3:J:362:ARG:H	3:J:365:GLN:HE21	1.43	0.67
3:D:514:THR:OG1	3:D:596:LEU:HB2	1.95	0.67
2:C:873:ILE:HG13	2:C:944:ARG:HH22	1.60	0.67
3:D:901:ARG:HA	3:D:908:ILE:HA	1.76	0.66
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.77	0.66
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.10	0.66
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.28	0.66
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.42	0.66
5:F:395:THR:OG1	5:F:396:ASN:N	2.27	0.66
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.28	0.66
3:J:527:LEU:HB2	3:J:550:VAL:HG12	1.78	0.66
5:F:467:SER:O	5:F:471:LEU:HB2	1.96	0.66
1:G:14:VAL:HG13	1:G:15:ASP:H	1.60	0.66
3:J:1167:LYS:HD3	3:J:1174:ARG:HH11	1.61	0.66
2:C:758:ARG:HH22	2:C:761:GLN:HG3	1.61	0.65
2:C:557:ARG:HB3	2:C:587:LEU:HD13	1.77	0.65
2:C:746:ALA:HA	2:C:974:ARG:HH21	1.61	0.65
2:I:176:ILE:HB	2:I:184:LEU:HB3	1.78	0.65
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.78	0.65
5:F:280:VAL:HG21	5:F:358:VAL:HG11	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:115:LYS:HD3	2:I:116:ASP:H	1.60	0.65
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.77	0.65
5:L:134:VAL:HG22	5:L:273:MET:HE3	1.78	0.65
3:D:131:PRO:HG2	3:D:134:ASP:HB2	1.79	0.65
3:D:479:GLU:OE1	3:D:1361:THR:OG1	2.13	0.65
2:C:802:VAL:HG11	2:C:1230:MET:HB3	1.78	0.65
3:J:827:GLU:O	3:J:829:GLY:N	2.29	0.65
2:C:471:VAL:HB	2:C:498:ILE:HD11	1.78	0.65
3:J:505:ASP:HB3	3:J:629:PHE:HE1	1.61	0.65
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.79	0.64
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.45	0.64
3:D:268:LEU:HD21	3:D:324:LEU:HD13	1.79	0.64
3:D:510:LEU:HD22	3:D:601:ILE:HD11	1.78	0.64
2:I:452:ARG:NH1	2:I:584:TYR:O	2.29	0.64
3:J:510:LEU:HD22	3:J:601:ILE:HD11	1.80	0.64
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.79	0.64
1:B:27:THR:HG22	1:B:202:VAL:HG22	1.79	0.64
1:B:86:LYS:HD3	1:B:174:ASP:HB2	1.79	0.64
3:D:844:THR:OG1	3:D:860:ARG:O	2.12	0.64
3:J:1221:LEU:HD12	3:J:1306:LEU:HB2	1.79	0.64
1:A:16:ILE:HG12	1:A:26:VAL:HG13	1.80	0.64
3:D:128:LEU:HD23	3:D:192:MET:HE3	1.80	0.64
2:I:996:ARG:NH1	2:I:999:GLU:OE2	2.31	0.64
3:J:514:THR:HA	3:J:576:ARG:HG2	1.80	0.64
2:I:1142:ARG:NH2	2:I:1165:SER:O	2.30	0.64
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.33	0.64
1:G:102:LEU:HD23	1:G:115:ILE:HG12	1.78	0.64
2:I:470:ARG:HA	2:I:473:ARG:HD2	1.79	0.64
2:I:1282:GLY:O	2:I:1284:ALA:N	2.29	0.64
3:D:473:THR:HG23	3:D:476:ALA:H	1.62	0.63
3:D:514:THR:HA	3:D:576:ARG:HG2	1.80	0.63
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.12	0.63
3:D:355:ILE:HD13	3:D:466:MET:HG3	1.78	0.63
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.80	0.63
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.80	0.63
5:F:461:ASN:O	5:F:465:ARG:HG2	1.98	0.63
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.79	0.63
1:A:162:GLU:HG3	1:A:165:GLU:HG2	1.81	0.63
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.80	0.63
2:C:363:LEU:HD13	2:C:382:GLU:HG2	1.79	0.63
3:D:614:LEU:HD23	4:E:7:GLN:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.78	0.63
5:F:571:TYR:HD1	5:F:575:GLU:HG2	1.64	0.63
2:C:808:ASN:H	3:D:633:ALA:HB2	1.64	0.62
1:A:57:THR:HG21	1:A:147:GLN:HE21	1.64	0.62
2:I:97:ARG:HB3	2:I:121:GLU:HB3	1.82	0.62
1:G:161:SER:O	1:G:163:GLU:N	2.30	0.62
1:H:57:THR:HG22	1:H:58:GLU:HG2	1.81	0.62
2:I:158:ASP:OD1	2:I:159:SER:N	2.33	0.62
5:F:598:LEU:O	5:F:604:SER:OG	2.17	0.62
1:G:231:PHE:HB3	1:H:218:ARG:HG2	1.82	0.62
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.64	0.62
2:C:551:HIS:ND1	2:C:553:THR:OG1	2.31	0.62
3:D:1280:VAL:O	3:D:1284:ARG:HB3	1.98	0.62
2:I:700:VAL:HG11	2:I:1114:GLU:HG2	1.81	0.62
1:A:102:LEU:HD11	1:A:110:VAL:HG11	1.81	0.62
3:J:903:LEU:HB3	3:J:905:ARG:H	1.64	0.62
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.32	0.61
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.33	0.61
1:H:44:ARG:HG3	1:H:183:ILE:HD13	1.82	0.61
2:I:564:PRO:HA	2:I:684:ASN:HD21	1.65	0.61
2:C:202:ARG:HD3	2:C:369:MET:HG2	1.81	0.61
2:C:1283:ALA:HB1	2:C:1286:THR:HB	1.80	0.61
2:C:41:GLN:NE2	2:C:73:TYR:O	2.34	0.61
5:F:137:TYR:HE1	5:F:351:THR:HB	1.64	0.61
1:H:102:LEU:O	1:H:141:SER:HA	2.00	0.61
2:C:762:ASN:O	2:C:833:ILE:N	2.32	0.61
2:C:28:LEU:HD21	2:C:524:ILE:HG13	1.83	0.61
2:I:176:ILE:HD11	2:I:428:VAL:HG21	1.81	0.61
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.83	0.60
2:I:5:TYR:HB2	2:I:781:ASP:OD2	2.00	0.60
2:I:357:ASN:ND2	2:I:358:ASP:OD2	2.34	0.60
3:J:514:THR:OG1	3:J:596:LEU:HB2	2.00	0.60
1:A:14:VAL:HG13	1:A:15:ASP:H	1.65	0.60
1:B:14:VAL:HB	1:B:28:LEU:HD13	1.83	0.60
2:C:700:VAL:HG11	2:C:1114:GLU:HG2	1.82	0.60
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.83	0.60
2:C:158:ASP:OD1	2:C:159:SER:N	2.34	0.60
3:D:77:ARG:HG3	3:D:79:LYS:H	1.65	0.60
1:H:64:VAL:HG11	1:H:69:SER:HB2	1.82	0.60
3:J:18:ASP:HB2	3:J:1373:ARG:NH2	2.16	0.60
1:A:7:GLU:OE1	1:B:150:ARG:NH2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.66	0.60
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.66	0.60
1:B:47:LEU:HB3	1:B:180:VAL:HG11	1.83	0.60
3:J:698:MET:O	3:J:702:GLN:HB3	2.01	0.60
1:A:133:LEU:HD21	1:A:140:ILE:HG21	1.83	0.60
2:I:363:LEU:HD13	2:I:382:GLU:HG2	1.82	0.60
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.83	0.60
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.36	0.60
5:F:561:MET:HG3	5:F:567:MET:HE1	1.83	0.60
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.33	0.60
1:A:187:VAL:HG22	1:A:201:LEU:HD13	1.83	0.60
4:E:15:ASN:HB3	4:E:18:ASP:H	1.66	0.60
2:I:1211:ARG:HB2	2:I:1220:GLN:HE21	1.66	0.60
3:D:615:LYS:HE2	3:D:616:PRO:HD3	1.83	0.60
3:D:1289:ASN:OD1	3:D:1290:ARG:NH1	2.34	0.60
1:A:102:LEU:HD23	1:A:115:ILE:HG12	1.83	0.59
3:J:843:VAL:HG13	3:J:883:ARG:HD3	1.84	0.59
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.84	0.59
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.38	0.59
5:F:343:LYS:HD2	5:F:343:LYS:H	1.67	0.59
2:I:1281:TYR:HE2	3:J:489:ASN:HD21	1.51	0.59
1:A:117:HIS:NE2	1:A:121:VAL:O	2.35	0.59
2:C:658:GLN:O	2:C:660:VAL:N	2.36	0.59
3:D:17:PHE:O	3:D:1369:ARG:NH2	2.36	0.59
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.38	0.59
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.84	0.59
1:H:16:ILE:HG13	1:H:26:VAL:HG22	1.84	0.59
2:I:1120:ALA:HB2	2:I:1199:LEU:HG	1.85	0.59
2:C:685:MET:HB3	2:C:1235:LEU:HD11	1.84	0.59
3:D:709:ARG:O	3:D:711:GLY:N	2.35	0.59
3:J:901:ARG:HA	3:J:908:ILE:HA	1.83	0.59
5:F:371:LYS:HA	5:F:374:ARG:NH1	2.17	0.59
1:G:191:ARG:HH12	1:G:197:ASP:HA	1.67	0.59
2:C:6:THR:HG21	2:C:782:VAL:HG23	1.84	0.59
3:D:362:ARG:H	3:D:365:GLN:HE21	1.49	0.59
2:I:168:GLY:O	2:I:170:VAL:N	2.29	0.59
3:J:268:LEU:HD21	3:J:324:LEU:HD13	1.83	0.59
3:J:858:VAL:HG21	3:J:864:LEU:HD21	1.85	0.59
4:K:26:ARG:NH1	4:K:29:GLN:OE1	2.35	0.59
5:L:557:LYS:HG2	5:L:580:PHE:HZ	1.66	0.59
1:A:83:LEU:HD23	2:C:694:ARG:HE	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:205:LEU:HD23	3:D:217:LEU:HD12	1.85	0.59
2:I:524:ILE:HD12	2:I:712:SER:HB2	1.84	0.59
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.82	0.59
2:I:811:ASN:HA	2:I:815:SER:HB2	1.85	0.59
2:C:735:LYS:HA	2:C:748:ILE:HG22	1.85	0.59
2:C:1253:LEU:O	3:D:99:ARG:NH2	2.36	0.59
3:J:804:ALA:O	3:J:806:ASP:N	2.35	0.59
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.38	0.58
2:C:1100:PRO:HB3	3:D:639:VAL:HG12	1.85	0.58
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.85	0.58
3:J:870:ASP:O	3:J:874:GLU:N	2.33	0.58
5:L:147:GLN:HE22	5:L:150:ARG:HH11	1.51	0.58
3:D:68:TYR:HA	3:D:92:VAL:HG23	1.85	0.58
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.85	0.58
1:G:133:LEU:HD21	1:G:140:ILE:HG21	1.85	0.58
2:I:1111:GLN:O	2:I:1115:THR:OG1	2.22	0.58
3:J:418:GLU:HG3	4:K:45:LYS:H	1.66	0.58
3:D:430:HIS:CE1	3:D:432:LEU:HB2	2.38	0.58
3:D:664:ILE:HG22	3:D:678:ARG:HG2	1.84	0.58
1:G:158:ARG:HB3	1:G:172:LEU:HD23	1.85	0.58
4:K:31:GLN:HB2	4:K:46:THR:HG21	1.85	0.58
5:L:316:PHE:HZ	5:L:334:SER:HA	1.67	0.58
3:D:1281:GLU:O	3:D:1285:VAL:HB	2.04	0.58
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.84	0.58
2:C:1302:THR:HG22	5:F:531:PRO:HB3	1.86	0.58
2:I:124:MET:HB3	2:I:493:ILE:HD12	1.86	0.58
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.84	0.58
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.29	0.58
3:J:418:GLU:HG3	4:K:44:ASP:HA	1.85	0.58
1:B:53:GLY:HA3	1:B:177:TYR:O	2.04	0.58
3:J:339:ARG:NH1	3:J:1323:ALA:O	2.36	0.58
3:J:506:VAL:HG23	3:J:628:GLY:HA3	1.85	0.58
2:C:548:ARG:NH2	2:C:567:PRO:O	2.37	0.58
1:H:35:PHE:HA	1:H:38:THR:HG22	1.85	0.58
3:D:804:ALA:O	3:D:806:ASP:N	2.37	0.58
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.85	0.58
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.86	0.58
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.84	0.57
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.39	0.57
2:I:1119:MET:HG3	2:I:1204:LEU:HD13	1.86	0.57
1:A:25:LYS:HG2	1:A:204:GLU:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.86	0.57
3:D:1347:LEU:HD12	3:D:1358:PRO:HG2	1.85	0.57
3:J:91:GLU:OE2	3:J:101:ARG:NH2	2.37	0.57
2:C:807:TRP:HB2	2:C:1097:VAL:HG11	1.86	0.57
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.85	0.57
5:F:262:VAL:HG12	5:F:264:LYS:H	1.69	0.57
2:C:736:VAL:HG23	2:C:748:ILE:HA	1.85	0.57
2:I:69:GLN:HE21	2:I:101:ARG:HD2	1.69	0.57
2:I:1296:ASP:HB3	2:I:1320:PRO:HB3	1.86	0.57
5:L:573:LEU:HD12	5:L:588:ARG:HG2	1.86	0.57
3:J:515:ARG:NH2	3:J:717:VAL:HB	2.20	0.57
3:J:536:LEU:HB3	3:J:542:ALA:HB3	1.86	0.57
2:C:1256:GLN:HB3	2:C:1301:ARG:HH22	1.68	0.57
3:D:708:ASN:OD1	3:D:708:ASN:N	2.37	0.57
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.87	0.57
2:I:992:LEU:HD11	2:I:1000:LEU:HD11	1.86	0.57
3:J:1263:LYS:HE2	3:J:1279:GLN:HE21	1.68	0.57
5:L:269:LEU:O	5:L:273:MET:HG3	2.05	0.57
3:D:189:LEU:HB3	3:D:234:PRO:HB2	1.85	0.57
5:F:231:THR:HG23	5:F:249:ILE:HG12	1.87	0.57
2:I:1255:THR:O	2:I:1257:GLN:N	2.37	0.57
3:J:148:GLU:H	3:J:156:ARG:HG3	1.70	0.57
1:A:133:LEU:HD12	1:A:138:ALA:HB3	1.87	0.57
1:B:62:ASP:OD2	1:B:71:LYS:NZ	2.34	0.57
2:C:243:PRO:HB2	2:C:278:GLU:HG3	1.85	0.57
1:G:218:ARG:NH1	1:H:231:PHE:O	2.37	0.57
1:H:62:ASP:OD1	1:H:62:ASP:N	2.27	0.57
2:I:710:VAL:HA	2:I:715:THR:HG21	1.85	0.57
2:I:1184:THR:HG23	2:I:1190:ALA:H	1.69	0.57
4:K:70:GLN:NE2	4:K:74:GLU:OE2	2.36	0.57
2:C:148:GLN:OE1	2:C:454:ARG:NH1	2.38	0.57
2:I:90:VAL:HG12	2:I:91:THR:H	1.70	0.57
1:B:191:ARG:HH12	3:D:370:LYS:HE3	1.70	0.56
3:D:1262:ARG:NH2	3:D:1312:ALA:O	2.36	0.56
3:D:1372:ARG:HE	3:J:854:ALA:HB2	1.70	0.56
2:I:972:PHE:HD1	2:I:994:ARG:HH21	1.52	0.56
3:J:800:LEU:HB3	3:J:920:ALA:HB1	1.86	0.56
1:A:113:ALA:HB2	1:A:126:PRO:HB3	1.86	0.56
2:C:678:ARG:NH2	2:C:1106:ARG:HG2	2.21	0.56
1:G:45:ARG:NH1	1:H:34:GLY:O	2.38	0.56
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:748:ILE:HD11	2:I:966:ILE:HG22	1.85	0.56
3:J:1289:ASN:OD1	3:J:1290:ARG:NH1	2.39	0.56
1:B:64:VAL:HG11	1:B:69:SER:CB	2.35	0.56
2:C:142:GLU:HB2	2:C:760:ASN:ND2	2.20	0.56
2:C:550:VAL:HG11	3:D:776:THR:HG22	1.86	0.56
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.87	0.56
2:I:208:ILE:HD13	2:I:365:GLU:HG2	1.87	0.56
2:I:556:GLY:HA2	2:I:659:GLN:O	2.04	0.56
3:J:320:ASN:OD1	3:J:322:ARG:HB3	2.05	0.56
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.04	0.56
1:G:58:GLU:OE2	1:G:170:ARG:NH1	2.39	0.56
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.87	0.56
2:I:849:GLU:HB2	2:I:887:VAL:HG23	1.87	0.56
3:J:205:LEU:HD23	3:J:217:LEU:HD12	1.88	0.56
5:F:420:GLU:OE1	5:F:423:ARG:NH2	2.39	0.56
1:G:226:GLU:OE1	1:H:10:LYS:HE2	2.06	0.56
3:J:850:LYS:HG2	3:J:857:LEU:HD23	1.86	0.56
1:A:47:LEU:O	1:A:180:VAL:HG21	2.06	0.56
2:C:30:ILE:HD11	2:C:575:LEU:HD22	1.87	0.56
2:C:811:ASN:HA	2:C:815:SER:HB2	1.87	0.56
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.87	0.56
2:I:1279:GLU:HG2	3:J:1357:ILE:HD13	1.88	0.56
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	1.87	0.56
1:B:59:VAL:HG21	1:B:85:LEU:HD13	1.86	0.56
2:C:515:MET:O	2:C:517:GLN:N	2.39	0.56
3:J:842:ARG:HD3	3:J:882:VAL:HG11	1.87	0.56
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.70	0.56
5:L:448:ARG:HH21	5:L:450:ILE:HG13	1.71	0.56
2:C:933:VAL:HG22	2:C:1050:VAL:HG22	1.86	0.56
3:D:259:ARG:NH1	5:F:505:ILE:HD11	2.19	0.56
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.86	0.56
1:G:73:GLY:HA3	1:G:138:ALA:HB1	1.88	0.56
1:G:221:ALA:HB1	1:H:228:LEU:HD22	1.88	0.56
2:I:41:GLN:NE2	2:I:73:TYR:O	2.38	0.56
3:J:16:GLU:HG3	3:J:17:PHE:HD2	1.71	0.56
3:J:77:ARG:HG3	3:J:79:LYS:H	1.71	0.56
3:D:836:ARG:HG3	3:D:869:CYS:HB3	1.87	0.56
2:I:742:TYR:O	2:I:974:ARG:NH2	2.38	0.56
3:J:140:TYR:OH	3:J:312:ARG:NH2	2.38	0.56
2:C:117:ILE:HG21	2:C:488:MET:HG2	1.87	0.56
3:D:378:LYS:NZ	3:D:382:TYR:OH	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:305:LEU:HD13	5:F:314:THR:HG22	1.87	0.56
2:I:590:PRO:HB2	2:I:655:VAL:HG21	1.88	0.56
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.88	0.56
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.88	0.56
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.88	0.55
3:D:322:ARG:NH1	3:D:322:ARG:HB2	2.21	0.55
3:J:516:ASP:HB3	3:J:573:THR:HG21	1.87	0.55
1:G:66:HIS:HB3	1:G:68:TYR:H	1.71	0.55
2:I:1004:ASP:OD1	2:I:1004:ASP:N	2.39	0.55
1:A:135:ASP:OD1	1:A:136:GLU:N	2.39	0.55
2:C:564:PRO:HA	2:C:684:ASN:HD21	1.71	0.55
2:C:1297:ASP:OD1	2:C:1300:GLY:N	2.26	0.55
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.89	0.55
3:D:201:LEU:HD12	3:D:221:ILE:HD13	1.88	0.55
3:D:709:ARG:C	3:D:711:GLY:H	2.10	0.55
5:F:111:LEU:HD11	5:F:119:ILE:HD12	1.88	0.55
1:G:62:ASP:HB2	1:G:141:SER:O	2.06	0.55
2:I:963:GLU:O	2:I:967:LEU:HB2	2.06	0.55
3:J:494:ALA:HB2	3:J:922:SER:HB3	1.88	0.55
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.41	0.55
2:C:1004:ASP:N	2:C:1004:ASP:OD1	2.38	0.55
3:D:809:VAL:HG21	3:D:909:ILE:HG12	1.88	0.55
3:D:198:CYS:HB3	3:D:202:ARG:HE	1.72	0.55
3:D:520:ALA:HB3	3:D:546:ALA:HB2	1.89	0.55
3:J:793:SER:O	3:J:797:THR:HG23	2.06	0.55
2:C:1087:TYR:HE1	2:C:1215:GLY:HA2	1.71	0.55
2:C:1137:GLU:HG2	2:C:1140:LYS:HG2	1.89	0.55
1:H:74:VAL:HG12	1:H:76:GLU:H	1.72	0.55
3:J:741:ALA:O	3:J:762:ASN:ND2	2.40	0.55
2:C:1151:LEU:HG	2:C:1198:LEU:HD23	1.89	0.55
3:D:707:ILE:HD11	3:D:716:GLN:HG2	1.89	0.55
1:G:57:THR:HG22	1:G:58:GLU:HG2	1.89	0.55
1:H:85:LEU:HD13	1:H:144:ILE:HD12	1.88	0.55
3:J:544:LEU:O	3:J:575:GLY:N	2.40	0.55
1:A:101:THR:HG23	1:A:116:THR:HB	1.89	0.55
5:F:137:TYR:CZ	5:F:139:GLU:HB2	2.42	0.55
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.89	0.55
2:C:1255:THR:O	2:C:1257:GLN:N	2.40	0.54
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.71	0.54
2:I:658:GLN:O	2:I:660:VAL:N	2.40	0.54
3:J:1149:ARG:HG3	3:J:1216:ALA:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:466:ILE:HG22	5:L:483:LEU:HD23	1.89	0.54
3:D:516:ASP:HB3	3:D:573:THR:HG21	1.88	0.54
3:D:800:LEU:HB3	3:D:920:ALA:HB1	1.88	0.54
1:B:19:VAL:O	1:B:23:HIS:HB3	2.07	0.54
1:B:195:ARG:HB3	1:B:198:LEU:HD21	1.89	0.54
2:I:1072:ASN:OD1	2:I:1072:ASN:N	2.40	0.54
1:B:86:LYS:NZ	3:D:532:GLU:OE2	2.40	0.54
3:D:418:GLU:HB2	4:E:45:LYS:HB2	1.89	0.54
4:E:31:GLN:HB2	4:E:46:THR:HG21	1.87	0.54
2:I:1100:PRO:HB3	3:J:639:VAL:HG12	1.88	0.54
1:A:12:ARG:H	1:A:30:PRO:HD2	1.72	0.54
3:D:290:ILE:HD12	3:D:290:ILE:H	1.72	0.54
3:D:421:VAL:HG13	3:D:439:PRO:HG3	1.89	0.54
3:D:903:LEU:HB3	3:D:905:ARG:H	1.72	0.54
1:B:102:LEU:O	1:B:141:SER:HA	2.07	0.54
1:B:176:CYS:HB3	3:D:535:ARG:HH12	1.72	0.54
1:G:50:SER:HB2	1:H:8:PHE:HZ	1.72	0.54
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.88	0.54
3:J:582:ILE:HG22	3:J:620:PHE:HE1	1.72	0.54
1:A:166:ARG:O	1:A:168:ILE:N	2.41	0.54
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.90	0.54
3:D:1181:ASP:OD1	3:D:1182:GLY:N	2.41	0.54
5:F:281:ARG:HD3	5:F:285:ARG:HH11	1.72	0.54
3:J:930:LEU:HB2	3:J:1138:LEU:HB2	1.89	0.54
1:A:92:VAL:HG12	1:A:121:VAL:HG22	1.89	0.54
2:C:1160:ASP:CG	2:C:1161:LEU:H	2.09	0.54
2:C:1287:LEU:HD13	3:D:1357:ILE:HD11	1.90	0.54
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.90	0.54
1:H:67:GLU:OE1	1:H:67:GLU:N	2.41	0.54
3:D:642:ASP:HA	3:D:764:ARG:HH21	1.73	0.54
2:I:185:ASP:OD2	2:I:200:ARG:NH1	2.38	0.54
1:A:50:SER:HB2	1:B:8:PHE:HZ	1.73	0.54
2:I:551:HIS:ND1	2:I:553:THR:OG1	2.38	0.54
1:B:133:LEU:HD11	1:B:140:ILE:HG21	1.90	0.53
2:C:1240:ASP:N	2:C:1240:ASP:OD1	2.38	0.53
2:I:61:SER:O	2:I:63:SER:N	2.41	0.53
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.72	0.53
