



Full wwPDB EM Validation Report ⓘ

Sep 29, 2025 – 12:26 PM EDT

PDB ID : 9NMR / pdb_00009nmr
EMDB ID : EMD-49538
Title : Structure of mouse RyR1 (including auxiliary transmembrane helix TMx; EGTA-only dataset)
Authors : Weninger, G.; Marks, A.R.
Deposited on : 2025-03-04
Resolution : 2.91 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:

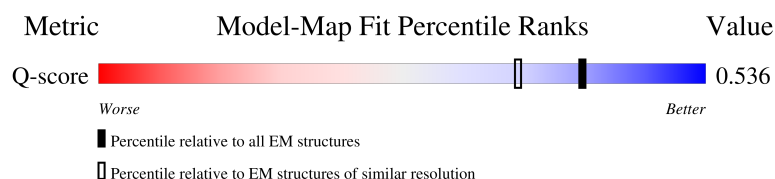
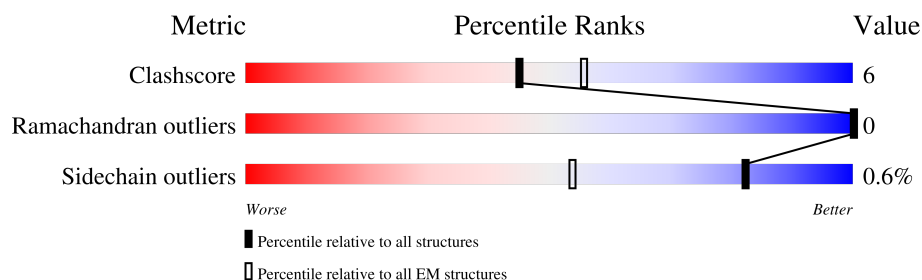
EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

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 2.91 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	12972 (2.41 - 3.41)

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	

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Mol	Chain	Length	Quality of chain
2	E	108	 91% 8% •
2	F	108	 89% 10% •
2	G	108	 90% 9% •
2	H	108	 91% 8% •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 143684 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4397	Total	C	N	O	S	1	0
			34983	22250	6021	6475	237		
1	B	4397	Total	C	N	O	S	1	0
			34983	22250	6021	6475	237		
1	C	4397	Total	C	N	O	S	1	0
			34983	22250	6021	6475	237		
1	D	4397	Total	C	N	O	S	1	0
			34983	22250	6021	6475	237		

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

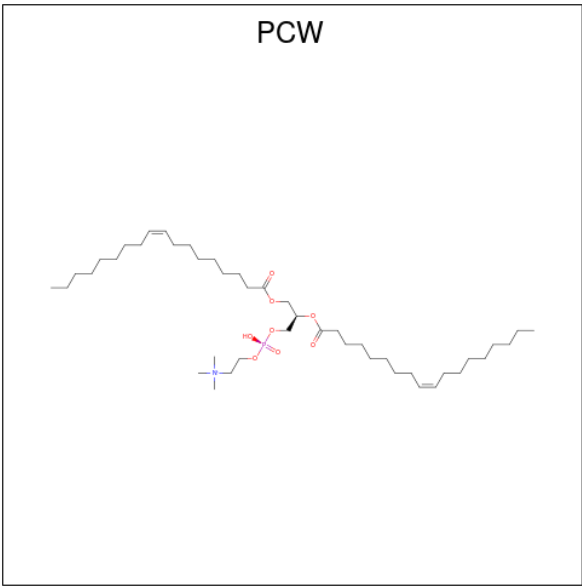
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
2	F	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
2	G	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
2	H	107	Total	C	N	O	S	0	0
			829	526	145	155	3		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW)

(formula: C₄₄H₈₅NO₈P).

