



Full wwPDB EM Validation Report ⓘ

Oct 15, 2024 – 02:09 AM EDT

PDB ID : 8VJJ
EMDB ID : EMD-43283
Title : Structure of mouse RyR1 (EGTA-only dataset)
Authors : Weninger, G.; Marks, A.R.
Deposited on : 2024-01-07
Resolution : 2.53 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

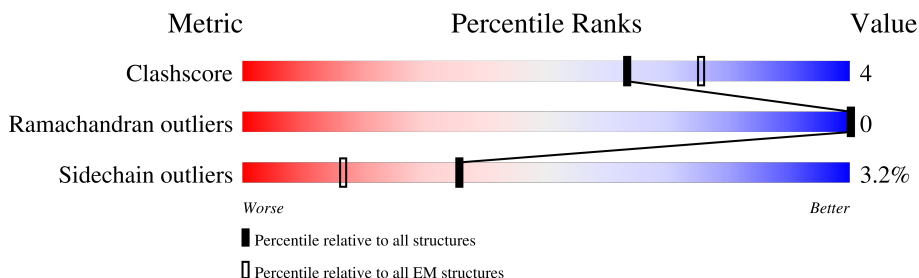
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.53 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	5035	
1	B	5035	
1	C	5035	
1	D	5035	
2	E	108	
2	F	108	
2	G	108	
2	H	108	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 284568 atoms, of which 141580 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	4374	Total	C	H	N	O	S	1	0
			69210	22140	34401	5985	6447	237		
1	D	4374	Total	C	H	N	O	S	1	0
			69210	22140	34401	5985	6447	237		
1	B	4374	Total	C	H	N	O	S	1	0
			69210	22140	34401	5985	6447	237		
1	C	4374	Total	C	H	N	O	S	1	0
			69210	22140	34401	5985	6447	237		

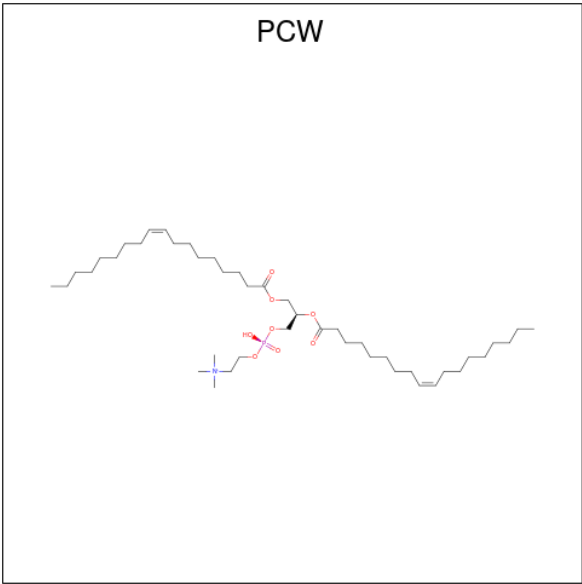
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	107	Total	C	H	N	O	S	0	0
			1655	526	826	145	155	3		
2	H	107	Total	C	H	N	O	S	0	0
			1655	526	826	145	155	3		
2	F	107	Total	C	H	N	O	S	0	0
			1655	526	826	145	155	3		
2	G	107	Total	C	H	N	O	S	0	0
			1655	526	826	145	155	3		

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

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

- Molecule 4 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: C₄₄H₈₅NO₈P).

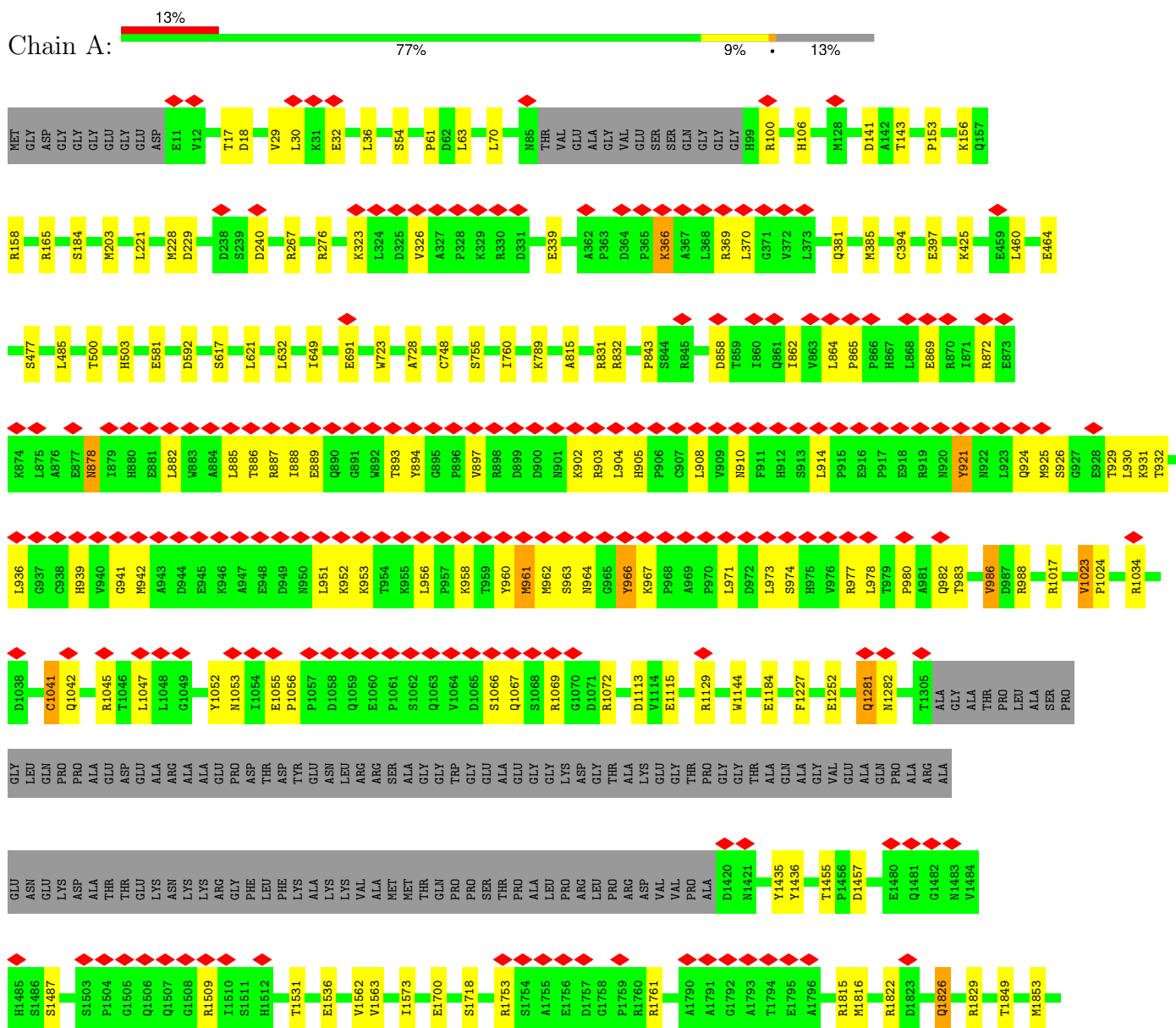


Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	H	N	O	P	0
			138	44	84	1	8	1	
4	A	1	Total	C	H	N	O	P	0
			138	44	84	1	8	1	
4	D	1	Total	C	H	N	O	P	0
			138	44	84	1	8	1	
4	D	1	Total	C	H	N	O	P	0
			138	44	84	1	8	1	
4	B	1	Total	C	H	N	O	P	0
			138	44	84	1	8	1	
4	B	1	Total	C	H	N	O	P	0
			138	44	84	1	8	1	
4	C	1	Total	C	H	N	O	P	0
			138	44	84	1	8	1	
4	C	1	Total	C	H	N	O	P	0
			138	44	84	1	8	1	

3 Residue-property plots

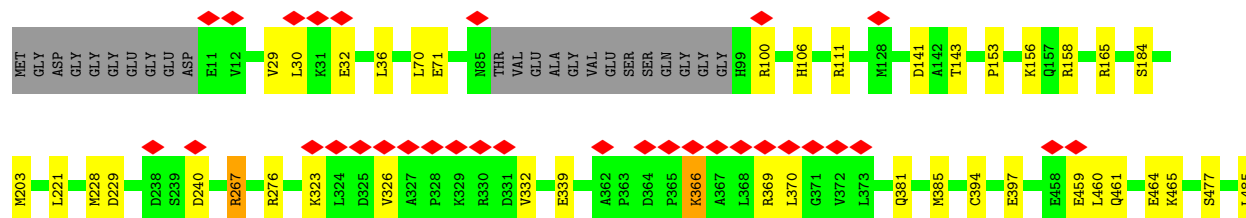
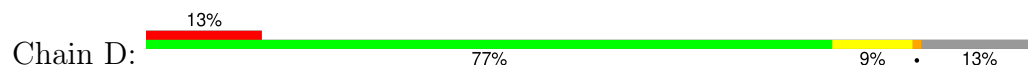
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

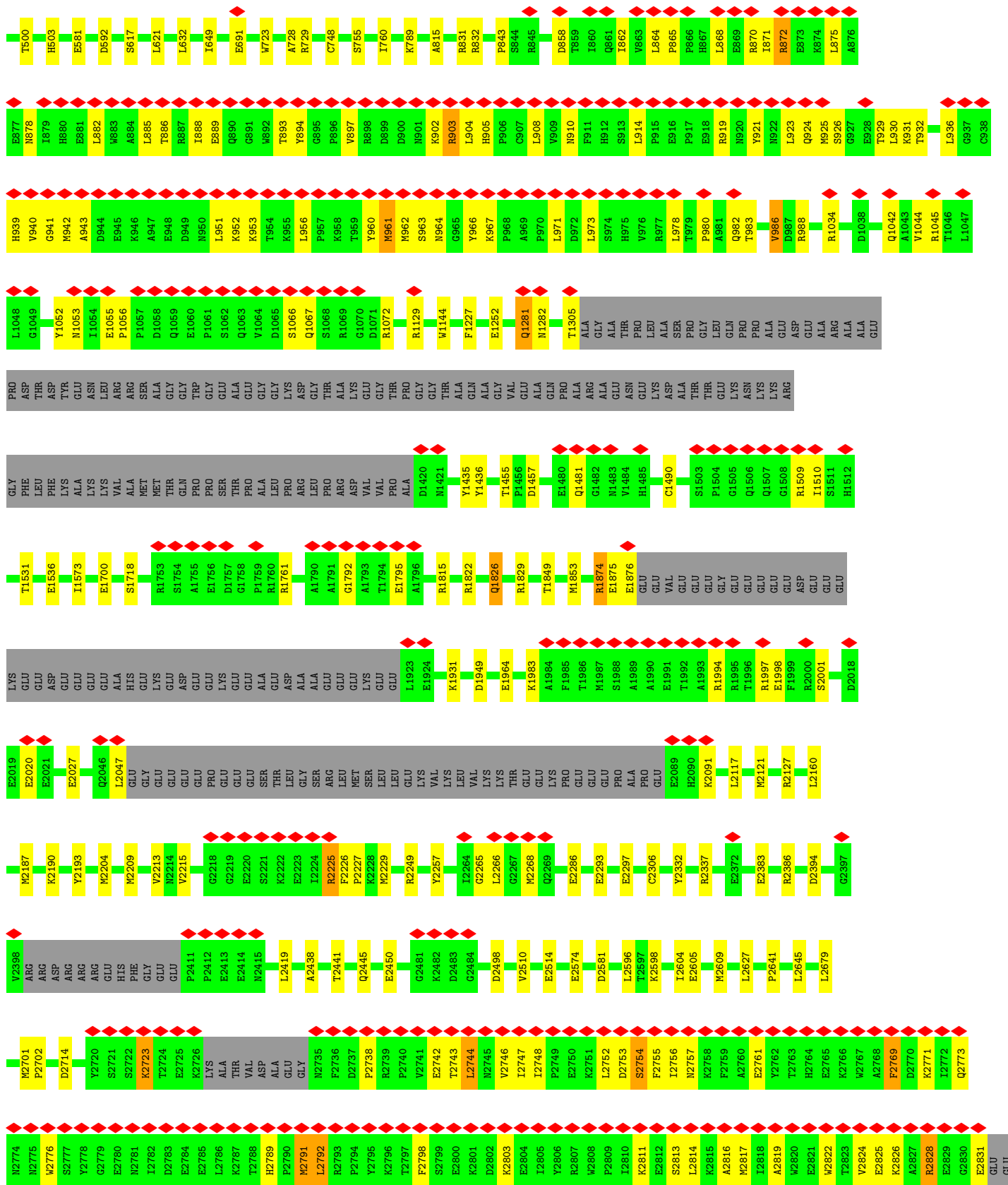
• Molecule 1: Ryanodine receptor 1





- Molecule 1: Ryanodine receptor 1



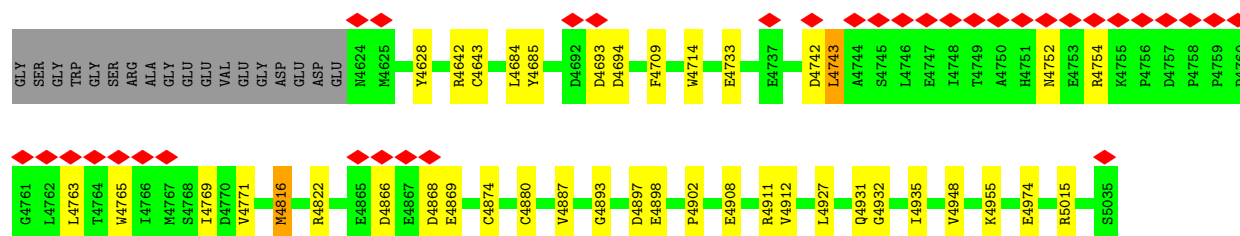


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PROTEIN DATA BANK

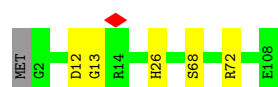




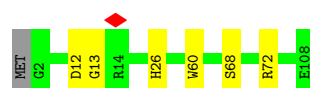
[illegible]



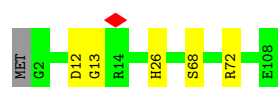
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