2:I:1116:HIS:CE1	3:J:641:ILE:H	2.26	0.53
3:J:210:SER:HB2	3:J:213:LYS:HB2	1.90	0.53
2:C:1212:LEU:HD22	2:C:1225:VAL:HG21	1.90	0.53
2:I:696:ASP:O	2:I:697:LYS:HB3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:THR:HG23	1:A:158:ARG:CZ	2.39	0.53
2:C:74:ARG:NH1	2:C:121:GLU:OE2	2.41	0.53
2:C:161:LYS:HA	2:C:170:VAL:HB	1.90	0.53
2:C:905:ILE:HG12	5:F:595:LEU:HD22	1.89	0.53
2:I:1287:LEU:HD22	3:J:1357:ILE:HG13	1.90	0.53
5:L:544:THR:HG22	5:L:607:LEU:HD21	1.91	0.53
5:L:571:TYR:CD1	5:L:575:GLU:HG2	2.40	0.53
1:H:228:LEU:HA	1:H:231:PHE:HD2	1.73	0.53
2:I:979:LEU:HD23	2:I:989:LEU:HD21	1.90	0.53
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.90	0.53
3:J:709:ARG:O	3:J:711:GLY:N	2.41	0.53
2:C:696:ASP:O	2:C:697:LYS:HB3	2.07	0.53
2:I:28:LEU:HD21	2:I:524:ILE:HG13	1.90	0.53
2:I:702:THR:N	2:I:705:GLU:OE2	2.38	0.53
3:J:290:ILE:H	3:J:290:ILE:HD12	1.73	0.53
5:L:532:LEU:HD12	5:L:532:LEU:H	1.74	0.53
2:C:1042:LEU:HB3	2:C:1046:VAL:HG13	1.89	0.53
3:D:94:GLN:HE21	3:D:96:LYS:HB2	1.74	0.53
2:I:724:VAL:HA	2:I:734:ILE:HD13	1.89	0.53
3:J:836:ARG:HD2	3:J:873:GLU:OE1	2.09	0.53
2:C:131:THR:HG22	2:C:135:THR:H	1.74	0.53
3:D:435:GLN:HE21	3:D:486:SER:HA	1.74	0.53
1:A:50:SER:HB2	1:B:8:PHE:CZ	2.42	0.53
3:D:864:LEU:HD13	3:D:872:LEU:HD11	1.90	0.53
1:G:52:PRO:HG2	1:G:219:ARG:HH21	1.74	0.53
2:I:5:TYR:O	2:I:8:LYS:HG2	2.09	0.53
2:I:241:LEU:HD11	2:I:246:LEU:HD11	1.90	0.53
1:A:54:CYS:HB3	1:A:148:ARG:HA	1.90	0.53
2:C:478:ARG:HG2	2:C:492:MET:HG2	1.90	0.53
3:D:930:LEU:HA	3:D:1244:GLN:HG3	1.91	0.53
2:I:1302:THR:HG22	5:L:531:PRO:HB3	1.91	0.53
3:J:748:ALA:O	3:J:777:HIS:HD2	1.92	0.53
3:J:750:PRO:HA	3:J:777:HIS:NE2	2.23	0.53
3:D:45:ASN:O	3:D:46:TYR:HB3	2.07	0.52
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.40	0.52
1:G:75:GLN:HA	2:I:729:ALA:N	2.24	0.52
2:C:74:ARG:HH12	2:C:121:GLU:CD	2.11	0.52
2:C:488:MET:O	2:C:490:GLN:N	2.40	0.52
3:J:154:LEU:HD22	3:J:160:LEU:HD11	1.92	0.52
2:C:400:VAL:HG13	2:C:584:TYR:HB3	1.92	0.52
3:D:515:ARG:NH2	3:D:717:VAL:HB	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:854:ILE:HD11	2:I:885:GLY:HA3	1.92	0.52
3:J:131:PRO:HG2	3:J:134:ASP:HB2	1.91	0.52
1:B:35:PHE:HA	1:B:38:THR:HG22	1.91	0.52
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.91	0.52
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.91	0.52
5:F:584:ARG:HA	5:F:584:ARG:HH11	1.75	0.52
3:J:45:ASN:HB3	3:J:48:THR:O	2.10	0.52
3:J:915:ILE:HA	3:J:918:ILE:HG23	1.90	0.52
3:J:1343:GLU:HG3	3:J:1373:ARG:CZ	2.40	0.52
5:L:395:THR:OG1	5:L:396:ASN:N	2.42	0.52
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.92	0.52
1:G:135:ASP:HB2	2:I:726:TYR:HE1	1.74	0.52
2:I:685:MET:HE1	2:I:1071:GLY:HA2	1.92	0.52
3:J:197:GLU:OE1	3:J:220:ARG:NH2	2.37	0.52
3:J:665:GLN:OE1	3:J:678:ARG:NH1	2.42	0.52
1:B:183:ILE:HG23	1:B:205:MET:HG3	1.90	0.52
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.92	0.52
2:C:1287:LEU:HD21	3:D:1351:VAL:HG22	1.90	0.52
3:D:750:PRO:HA	3:D:777:HIS:NE2	2.25	0.52
1:G:47:LEU:O	1:G:51:MET:HG3	2.10	0.52
1:G:85:LEU:HD23	1:G:130:ILE:HD12	1.92	0.52
2:I:1073:LYS:HE3	3:J:462:ASP:HB2	1.91	0.52
2:I:1116:HIS:HE1	3:J:641:ILE:N	2.08	0.52
2:I:1312:ASN:OD1	2:I:1314:GLN:HG3	2.10	0.52
2:C:993:PRO:HG2	2:C:996:ARG:HB2	1.92	0.52
3:D:88:CYS:O	3:D:90:VAL:N	2.40	0.52
3:D:495:ASN:C	3:D:497:GLU:H	2.11	0.52
1:H:86:LYS:HD3	1:H:174:ASP:HB2	1.90	0.52
2:I:148:GLN:NE2	2:I:535:PRO:O	2.23	0.52
2:I:260:LYS:HE3	2:I:262:TYR:CE1	2.45	0.52
5:L:281:ARG:HG2	5:L:285:ARG:HD2	1.91	0.52
1:B:79:LEU:HD23	1:B:79:LEU:H	1.74	0.52
3:D:582:ILE:HG22	3:D:620:PHE:HE1	1.75	0.52
2:C:378:ARG:NH1	2:C:382:GLU:OE2	2.43	0.52
3:J:27:PRO:HB3	3:J:241:VAL:HG23	1.92	0.52
5:L:561:MET:HG3	5:L:567:MET:HE1	1.91	0.52
2:C:168:GLY:O	2:C:170:VAL:N	2.35	0.51
2:C:518:ASN:HD21	2:C:787:PRO:HG3	1.75	0.51
2:C:632:ASP:O	2:C:647:ARG:HB2	2.10	0.51
3:D:43:THR:OG1	5:F:449:THR:O	2.21	0.51
5:F:600:HIS:O	5:F:602:SER:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:338:THR:HG22	2:I:345:PRO:HB3	1.91	0.51
3:J:526:VAL:HG12	3:J:549:LYS:HB2	1.92	0.51
2:C:315:MET:HA	2:C:352:ARG:HH12	1.74	0.51
2:C:764:CYS:SG	2:C:765:ILE:N	2.82	0.51
1:H:61:ILE:HB	1:H:64:VAL:O	2.10	0.51
2:I:122:VAL:HG23	5:L:472:GLN:HG3	1.92	0.51
2:C:606:LEU:HD21	2:C:614:TYR:HD1	1.74	0.51
5:F:306:PHE:CE1	5:F:310:GLU:HA	2.46	0.51
1:H:56:VAL:HG21	1:H:144:ILE:HD11	1.92	0.51
3:J:104:HIS:HA	3:J:243:PRO:HA	1.92	0.51
1:A:59:VAL:HG22	1:A:144:ILE:HG23	1.91	0.51
5:F:251:LYS:HA	5:F:254:GLU:HG2	1.93	0.51
5:F:571:TYR:CD1	5:F:575:GLU:HG2	2.45	0.51
1:H:47:LEU:HD22	1:H:180:VAL:HG11	1.91	0.51
3:J:850:LYS:HB2	3:J:852:GLY:O	2.09	0.51
5:L:461:ASN:O	5:L:465:ARG:HG2	2.09	0.51
2:C:620:ASN:O	2:C:620:ASN:ND2	2.44	0.51
5:F:281:ARG:HD3	5:F:285:ARG:NH1	2.26	0.51
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.92	0.51
2:C:568:ASN:N	2:C:568:ASN:OD1	2.44	0.51
1:H:125:LYS:HB3	1:H:128:HIS:HB2	1.91	0.51
2:I:228:VAL:HG22	2:I:245:ARG:HE	1.75	0.51
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.76	0.51
2:I:802:VAL:HG11	2:I:1230:MET:HB3	1.92	0.51
2:I:1115:THR:O	2:I:1228:GLY:HA3	2.09	0.51
3:J:518:VAL:HG11	3:J:707:ILE:HB	1.92	0.51
3:D:697:MET:SD	3:D:741:ALA:HB3	2.50	0.51
3:J:128:LEU:HD23	3:J:192:MET:HE1	1.93	0.51
1:B:57:THR:O	1:B:173:VAL:HG23	2.10	0.51
1:G:65:LEU:HD22	1:G:65:LEU:H	1.76	0.51
2:I:834:GLN:HE21	2:I:1056:VAL:HG21	1.76	0.51
2:I:1149:TYR:CD1	2:I:1159:VAL:HG11	2.46	0.51
2:I:161:LYS:HA	2:I:170:VAL:HB	1.93	0.51
2:I:778:GLU:HG3	2:I:779:ARG:N	2.26	0.51
3:J:174:ASP:O	3:J:175:GLU:HG2	2.11	0.51
3:J:355:ILE:HD13	3:J:466:MET:HG3	1.93	0.51
3:J:709:ARG:C	3:J:711:GLY:H	2.14	0.51
1:A:22:THR:O	1:A:206:GLU:HA	2.11	0.50
2:I:598:VAL:HG22	2:I:628:HIS:CE1	2.46	0.50
2:I:620:ASN:ND2	2:I:620:ASN:O	2.43	0.50
3:J:707:ILE:HG22	3:J:708:ASN:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1158:GLU:HG3	3:J:1186:TYR:CZ	2.46	0.50
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.93	0.50
2:C:541:GLU:OE1	2:C:541:GLU:N	2.43	0.50
2:C:1142:ARG:HH22	2:C:1165:SER:CA	2.21	0.50
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.92	0.50
5:F:586:ARG:O	5:F:590:ILE:HG13	2.12	0.50
1:G:74:VAL:HG12	1:G:76:GLU:H	1.76	0.50
2:I:471:VAL:HB	2:I:498:ILE:HD11	1.92	0.50
3:J:81:ARG:HG3	3:J:82:GLY:H	1.76	0.50
3:J:644:MET:HB2	3:J:764:ARG:HG3	1.91	0.50
3:J:930:LEU:HD12	3:J:1138:LEU:HD13	1.93	0.50
1:B:100:LEU:O	1:B:143:ARG:HA	2.11	0.50
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.46	0.50
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.92	0.50
2:C:716:ALA:HB3	2:C:784:ALA:HB3	1.93	0.50
2:I:179:TYR:OH	2:I:458:GLU:OE2	2.17	0.50
3:J:495:ASN:C	3:J:497:GLU:H	2.14	0.50
5:L:147:GLN:O	5:L:151:VAL:HG23	2.11	0.50
2:C:1065:LYS:HD3	2:C:1235:LEU:HD12	1.92	0.50
2:C:1222:GLU:OE2	3:D:537:TYR:OH	2.21	0.50
5:F:227:GLN:HG3	5:F:252:LEU:HA	1.94	0.50
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.93	0.50
5:L:357:GLN:HA	5:L:360:ASP:HB2	1.92	0.50
3:D:294:ASN:HD22	5:F:406:GLN:NE2	2.09	0.50
2:I:452:ARG:NH2	2:I:458:GLU:OE1	2.44	0.50
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.77	0.50
3:J:88:CYS:O	3:J:90:VAL:N	2.42	0.50
2:C:637:ARG:HB3	2:C:642:SER:HB3	1.92	0.50
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.92	0.50
3:D:174:ASP:O	3:D:175:GLU:HG2	2.12	0.50
2:I:1210:ILE:HD11	2:I:1227:VAL:HG21	1.94	0.50
1:A:218:ARG:HG3	1:B:231:PHE:O	2.12	0.50
2:C:798:GLN:OE1	2:C:827:ARG:HB2	2.12	0.50
3:D:865:HIS:CE1	3:D:867:GLN:HB2	2.47	0.50
1:G:47:LEU:O	1:G:180:VAL:HG21	2.11	0.50
2:I:4:SER:OG	2:I:5:TYR:N	2.42	0.50
2:I:1268:GLN:HE22	3:J:352:ARG:HH12	1.59	0.50
3:J:201:LEU:HB2	3:J:221:ILE:HD13	1.94	0.50
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.94	0.50
3:D:748:ALA:O	3:D:777:HIS:HD2	1.94	0.50
2:I:119:GLU:HG2	2:I:488:MET:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:746:LEU:HD22	3:J:754:ILE:HD11	1.94	0.50
2:C:323:ALA:O	2:C:327:GLN:HG3	2.11	0.50
2:C:1116:HIS:CE1	3:D:641:ILE:H	2.27	0.50
2:C:1279:GLU:HG2	3:D:1357:ILE:HD13	1.93	0.50
2:C:1312:ASN:OD1	2:C:1314:GLN:HG3	2.12	0.50
3:D:810:THR:HG23	3:D:811:GLU:H	1.76	0.50
2:I:722:GLY:HA2	2:I:737:ASN:OD1	2.12	0.50
2:I:976:ARG:NH2	2:I:990:ASP:OD2	2.45	0.50
3:J:210:SER:O	3:J:214:ARG:HG2	2.12	0.50
3:J:311:ARG:NH2	3:J:1329:THR:HG21	2.27	0.50
1:B:149:GLY:HA3	1:B:177:TYR:CD2	2.48	0.49
2:C:746:ALA:HB2	2:C:974:ARG:HE	1.77	0.49
3:D:45:ASN:HB3	3:D:48:THR:O	2.12	0.49
3:D:317:THR:HG22	3:D:322:ARG:O	2.12	0.49
3:D:352:ARG:HD2	3:D:465:GLN:NE2	2.26	0.49
1:H:158:ARG:HB3	1:H:172:LEU:HD23	1.94	0.49
2:I:30:ILE:HD12	2:I:30:ILE:H	1.77	0.49
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.92	0.49
3:J:41:PRO:HB2	3:J:270:ARG:HG3	1.92	0.49
3:J:515:ARG:O	3:J:545:HIS:HB3	2.11	0.49
3:J:1326:GLN:OE1	3:J:1330:ARG:NH2	2.45	0.49
3:D:850:LYS:HG2	3:D:857:LEU:HD23	1.93	0.49
1:H:187:VAL:HG22	1:H:201:LEU:HD13	1.93	0.49
2:I:31:GLN:HG3	2:I:527:LYS:HB3	1.94	0.49
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.94	0.49
1:B:104:LYS:HG2	1:B:110:VAL:HG22	1.92	0.49
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.94	0.49
2:C:661:VAL:HB	2:C:665:ALA:HB3	1.94	0.49
1:H:228:LEU:HA	1:H:231:PHE:CD2	2.47	0.49
3:J:1146:GLU:HB3	3:J:1148:ARG:HG3	1.94	0.49
2:C:406:ASN:HD22	2:C:413:GLU:HB2	1.77	0.49
2:C:520:PRO:HG3	2:C:714:VAL:HG21	1.95	0.49
2:C:658:GLN:HE21	2:C:1186:VAL:HG23	1.76	0.49
5:F:394:TYR:HE2	5:F:436:ARG:HG3	1.77	0.49
1:H:53:GLY:HA3	1:H:177:TYR:O	2.12	0.49
1:H:59:VAL:HG21	1:H:85:LEU:HD13	1.94	0.49
2:I:727:VAL:HG13	2:I:732:ILE:HG12	1.94	0.49
3:J:824:PRO:HD3	3:J:835:LEU:HD13	1.94	0.49
1:B:49:SER:O	1:B:151:GLY:HA3	2.12	0.49
2:C:115:LYS:HD3	2:C:116:ASP:H	1.78	0.49
2:C:959:ASP:O	2:C:963:GLU:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:518:VAL:HG11	3:D:707:ILE:HB	1.94	0.49
1:G:16:ILE:HG23	1:G:26:VAL:HG22	1.94	0.49
2:I:1065:LYS:HD3	2:I:1235:LEU:HD12	1.93	0.49
2:I:1281:TYR:HE2	3:J:489:ASN:ND2	2.09	0.49
3:D:585:LYS:HB2	3:D:612:LEU:HD21	1.94	0.49
1:G:102:LEU:HB3	1:G:142:MET:HG2	1.94	0.49
2:I:960:LEU:HD11	2:I:1028:LYS:HE2	1.95	0.49
4:K:50:ALA:O	4:K:54:ILE:HG12	2.11	0.49
1:A:161:SER:O	1:A:163:GLU:N	2.46	0.49
2:C:176:ILE:HD11	2:C:428:VAL:HG21	1.94	0.49
2:C:1327:LEU:O	2:C:1331:ARG:HB2	2.12	0.49
2:I:478:ARG:NH1	2:I:482:GLY:HA2	2.27	0.49
2:I:802:VAL:HG21	2:I:1098:LEU:HD22	1.95	0.49
2:I:885:GLY:HA2	2:I:917:SER:HB3	1.94	0.49
3:J:362:ARG:H	3:J:365:GLN:NE2	2.08	0.49
5:L:337:VAL:O	5:L:341:LEU:HD12	2.12	0.49
1:A:74:VAL:HG12	1:A:76:GLU:H	1.77	0.49
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.95	0.49
2:C:1083:GLU:O	2:C:1215:GLY:HA3	2.13	0.49
3:D:701:LEU:CD1	3:D:723:TYR:HB2	2.43	0.49
3:D:708:ASN:HB3	3:D:712:GLN:O	2.13	0.49
3:J:347:VAL:HG12	3:J:348:ASP:O	2.12	0.49
3:J:510:LEU:HA	3:J:513:MET:HE2	1.95	0.49
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.94	0.49
2:C:218:GLU:HG3	2:C:299:LYS:HA	1.94	0.49
2:C:885:GLY:HA2	2:C:917:SER:HB3	1.95	0.49
2:C:936:ARG:NH1	5:F:495:ARG:HD3	2.27	0.49
2:C:975:ILE:O	2:C:979:LEU:HB2	2.12	0.49
3:D:81:ARG:HG3	3:D:82:GLY:H	1.77	0.49
3:D:452:LEU:HB3	3:D:500:ILE:HG23	1.95	0.49
3:D:510:LEU:HA	3:D:513:MET:HE2	1.94	0.49
2:I:125:GLY:HA2	2:I:499:SER:HB2	1.95	0.49
2:I:730:SER:O	2:I:753:LEU:HB2	2.13	0.49
1:B:101:THR:H	1:B:116:THR:HG22	1.78	0.49
3:D:363:LEU:HD23	3:D:487:THR:HG22	1.94	0.49
1:G:155:ALA:N	1:G:174:ASP:OD1	2.40	0.49
2:I:798:GLN:OE1	2:I:827:ARG:HB2	2.13	0.49
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.12	0.49
3:J:708:ASN:OD1	3:J:708:ASN:N	2.46	0.49
1:A:27:THR:HG23	1:A:202:VAL:HG22	1.95	0.48
1:B:12:ARG:O	1:B:13:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:470:ARG:CZ	2:C:497:PRO:HB3	2.43	0.48
2:C:551:HIS:HD1	2:C:553:THR:H	1.59	0.48
3:D:18:ASP:HB2	3:D:1373:ARG:NH2	2.28	0.48
3:D:848:VAL:HB	3:D:857:LEU:HD11	1.93	0.48
4:K:58:LEU:HD12	4:K:59:ILE:HG12	1.95	0.48
1:A:194:GLN:O	1:A:195:ARG:HB2	2.13	0.48
2:C:90:VAL:HG12	2:C:91:THR:H	1.78	0.48
2:C:815:SER:HB3	2:C:1077:SER:HB3	1.94	0.48
3:D:210:SER:HB2	3:D:213:LYS:HB2	1.94	0.48
3:D:279:LEU:HD11	3:D:296:LYS:HG2	1.94	0.48
3:D:744:ARG:O	3:D:744:ARG:HG3	2.13	0.48
3:D:848:VAL:HG11	3:D:880:VAL:HG22	1.95	0.48
1:G:57:THR:HG21	1:G:158:ARG:HH21	1.78	0.48
2:I:75:LEU:HD11	2:I:127:ILE:HD11	1.95	0.48
2:I:250:THR:HA	2:I:268:ARG:HA	1.96	0.48
2:I:1087:TYR:CE1	2:I:1215:GLY:HA2	2.48	0.48
1:B:59:VAL:HG22	1:B:144:ILE:HG13	1.94	0.48
1:G:99:ILE:HG12	1:G:145:LYS:HG3	1.94	0.48
2:I:208:ILE:HG23	2:I:362:ALA:HB1	1.94	0.48
2:I:223:LEU:HD11	2:I:426:ILE:HD13	1.95	0.48
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.95	0.48
3:J:849:LEU:H	3:J:849:LEU:HD22	1.78	0.48
1:A:39:LEU:O	1:A:43:LEU:HB2	2.13	0.48
1:B:74:VAL:HG12	1:B:76:GLU:H	1.78	0.48
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.13	0.48
3:J:1181:ASP:OD1	3:J:1182:GLY:N	2.46	0.48
2:C:1280:ALA:HB3	3:D:431:ARG:HB3	1.96	0.48
3:D:621:ALA:HA	3:D:624:ILE:HD12	1.95	0.48
3:J:555:TYR:HB2	3:J:586:GLY:HA2	1.95	0.48
5:L:137:TYR:HE1	5:L:351:THR:HB	1.79	0.48
2:C:613:ASN:OD1	2:C:639:LYS:NZ	2.46	0.48
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.94	0.48
1:G:134:THR:HG23	1:G:135:ASP:H	1.79	0.48
1:H:23:HIS:ND1	1:H:206:GLU:HG2	2.28	0.48
4:K:25:ARG:NH1	4:K:65:ASP:OD1	2.34	0.48
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.96	0.48
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.94	0.48
3:D:905:ARG:HH12	4:E:10:VAL:HG11	1.79	0.48
5:F:142:THR:O	5:F:146:GLU:N	2.40	0.48
2:I:241:LEU:HD21	2:I:277:LEU:HD13	1.95	0.48
2:I:448:LEU:HB2	2:I:553:THR:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:724:VAL:HG23	2:I:775:GLU:O	2.14	0.48
2:I:841:ARG:NE	3:J:256:ASP:HB3	2.28	0.48
2:I:990:ASP:HA	2:I:997:TRP:HZ2	1.78	0.48
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.94	0.48
2:C:761:GLN:HA	2:C:762:ASN:HA	1.56	0.48
2:C:871:VAL:O	2:C:944:ARG:NH1	2.47	0.48
3:D:827:GLU:O	3:D:829:GLY:N	2.47	0.48
3:D:842:ARG:HD3	3:D:882:VAL:HG11	1.96	0.48
3:D:1301:THR:HG23	3:J:1301:THR:HG23	1.96	0.48
5:F:478:PRO:HB2	5:F:483:LEU:HG	1.95	0.48
3:J:744:ARG:O	3:J:744:ARG:HG3	2.13	0.48
3:J:749:LYS:HB3	3:J:755:ILE:HG12	1.95	0.48
5:L:586:ARG:O	5:L:590:ILE:HG13	2.13	0.48
1:A:26:VAL:HG11	1:A:217:ILE:HD12	1.96	0.48
2:C:483:ASP:HB2	2:C:486:THR:HG21	1.95	0.48
5:F:583:THR:HG22	5:F:584:ARG:HG2	1.95	0.48
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.49	0.48
2:C:672:GLU:HB3	3:D:767:LEU:O	2.14	0.48
2:C:1129:ASN:OD1	2:C:1177:ARG:NH2	2.47	0.48
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.13	0.48
3:D:1348:LYS:O	3:D:1352:ILE:HG12	2.12	0.48
2:I:720:ARG:HH21	2:I:741:MET:HA	1.79	0.48
2:C:582:ASN:HB3	2:C:586:PHE:H	1.78	0.47
2:C:724:VAL:HG11	2:C:727:VAL:HG22	1.96	0.47
2:C:758:ARG:NH2	2:C:761:GLN:HG3	2.28	0.47
2:I:484:LEU:HB2	2:I:485:ASP:H	1.40	0.47
2:I:518:ASN:HD22	2:I:691:PRO:HG2	1.78	0.47
2:I:778:GLU:HG3	2:I:779:ARG:H	1.78	0.47
2:I:1240:ASP:OD1	2:I:1240:ASP:N	2.38	0.47
2:C:911:SER:OG	2:C:913:VAL:HG12	2.14	0.47
3:D:210:SER:O	3:D:214:ARG:HG2	2.14	0.47
3:D:654:ILE:O	3:D:658:GLU:HB2	2.14	0.47
5:F:493:LYS:HA	5:F:496:LYS:HE3	1.96	0.47
2:I:516:ASP:O	2:I:517:GLN:HG2	2.14	0.47
3:J:177:ASP:OD2	3:J:179:LYS:NZ	2.47	0.47
2:C:1122:LYS:HG2	2:C:1229:TYR:CE1	2.49	0.47
3:D:1221:LEU:HD11	3:D:1304:ARG:O	2.14	0.47
3:D:1344:LEU:O	3:D:1346:GLY:N	2.44	0.47
3:J:1344:LEU:HB3	3:J:1350:ASN:HD21	1.80	0.47
1:A:56:VAL:HG22	1:A:173:VAL:HG21	1.96	0.47
1:B:48:LEU:HD11	3:D:538:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:88:ARG:HH11	2:C:88:ARG:HB2	1.79	0.47
2:C:297:VAL:HG12	2:C:315:MET:O	2.14	0.47
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.97	0.47
3:J:801:VAL:O	3:J:805:GLN:HB2	2.13	0.47
3:J:814:CYS:HB3	3:J:890:THR:OG1	2.14	0.47
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.96	0.47
1:B:190:ALA:HB2	1:B:200:LYS:HB2	1.96	0.47
2:C:1115:THR:O	2:C:1228:GLY:HA3	2.15	0.47
2:C:1116:HIS:HE1	3:D:641:ILE:N	2.11	0.47
1:G:102:LEU:HD11	1:G:110:VAL:HG11	1.96	0.47
2:I:157:PHE:CZ	2:I:431:LYS:HG2	2.49	0.47
2:I:812:PHE:HZ	3:J:503:SER:HB2	1.79	0.47
2:I:1176:LEU:HD13	2:I:1180:MET:HG2	1.96	0.47
3:J:502:PRO:HB2	3:J:507:VAL:HG12	1.97	0.47
3:J:682:VAL:O	3:J:685:ILE:HG12	2.14	0.47
5:L:245:ALA:O	5:L:249:ILE:HG13	2.14	0.47
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.50	0.47
3:D:892:PHE:H	3:D:1281:GLU:HG2	1.80	0.47
3:D:1194:ARG:HD2	3:D:1194:ARG:N	2.30	0.47
2:I:6:THR:HG21	2:I:782:VAL:HG23	1.97	0.47
2:I:159:SER:O	2:I:160:ASP:HB2	2.15	0.47
2:I:367:TYR:CD2	2:I:376:PRO:HB3	2.50	0.47