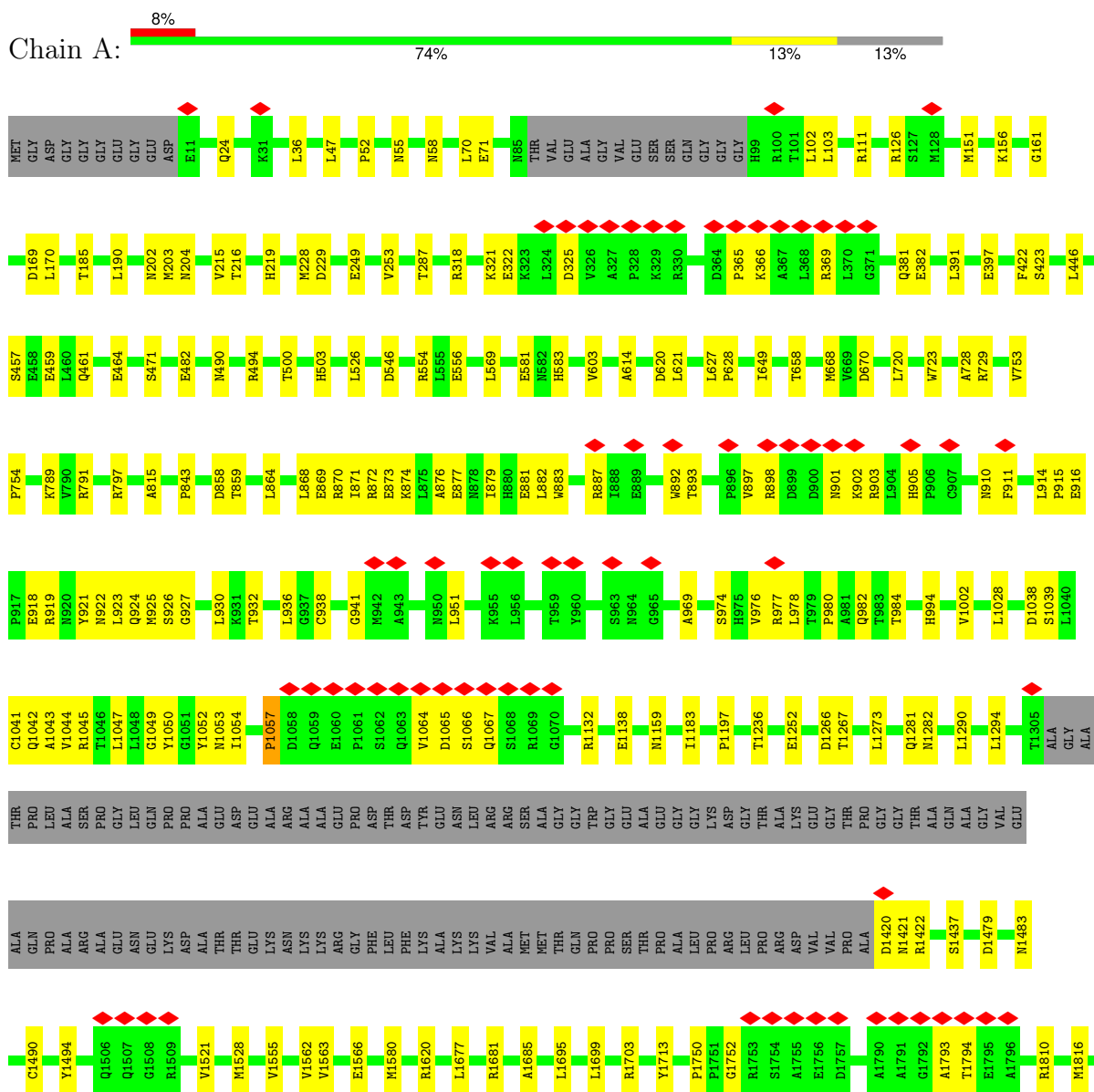


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
4	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
4	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
4	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
4	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
4	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
4	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
4	D	1	Total	C	N	O	P	0
			54	44	1	8	1	

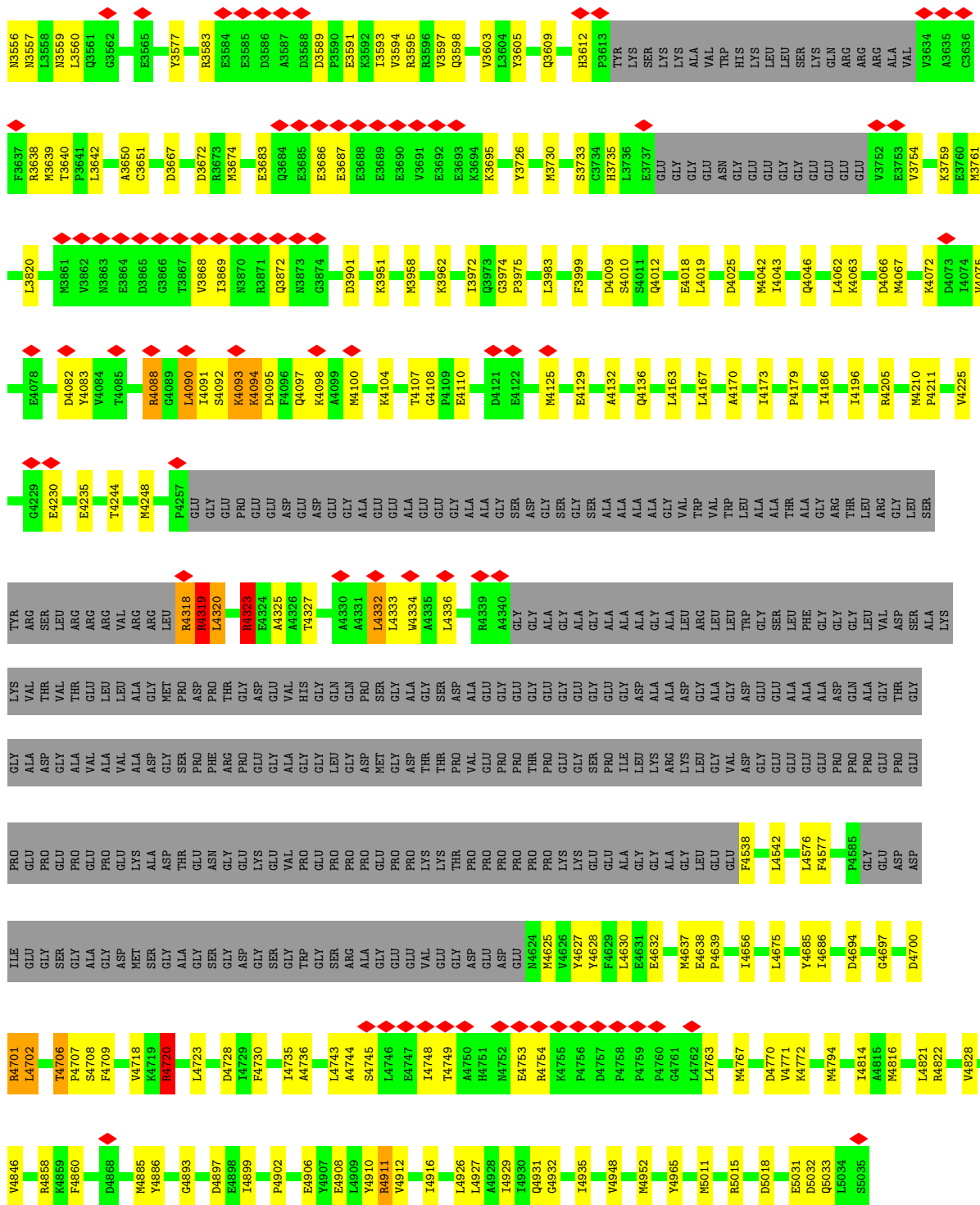
3 Residue-property plots

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.