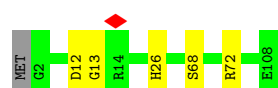
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	336237	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.804	Depositor
Minimum map value	0.000	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	428.544, 428.544, 428.544	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.28	0/35601	0.50	2/48224 (0.0%)
1	B	0.28	0/35601	0.50	1/48224 (0.0%)
1	C	0.28	0/35601	0.50	1/48224 (0.0%)
1	D	0.28	0/35601	0.50	1/48224 (0.0%)
2	E	0.28	0/847	0.52	0/1142
2	F	0.28	0/847	0.51	0/1142
2	G	0.28	0/847	0.52	0/1142
2	H	0.28	0/847	0.52	0/1142
All	All	0.28	0/145792	0.50	5/197464 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	4584	PRO	CA-N-CD	-9.17	98.66	111.50
1	C	4584	PRO	CA-N-CD	-9.10	98.76	111.50
1	B	4584	PRO	CA-N-CD	-8.99	98.91	111.50
1	A	4584	PRO	CA-N-CD	-8.94	98.99	111.50
1	A	3568	PRO	CA-N-CD	-5.20	104.22	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	3230	ILE	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	34809	34401	34401	286	0
1	B	34809	34401	34401	278	0
1	C	34809	34401	34401	283	0
1	D	34809	34401	34401	281	0
2	E	829	826	826	1	0
2	F	829	826	826	1	0
2	G	829	826	826	1	0
2	H	829	826	826	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	108	168	167	0	0
4	B	108	168	167	3	0
4	C	108	168	168	3	0
4	D	108	168	167	1	0
All	All	142988	141580	141577	1133	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (1133) 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:D:2828:ARG:NH1	1:D:2935:GLY:O	1.99	0.93
1:C:4110:GLU:O	1:C:4114:LEU:HD12	1.70	0.91
1:B:4110:GLU:O	1:B:4114:LEU:HD12	1.70	0.90
1:A:4110:GLU:O	1:A:4114:LEU:HD12	1.70	0.90
1:C:893:THR:HG23	1:C:904:LEU:HD23	1.50	0.89
1:D:4110:GLU:O	1:D:4114:LEU:HD12	1.71	0.89
1:B:893:THR:HG23	1:B:904:LEU:HD23	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:893:THR:HG23	1:D:904:LEU:HD23	1.55	0.88
1:B:2813:SER:OG	1:B:2883:TYR:OH	1.91	0.87
1:C:2813:SER:OG	1:C:2883:TYR:OH	1.92	0.85
1:B:32:GLU:OE1	1:B:32:GLU:N	2.11	0.84
1:A:2948:ASP:O	1:A:2949:THR:OG1	1.98	0.82
1:B:2828:ARG:NH1	1:B:2935:GLY:O	2.12	0.82
1:C:2813:SER:HG	1:C:2883:TYR:HH	1.26	0.82
1:A:893:THR:HG23	1:A:904:LEU:HD23	1.62	0.81
1:A:2813:SER:OG	1:A:2883:TYR:OH	1.93	0.81
1:D:2813:SER:OG	1:D:2883:TYR:OH	1.95	0.81
1:A:1700:GLU:OE2	1:A:1815:ARG:NH1	2.14	0.81
1:D:1700:GLU:OE2	1:D:1815:ARG:NH1	2.14	0.80
1:C:1700:GLU:OE2	1:C:1815:ARG:NH1	2.14	0.80
1:B:1700:GLU:OE2	1:B:1815:ARG:NH1	2.15	0.80
1:C:3944:ASP:OD1	1:C:3945:VAL:N	2.15	0.80
1:B:3944:ASP:OD1	1:B:3945:VAL:N	2.15	0.80
1:A:3944:ASP:OD1	1:A:3945:VAL:N	2.15	0.80
1:D:2187:MET:O	1:D:2193:TYR:OH	2.00	0.80
1:D:3944:ASP:OD1	1:D:3945:VAL:N	2.15	0.80
1:B:1252:GLU:N	1:B:1252:GLU:OE1	2.15	0.79
1:B:3608:ASP:OD1	1:B:3612:HIS:NE2	2.15	0.79
1:D:4009:ASP:OD1	1:D:4010:SER:N	2.16	0.79
1:C:3608:ASP:OD1	1:C:3612:HIS:NE2	2.15	0.79
1:C:2187:MET:O	1:C:2193:TYR:OH	1.99	0.79
1:A:4009:ASP:OD1	1:A:4010:SER:N	2.16	0.79
1:A:3608:ASP:OD2	1:A:3612:HIS:NE2	2.16	0.79
1:B:2872:LEU:HD22	1:B:2928:LEU:HD11	1.65	0.79
1:D:1252:GLU:N	1:D:1252:GLU:OE1	2.17	0.78
1:C:4009:ASP:OD1	1:C:4010:SER:N	2.16	0.78
1:A:1252:GLU:OE1	1:A:1252:GLU:N	2.17	0.78
1:C:2825:GLU:O	1:C:2828:ARG:NH1	2.17	0.78
1:B:4009:ASP:OD1	1:B:4010:SER:N	2.16	0.78
1:C:1252:GLU:OE1	1:C:1252:GLU:N	2.16	0.78
1:C:2828:ARG:NH1	1:C:2935:GLY:O	2.16	0.78
1:D:3608:ASP:OD1	1:D:3612:HIS:NE2	2.17	0.77
1:C:2872:LEU:HD22	1:C:2928:LEU:HD11	1.66	0.77
1:C:894:TYR:O	1:C:904:LEU:HD22	1.84	0.77
1:A:2187:MET:O	1:A:2193:TYR:OH	2.00	0.77
1:B:894:TYR:O	1:B:904:LEU:HD22	1.86	0.76
1:C:897:VAL:O	1:C:902:LYS:NZ	2.19	0.76
1:B:2187:MET:O	1:B:2193:TYR:OH	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:894:TYR:O	1:D:904:LEU:HD22	1.85	0.76
1:D:2383:GLU:OE1	1:D:2386:ARG:NH1	2.19	0.76
1:A:2828:ARG:NH1	1:A:2935:GLY:O	2.18	0.75
1:D:897:VAL:O	1:D:902:LYS:NZ	2.18	0.75
1:B:2383:GLU:OE1	1:B:2386:ARG:NH1	2.19	0.75
1:C:3556:ASN:OD1	1:C:3557:ASN:N	2.19	0.75
1:D:3556:ASN:OD1	1:D:3557:ASN:N	2.20	0.75
1:C:2383:GLU:OE1	1:C:2386:ARG:NH1	2.20	0.75
1:A:2383:GLU:OE1	1:A:2386:ARG:NH1	2.20	0.75
1:A:3556:ASN:OD1	1:A:3557:ASN:N	2.20	0.75
1:A:2871:GLU:O	1:A:2940:ARG:NH1	2.20	0.74
1:B:3556:ASN:OD1	1:B:3557:ASN:N	2.20	0.74
1:A:894:TYR:O	1:A:904:LEU:HD22	1.86	0.74
1:D:460:LEU:HD13	1:D:464:GLU:OE2	1.88	0.73
1:A:2027:GLU:OE1	1:A:2027:GLU:N	2.20	0.73
1:D:2938:VAL:O	1:D:2940:ARG:NH2	2.22	0.73
1:B:897:VAL:O	1:B:902:LYS:NZ	2.18	0.73
1:C:141:ASP:OD2	1:C:143:THR:OG1	2.04	0.72
1:A:897:VAL:O	1:A:902:LYS:NZ	2.22	0.71
1:B:1998:GLU:O	1:B:2001:SER:OG	2.09	0.71
1:C:2948:ASP:O	1:C:2949:THR:OG1	2.09	0.71
1:A:2825:GLU:O	1:A:2828:ARG:NH1	2.23	0.70
1:D:956:LEU:O	1:D:967:LYS:NZ	2.20	0.70
1:D:2872:LEU:HD22	1:D:2928:LEU:HD11	1.72	0.69
1:C:1998:GLU:O	1:C:2001:SER:OG	2.11	0.69
1:A:951:LEU:HD23	1:A:971:LEU:HD11	1.75	0.69
1:D:3088:ILE:HD12	1:D:3088:ILE:H	1.58	0.69
1:B:2825:GLU:O	1:B:2828:ARG:NH1	2.26	0.69
1:B:3088:ILE:HD12	1:B:3088:ILE:H	1.58	0.69
1:C:3088:ILE:HD12	1:C:3088:ILE:H	1.58	0.69
1:B:2948:ASP:O	1:B:2949:THR:OG1	2.09	0.69
1:D:951:LEU:HD23	1:D:971:LEU:HD11	1.75	0.69
1:D:2027:GLU:OE1	1:D:2027:GLU:N	2.20	0.68
1:D:2875:MET:SD	1:D:2940:ARG:NE	2.66	0.68
1:A:3088:ILE:H	1:A:3088:ILE:HD12	1.58	0.68
1:B:951:LEU:HD23	1:B:971:LEU:HD11	1.74	0.68
1:B:2027:GLU:OE1	1:B:2027:GLU:N	2.22	0.67
1:C:2027:GLU:OE1	1:C:2027:GLU:N	2.22	0.67
1:A:956:LEU:O	1:A:967:LYS:NZ	2.20	0.67
1:D:1998:GLU:O	1:D:2001:SER:OG	2.09	0.67
1:A:2868:LEU:HD12	1:A:2873:GLN:HG3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4908:GLU:O	1:D:4912:VAL:HG13	1.95	0.67
1:B:956:LEU:O	1:B:967:LYS:NZ	2.22	0.67
1:A:2268:MET:SD	1:A:2268:MET:N	2.68	0.67
1:A:1998:GLU:O	1:A:2001:SER:OG	2.11	0.67
1:C:70:LEU:HD21	1:C:203:MET:CE	2.25	0.67
1:A:3690:GLU:N	1:A:3690:GLU:OE1	2.28	0.67
1:C:1055:GLU:N	1:C:1055:GLU:OE1	2.27	0.67
1:C:4816:MET:SD	1:C:4816:MET:N	2.68	0.67
1:C:926:SER:O	1:C:930:LEU:HD22	1.95	0.67
1:B:1023:VAL:HG22	1:B:1024:PRO:HD2	1.77	0.66
1:B:1055:GLU:N	1:B:1055:GLU:OE1	2.27	0.66
1:C:4908:GLU:O	1:C:4912:VAL:HG13	1.95	0.66
1:A:141:ASP:OD2	1:A:143:THR:OG1	2.08	0.66
1:D:4816:MET:SD	1:D:4816:MET:N	2.68	0.66
1:C:885:LEU:HD12	1:C:886:THR:N	2.11	0.66
1:A:4908:GLU:O	1:A:4912:VAL:HG13	1.95	0.66
1:D:1055:GLU:OE1	1:D:1055:GLU:N	2.29	0.66
1:B:885:LEU:HD12	1:B:886:THR:N	2.11	0.66
1:B:4816:MET:SD	1:B:4816:MET:N	2.68	0.66
1:D:2948:ASP:O	1:D:2949:THR:OG1	2.09	0.66
1:A:2868:LEU:HD13	1:A:2869:SER:N	2.11	0.65
1:A:1023:VAL:HG22	1:A:1024:PRO:HD2	1.77	0.65
1:B:2868:LEU:HD13	1:B:2869:SER:O	1.97	0.65
1:B:3690:GLU:N	1:B:3690:GLU:OE1	2.29	0.65
1:B:4908:GLU:O	1:B:4912:VAL:HG13	1.95	0.65
1:C:951:LEU:HD23	1:C:971:LEU:HD11	1.78	0.65
1:A:2249:ARG:NH2	1:A:2286:GLU:OE2	2.29	0.65
1:C:925:MET:O	1:C:929:THR:HG23	1.97	0.65
1:A:2872:LEU:HD13	1:A:2928:LEU:HD11	1.78	0.65
1:A:893:THR:O	1:A:905:HIS:N	2.29	0.65
1:C:2868:LEU:HD13	1:C:2869:SER:O	1.97	0.65
1:D:3690:GLU:N	1:D:3690:GLU:OE1	2.29	0.65
1:B:926:SER:O	1:B:930:LEU:HD22	1.97	0.65
1:D:2645:LEU:HD13	1:D:2679:LEU:HD21	1.79	0.65
1:A:70:LEU:HD21	1:A:203:MET:CE	2.26	0.64
1:A:2645:LEU:HD13	1:A:2679:LEU:HD21	1.79	0.64
1:A:3548:GLU:OE1	1:A:3551:ARG:NH1	2.30	0.64
1:C:2875:MET:SD	1:C:2940:ARG:NE	2.71	0.64
1:D:2249:ARG:NH2	1:D:2286:GLU:OE2	2.30	0.64
1:D:2868:LEU:HD13	1:D:2869:SER:O	1.97	0.64
1:A:2868:LEU:HD21	1:A:2928:LEU:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ASP:OD2	1:B:143:THR:OG1	2.11	0.64
1:A:885:LEU:HD12	1:A:886:THR:N	2.12	0.64
1:D:3548:GLU:OE1	1:D:3551:ARG:NH1	2.31	0.64
1:B:2742:GLU:OE1	1:B:2742:GLU:N	2.30	0.64
1:D:885:LEU:HD12	1:D:886:THR:N	2.11	0.64
1:C:2249:ARG:NH2	1:C:2286:GLU:OE2	2.30	0.64
1:C:2645:LEU:HD13	1:C:2679:LEU:HD21	1.80	0.64
1:C:962:MET:SD	1:C:963:SER:N	2.71	0.64
1:D:2817:MET:HE1	1:D:2938:VAL:HG21	1.80	0.64
1:B:70:LEU:HD21	1:B:203:MET:CE	2.27	0.64
1:C:2742:GLU:N	1:C:2742:GLU:OE1	2.30	0.64
1:A:1055:GLU:OE1	1:A:1055:GLU:N	2.30	0.64
1:B:3972:ILE:HG21	1:B:3983:LEU:HD12	1.79	0.64
1:C:3369:ARG:NH2	1:C:3405:ASP:OD2	2.31	0.64
1:B:2645:LEU:HD13	1:B:2679:LEU:HD21	1.79	0.64
1:C:2789:HIS:HB2	1:C:2792:LEU:HD23	1.79	0.63
1:D:3972:ILE:HG21	1:D:3983:LEU:HD12	1.80	0.63
1:D:926:SER:O	1:D:930:LEU:HD22	1.98	0.63
1:A:878:ASN:HD22	1:A:878:ASN:C	1.98	0.63
1:A:926:SER:O	1:A:930:LEU:HD22	1.97	0.63
1:B:2938:VAL:O	1:B:2940:ARG:NH2	2.31	0.63
1:D:141:ASP:OD2	1:D:143:THR:OG1	2.07	0.63
1:C:3972:ILE:HG21	1:C:3983:LEU:HD12	1.79	0.63
1:D:2742:GLU:OE1	1:D:2742:GLU:N	2.32	0.63
1:B:3230:ILE:HD12	1:B:3231:LEU:HD12	1.81	0.63
1:D:3369:ARG:NH2	1:D:3405:ASP:OD2	2.32	0.62
1:B:2268:MET:SD	1:B:2268:MET:N	2.72	0.62
1:B:2789:HIS:HB2	1:B:2792:LEU:HD23	1.81	0.62
1:C:893:THR:O	1:C:905:HIS:N	2.33	0.62
1:D:381:GLN:N	1:D:381:GLN:OE1	2.33	0.62
1:B:2875:MET:SD	1:B:2940:ARG:NE	2.72	0.62
1:A:3962:LYS:NZ	1:A:4021:ASP:OD2	2.28	0.62
1:B:2293:GLU:O	1:B:2297:GLU:HG3	1.99	0.62
4:C:5103:PCW:O4P	4:C:5103:PCW:H63	2.00	0.62
1:D:2824:VAL:CG1	1:D:2938:VAL:HG22	2.30	0.62
1:C:2268:MET:SD	1:C:2268:MET:N	2.73	0.62
1:A:3972:ILE:HG21	1:A:3983:LEU:HD12	1.80	0.61
1:D:2268:MET:N	1:D:2268:MET:SD	2.73	0.61
1:B:2249:ARG:NH2	1:B:2286:GLU:OE2	2.30	0.61
1:A:2742:GLU:N	1:A:2742:GLU:OE1	2.33	0.61
1:A:2782:ILE:HD12	1:A:2789:HIS:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:460:LEU:HD22	1:D:464:GLU:OE2	1.99	0.61
1:A:2293:GLU:O	1:A:2297:GLU:HG3	2.01	0.60
1:D:2789:HIS:HB2	1:D:2792:LEU:HD23	1.83	0.60
1:C:2938:VAL:O	1:C:2940:ARG:NH2	2.34	0.60
1:D:4235:GLU:OE2	1:D:5015:ARG:NH2	2.35	0.60
1:A:4235:GLU:OE2	1:A:5015:ARG:NH2	2.34	0.60
1:A:893:THR:CG2	1:A:904:LEU:HD23	2.32	0.60
1:C:381:GLN:OE1	1:C:381:GLN:N	2.33	0.60
1:C:2293:GLU:O	1:C:2297:GLU:HG3	2.02	0.59
1:B:4235:GLU:OE2	1:B:5015:ARG:NH2	2.35	0.59
1:A:3730:MET:O	1:A:3733:SER:OG	2.20	0.59
1:C:4235:GLU:OE2	1:C:5015:ARG:NH2	2.35	0.59
1:A:3236:SER:OG	1:A:3239:GLU:OE2	2.20	0.59
1:B:381:GLN:OE1	1:B:381:GLN:N	2.33	0.59
1:D:71:GLU:OE1	1:D:111:ARG:NE	2.35	0.59
1:A:941:GLY:O	1:A:1053:ASN:ND2	2.36	0.59
1:C:71:GLU:OE1	1:C:111:ARG:NE	2.35	0.59
1:D:3865:ASP:OD2	1:D:3870:ASN:ND2	2.35	0.58
1:D:4632:GLU:OE2	1:D:4634:THR:OG1	2.18	0.58
1:B:2117:LEU:O	1:B:2121:MET:HG3	2.03	0.58
1:B:3865:ASP:OD2	1:B:3870:ASN:ND2	2.35	0.58
1:B:908:LEU:HD23	1:B:964:ASN:OD1	2.02	0.58
1:A:2738:PRO:O	1:A:2889:ARG:NH2	2.36	0.58
1:D:691:GLU:OE1	1:D:691:GLU:HA	2.03	0.58
1:C:460:LEU:HD22	1:C:464:GLU:OE1	2.02	0.58
1:A:4887:VAL:HG12	1:A:4898:GLU:HG3	1.84	0.58
1:D:956:LEU:HD22	1:D:960:TYR:CD2	2.38	0.58
1:B:3568:PRO:HD2	1:B:3569:SER:H	1.68	0.58
1:C:4887:VAL:HG12	1:C:4898:GLU:HG3	1.84	0.58
1:C:2761:GLU:OE1	1:C:2803:LYS:NZ	2.27	0.58
1:C:3457:GLN:O	1:C:3461:VAL:HG12	2.03	0.58
1:A:1069:ARG:NE	1:A:1115:GLU:OE1	2.36	0.58
1:C:2789:HIS:CB	1:C:2792:LEU:HD23	2.33	0.58
1:C:3568:PRO:HD2	1:C:3569:SER:H	1.69	0.58
1:D:893:THR:O	1:D:905:HIS:N	2.37	0.58
1:C:4816:MET:O	1:C:4822:ARG:NH1	2.37	0.58
1:A:1562:VAL:HG12	1:A:1563:VAL:HG13	1.86	0.57
1:B:893:THR:O	1:B:905:HIS:N	2.37	0.57
1:A:2117:LEU:O	1:A:2121:MET:HG3	2.04	0.57
1:C:1949:ASP:OD1	1:C:2127:ARG:NH2	2.37	0.57
1:C:2117:LEU:O	1:C:2121:MET:HG3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:8002:PCW:O4P	4:B:8002:PCW:H63	2.05	0.57
1:D:4887:VAL:HG12	1:D:4898:GLU:HG3	1.85	0.57
1:B:4887:VAL:HG12	1:B:4898:GLU:HG3	1.84	0.57
1:C:3369:ARG:O	1:C:3373:VAL:HG23	2.05	0.57
1:A:956:LEU:HD22	1:A:960:TYR:CD2	2.39	0.57
1:A:2978:LEU:HD22	1:A:3057:LEU:HD21	1.85	0.57
1:D:3457:GLN:O	1:D:3461:VAL:HG12	2.04	0.57
1:D:2931:LEU:O	1:D:2936:TYR:N	2.36	0.57
1:D:3730:MET:O	1:D:3733:SER:OG	2.20	0.57
1:B:2929:LYS:O	1:B:2933:MET:SD	2.63	0.57
1:C:2929:LYS:O	1:C:2933:MET:SD	2.63	0.57
1:A:3590:PRO:O	1:A:3594:VAL:HG23	2.05	0.57
1:D:2117:LEU:O	1:D:2121:MET:HG3	2.03	0.57
1:D:3369:ARG:O	1:D:3373:VAL:HG23	2.05	0.57
1:B:581:GLU:HG3	1:B:621:LEU:HD22	1.87	0.57
1:C:3730:MET:O	1:C:3733:SER:OG	2.21	0.57
1:A:581:GLU:HG3	1:A:621:LEU:HD22	1.86	0.56
1:D:581:GLU:HG3	1:D:621:LEU:HD22	1.86	0.56
1:C:581:GLU:HG3	1:C:621:LEU:HD22	1.86	0.56
1:C:2978:LEU:HD22	1:C:3057:LEU:HD21	1.86	0.56
1:B:956:LEU:HD22	1:B:960:TYR:CD2	2.40	0.56
1:B:1949:ASP:OD1	1:B:2127:ARG:NH2	2.37	0.56
1:A:2753:ASP:HA	1:A:2756:ILE:HD12	1.88	0.56
1:A:381:GLN:OE1	1:A:381:GLN:N	2.33	0.56
1:D:1949:ASP:OD1	1:D:2127:ARG:NH2	2.37	0.56
1:D:3568:PRO:HD2	1:D:3569:SER:H	1.69	0.56
1:B:2978:LEU:HD22	1:B:3057:LEU:HD21	1.87	0.56
1:B:3369:ARG:O	1:B:3373:VAL:HG23	2.06	0.56
1:C:936:LEU:HD12	1:C:988:ARG:NH2	2.21	0.56
1:D:2929:LYS:O	1:D:2933:MET:SD	2.64	0.56
1:B:4578:TYR:HE2	1:B:4628:TYR:HB3	1.70	0.56
1:D:4816:MET:O	1:D:4822:ARG:NH1	2.36	0.56
1:C:902:LYS:HZ2	1:C:904:LEU:HB2	1.71	0.56
1:C:2743:THR:OG1	1:C:2816:ALA:N	2.39	0.56
1:A:4874:CYS:HA	1:A:4880:CYS:HB2	1.87	0.56
1:B:3076:LEU:O	1:B:3147:HIS:NE2	2.36	0.56
1:B:4874:CYS:HA	1:B:4880:CYS:HB2	1.88	0.56
1:C:4578:TYR:HE2	1:C:4628:TYR:HB3	1.70	0.56
1:A:3076:LEU:O	1:A:3147:HIS:NE2	2.36	0.55
1:C:4874:CYS:HA	1:C:4880:CYS:HB2	1.88	0.55
1:D:3590:PRO:O	1:D:3594:VAL:HG23	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:PRO:HG2	1:A:63:LEU:HD13	1.88	0.55
1:A:4578:TYR:HE2	1:A:4628:TYR:HB3	1.70	0.55
1:B:2743:THR:OG1	1:B:2816:ALA:N	2.38	0.55
1:D:2756:ILE:HD13	1:D:2811:LYS:HG2	1.89	0.55
1:D:2978:LEU:HD22	1:D:3057:LEU:HD21	1.87	0.55
1:B:3088:ILE:HD12	1:B:3088:ILE:N	2.22	0.55
1:C:2824:VAL:CG1	1:C:2938:VAL:HG22	2.37	0.55
1:A:1949:ASP:OD1	1:A:2127:ARG:NH2	2.37	0.55
1:A:3369:ARG:O	1:A:3373:VAL:HG23	2.06	0.55
1:B:3041:THR:HA	1:B:3076:LEU:HD11	1.89	0.55
1:A:3541:TYR:OH	1:A:3547:ASP:OD1	2.16	0.55
1:A:4582:ASP:OD1	1:A:4583:SER:N	2.40	0.55
1:B:3730:MET:O	1:B:3733:SER:OG	2.22	0.55
1:C:3041:THR:HA	1:C:3076:LEU:HD11	1.89	0.55
1:A:862:ILE:O	1:A:931:LYS:NZ	2.40	0.55
1:C:4765:TRP:O	1:C:4769:ILE:HG23	2.06	0.55
1:B:902:LYS:HZ2	1:B:904:LEU:HB2	1.72	0.55
1:C:908:LEU:HD22	1:C:962:MET:CE	2.37	0.55
1:C:942:MET:HA	1:C:942:MET:HE3	1.88	0.55
1:C:4163:LEU:O	1:C:4167:LEU:HD23	2.07	0.55
1:D:4256:GLU:N	1:D:4256:GLU:OE1	2.40	0.54
1:B:936:LEU:HD12	1:B:988:ARG:NH2	2.22	0.54
1:C:2753:ASP:HA	1:C:2756:ILE:HD12	1.89	0.54
1:C:3524:ASN:O	1:C:3583:ARG:NH1	2.40	0.54
1:A:936:LEU:HD12	1:A:988:ARG:NH2	2.22	0.54
1:A:2089:GLU:OE2	1:A:2090:HIS:ND1	2.40	0.54
1:B:3524:ASN:O	1:B:3583:ARG:NH1	2.41	0.54
1:C:3088:ILE:HD12	1:C:3088:ILE:N	2.22	0.54
1:D:902:LYS:HZ2	1:D:904:LEU:HB2	1.71	0.54
1:D:3524:ASN:O	1:D:3583:ARG:NH1	2.41	0.54
1:B:2753:ASP:HA	1:B:2756:ILE:HD12	1.88	0.54
1:B:3378:GLU:OE2	1:B:3378:GLU:HA	2.08	0.54
1:C:3170:LEU:HD12	1:C:3195:LEU:HD11	1.88	0.54
1:B:4163:LEU:O	1:B:4167:LEU:HD23	2.07	0.54
1:B:4582:ASP:OD1	1:B:4583:SER:N	2.41	0.54
1:C:3378:GLU:HA	1:C:3378:GLU:OE2	2.08	0.54
1:C:4155:GLU:OE1	1:C:4197:TYR:OH	2.17	0.54
1:C:4582:ASP:OD1	1:C:4583:SER:N	2.40	0.54
1:A:1874:ARG:HB3	1:A:1874:ARG:CZ	2.38	0.54
1:A:2929:LYS:O	1:A:2933:MET:SD	2.65	0.54
1:D:3378:GLU:OE2	1:D:3378:GLU:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2738:PRO:O	1:C:2889:ARG:NH2	2.40	0.54
1:D:936:LEU:HD12	1:D:988:ARG:NH2	2.23	0.54
1:D:3170:LEU:HD12	1:D:3195:LEU:HD11	1.88	0.54
1:D:4163:LEU:O	1:D:4167:LEU:HD23	2.07	0.54
1:C:2756:ILE:HD13	1:C:2811:LYS:HG2	1.90	0.54
1:C:3683:GLU:HB3	1:C:3686:GLU:HB3	1.89	0.54
1:D:868:LEU:HD21	1:D:940:VAL:HG21	1.88	0.54
1:D:2753:ASP:HA	1:D:2756:ILE:HD12	1.90	0.54
1:B:366:LYS:NZ	1:B:370:LEU:HD11	2.23	0.54
1:B:2746:VAL:HG21	1:B:2819:ALA:HB2	1.88	0.54
1:B:4816:MET:O	1:B:4822:ARG:NH1	2.40	0.54
1:B:2738:PRO:O	1:B:2889:ARG:NH2	2.40	0.54
1:B:2756:ILE:HD13	1:B:2811:LYS:HG2	1.89	0.54
1:C:366:LYS:NZ	1:C:370:LEU:HD11	2.23	0.54
1:A:4163:LEU:O	1:A:4167:LEU:HD23	2.07	0.54
1:B:2824:VAL:CG1	1:B:2938:VAL:HG22	2.38	0.54
1:D:3088:ILE:HD12	1:D:3088:ILE:N	2.22	0.53
1:D:4582:ASP:OD1	1:D:4583:SER:N	2.41	0.53
1:C:956:LEU:O	1:C:967:LYS:NZ	2.31	0.53
1:A:2746:VAL:HG21	1:A:2819:ALA:HB2	1.90	0.53
1:B:3325:VAL:HG12	1:B:3362:THR:HG23	1.90	0.53
1:D:1510:ILE:HD12	1:D:1510:ILE:H	1.73	0.53
1:D:1874:ARG:CZ	1:D:1874:ARG:HB3	2.38	0.53
1:C:2746:VAL:HG21	1:C:2819:ALA:HB2	1.89	0.53
1:C:4868:ASP:OD1	1:C:4869:GLU:N	2.42	0.53
1:A:2761:GLU:OE1	1:A:2803:LYS:NZ	2.36	0.53
1:A:3524:ASN:O	1:A:3583:ARG:NH1	2.41	0.53
1:D:3041:THR:HA	1:D:3076:LEU:HD11	1.89	0.53
1:B:228:MET:SD	1:B:228:MET:N	2.81	0.53
1:D:2738:PRO:O	1:D:2889:ARG:NH2	2.40	0.53
1:B:862:ILE:O	1:B:931:LYS:NZ	2.41	0.53
1:B:4902:PRO:HB3	1:B:4911:ARG:HG2	1.91	0.53
1:A:2678:LYS:NZ	1:A:2910:ASP:OD2	2.42	0.53
1:D:366:LYS:NZ	1:D:370:LEU:HD11	2.23	0.53
1:D:4868:ASP:OD1	1:D:4869:GLU:N	2.41	0.53
4:D:5103:PCW:O4P	4:D:5103:PCW:H63	2.07	0.53
1:C:908:LEU:HD22	1:C:962:MET:HE1	1.90	0.53
1:A:4816:MET:O	1:A:4822:ARG:NH1	2.39	0.53
1:B:2089:GLU:OE2	1:B:2090:HIS:ND1	2.41	0.53
1:B:4868:ASP:OD1	1:B:4869:GLU:N	2.42	0.53
1:A:2789:HIS:HB3	1:A:2792:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3176:LEU:HD13	1:A:3176:LEU:C	2.30	0.53
1:A:3568:PRO:HD2	1:A:3569:SER:H	1.72	0.53
1:C:862:ILE:O	1:C:931:LYS:NZ	2.42	0.53
1:A:4112:GLN:OE1	1:A:4112:GLN:HA	2.08	0.52
1:D:925:MET:O	1:D:929:THR:HG23	2.08	0.52
1:C:3076:LEU:O	1:C:3147:HIS:NE2	2.36	0.52
1:A:2215:VAL:HG21	1:A:2229:MET:HE2	1.91	0.52
1:A:4868:ASP:OD1	1:A:4869:GLU:N	2.42	0.52
1:A:4902:PRO:HB3	1:A:4911:ARG:HG2	1.91	0.52
1:D:3076:LEU:O	1:D:3147:HIS:NE2	2.36	0.52
1:A:3041:THR:HA	1:A:3076:LEU:HD11	1.89	0.52
1:A:3325:VAL:HG12	1:A:3362:THR:HG23	1.90	0.52
1:B:925:MET:O	1:B:929:THR:HG23	2.09	0.52
1:B:2761:GLU:OE1	1:B:2803:LYS:NZ	2.31	0.52
1:C:4256:GLU:OE1	1:C:4256:GLU:N	2.40	0.52
1:D:910:ASN:O	1:D:914:LEU:N	2.43	0.52
1:A:4256:GLU:OE1	1:A:4256:GLU:N	2.40	0.52
1:B:3170:LEU:HD12	1:B:3195:LEU:HD11	1.91	0.52
1:C:868:LEU:HD21	1:C:940:VAL:HG21	1.91	0.52
1:C:4902:PRO:HB3	1:C:4911:ARG:HG2	1.91	0.52
1:A:240:ASP:OD2	1:A:240:ASP:N	2.41	0.52
1:A:3378:GLU:HA	1:A:3378:GLU:OE2	2.08	0.52
1:D:4902:PRO:HB3	1:D:4911:ARG:HG2	1.92	0.52
1:A:925:MET:O	1:A:929:THR:HG23	2.09	0.52
1:A:3683:GLU:O	1:A:3686:GLU:N	2.43	0.52
1:B:2020:GLU:OE1	1:B:2020:GLU:HA	2.10	0.52
1:C:322:GLU:OE1	1:C:322:GLU:HA	2.10	0.52
1:C:2020:GLU:OE2	1:C:2020:GLU:HA	2.09	0.52
1:A:366:LYS:NZ	1:A:370:LEU:HD11	2.24	0.51
1:A:3088:ILE:HD12	1:A:3088:ILE:N	2.22	0.51
1:C:2215:VAL:HG21	1:C:2229:MET:HE2	1.92	0.51
1:A:2413:GLU:OE1	1:A:2413:GLU:O	2.28	0.51
1:A:2756:ILE:HD13	1:A:2811:LYS:HG2	1.91	0.51
1:D:2771:LYS:HB3	1:D:2776:TRP:HB2	1.92	0.51
1:B:322:GLU:HA	1:B:322:GLU:OE1	2.10	0.51
1:C:2767:TRP:O	1:C:2771:LYS:HG3	2.10	0.51
1:D:4733:GLU:OE2	1:D:4733:GLU:HA	2.11	0.51
1:B:868:LEU:HD21	1:B:940:VAL:HG21	1.91	0.51
1:B:4733:GLU:OE2	1:B:4733:GLU:HA	2.11	0.51
1:B:4743:LEU:HD22	1:B:4743:LEU:H	1.76	0.51
1:D:3236:SER:OG	1:D:3239:GLU:OE2	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2020:GLU:OE1	1:A:2020:GLU:HA	2.11	0.51
1:D:893:THR:CG2	1:D:904:LEU:HD23	2.35	0.51
1:D:2944:ASP:OD1	1:D:2945:MET:N	2.44	0.51
1:B:2944:ASP:OD1	1:B:2945:MET:N	2.44	0.51
1:B:4256:GLU:OE1	1:B:4256:GLU:N	2.40	0.51
1:C:240:ASP:OD1	1:C:240:ASP:N	2.44	0.51
1:A:2743:THR:OG1	1:A:2816:ALA:N	2.44	0.50
1:B:1874:ARG:CZ	1:B:1874:ARG:HB3	2.41	0.50
1:D:70:LEU:HD21	1:D:203:MET:HE1	1.92	0.50
1:D:864:LEU:HD13	1:D:865:PRO:O	2.12	0.50
1:C:70:LEU:HD21	1:C:203:MET:HE1	1.92	0.50
1:C:910:ASN:O	1:C:914:LEU:N	2.44	0.50
1:C:3955:SER:OG	1:C:4018:GLU:OE1	2.28	0.50
1:C:4112:GLN:HA	1:C:4112:GLN:OE1	2.11	0.50
1:D:1066:SER:OG	1:D:1067:GLN:OE1	2.29	0.50
1:B:4142:ILE:HD12	1:B:4142:ILE:H	1.77	0.50
1:A:4733:GLU:OE2	1:A:4733:GLU:HA	2.11	0.50
1:B:3683:GLU:HB3	1:B:3686:GLU:HB3	1.94	0.50
1:C:2944:ASP:OD1	1:C:2945:MET:N	2.43	0.50
1:C:4733:GLU:HA	1:C:4733:GLU:OE2	2.11	0.50
1:A:2874:ALA:HB3	1:A:2940:ARG:HH12	1.76	0.50
1:B:942:MET:HE3	1:B:942:MET:HA	1.93	0.50
1:A:2215:VAL:HG21	1:A:2229:MET:CE	2.42	0.50
1:A:2868:LEU:HD21	1:A:2928:LEU:CD1	2.40	0.50
1:C:3282:LEU:HD12	1:C:3316:LEU:HD22	1.94	0.50
1:A:32:GLU:OE2	1:A:32:GLU:HA	2.12	0.50
1:B:4112:GLN:OE1	1:B:4112:GLN:HA	2.11	0.50
1:C:32:GLU:OE2	1:C:32:GLU:HA	2.12	0.50
1:A:3362:THR:HG21	1:A:3409:LEU:HD22	1.94	0.50
1:A:4743:LEU:H	1:A:4743:LEU:HD22	1.76	0.50
1:D:4112:GLN:OE1	1:D:4112:GLN:HA	2.11	0.50
1:B:3362:THR:HG21	1:B:3409:LEU:HD22	1.94	0.50
1:C:3828:GLU:OE1	1:C:3828:GLU:N	2.37	0.50
1:B:2215:VAL:HG21	1:B:2229:MET:CE	2.42	0.50
1:A:908:LEU:HD23	1:A:964:ASN:OD1	2.12	0.49
1:A:910:ASN:O	1:A:914:LEU:N	2.44	0.49
1:A:2870:ARG:NH2	1:A:2873:GLN:OE1	2.45	0.49
1:D:2813:SER:O	1:D:2817:MET:HG3	2.12	0.49
1:B:2767:TRP:C	1:B:2771:LYS:HZ2	2.15	0.49
1:C:2215:VAL:HG21	1:C:2229:MET:CE	2.42	0.49
1:C:4142:ILE:HD12	1:C:4142:ILE:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:ARG:NH1	1:D:339:GLU:OE2	2.45	0.49
1:D:2215:VAL:HG21	1:D:2229:MET:HE2	1.93	0.49
1:D:4142:ILE:HD12	1:D:4142:ILE:H	1.77	0.49
1:B:868:LEU:HD23	1:B:871:ILE:HD11	1.93	0.49
1:C:1874:ARG:CZ	1:C:1874:ARG:HB3	2.42	0.49
1:C:4743:LEU:HD22	1:C:4743:LEU:H	1.76	0.49
1:A:3282:LEU:HD12	1:A:3316:LEU:HD22	1.94	0.49
1:D:2755:PHE:HD2	1:D:2814:LEU:HD11	1.77	0.49
1:B:3683:GLU:O	1:B:3686:GLU:N	2.45	0.49
1:D:2828:ARG:HH12	1:D:2936:TYR:HA	1.76	0.49
1:D:3282:LEU:HD12	1:D:3316:LEU:HD22	1.94	0.49
1:D:4765:TRP:O	1:D:4769:ILE:HG23	2.12	0.49
1:C:926:SER:O	1:C:929:THR:OG1	2.26	0.49
1:C:2091:LYS:HD2	1:C:2091:LYS:N	2.28	0.49
1:A:276:ARG:NH1	1:A:339:GLU:OE2	2.45	0.49
1:A:4142:ILE:HD12	1:A:4142:ILE:H	1.77	0.49
1:A:4765:TRP:O	1:A:4769:ILE:HG23	2.13	0.49
1:D:3683:GLU:O	1:D:3686:GLU:N	2.45	0.49
1:B:1849:THR:O	1:B:1853:MET:HG3	2.13	0.49
1:C:1066:SER:OG	1:C:1067:GLN:OE1	2.31	0.49
1:D:4866:ASP:N	1:D:4866:ASP:OD1	2.46	0.49
1:B:2596:LEU:HD21	1:B:2604:ILE:CD1	2.43	0.49
1:B:3282:LEU:HD12	1:B:3316:LEU:HD22	1.94	0.49
1:C:908:LEU:HD23	1:C:964:ASN:OD1	2.13	0.49
1:A:962:MET:O	1:A:964:ASN:N	2.45	0.49
1:A:3683:GLU:HB3	1:A:3686:GLU:HB3	1.94	0.49
1:D:2746:VAL:HG21	1:D:2819:ALA:HB2	1.94	0.49
1:B:70:LEU:HD21	1:B:203:MET:HE1	1.94	0.49
1:C:1849:THR:O	1:C:1853:MET:HG3	2.13	0.49
1:A:2982:VAL:O	1:A:2986:ARG:NE	2.46	0.49
1:D:4743:LEU:H	1:D:4743:LEU:HD22	1.76	0.49
1:B:4765:TRP:O	1:B:4769:ILE:HG23	2.12	0.49
1:A:1227:PHE:O	1:A:1829:ARG:NH2	2.45	0.49
1:D:29:VAL:HG12	1:D:30:LEU:HD22	1.94	0.49
1:B:1227:PHE:O	1:B:1829:ARG:NH2	2.45	0.49
1:B:2091:LYS:N	1:B:2091:LYS:HD2	2.28	0.49
1:B:3590:PRO:O	1:B:3594:VAL:HG23	2.13	0.49
1:B:4866:ASP:N	1:B:4866:ASP:OD1	2.46	0.49
1:C:4769:ILE:HD11	1:C:4771:VAL:HG23	1.94	0.49
1:D:2215:VAL:HG21	1:D:2229:MET:CE	2.42	0.49
1:D:2791:MET:SD	1:D:2792:LEU:N	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3683:GLU:HB3	1:D:3686:GLU:HB3	1.94	0.49
1:D:4874:CYS:HA	1:D:4880:CYS:HB2	1.93	0.49
1:B:240:ASP:OD1	1:B:240:ASP:N	2.44	0.49
4:B:8002:PCW:H2O	4:B:8002:PCW:H462	1.95	0.49
1:A:691:GLU:OE2	1:A:691:GLU:HA	2.12	0.48
1:A:2091:LYS:HD2	1:A:2091:LYS:N	2.27	0.48
1:A:2789:HIS:CB	1:A:2792:LEU:HD23	2.43	0.48
1:A:3170:LEU:HD12	1:A:3195:LEU:HD11	1.94	0.48
1:A:1113:ASP:OD1	1:A:1113:ASP:N	2.45	0.48
1:D:1822:ARG:NH1	1:D:1822:ARG:HB3	2.28	0.48
1:D:3789:CYS:SG	1:D:3834:SER:OG	2.71	0.48
1:B:1066:SER:OG	1:B:1067:GLN:OE1	2.31	0.48
1:B:3789:CYS:SG	1:B:3834:SER:OG	2.71	0.48
1:C:868:LEU:HD23	1:C:871:ILE:HD11	1.93	0.48
1:C:2791:MET:SD	1:C:2792:LEU:N	2.86	0.48
1:D:2743:THR:OG1	1:D:2816:ALA:N	2.46	0.48
1:C:1822:ARG:HB3	1:C:1822:ARG:NH1	2.28	0.48
1:A:70:LEU:HD21	1:A:203:MET:HE1	1.95	0.48
1:A:2753:ASP:O	1:A:2757:ASN:OD1	2.31	0.48
1:B:29:VAL:HG12	1:B:30:LEU:HD22	1.94	0.48
1:C:1227:PHE:O	1:C:1829:ARG:NH2	2.44	0.48
1:C:3789:CYS:SG	1:C:3834:SER:OG	2.71	0.48
1:A:4866:ASP:OD1	1:A:4866:ASP:N	2.46	0.48
1:D:862:ILE:O	1:D:931:LYS:NZ	2.46	0.48
1:B:366:LYS:HZ2	1:B:370:LEU:HD11	1.78	0.48
1:B:1822:ARG:HB3	1:B:1822:ARG:NH1	2.28	0.48
1:B:3230:ILE:CD1	1:B:3231:LEU:HD12	2.42	0.48
1:C:592:ASP:HA	1:C:632:LEU:HD21	1.95	0.48
1:D:240:ASP:OD2	1:D:240:ASP:N	2.45	0.48
1:D:1849:THR:O	1:D:1853:MET:HG3	2.13	0.48
1:D:2910:ASP:OD1	1:D:2911:THR:N	2.47	0.48
1:B:3869:ILE:HD11	1:B:3872:GLN:O	2.14	0.48
1:A:3457:GLN:OE1	1:A:3457:GLN:HA	2.14	0.48
1:A:3556:ASN:OD1	1:A:3556:ASN:C	2.52	0.48
1:A:3789:CYS:SG	1:A:3834:SER:OG	2.72	0.48
1:C:3590:PRO:O	1:C:3594:VAL:HG23	2.13	0.48
1:D:941:GLY:O	1:D:1053:ASN:ND2	2.47	0.48
1:D:2752:LEU:HD13	1:D:2814:LEU:HD13	1.96	0.48
1:B:910:ASN:O	1:B:914:LEU:N	2.46	0.48
1:B:941:GLY:O	1:B:1053:ASN:ND2	2.47	0.48
1:B:962:MET:HG3	1:B:963:SER:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:871:ILE:HD13	1:C:1052:TYR:CZ	2.49	0.48
1:C:3556:ASN:OD1	1:C:3556:ASN:C	2.52	0.48
1:A:1822:ARG:HB3	1:A:1822:ARG:NH1	2.28	0.48
1:A:2944:ASP:OD1	1:A:2945:MET:N	2.47	0.48
1:D:858:ASP:OD1	1:D:858:ASP:N	2.47	0.48
1:D:1227:PHE:O	1:D:1829:ARG:NH2	2.45	0.48
1:D:2091:LYS:N	1:D:2091:LYS:HD2	2.29	0.48
1:D:4207:GLN:HB3	1:D:4248:MET:HG2	1.96	0.48
1:C:941:GLY:O	1:C:1053:ASN:ND2	2.47	0.48
1:A:592:ASP:HA	1:A:632:LEU:HD21	1.96	0.47
1:A:1849:THR:O	1:A:1853:MET:HG3	2.13	0.47
1:D:3556:ASN:OD1	1:D:3556:ASN:C	2.52	0.47
1:D:3869:ILE:HD11	1:D:3872:GLN:O	2.14	0.47
1:A:1066:SER:OG	1:A:1067:GLN:OE1	2.32	0.47
2:H:12:ASP:OD1	2:H:13:GLY:N	2.47	0.47
1:D:2879:LEU:CD1	1:D:2883:TYR:CE2	2.97	0.47
1:C:3108:VAL:HG13	1:C:3176:LEU:HB2	1.96	0.47
1:A:2978:LEU:O	1:A:2978:LEU:HD23	2.14	0.47
1:A:3714:LYS:NZ	1:A:3716:LYS:O	2.47	0.47
1:D:592:ASP:HA	1:D:632:LEU:HD21	1.97	0.47
1:D:3457:GLN:OE1	1:D:3457:GLN:HA	2.15	0.47
1:B:592:ASP:HA	1:B:632:LEU:HD21	1.96	0.47
1:B:1455:THR:OG1	1:B:1457:ASP:OD1	2.31	0.47
1:B:2910:ASP:OD1	1:B:2911:THR:N	2.47	0.47
1:B:3714:LYS:NZ	1:B:3716:LYS:O	2.47	0.47
1:C:4866:ASP:OD1	1:C:4866:ASP:N	2.46	0.47
2:E:12:ASP:OD1	2:E:13:GLY:N	2.47	0.47
1:D:921:TYR:O	1:D:924:GLN:HG3	2.15	0.47
1:D:2824:VAL:HG11	1:D:2938:VAL:HG22	1.95	0.47
1:B:2826:LYS:NZ	1:B:2934:ASN:O	2.42	0.47
1:A:893:THR:HA	1:A:962:MET:SD	2.55	0.47
1:C:2047:LEU:N	1:C:2047:LEU:HD22	2.29	0.47
1:C:4752:ASN:O	1:C:4754:ARG:NH1	2.47	0.47
1:A:858:ASP:OD1	1:A:858:ASP:N	2.46	0.47
1:A:2047:LEU:N	1:A:2047:LEU:HD22	2.30	0.47
1:A:3004:LEU:HB2	1:A:3005:PRO:HD3	1.97	0.47
1:D:2020:GLU:HA	1:D:2020:GLU:OE2	2.14	0.47
1:D:2047:LEU:HD22	1:D:2047:LEU:N	2.30	0.47
1:D:2306:CYS:HG	1:D:2332:TYR:HE2	1.63	0.47
1:B:2047:LEU:N	1:B:2047:LEU:HD22	2.29	0.47
1:B:3588:ASP:OD1	1:B:3588:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3955:SER:OG	1:B:4018:GLU:OE1	2.28	0.47
1:B:4579:LYS:HG2	1:B:4580:VAL:N	2.30	0.47
1:B:4752:ASN:O	1:B:4754:ARG:NH1	2.48	0.47
1:C:858:ASP:OD1	1:C:858:ASP:N	2.47	0.47
1:C:2306:CYS:HG	1:C:2332:TYR:HE2	1.63	0.47
2:F:12:ASP:OD1	2:F:13:GLY:N	2.47	0.47
1:B:858:ASP:OD1	1:B:858:ASP:N	2.47	0.47
1:C:3457:GLN:HA	1:C:3457:GLN:OE1	2.14	0.47
1:C:4207:GLN:HB3	1:C:4248:MET:HG2	1.97	0.47
1:D:2769:PHE:O	1:D:2773:GLN:HG2	2.15	0.47
1:D:3004:LEU:HB2	1:D:3005:PRO:HD3	1.97	0.47
1:D:3588:ASP:OD1	1:D:3588:ASP:N	2.48	0.47
1:B:871:ILE:HD13	1:B:1052:TYR:CZ	2.50	0.47
1:B:893:THR:CG2	1:B:904:LEU:HD23	2.36	0.47
1:B:3556:ASN:OD1	1:B:3556:ASN:C	2.53	0.47
1:C:4742:ASP:OD1	1:C:4742:ASP:C	2.54	0.47
1:A:228:MET:SD	1:A:228:MET:N	2.88	0.47
1:A:878:ASN:C	1:A:878:ASN:ND2	2.67	0.47
1:A:3588:ASP:OD1	1:A:3588:ASP:N	2.48	0.47
1:D:914:LEU:O	1:D:919:ARG:NH2	2.41	0.47