2:I:397:LEU:HB3	2:I:401:GLY:HA3	1.96	0.47
2:I:629:PHE:CE2	2:I:634:VAL:HG11	2.49	0.47
5:L:381:GLU:HA	5:L:384:LEU:HG	1.95	0.47
2:C:61:SER:O	2:C:63:SER:N	2.47	0.47
2:C:156:PHE:CE2	2:C:158:ASP:HB2	2.50	0.47
5:F:409:ASN:O	5:F:413:MET:HG3	2.14	0.47
2:I:924:VAL:HG12	2:I:1058:ARG:HH22	1.78	0.47
2:I:1205:PRO:HG3	2:I:1210:ILE:HG23	1.96	0.47
4:K:53:GLU:HB3	4:K:59:ILE:HB	1.97	0.47
5:L:134:VAL:HG21	5:L:266:PHE:CE1	2.50	0.47
5:L:262:VAL:HG12	5:L:264:LYS:H	1.79	0.47
2:C:1142:ARG:O	2:C:1146:GLN:HB2	2.14	0.47
3:D:24:LEU:HD13	3:D:24:LEU:HA	1.80	0.47
3:D:368:LEU:HD23	3:D:369:PRO:HD2	1.96	0.47
3:D:384:LYS:HD2	3:D:387:LEU:HD23	1.97	0.47
3:D:770:LEU:HD12	3:D:770:LEU:HA	1.79	0.47
3:D:902:ASP:OD1	3:D:903:LEU:N	2.47	0.47
1:H:107:ILE:HG23	1:H:134:THR:O	2.15	0.47
2:I:9:LYS:HD3	2:I:1171:ARG:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:323:ALA:O	2:I:327:GLN:HG3	2.15	0.47
2:I:483:ASP:HB2	2:I:486:THR:HG21	1.96	0.47
2:I:1248:THR:HG21	5:L:531:PRO:CG	2.44	0.47
3:J:24:LEU:HB2	3:J:232:ASN:CG	2.35	0.47
3:J:1153:PRO:HA	3:J:1214:PRO:O	2.15	0.47
5:L:248:GLU:HA	5:L:251:LYS:HZ2	1.80	0.47
5:L:557:LYS:HG2	5:L:580:PHE:CZ	2.49	0.47
1:A:57:THR:HG21	1:A:147:GLN:NE2	2.28	0.47
1:A:104:LYS:HG2	1:A:110:VAL:HG22	1.96	0.47
2:C:382:GLU:O	2:C:386:GLU:HG2	2.15	0.47
2:C:592:ARG:O	2:C:652:TYR:HA	2.15	0.47
3:D:517:CYS:SG	3:D:518:VAL:N	2.88	0.47
4:E:60:ASN:HD21	4:E:63:ILE:HD13	1.80	0.47
1:H:98:VAL:HG11	1:H:121:VAL:HG22	1.97	0.47
3:J:416:ILE:HG21	3:J:441:LEU:HD23	1.96	0.47
3:J:518:VAL:N	3:J:716:GLN:HE22	2.12	0.47
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.79	0.47
2:C:271:ALA:O	2:C:275:ARG:N	2.31	0.47
2:C:1117:LEU:HD12	2:C:1195:ILE:HG12	1.97	0.47
3:D:133:ARG:HD2	3:D:133:ARG:HA	1.67	0.47
5:F:439:ILE:O	5:F:443:ILE:HG13	2.15	0.47
2:I:799:ASN:HA	2:I:1231:TYR:HA	1.97	0.47
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.97	0.47
3:J:808:VAL:O	3:J:810:THR:HG22	2.15	0.47
5:L:561:MET:HA	5:L:567:MET:HE1	1.97	0.47
1:B:125:LYS:HB3	1:B:128:HIS:HB2	1.97	0.46
2:C:468:LEU:O	2:C:471:VAL:HG12	2.15	0.46
2:C:553:THR:O	2:C:557:ARG:HD2	2.16	0.46
2:C:1099:ASN:ND2	3:D:505:ASP:OD2	2.47	0.46
3:D:322:ARG:HG3	3:D:323:PRO:HD2	1.97	0.46
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.97	0.46
2:I:623:LEU:HD12	2:I:627:GLY:HA2	1.96	0.46
3:J:482:ALA:HB3	4:K:20:VAL:HG22	1.96	0.46
1:A:191:ARG:NH1	1:A:197:ASP:HA	2.29	0.46
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.46	0.46
2:C:1331:ARG:HG2	3:D:33:TRP:CH2	2.50	0.46
5:F:135:ALA:HB1	5:F:253:SER:HA	1.97	0.46
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.50	0.46
2:C:617:ALA:HA	2:C:636:CYS:SG	2.56	0.46
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.51	0.46
2:C:833:ILE:HA	2:C:1054:LEU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1372:ARG:NE	3:J:854:ALA:HB2	2.29	0.46
5:F:562:ARG:NH2	5:F:573:LEU:HD22	2.30	0.46
2:I:20:GLN:HG2	2:I:1156:ARG:HH22	1.79	0.46
2:I:495:ALA:HB3	5:L:471:LEU:HD13	1.97	0.46
2:I:496:LYS:HB3	2:I:496:LYS:HE3	1.68	0.46
5:L:141:ILE:HG23	5:L:224:LEU:HD11	1.97	0.46
1:A:64:VAL:HG12	1:A:66:HIS:H	1.81	0.46
2:C:1247:SER:HB3	3:D:375:GLU:O	2.15	0.46
1:G:66:HIS:CE1	2:I:874:GLY:HA2	2.50	0.46
3:J:47:ARG:HD2	3:J:47:ARG:HA	1.43	0.46
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.97	0.46
1:B:67:GLU:N	1:B:67:GLU:OE1	2.48	0.46
2:C:741:MET:HG2	2:C:974:ARG:NH2	2.31	0.46
5:F:137:TYR:CD2	5:F:273:MET:HG2	2.50	0.46
1:G:152:TYR:CD1	2:I:824:GLN:HG2	2.49	0.46
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.97	0.46
2:I:465:ARG:O	2:I:469:VAL:HG13	2.15	0.46
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.97	0.46
3:J:527:LEU:HD23	3:J:532:GLU:HG2	1.98	0.46
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.16	0.46
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.80	0.46
2:C:499:SER:O	2:C:503:LYS:HB2	2.15	0.46
2:C:724:VAL:HG23	2:C:775:GLU:O	2.15	0.46
2:C:836:LEU:HD13	2:C:1054:LEU:HD22	1.96	0.46
3:D:694:SER:OG	3:D:738:ARG:NE	2.48	0.46
3:D:802:ASP:OD1	3:D:1348:LYS:NZ	2.39	0.46
3:D:1361:THR:HG22	4:E:21:LEU:HD13	1.97	0.46
5:F:348:GLU:HG2	5:F:354:THR:HA	1.97	0.46
2:I:1211:ARG:HE	2:I:1220:GLN:NE2	2.12	0.46
3:J:505:ASP:HB3	3:J:629:PHE:CE1	2.46	0.46
3:D:511:TYR:CG	3:D:728:SER:HB3	2.51	0.46
3:D:741:ALA:O	3:D:762:ASN:ND2	2.49	0.46
2:I:1035:LYS:O	2:I:1038:GLN:HG2	2.15	0.46
3:J:31:ARG:NH2	3:J:106:GLU:OE2	2.28	0.46
3:J:422:LEU:HB2	3:J:469:HIS:HB2	1.96	0.46
3:J:1347:LEU:HG	3:J:1357:ILE:HG23	1.97	0.46
1:A:155:ALA:HA	1:A:158:ARG:HG3	1.97	0.46
2:C:667:LEU:HD11	2:C:708:VAL:HG21	1.97	0.46
2:C:972:PHE:HD2	2:C:975:ILE:HD12	1.79	0.46
5:F:458:GLU:O	5:F:462:LYS:HG3	2.16	0.46
2:I:967:LEU:HB3	2:I:1021:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ILE:HG23	1:A:26:VAL:HG22	1.98	0.46
1:A:228:LEU:HA	1:A:231:PHE:HD2	1.80	0.46
2:C:50:GLU:HG2	2:C:73:TYR:HE1	1.81	0.46
2:C:726:TYR:CE2	2:C:728:ASP:HB2	2.50	0.46
2:C:744:GLY:C	2:C:746:ALA:H	2.19	0.46
2:C:1090:ASN:HB3	2:C:1092:THR:HG23	1.98	0.46
3:D:720:ASN:HD21	3:D:722:ILE:HG22	1.80	0.46
2:I:463:GLN:NE2	2:I:501:ALA:O	2.48	0.46
3:J:45:ASN:O	3:J:46:TYR:HB3	2.15	0.46
3:D:870:ASP:O	3:D:874:GLU:N	2.47	0.46
5:F:444:ALA:HB1	5:F:454:VAL:HG22	1.98	0.46
1:G:76:GLU:N	1:G:76:GLU:OE2	2.49	0.46
2:I:1117:LEU:HD21	2:I:1182:ILE:HG21	1.97	0.46
2:I:1296:ASP:OD2	3:J:345:LYS:HD2	2.16	0.46
1:B:197:ASP:O	1:B:198:LEU:HD13	2.16	0.45
2:C:1024:GLU:HA	2:C:1027:LYS:HD3	1.98	0.45
2:C:1184:THR:HG23	2:C:1190:ALA:H	1.80	0.45
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.51	0.45
1:G:218:ARG:HG3	1:H:231:PHE:O	2.16	0.45
1:H:48:LEU:CD2	3:J:535:ARG:HG3	2.47	0.45
1:H:109:PRO:HB3	1:H:132:HIS:CD2	2.51	0.45
2:I:499:SER:O	2:I:503:LYS:HB2	2.16	0.45
2:I:1283:ALA:HB1	2:I:1286:THR:HB	1.97	0.45
3:J:18:ASP:HB2	3:J:1373:ARG:HH21	1.81	0.45
3:J:357:VAL:HA	3:J:461:PHE:CE1	2.50	0.45
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.98	0.45
3:J:621:ALA:HA	3:J:624:ILE:HD12	1.98	0.45
2:C:819:SER:HB2	2:C:1085:MET:HG3	1.97	0.45
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.98	0.45
3:D:552:ILE:HG21	3:D:589:TYR:CE1	2.51	0.45
3:D:560:ASN:ND2	3:D:560:ASN:O	2.48	0.45
3:D:810:THR:HG21	3:D:892:PHE:O	2.15	0.45
2:I:582:ASN:HB3	2:I:586:PHE:H	1.82	0.45
5:L:135:ALA:HB1	5:L:253:SER:HA	1.98	0.45
1:A:41:ASN:HB2	1:A:185:TYR:OH	2.16	0.45
1:A:103:ASN:OD1	1:A:141:SER:HB2	2.17	0.45
1:B:75:GLN:HG3	1:B:76:GLU:OE1	2.16	0.45
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.97	0.45
3:D:707:ILE:HD12	3:D:714:GLU:O	2.16	0.45
2:I:411:ARG:HH22	2:I:424:ASP:HA	1.80	0.45
3:J:1257:VAL:HA	3:J:1260:MET:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1135:THR:HB	3:D:1136:GLY:H	1.36	0.45
3:D:1157:ALA:HB3	3:D:1208:ASP:H	1.80	0.45
2:I:519:ASN:O	2:I:521:LEU:N	2.49	0.45
2:I:811:ASN:ND2	2:I:1097:VAL:HG12	2.31	0.45
2:C:157:PHE:CZ	2:C:431:LYS:HG2	2.51	0.45
2:C:1268:GLN:HE22	3:D:352:ARG:NH1	2.15	0.45
3:D:425:ARG:HG2	3:D:426:ALA:H	1.80	0.45
5:F:279:ARG:NH2	5:F:350:GLU:OE2	2.33	0.45
2:I:5:TYR:HA	2:I:8:LYS:HD3	1.98	0.45
3:J:702:GLN:HG2	3:J:703:THR:N	2.31	0.45
2:I:359:ARG:NH1	2:I:382:GLU:OE2	2.49	0.45
2:I:801:ARG:HG2	2:I:1094:VAL:HG23	1.98	0.45
2:I:968:GLU:HG3	2:I:1018:TYR:CE1	2.51	0.45
3:J:279:LEU:O	3:J:283:LEU:HG	2.16	0.45
3:J:282:LEU:HD21	5:L:410:ILE:HG12	1.99	0.45
3:J:355:ILE:HG12	3:J:464:ASP:O	2.17	0.45
2:C:510:GLN:OE1	2:C:534:GLY:HA2	2.17	0.45
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.51	0.45
5:F:97:PRO:HA	5:F:100:MET:HG3	1.97	0.45
2:I:804:PHE:HE2	2:I:1115:THR:HG21	1.82	0.45
2:I:1240:ASP:HB3	3:J:445:LYS:HD2	1.97	0.45
3:J:902:ASP:OD1	3:J:903:LEU:N	2.50	0.45
3:J:1349:GLU:OE2	3:J:1349:GLU:N	2.41	0.45
1:A:13:LEU:HD13	1:A:16:ILE:HD11	1.99	0.45
1:B:228:LEU:HA	1:B:231:PHE:HD2	1.82	0.45
2:C:97:ARG:NH2	5:F:475:GLY:HA3	2.31	0.45
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.98	0.45
2:C:1042:LEU:HD13	2:C:1046:VAL:HG22	1.99	0.45
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.99	0.45
5:F:108:VAL:HG11	5:F:381:GLU:HB3	1.98	0.45
5:F:452:ILE:HD11	5:F:457:ILE:HG12	1.97	0.45
1:G:66:HIS:HE1	2:I:928:VAL:O	1.99	0.45
2:I:833:ILE:HA	2:I:1054:LEU:O	2.17	0.45
2:I:898:GLU:HB3	5:L:540:LEU:HD22	1.98	0.45
3:J:572:THR:OG1	3:J:573:THR:N	2.48	0.45
3:J:709:ARG:HA	3:J:709:ARG:HD2	1.83	0.45
5:L:573:LEU:HD23	5:L:573:LEU:H	1.82	0.45
2:C:699:LEU:HD23	2:C:699:LEU:HA	1.83	0.45
3:D:858:VAL:HG21	3:D:864:LEU:HD21	1.99	0.45
2:I:59:ILE:HG23	2:I:476:LYS:HE3	1.99	0.45
2:I:1043:ALA:HB1	2:I:1044:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:522:GLY:O	3:J:525:MET:HG2	2.17	0.45
3:J:596:LEU:HD12	3:J:601:ILE:HG13	1.97	0.45
3:J:930:LEU:HD11	3:J:1241:TYR:CE2	2.52	0.45
1:A:211:ILE:HA	1:A:211:ILE:HD13	1.71	0.45
2:C:903:ARG:HE	2:C:910:ALA:HB2	1.82	0.45
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.47	0.45
3:D:34:SER:HB2	3:D:104:HIS:HB3	1.99	0.45
5:F:137:TYR:O	5:F:141:ILE:HG12	2.17	0.45
1:G:124:VAL:HG21	1:G:209:GLY:C	2.37	0.45
3:J:146:VAL:HB	3:J:156:ARG:O	2.17	0.45
2:C:120:GLN:HG3	2:C:121:GLU:HG3	1.99	0.44
3:D:347:VAL:HG12	3:D:348:ASP:O	2.17	0.44
3:D:572:THR:OG1	3:D:573:THR:N	2.50	0.44
3:D:847:ASP:HB3	3:D:856:ILE:HG23	1.99	0.44
3:D:915:ILE:HA	3:D:918:ILE:HG23	1.98	0.44
5:F:391:ALA:HB3	5:F:405:ILE:HG22	1.97	0.44
2:I:115:LYS:HD3	2:I:116:ASP:N	2.31	0.44
2:I:488:MET:O	2:I:490:GLN:N	2.50	0.44
3:J:465:GLN:HB2	6:J:1501:ECJ:N27	2.32	0.44
3:J:1348:LYS:O	3:J:1352:ILE:HG12	2.17	0.44
1:B:205:MET:HE3	1:B:213:PRO:HB3	1.99	0.44
2:C:466:VAL:O	2:C:469:VAL:HG22	2.17	0.44
2:C:930:ASP:OD2	2:C:931:VAL:N	2.51	0.44
5:F:388:ILE:O	5:F:392:LYS:HG3	2.16	0.44
5:F:479:THR:HG22	5:F:482:GLU:HB2	1.99	0.44
1:G:231:PHE:HB3	1:H:218:ARG:HA	1.99	0.44
2:I:743:PRO:O	2:I:974:ARG:NH2	2.50	0.44
3:J:797:THR:O	3:J:801:VAL:HG13	2.17	0.44
5:L:556:ALA:HB1	5:L:560:ARG:HE	1.82	0.44
5:L:562:ARG:HH21	5:L:573:LEU:HD22	1.81	0.44
2:C:357:ASN:ND2	2:C:358:ASP:OD2	2.51	0.44
2:C:602:GLU:O	2:C:602:GLU:HG3	2.16	0.44
2:C:730:SER:O	2:C:753:LEU:HB2	2.18	0.44
3:D:853:THR:HG22	3:D:854:ALA:H	1.82	0.44
5:F:245:ALA:O	5:F:249:ILE:HG13	2.17	0.44
5:F:371:LYS:HA	5:F:374:ARG:HH12	1.80	0.44
3:J:363:LEU:HA	3:J:450:HIS:CD2	2.52	0.44
3:J:482:ALA:HA	4:K:6:VAL:HG11	1.98	0.44
3:D:349:TYR:CD1	3:D:472:LEU:HD11	2.52	0.44
3:D:507:VAL:HG21	3:D:598:LYS:HB2	2.00	0.44
4:E:39:VAL:HG21	4:E:56:GLU:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:274:ARG:NH2	5:F:369:GLU:OE2	2.50	0.44
2:I:158:ASP:HB3	2:I:173:ASN:OD1	2.17	0.44
2:I:213:LEU:HD13	2:I:422:LYS:HG2	1.99	0.44
2:I:1013:GLN:O	2:I:1017:GLN:HG2	2.18	0.44
3:J:1167:LYS:NZ	3:J:1170:LYS:HB2	2.32	0.44
1:A:76:GLU:OE2	1:A:76:GLU:N	2.50	0.44
1:B:152:TYR:HD1	1:B:176:CYS:HA	1.83	0.44
1:B:211:ILE:HD12	1:B:211:ILE:HA	1.87	0.44
2:C:496:LYS:HE3	2:C:496:LYS:HB3	1.63	0.44
2:C:1225:VAL:HA	3:D:638:SER:HB2	1.99	0.44
3:D:10:ALA:O	3:D:11:GLN:HB2	2.16	0.44
3:D:322:ARG:HB2	3:D:322:ARG:HH11	1.83	0.44
3:D:849:LEU:HD22	3:D:849:LEU:H	1.83	0.44
3:D:866:GLU:OE2	3:D:901:ARG:NH2	2.48	0.44
1:H:183:ILE:HG23	1:H:205:MET:HG3	1.99	0.44
2:I:541:GLU:OE1	2:I:541:GLU:N	2.43	0.44
3:J:24:LEU:HD13	3:J:24:LEU:HA	1.84	0.44
3:J:1168:GLU:HB3	3:J:1169:THR:H	1.61	0.44
4:K:4:VAL:HG22	4:K:5:THR:HG23	1.99	0.44
1:B:31:LEU:HB3	1:B:35:PHE:HB2	2.00	0.44
2:C:159:SER:O	2:C:160:ASP:HB2	2.18	0.44
2:C:486:THR:HG23	2:C:487:LEU:H	1.82	0.44
2:C:1288:GLN:HE21	3:D:1355:ARG:HA	1.82	0.44
3:D:131:PRO:O	3:D:135:ILE:HG13	2.18	0.44
3:D:1167:LYS:NZ	3:D:1170:LYS:HB2	2.33	0.44
3:D:1226:VAL:HG13	3:D:1261:LEU:HD22	2.00	0.44
1:G:227:GLN:HB3	1:H:39:LEU:HD11	1.99	0.44
2:I:1327:LEU:O	2:I:1331:ARG:HB2	2.16	0.44
3:J:478:LEU:HD21	4:K:47:THR:O	2.18	0.44
3:J:536:LEU:HB3	3:J:542:ALA:CB	2.48	0.44
3:J:598:LYS:O	3:J:601:ILE:HG22	2.18	0.44
3:J:1280:VAL:HA	3:J:1283:SER:HB3	1.99	0.44
5:L:261:LEU:HD12	5:L:261:LEU:H	1.83	0.44
5:L:572:THR:HG23	5:L:575:GLU:HB2	1.99	0.44
2:C:591:TYR:CE1	2:C:616:ILE:HG21	2.53	0.44
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.53	0.44
5:F:234:THR:O	5:F:245:ALA:HB2	2.18	0.44
1:G:12:ARG:HA	1:H:231:PHE:CE1	2.53	0.44
2:I:1142:ARG:O	2:I:1146:GLN:HB2	2.17	0.44
3:J:253:VAL:HG21	5:L:523:ILE:HG21	2.00	0.44
1:A:45:ARG:HH21	2:C:1216:ARG:HA	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:LEU:HD11	1:B:130:ILE:HD13	2.00	0.44
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.99	0.44
2:C:798:GLN:HB2	2:C:828:PHE:CE1	2.53	0.44
2:C:1326:LEU:HD11	3:D:331:ILE:HG23	1.98	0.44
3:D:814:CYS:H	3:D:895:CYS:CB	2.30	0.44
3:D:1329:THR:O	3:D:1333:THR:OG1	2.35	0.44
1:G:32:GLU:HB2	1:G:35:PHE:CD2	2.51	0.44
1:H:134:THR:OG1	1:H:135:ASP:N	2.48	0.44
2:I:761:GLN:HA	2:I:762:ASN:HA	1.53	0.44
3:J:420:PRO:O	3:J:471:PRO:HD2	2.17	0.44
3:J:702:GLN:HG2	3:J:703:THR:HB	1.99	0.44
5:L:316:PHE:CZ	5:L:334:SER:HA	2.51	0.44
3:D:27:PRO:HB3	3:D:241:VAL:HG23	2.00	0.44
3:D:801:VAL:O	3:D:805:GLN:HB2	2.17	0.44
1:G:76:GLU:OE1	1:G:132:HIS:N	2.51	0.44
1:G:83:LEU:HB3	2:I:694:ARG:HH21	1.83	0.44
1:G:228:LEU:HD22	1:H:221:ALA:HB1	2.00	0.44
2:I:816:ILE:O	2:I:1076:ILE:HD12	2.17	0.44
3:J:367:GLY:HA3	3:J:448:GLN:HB2	2.00	0.44
3:J:1356:LEU:HD23	3:J:1356:LEU:HA	1.77	0.44
1:A:168:ILE:H	1:A:168:ILE:HG12	1.64	0.43
2:C:873:ILE:HG13	2:C:944:ARG:NH2	2.29	0.43
3:D:140:TYR:O	3:D:297:ARG:NH1	2.51	0.43
3:D:1356:LEU:HD23	3:D:1356:LEU:HA	1.77	0.43
5:F:105:MET:HE3	5:F:385:ARG:HG2	2.00	0.43
5:F:402:LEU:HA	5:F:405:ILE:HG12	2.00	0.43
2:I:12:ARG:NH1	2:I:698:PRO:O	2.46	0.43
2:I:819:SER:HB2	2:I:1085:MET:HG3	1.99	0.43
3:J:903:LEU:HD21	3:J:909:ILE:HD12	2.00	0.43
2:C:796:LEU:HD12	2:C:796:LEU:H	1.82	0.43
2:C:798:GLN:HB2	2:C:828:PHE:HE1	1.83	0.43
2:C:1103:VAL:HG11	2:C:1112:ILE:HD11	1.98	0.43
3:D:359:PRO:HB3	3:D:629:PHE:CE2	2.53	0.43
3:D:1279:GLN:H	3:D:1279:GLN:HG2	1.52	0.43
1:G:13:LEU:H	1:G:13:LEU:HD23	1.83	0.43
2:I:11:ILE:HD13	2:I:11:ILE:HA	1.88	0.43
5:L:591:GLU:O	5:L:595:LEU:HG	2.18	0.43
2:C:27:LEU:O	2:C:528:ARG:NH1	2.50	0.43
2:C:37:LYS:HD3	2:C:37:LYS:HA	1.74	0.43
2:C:281:ASP:OD1	2:C:283:LYS:HE3	2.19	0.43
2:C:1103:VAL:HB	2:C:1104:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:140:TYR:OH	3:D:312:ARG:NH1	2.51	0.43
3:D:292:VAL:O	3:D:296:LYS:HG3	2.17	0.43
3:D:310:GLY:HA2	3:D:314:ARG:CD	2.46	0.43
5:F:143:TYR:HA	5:F:146:GLU:HB2	1.99	0.43
1:B:63:GLY:HA3	1:B:71:LYS:HE3	2.00	0.43
2:C:31:GLN:HG3	2:C:527:LYS:HB3	1.99	0.43
2:C:741:MET:HG2	2:C:974:ARG:HH22	1.82	0.43
3:D:363:LEU:HA	3:D:450:HIS:CD2	2.53	0.43
3:D:514:THR:HG21	3:D:596:LEU:HG	2.00	0.43
3:D:1163:VAL:HG23	3:D:1177:ILE:HG12	2.01	0.43
2:I:406:ASN:OD1	2:I:411:ARG:NH1	2.52	0.43
2:I:462:ASN:O	2:I:465:ARG:HB3	2.18	0.43
2:I:1104:PRO:O	2:I:1107:MET:HG2	2.18	0.43
2:I:1151:LEU:HD11	2:I:1198:LEU:HG	1.99	0.43
2:I:1326:LEU:HD11	3:J:331:ILE:HG23	2.01	0.43
3:J:317:THR:HG22	3:J:322:ARG:O	2.18	0.43
2:C:799:ASN:ND2	2:C:799:ASN:H	2.16	0.43
3:D:245:LEU:HD12	3:D:246:PRO:HD2	2.00	0.43
3:D:746:LEU:HD22	3:D:754:ILE:HD11	2.00	0.43
3:D:1355:ARG:HH12	3:D:1369:ARG:HH22	1.66	0.43
5:F:316:PHE:O	5:F:320:ILE:HG13	2.17	0.43
1:G:41:ASN:HD22	1:H:41:ASN:HD22	1.65	0.43
1:G:195:ARG:HD2	1:G:195:ARG:HA	1.80	0.43
2:I:1148:ALA:O	2:I:1151:LEU:HB2	2.18	0.43
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.65	0.43
2:I:1314:GLN:HG2	4:K:28:ARG:CZ	2.49	0.43
3:J:94:GLN:O	3:J:97:VAL:HG23	2.18	0.43
4:K:60:ASN:OD1	4:K:62:GLN:HB3	2.17	0.43
5:L:99:ARG:HD3	5:L:99:ARG:HA	1.88	0.43
1:B:134:THR:OG1	1:B:135:ASP:N	2.48	0.43
2:C:1176:LEU:HD13	2:C:1180:MET:HG3	1.99	0.43
3:D:215:LYS:HB3	3:D:215:LYS:HE2	1.69	0.43
3:D:282:LEU:HD21	5:F:410:ILE:HG12	1.99	0.43
3:D:596:LEU:HD11	3:D:604:MET:CE	2.48	0.43
3:D:1257:VAL:HA	3:D:1260:MET:HG3	2.00	0.43
4:E:25:ARG:NH2	4:E:65:ASP:OD1	2.45	0.43
5:F:555:GLU:HA	5:F:558:VAL:HG12	1.99	0.43
5:F:593:LYS:HD2	5:F:596:ARG:HD3	2.01	0.43
1:G:195:ARG:HH21	1:G:198:LEU:HD21	1.83	0.43
2:I:621:SER:O	2:I:623:LEU:HD23	2.19	0.43
2:I:1090:ASN:HB3	2:I:1092:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1276:TRP:CE2	3:J:801:VAL:HG21	2.54	0.43
3:J:57:PHE:CZ	3:J:252:LEU:HB2	2.54	0.43
3:J:516:ASP:OD1	3:J:516:ASP:N	2.52	0.43
1:A:91:ARG:HD2	1:A:210:THR:HA	2.00	0.43
2:C:125:GLY:HA2	2:C:499:SER:HB2	2.01	0.43
2:C:235:ASN:OD1	2:C:236:LYS:HG2	2.18	0.43
3:D:233:LYS:HB3	3:D:235:GLU:OE2	2.19	0.43
3:D:853:THR:O	3:D:854:ALA:HB3	2.19	0.43
4:E:50:ALA:O	4:E:54:ILE:HG12	2.19	0.43
5:F:399:LEU:HD12	5:F:399:LEU:HA	1.88	0.43
2:I:699:LEU:HD23	2:I:699:LEU:HA	1.82	0.43
5:L:513:ASP:C	5:L:515:GLU:H	2.20	0.43
1:A:14:VAL:HG22	1:A:15:ASP:N	2.34	0.43