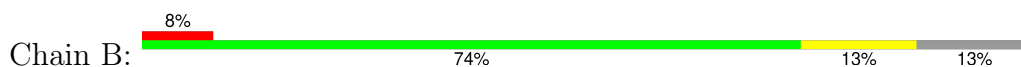
• Molecule 1: Ryanodine receptor 1





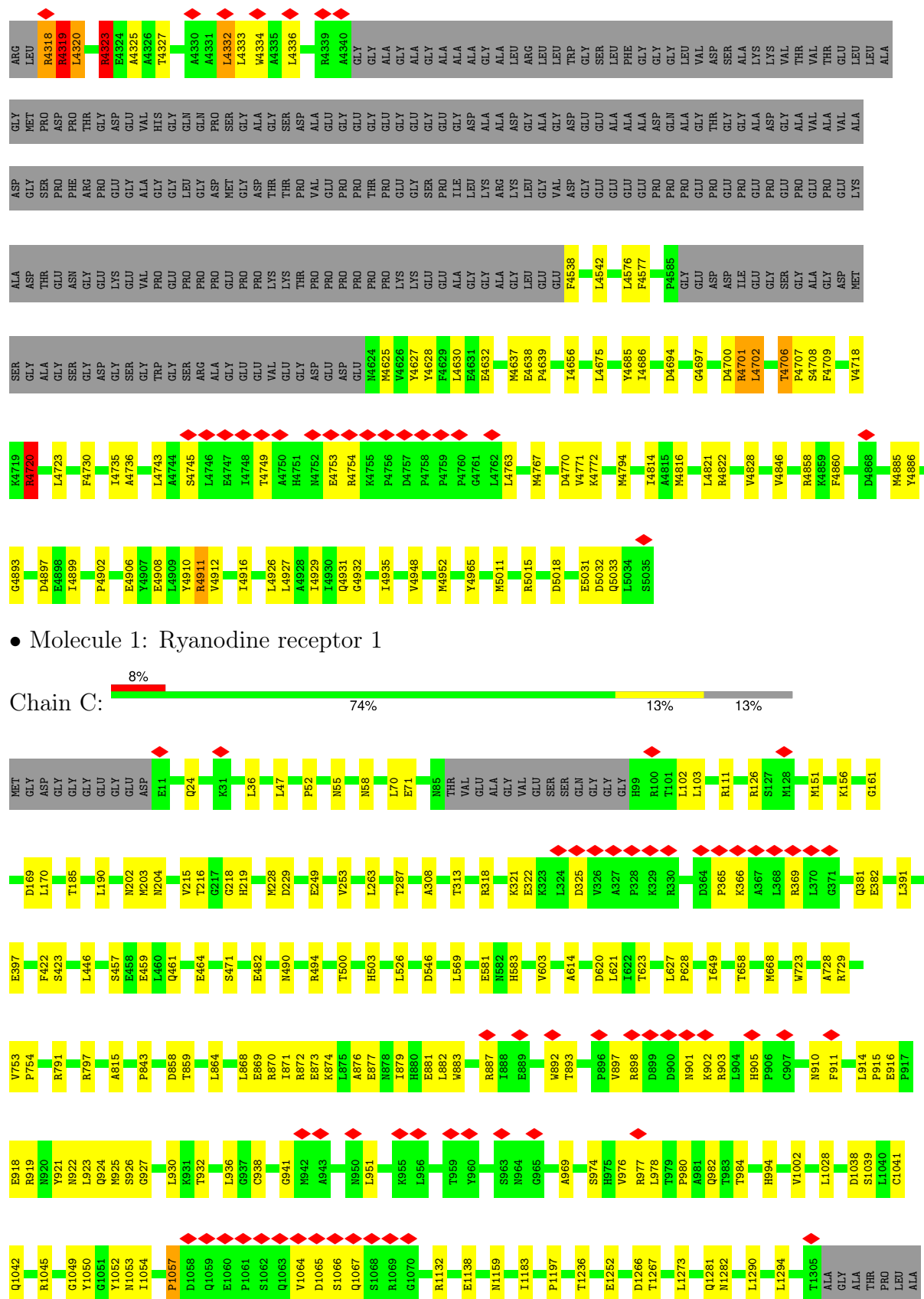


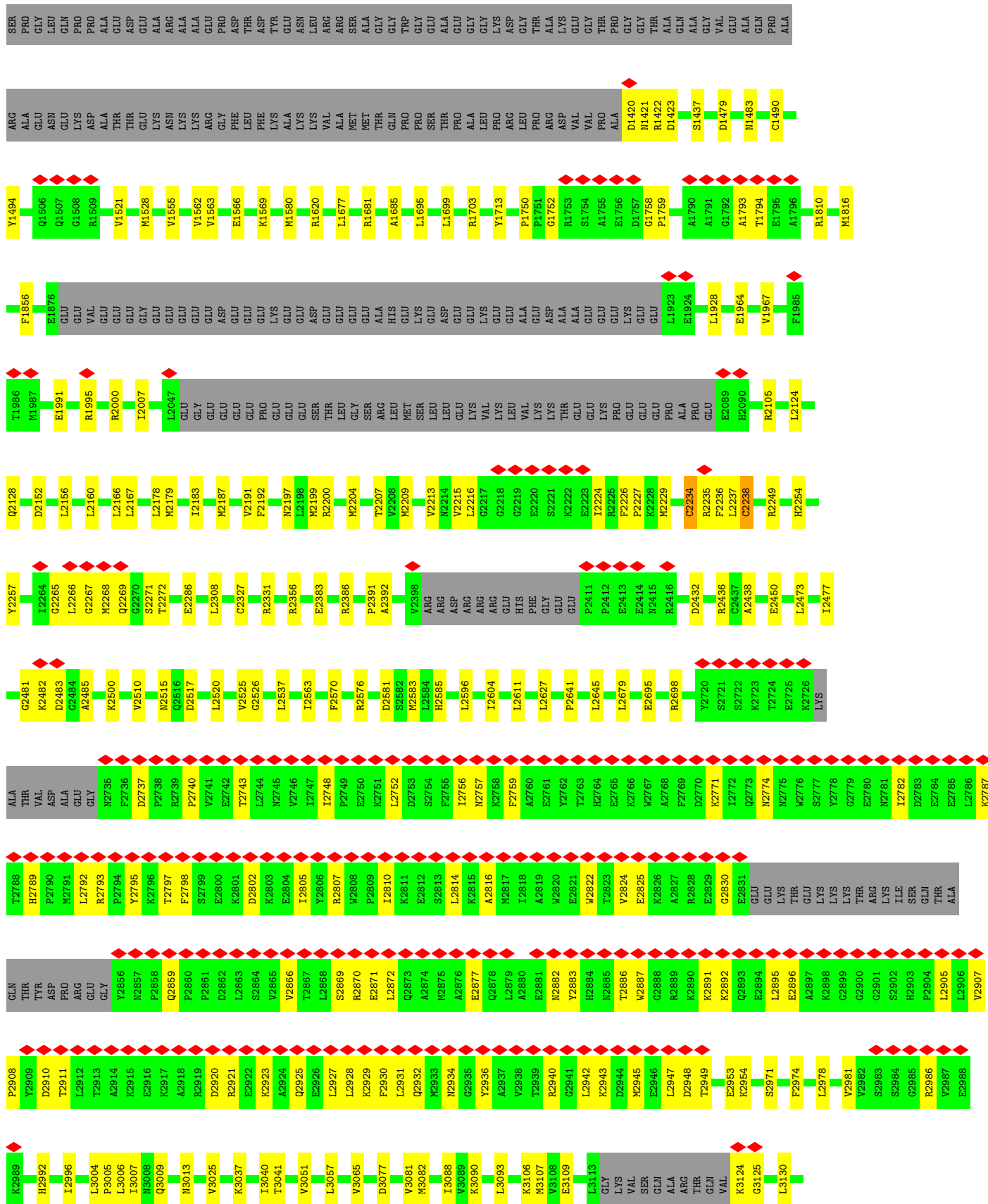
- Molecule 1: Ryanodine receptor 1



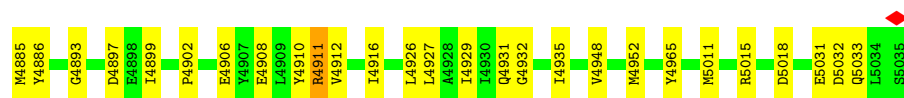




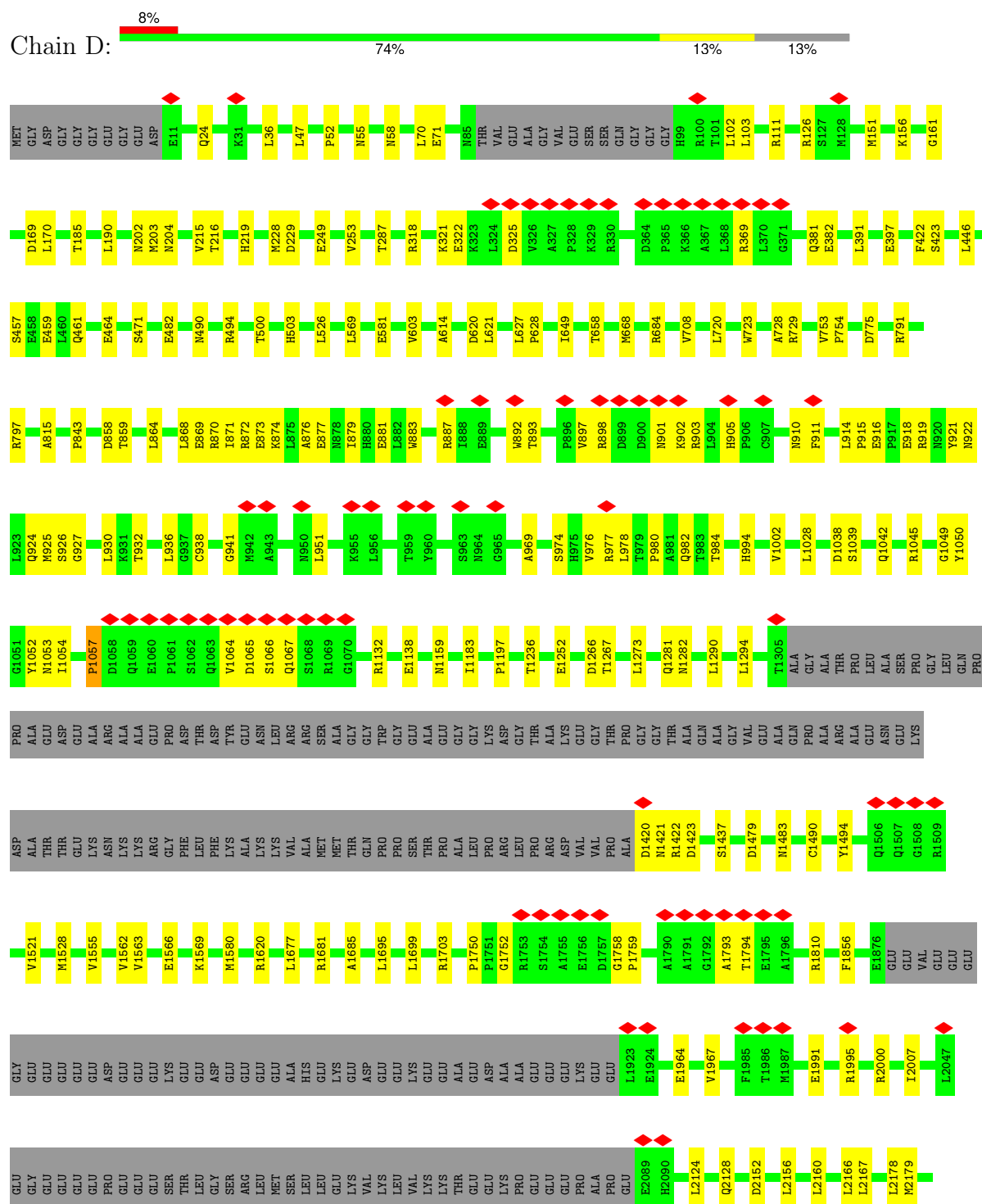




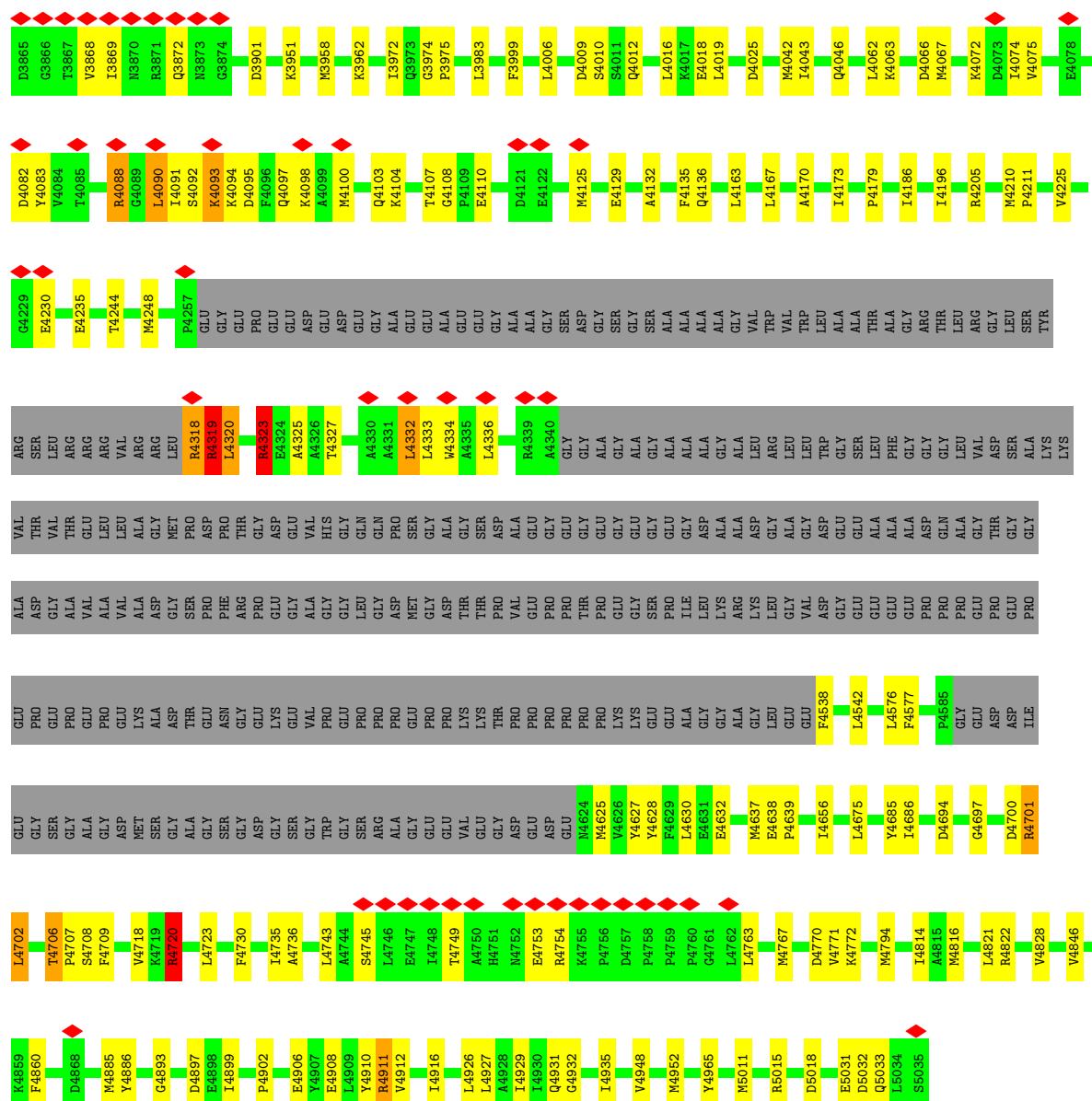





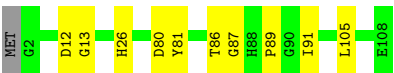
Molecule 1: Ryanodine receptor 1








Chain G:  90% 9% .



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

Chain H:  91% 8% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	129073	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS 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	0.613	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	427.008, 427.008, 427.008	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	0/35776	0.41	5/48462 (0.0%)
1	B	0.23	0/35776	0.41	5/48462 (0.0%)
1	C	0.23	0/35776	0.41	5/48462 (0.0%)
1	D	0.23	0/35776	0.41	5/48462 (0.0%)
2	E	0.18	0/847	0.32	0/1142
2	F	0.18	0/847	0.32	0/1142
2	G	0.18	0/847	0.31	0/1142
2	H	0.18	0/847	0.31	0/1142