1:B:2769:PHE:O	1:B:2773:GLN:HG2	2.15	0.47
1:C:3362:THR:HG21	1:C:3409:LEU:HD22	1.97	0.47
1:C:3588:ASP:N	1:C:3588:ASP:OD1	2.48	0.47
1:A:908:LEU:O	1:A:966:TYR:OH	2.20	0.46
1:A:2767:TRP:O	1:A:2771:LYS:HG3	2.15	0.46
1:A:2879:LEU:CD1	1:A:2883:TYR:CE2	2.98	0.46
1:D:3559:ASN:O	1:D:3560:LEU:HB2	2.15	0.46
1:B:921:TYR:O	1:B:924:GLN:HG3	2.15	0.46
1:B:2978:LEU:HD23	1:B:2978:LEU:O	2.15	0.46
1:B:3559:ASN:O	1:B:3560:LEU:HB2	2.15	0.46
1:C:1510:ILE:HD12	1:C:1510:ILE:H	1.80	0.46
1:C:2817:MET:HE2	1:C:2822:TRP:HE3	1.79	0.46
1:C:4579:LYS:HG2	1:C:4580:VAL:N	2.30	0.46
1:A:460:LEU:HD22	1:A:464:GLU:OE2	2.15	0.46
1:A:4742:ASP:OD1	1:A:4742:ASP:C	2.54	0.46
1:D:980:PRO:O	1:D:983:THR:OG1	2.28	0.46
1:B:4742:ASP:C	1:B:4742:ASP:OD1	2.53	0.46
1:C:2978:LEU:O	1:C:2978:LEU:HD23	2.15	0.46
1:C:3559:ASN:O	1:C:3560:LEU:HB2	2.15	0.46
1:C:3714:LYS:NZ	1:C:3716:LYS:O	2.46	0.46
1:A:29:VAL:HG12	1:A:30:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:MET:SD	1:D:228:MET:N	2.88	0.46
1:D:3828:GLU:OE1	1:D:3828:GLU:N	2.40	0.46
1:B:3004:LEU:HB2	1:B:3005:PRO:HD3	1.97	0.46
1:B:3369:ARG:NH2	1:B:3405:ASP:OD2	2.48	0.46
1:B:3457:GLN:HA	1:B:3457:GLN:OE1	2.14	0.46
1:C:1792:GLY:N	1:C:1795:GLU:OE2	2.43	0.46
1:C:3004:LEU:HB2	1:C:3005:PRO:HD3	1.97	0.46
1:A:903:ARG:O	1:A:904:LEU:HD23	2.14	0.46
1:A:980:PRO:O	1:A:983:THR:OG1	2.26	0.46
1:D:4742:ASP:OD1	1:D:4742:ASP:C	2.54	0.46
1:B:2755:PHE:HD2	1:B:2814:LEU:HD11	1.81	0.46
1:B:2822:TRP:CD2	1:B:2875:MET:HE1	2.50	0.46
1:B:4207:GLN:HB3	1:B:4248:MET:HG2	1.97	0.46
1:C:894:TYR:HA	1:C:905:HIS:O	2.14	0.46
1:B:3112:ARG:HG3	1:B:3112:ARG:HH11	1.81	0.46
1:A:2747:ILE:C	1:A:2747:ILE:HD12	2.36	0.46
1:A:4207:GLN:HB3	1:A:4248:MET:HG2	1.96	0.46
1:D:2978:LEU:HD23	1:D:2978:LEU:O	2.15	0.46
1:C:3526:CYS:SG	1:C:3600:VAL:HG21	2.56	0.46
1:D:908:LEU:HD23	1:D:964:ASN:OD1	2.16	0.46
1:D:3112:ARG:HH11	1:D:3112:ARG:HG3	1.81	0.46
1:D:3362:THR:HG21	1:D:3409:LEU:HD22	1.97	0.46
1:D:3952:ARG:CZ	1:D:3952:ARG:HB3	2.46	0.46
1:B:3762:GLU:OE2	1:B:3765:ARG:NH2	2.49	0.46
1:C:2910:ASP:OD1	1:C:2911:THR:N	2.47	0.46
1:B:2753:ASP:O	1:B:2757:ASN:OD1	2.34	0.46
1:C:1455:THR:OG1	1:C:1457:ASP:OD1	2.32	0.46
1:A:2756:ILE:HD11	1:A:2814:LEU:HD12	1.98	0.46
1:A:3559:ASN:O	1:A:3560:LEU:HB2	2.15	0.46
1:D:460:LEU:CD1	1:D:464:GLU:OE2	2.61	0.46
1:D:3762:GLU:OE2	1:D:3765:ARG:NH2	2.49	0.46
1:B:2817:MET:HE2	1:B:2822:TRP:HE3	1.80	0.46
1:C:2755:PHE:HD2	1:C:2814:LEU:HD11	1.81	0.46
2:G:12:ASP:OD1	2:G:13:GLY:N	2.49	0.46
1:B:2394:ASP:OD1	1:B:2419:LEU:N	2.48	0.46
1:B:2879:LEU:CD1	1:B:2883:TYR:CE2	2.99	0.46
1:C:885:LEU:O	1:C:889:GLU:HG2	2.16	0.46
1:C:2822:TRP:CD2	1:C:2875:MET:HE1	2.51	0.46
1:A:153:PRO:HB3	1:A:158:ARG:HB2	1.98	0.45
1:A:921:TYR:O	1:A:924:GLN:HG3	2.17	0.45
1:A:3369:ARG:NH2	1:A:3405:ASP:OD2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3952:ARG:CZ	1:A:3952:ARG:HB3	2.46	0.45
1:D:2942:LEU:HA	1:D:2945:MET:HE2	1.99	0.45
1:C:2879:LEU:CD1	1:C:2883:TYR:CE2	2.99	0.45
1:C:2971:SER:HA	1:C:2974:PHE:CE2	2.51	0.45
1:A:1875:GLU:OE1	1:A:1876:GLU:N	2.49	0.45
1:D:2872:LEU:HD13	1:D:2928:LEU:HD11	1.98	0.45
1:B:3526:CYS:SG	1:B:3600:VAL:HG21	2.56	0.45
1:B:4155:GLU:OE1	1:B:4197:TYR:OH	2.16	0.45
1:C:366:LYS:HZ2	1:C:370:LEU:HD11	1.81	0.45
1:A:2931:LEU:O	1:A:2936:TYR:N	2.45	0.45
1:D:962:MET:O	1:D:964:ASN:N	2.49	0.45
1:D:973:LEU:HD13	1:D:1045:ARG:HB3	1.97	0.45
1:D:3526:CYS:SG	1:D:3600:VAL:HG21	2.56	0.45
1:B:4632:GLU:OE2	1:B:4634:THR:OG1	2.25	0.45
1:C:1281:GLN:O	1:C:1282:ASN:OD1	2.35	0.45
1:A:885:LEU:HA	1:A:888:ILE:HG12	1.98	0.45
1:A:4752:ASN:O	1:A:4754:ARG:NH1	2.49	0.45
1:D:1129:ARG:HB2	1:D:1129:ARG:NH1	2.32	0.45
1:D:1875:GLU:OE1	1:D:1876:GLU:N	2.49	0.45
1:B:2931:LEU:O	1:B:2936:TYR:N	2.45	0.45
1:C:2871:GLU:O	1:C:2875:MET:HG2	2.16	0.45
1:C:3112:ARG:HG3	1:C:3112:ARG:HH11	1.81	0.45
1:A:2441:THR:O	1:A:2445:GLN:HG2	2.16	0.45
1:A:2627:LEU:HD22	1:A:2641:PRO:HB3	1.98	0.45
1:A:4579:LYS:HG2	1:A:4580:VAL:N	2.30	0.45
1:D:885:LEU:HA	1:D:888:ILE:HG12	1.97	0.45
1:D:1281:GLN:O	1:D:1282:ASN:OD1	2.35	0.45
1:D:3714:LYS:NZ	1:D:3716:LYS:O	2.47	0.45
1:D:3955:SER:OG	1:D:4018:GLU:OE1	2.28	0.45
1:B:926:SER:O	1:B:929:THR:OG1	2.25	0.45
1:B:3108:VAL:HG22	1:B:3176:LEU:HB2	1.99	0.45
1:A:2394:ASP:OD1	1:A:2419:LEU:N	2.50	0.45
1:D:903:ARG:CZ	1:D:903:ARG:HA	2.46	0.45
1:D:1826:GLN:OE1	1:D:1826:GLN:HA	2.17	0.45
1:B:2974:PHE:CD1	1:B:2974:PHE:C	2.90	0.45
1:C:3380:LEU:C	1:C:3380:LEU:HD23	2.37	0.45
1:A:1129:ARG:NH1	1:A:1129:ARG:HB2	2.32	0.45
1:A:2213:VAL:HG11	1:A:2257:TYR:OH	2.17	0.45
1:A:2978:LEU:HD23	1:A:2982:VAL:HG23	1.99	0.45
1:D:885:LEU:O	1:D:889:GLU:HG2	2.15	0.45
1:D:978:LEU:CD1	1:D:982:GLN:HB3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:885:LEU:HA	1:B:888:ILE:HG12	1.99	0.45
1:B:894:TYR:HA	1:B:905:HIS:O	2.17	0.45
1:B:3683:GLU:O	1:B:3687:GLU:OE2	2.34	0.45
1:B:3952:ARG:CZ	1:B:3952:ARG:HB3	2.46	0.45
1:C:3762:GLU:OE2	1:C:3765:ARG:NH2	2.49	0.45
1:A:2974:PHE:CD1	1:A:2974:PHE:C	2.90	0.45
1:A:3526:CYS:SG	1:A:3600:VAL:HG21	2.56	0.45
1:B:2441:THR:O	1:B:2445:GLN:HG2	2.17	0.45
1:C:29:VAL:HG12	1:C:30:LEU:HD22	1.98	0.45
1:C:3952:ARG:CZ	1:C:3952:ARG:HB3	2.46	0.45
1:A:942:MET:HE3	1:A:942:MET:HA	1.98	0.45
1:A:2771:LYS:HB3	1:A:2776:TRP:HB2	1.99	0.45
1:A:3955:SER:OG	1:A:4018:GLU:OE1	2.28	0.45
1:D:894:TYR:HA	1:D:905:HIS:O	2.16	0.45
1:A:882:LEU:HD23	1:A:885:LEU:HD21	1.99	0.45
1:A:988:ARG:HG3	1:A:988:ARG:HH11	1.82	0.45
1:A:2971:SER:HA	1:A:2974:PHE:CE2	2.52	0.45
1:D:2394:ASP:OD1	1:D:2419:LEU:N	2.50	0.45
1:D:2441:THR:O	1:D:2445:GLN:HG2	2.16	0.45
1:D:2971:SER:HA	1:D:2974:PHE:CE2	2.52	0.45
1:D:4752:ASN:O	1:D:4754:ARG:NH1	2.50	0.45
1:B:885:LEU:O	1:B:889:GLU:HG2	2.16	0.45
1:B:2215:VAL:HG21	1:B:2229:MET:HE2	1.99	0.45
1:B:4769:ILE:HD11	1:B:4771:VAL:HG23	1.99	0.45
1:C:2441:THR:O	1:C:2445:GLN:HG2	2.17	0.45
1:D:988:ARG:HG3	1:D:988:ARG:HH11	1.82	0.44
1:D:3861:MET:SD	1:D:3868:VAL:CG2	3.06	0.44
1:B:988:ARG:HG3	1:B:988:ARG:HH11	1.82	0.44
1:B:1113:ASP:OD1	1:B:1113:ASP:N	2.45	0.44
1:B:2944:ASP:OD1	1:B:2945:MET:SD	2.76	0.44
1:C:2929:LYS:HB3	1:C:2933:MET:HE1	1.99	0.44
1:C:2974:PHE:CD1	1:C:2974:PHE:C	2.90	0.44
1:A:894:TYR:HA	1:A:905:HIS:O	2.17	0.44
1:A:1455:THR:OG1	1:A:1457:ASP:OD1	2.32	0.44
1:D:267:ARG:NH2	1:D:332:VAL:O	2.47	0.44
1:D:2747:ILE:HD12	1:D:2747:ILE:C	2.38	0.44
1:D:2761:GLU:OE1	1:D:2803:LYS:NZ	2.38	0.44
1:D:3683:GLU:O	1:D:3687:GLU:OE2	2.34	0.44
1:B:1281:GLN:O	1:B:1282:ASN:OD1	2.35	0.44
1:B:2747:ILE:HD12	1:B:2747:ILE:C	2.38	0.44
1:A:2246:GLN:OE1	1:A:3868:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3683:GLU:O	1:A:3687:GLU:OE2	2.34	0.44
1:A:4155:GLU:OE1	1:A:4197:TYR:OH	2.16	0.44
1:D:2822:TRP:CD2	1:D:2875:MET:HE1	2.53	0.44
1:D:3447:SER:O	1:D:3453:LYS:NZ	2.44	0.44
1:B:153:PRO:HB3	1:B:158:ARG:HB2	1.98	0.44
1:C:3088:ILE:H	1:C:3088:ILE:CD1	2.28	0.44
1:A:864:LEU:HD13	1:A:865:PRO:O	2.18	0.44
1:D:153:PRO:HB3	1:D:158:ARG:HB2	1.98	0.44
1:D:2944:ASP:OD1	1:D:2945:MET:SD	2.76	0.44
1:B:2971:SER:HA	1:B:2974:PHE:CE2	2.52	0.44
1:C:2747:ILE:C	1:C:2747:ILE:HD12	2.38	0.44
1:A:1826:GLN:OE1	1:A:1826:GLN:HA	2.17	0.44
1:D:882:LEU:HD23	1:D:885:LEU:HD21	1.98	0.44
1:D:2226:PHE:N	1:D:2227:PRO:HD3	2.33	0.44
1:D:3736:LEU:HD12	1:D:3766:LEU:HD22	2.00	0.44
1:D:4684:LEU:HD12	1:D:4685:TYR:CE2	2.53	0.44
1:B:908:LEU:O	1:B:966:TYR:OH	2.30	0.44
1:B:2627:LEU:HD22	1:B:2641:PRO:HB3	1.99	0.44
1:C:153:PRO:HB3	1:C:158:ARG:HB2	1.99	0.44
1:C:885:LEU:HA	1:C:888:ILE:HG12	2.00	0.44
1:C:2944:ASP:OD1	1:C:2945:MET:SD	2.76	0.44
1:A:2438:ALA:HB2	1:A:2510:VAL:HG22	1.99	0.44
1:D:2974:PHE:CD1	1:D:2974:PHE:C	2.90	0.44
1:C:893:THR:CG2	1:C:904:LEU:HD23	2.35	0.44
1:C:988:ARG:HG3	1:C:988:ARG:HH11	1.82	0.44
1:C:2438:ALA:HB2	1:C:2510:VAL:HG22	1.99	0.44
1:B:3088:ILE:H	1:B:3088:ILE:CD1	2.29	0.44
1:B:3861:MET:SD	1:B:3868:VAL:CG2	3.05	0.44
1:D:2627:LEU:HD22	1:D:2641:PRO:HB3	1.99	0.44
1:D:4769:ILE:HD11	1:D:4771:VAL:HG23	1.99	0.44
1:C:3410:TYR:N	1:C:3411:PRO:HD2	2.33	0.44
1:B:3684:GLN:HA	1:B:3687:GLU:OE2	2.18	0.44
1:C:956:LEU:HD22	1:C:960:TYR:CD2	2.52	0.44
1:C:2949:THR:OG1	1:C:2954:LYS:NZ	2.51	0.44
1:A:974:SER:O	1:A:977:ARG:NH2	2.50	0.43
1:A:3240:MET:HA	1:A:3240:MET:HE2	2.00	0.43
1:B:2213:VAL:HG11	1:B:2257:TYR:OH	2.18	0.43
1:B:4684:LEU:HD12	1:B:4685:TYR:CE2	2.53	0.43
1:C:2394:ASP:OD1	1:C:2419:LEU:N	2.51	0.43
1:C:4684:LEU:HD12	1:C:4685:TYR:CE2	2.53	0.43
1:D:868:LEU:HD23	1:D:871:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:980:PRO:O	1:B:983:THR:OG1	2.27	0.43
1:B:3176:LEU:HD11	1:B:3184:VAL:HG22	2.00	0.43
4:B:8003:PCW:H483	4:C:5103:PCW:H271	1.99	0.43
1:C:882:LEU:HD23	1:C:885:LEU:HD21	2.00	0.43
1:C:893:THR:HA	1:C:962:MET:HE3	1.99	0.43
1:C:2226:PHE:N	1:C:2227:PRO:HD3	2.33	0.43
1:C:2246:GLN:OE1	1:C:3868:VAL:HG12	2.18	0.43
1:C:3541:TYR:OH	1:C:3547:ASP:OD1	2.17	0.43
1:A:2265:GLY:C	1:A:2266:LEU:HD12	2.38	0.43
1:D:893:THR:HA	1:D:962:MET:SD	2.58	0.43
1:D:3684:GLN:HA	1:D:3687:GLU:OE2	2.18	0.43
1:B:1129:ARG:HB2	1:B:1129:ARG:NH1	2.32	0.43
1:B:1826:GLN:HA	1:B:1826:GLN:OE1	2.18	0.43
1:B:4090:LEU:N	1:B:4090:LEU:HD12	2.33	0.43
1:C:926:SER:O	1:C:930:LEU:CD2	2.66	0.43
1:C:1129:ARG:NH1	1:C:1129:ARG:HB2	2.32	0.43
1:C:1826:GLN:HA	1:C:1826:GLN:OE1	2.17	0.43
1:C:2940:ARG:CB	1:C:2944:ASP:HB3	2.48	0.43
1:C:4090:LEU:HD12	1:C:4090:LEU:N	2.33	0.43
1:A:973:LEU:HD13	1:A:1045:ARG:HB3	2.00	0.43
1:A:978:LEU:CD2	1:A:1045:ARG:HD3	2.48	0.43
1:A:978:LEU:HD23	1:A:1045:ARG:HD3	1.98	0.43
1:A:2755:PHE:HD2	1:A:2814:LEU:HD11	1.83	0.43
1:D:2978:LEU:HD23	1:D:2982:VAL:HG23	2.01	0.43
1:A:1435:TYR:HB2	1:A:1573:ILE:HG21	2.00	0.43
1:A:1964:GLU:HA	1:A:3651:CYS:SG	2.59	0.43
1:A:4684:LEU:HD12	1:A:4685:TYR:CE2	2.54	0.43
1:D:723:TRP:CZ2	1:D:728:ALA:HB2	2.54	0.43
1:B:1435:TYR:HB2	1:B:1573:ILE:HG21	2.01	0.43
1:B:2226:PHE:N	1:B:2227:PRO:HD3	2.33	0.43
1:B:2871:GLU:O	1:B:2875:MET:HG2	2.17	0.43
1:B:3236:SER:OG	1:B:3239:GLU:OE2	2.34	0.43
1:C:872:ARG:NH2	1:C:923:LEU:O	2.47	0.43
1:C:2596:LEU:HD21	1:C:2604:ILE:CD1	2.49	0.43
1:C:2627:LEU:HD22	1:C:2641:PRO:HB3	1.98	0.43
1:C:2931:LEU:O	1:C:2936:TYR:N	2.49	0.43
1:C:3974:GLY:N	1:C:3975:PRO:HA	2.34	0.43
1:A:723:TRP:CZ2	1:A:728:ALA:HB2	2.54	0.43
1:A:3684:GLN:HA	1:A:3687:GLU:OE2	2.18	0.43
1:D:843:PRO:HG2	1:D:1072:ARG:O	2.19	0.43
1:D:1964:GLU:HA	1:D:3651:CYS:SG	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2213:VAL:HG11	1:D:2257:TYR:OH	2.18	0.43
1:D:3410:TYR:N	1:D:3411:PRO:HD2	2.34	0.43
1:B:3974:GLY:N	1:B:3975:PRO:HA	2.33	0.43
1:D:2438:ALA:HB2	1:D:2510:VAL:HG22	1.99	0.43
1:D:4932:GLY:HA2	1:C:4935:ILE:HG12	2.01	0.43
1:B:729:ARG:NH2	1:B:1490:CYS:SG	2.92	0.43
1:B:1964:GLU:HA	1:B:3651:CYS:SG	2.59	0.43
1:C:4225:VAL:HG11	1:C:4948:VAL:HA	2.00	0.43
1:A:1531:THR:HG22	1:A:1536:GLU:HA	2.00	0.43
1:A:2927:LEU:C	1:A:2927:LEU:HD23	2.39	0.43
1:A:3410:TYR:N	1:A:3411:PRO:HD2	2.33	0.43
1:A:4090:LEU:N	1:A:4090:LEU:HD12	2.33	0.43
1:A:4932:GLY:HA2	1:D:4935:ILE:HG12	2.01	0.43
1:D:2940:ARG:CB	1:D:2944:ASP:HB3	2.49	0.43
1:B:2940:ARG:CB	1:B:2944:ASP:HB3	2.48	0.43
1:B:4225:VAL:HG11	1:B:4948:VAL:HA	1.99	0.43
1:C:1964:GLU:HA	1:C:3651:CYS:SG	2.59	0.43
1:A:2922:GLU:OE1	1:A:2925:GLN:NE2	2.50	0.43
1:A:2950:SER:OG	1:A:2951:SER:N	2.52	0.43
1:A:3974:GLY:N	1:A:3975:PRO:HA	2.33	0.43
1:D:872:ARG:HE	1:D:923:LEU:HB3	1.84	0.43
1:D:2265:GLY:C	1:D:2266:LEU:HD12	2.39	0.43
1:D:3952:ARG:HB3	1:D:3952:ARG:NH1	2.34	0.43
1:B:500:THR:HG23	1:B:503:HIS:H	1.84	0.43
1:B:2265:GLY:C	1:B:2266:LEU:HD12	2.39	0.43
1:B:2949:THR:OG1	1:B:2954:LYS:NZ	2.51	0.43
1:C:2777:SER:C	1:C:2792:LEU:HD21	2.38	0.43
1:C:2868:LEU:HD21	1:C:2928:LEU:HD12	2.01	0.43
1:C:2950:SER:OG	1:C:2951:SER:N	2.52	0.43
1:A:843:PRO:HG2	1:A:1072:ARG:O	2.19	0.43
1:A:932:THR:O	1:A:936:LEU:HD23	2.19	0.43
1:A:2226:PHE:N	1:A:2227:PRO:HD3	2.33	0.43
1:A:4935:ILE:HG12	1:B:4932:GLY:HA2	2.01	0.43
1:D:366:LYS:HZ2	1:D:370:LEU:HD11	1.83	0.43
1:D:3088:ILE:H	1:D:3088:ILE:CD1	2.29	0.43
1:B:267:ARG:NH2	1:B:332:VAL:O	2.48	0.43
1:B:2868:LEU:HD21	1:B:2928:LEU:HD12	2.00	0.43
1:B:2927:LEU:C	1:B:2927:LEU:HD23	2.40	0.43
1:B:3410:TYR:N	1:B:3411:PRO:HD2	2.34	0.43
1:C:872:ARG:HD3	1:C:923:LEU:HD22	2.01	0.43
1:C:1113:ASP:OD1	1:C:1113:ASP:N	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:GLU:O	1:A:1056:PRO:C	2.57	0.42
1:D:871:ILE:HD13	1:D:1052:TYR:CZ	2.54	0.42
1:D:2723:LYS:H	1:D:2723:LYS:HD3	1.84	0.42
1:D:2949:THR:OG1	1:D:2954:LYS:NZ	2.51	0.42
1:B:1055:GLU:O	1:B:1056:PRO:C	2.57	0.42
1:B:2723:LYS:HD3	1:B:2723:LYS:H	1.84	0.42
1:C:323:LYS:NZ	1:C:326:VAL:HG13	2.34	0.42
1:C:649:ILE:HG23	1:C:815:ALA:HB3	2.01	0.42
1:C:2265:GLY:C	1:C:2266:LEU:HD12	2.39	0.42
1:A:893:THR:HG23	1:A:904:LEU:CD2	2.38	0.42
1:A:2445:GLN:HA	1:A:2445:GLN:OE1	2.19	0.42
1:A:2723:LYS:H	1:A:2723:LYS:HD3	1.85	0.42
1:A:4059:GLU:HG2	1:A:4169:LEU:HD13	2.01	0.42
1:D:729:ARG:NH2	1:D:1490:CYS:SG	2.92	0.42
1:D:4059:GLU:HG2	1:D:4169:LEU:HD13	2.01	0.42
1:B:760:ILE:O	1:B:760:ILE:HG23	2.19	0.42
1:B:2825:GLU:O	1:B:2828:ARG:CZ	2.66	0.42
1:B:2872:LEU:HD13	1:B:2928:LEU:HD11	2.00	0.42
1:B:3952:ARG:HB3	1:B:3952:ARG:NH1	2.34	0.42
1:C:500:THR:HG23	1:C:503:HIS:H	1.84	0.42
1:C:2605:GLU:O	1:C:2609:MET:HG2	2.20	0.42
1:C:3736:LEU:HD12	1:C:3766:LEU:HD22	2.01	0.42
1:A:3108:VAL:HG22	1:A:3176:LEU:HB2	2.01	0.42
1:A:3952:ARG:HB3	1:A:3952:ARG:NH1	2.34	0.42
1:D:760:ILE:O	1:D:760:ILE:HG23	2.19	0.42
1:D:1055:GLU:O	1:D:1056:PRO:C	2.57	0.42
1:D:2871:GLU:O	1:D:2875:MET:HG2	2.19	0.42
1:D:3736:LEU:HD13	1:D:3809:ASN:HB3	2.02	0.42
1:B:2908:PRO:O	1:B:2911:THR:OG1	2.28	0.42
1:C:723:TRP:CZ2	1:C:728:ALA:HB2	2.54	0.42
1:C:2771:LYS:HB3	1:C:2776:TRP:HB2	2.01	0.42
1:C:2978:LEU:HD23	1:C:2982:VAL:HG23	2.01	0.42
1:C:4161:PRO:N	1:C:4164:ARG:NH2	2.67	0.42
1:A:460:LEU:HD13	1:A:464:GLU:HG2	2.02	0.42
1:A:902:LYS:HZ2	1:A:904:LEU:HB2	1.83	0.42
1:A:978:LEU:CD1	1:A:982:GLN:HB3	2.50	0.42
1:A:3108:VAL:HG13	1:A:3176:LEU:HB2	2.00	0.42
1:A:4161:PRO:N	1:A:4164:ARG:NH2	2.67	0.42
1:B:864:LEU:HD21	1:B:868:LEU:HB3	2.01	0.42
1:B:882:LEU:HD23	1:B:885:LEU:HD21	2.00	0.42
1:B:2438:ALA:HB2	1:B:2510:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:MET:SD	1:C:228:MET:N	2.93	0.42
1:C:2744:LEU:HD13	1:C:2744:LEU:O	2.20	0.42
1:C:3227:GLU:O	1:C:3228:ARG:HB2	2.19	0.42
1:C:3952:ARG:HB3	1:C:3952:ARG:NH1	2.34	0.42
1:A:962:MET:HE3	1:A:963:SER:OG	2.19	0.42
1:A:2605:GLU:O	1:A:2609:MET:HG2	2.20	0.42
1:A:3736:LEU:HD12	1:A:3766:LEU:HD22	2.01	0.42
1:D:649:ILE:HG23	1:D:815:ALA:HB3	2.01	0.42
1:D:864:LEU:HD21	1:D:868:LEU:HB3	2.01	0.42
1:D:942:MET:HE3	1:D:942:MET:HA	2.01	0.42
1:D:1822:ARG:HB3	1:D:1822:ARG:HH11	1.85	0.42
1:D:2605:GLU:O	1:D:2609:MET:HG2	2.20	0.42
1:D:4090:LEU:N	1:D:4090:LEU:HD12	2.33	0.42
1:B:691:GLU:OE1	1:B:691:GLU:HA	2.20	0.42
1:B:878:ASN:C	1:B:878:ASN:HD22	2.22	0.42
1:B:2445:GLN:OE1	1:B:2445:GLN:HA	2.19	0.42
1:B:4935:ILE:HG12	1:C:4932:GLY:HA2	2.01	0.42
1:C:978:LEU:CD2	1:C:1045:ARG:HD3	2.50	0.42
1:C:1822:ARG:HB3	1:C:1822:ARG:HH11	1.85	0.42
1:C:2872:LEU:HD13	1:C:2928:LEU:HD11	2.00	0.42
1:A:156:LYS:HE2	1:A:156:LYS:HA	2.02	0.42
1:A:760:ILE:HG23	1:A:760:ILE:O	2.19	0.42
1:A:983:THR:O	1:A:986:VAL:HG12	2.19	0.42
1:A:2767:TRP:CZ3	1:A:2791:MET:HE1	2.54	0.42
1:A:2866:VAL:HG21	1:A:2933:MET:HE3	2.01	0.42
1:A:3227:GLU:O	1:A:3228:ARG:HB2	2.19	0.42
1:A:3861:MET:SD	1:A:3870:ASN:OD1	2.78	0.42
1:A:4769:ILE:HD11	1:A:4771:VAL:HG23	2.02	0.42
1:D:323:LYS:NZ	1:D:326:VAL:HG13	2.35	0.42
1:D:2927:LEU:C	1:D:2927:LEU:HD23	2.40	0.42
1:B:323:LYS:NZ	1:B:326:VAL:HG13	2.34	0.42
1:B:2605:GLU:O	1:B:2609:MET:HG2	2.20	0.42
1:C:843:PRO:HG2	1:C:1072:ARG:O	2.19	0.42
1:C:914:LEU:O	1:C:919:ARG:NH2	2.41	0.42
1:C:980:PRO:O	1:C:983:THR:OG1	2.27	0.42
1:C:1435:TYR:HB2	1:C:1573:ILE:HG21	2.01	0.42
1:C:2445:GLN:HA	1:C:2445:GLN:OE1	2.19	0.42
1:C:3869:ILE:HD11	1:C:3872:GLN:O	2.20	0.42
1:A:2940:ARG:HB2	1:A:2944:ASP:HB3	2.00	0.42
1:D:932:THR:O	1:D:936:LEU:HD23	2.20	0.42
1:D:983:THR:O	1:D:986:VAL:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:986:VAL:HG23	1:D:1044:VAL:HG21	2.02	0.42
1:D:2950:SER:OG	1:D:2951:SER:N	2.53	0.42
1:D:3176:LEU:HD11	1:D:3184:VAL:HG22	2.02	0.42
1:B:723:TRP:CZ2	1:B:728:ALA:HB2	2.54	0.42
1:B:3227:GLU:O	1:B:3228:ARG:HB2	2.20	0.42
1:B:4161:PRO:N	1:B:4164:ARG:NH2	2.67	0.42
1:C:2938:VAL:HB	1:C:2940:ARG:NH2	2.35	0.42
1:A:961:MET:HG2	1:A:967:LYS:HE2	2.01	0.42
1:A:2944:ASP:OD1	1:A:2945:MET:SD	2.78	0.42
1:A:3160:ASP:OD2	1:A:3223:LYS:NZ	2.52	0.42
1:A:4225:VAL:HG11	1:A:4948:VAL:HA	2.00	0.42
1:D:276:ARG:HG2	1:D:276:ARG:HH11	1.84	0.42
1:D:870:ARG:NH2	1:D:1052:TYR:OH	2.53	0.42
1:D:2225:ARG:HD3	1:D:2225:ARG:N	2.34	0.42
1:D:2596:LEU:HD21	1:D:2604:ILE:CD1	2.50	0.42
1:D:3227:GLU:O	1:D:3228:ARG:HB2	2.19	0.42
1:D:4225:VAL:HG11	1:D:4948:VAL:HA	2.01	0.42
1:B:2978:LEU:HD23	1:B:2982:VAL:HG23	2.01	0.42
1:C:729:ARG:NH2	1:C:1490:CYS:SG	2.93	0.42
1:C:760:ILE:HG23	1:C:760:ILE:O	2.20	0.42
1:C:4769:ILE:C	1:C:4769:ILE:HD12	2.40	0.42
1:A:3736:LEU:HD13	1:A:3809:ASN:HB3	2.02	0.42
1:D:961:MET:HG2	1:D:967:LYS:HE2	2.01	0.42
1:D:2825:GLU:O	1:D:2828:ARG:CZ	2.68	0.42
1:D:3974:GLY:N	1:D:3975:PRO:HA	2.33	0.42
1:B:156:LYS:HE2	1:B:156:LYS:HA	2.02	0.42
1:B:868:LEU:HD13	1:B:930:LEU:HB3	2.02	0.42
1:B:932:THR:O	1:B:936:LEU:HD23	2.20	0.42
1:B:2938:VAL:HB	1:B:2940:ARG:NH2	2.35	0.42
1:B:2950:SER:OG	1:B:2951:SER:N	2.52	0.42
1:C:1055:GLU:O	1:C:1056:PRO:C	2.57	0.42
1:C:1531:THR:HG22	1:C:1536:GLU:HA	2.01	0.42
1:C:2927:LEU:C	1:C:2927:LEU:HD23	2.40	0.42
1:C:4893:GLY:N	1:C:4897:ASP:OD2	2.46	0.42
1:A:500:THR:HG23	1:A:503:HIS:H	1.84	0.42
1:A:2225:ARG:HD3	1:A:2225:ARG:N	2.35	0.42
1:A:2940:ARG:O	1:A:2943:LYS:NZ	2.53	0.42
1:D:942:MET:HE2	1:D:943:ALA:H	1.85	0.42
1:D:978:LEU:HD23	1:D:1045:ARG:HD3	2.01	0.42
1:D:1435:TYR:HB2	1:D:1573:ILE:HG21	2.01	0.42
1:D:2293:GLU:O	1:D:2297:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2714:ASP:OD1	1:D:2714:ASP:N	2.50	0.42
1:D:3366:LEU:HD13	1:D:3406:LEU:HD23	2.02	0.42
1:D:4161:PRO:N	1:D:4164:ARG:NH2	2.67	0.42
1:B:2942:LEU:HA	1:B:2945:MET:HE2	2.01	0.42
1:C:864:LEU:HD21	1:C:868:LEU:HB3	2.01	0.42
1:C:2213:VAL:HG11	1:C:2257:TYR:OH	2.19	0.42
4:C:5103:PCW:H2O	4:C:5103:PCW:H462	2.01	0.42
1:D:500:THR:HG23	1:D:503:HIS:H	1.84	0.41
1:D:2744:LEU:HD13	1:D:2744:LEU:O	2.20	0.41
1:C:3861:MET:SD	1:C:3870:ASN:OD1	2.78	0.41
1:A:276:ARG:HG2	1:A:276:ARG:HH11	1.85	0.41
1:D:1455:THR:OG1	1:D:1457:ASP:OD1	2.32	0.41
1:B:1531:THR:HG22	1:B:1536:GLU:HA	2.01	0.41
1:C:156:LYS:HA	1:C:156:LYS:HE2	2.02	0.41
1:C:878:ASN:C	1:C:878:ASN:HD22	2.22	0.41
1:C:932:THR:O	1:C:936:LEU:HD23	2.20	0.41
1:C:947:ALA:O	1:C:951:LEU:HD13	2.18	0.41
1:C:2723:LYS:H	1:C:2723:LYS:HD3	1.84	0.41
1:A:885:LEU:O	1:A:889:GLU:HG2	2.21	0.41
1:A:2872:LEU:HD22	1:A:2928:LEU:HD11	2.02	0.41
1:D:1481:GLN:O	1:D:1481:GLN:HG2	2.20	0.41
1:D:1531:THR:HG22	1:D:1536:GLU:HA	2.01	0.41
1:D:2868:LEU:HD21	1:D:2928:LEU:HD12	2.02	0.41
1:B:843:PRO:HG2	1:B:1072:ARG:O	2.19	0.41
1:B:870:ARG:NH2	1:B:1052:TYR:OH	2.53	0.41
1:B:914:LEU:O	1:B:919:ARG:NH2	2.41	0.41
1:C:139:GLN:NE2	1:C:141:ASP:O	2.53	0.41
1:C:2942:LEU:HA	1:C:2945:MET:HE2	2.02	0.41
1:A:2769:PHE:O	1:A:2773:GLN:HG2	2.21	0.41
1:A:4833:LYS:O	1:A:4837:MET:HG2	2.19	0.41
1:D:32:GLU:OE1	1:D:32:GLU:N	2.54	0.41
1:D:2160:LEU:HD13	1:D:2204:MET:HG2	2.02	0.41
1:B:2480:LEU:HD23	1:B:2480:LEU:HA	1.96	0.41
1:B:2768:ALA:O	1:B:2772:ILE:HG12	2.21	0.41
1:C:1481:GLN:HG2	1:C:1481:GLN:O	2.20	0.41
1:C:3919:ILE:N	1:C:3919:ILE:HD12	2.36	0.41
1:A:366:LYS:HZ2	1:A:370:LEU:HD11	1.85	0.41
1:D:882:LEU:O	1:D:885:LEU:HG	2.21	0.41
1:B:1822:ARG:HB3	1:B:1822:ARG:HH11	1.85	0.41
1:B:2225:ARG:HD3	1:B:2225:ARG:N	2.35	0.41
1:C:691:GLU:HA	1:C:691:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2225:ARG:HD3	1:C:2225:ARG:N	2.35	0.41
1:C:2752:LEU:HD13	1:C:2814:LEU:HD13	2.01	0.41
1:A:887:ARG:HA	1:A:887:ARG:NE	2.36	0.41
1:A:2825:GLU:O	1:A:2828:ARG:CZ	2.68	0.41
1:A:3365:ARG:HE	1:A:3365:ARG:HB3	1.77	0.41
1:B:2791:MET:SD	1:B:2792:LEU:N	2.93	0.41
1:B:2863:LEU:CD2	1:B:2933:MET:HE1	2.51	0.41
1:B:3757:GLU:HA	1:B:3757:GLU:OE1	2.21	0.41
1:B:3919:ILE:HD12	1:B:3919:ILE:N	2.36	0.41
1:C:868:LEU:HD13	1:C:930:LEU:HB3	2.03	0.41
1:C:2754:SER:HA	1:C:2757:ASN:OD1	2.20	0.41
1:C:4578:TYR:CE2	1:C:4628:TYR:HB3	2.53	0.41
1:A:3291:GLU:O	1:A:3291:GLU:CG	2.68	0.41
1:D:461:GLN:O	1:D:465:LYS:HB2	2.20	0.41
1:D:2445:GLN:OE1	1:D:2445:GLN:HA	2.20	0.41
1:D:2931:LEU:HD22	1:D:2936:TYR:CB	2.51	0.41
1:D:3291:GLU:O	1:D:3291:GLU:CG	2.68	0.41
1:B:962:MET:O	1:B:964:ASN:N	2.54	0.41
1:B:3111:LEU:HD21	1:B:3187:LEU:HD22	2.03	0.41
1:B:4059:GLU:HG2	1:B:4169:LEU:HD13	2.01	0.41
1:C:903:ARG:O	1:C:904:LEU:HD23	2.20	0.41
1:C:3366:LEU:HD13	1:C:3406:LEU:HD23	2.03	0.41
1:C:3736:LEU:HD13	1:C:3809:ASN:HB3	2.02	0.41
1:C:3757:GLU:OE1	1:C:3757:GLU:HA	2.21	0.41
1:A:649:ILE:HG23	1:A:815:ALA:HB3	2.01	0.41
1:A:2701:MET:HB3	1:A:2702:PRO:HD3	2.03	0.41
1:A:3919:ILE:HD12	1:A:3919:ILE:N	2.36	0.41
1:D:156:LYS:HE2	1:D:156:LYS:HA	2.02	0.41
1:D:1874:ARG:HB3	1:D:1874:ARG:NH1	2.36	0.41
1:D:2701:MET:HB3	1:D:2702:PRO:HD3	2.03	0.41
1:D:3944:ASP:OD1	1:D:3944:ASP:C	2.59	0.41
1:B:903:ARG:O	1:B:904:LEU:HD23	2.21	0.41
1:B:2767:TRP:O	1:B:2771:LYS:HG3	2.20	0.41
1:B:3291:GLU:O	1:B:3291:GLU:CG	2.68	0.41
1:C:4059:GLU:HG2	1:C:4169:LEU:HD13	2.02	0.41
1:A:958:LYS:HA	1:A:961:MET:HB2	2.02	0.41
1:A:986:VAL:HG21	1:A:1041:CYS:HA	2.02	0.41
1:A:3294:PRO:HB2	1:A:3297:LEU:HB2	2.03	0.41
1:A:3366:LEU:HD13	1:A:3406:LEU:HD23	2.03	0.41
1:A:3944:ASP:OD1	1:A:3944:ASP:C	2.59	0.41
1:D:903:ARG:O	1:D:904:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2789:HIS:CB	1:D:2792:LEU:HD23	2.50	0.41
1:B:649:ILE:HG23	1:B:815:ALA:HB3	2.02	0.41
1:B:882:LEU:O	1:B:885:LEU:HG	2.21	0.41
1:B:958:LYS:HA	1:B:961:MET:HB2	2.02	0.41
1:B:986:VAL:HG23	1:B:1044:VAL:HG21	2.02	0.41
1:B:2883:TYR:CE2	1:B:2923:LYS:HE3	2.56	0.41
1:B:3076:LEU:HD12	1:B:3076:LEU:HA	1.96	0.41
1:B:3366:LEU:HD13	1:B:3406:LEU:HD23	2.03	0.41
1:B:3736:LEU:HD12	1:B:3766:LEU:HD22	2.02	0.41
1:B:4927:LEU:O	1:B:4931:GLN:OE1	2.39	0.41
1:C:2701:MET:HB3	1:C:2702:PRO:HD3	2.03	0.41
1:C:2748:ILE:O	1:C:2748:ILE:HG23	2.21	0.41
1:C:2817:MET:CE	1:C:2938:VAL:HG11	2.50	0.41
1:C:2873:GLN:O	1:C:2877:GLU:HG2	2.21	0.41
1:C:3294:PRO:HB2	1:C:3297:LEU:HB2	2.03	0.41
1:C:4575:LEU:O	1:C:4578:TYR:HB2	2.21	0.41
1:A:869:GLU:O	1:A:869:GLU:OE2	2.39	0.41
1:A:882:LEU:O	1:A:885:LEU:HG	2.21	0.41
1:A:926:SER:O	1:A:929:THR:OG1	2.25	0.41
1:A:1034:ARG:HH11	1:A:1034:ARG:HB3	1.86	0.41
1:A:2941:GLY:O	1:A:2945:MET:SD	2.79	0.41
1:A:3828:GLU:OE1	1:A:3828:GLU:N	2.40	0.41
1:A:4578:TYR:CE2	1:A:4628:TYR:HB3	2.53	0.41
1:A:4642:ARG:NH1	1:A:4642:ARG:HG2	2.36	0.41
1:D:962:MET:HE3	1:D:963:SER:OG	2.20	0.41
1:D:2754:SER:HA	1:D:2757:ASN:OD1	2.21	0.41
1:D:2873:GLN:O	1:D:2877:GLU:HG2	2.21	0.41
1:D:3160:ASP:OD2	1:D:3223:LYS:NZ	2.52	0.41
1:B:1997:ARG:HB2	1:B:1997:ARG:NH1	2.36	0.41
1:B:2873:GLN:O	1:B:2877:GLU:HG2	2.21	0.41
1:B:3294:PRO:HB2	1:B:3297:LEU:HB2	2.03	0.41
1:B:3736:LEU:HD13	1:B:3809:ASN:HB3	2.03	0.41
1:C:986:VAL:HG23	1:C:1044:VAL:HG21	2.02	0.41
1:C:1034:ARG:HB3	1:C:1034:ARG:HH11	1.86	0.41
1:C:1997:ARG:HB2	1:C:1997:ARG:NH1	2.36	0.41
1:C:2160:LEU:HD13	1:C:2204:MET:HG2	2.03	0.41
1:C:3037:LYS:O	1:C:3040:ILE:HG22	2.21	0.41
1:C:4869:GLU:OE2	1:C:4869:GLU:HA	2.21	0.41
1:A:323:LYS:NZ	1:A:326:VAL:HG13	2.35	0.40
1:A:3037:LYS:O	1:A:3040:ILE:HG22	2.21	0.40
1:A:3568:PRO:HD2	1:A:3569:SER:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3576:LEU:HD23	1:B:1220:LEU:HD22	2.03	0.40
1:A:4869:GLU:HA	1:A:4869:GLU:OE2	2.22	0.40
1:D:1034:ARG:HH11	1:D:1034:ARG:HB3	1.86	0.40
1:D:2748:ILE:HG23	1:D:2748:ILE:O	2.21	0.40
1:D:2826:LYS:NZ	1:D:2934:ASN:O	2.46	0.40
1:B:2259:LEU:HA	1:B:2262:SER:HG	1.86	0.40
1:B:2306:CYS:HG	1:B:2332:TYR:HE2	1.69	0.40
1:B:2514:GLU:OE1	1:B:2514:GLU:N	2.49	0.40
1:B:2817:MET:CE	1:B:2938:VAL:HG11	2.50	0.40
1:C:2769:PHE:O	1:C:2773:GLN:HG2	2.21	0.40
1:A:1874:ARG:HB3	1:A:1874:ARG:NH1	2.36	0.40
1:A:2160:LEU:HD13	1:A:2204:MET:HG2	2.02	0.40
1:A:3545:ASP:OD2	1:A:3550:VAL:HG23	2.22	0.40
1:A:3757:GLU:OE1	1:A:3757:GLU:CA	2.70	0.40
1:A:3757:GLU:OE1	1:A:3757:GLU:HA	2.21	0.40
1:A:3869:ILE:HD11	1:A:3872:GLN:O	2.21	0.40
1:B:865:PRO:HD2	1:B:868:LEU:HD12	2.03	0.40
1:B:2701:MET:HB3	1:B:2702:PRO:HD3	2.03	0.40
1:B:3176:LEU:HD12	1:B:3176:LEU:O	2.21	0.40
1:B:4869:GLU:OE2	1:B:4869:GLU:HA	2.21	0.40
1:C:882:LEU:O	1:C:885:LEU:HG	2.21	0.40
1:C:1156:LEU:HD22	1:C:1185:ILE:HD12	2.03	0.40
1:C:1793:ALA:O	1:C:1794:THR:OG1	2.35	0.40
1:C:2866:VAL:HG21	1:C:2933:MET:CE	2.51	0.40
1:C:3291:GLU:O	1:C:3291:GLU:CG	2.68	0.40
1:C:4927:LEU:O	1:C:4931:GLN:OE1	2.39	0.40
1:A:2922:GLU:O	1:A:2926:GLU:HG2	2.22	0.40
1:D:1792:GLY:N	1:D:1795:GLU:OE2	2.43	0.40
1:D:1994:ARG:HA	1:D:1997:ARG:HH12	1.86	0.40
1:D:2755:PHE:CD2	1:D:2814:LEU:HD11	2.55	0.40
1:D:3757:GLU:HA	1:D:3757:GLU:OE1	2.21	0.40
1:D:3919:ILE:HD12	1:D:3919:ILE:N	2.36	0.40
1:D:4869:GLU:HA	1:D:4869:GLU:OE2	2.21	0.40
1:B:978:LEU:CD2	1:B:1045:ARG:HD3	2.50	0.40
1:B:4578:TYR:CE2	1:B:4628:TYR:HB3	2.53	0.40
1:C:978:LEU:CD1	1:C:982:GLN:HB3	2.52	0.40
1:C:2259:LEU:HA	1:C:2262:SER:HG	1.86	0.40
1:C:4642:ARG:NH1	1:C:4642:ARG:HG2	2.36	0.40
1:C:4693:ASP:OD1	1:C:4694:ASP:N	2.54	0.40
1:C:4763:LEU:HD13	1:C:4763:LEU:C	2.41	0.40
1:A:2910:ASP:OD1	1:A:2911:THR:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2931:LEU:HD22	1:A:2936:TYR:CB	2.52	0.40
1:A:4687:THR:HG22	1:A:4730:PHE:CZ	2.57	0.40
1:D:3037:LYS:O	1:D:3040:ILE:HG22	2.21	0.40
1:D:3294:PRO:HB2	1:D:3297:LEU:HB2	2.03	0.40
1:D:3545:ASP:OD2	1:D:3550:VAL:HG23	2.22	0.40
1:D:4575:LEU:O	1:D:4578:TYR:HB2	2.21	0.40
1:B:29:VAL:HG12	1:B:30:LEU:CD2	2.52	0.40
1:B:4693:ASP:OD1	1:B:4694:ASP:N	2.54	0.40
1:C:267:ARG:NH2	1:C:332:VAL:O	2.49	0.40
1:C:2824:VAL:HG11	1:C:2938:VAL:HG22	2.03	0.40
1:C:3732:LYS:HE2	1:C:3732:LYS:HB3	1.98	0.40
1:A:17:THR:O	1:A:18:ASP:HB2	2.22	0.40
1:A:1281:GLN:O	1:A:1282:ASN:OD1	2.40	0.40
1:A:2480:LEU:HD23	1:A:2480:LEU:HA	1.95	0.40
1:D:3757:GLU:OE1	1:D:3757:GLU:CA	2.70	0.40
1:B:1007:SER:CA	1:B:1022:LEU:HD23	2.52	0.40
1:B:2817:MET:HE3	1:B:2938:VAL:HG11	2.03	0.40
1:B:4642:ARG:NH1	1:B:4642:ARG:HG2	2.36	0.40
1:C:4133:ASN:OD1	1:C:4133:ASN:O	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4347/5035 (86%)	4240 (98%)	107 (2%)	0	100	100
1	B	4347/5035 (86%)	4238 (98%)	109 (2%)	0	100	100
1	C	4347/5035 (86%)	4236 (97%)	111 (3%)	0	100	100
1	D	4347/5035 (86%)	4241 (98%)	106 (2%)	0	100	100
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
All	All	17808/20572 (87%)	17363 (98%)	445 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3808/4296 (89%)	3681 (97%)	127 (3%)	33	57
1	B	3808/4296 (89%)	3694 (97%)	114 (3%)	36	61
1	C	3808/4296 (89%)	3690 (97%)	118 (3%)	35	59
1	D	3808/4296 (89%)	3689 (97%)	119 (3%)	35	59
2	E	89/90 (99%)	86 (97%)	3 (3%)	32	56
2	F	89/90 (99%)	86 (97%)	3 (3%)	32	56
2	G	89/90 (99%)	86 (97%)	3 (3%)	32	56
2	H	89/90 (99%)	85 (96%)	4 (4%)	23	43
All	All	15588/17544 (89%)	15097 (97%)	491 (3%)	36	59