2:C:516:ASP:OD1	2:C:516:ASP:N	2.50	0.43
2:C:538:LEU:H	2:C:538:LEU:HG	1.61	0.43
2:C:1304:MET:HE2	2:C:1315:MET:HB3	2.00	0.43
3:D:304:ASP:OD2	3:D:312:ARG:NH2	2.51	0.43
3:D:491:LEU:HD11	3:D:609:TYR:CE1	2.53	0.43
2:I:38:PHE:HB2	2:I:457:GLY:HA2	2.01	0.43
2:I:601:ASP:OD1	2:I:601:ASP:N	2.52	0.43
3:J:646:ILE:HD11	3:J:764:ARG:HD2	2.01	0.43
3:J:706:VAL:HG13	3:J:715:LYS:HB3	2.00	0.43
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.18	0.43
1:A:179:PRO:HA	1:A:208:ASN:ND2	2.33	0.43
4:E:15:ASN:O	4:E:16:ARG:HB3	2.18	0.43
5:F:394:TYR:CE2	5:F:436:ARG:HG3	2.54	0.43
1:G:124:VAL:HG13	1:G:125:LYS:HG3	2.01	0.43
2:I:661:VAL:HB	2:I:665:ALA:HB3	2.01	0.43
2:I:1024:GLU:HG2	2:I:1028:LYS:HD3	2.01	0.43
2:C:672:GLU:HG2	2:C:1187:PHE:HA	2.01	0.43
3:D:1353:VAL:HG13	3:D:1355:ARG:HG2	2.00	0.43
5:F:269:LEU:O	5:F:273:MET:HG3	2.19	0.43
2:I:930:ASP:OD2	2:I:931:VAL:N	2.52	0.43
3:J:1344:LEU:O	3:J:1346:GLY:N	2.48	0.43
1:B:48:LEU:HA	1:B:180:VAL:HG21	2.01	0.42
1:B:98:VAL:HG12	1:B:146:VAL:HG22	2.01	0.42
2:C:5:TYR:O	2:C:8:LYS:HG2	2.19	0.42
3:D:557:LYS:HE3	3:D:557:LYS:HB2	1.79	0.42
1:G:11:PRO:HB3	1:G:30:PRO:O	2.19	0.42
2:I:94:ALA:HB2	2:I:129:LEU:HD11	2.01	0.42
2:I:231:GLU:HG2	2:I:332:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1032:LYS:O	2:I:1036:ILE:HG13	2.18	0.42
3:J:576:ARG:H	3:J:576:ARG:HG3	1.64	0.42
2:C:123:TYR:H	5:F:472:GLN:HG2	1.84	0.42
2:C:246:LEU:HB2	2:C:269:ILE:HG21	2.01	0.42
2:C:367:TYR:CD2	2:C:376:PRO:HB3	2.54	0.42
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.19	0.42
3:D:362:ARG:H	3:D:365:GLN:NE2	2.15	0.42
3:D:1198:VAL:HB	3:D:1210:ILE:HA	2.01	0.42
5:F:562:ARG:NE	5:F:573:LEU:HB3	2.34	0.42
1:H:76:GLU:N	1:H:76:GLU:OE1	2.52	0.42
2:I:559:CYS:CB	2:I:662:SER:HB3	2.48	0.42
2:I:1314:GLN:HG2	4:K:28:ARG:NE	2.34	0.42
3:J:339:ARG:HB3	3:J:340:GLN:H	1.60	0.42
3:J:507:VAL:HG21	3:J:598:LYS:HB2	2.01	0.42
5:L:354:THR:O	5:L:358:VAL:HG23	2.20	0.42
1:A:152:TYR:CG	2:C:824:GLN:HG2	2.55	0.42
2:C:732:ILE:HD11	2:C:769:PRO:HB3	2.01	0.42
2:C:1294:LYS:HB3	3:D:347:VAL:HG13	2.01	0.42
3:D:94:GLN:O	3:D:97:VAL:HG23	2.20	0.42
3:D:930:LEU:HD11	3:D:1241:TYR:CE2	2.54	0.42
5:F:306:PHE:HD1	5:F:306:PHE:HA	1.73	0.42
5:F:484:ALA:HB1	5:F:491:GLU:CB	2.50	0.42
5:F:557:LYS:O	5:F:561:MET:HB2	2.19	0.42
1:H:27:THR:HG22	1:H:202:VAL:HG22	2.00	0.42
2:I:339:ASN:HB3	2:I:343:HIS:H	1.83	0.42
2:I:486:THR:HG23	2:I:487:LEU:H	1.84	0.42
2:I:642:SER:OG	3:J:770:LEU:HD21	2.19	0.42
2:I:975:ILE:O	2:I:979:LEU:HB2	2.19	0.42
2:I:1127:LYS:O	2:I:1131:MET:HG3	2.19	0.42
3:J:537:TYR:HE2	3:J:631:TYR:HE1	1.68	0.42
3:J:800:LEU:HB3	3:J:920:ALA:CB	2.49	0.42
1:A:79:LEU:O	1:A:83:LEU:HD13	2.19	0.42
1:A:166:ARG:O	1:A:167:PRO:C	2.57	0.42
2:C:136:PHE:CE2	2:C:456:VAL:HG11	2.54	0.42
2:C:1073:LYS:HB2	3:D:462:ASP:HB2	2.01	0.42
3:D:598:LYS:HA	3:D:601:ILE:HG22	2.01	0.42
1:G:66:HIS:NE2	2:I:929:ILE:HA	2.35	0.42
2:I:229:ILE:HB	2:I:240:GLU:HB2	2.01	0.42
2:I:387:ASN:O	2:I:394:ARG:HB2	2.19	0.42
2:I:483:ASP:HB2	2:I:486:THR:CG2	2.50	0.42
2:I:735:LYS:HA	2:I:748:ILE:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1142:ARG:NH1	2:I:1169:VAL:HG21	2.34	0.42
3:J:62:PHE:CD1	3:J:247:PRO:HD3	2.54	0.42
3:J:514:THR:HG21	3:J:596:LEU:HG	2.00	0.42
3:J:515:ARG:HH21	3:J:717:VAL:HB	1.83	0.42
3:J:925:GLU:HB3	3:J:926:PRO:HD3	2.00	0.42
3:J:1217:PRO:HG3	3:J:1232:TYR:HE2	1.84	0.42
1:A:64:VAL:HG13	1:A:69:SER:HB2	2.01	0.42
1:B:125:LYS:CB	1:B:128:HIS:HB2	2.49	0.42
2:C:49:LEU:HD23	2:C:49:LEU:HA	1.83	0.42
3:D:810:THR:CG2	3:D:893:GLY:HA3	2.50	0.42
3:D:1295:ASN:OD1	3:J:1206:ARG:NH2	2.53	0.42
1:H:49:SER:O	1:H:151:GLY:HA2	2.19	0.42
2:I:13:LYS:HD3	2:I:1149:TYR:HA	2.01	0.42
2:I:555:TYR:OH	2:I:618:GLN:NE2	2.44	0.42
2:I:1247:SER:HB3	3:J:375:GLU:O	2.20	0.42
3:J:740:LEU:O	3:J:764:ARG:HB2	2.19	0.42
5:L:118:ASP:O	5:L:122:ARG:HG3	2.20	0.42
5:L:343:LYS:H	5:L:343:LYS:HD2	1.85	0.42
2:C:124:MET:HB3	2:C:493:ILE:CD1	2.47	0.42
2:C:615:VAL:HG13	2:C:651:ASP:H	1.85	0.42
2:C:852:ALA:HB2	2:C:869:GLY:HA2	2.01	0.42
3:D:530:PRO:HB2	3:D:581:MET:HG2	2.02	0.42
3:D:793:SER:O	3:D:797:THR:HG23	2.20	0.42
1:G:135:ASP:OD1	1:G:136:GLU:N	2.52	0.42
2:I:32:LEU:HD23	2:I:130:MET:SD	2.59	0.42
2:I:131:THR:HG22	2:I:132:ASP:H	1.84	0.42
2:I:1285:TYR:CZ	3:J:1356:LEU:HD11	2.53	0.42
3:J:794:GLY:O	3:J:798:ARG:HB2	2.20	0.42
2:C:371:ARG:HB3	2:C:374:GLU:OE2	2.19	0.42
2:C:556:GLY:HA2	2:C:659:GLN:O	2.18	0.42
2:C:629:PHE:CE2	2:C:634:VAL:HG11	2.55	0.42
2:C:637:ARG:HA	2:C:642:SER:HA	2.02	0.42
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.54	0.42
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	2.02	0.42
3:D:62:PHE:CD1	3:D:247:PRO:HD3	2.55	0.42
3:D:615:LYS:HB2	3:D:616:PRO:HD3	2.01	0.42
3:D:810:THR:HG22	3:D:893:GLY:HA3	2.01	0.42
3:D:861:ASN:OD1	3:D:861:ASN:N	2.51	0.42
3:D:863:LEU:HD21	3:D:901:ARG:HB3	2.01	0.42
1:G:85:LEU:HD21	1:G:130:ILE:HG23	2.01	0.42
1:G:166:ARG:N	1:G:167:PRO:HD2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:56:VAL:HG22	1:H:146:VAL:HG12	2.02	0.42
2:I:936:ARG:HH12	5:L:495:ARG:HD3	1.84	0.42
2:I:1256:GLN:HB3	2:I:1301:ARG:NH2	2.27	0.42
2:I:1323:PHE:CE1	3:J:1353:VAL:HG23	2.55	0.42
3:J:1251:LYS:O	3:J:1255:VAL:HG12	2.20	0.42
1:A:11:PRO:HB3	1:A:31:LEU:HG	2.02	0.42
2:C:906:PHE:HZ	5:F:604:SER:HB3	1.85	0.42
3:D:531:LYS:HG2	3:D:581:MET:HE1	2.01	0.42
3:D:903:LEU:HD21	3:D:909:ILE:HD12	2.00	0.42
3:D:1282:TYR:O	3:D:1285:VAL:HG12	2.20	0.42
5:F:309:ASN:HB3	5:F:310:GLU:H	1.71	0.42
5:F:309:ASN:HD21	5:F:312:SER:HB3	1.85	0.42
1:G:51:MET:HE1	1:G:216:ALA:HB1	2.02	0.42
2:I:303:ASP:OD2	2:I:328:SER:HB2	2.19	0.42
2:I:518:ASN:ND2	2:I:691:PRO:HG2	2.35	0.42
2:I:1106:ARG:CZ	3:J:731:ARG:HH21	2.33	0.42
3:J:138:VAL:HG21	3:J:145:VAL:HB	2.01	0.42
3:J:213:LYS:O	3:J:217:LEU:HB2	2.20	0.42
3:J:733:SER:O	3:J:736:GLN:N	2.53	0.42
3:J:1174:ARG:HG2	3:J:1189:MET:SD	2.60	0.42
2:C:360:LEU:HA	2:C:363:LEU:HD12	2.01	0.42
3:D:209:ASN:HA	3:D:214:ARG:HE	1.85	0.42
3:D:395:LYS:NZ	5:F:612:ASP:OD2	2.43	0.42
3:D:665:GLN:HG3	3:D:669:GLN:HE21	1.83	0.42
5:F:575:GLU:OE2	5:F:578:LYS:NZ	2.53	0.42
2:I:168:GLY:C	2:I:170:VAL:H	2.17	0.42
2:I:1128:ILE:HG12	2:I:1145:ILE:HD11	2.02	0.42
2:I:1272:GLU:HB2	3:J:342:LEU:O	2.19	0.42
1:A:77:ASP:OD2	2:C:755:LYS:NZ	2.30	0.42
1:B:179:PRO:HA	1:B:208:ASN:ND2	2.35	0.42
2:C:300:ASP:OD1	2:C:313:ALA:N	2.53	0.42
2:C:1285:TYR:CZ	3:D:1356:LEU:HD11	2.55	0.42
3:D:647:PRO:HG3	3:D:697:MET:CA	2.49	0.42
5:F:105:MET:HE2	5:F:105:MET:HB2	1.86	0.42
2:I:1117:LEU:HD12	2:I:1195:ILE:HG12	2.01	0.42
3:J:382:TYR:CE1	3:J:398:LYS:HA	2.55	0.42
2:C:245:ARG:HG2	2:C:337:PHE:CE2	2.55	0.41
5:F:528:LEU:HD23	5:F:528:LEU:HA	1.90	0.41
2:I:802:VAL:HA	2:I:1096:ILE:O	2.20	0.41
2:I:857:VAL:HG21	2:I:862:LEU:HD21	2.00	0.41
3:J:71:LEU:HB3	3:J:88:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:615:LYS:HE2	3:J:616:PRO:HD3	2.01	0.41
3:J:1221:LEU:HG	3:J:1229:VAL:HG11	2.02	0.41
1:A:43:LEU:HD23	1:A:43:LEU:HA	1.93	0.41
2:C:242:VAL:HB	2:C:245:ARG:HD2	2.00	0.41
3:D:1151:LYS:O	3:D:1153:PRO:HD3	2.20	0.41
1:H:185:TYR:HB2	1:H:201:LEU:HD11	2.02	0.41
3:J:70:CYS:SG	3:J:71:LEU:N	2.93	0.41
3:J:113:HIS:CE1	3:J:115:TRP:HB2	2.55	0.41
3:J:131:PRO:O	3:J:135:ILE:HG13	2.20	0.41
3:J:615:LYS:HB2	3:J:616:PRO:HD3	2.03	0.41
5:L:448:ARG:HE	5:L:448:ARG:HB3	1.52	0.41
1:A:12:ARG:H	1:A:30:PRO:CD	2.33	0.41
1:A:166:ARG:N	1:A:167:PRO:HD2	2.34	0.41
1:B:64:VAL:HG11	1:B:69:SER:HB2	2.03	0.41
1:B:182:ARG:HD2	3:D:581:MET:HE1	2.02	0.41
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.39	0.41
2:C:202:ARG:H	2:C:202:ARG:HG3	1.59	0.41
2:C:724:VAL:HA	2:C:734:ILE:HD13	2.01	0.41
2:C:842:ASP:N	2:C:1045:GLY:O	2.52	0.41
3:D:504:GLN:HG3	3:D:505:ASP:H	1.85	0.41
5:F:150:ARG:HE	5:F:150:ARG:HB3	1.68	0.41
5:F:555:GLU:O	5:F:559:LEU:HB2	2.19	0.41
1:G:51:MET:HE3	1:G:51:MET:HB3	1.82	0.41
1:H:41:ASN:O	1:H:45:ARG:HG3	2.20	0.41
2:I:528:ARG:NH2	2:I:576:SER:O	2.53	0.41
2:I:587:LEU:HD23	2:I:587:LEU:HA	1.91	0.41
3:J:250:ARG:HB3	3:J:265:LEU:HD12	2.02	0.41
3:J:500:ILE:O	3:J:500:ILE:HG22	2.21	0.41
3:J:1215:GLU:HG3	3:J:1220:ILE:HD11	2.02	0.41
3:J:1278:GLU:CD	3:J:1279:GLN:H	2.23	0.41
1:A:48:LEU:HA	1:A:180:VAL:HG21	2.02	0.41
2:C:28:LEU:HD22	2:C:527:LYS:HD2	2.02	0.41
2:C:120:GLN:HE21	2:C:120:GLN:HB2	1.54	0.41
2:C:215:TYR:HE2	2:C:426:ILE:HD11	1.85	0.41
2:C:1275:VAL:HG13	2:C:1287:LEU:CD1	2.50	0.41
3:D:248:ASP:O	3:D:251:PRO:HG3	2.20	0.41
3:D:796:LEU:HG	3:D:800:LEU:HD13	2.03	0.41
3:D:884:SER:OG	3:D:1254:GLU:OE1	2.25	0.41
2:I:237:LEU:HD13	2:I:237:LEU:HA	1.78	0.41
2:I:933:VAL:HG22	2:I:1050:VAL:HG22	2.02	0.41
3:J:860:ARG:HB3	3:J:861:ASN:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:908:ILE:HG12	3:J:909:ILE:N	2.35	0.41
3:J:1344:LEU:CD2	3:J:1355:ARG:HD2	2.51	0.41
5:L:559:LEU:HD12	5:L:559:LEU:HA	1.87	0.41
2:C:208:ILE:HG23	2:C:362:ALA:HB1	2.03	0.41
2:C:960:LEU:HD11	2:C:1028:LYS:HE2	2.02	0.41
2:C:1106:ARG:CZ	3:D:731:ARG:HH21	2.34	0.41
3:D:522:GLY:O	3:D:525:MET:HG2	2.21	0.41
3:D:638:SER:OG	3:D:639:VAL:N	2.50	0.41
3:D:853:THR:C	3:D:855:ASP:H	2.23	0.41
4:E:29:GLN:O	4:E:35:LYS:N	2.54	0.41
1:G:29:GLU:OE1	1:G:200:LYS:HE2	2.20	0.41
1:G:107:ILE:HG23	1:G:134:THR:O	2.20	0.41
2:I:35:PHE:CD2	2:I:130:MET:HB3	2.55	0.41
3:J:442:ILE:HD13	3:J:442:ILE:HA	1.76	0.41
5:L:409:ASN:O	5:L:413:MET:HG3	2.21	0.41
1:A:102:LEU:O	1:A:141:SER:HA	2.21	0.41
1:A:156:SER:CB	2:C:1059:ARG:HH22	2.33	0.41
2:C:688:GLN:OE1	2:C:1237:HIS:HE1	2.03	0.41
3:D:507:VAL:HG22	3:D:730:ALA:HB2	2.03	0.41
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.35	0.41
3:D:1262:ARG:HD2	3:D:1279:GLN:OE1	2.20	0.41
5:F:599:ARG:HE	5:F:599:ARG:HB2	1.40	0.41
2:I:387:ASN:HA	2:I:391:SER:HB2	2.03	0.41
2:I:550:VAL:HG11	3:J:776:THR:HG22	2.03	0.41
3:J:1205:GLU:O	3:J:1208:ASP:HB2	2.20	0.41
5:L:412:LEU:HB2	5:L:435:ILE:HD11	2.03	0.41
2:C:230:PHE:CE1	2:C:239:MET:HB2	2.55	0.41
2:C:818:VAL:HB	2:C:1076:ILE:HD13	2.02	0.41
3:D:429:LEU:HD13	3:D:429:LEU:HA	1.80	0.41
3:D:526:VAL:HA	3:D:549:LYS:O	2.21	0.41
5:F:568:ASN:O	5:F:569:THR:HG22	2.20	0.41
1:G:188:GLU:OE2	1:G:200:LYS:HD2	2.21	0.41
2:I:373:GLY:O	5:L:99:ARG:HD2	2.20	0.41
2:I:700:VAL:HB	2:I:1069:ARG:HH22	1.85	0.41
3:J:638:SER:OG	3:J:639:VAL:N	2.53	0.41
3:J:1155:ILE:O	3:J:1210:ILE:HB	2.21	0.41
1:B:7:GLU:H	1:B:7:GLU:CD	2.24	0.41
2:C:657:THR:OG1	2:C:1187:PHE:HB2	2.20	0.41
2:C:870:ILE:HG21	2:C:931:VAL:HG11	2.01	0.41
3:D:42:GLU:HG3	5:F:451:ARG:HE	1.86	0.41
3:D:412:LEU:O	3:D:416:ILE:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:324:LYS:HG3	5:F:326:TRP:CZ2	2.56	0.41
2:I:1230:MET:HG2	2:I:1232:MET:HG3	2.03	0.41
3:J:245:LEU:HD12	3:J:246:PRO:HD2	2.03	0.41
3:J:1343:GLU:HB3	3:J:1345:ARG:HG3	2.02	0.41
1:A:64:VAL:HG11	1:A:78:ILE:HG21	2.02	0.41
1:A:195:ARG:HD2	1:A:195:ARG:HA	1.79	0.41
1:A:228:LEU:O	1:A:232:VAL:HG23	2.20	0.41
1:B:89:ALA:HB3	1:B:124:VAL:HB	2.03	0.41
2:C:321:LEU:HD23	2:C:321:LEU:HA	1.88	0.41
2:C:634:VAL:HG13	2:C:636:CYS:SG	2.61	0.41
2:C:949:GLU:HG2	2:C:1036:ILE:HG22	2.02	0.41
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	2.03	0.41
2:C:1217:THR:OG1	2:C:1219:GLU:HG2	2.20	0.41
3:D:165:TYR:CE2	3:D:178:ALA:HB3	2.56	0.41
3:D:339:ARG:HA	3:D:1324:SER:O	2.21	0.41
3:D:516:ASP:OD1	3:D:516:ASP:N	2.53	0.41
3:D:591:ILE:HD12	3:D:591:ILE:HA	1.94	0.41
5:F:119:ILE:HG21	5:F:379:MET:HB2	2.03	0.41
5:F:147:GLN:O	5:F:151:VAL:HG23	2.21	0.41
1:G:143:ARG:HH11	1:G:143:ARG:HB2	1.85	0.41
2:I:149:LEU:HD12	2:I:452:ARG:O	2.21	0.41
2:I:516:ASP:OD2	2:I:516:ASP:N	2.53	0.41
2:I:528:ARG:HD3	2:I:663:VAL:HG21	2.02	0.41
2:I:764:CYS:SG	2:I:765:ILE:N	2.94	0.41
2:I:974:ARG:HB3	2:I:1014:LEU:HD21	2.02	0.41
3:J:41:PRO:CB	3:J:270:ARG:HG3	2.51	0.41
3:J:60:ARG:HA	3:J:89:GLY:O	2.21	0.41
3:J:322:ARG:NH1	3:J:322:ARG:HB2	2.36	0.41
3:J:585:LYS:HD3	3:J:585:LYS:HA	1.86	0.41
3:J:599:LYS:HA	3:J:599:LYS:HD3	1.63	0.41
3:J:611:ILE:HG22	3:J:612:LEU:HD12	2.03	0.41
3:J:708:ASN:HB3	3:J:712:GLN:O	2.21	0.41
3:J:1199:PHE:HB2	3:J:1202:GLU:HB3	2.02	0.41
5:L:137:TYR:CE2	5:L:139:GLU:HB2	2.56	0.41
2:C:685:MET:HE3	2:C:685:MET:HB2	1.84	0.41
2:C:700:VAL:HB	2:C:1069:ARG:HH22	1.86	0.41
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	2.03	0.41
2:C:1114:GLU:OE1	2:C:1230:MET:HA	2.21	0.41
3:D:318:GLY:C	3:D:320:ASN:H	2.24	0.41
3:D:505:ASP:HB3	3:D:629:PHE:HE1	1.86	0.41
3:D:518:VAL:O	3:D:547:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:520:ALA:HB1	3:D:543:SER:HB3	2.03	0.41
2:I:142:GLU:HB2	2:I:760:ASN:ND2	2.32	0.41
2:I:202:ARG:HD3	2:I:369:MET:HG2	2.03	0.41
2:I:816:ILE:HB	2:I:1076:ILE:HA	2.03	0.41
2:I:1111:GLN:HB2	2:I:1230:MET:CE	2.51	0.41
3:J:148:GLU:HG2	3:J:156:ARG:HE	1.86	0.41
3:J:614:LEU:HB3	3:J:615:LYS:HZ3	1.86	0.41
5:L:600:HIS:CG	5:L:601:PRO:HD2	2.56	0.41
1:B:76:GLU:OE1	1:B:76:GLU:N	2.54	0.40
3:D:349:TYR:HE2	3:D:379:PRO:HG2	1.86	0.40
3:D:1221:LEU:HD21	3:D:1304:ARG:HB2	2.03	0.40
1:G:12:ARG:HG3	1:H:230:ALA:HB1	2.02	0.40
1:H:211:ILE:HD12	1:H:211:ILE:HA	1.94	0.40
2:I:185:ASP:HB2	2:I:197:ARG:HG3	2.04	0.40
2:I:953:LEU:HD11	2:I:1033:ARG:HG3	2.01	0.40
3:J:133:ARG:HA	3:J:133:ARG:HD2	1.88	0.40
3:J:1155:ILE:H	3:J:1155:ILE:HG13	1.51	0.40
1:B:91:ARG:HG3	1:B:122:GLU:HB3	2.02	0.40
2:C:75:LEU:HD13	2:C:75:LEU:HA	1.91	0.40
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.50	0.40
2:C:1308:ILE:HG21	3:D:379:PRO:HB2	2.03	0.40
3:D:357:VAL:HG22	3:D:461:PHE:CD1	2.56	0.40
3:D:814:CYS:HB3	3:D:890:THR:OG1	2.21	0.40
5:F:585:GLU:HA	5:F:588:ARG:HG3	2.04	0.40
1:G:108:GLY:O	1:G:133:LEU:HB2	2.20	0.40
1:G:135:ASP:HB2	2:I:726:TYR:CE1	2.54	0.40
2:I:68:LEU:HD11	2:I:100:LEU:HB3	2.03	0.40
2:I:559:CYS:SG	2:I:662:SER:HB3	2.61	0.40
2:I:840:SER:HB2	2:I:850:ILE:HD11	2.03	0.40
2:I:1103:VAL:HG11	2:I:1112:ILE:HD11	2.02	0.40
3:J:322:ARG:HG3	3:J:323:PRO:HD2	2.03	0.40
3:J:491:LEU:HB2	3:J:904:ALA:HA	2.02	0.40
3:J:861:ASN:OD1	3:J:861:ASN:N	2.55	0.40
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.56	0.40
5:L:458:GLU:O	5:L:462:LYS:HG3	2.21	0.40
5:L:568:ASN:O	5:L:569:THR:HG22	2.21	0.40
2:C:119:GLU:CG	2:C:488:MET:HB3	2.51	0.40
3:D:197:GLU:O	3:D:201:LEU:HG	2.22	0.40
3:D:1221:LEU:HD13	3:D:1222:ARG:N	2.36	0.40
5:F:558:VAL:HG21	5:F:587:ILE:HG12	2.02	0.40
1:G:18:GLN:HG3	1:G:23:HIS:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:538:LEU:H	2:I:538:LEU:HG	1.57	0.40
2:I:1139:ALA:O	2:I:1143:GLU:HB2	2.21	0.40
2:I:1160:ASP:HB2	2:I:1163:THR:OG1	2.22	0.40
2:I:1192:GLU:OE2	3:J:764:ARG:HD3	2.21	0.40
2:I:1334:GLY:H	3:J:113:HIS:HE2	1.68	0.40
5:L:452:ILE:HD11	5:L:457:ILE:HG12	2.03	0.40
2:C:147:SER:HB3	2:C:454:ARG:O	2.22	0.40
2:C:590:PRO:HG3	2:C:605:TYR:CE1	2.57	0.40
2:C:882:ILE:H	2:C:882:ILE:HD12	1.85	0.40
2:C:1303:LYS:HA	2:C:1303:LYS:HD3	1.95	0.40
2:C:1327:LEU:HD23	2:C:1331:ARG:HH21	1.86	0.40
4:E:21:LEU:HD12	4:E:21:LEU:HA	1.82	0.40
2:I:452:ARG:NH1	2:I:585:GLY:HA3	2.37	0.40
2:I:452:ARG:HG2	2:I:453:ILE:N	2.37	0.40
2:I:809:GLY:O	3:J:357:VAL:HG11	2.21	0.40
3:J:123:ARG:HA	3:J:123:ARG:HD3	1.93	0.40
3:J:504:GLN:HG3	3:J:505:ASP:H	1.86	0.40
3:J:847:ASP:HB3	3:J:856:ILE:HG21	2.04	0.40
3:J:1261:LEU:H	3:J:1261:LEU:HG	1.67	0.40
5:L:603:ARG:H	5:L:603:ARG:HG2	1.66	0.40
1:B:57:THR:HG21	1:B:147:GLN:OE1	2.21	0.40
2:C:88:ARG:HB2	2:C:88:ARG:NH1	2.37	0.40
2:C:158:ASP:HB3	2:C:173:ASN:OD1	2.22	0.40
3:D:9:LYS:NZ	3:D:11:GLN:HA	2.37	0.40
3:D:259:ARG:HD3	5:F:502:LYS:HD2	2.02	0.40
3:D:357:VAL:HB	3:D:358:GLY:H	1.67	0.40
3:D:803:VAL:HG22	3:D:1259:GLN:HB3	2.04	0.40
1:G:167:PRO:HB2	1:G:170:ARG:HB2	2.02	0.40
1:H:79:LEU:HD23	1:H:79:LEU:H	1.86	0.40
2:I:175:ARG:HG3	2:I:185:ASP:OD1	2.22	0.40
2:I:675:ASP:OD2	2:I:677:ASN:HB2	2.22	0.40
3:J:318:GLY:C	3:J:320:ASN:H	2.25	0.40
5:L:512:GLY:C	5:L:514:ASP:H	2.23	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:219:GLU:OE1	5:L:232:ARG:NH2[1_565]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	226/329 (69%)	202 (89%)	16 (7%)	8 (4%)	3	24
1	B	213/329 (65%)	195 (92%)	16 (8%)	2 (1%)	14	48
1	G	222/329 (68%)	196 (88%)	20 (9%)	6 (3%)	4	28
1	H	213/329 (65%)	194 (91%)	17 (8%)	2 (1%)	14	48
2	C	1338/1342 (100%)	1203 (90%)	114 (8%)	21 (2%)	8	38
2	I	1338/1342 (100%)	1203 (90%)	112 (8%)	23 (2%)	7	37
3	D	1157/1407 (82%)	1038 (90%)	101 (9%)	18 (2%)	8	38
3	J	1151/1407 (82%)	1036 (90%)	100 (9%)	15 (1%)	10	41
4	E	87/91 (96%)	81 (93%)	4 (5%)	2 (2%)	5	31
4	K	77/91 (85%)	72 (94%)	4 (5%)	1 (1%)	10	41
5	F	461/613 (75%)	432 (94%)	25 (5%)	4 (1%)	14	48
5	L	463/613 (76%)	426 (92%)	33 (7%)	4 (1%)	14	48
All	All	6946/8222 (84%)	6278 (90%)	562 (8%)	106 (2%)	8	39