All	All	0.23	0/146492	0.40	20/198416 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	8
1	C	0	8
1	D	0	8
All	All	0	32

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2238	CYS	CA-CB-SG	9.06	135.23	114.40
1	A	2238	CYS	CA-CB-SG	9.05	135.21	114.40
1	D	2238	CYS	CA-CB-SG	9.05	135.21	114.40
1	C	2238	CYS	CA-CB-SG	9.04	135.19	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2238	CYS	CB-CA-C	6.19	120.63	110.17
1	A	2238	CYS	CB-CA-C	6.17	120.59	110.17
1	C	2238	CYS	CB-CA-C	6.17	120.59	110.17
1	D	2238	CYS	CB-CA-C	6.17	120.59	110.17
1	D	2238	CYS	N-CA-CB	-5.83	101.81	110.61
1	A	2238	CYS	N-CA-CB	-5.82	101.83	110.61
1	C	2238	CYS	N-CA-CB	-5.82	101.83	110.61
1	B	2238	CYS	N-CA-CB	-5.79	101.86	110.61
1	B	1057	PRO	CA-N-CD	-5.75	103.96	112.00
1	A	1057	PRO	CA-N-CD	-5.72	103.99	112.00
1	C	1057	PRO	CA-N-CD	-5.72	103.99	112.00
1	D	1057	PRO	CA-N-CD	-5.72	103.99	112.00
1	C	2234	CYS	N-CA-CB	5.39	119.59	110.49
1	A	2234	CYS	N-CA-CB	5.37	119.57	110.49
1	B	2234	CYS	N-CA-CB	5.37	119.57	110.49
1	D	2234	CYS	N-CA-CB	5.37	119.57	110.49

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2238	CYS	Peptide
1	A	4088	ARG	Sidechain
1	A	4318	ARG	Sidechain