All (491) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	54	SER
1	A	100	ARG
1	A	106	HIS
1	A	165	ARG
1	A	184	SER
1	A	221	LEU
1	A	229	ASP

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Mol	Chain	Res	Type
1	A	267	ARG
1	A	366	LYS
1	A	369	ARG
1	A	385	MET
1	A	394	CYS
1	A	397	GLU
1	A	425	LYS
1	A	477	SER
1	A	485	LEU
1	A	617	SER
1	A	748	CYS
1	A	755	SER
1	A	789	LYS
1	A	831	ARG
1	A	832	ARG
1	A	872	ARG
1	A	878	ASN
1	A	921	TYR
1	A	939	HIS
1	A	952	LYS
1	A	953	LYS
1	A	961	MET
1	A	966	TYR
1	A	986	VAL
1	A	1017	ARG
1	A	1023	VAL
1	A	1041	CYS
1	A	1042	GLN
1	A	1047	LEU
1	A	1052	TYR
1	A	1144	TRP
1	A	1184	GLU
1	A	1281	GLN
1	A	1436	TYR
1	A	1487	SER
1	A	1509	ARG
1	A	1718	SER
1	A	1753	ARG
1	A	1761	ARG
1	A	1816	MET
1	A	1826	GLN
1	A	1874	ARG