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	PRO
1	A	195	ARG
2	C	62	TYR
2	C	170	VAL
2	C	516	ASP
2	C	697	LYS
2	C	1151	LEU
2	C	1283	ALA
2	C	1317	PRO
3	D	10	ALA
3	D	357	VAL
3	D	426	ALA

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Mol	Chain	Res	Type
3	D	496	GLY
3	D	710	ASP
3	D	745	GLY
3	D	805	GLN
3	D	831	VAL
4	E	33	GLY
5	F	96	ASP
1	G	167	PRO
1	G	178	SER
1	H	138	ALA
2	I	62	TYR
2	I	111	GLU
2	I	484	LEU
2	I	519	ASN
2	I	697	LYS
2	I	1136	GLN
2	I	1151	LEU
2	I	1283	ALA
2	I	1317	PRO
3	J	357	VAL
3	J	710	ASP
3	J	745	GLY
3	J	805	GLN
3	J	826	ILE
3	J	828	GLY
3	J	831	VAL
4	K	33	GLY
5	L	96	ASP
1	A	162	GLU
2	C	111	GLU
2	C	484	LEU
2	C	756	TYR
2	C	761	GLN
2	C	1136	GLN
2	C	1159	VAL
3	D	46	TYR
3	D	332	LYS
3	D	705	THR
3	D	714	GLU
3	D	828	GLY
2	I	170	VAL
2	I	756	TYR