1	A	4319	ARG	Sidechain
1	A	4323	ARG	Sidechain
1	A	4701	ARG	Sidechain
1	A	4720	ARG	Sidechain
1	A	4911	ARG	Sidechain
1	B	2238	CYS	Peptide
1	B	4088	ARG	Sidechain
1	B	4318	ARG	Sidechain
1	B	4319	ARG	Sidechain
1	B	4323	ARG	Sidechain
1	B	4701	ARG	Sidechain
1	B	4720	ARG	Sidechain
1	B	4911	ARG	Sidechain
1	C	2238	CYS	Peptide
1	C	4088	ARG	Sidechain
1	C	4318	ARG	Sidechain
1	C	4319	ARG	Sidechain
1	C	4323	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	4701	ARG	Sidechain
1	C	4720	ARG	Sidechain
1	C	4911	ARG	Sidechain
1	D	2238	CYS	Peptide
1	D	4088	ARG	Sidechain
1	D	4318	ARG	Sidechain
1	D	4319	ARG	Sidechain
1	D	4323	ARG	Sidechain
1	D	4701	ARG	Sidechain
1	D	4720	ARG	Sidechain
1	D	4911	ARG	Sidechain

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	34983	0	34589	445	0
1	B	34983	0	34589	438	0
1	C	34983	0	34589	437	0
1	D	34983	0	34589	432	0
2	E	829	0	826	8	0
2	F	829	0	826	10	0
2	G	829	0	826	9	0
2	H	829	0	826	9	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	0	168	0	0
4	B	108	0	168	0	0
4	C	108	0	168	0	0
4	D	108	0	168	0	0
All	All	143684	0	142332	1748	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 6.