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Mol	Chain	Res	Type
1	A	1931	LYS
1	A	1983	LYS
1	A	2190	LYS
1	A	2209	MET
1	A	2225	ARG
1	A	2337	ARG
1	A	2413	GLU
1	A	2450	GLU
1	A	2498	ASP
1	A	2514	GLU
1	A	2574	GLU
1	A	2581	ASP
1	A	2598	LYS
1	A	2721	SER
1	A	2723	LYS
1	A	2744	LEU
1	A	2769	PHE
1	A	2789	HIS
1	A	2791	MET
1	A	2798	PHE
1	A	2817	MET
1	A	2828	ARG
1	A	2831	GLU
1	A	2856	TYR
1	A	2875	MET
1	A	2915	LYS
1	A	2923	LYS
1	A	2933	MET
1	A	2934	ASN
1	A	2945	MET
1	A	2948	ASP
1	A	2974	PHE
1	A	2983	SER
1	A	2986	ARG
1	A	3083	LYS
1	A	3109	GLU
1	A	3160	ASP
1	A	3175	SER
1	A	3226	ARG
1	A	3241	CYS
1	A	3284	ARG
1	A	3331	ASP

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Mol	Chain	Res	Type
1	A	3385	LYS
1	A	3410	TYR
1	A	3452	PHE
1	A	3454	ARG
1	A	3456	GLU
1	A	3509	SER
1	A	3525	MET
1	A	3545	ASP
1	A	3578	ARG
1	A	3583	ARG
1	A	3586	ASP
1	A	3588	ASP
1	A	3649	ARG
1	A	3669	SER
1	A	3755	SER
1	A	3761	MET
1	A	3873	ASN
1	A	3902	PHE
1	A	3936	PHE
1	A	3952	ARG
1	A	3954	PHE
1	A	3955	SER
1	A	4024	LYS
1	A	4073	ASP
1	A	4114	LEU
1	A	4154	SER
1	A	4164	ARG
1	A	4183	ARG
1	A	4538	PHE
1	A	4643	CYS
1	A	4709	PHE
1	A	4714	TRP
1	A	4743	LEU
1	A	4816	MET
1	A	4974	GLU
2	E	26	HIS
2	E	68	SER
2	E	72	ARG
2	H	26	HIS
2	H	60	TRP
2	H	68	SER
2	H	72	ARG

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Mol	Chain	Res	Type
2	F	26	HIS
2	F	68	SER
2	F	72	ARG
2	G	26	HIS
2	G	68	SER
2	G	72	ARG
1	D	36	LEU
1	D	100	ARG
1	D	106	HIS
1	D	165	ARG
1	D	184	SER
1	D	221	LEU
1	D	229	ASP
1	D	267	ARG
1	D	366	LYS
1	D	369	ARG
1	D	385	MET
1	D	394	CYS
1	D	397	GLU
1	D	459	GLU
1	D	477	SER
1	D	485	LEU
1	D	617	SER
1	D	748	CYS
1	D	755	SER
1	D	789	LYS
1	D	831	ARG
1	D	832	ARG
1	D	872	ARG
1	D	875	LEU
1	D	878	ASN
1	D	903	ARG
1	D	939	HIS
1	D	952	LYS
1	D	953	LYS
1	D	961	MET
1	D	966	TYR
1	D	986	VAL
1	D	1042	GLN
1	D	1144	TRP
1	D	1281	GLN
1	D	1305	THR

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Mol	Chain	Res	Type
1	D	1436	TYR
1	D	1509	ARG
1	D	1718	SER
1	D	1761	ARG
1	D	1826	GLN
1	D	1874	ARG
1	D	1931	LYS
1	D	1983	LYS
1	D	2190	LYS
1	D	2209	MET
1	D	2225	ARG
1	D	2337	ARG
1	D	2450	GLU
1	D	2498	ASP
1	D	2514	GLU
1	D	2574	GLU
1	D	2581	ASP
1	D	2598	LYS
1	D	2723	LYS
1	D	2744	LEU
1	D	2754	SER
1	D	2769	PHE
1	D	2791	MET
1	D	2792	LEU
1	D	2798	PHE
1	D	2828	ARG
1	D	2831	GLU
1	D	2856	TYR
1	D	2867	THR
1	D	2915	LYS
1	D	2923	LYS
1	D	2933	MET
1	D	2934	ASN
1	D	2945	MET
1	D	2974	PHE
1	D	2983	SER
1	D	3083	LYS
1	D	3160	ASP
1	D	3175	SER
1	D	3202	MET
1	D	3226	ARG
1	D	3284	ARG

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Mol	Chain	Res	Type
1	D	3331	ASP
1	D	3356	ARG
1	D	3385	LYS
1	D	3410	TYR
1	D	3452	PHE
1	D	3453	LYS
1	D	3454	ARG
1	D	3456	GLU
1	D	3509	SER
1	D	3525	MET
1	D	3545	ASP
1	D	3578	ARG
1	D	3583	ARG
1	D	3586	ASP
1	D	3588	ASP
1	D	3649	ARG
1	D	3669	SER
1	D	3755	SER
1	D	3861	MET
1	D	3873	ASN
1	D	3902	PHE
1	D	3936	PHE
1	D	3952	ARG
1	D	3954	PHE
1	D	3955	SER
1	D	4024	LYS
1	D	4073	ASP
1	D	4114	LEU
1	D	4154	SER
1	D	4164	ARG
1	D	4183	ARG
1	D	4538	PHE
1	D	4578	TYR
1	D	4643	CYS
1	D	4663	LYS
1	D	4709	PHE
1	D	4714	TRP
1	D	4743	LEU
1	D	4816	MET
1	D	4955	LYS
1	D	4974	GLU
1	B	36	LEU

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Mol	Chain	Res	Type
1	B	100	ARG
1	B	106	HIS
1	B	165	ARG
1	B	184	SER
1	B	221	LEU
1	B	229	ASP
1	B	267	ARG
1	B	366	LYS
1	B	369	ARG
1	B	385	MET
1	B	394	CYS
1	B	397	GLU
1	B	477	SER
1	B	485	LEU
1	B	617	SER
1	B	748	CYS
1	B	755	SER
1	B	789	LYS
1	B	831	ARG
1	B	832	ARG
1	B	872	ARG
1	B	878	ASN
1	B	903	ARG
1	B	921	TYR
1	B	926	SER
1	B	939	HIS
1	B	952	LYS
1	B	953	LYS
1	B	961	MET
1	B	962	MET
1	B	966	TYR
1	B	986	VAL
1	B	1023	VAL
1	B	1042	GLN
1	B	1144	TRP
1	B	1281	GLN
1	B	1305	THR
1	B	1436	TYR
1	B	1509	ARG
1	B	1761	ARG
1	B	1816	MET
1	B	1826	GLN

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Mol	Chain	Res	Type
1	B	1874	ARG
1	B	1931	LYS
1	B	1983	LYS
1	B	2190	LYS
1	B	2209	MET
1	B	2225	ARG
1	B	2337	ARG
1	B	2450	GLU
1	B	2476	GLN
1	B	2498	ASP
1	B	2514	GLU
1	B	2574	GLU
1	B	2581	ASP
1	B	2723	LYS
1	B	2744	LEU
1	B	2769	PHE
1	B	2791	MET
1	B	2798	PHE
1	B	2828	ARG
1	B	2831	GLU
1	B	2856	TYR
1	B	2867	THR
1	B	2915	LYS
1	B	2923	LYS
1	B	2934	ASN
1	B	2945	MET
1	B	2974	PHE
1	B	2983	SER
1	B	3083	LYS
1	B	3109	GLU
1	B	3160	ASP
1	B	3175	SER
1	B	3284	ARG
1	B	3331	ASP
1	B	3385	LYS
1	B	3410	TYR
1	B	3452	PHE
1	B	3454	ARG
1	B	3456	GLU
1	B	3509	SER
1	B	3525	MET
1	B	3545	ASP

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Mol	Chain	Res	Type
1	B	3578	ARG
1	B	3583	ARG
1	B	3586	ASP
1	B	3588	ASP
1	B	3649	ARG
1	B	3669	SER
1	B	3755	SER
1	B	3861	MET
1	B	3873	ASN
1	B	3902	PHE
1	B	3936	PHE
1	B	3952	ARG
1	B	3954	PHE
1	B	3955	SER
1	B	4024	LYS
1	B	4073	ASP
1	B	4114	LEU
1	B	4137	GLU
1	B	4154	SER
1	B	4164	ARG
1	B	4183	ARG
1	B	4538	PHE
1	B	4643	CYS
1	B	4709	PHE
1	B	4714	TRP
1	B	4743	LEU
1	B	4816	MET
1	B	4955	LYS
1	B	4974	GLU
1	C	36	LEU
1	C	54	SER
1	C	100	ARG
1	C	106	HIS
1	C	165	ARG
1	C	184	SER
1	C	221	LEU
1	C	229	ASP
1	C	267	ARG
1	C	366	LYS
1	C	369	ARG
1	C	385	MET
1	C	394	CYS

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Mol	Chain	Res	Type
1	C	397	GLU
1	C	459	GLU
1	C	464	GLU
1	C	477	SER
1	C	485	LEU
1	C	617	SER
1	C	748	CYS
1	C	755	SER
1	C	789	LYS
1	C	831	ARG
1	C	832	ARG
1	C	872	ARG
1	C	878	ASN
1	C	921	TYR
1	C	926	SER
1	C	939	HIS
1	C	952	LYS
1	C	953	LYS
1	C	962	MET
1	C	966	TYR
1	C	967	LYS
1	C	986	VAL
1	C	1042	GLN
1	C	1144	TRP
1	C	1281	GLN
1	C	1305	THR
1	C	1436	TYR
1	C	1509	ARG
1	C	1718	SER
1	C	1753	ARG
1	C	1761	ARG
1	C	1826	GLN
1	C	1874	ARG
1	C	1931	LYS
1	C	1983	LYS
1	C	2190	LYS
1	C	2204	MET
1	C	2209	MET
1	C	2225	ARG
1	C	2337	ARG
1	C	2450	GLU
1	C	2476	GLN

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Mol	Chain	Res	Type
1	C	2498	ASP
1	C	2514	GLU
1	C	2574	GLU
1	C	2721	SER
1	C	2723	LYS
1	C	2744	LEU
1	C	2754	SER
1	C	2769	PHE
1	C	2791	MET
1	C	2792	LEU
1	C	2798	PHE
1	C	2828	ARG
1	C	2831	GLU
1	C	2856	TYR
1	C	2915	LYS
1	C	2923	LYS
1	C	2933	MET
1	C	2934	ASN
1	C	2945	MET
1	C	2974	PHE
1	C	2983	SER
1	C	3083	LYS
1	C	3160	ASP
1	C	3175	SER
1	C	3226	ARG
1	C	3284	ARG
1	C	3331	ASP
1	C	3385	LYS
1	C	3410	TYR
1	C	3452	PHE
1	C	3454	ARG
1	C	3509	SER
1	C	3525	MET
1	C	3545	ASP
1	C	3578	ARG
1	C	3583	ARG
1	C	3586	ASP
1	C	3588	ASP
1	C	3649	ARG
1	C	3669	SER
1	C	3755	SER
1	C	3873	ASN

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Mol	Chain	Res	Type
1	C	3902	PHE
1	C	3936	PHE
1	C	3952	ARG
1	C	3954	PHE
1	C	3955	SER
1	C	4024	LYS
1	C	4073	ASP
1	C	4114	LEU
1	C	4137	GLU
1	C	4154	SER
1	C	4164	ARG
1	C	4183	ARG
1	C	4538	PHE
1	C	4541	GLU
1	C	4643	CYS
1	C	4709	PHE
1	C	4714	TRP
1	C	4743	LEU
1	C	4816	MET
1	C	4955	LYS
1	C	4974	GLU

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

Mol	Chain	Res	Type
1	A	1546	ASN
1	A	2757	ASN
1	A	3450	HIS
1	A	3557	ASN
1	A	3870	ASN
1	D	1546	ASN
1	D	3450	HIS
1	D	3557	ASN
1	B	3450	HIS
1	B	3557	ASN
1	C	2585	HIS
1	C	3450	HIS
1	C	3557	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	PCW	C	5101	-	53,53,53	1.18	5 (9%)	59,61,61	2.27	9 (15%)
4	PCW	B	8002	-	53,53,53	1.16	5 (9%)	59,61,61	2.39	9 (15%)
4	PCW	A	8003	-	53,53,53	1.17	5 (9%)	59,61,61	2.27	9 (15%)
4	PCW	A	8002	-	53,53,53	1.17	4 (7%)	59,61,61	2.34	9 (15%)
4	PCW	D	5103	-	53,53,53	1.18	6 (11%)	59,61,61	2.37	10 (16%)
4	PCW	B	8003	-	53,53,53	1.18	5 (9%)	59,61,61	2.28	9 (15%)
4	PCW	C	5103	-	53,53,53	1.17	5 (9%)	59,61,61	2.36	9 (15%)
4	PCW	D	5101	-	53,53,53	1.18	5 (9%)	59,61,61	2.29	9 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCW	C	5101	-	-	26/57/57/57	-
4	PCW	B	8002	-	-	22/57/57/57	-
4	PCW	A	8003	-	-	22/57/57/57	-
4	PCW	A	8002	-	-	25/57/57/57	-
4	PCW	D	5103	-	-	25/57/57/57	-
4	PCW	B	8003	-	-	23/57/57/57	-
4	PCW	C	5103	-	-	24/57/57/57	-
4	PCW	D	5101	-	-	20/57/57/57	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5103	PCW	O3-C11	3.12	1.42	1.33
4	B	8002	PCW	O3-C11	3.10	1.42	1.33
4	C	5103	PCW	O3-C11	3.09	1.42	1.33
4	D	5101	PCW	O3-C11	3.04	1.42	1.33
4	B	8003	PCW	O3-C11	3.04	1.42	1.33
4	A	8002	PCW	O3-C11	3.00	1.42	1.33
4	C	5101	PCW	O3-C11	3.00	1.42	1.33
4	A	8003	PCW	O3-C11	3.00	1.42	1.33
4	B	8002	PCW	O2-C2	-2.85	1.39	1.46
4	A	8003	PCW	O2-C31	2.84	1.42	1.34
4	D	5103	PCW	O2-C2	-2.84	1.39	1.46
4	C	5101	PCW	O2-C31	2.83	1.42	1.34
4	B	8003	PCW	O2-C31	2.83	1.42	1.34
4	D	5101	PCW	O2-C31	2.82	1.42	1.34
4	C	5103	PCW	O2-C2	-2.80	1.40	1.46
4	C	5103	PCW	O2-C31	2.80	1.42	1.34
4	D	5101	PCW	O2-C2	-2.80	1.40	1.46
4	A	8002	PCW	O2-C2	-2.80	1.40	1.46
4	B	8003	PCW	O2-C2	-2.78	1.40	1.46
4	C	5101	PCW	O2-C2	-2.77	1.40	1.46
4	A	8002	PCW	O2-C31	2.75	1.42	1.34
4	A	8003	PCW	O2-C2	-2.73	1.40	1.46
4	B	8002	PCW	O2-C31	2.72	1.42	1.34
4	D	5103	PCW	O2-C31	2.68	1.41	1.34
4	B	8002	PCW	C5-C4	2.10	1.57	1.51
4	C	5103	PCW	C5-C4	2.10	1.57	1.51
4	D	5103	PCW	C5-C4	2.07	1.57	1.51
4	B	8003	PCW	P-O4P	2.07	1.67	1.59
4	A	8002	PCW	P-O4P	2.07	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	5101	PCW	P-O4P	2.05	1.67	1.59
4	C	5103	PCW	P-O4P	2.05	1.67	1.59
4	A	8003	PCW	C5-C4	2.04	1.57	1.51
4	D	5101	PCW	P-O4P	2.04	1.67	1.59
4	D	5103	PCW	P-O4P	2.04	1.67	1.59
4	D	5101	PCW	C5-C4	2.04	1.57	1.51
4	B	8003	PCW	C5-C4	2.03	1.57	1.51
4	A	8003	PCW	P-O4P	2.02	1.67	1.59
4	B	8002	PCW	P-O4P	2.02	1.67	1.59
4	C	5101	PCW	C5-C4	2.01	1.57	1.51
4	D	5103	PCW	P-O3P	2.01	1.67	1.59

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	5103	PCW	C8-N-C6	12.12	140.80	108.98
4	B	8002	PCW	C8-N-C6	12.05	140.63	108.98
4	C	5103	PCW	C8-N-C6	11.88	140.18	108.98
4	A	8002	PCW	C8-N-C6	11.74	139.82	108.98
4	D	5101	PCW	C8-N-C6	10.63	136.90	108.98
4	B	8003	PCW	C8-N-C6	10.62	136.87	108.98
4	C	5101	PCW	C8-N-C6	10.61	136.84	108.98
4	A	8003	PCW	C8-N-C6	10.51	136.59	108.98
4	B	8003	PCW	C7-N-C5	7.90	141.30	109.91
4	D	5101	PCW	C7-N-C5	7.89	141.28	109.91
4	C	5101	PCW	C7-N-C5	7.87	141.20	109.91
4	A	8003	PCW	C7-N-C5	7.76	140.78	109.91
4	A	8002	PCW	C7-N-C5	7.39	139.29	109.91
4	B	8002	PCW	C7-N-C5	7.16	138.37	109.91
4	C	5103	PCW	C7-N-C5	7.13	138.26	109.91
4	D	5103	PCW	C7-N-C5	7.12	138.20	109.91
4	C	5103	PCW	C8-N-C7	-5.81	93.71	108.98
4	D	5103	PCW	C8-N-C7	-5.60	94.26	108.98
4	B	8002	PCW	C8-N-C7	-5.59	94.28	108.98
4	A	8002	PCW	C8-N-C7	-5.37	94.86	108.98
4	A	8003	PCW	C8-N-C7	-5.23	95.24	108.98
4	C	5103	PCW	C7-N-C6	-5.05	95.72	108.98
4	B	8003	PCW	C8-N-C7	-4.98	95.90	108.98
4	D	5101	PCW	C8-N-C7	-4.97	95.92	108.98
4	C	5101	PCW	C8-N-C7	-4.96	95.94	108.98
4	B	8002	PCW	C7-N-C6	-4.89	96.13	108.98
4	D	5103	PCW	C7-N-C6	-4.85	96.23	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	8003	PCW	C7-N-C6	-4.82	96.32	108.98
4	B	8003	PCW	C7-N-C6	-4.76	96.47	108.98
4	D	5101	PCW	C7-N-C6	-4.76	96.47	108.98
4	C	5101	PCW	C7-N-C6	-4.76	96.47	108.98
4	A	8002	PCW	C7-N-C6	-4.69	96.66	108.98
4	D	5101	PCW	C21-C20-C19	4.21	156.35	124.83
4	B	8003	PCW	C21-C20-C19	4.11	155.64	124.83
4	A	8003	PCW	C21-C20-C19	3.98	154.69	124.83
4	A	8002	PCW	C21-C20-C19	3.93	154.24	124.83
4	C	5101	PCW	C21-C20-C19	3.84	153.63	124.83
4	C	5103	PCW	C21-C20-C19	3.84	153.57	124.83
4	D	5103	PCW	O2-C31-C32	3.83	119.76	111.48
4	B	8002	PCW	C21-C20-C19	3.80	153.31	124.83
4	B	8002	PCW	O2-C31-C32	3.77	119.63	111.48
4	D	5103	PCW	C21-C20-C19	3.75	152.92	124.83
4	A	8002	PCW	O2-C31-C32	3.75	119.59	111.48
4	C	5103	PCW	O2-C31-C32	3.64	119.35	111.48
4	B	8003	PCW	C8-N-C5	-3.57	95.71	109.91
4	D	5101	PCW	C8-N-C5	-3.57	95.72	109.91
4	A	8003	PCW	C8-N-C5	-3.56	95.75	109.91
4	C	5101	PCW	O2-C31-C32	3.56	119.18	111.48
4	C	5101	PCW	C8-N-C5	-3.55	95.81	109.91
4	D	5101	PCW	O2-C31-C32	3.40	118.84	111.48
4	A	8003	PCW	O2-C31-C32	3.37	118.76	111.48
4	A	8002	PCW	C8-N-C5	-3.33	96.65	109.91
4	B	8003	PCW	O2-C31-C32	3.32	118.65	111.48
4	D	5103	PCW	C8-N-C5	-3.16	97.34	109.91
4	B	8002	PCW	C8-N-C5	-3.13	97.47	109.91
4	C	5103	PCW	C8-N-C5	-3.02	97.89	109.91
4	C	5101	PCW	O3-C11-C12	2.79	120.36	111.83
4	D	5101	PCW	O3-C11-C12	2.79	120.33	111.83
4	A	8002	PCW	C6-N-C5	-2.70	99.19	109.91
4	A	8003	PCW	O3-C11-C12	2.67	119.97	111.83
4	B	8002	PCW	C6-N-C5	-2.62	99.48	109.91
4	D	5103	PCW	C6-N-C5	-2.61	99.54	109.91
4	B	8003	PCW	O3-C11-C12	2.58	119.71	111.83
4	C	5101	PCW	C6-N-C5	-2.55	99.78	109.91
4	D	5101	PCW	C6-N-C5	-2.55	99.79	109.91
4	B	8003	PCW	C6-N-C5	-2.54	99.83	109.91
4	C	5103	PCW	C6-N-C5	-2.41	100.33	109.91
4	C	5103	PCW	O3-C11-C12	2.34	118.97	111.83
4	B	8002	PCW	O3-C11-C12	2.34	118.97	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	8002	PCW	O3-C11-C12	2.29	118.81	111.83
4	D	5103	PCW	O3-C11-C12	2.27	118.75	111.83
4	A	8003	PCW	C6-N-C5	-2.23	101.06	109.91
4	D	5103	PCW	C2-O2-C31	-2.16	112.62	117.80

There are no chirality outliers.