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Mol	Chain	Res	Type
3	J	46	TYR
3	J	426	ALA
3	J	496	GLY
3	J	705	THR
3	J	714	GLU
5	L	581	ASP
5	L	584	ARG
1	B	138	ALA
2	C	519	ASN
3	D	13	LYS
5	F	569	THR
5	F	581	ASP
5	F	584	ARG
1	G	162	GLU
2	I	489	PRO
2	I	490	GLN
2	I	761	GLN
1	A	19	VAL
1	A	136	GLU
2	C	490	GLN
2	C	659	GLN
2	C	1107	MET
2	C	1158	LYS
3	D	89	GLY
3	D	639	VAL
2	I	237	LEU
2	I	516	ASP
2	I	1159	VAL
2	I	1256	GLN
3	J	89	GLY
5	L	569	THR
1	A	14	VAL
2	C	489	PRO
3	D	826	ILE
1	G	93	GLN
2	I	813	GLU
2	I	892	GLU
2	I	1158	LYS
3	J	639	VAL
2	C	237	LEU
2	I	696	ASP
2	I	1104	PRO

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Mol	Chain	Res	Type
3	J	1344	LEU
1	A	107	ILE
1	B	107	ILE
2	C	1104	PRO
1	G	107	ILE
4	E	86	ILE
1	H	107	ILE
1	A	29	GLU
1	G	19	VAL
3	D	1184	ASP