All (1748) 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:C:2752:LEU:HD13	1:C:2814:LEU:HD21	1.43	1.00
1:B:2752:LEU:HD13	1:B:2814:LEU:HD21	1.43	0.98
1:C:1991:GLU:OE2	1:C:1995:ARG:NH1	1.97	0.97
1:D:2752:LEU:HD13	1:D:2814:LEU:HD21	1.43	0.97
1:A:1991:GLU:OE2	1:A:1995:ARG:NH1	1.97	0.96
1:B:1991:GLU:OE2	1:B:1995:ARG:NH1	1.97	0.96
1:A:2752:LEU:HD13	1:A:2814:LEU:HD21	1.43	0.96
1:D:1991:GLU:OE2	1:D:1995:ARG:NH1	1.97	0.95
1:B:3009:GLN:NE2	1:B:3013:ASN:OD1	2.02	0.92
1:D:3009:GLN:NE2	1:D:3013:ASN:OD1	2.02	0.92
1:C:3009:GLN:NE2	1:C:3013:ASN:OD1	2.02	0.92
1:A:3009:GLN:NE2	1:A:3013:ASN:OD1	2.02	0.91
1:D:3322:ARG:NH1	1:D:3326:ASN:OD1	2.06	0.88
1:B:3322:ARG:NH1	1:B:3326:ASN:OD1	2.06	0.87
1:C:3322:ARG:NH1	1:C:3326:ASN:OD1	2.06	0.87
1:A:3322:ARG:NH1	1:A:3326:ASN:OD1	2.06	0.87
1:C:4816:MET:O	1:C:4822:ARG:NH2	2.09	0.85
1:C:926:SER:O	1:C:930:LEU:HD12	1.77	0.85
1:B:914:LEU:O	1:B:919:ARG:NH2	2.10	0.84
1:A:2249:ARG:NH2	1:A:2286:GLU:OE2	2.10	0.84
1:A:4816:MET:O	1:A:4822:ARG:NH2	2.09	0.84
1:D:914:LEU:O	1:D:919:ARG:NH2	2.10	0.84
1:D:926:SER:O	1:D:930:LEU:HD12	1.77	0.84
1:A:914:LEU:O	1:A:919:ARG:NH2	2.10	0.84
1:B:2249:ARG:NH2	1:B:2286:GLU:OE2	2.10	0.84
1:C:2249:ARG:NH2	1:C:2286:GLU:OE2	2.10	0.84
1:D:2249:ARG:NH2	1:D:2286:GLU:OE2	2.10	0.84
1:B:4816:MET:O	1:B:4822:ARG:NH2	2.09	0.84
1:D:2825:GLU:O	1:D:2936:TYR:HA	1.78	0.84
1:B:3170:LEU:HD12	1:B:3195:LEU:HD11	1.60	0.84
1:D:4816:MET:O	1:D:4822:ARG:NH2	2.09	0.84
1:B:926:SER:O	1:B:930:LEU:HD12	1.77	0.84
1:C:914:LEU:O	1:C:919:ARG:NH2	2.10	0.84
1:D:3170:LEU:HD12	1:D:3195:LEU:HD11	1.60	0.84
1:C:2825:GLU:O	1:C:2936:TYR:HA	1.78	0.83
1:A:926:SER:O	1:A:930:LEU:HD12	1.77	0.83
1:C:3170:LEU:HD12	1:C:3195:LEU:HD11	1.60	0.83
1:A:3170:LEU:HD12	1:A:3195:LEU:HD11	1.60	0.82
1:B:2825:GLU:O	1:B:2936:TYR:HA	1.78	0.82
1:A:2825:GLU:O	1:A:2936:TYR:HA	1.78	0.82
1:B:4042:MET:SD	1:B:4046:GLN:NE2	2.54	0.81
1:A:4042:MET:SD	1:A:4046:GLN:NE2	2.54	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4042:MET:SD	1:C:4046:GLN:NE2	2.54	0.80
1:D:4042:MET:SD	1:D:4046:GLN:NE2	2.54	0.79
1:A:2234:CYS:O	1:A:2235:ARG:C	2.26	0.78
1:D:1793:ALA:O	1:D:1794:THR:OG1	2.02	0.78
1:B:2234:CYS:O	1:B:2235:ARG:C	2.26	0.77
1:A:1793:ALA:O	1:A:1794:THR:OG1	2.02	0.77
1:B:4091:ILE:HG12	1:B:4095:ASP:HB3	1.67	0.77
1:B:4632:GLU:HG2	1:B:4637:MET:HG3	1.67	0.76
1:B:1793:ALA:O	1:B:1794:THR:OG1	2.02	0.76
1:C:2234:CYS:O	1:C:2235:ARG:C	2.26	0.76
1:C:1793:ALA:O	1:C:1794:THR:OG1	2.02	0.76
1:B:4952:MET:HE2	1:B:4952:MET:HA	1.67	0.76
1:D:2234:CYS:O	1:D:2235:ARG:C	2.26	0.76
1:D:4091:ILE:HG12	1:D:4095:ASP:HB3	1.67	0.75
1:C:4091:ILE:HG12	1:C:4095:ASP:HB3	1.67	0.75
1:A:2948:ASP:OD2	1:A:2949:THR:N	2.20	0.75
1:B:2948:ASP:OD2	1:B:2949:THR:N	2.20	0.75
1:C:2948:ASP:OD2	1:C:2949:THR:N	2.20	0.75
1:C:4952:MET:HA	1:C:4952:MET:HE2	1.67	0.75
1:D:2948:ASP:OD2	1:D:2949:THR:N	2.20	0.75
1:D:4952:MET:HE2	1:D:4952:MET:HA	1.67	0.75
1:A:4632:GLU:HG2	1:A:4637:MET:HG3	1.67	0.75
1:B:4066:ASP:OD1	1:B:4067:MET:N	2.20	0.75
1:D:4066:ASP:OD1	1:D:4067:MET:N	2.20	0.74
1:A:4952:MET:HE2	1:A:4952:MET:HA	1.67	0.74
1:A:4066:ASP:OD1	1:A:4067:MET:N	2.20	0.74
1:A:4091:ILE:HG12	1:A:4095:ASP:HB3	1.67	0.74
1:C:4632:GLU:HG2	1:C:4637:MET:HG3	1.67	0.74
1:D:4632:GLU:HG2	1:D:4637:MET:HG3	1.67	0.74
1:B:2215:VAL:HG21	1:B:2229:MET:HE2	1.70	0.74