All (187) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	8002	PCW	O4P-C4-C5-N
4	A	8002	PCW	C1-O3P-P-O4P
4	D	5101	PCW	O4P-C4-C5-N
4	D	5103	PCW	O4P-C4-C5-N
4	D	5103	PCW	C1-O3P-P-O4P
4	B	8002	PCW	O4P-C4-C5-N
4	B	8002	PCW	C1-O3P-P-O4P
4	B	8002	PCW	C4-O4P-P-O2P
4	B	8003	PCW	O4P-C4-C5-N
4	C	5101	PCW	O4P-C4-C5-N
4	C	5103	PCW	O4P-C4-C5-N
4	C	5103	PCW	C1-O3P-P-O1P
4	C	5103	PCW	C1-O3P-P-O4P
4	C	5103	PCW	C4-O4P-P-O2P
4	A	8002	PCW	C13-C14-C15-C16
4	D	5103	PCW	C13-C14-C15-C16
4	D	5101	PCW	C11-C12-C13-C14
4	C	5103	PCW	C13-C14-C15-C16
4	B	8003	PCW	C44-C45-C46-C47
4	A	8002	PCW	C33-C34-C35-C36
4	C	5103	PCW	C44-C45-C46-C47
4	B	8003	PCW	C11-C12-C13-C14
4	D	5103	PCW	C32-C31-O2-C2
4	A	8003	PCW	C41-C42-C43-C44
4	B	8003	PCW	C32-C33-C34-C35
4	C	5103	PCW	C11-C12-C13-C14
4	A	8002	PCW	C35-C36-C37-C38
4	B	8002	PCW	C44-C45-C46-C47
4	C	5103	PCW	C32-C33-C34-C35
4	A	8003	PCW	C21-C22-C23-C24
4	D	5103	PCW	C44-C45-C46-C47
4	D	5103	PCW	C22-C23-C24-C25
4	B	8002	PCW	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
4	C	5101	PCW	C41-C42-C43-C44
4	B	8002	PCW	C32-C31-O2-C2
4	C	5103	PCW	C32-C31-O2-C2
4	A	8002	PCW	C40-C41-C42-C43
4	D	5101	PCW	C20-C21-C22-C23
4	B	8003	PCW	C15-C16-C17-C18
4	D	5103	PCW	O31-C31-O2-C2
4	D	5101	PCW	C43-C44-C45-C46
4	A	8003	PCW	C43-C44-C45-C46
4	C	5101	PCW	C43-C44-C45-C46
4	A	8003	PCW	C24-C25-C26-C27
4	A	8002	PCW	C32-C31-O2-C2
4	B	8003	PCW	C32-C31-O2-C2
4	A	8002	PCW	O31-C31-O2-C2
4	B	8002	PCW	O31-C31-O2-C2
4	B	8003	PCW	O31-C31-O2-C2
4	B	8003	PCW	C20-C21-C22-C23
4	A	8002	PCW	C44-C45-C46-C47
4	C	5103	PCW	C43-C44-C45-C46
4	C	5103	PCW	O31-C31-O2-C2
4	A	8002	PCW	C43-C44-C45-C46
4	C	5101	PCW	C13-C14-C15-C16
4	D	5101	PCW	C16-C17-C18-C19
4	B	8003	PCW	C13-C14-C15-C16
4	C	5101	PCW	C2-C1-O3P-P
4	B	8003	PCW	C35-C36-C37-C38
4	B	8003	PCW	C12-C13-C14-C15
4	A	8002	PCW	C24-C25-C26-C27
4	D	5101	PCW	C35-C36-C37-C38
4	A	8003	PCW	O3P-C1-C2-C3
4	C	5101	PCW	O3P-C1-C2-C3
4	B	8002	PCW	C15-C16-C17-C18
4	C	5101	PCW	C24-C25-C26-C27
4	C	5101	PCW	C20-C21-C22-C23
4	C	5103	PCW	C15-C16-C17-C18
4	D	5101	PCW	C12-C11-O3-C3
4	D	5103	PCW	C33-C34-C35-C36
4	A	8002	PCW	C11-C12-C13-C14
4	C	5101	PCW	C42-C43-C44-C45
4	B	8002	PCW	C24-C25-C26-C27
4	A	8003	PCW	C20-C21-C22-C23
4	C	5101	PCW	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
4	B	8002	PCW	C33-C34-C35-C36
4	C	5101	PCW	C35-C36-C37-C38
4	C	5101	PCW	C11-C12-C13-C14
4	A	8002	PCW	C32-C33-C34-C35
4	C	5103	PCW	C40-C41-C42-C43
4	A	8002	PCW	C12-C11-O3-C3
4	B	8002	PCW	C11-C12-C13-C14
4	C	5103	PCW	C41-C42-C43-C44
4	B	8003	PCW	C19-C20-C21-C22
4	B	8003	PCW	C2-C1-O3P-P
4	D	5101	PCW	C14-C15-C16-C17
4	C	5103	PCW	C24-C25-C26-C27
4	B	8003	PCW	O3P-C1-C2-C3
4	D	5101	PCW	O11-C11-O3-C3
4	B	8002	PCW	C32-C33-C34-C35
4	B	8003	PCW	C41-C42-C43-C44
4	D	5103	PCW	C32-C33-C34-C35
4	A	8002	PCW	C1-C2-C3-O3
4	B	8002	PCW	C1-C2-C3-O3
4	C	5103	PCW	C1-C2-C3-O3
4	A	8003	PCW	C35-C36-C37-C38
4	A	8003	PCW	C4-C5-N-C8
4	D	5103	PCW	O2-C2-C3-O3
4	B	8002	PCW	O2-C2-C3-O3
4	D	5103	PCW	C11-C12-C13-C14
4	C	5101	PCW	C21-C22-C23-C24
4	D	5103	PCW	C12-C11-O3-C3
4	B	8003	PCW	C12-C11-O3-C3
4	D	5101	PCW	O3P-C1-C2-C3
4	A	8002	PCW	O11-C11-O3-C3
4	D	5103	PCW	O11-C11-O3-C3
4	B	8003	PCW	O11-C11-O3-C3
4	B	8003	PCW	C1-C2-O2-C31
4	D	5101	PCW	C44-C45-C46-C47
4	A	8003	PCW	O3P-C1-C2-O2
4	C	5101	PCW	O3P-C1-C2-O2
4	A	8002	PCW	O2-C2-C3-O3
4	D	5103	PCW	C40-C41-C42-C43
4	C	5103	PCW	O2-C2-C3-O3
4	D	5103	PCW	C35-C36-C37-C38
4	D	5101	PCW	C13-C14-C15-C16
4	A	8003	PCW	C45-C46-C47-C48

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Mol	Chain	Res	Type	Atoms
4	D	5101	PCW	C19-C20-C21-C22
4	D	5101	PCW	O3P-C1-C2-O2
4	B	8003	PCW	O3P-C1-C2-O2
4	C	5101	PCW	C4-C5-N-C8
4	D	5103	PCW	C1-C2-C3-O3
4	A	8002	PCW	C1-O3P-P-O2P
4	D	5103	PCW	C1-O3P-P-O2P
4	D	5103	PCW	C4-O4P-P-O2P
4	B	8002	PCW	C1-O3P-P-O2P
4	C	5103	PCW	C1-O3P-P-O2P
4	C	5101	PCW	C45-C46-C47-C48
4	A	8003	PCW	C2-C1-O3P-P
4	D	5101	PCW	C2-C1-O3P-P
4	C	5103	PCW	C2-C1-O3P-P
4	A	8003	PCW	C1-C2-O2-C31
4	D	5103	PCW	C24-C25-C26-C27
4	D	5101	PCW	C4-C5-N-C8
4	B	8003	PCW	C4-C5-N-C8
4	C	5103	PCW	O3P-C1-C2-C3
4	A	8003	PCW	C15-C16-C17-C18
4	A	8003	PCW	O11-C11-O3-C3
4	D	5101	PCW	C12-C13-C14-C15
4	A	8003	PCW	C12-C11-O3-C3
4	B	8002	PCW	C37-C38-C39-C40
4	C	5101	PCW	C19-C20-C21-C22
4	D	5103	PCW	C25-C26-C27-C28
4	A	8002	PCW	C2-C1-O3P-P
4	B	8002	PCW	C41-C42-C43-C44
4	C	5103	PCW	C25-C26-C27-C28
4	A	8003	PCW	C17-C18-C19-C20
4	D	5101	PCW	C3-C2-O2-C31
4	C	5101	PCW	C1-C2-O2-C31
4	C	5101	PCW	C3-C2-O2-C31
4	D	5103	PCW	C41-C42-C43-C44
4	A	8003	PCW	C19-C20-C21-C22
4	B	8003	PCW	C37-C38-C39-C40
4	A	8002	PCW	C45-C46-C47-C48
4	C	5101	PCW	O31-C31-O2-C2
4	C	5103	PCW	O3P-C1-C2-O2
4	D	5103	PCW	C19-C20-C21-C22
4	C	5101	PCW	C32-C31-O2-C2
4	A	8002	PCW	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
4	A	8003	PCW	C42-C43-C44-C45
4	B	8003	PCW	C17-C18-C19-C20
4	C	5101	PCW	O11-C11-O3-C3
4	D	5101	PCW	C1-C2-O2-C31
4	B	8002	PCW	C19-C20-C21-C22
4	C	5103	PCW	C37-C38-C39-C40
4	A	8003	PCW	C14-C15-C16-C17
4	A	8002	PCW	C37-C38-C39-C40
4	B	8003	PCW	C14-C15-C16-C17
4	B	8002	PCW	C2-C1-O3P-P
4	C	5101	PCW	C12-C11-O3-C3
4	D	5103	PCW	C39-C40-C41-C42
4	A	8002	PCW	C4-C5-N-C8
4	C	5103	PCW	C19-C20-C21-C22
4	B	8002	PCW	C40-C41-C42-C43
4	A	8002	PCW	C17-C18-C19-C20
4	A	8003	PCW	C11-C12-C13-C14
4	A	8003	PCW	C39-C40-C41-C42
4	D	5101	PCW	C15-C16-C17-C18
4	C	5101	PCW	C44-C45-C46-C47
4	A	8003	PCW	C3-C2-O2-C31
4	A	8002	PCW	C23-C24-C25-C26
4	C	5101	PCW	C37-C38-C39-C40
4	C	5101	PCW	C33-C34-C35-C36
4	B	8002	PCW	O3P-C1-C2-C3
4	D	5103	PCW	C45-C46-C47-C48
4	B	8002	PCW	C13-C14-C15-C16
4	D	5103	PCW	C17-C18-C19-C20

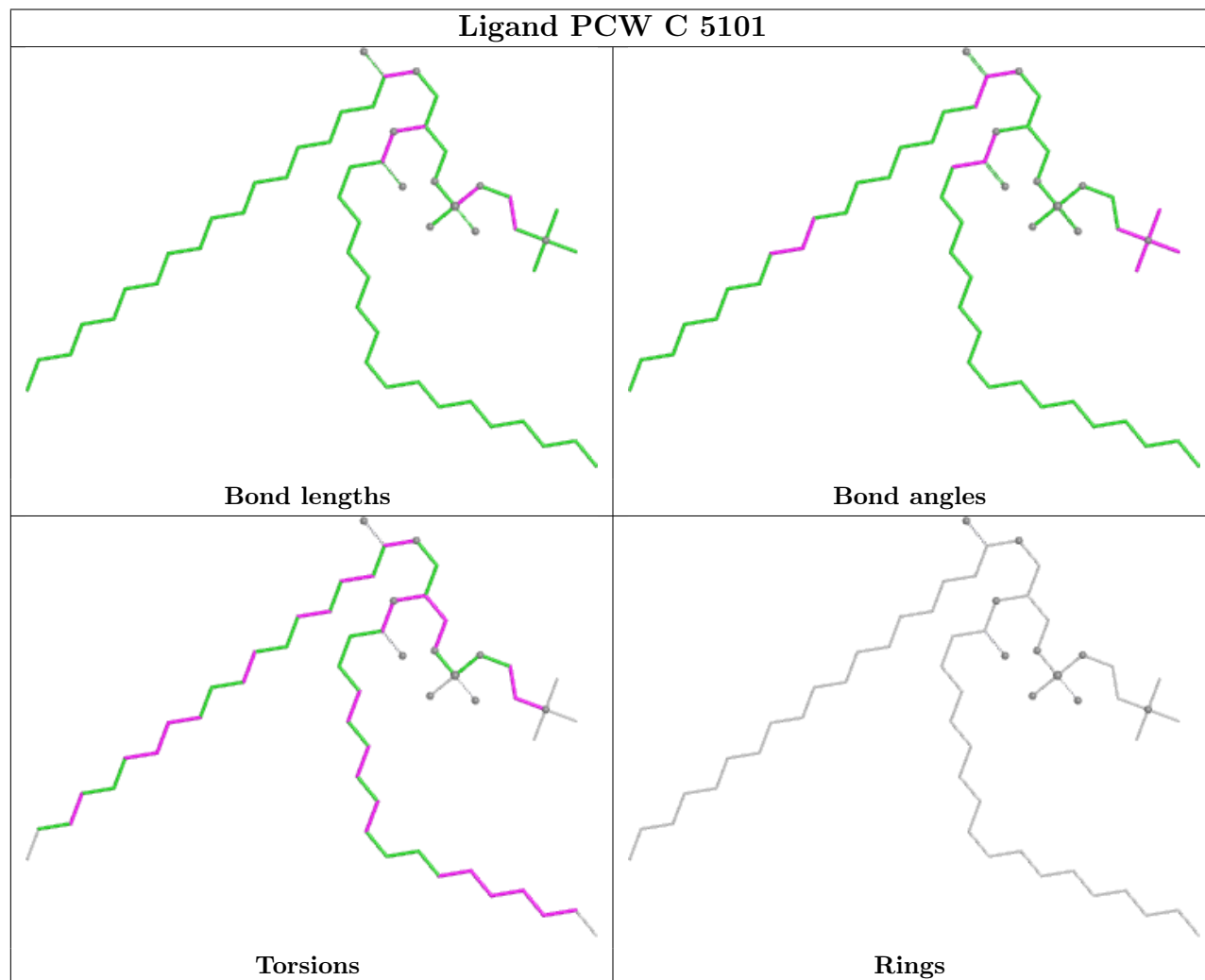
There are no ring outliers.

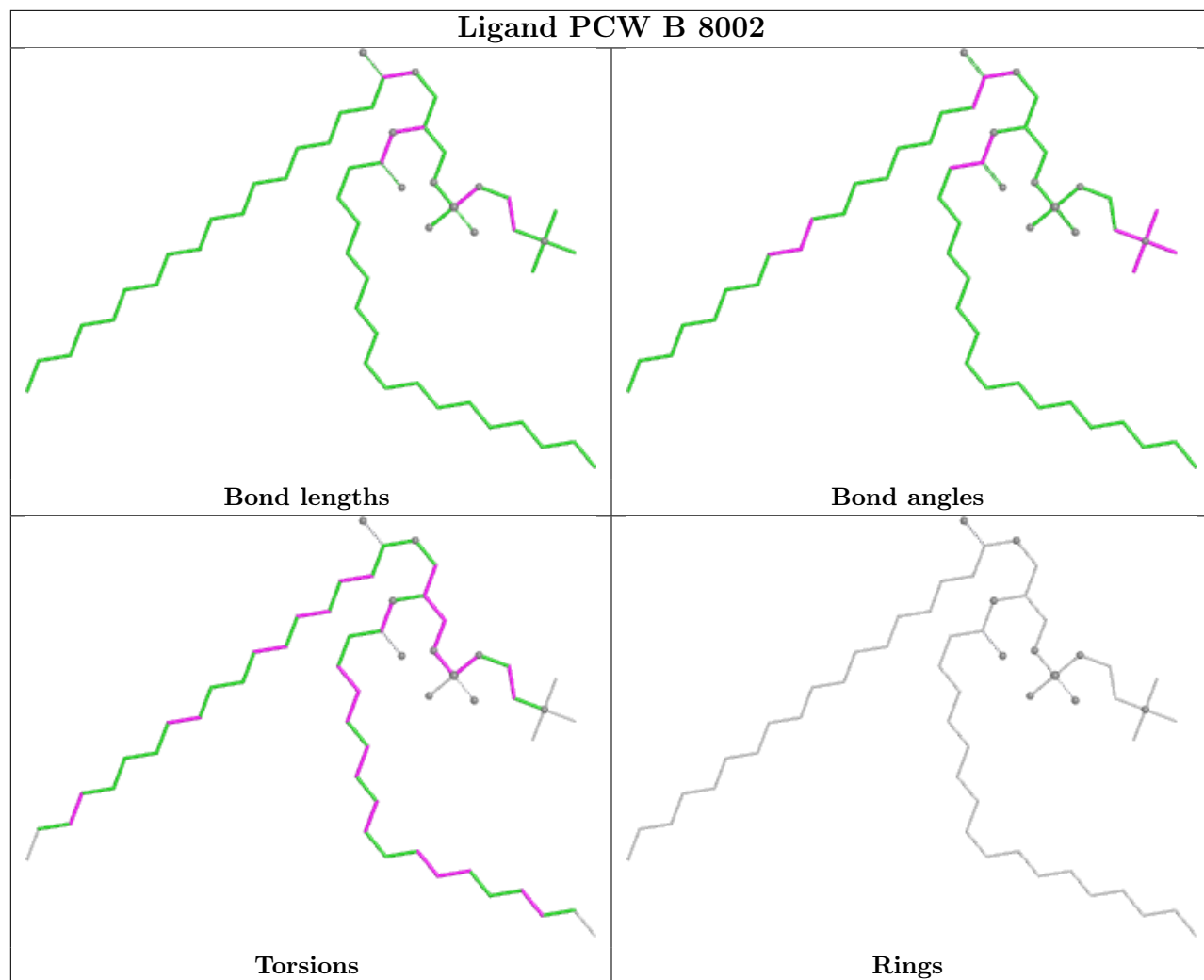
4 monomers are involved in 6 short contacts:

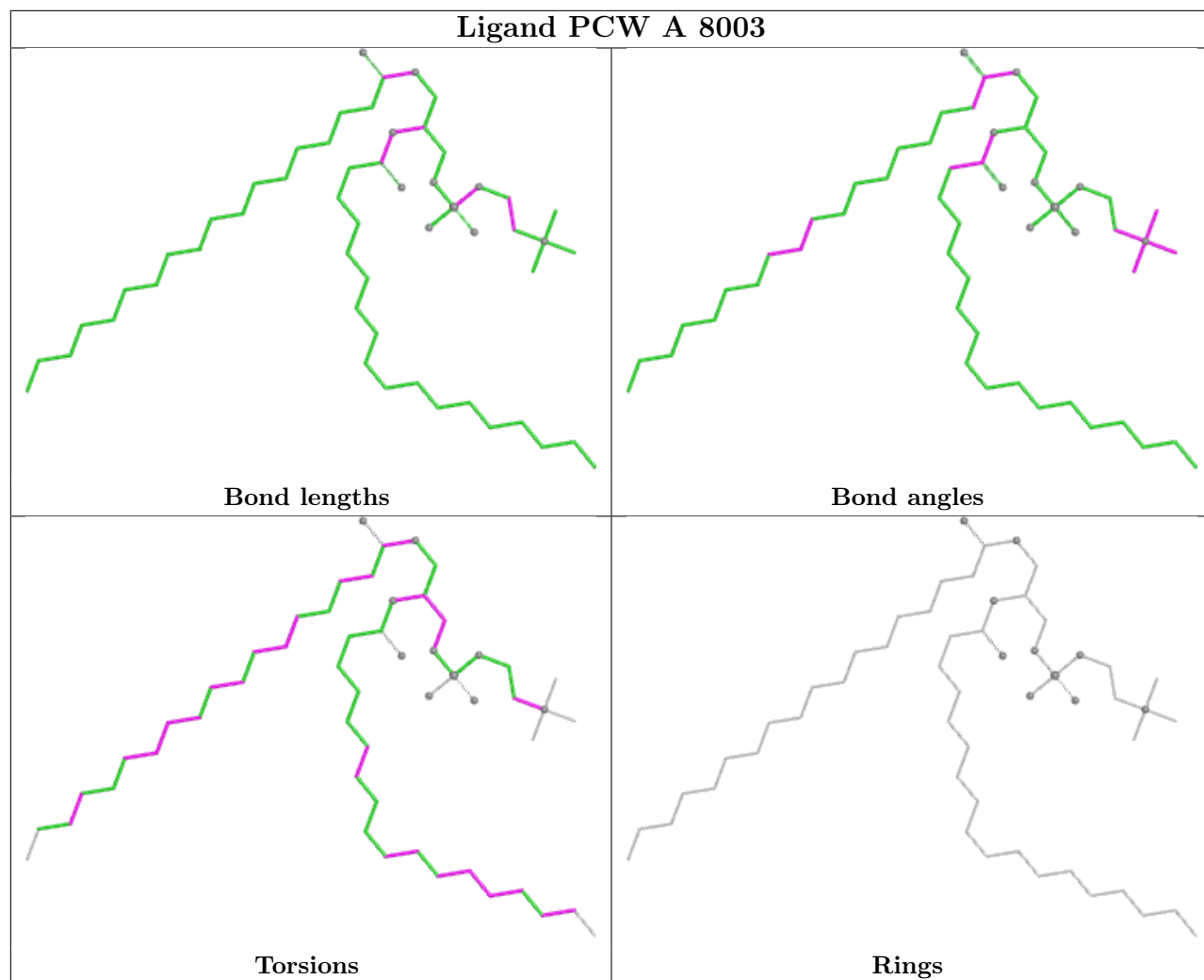
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	8002	PCW	2	0
4	D	5103	PCW	1	0
4	B	8003	PCW	1	0
4	C	5103	PCW	3	0

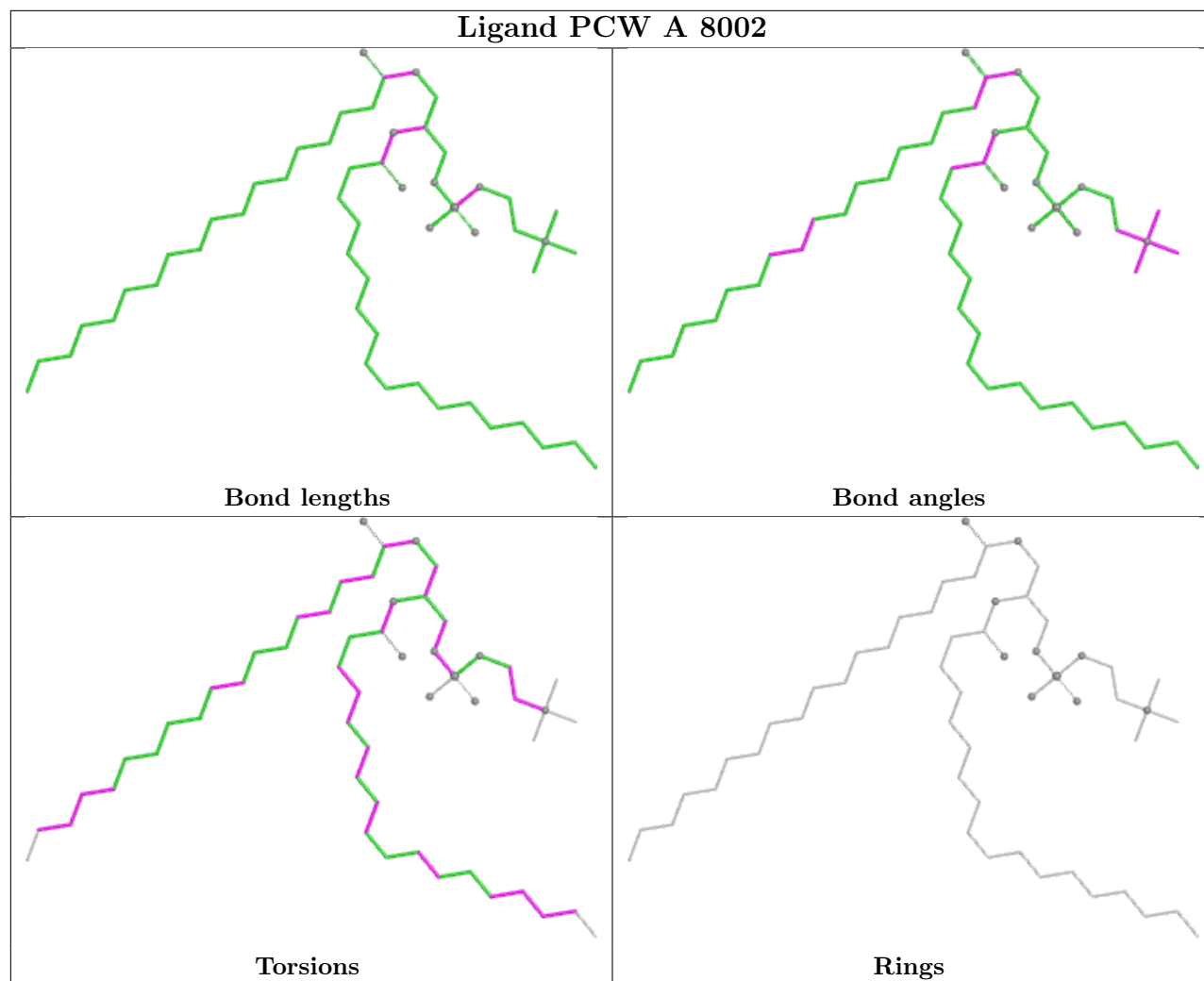
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