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	196/286 (68%)	180 (92%)	16 (8%)	9	34
1	B	184/286 (64%)	173 (94%)	11 (6%)	16	45
1	G	191/286 (67%)	180 (94%)	11 (6%)	17	46
1	H	183/286 (64%)	167 (91%)	16 (9%)	8	33
2	C	1152/1157 (100%)	1047 (91%)	105 (9%)	7	31
2	I	1151/1157 (100%)	1049 (91%)	102 (9%)	8	32
3	D	968/1168 (83%)	869 (90%)	99 (10%)	6	27
3	J	959/1168 (82%)	864 (90%)	95 (10%)	6	28
4	E	71/75 (95%)	66 (93%)	5 (7%)	12	40
4	K	67/75 (89%)	60 (90%)	7 (10%)	5	26
5	F	413/540 (76%)	389 (94%)	24 (6%)	17	46
5	L	410/540 (76%)	384 (94%)	26 (6%)	15	44
All	All	5945/7024 (85%)	5428 (91%)	517 (9%)	8	33

All (517) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	43	LEU
1	A	56	VAL
1	A	67	GLU
1	A	72	GLU
1	A	96	ASP
1	A	101	THR
1	A	124	VAL
1	A	140	ILE
1	A	145	LYS
1	A	147	GLN
1	A	158	ARG
1	A	178	SER
1	A	186	ASN
1	A	207	THR
1	A	211	ILE
1	B	38	THR
1	B	60	GLU
1	B	62	ASP
1	B	65	LEU
1	B	92	VAL
1	B	135	ASP
1	B	173	VAL
1	B	176	CYS
1	B	183	ILE
1	B	186	ASN
1	B	203	ILE
2	C	4	SER
2	C	22	LEU
2	C	39	ILE
2	C	46	GLN
2	C	60	GLN
2	C	66	SER
2	C	115	LYS
2	C	116	ASP
2	C	119	GLU
2	C	120	GLN
2	C	132	ASP
2	C	138	ILE
2	C	164	THR
2	C	170	VAL
2	C	179	TYR
2	C	223	LEU

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Mol	Chain	Res	Type
2	C	316	GLU
2	C	369	MET
2	C	377	THR
2	C	400	VAL
2	C	419	ILE
2	C	434	ASP
2	C	442	VAL
2	C	443	ASP
2	C	455	SER
2	C	463	GLN
2	C	471	VAL
2	C	484	LEU
2	C	485	ASP
2	C	487	LEU
2	C	493	ILE
2	C	496	LYS
2	C	512	SER
2	C	514	PHE
2	C	525	THR
2	C	538	LEU
2	C	542	ARG
2	C	553	THR
2	C	554	HIS
2	C	558	VAL
2	C	563	THR
2	C	568	ASN
2	C	615	VAL
2	C	623	LEU
2	C	637	ARG
2	C	657	THR
2	C	660	VAL
2	C	663	VAL
2	C	672	GLU
2	C	697	LYS
2	C	700	VAL
2	C	705	GLU
2	C	706	ARG
2	C	714	VAL
2	C	727	VAL
2	C	748	ILE
2	C	764	CYS
2	C	765	ILE

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Mol	Chain	Res	Type
2	C	781	ASP
2	C	782	VAL
2	C	791	LEU
2	C	799	ASN
2	C	839	VAL
2	C	864	LYS
2	C	866	ASP
2	C	867	GLU
2	C	890	LYS
2	C	892	GLU
2	C	895	LEU
2	C	913	VAL
2	C	919	ARG
2	C	990	ASP
2	C	992	LEU
2	C	995	ASP
2	C	1002	LEU
2	C	1029	LEU
2	C	1037	THR
2	C	1054	LEU
2	C	1072	ASN
2	C	1076	ILE
2	C	1082	ILE
2	C	1083	GLU
2	C	1106	ARG
2	C	1109	ILE
2	C	1114	GLU
2	C	1115	THR
2	C	1146	GLN
2	C	1151	LEU
2	C	1156	ARG
2	C	1158	LYS
2	C	1159	VAL
2	C	1164	PHE
2	C	1177	ARG
2	C	1198	LEU
2	C	1206	THR
2	C	1233	LEU
2	C	1240	ASP
2	C	1248	THR
2	C	1253	LEU
2	C	1255	THR

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Mol	Chain	Res	Type
2	C	1296	ASP
2	C	1299	ASN
2	C	1304	MET
2	C	1310	ASP
2	C	1341	ASP
3	D	8	LEU
3	D	24	LEU
3	D	42	GLU
3	D	46	TYR
3	D	47	ARG
3	D	52	GLU
3	D	70	CYS
3	D	83	VAL
3	D	92	VAL
3	D	93	THR
3	D	97	VAL
3	D	126	LEU
3	D	132	LEU
3	D	139	LEU
3	D	172	PHE
3	D	176	PHE
3	D	215	LYS
3	D	217	LEU
3	D	244	VAL
3	D	252	LEU
3	D	259	ARG
3	D	264	ASP
3	D	306	LEU
3	D	324	LEU
3	D	332	LYS
3	D	374	LEU
3	D	392	THR
3	D	416	ILE
3	D	425	ARG
3	D	429	LEU
3	D	430	HIS
3	D	442	ILE
3	D	474	LEU
3	D	486	SER
3	D	505	ASP
3	D	506	VAL
3	D	517	CYS

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Mol	Chain	Res	Type
3	D	526	VAL
3	D	545	HIS
3	D	547	ARG
3	D	570	LYS
3	D	593	ASN
3	D	605	LEU
3	D	641	ILE
3	D	646	ILE
3	D	678	ARG
3	D	701	LEU
3	D	702	GLN
3	D	706	VAL
3	D	707	ILE
3	D	708	ASN
3	D	710	ASP
3	D	712	GLN
3	D	717	VAL
3	D	720	ASN
3	D	731	ARG
3	D	746	LEU
3	D	749	LYS
3	D	754	ILE
3	D	764	ARG
3	D	769	VAL
3	D	770	LEU
3	D	797	THR
3	D	810	THR
3	D	830	ASP
3	D	832	LYS
3	D	848	VAL
3	D	849	LEU
3	D	853	THR
3	D	857	LEU
3	D	885	VAL
3	D	903	LEU
3	D	908	ILE
3	D	918	ILE
3	D	1135	THR
3	D	1155	ILE
3	D	1162	ILE
3	D	1163	VAL
3	D	1170	LYS

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Mol	Chain	Res	Type
3	D	1186	TYR
3	D	1194	ARG
3	D	1199	PHE
3	D	1208	ASP
3	D	1209	VAL
3	D	1215	GLU
3	D	1221	LEU
3	D	1237	VAL
3	D	1255	VAL
3	D	1261	LEU
3	D	1266	ILE
3	D	1275	LEU
3	D	1278	GLU
3	D	1284	ARG
3	D	1285	VAL
3	D	1290	ARG
3	D	1293	GLU
3	D	1333	THR
3	D	1348	LYS
3	D	1361	THR
4	E	13	ILE
4	E	21	LEU
4	E	39	VAL
4	E	58	LEU
4	E	67	ARG
5	F	98	VAL
5	F	163	THR
5	F	266	PHE
5	F	267	ASP
5	F	277	MET
5	F	306	PHE
5	F	310	GLU
5	F	360	ASP
5	F	395	THR
5	F	417	ASP
5	F	429	THR
5	F	471	LEU
5	F	483	LEU
5	F	488	LEU
5	F	491	GLU
5	F	492	ASP
5	F	536	THR

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Mol	Chain	Res	Type
5	F	547	VAL
5	F	569	THR
5	F	572	THR
5	F	587	ILE
5	F	599	ARG
5	F	603	ARG
5	F	612	ASP
1	G	65	LEU
1	G	70	THR
1	G	79	LEU
1	G	96	ASP
1	G	101	THR
1	G	123	ILE
1	G	124	VAL
1	G	157	THR
1	G	168	ILE
1	G	171	LEU
1	G	186	ASN
1	H	7	GLU
1	H	8	PHE
1	H	18	GLN
1	H	58	GLU
1	H	60	GLU
1	H	62	ASP
1	H	65	LEU
1	H	70	THR
1	H	75	GLN
1	H	95	LYS
1	H	116	THR
1	H	135	ASP
1	H	157	THR
1	H	176	CYS
1	H	183	ILE
1	H	186	ASN
2	I	23	ASP
2	I	39	ILE
2	I	44	GLU
2	I	46	GLN
2	I	60	GLN
2	I	66	SER
2	I	81	ASP
2	I	115	LYS

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Mol	Chain	Res	Type
2	I	131	THR
2	I	132	ASP
2	I	138	ILE
2	I	170	VAL
2	I	179	TYR
2	I	223	LEU
2	I	302	ILE
2	I	316	GLU
2	I	353	VAL
2	I	369	MET
2	I	377	THR
2	I	400	VAL
2	I	419	ILE
2	I	434	ASP
2	I	442	VAL
2	I	443	ASP
2	I	455	SER
2	I	463	GLN
2	I	484	LEU
2	I	485	ASP
2	I	487	LEU
2	I	493	ILE
2	I	496	LYS
2	I	514	PHE
2	I	525	THR
2	I	538	LEU
2	I	542	ARG
2	I	553	THR
2	I	554	HIS
2	I	558	VAL
2	I	561	ILE
2	I	563	THR
2	I	568	ASN
2	I	609	ILE
2	I	615	VAL
2	I	620	ASN
2	I	637	ARG
2	I	657	THR
2	I	660	VAL
2	I	663	VAL
2	I	672	GLU
2	I	697	LYS

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Mol	Chain	Res	Type
2	I	700	VAL
2	I	705	GLU
2	I	714	VAL
2	I	727	VAL
2	I	748	ILE
2	I	750	ILE
2	I	757	THR
2	I	765	ILE
2	I	781	ASP
2	I	782	VAL
2	I	791	LEU
2	I	799	ASN
2	I	839	VAL
2	I	864	LYS
2	I	866	ASP
2	I	867	GLU
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
2	I	990	ASP
2	I	992	LEU
2	I	995	ASP
2	I	1002	LEU
2	I	1029	LEU
2	I	1037	THR
2	I	1072	ASN
2	I	1076	ILE
2	I	1082	ILE
2	I	1083	GLU
2	I	1106	ARG
2	I	1114	GLU
2	I	1115	THR
2	I	1132	LEU
2	I	1146	GLN
2	I	1151	LEU
2	I	1154	ASP
2	I	1156	ARG
2	I	1159	VAL
2	I	1164	PHE
2	I	1180	MET
2	I	1198	LEU
2	I	1233	LEU

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Mol	Chain	Res	Type
2	I	1240	ASP
2	I	1250	SER
2	I	1253	LEU
2	I	1255	THR
2	I	1287	LEU
2	I	1293	VAL
2	I	1296	ASP
2	I	1299	ASN
2	I	1304	MET
2	I	1341	ASP
3	J	24	LEU
3	J	42	GLU
3	J	46	TYR
3	J	47	ARG
3	J	52	GLU
3	J	70	CYS
3	J	83	VAL
3	J	92	VAL
3	J	93	THR
3	J	126	LEU
3	J	132	LEU
3	J	139	LEU
3	J	159	ILE
3	J	162	GLU
3	J	172	PHE
3	J	176	PHE
3	J	217	LEU
3	J	222	LYS
3	J	252	LEU
3	J	264	ASP
3	J	306	LEU
3	J	324	LEU
3	J	352	ARG
3	J	374	LEU
3	J	384	LYS
3	J	392	THR
3	J	408	VAL
3	J	416	ILE
3	J	425	ARG
3	J	429	LEU
3	J	430	HIS
3	J	474	LEU

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Mol	Chain	Res	Type
3	J	486	SER
3	J	505	ASP
3	J	506	VAL
3	J	507	VAL
3	J	545	HIS
3	J	567	THR
3	J	571	ASP
3	J	605	LEU
3	J	615	LYS
3	J	641	ILE
3	J	646	ILE
3	J	660	GLU
3	J	678	ARG
3	J	680	ASN
3	J	683	ILE
3	J	702	GLN
3	J	706	VAL
3	J	707	ILE
3	J	708	ASN
3	J	710	ASP
3	J	712	GLN
3	J	717	VAL
3	J	720	ASN
3	J	731	ARG
3	J	746	LEU
3	J	749	LYS
3	J	754	ILE
3	J	764	ARG
3	J	765	GLU
3	J	769	VAL
3	J	770	LEU
3	J	797	THR
3	J	810	THR
3	J	830	ASP
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	858	VAL
3	J	885	VAL
3	J	903	LEU
3	J	908	ILE
3	J	910	ASN

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Mol	Chain	Res	Type
3	J	918	ILE
3	J	1155	ILE
3	J	1162	ILE
3	J	1163	VAL
3	J	1186	TYR
3	J	1194	ARG
3	J	1199	PHE
3	J	1208	ASP
3	J	1209	VAL
3	J	1215	GLU
3	J	1221	LEU
3	J	1237	VAL
3	J	1255	VAL
3	J	1261	LEU
3	J	1278	GLU
3	J	1285	VAL
3	J	1290	ARG
3	J	1293	GLU
3	J	1305	ASP
3	J	1333	THR
3	J	1361	THR
4	K	3	ARG
4	K	13	ILE
4	K	15	ASN
4	K	21	LEU
4	K	36	ASP
4	K	39	VAL
4	K	67	ARG
5	L	98	VAL
5	L	154	GLU
5	L	163	THR
5	L	266	PHE
5	L	267	ASP
5	L	277	MET
5	L	310	GLU
5	L	341	LEU
5	L	360	ASP
5	L	395	THR
5	L	417	ASP
5	L	429	THR
5	L	471	LEU
5	L	482	GLU

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Mol	Chain	Res	Type
5	L	483	LEU
5	L	488	LEU
5	L	491	GLU
5	L	492	ASP
5	L	536	THR
5	L	547	VAL
5	L	557	LYS
5	L	569	THR
5	L	572	THR
5	L	603	ARG
5	L	612	ASP
5	L	613	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
2	C	31	GLN
2	C	69	GLN
2	C	120	GLN
2	C	357	ASN
2	C	463	GLN
2	C	518	ASN
2	C	658	GLN
2	C	684	ASN
2	C	952	GLN
2	C	1116	HIS
2	C	1134	GLN
2	C	1136	GLN
2	C	1146	GLN
2	C	1237	HIS
2	C	1288	GLN
3	D	11	GLN
3	D	94	GLN
3	D	200	GLN
3	D	365	GLN
3	D	435	GLN
3	D	465	GLN
3	D	594	GLN
3	D	702	GLN
3	D	716	GLN
3	D	929	GLN