1:C:2215:VAL:HG21	1:C:2229:MET:HE2	1.70	0.74
1:D:2215:VAL:HG21	1:D:2229:MET:HE2	1.70	0.74
1:C:4066:ASP:OD1	1:C:4067:MET:N	2.20	0.73
1:A:2215:VAL:HG21	1:A:2229:MET:HE2	1.70	0.73
1:B:2213:VAL:HG21	1:B:2257:TYR:CE2	2.24	0.73
1:C:2213:VAL:HG21	1:C:2257:TYR:CE2	2.24	0.73
1:B:911:PHE:O	1:B:919:ARG:NH1	2.22	0.73
1:D:911:PHE:O	1:D:919:ARG:NH1	2.22	0.72
1:A:3366:LEU:HD21	1:A:3406:LEU:HD23	1.72	0.72
1:B:3366:LEU:HD21	1:B:3406:LEU:HD23	1.72	0.72
1:A:2213:VAL:HG21	1:A:2257:TYR:CE2	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:911:PHE:O	1:C:919:ARG:NH1	2.22	0.72
1:D:2213:VAL:HG21	1:D:2257:TYR:CE2	2.24	0.72
1:D:3868:VAL:HG12	1:D:3869:ILE:H	1.56	0.71
1:B:2234:CYS:O	1:B:2236:PHE:N	2.23	0.71
1:A:3082:MET:HE3	1:A:3093:LEU:HD23	1.72	0.71
1:A:3868:VAL:HG12	1:A:3869:ILE:H	1.56	0.71
1:A:3962:LYS:NZ	1:A:4025:ASP:OD2	2.21	0.71
1:B:3868:VAL:HG12	1:B:3869:ILE:H	1.56	0.71
1:A:911:PHE:O	1:A:919:ARG:NH1	2.22	0.71
1:A:2887:TRP:CD1	1:A:2891:LYS:HZ1	2.09	0.71
1:C:1236:THR:OG1	1:C:1703:ARG:NH1	2.24	0.71
1:D:3366:LEU:HD21	1:D:3406:LEU:HD23	1.72	0.71
1:B:1236:THR:OG1	1:B:1703:ARG:NH1	2.24	0.71
1:C:3868:VAL:HG12	1:C:3869:ILE:H	1.56	0.71
1:A:1236:THR:OG1	1:A:1703:ARG:NH1	2.24	0.70
1:B:2748:ILE:CD1	1:B:2814:LEU:HD22	2.21	0.70
1:C:2748:ILE:CD1	1:C:2814:LEU:HD22	2.21	0.70
1:B:2992:HIS:O	1:B:2996:ILE:HD12	1.91	0.70
1:C:2887:TRP:CD1	1:C:2891:LYS:HZ1	2.08	0.70
1:D:3082:MET:HE3	1:D:3093:LEU:HD23	1.72	0.70
1:A:2234:CYS:O	1:A:2236:PHE:N	2.23	0.70
1:C:2234:CYS:O	1:C:2236:PHE:N	2.23	0.70
1:D:1236:THR:OG1	1:D:1703:ARG:NH1	2.24	0.70
1:B:3082:MET:HE3	1:B:3093:LEU:HD23	1.72	0.70
1:C:3366:LEU:HD21	1:C:3406:LEU:HD23	1.72	0.70
1:A:2992:HIS:O	1:A:2996:ILE:HD12	1.91	0.70
1:D:2234:CYS:O	1:D:2236:PHE:N	2.23	0.70
1:B:3451:ASN:OD1	1:B:3454:ARG:NH2	2.25	0.70
1:D:2748:ILE:CD1	1:D:2814:LEU:HD22	2.21	0.70
1:D:4210:MET:HE3	1:D:4211:PRO:HD2	1.74	0.70
1:D:2992:HIS:O	1:D:2996:ILE:HD12	1.91	0.69
1:B:2887:TRP:CD1	1:B:2891:LYS:HZ1	2.10	0.69
1:B:4210:MET:HE3	1:B:4211:PRO:HD2	1.74	0.69
1:B:3612:HIS:ND1	1:B:3612:HIS:O	2.26	0.69
1:C:3451:ASN:OD1	1:C:3454:ARG:NH2	2.25	0.69
1:B:3589:ASP:O	1:B:3593:ILE:HD12	1.93	0.69
1:C:1420:ASP:O	1:C:1422:ARG:NH1	2.26	0.69
1:A:2748:ILE:CD1	1:A:2814:LEU:HD22	2.21	0.69
1:D:3589:ASP:O	1:D:3593:ILE:HD12	1.93	0.69
1:A:1420:ASP:O	1:A:1422:ARG:NH1	2.26	0.69
1:C:2992:HIS:O	1:C:2996:ILE:HD12	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4210:MET:HE3	1:C:4211:PRO:HD2	1.74	0.69
1:B:1420:ASP:O	1:B:1422:ARG:NH1	2.26	0.69
1:C:3612:HIS:ND1	1:C:3612:HIS:O	2.26	0.69
1:D:3451:ASN:OD1	1:D:3454:ARG:NH2	2.25	0.69
1:C:3082:MET:HE3	1:C:3093:LEU:HD23	1.72	0.69
1:D:24:GLN:OE1	1:D:204:ASN:ND2	2.26	0.69
1:A:3612:HIS:ND1	1:A:3612:HIS:O	2.26	0.68
1:C:287:THR:HG21	1:C:482:GLU:OE2	1.93	0.68
1:A:4210:MET:HE3	1:A:4211:PRO:HD2	1.74	0.68
1:D:287:THR:HG21	1:D:482:GLU:OE2	1.94	0.68
1:D:1420:ASP:O	1:D:1422:ARG:NH1	2.26	0.68
1:B:24:GLN:OE1	1:B:204:ASN:ND2	2.26	0.68
1:C:24:GLN:OE1	1:C:204:ASN:ND2	2.26	0.68
1:A:24:GLN:OE1	1:A:204:ASN:ND2	2.26	0.68
1:C:3589:ASP:O	1:C:3593:ILE:HD12	1.93	0.68
1:D:3612:HIS:ND1	1:D:3612:HIS:O	2.26	0.68
1:A:3451:ASN:OD1	1:A:3454:ARG:NH2	2.25	0.68
2:G:26:HIS:CE1	2:G:105:LEU:HD11	2.29	0.68
2:F:26:HIS:CE1	2:F:105:LEU:HD11	2.29	0.68
2:H:26:HIS:CE1	2:H:105:LEU:HD11	2.29	0.68
1:C:169:ASP:OD1	1:C:202:ASN:ND2	2.27	0.68