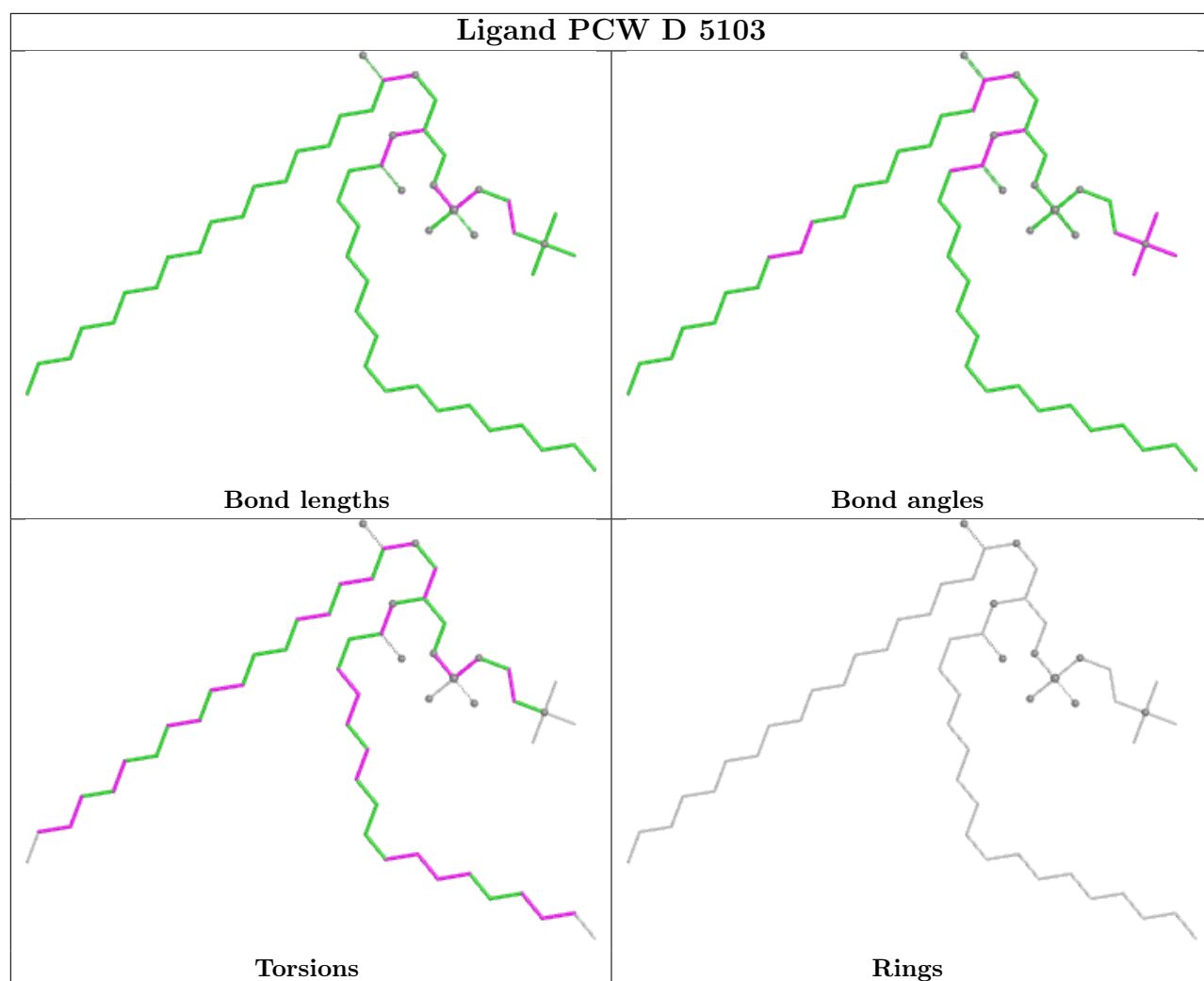
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

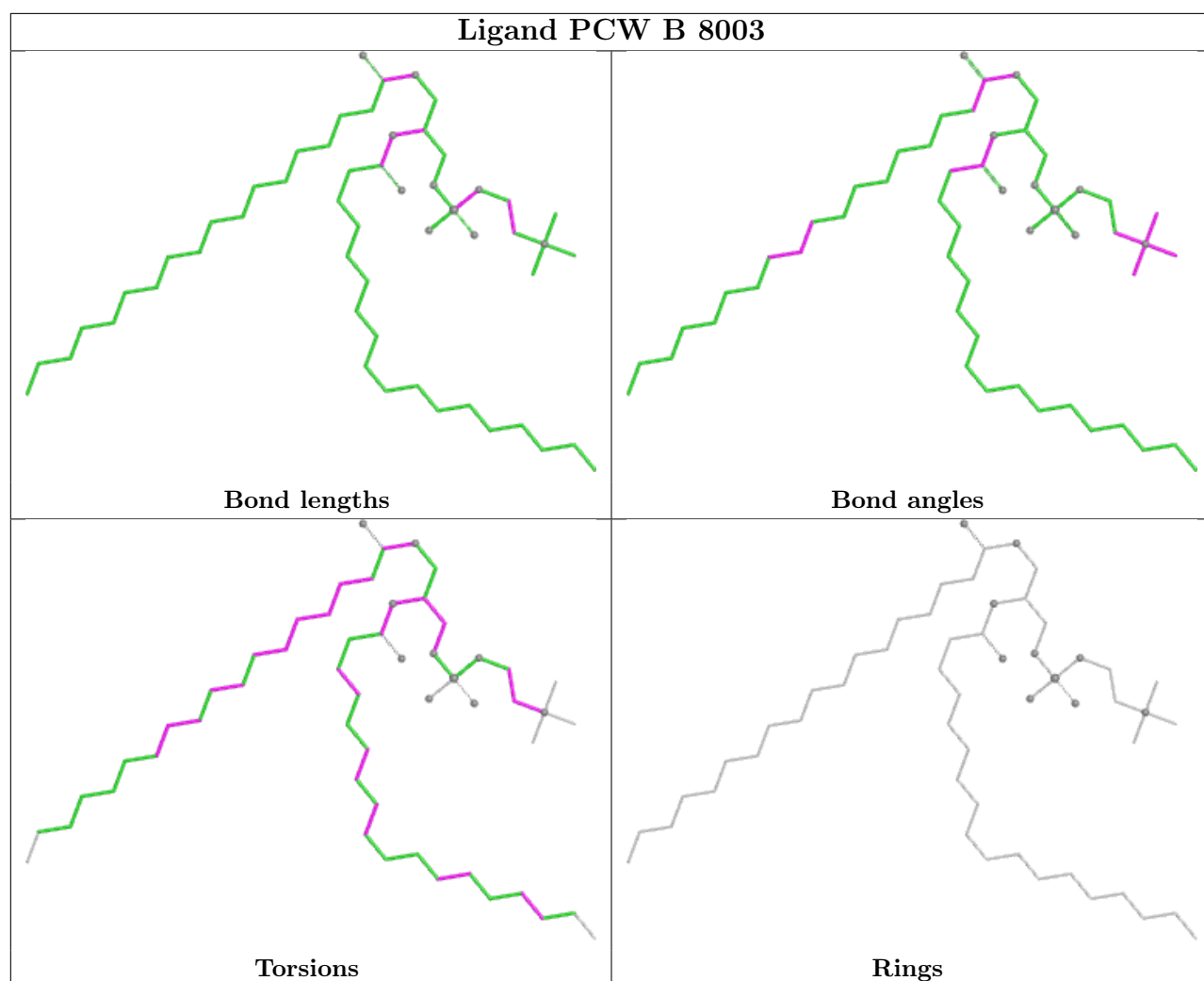


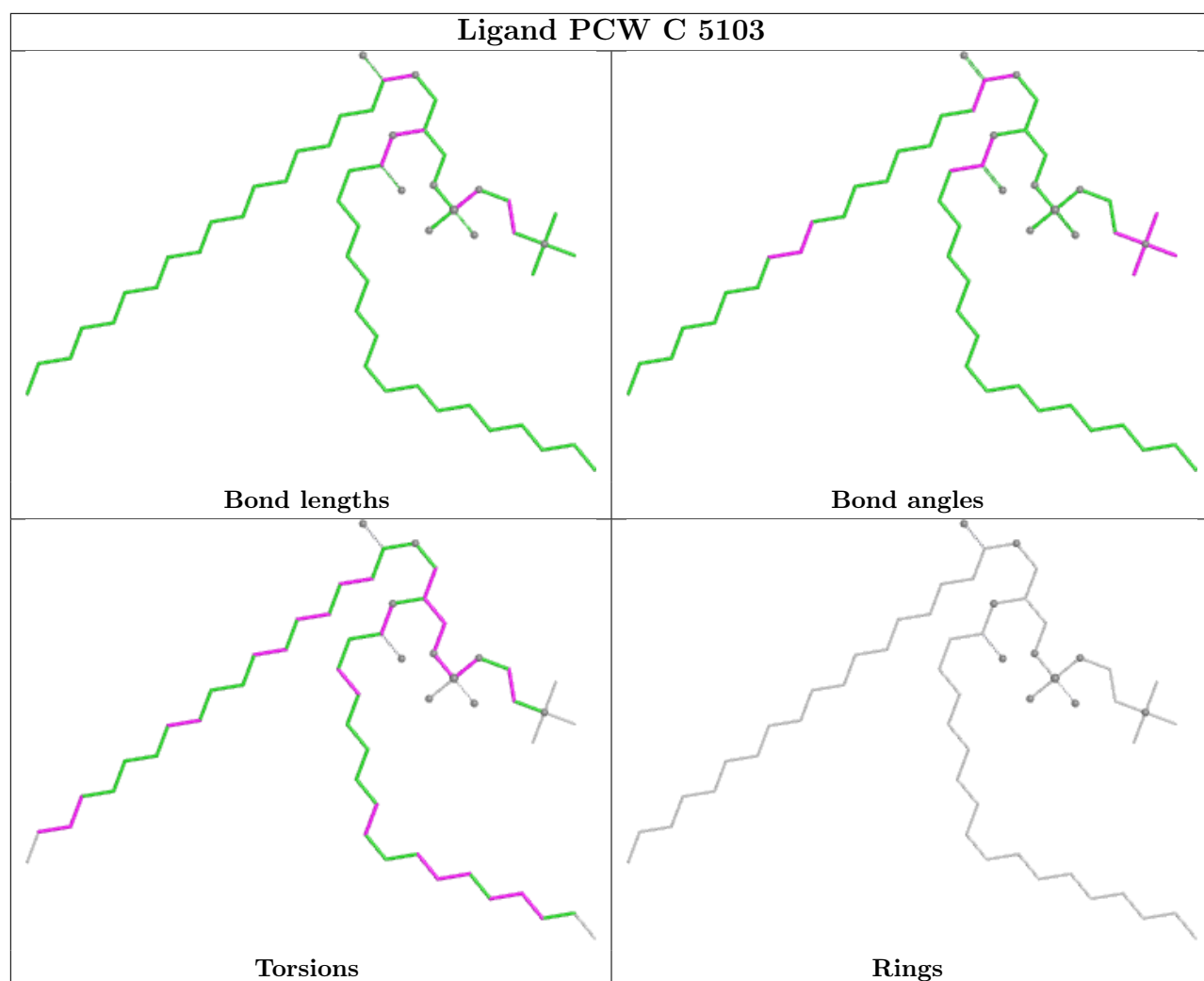


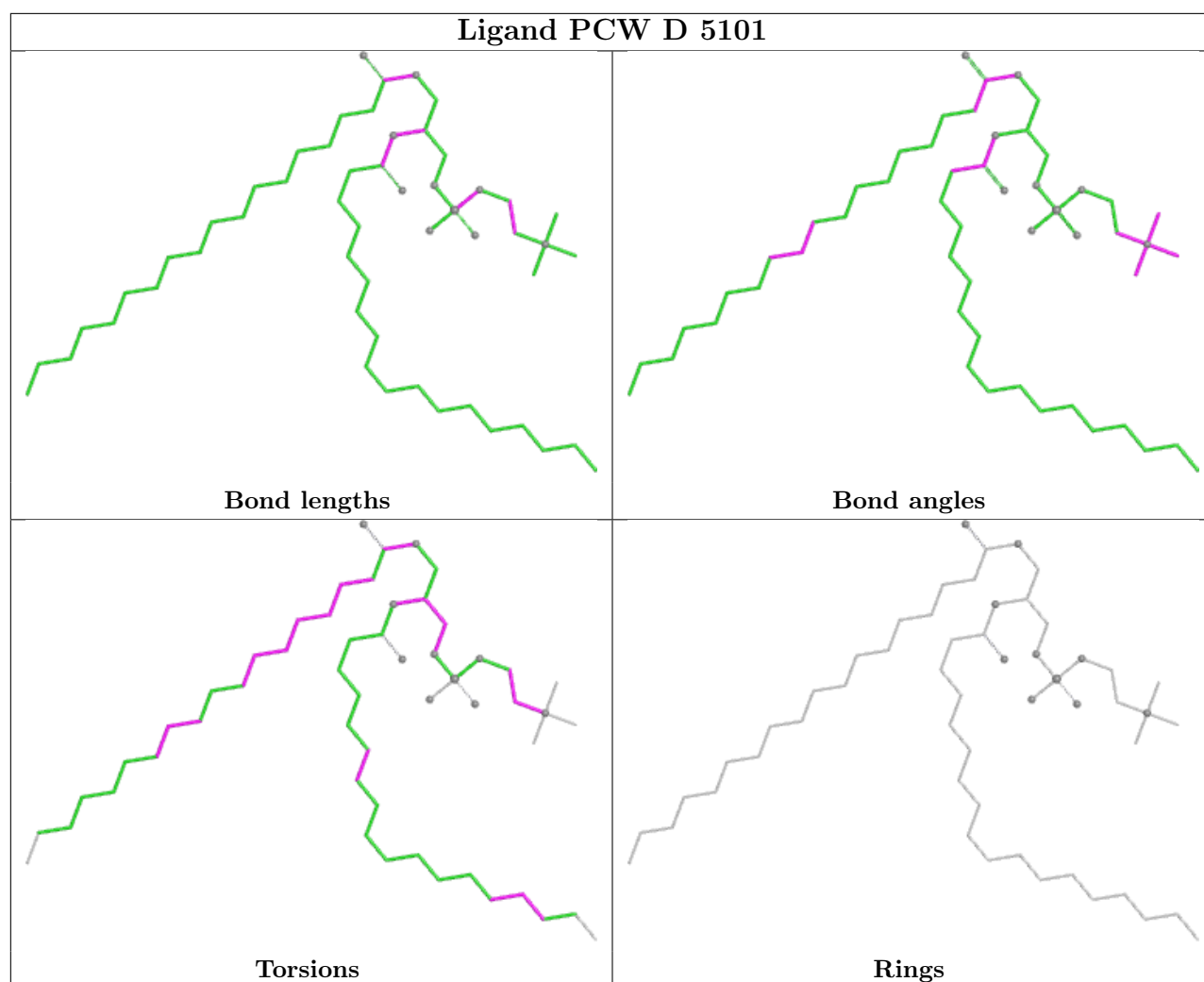












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

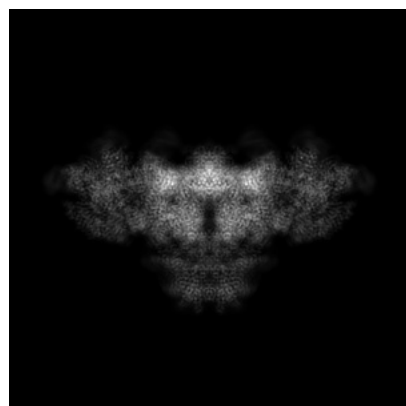
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43283. These allow visual inspection of the internal detail of the map and identification of artifacts.

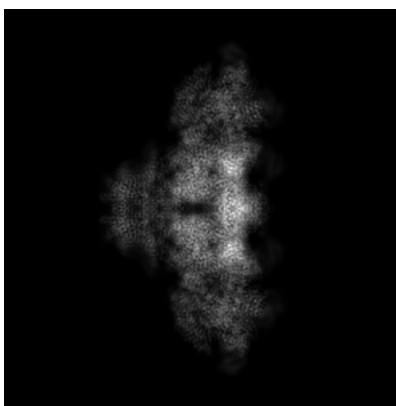
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

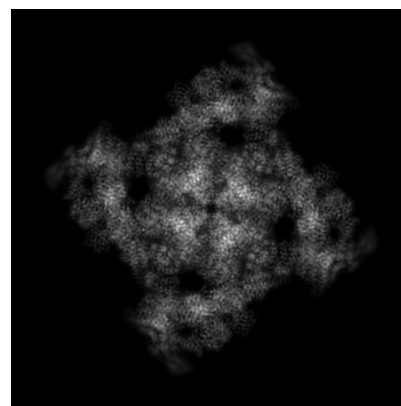
6.1.1 Primary map



X

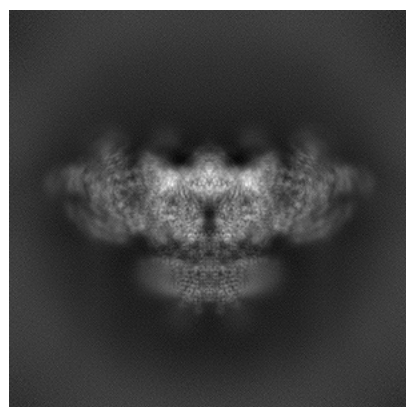


Y

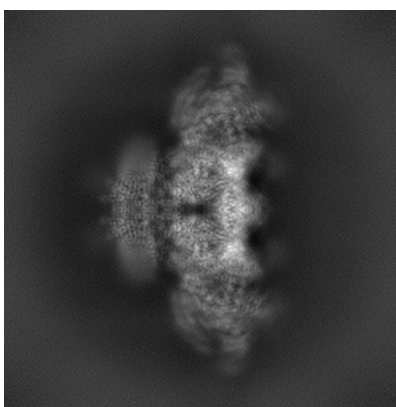


Z

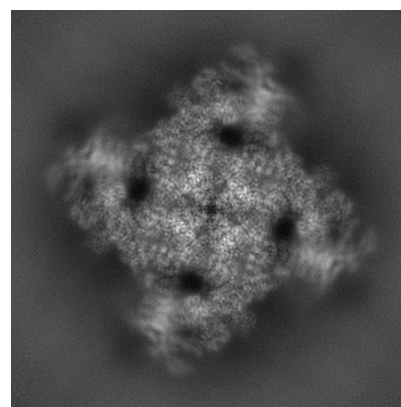
6.1.2 Raw map



X



Y



Z

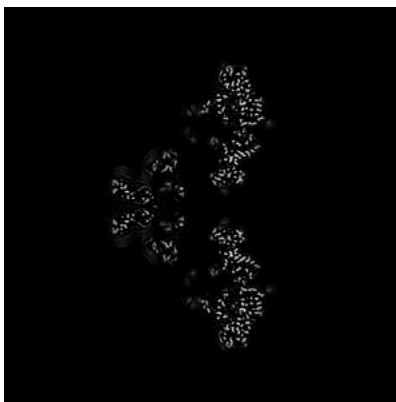
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

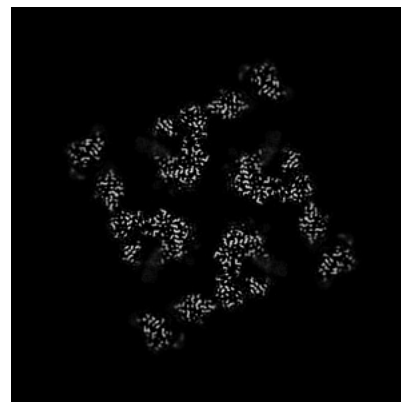
6.2.1 Primary map



X Index: 256

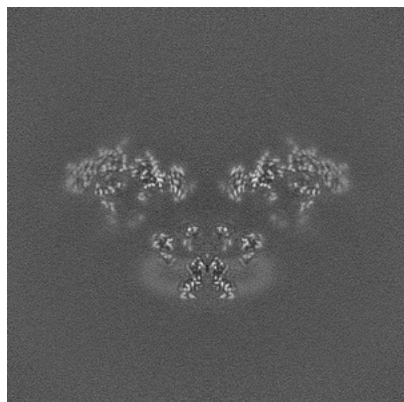


Y Index: 256

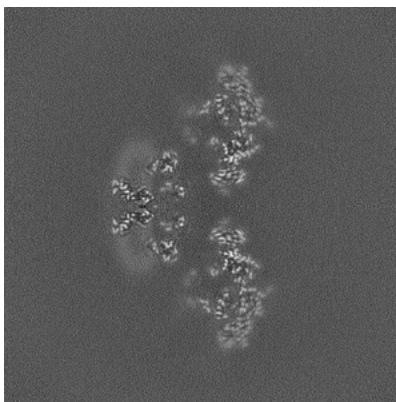


Z Index: 256

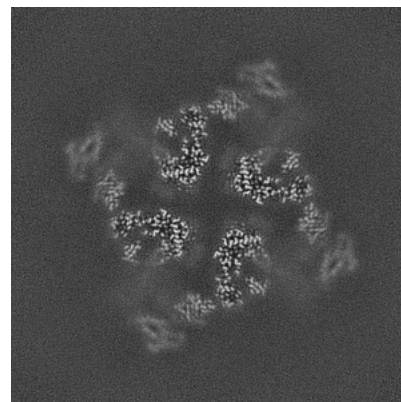
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

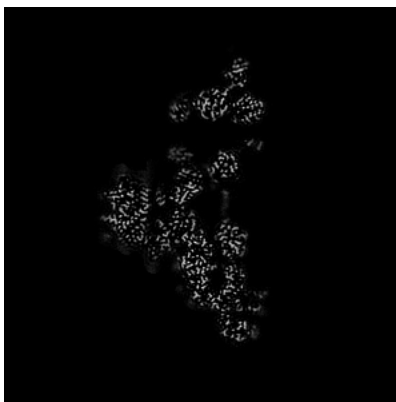
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

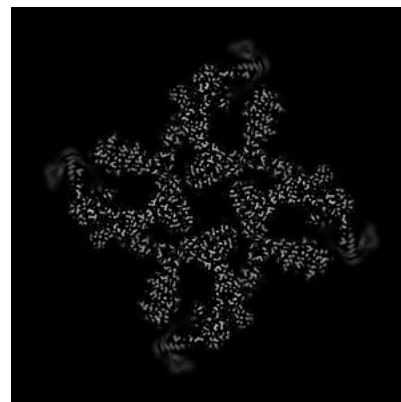
6.3.1 Primary map



X Index: 238

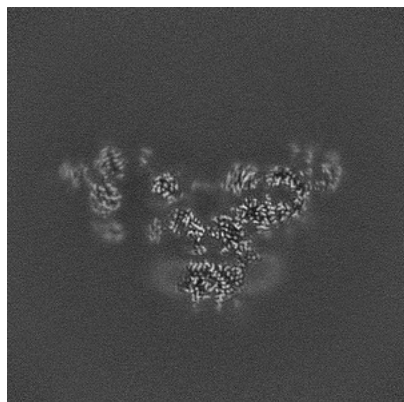


Y Index: 238

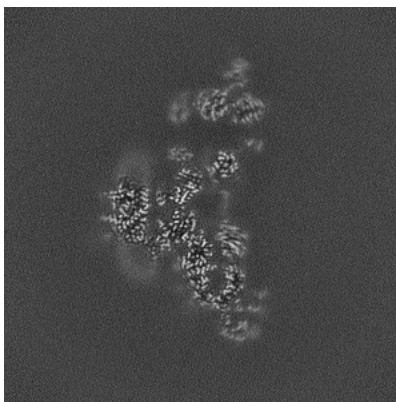


Z Index: 289

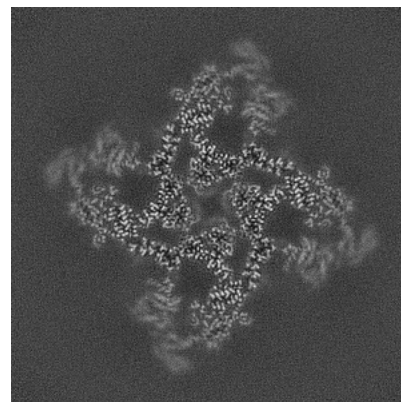
6.3.2 Raw map



X Index: 238



Y Index: 238

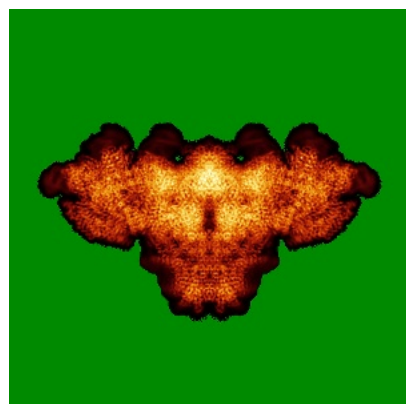


Z Index: 285

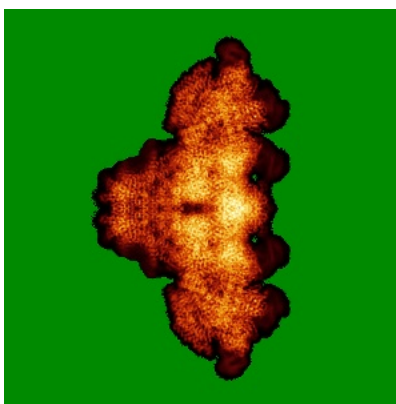
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

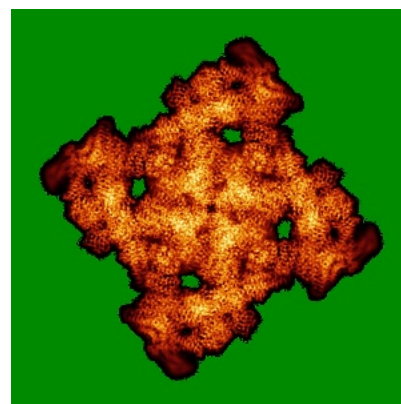
6.4.1 Primary map



X



Y

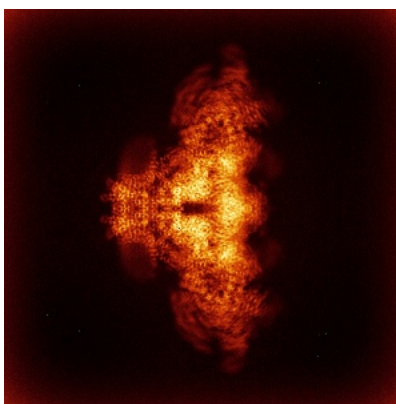


Z

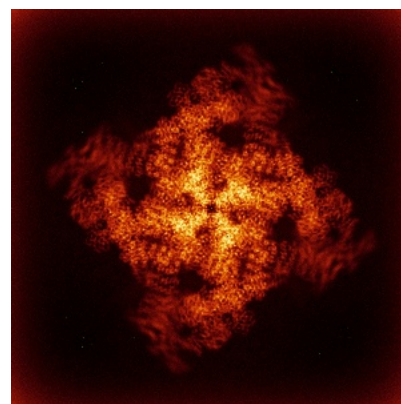
6.4.2 Raw map



X



Y

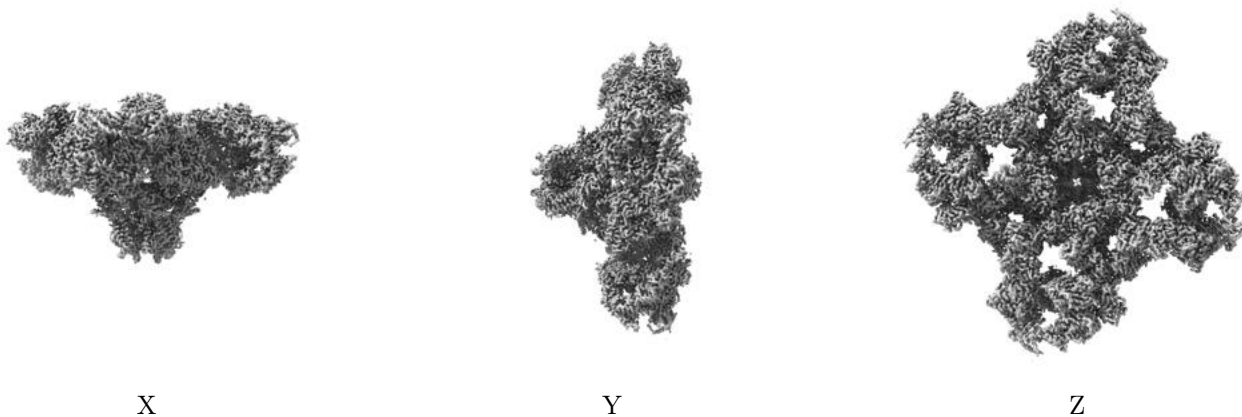


Z

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

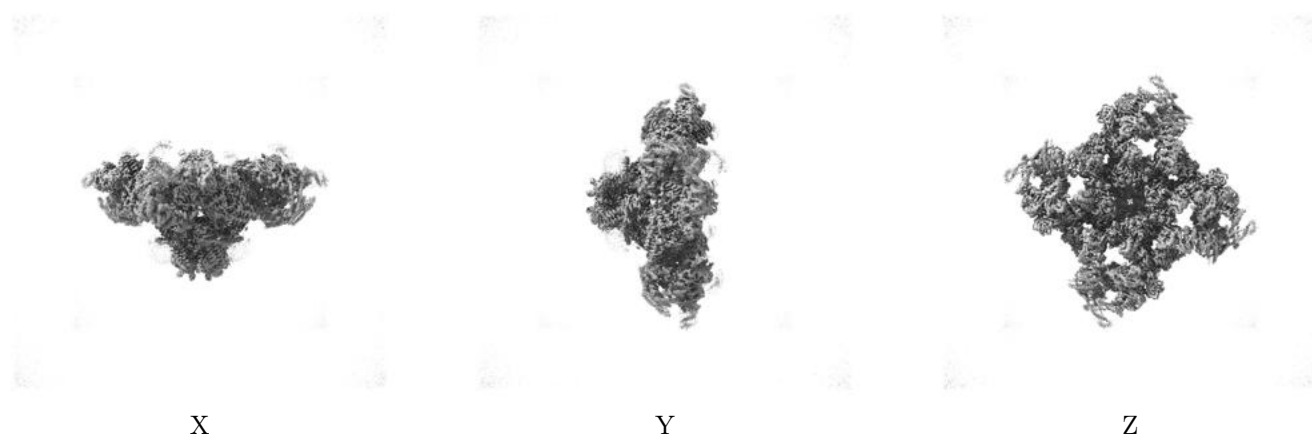
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