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Mol	Chain	Res	Type
3	D	1227	HIS
4	E	61	ASN
5	F	131	GLN
5	F	258	GLN
5	F	362	ASN
5	F	383	ASN
5	F	406	GLN
5	F	446	GLN
1	G	41	ASN
1	G	66	HIS
1	G	84	ASN
1	G	227	GLN
1	H	84	ASN
1	H	128	HIS
2	I	69	GLN
2	I	518	ASN
2	I	628	HIS
2	I	684	ASN
2	I	834	GLN
2	I	1116	HIS
2	I	1136	GLN
2	I	1146	GLN
2	I	1220	GLN
2	I	1288	GLN
2	I	1314	GLN
3	J	94	GLN
3	J	200	GLN
3	J	206	ASN
3	J	365	GLN
3	J	424	ASN
3	J	477	GLN
3	J	594	GLN
3	J	716	GLN
3	J	910	ASN
3	J	929	GLN
3	J	1279	GLN
5	L	131	GLN
5	L	258	GLN
5	L	406	GLN
5	L	446	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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
6	ECJ	C	1401	-	30,37,37	2.97	10 (33%)	34,59,59	2.84	6 (17%)
6	ECJ	J	1501	-	30,37,37	2.97	9 (30%)	34,59,59	3.18	5 (14%)

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
6	ECJ	C	1401	-	-	5/21/43/43	0/3/3/3
6	ECJ	J	1501	-	-	5/21/43/43	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1401	ECJ	O16-C15	9.99	1.39	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	1501	ECJ	O16-C15	9.86	1.39	1.22
6	C	1401	ECJ	C13-C11	7.23	1.49	1.35
6	J	1501	ECJ	C13-C11	7.10	1.49	1.35
6	J	1501	ECJ	P29-O32	5.86	1.65	1.59
6	C	1401	ECJ	P29-O32	5.74	1.65	1.59
6	J	1501	ECJ	O12-C11	4.69	1.45	1.36
6	C	1401	ECJ	O12-C11	4.64	1.44	1.36
6	J	1501	ECJ	P29-O14	-3.15	1.54	1.60
6	C	1401	ECJ	P29-O14	-3.01	1.54	1.60
6	J	1501	ECJ	C22-N23	2.66	1.43	1.34
6	C	1401	ECJ	C22-N23	2.65	1.43	1.34
6	J	1501	ECJ	P06-O05	-2.62	1.56	1.59
6	C	1401	ECJ	C17-N18	-2.60	1.42	1.49
6	J	1501	ECJ	C17-N18	-2.50	1.42	1.49
6	C	1401	ECJ	P06-O05	-2.24	1.57	1.59
6	C	1401	ECJ	C10-C11	2.13	1.51	1.48
6	C	1401	ECJ	P01-O04	-2.02	1.47	1.54
6	J	1501	ECJ	P01-O04	-2.01	1.47	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	1501	ECJ	O16-C15-C13	-13.92	109.93	126.89
6	C	1401	ECJ	O16-C15-C13	-12.82	111.27	126.89
6	J	1501	ECJ	C15-C13-C11	-8.53	100.82	109.40
6	C	1401	ECJ	C15-C13-C11	-7.30	102.06	109.40
6	J	1501	ECJ	N27-C25-N24	-6.67	119.61	128.67
6	C	1401	ECJ	N27-C25-N24	-4.35	122.76	128.67
6	C	1401	ECJ	C28-C21-N20	-2.98	106.19	109.34
6	J	1501	ECJ	C17-O12-C11	-2.70	106.59	111.41
6	C	1401	ECJ	C17-O12-C11	-2.55	106.86	111.41
6	J	1501	ECJ	C28-C21-N20	-2.40	106.80	109.34
6	C	1401	ECJ	P29-O14-C13	-2.13	118.37	123.01

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1401	ECJ	O09-C10-C11-C13
6	J	1501	ECJ	O09-C10-C11-C13
6	J	1501	ECJ	P01-O05-P06-O09
6	J	1501	ECJ	C10-O09-P06-O05

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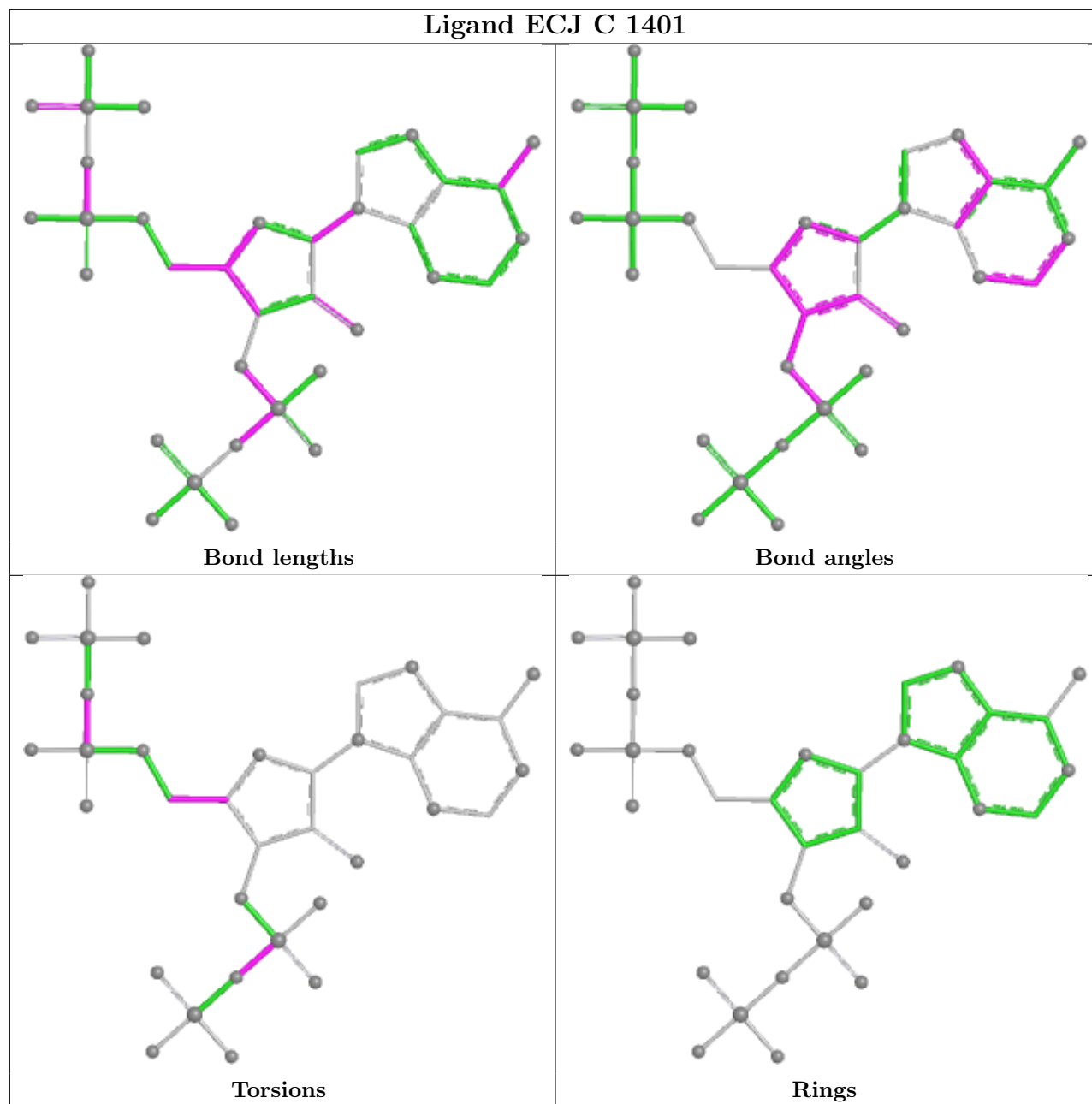
Mol	Chain	Res	Type	Atoms
6	J	1501	ECJ	C10-O09-P06-O08
6	C	1401	ECJ	O09-C10-C11-O12
6	C	1401	ECJ	P01-O05-P06-O09
6	C	1401	ECJ	P33-O32-P29-O14
6	C	1401	ECJ	P33-O32-P29-O31
6	J	1501	ECJ	C13-O14-P29-O32

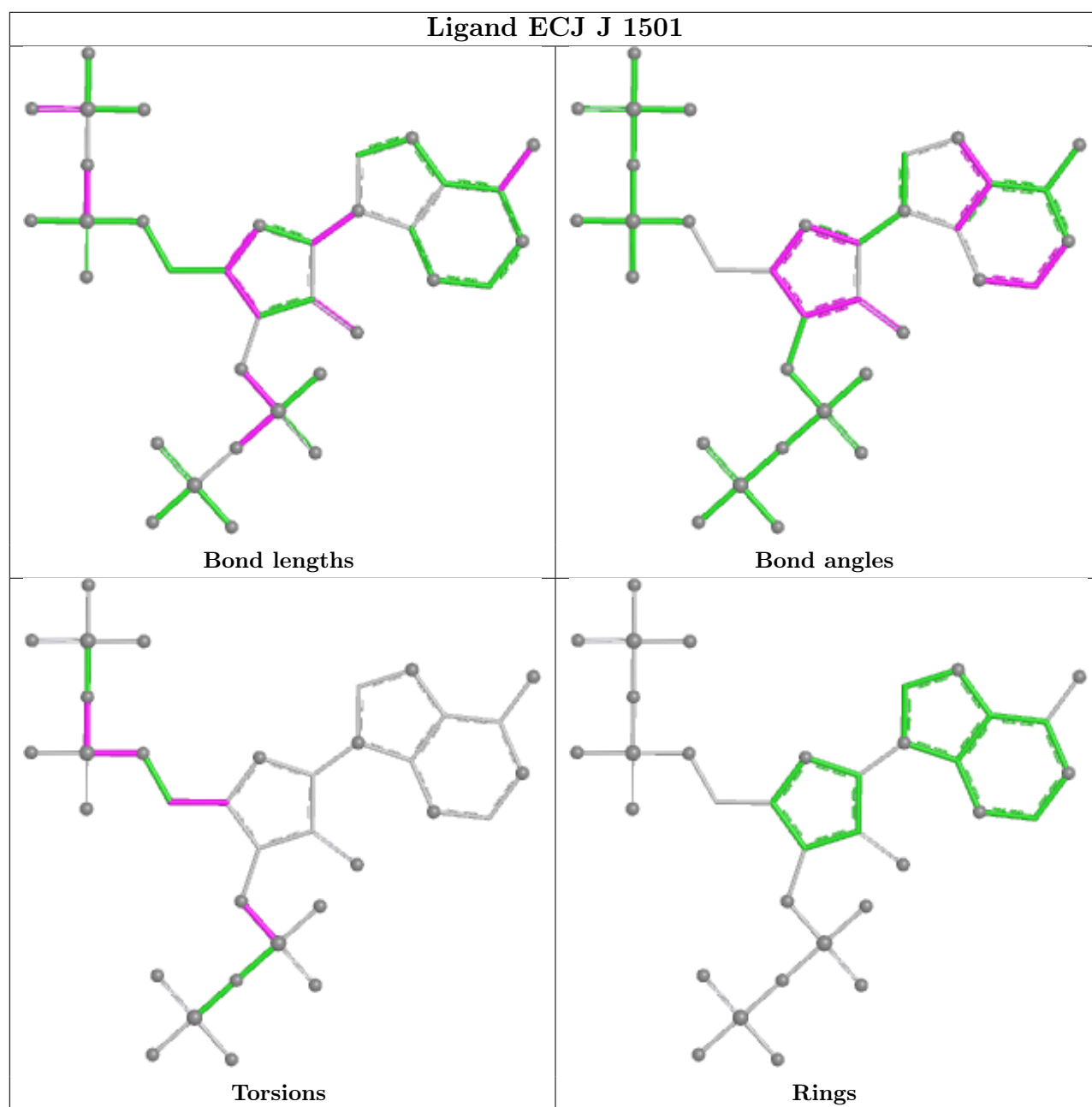
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	1501	ECJ	1	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.





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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	228/329 (69%)	-0.78	0 100 100	90, 124, 199, 234	0
1	B	217/329 (65%)	-0.65	0 100 100	85, 176, 231, 252	0
1	G	224/329 (68%)	-0.69	0 100 100	137, 176, 229, 280	0
1	H	217/329 (65%)	-0.60	0 100 100	150, 198, 235, 274	0
2	C	1340/1342 (99%)	-0.72	0 100 100	67, 119, 204, 265	0
2	I	1340/1342 (99%)	-0.70	1 (0%) 92 88	100, 147, 231, 373	0
3	D	1163/1407 (82%)	-0.73	0 100 100	63, 114, 199, 265	0
3	J	1155/1407 (82%)	-0.71	0 100 100	82, 145, 217, 279	0
4	E	89/91 (97%)	-0.63	0 100 100	107, 148, 174, 186	0
4	K	79/91 (86%)	-0.51	1 (1%) 74 53	182, 265, 298, 321	0
5	F	467/613 (76%)	-0.66	0 100 100	97, 182, 330, 392	0
5	L	469/613 (76%)	-0.71	0 100 100	121, 192, 300, 372	0
All	All	6988/8222 (84%)	-0.70	2 (0%) 100 100	63, 145, 240, 392	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	K	16	ARG	2.4
2	I	1264	GLN	2.2

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

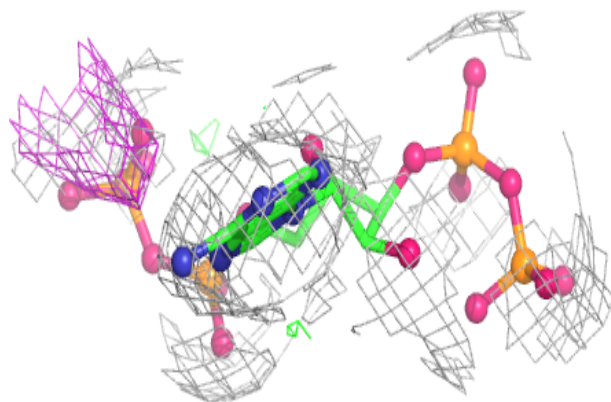
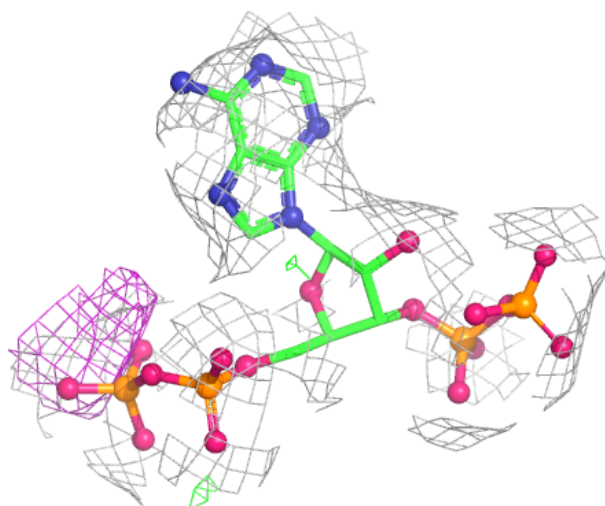
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	ECJ	J	1501	35/35	0.84	0.08	63,90,174,177	35
8	ZN	D	2003	1/1	0.86	0.30	377,377,377,377	0
6	ECJ	C	1401	35/35	0.89	0.08	74,99,183,185	35
7	MG	J	1502	1/1	0.96	0.05	81,81,81,81	0
8	ZN	D	2002	1/1	0.99	0.06	152,152,152,152	0
7	MG	D	2001	1/1	0.99	0.03	47,47,47,47	0
8	ZN	J	1503	1/1	0.99	0.01	155,155,155,155	0
8	ZN	J	1504	1/1	0.99	0.03	128,128,128,128	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

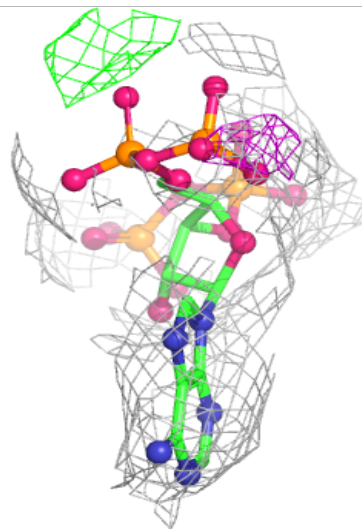
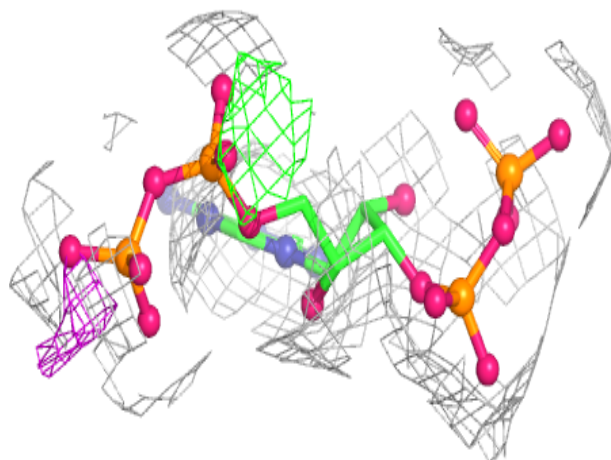
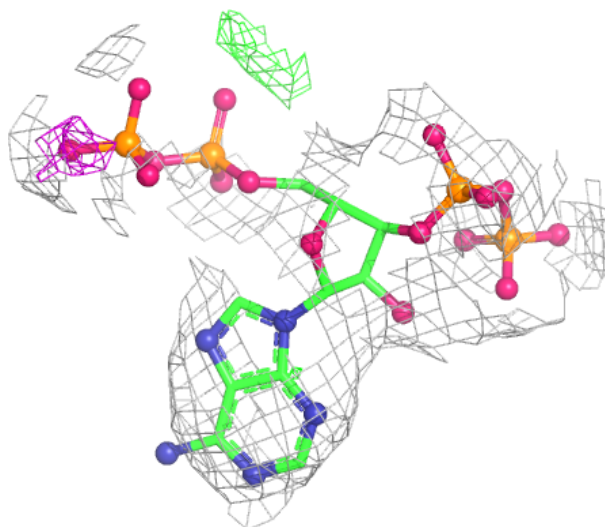
Electron density around ECJ J 1501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ECJ C 1401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.