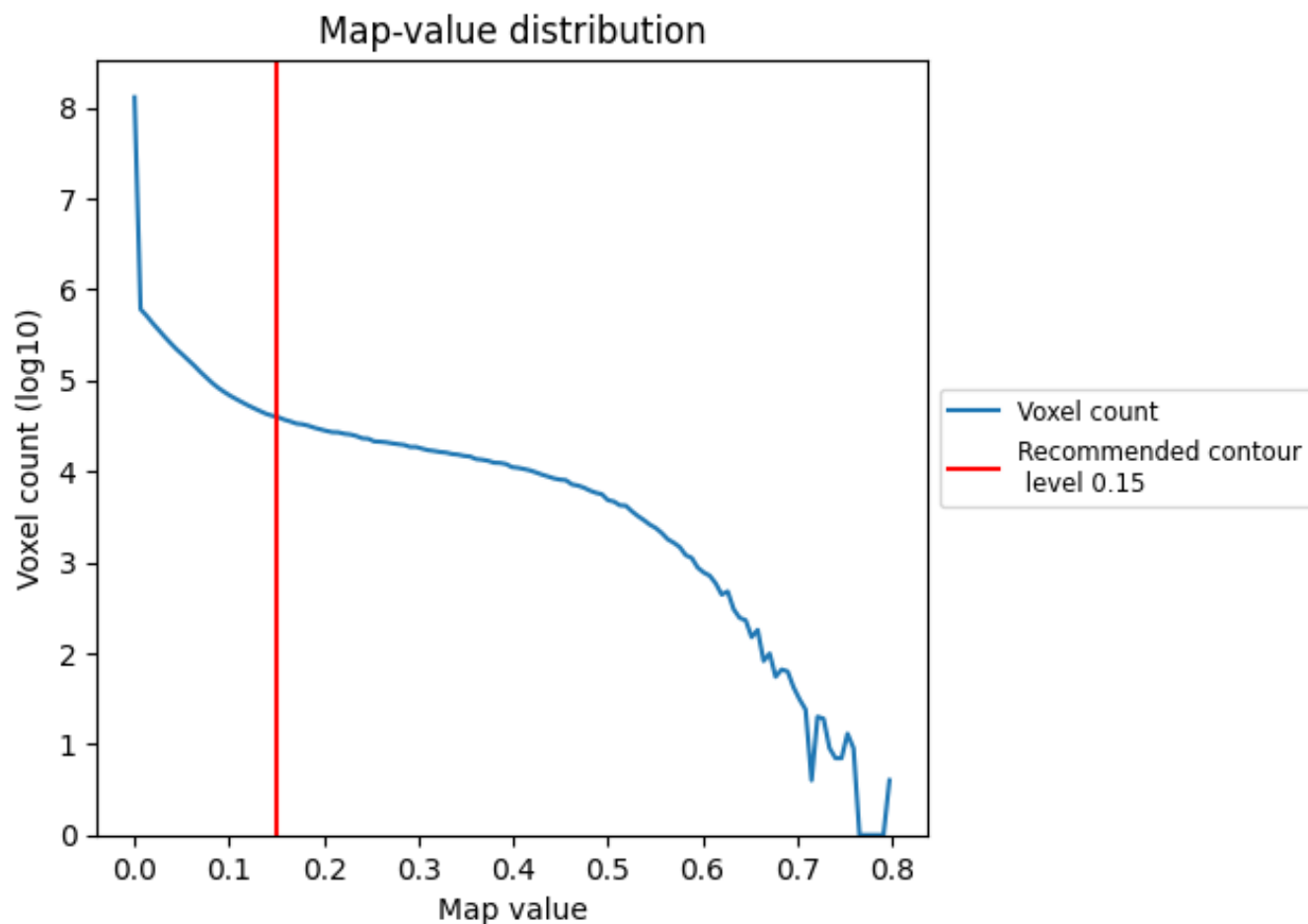
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

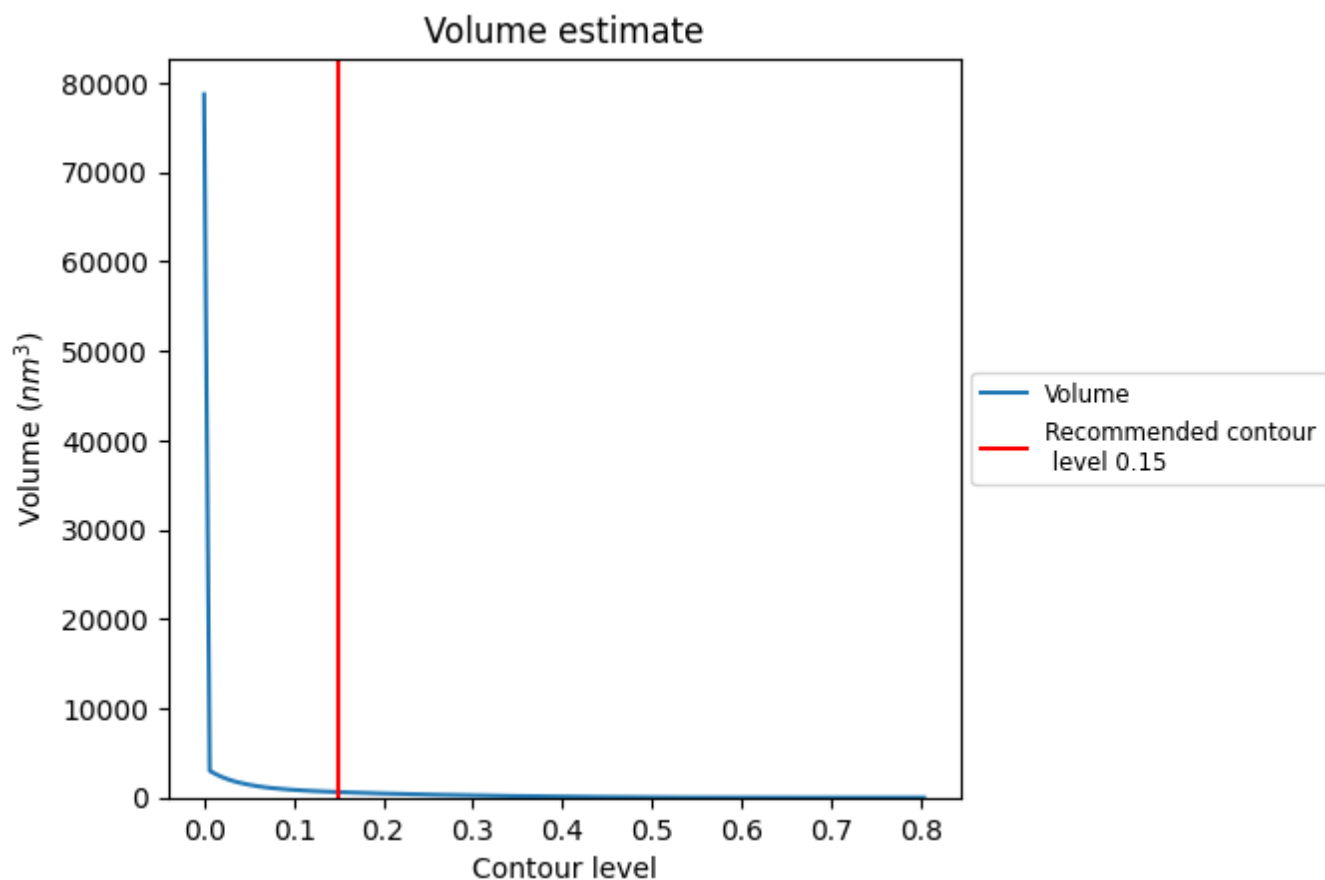
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

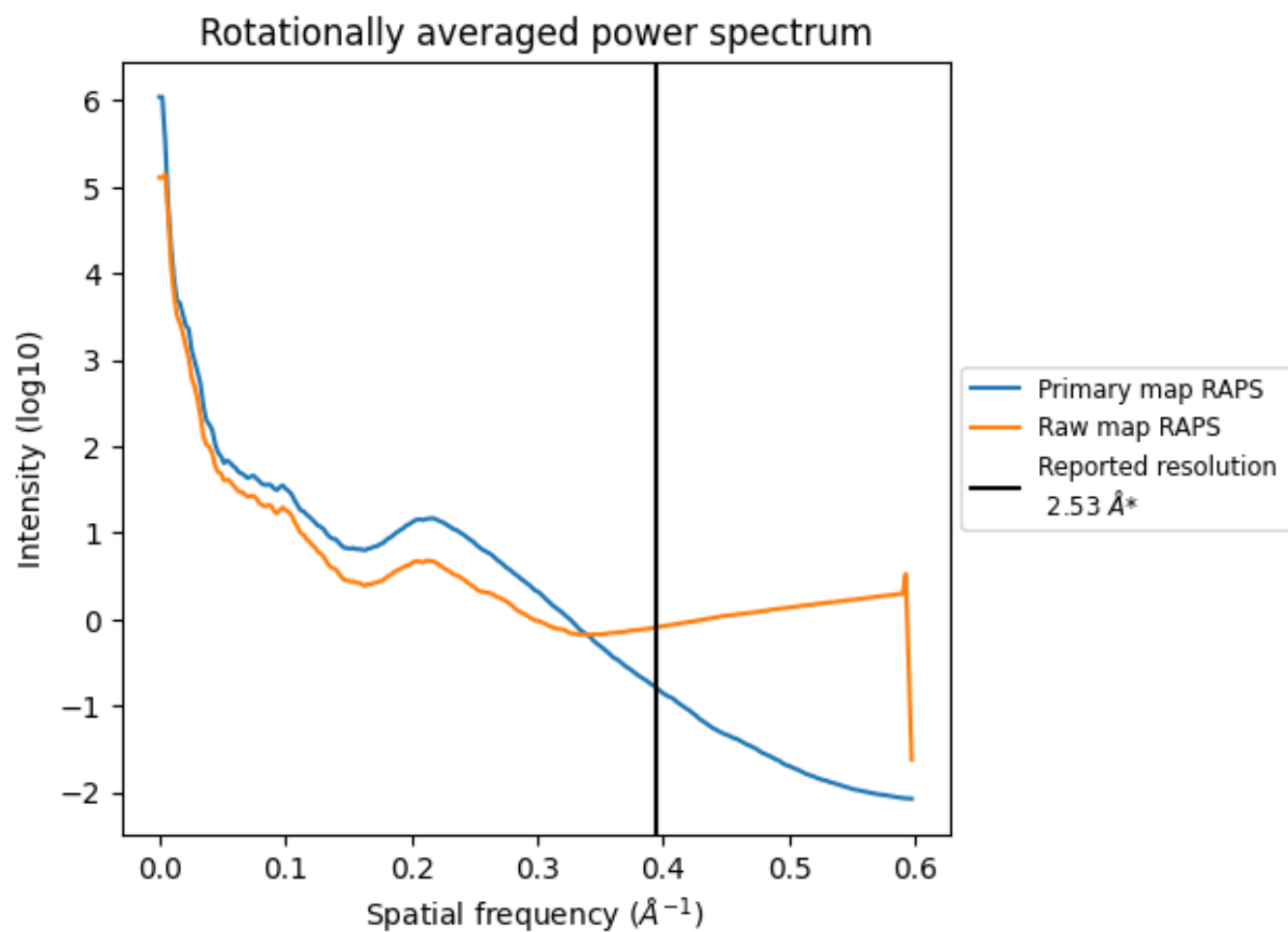
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 612 nm^3 ; this corresponds to an approximate mass of 552 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

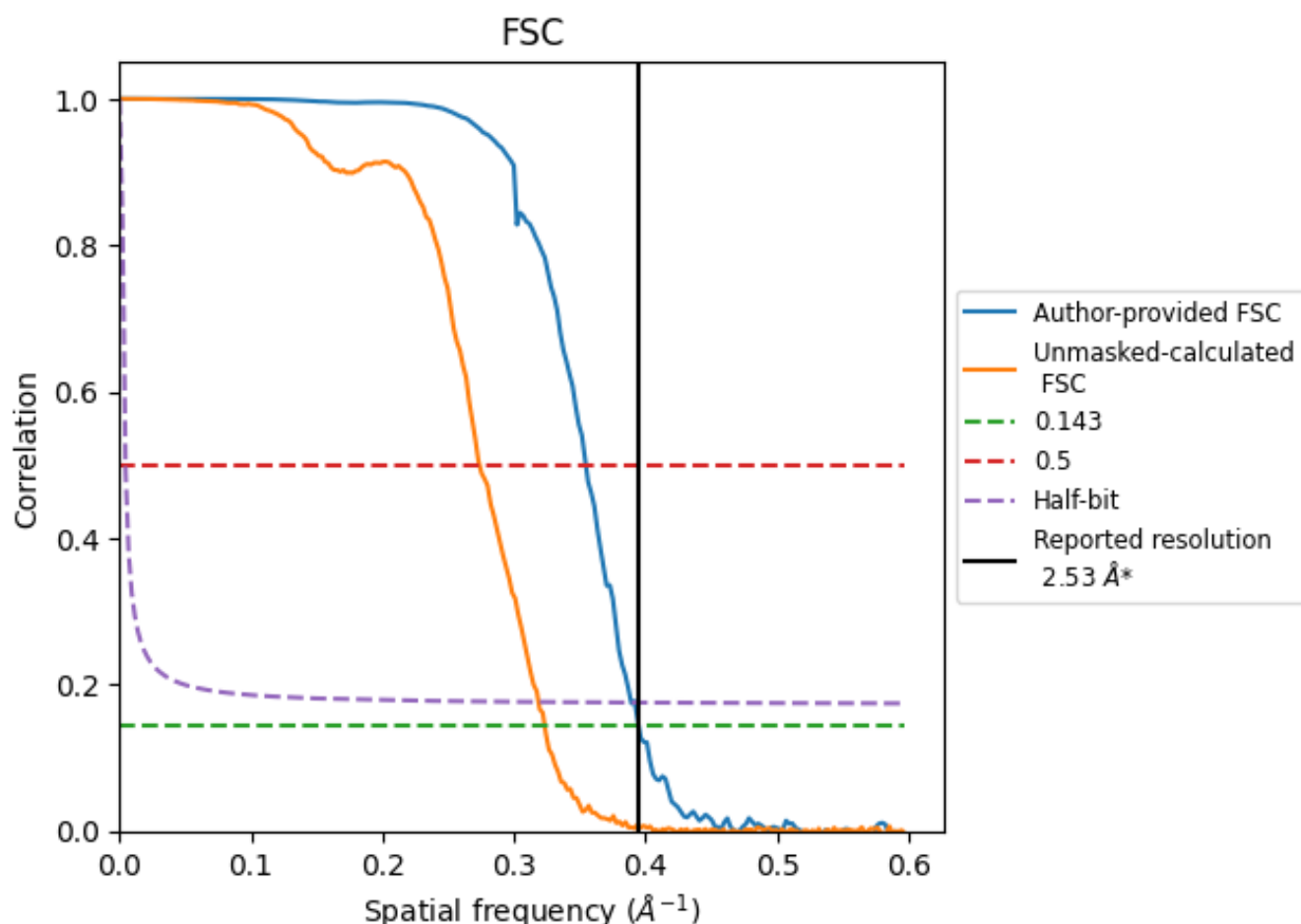


*Reported resolution corresponds to spatial frequency of 0.395 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.395 Å⁻¹

8.2 Resolution estimates [i](#)

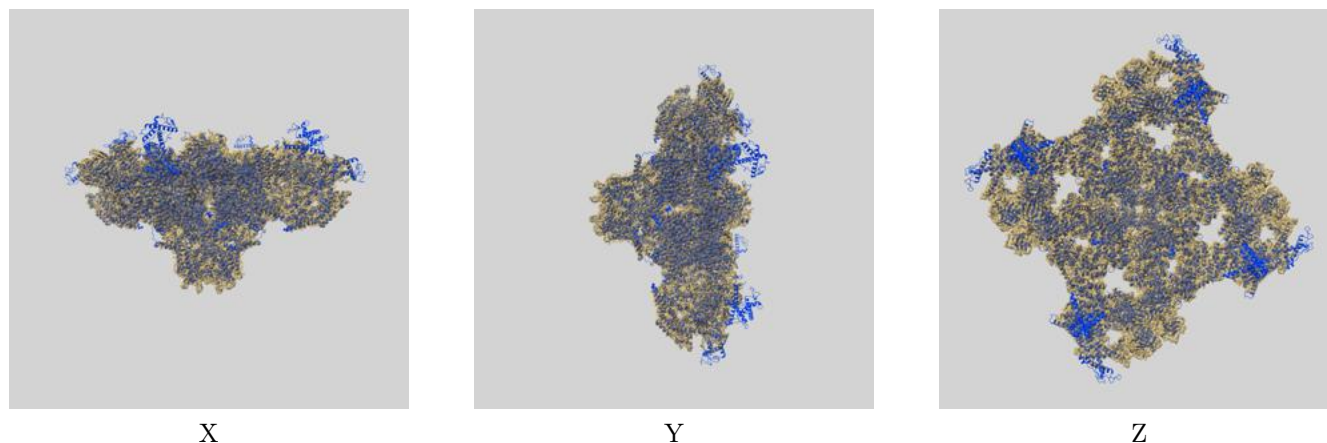
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.53	-	-
Author-provided FSC curve	2.53	2.82	2.57
Unmasked-calculated*	3.09	3.65	3.14

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.09 differs from the reported value 2.53 by more than 10 %

9 Map-model fit [i](#)

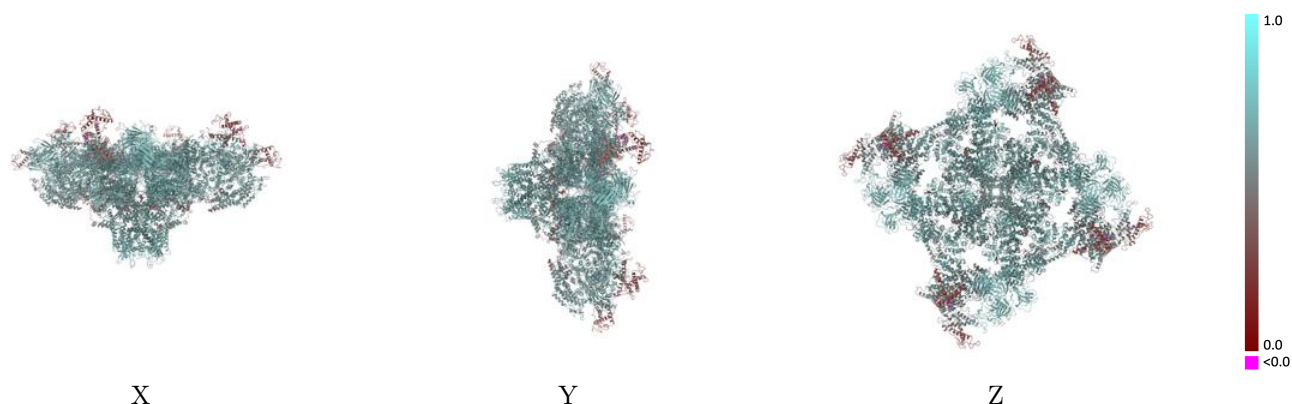
This section contains information regarding the fit between EMDB map EMD-43283 and PDB model 8VJJ. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



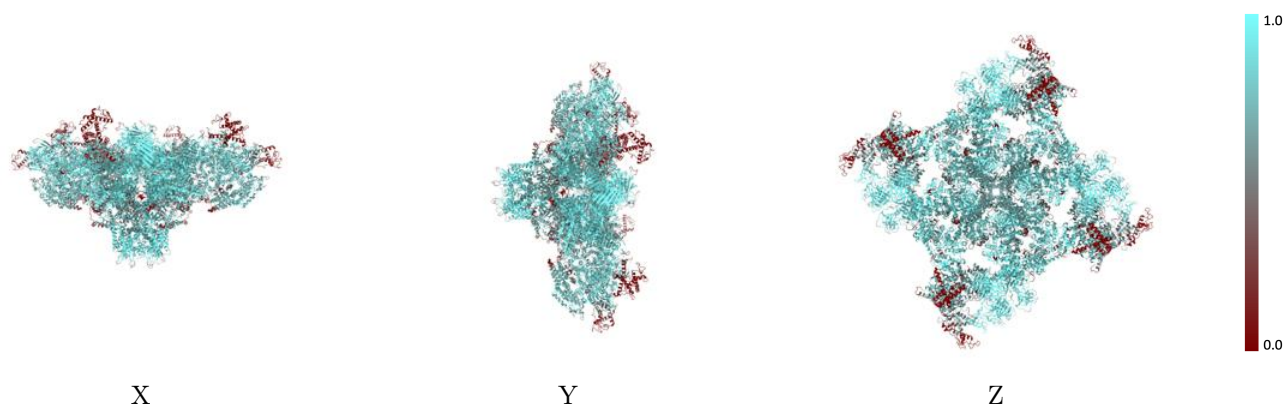
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



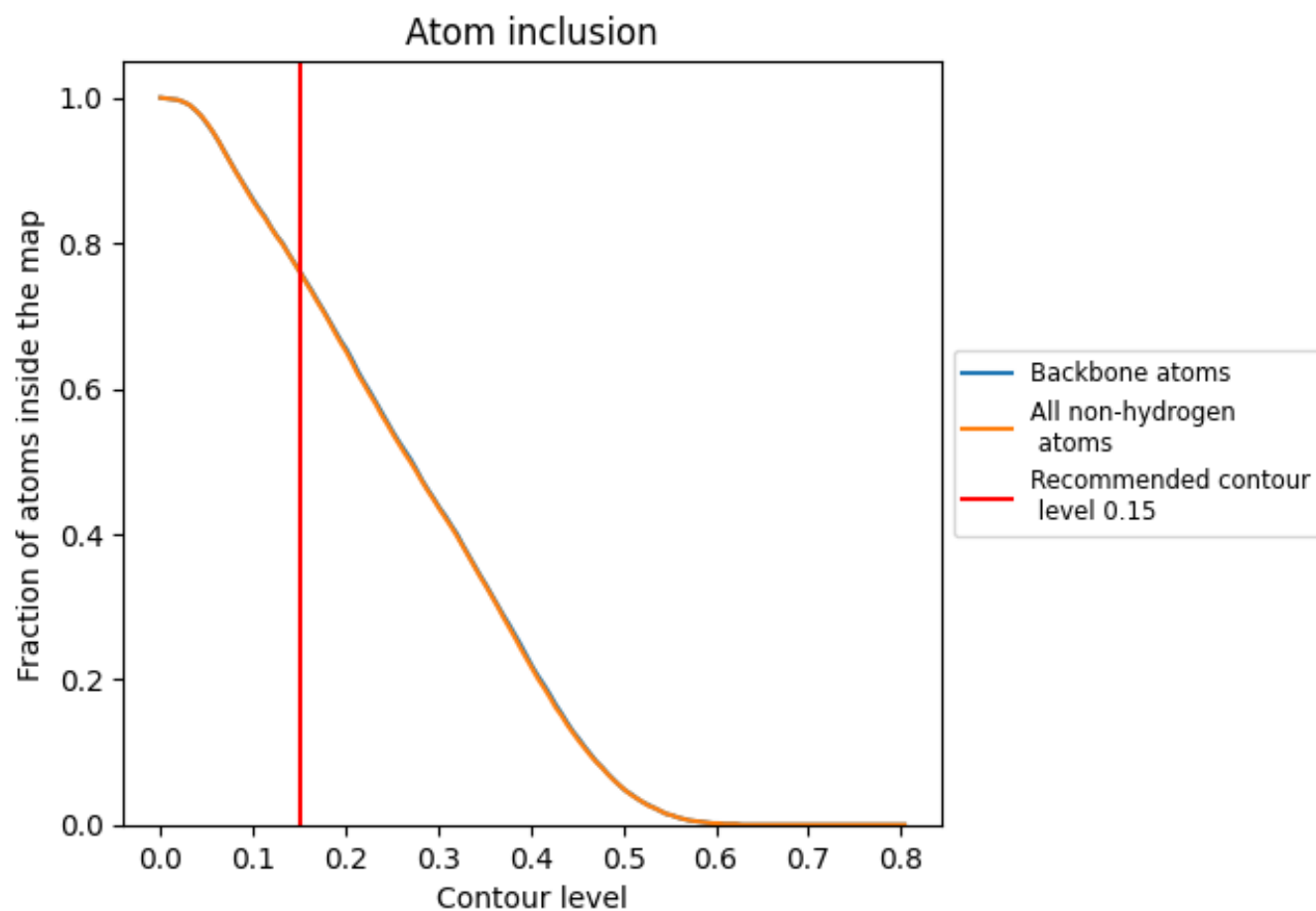
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7610	<div><div></div></div> 0.5970
A	<div><div></div></div> 0.7630	<div><div></div></div> 0.5960
B	<div><div></div></div> 0.7640	<div><div></div></div> 0.5950
C	<div><div></div></div> 0.7630	<div><div></div></div> 0.5960
D	<div><div></div></div> 0.7640	<div><div></div></div> 0.5960
E	<div><div></div></div> 0.8670	<div><div></div></div> 0.6550
F	<div><div></div></div> 0.8660	<div><div></div></div> 0.6530
G	<div><div></div></div> 0.8650	<div><div></div></div> 0.6530
H	<div><div></div></div> 0.8680	<div><div></div></div> 0.6540

1.0

0.0

<0.0