1:A:2774:ASN:O	1:A:2787:LYS:NZ	2.21	0.67
1:A:2971:SER:HA	1:A:2974:PHE:CE1	2.29	0.67
1:A:3589:ASP:O	1:A:3593:ILE:HD12	1.93	0.67
1:D:169:ASP:OD1	1:D:202:ASN:ND2	2.27	0.67
1:D:2908:PRO:O	1:D:2911:THR:OG1	2.12	0.67
2:E:26:HIS:CE1	2:E:105:LEU:HD11	2.30	0.67
1:A:287:THR:HG21	1:A:482:GLU:OE2	1.93	0.67
1:C:2908:PRO:O	1:C:2911:THR:OG1	2.12	0.67
1:D:2971:SER:HA	1:D:2974:PHE:CE1	2.29	0.67
1:B:2971:SER:HA	1:B:2974:PHE:CE1	2.29	0.67
1:B:1038:ASP:OD1	1:B:1039:SER:N	2.28	0.67
1:A:1038:ASP:OD1	1:A:1039:SER:N	2.28	0.67
1:A:974:SER:O	1:A:977:ARG:NH1	2.28	0.67
1:B:974:SER:O	1:B:977:ARG:NH1	2.28	0.67
1:C:3593:ILE:O	1:C:3597:VAL:HG23	1.95	0.67
1:C:2971:SER:HA	1:C:2974:PHE:CE1	2.29	0.67
1:C:1038:ASP:OD1	1:C:1039:SER:N	2.28	0.66
1:D:2920:ASP:OD1	1:D:2923:LYS:NZ	2.28	0.66
1:B:287:THR:HG21	1:B:482:GLU:OE2	1.93	0.66
1:B:2197:ASN:OD1	1:B:2200:ARG:NH2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2197:ASN:OD1	1:A:2200:ARG:NH2	2.28	0.66
1:B:2520:LEU:HD13	1:B:2576:ARG:HD3	1.77	0.66
1:B:318:ARG:NH2	1:B:322:GLU:O	2.28	0.66
1:B:3577:TYR:OH	1:B:3583:ARG:NH2	2.29	0.66
1:B:3962:LYS:NZ	1:B:4025:ASP:OD2	2.21	0.66
1:D:318:ARG:NH2	1:D:322:GLU:O	2.28	0.66
1:D:2520:LEU:HD13	1:D:2576:ARG:HD3	1.77	0.66
1:A:2920:ASP:OD1	1:A:2923:LYS:NZ	2.28	0.66
1:D:2197:ASN:OD1	1:D:2200:ARG:NH2	2.28	0.66
1:D:3167:TYR:CD2	1:D:3240:MET:HE2	2.31	0.66
1:A:3577:TYR:OH	1:A:3583:ARG:NH2	2.29	0.66
1:B:2908:PRO:O	1:B:2911:THR:OG1	2.12	0.66
1:C:974:SER:O	1:C:977:ARG:NH1	2.28	0.66
1:D:1038:ASP:OD1	1:D:1039:SER:N	2.28	0.66
1:D:3962:LYS:NZ	1:D:4025:ASP:OD2	2.21	0.66
1:C:2197:ASN:OD1	1:C:2200:ARG:NH2	2.28	0.66
1:C:3167:TYR:CD2	1:C:3240:MET:HE2	2.31	0.66
1:D:974:SER:O	1:D:977:ARG:NH1	2.28	0.66
1:D:3593:ILE:O	1:D:3597:VAL:HG23	1.95	0.66
1:A:169:ASP:OD1	1:A:202:ASN:ND2	2.27	0.66
1:A:3167:TYR:CD2	1:A:3240:MET:HE2	2.31	0.66
1:B:3593:ILE:O	1:B:3597:VAL:HG23	1.95	0.66
1:A:3593:ILE:O	1:A:3597:VAL:HG23	1.95	0.65
1:B:2920:ASP:OD1	1:B:2923:LYS:NZ	2.28	0.65
1:C:2920:ASP:OD1	1:C:2923:LYS:NZ	2.28	0.65
1:D:3577:TYR:OH	1:D:3583:ARG:NH2	2.29	0.65
1:C:318:ARG:NH2	1:C:322:GLU:O	2.28	0.65
1:C:3577:TYR:OH	1:C:3583:ARG:NH2	2.29	0.65
1:A:318:ARG:NH2	1:A:322:GLU:O	2.28	0.65
1:A:2520:LEU:HD13	1:A:2576:ARG:HD3	1.77	0.65
1:C:2520:LEU:HD13	1:C:2576:ARG:HD3	1.77	0.65
1:B:901:ASN:OD1	1:B:902:LYS:N	2.30	0.64
1:C:2583:MET:HE3	1:C:2611:LEU:HD13	1.80	0.64
1:A:901:ASN:OD1	1:A:902:LYS:N	2.30	0.64
1:B:3167:TYR:CD2	1:B:3240:MET:HE2	2.31	0.64
1:C:2871:GLU:OE2	1:C:2940:ARG:NH1	2.31	0.64
1:C:2752:LEU:HD11	1:C:2824:VAL:HG23	1.80	0.64
1:C:3235:ASN:OD1	1:C:3236:SER:N	2.30	0.64
1:A:2583:MET:HE3	1:A:2611:LEU:HD13	1.80	0.64
1:A:2871:GLU:OE2	1:A:2940:ARG:NH1	2.31	0.64
1:B:169:ASP:OD1	1:B:202:ASN:ND2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2752:LEU:HD11	1:B:2824:VAL:HG23	1.80	0.64
1:D:2583:MET:HE3	1:D:2611:LEU:HD13	1.80	0.64
1:D:2887:TRP:CD1	1:D:2891:LYS:HZ1	2.16	0.64
1:B:2871:GLU:OE2	1:B:2940:ARG:NH1	2.31	0.64
1:C:3556:ASN:OD1	1:C:3557:ASN:N	2.31	0.64
1:D:901:ASN:OD1	1:D:902:LYS:N	2.30	0.64
1:D:2871:GLU:OE2	1:D:2940:ARG:NH1	2.31	0.64
1:A:4908:GLU:O	1:A:4912:VAL:HG13	1.98	0.64
1:D:2752:LEU:HD11	1:D:2824:VAL:HG23	1.80	0.64
1:D:3235:ASN:OD1	1:D:3236:SER:N	2.30	0.64
1:B:2583:MET:HE3	1:B:2611:LEU:HD13	1.80	0.64
1:A:2908:PRO:O	1:A:2911:THR:OG1	2.12	0.63
1:B:3235:ASN:OD1	1:B:3236:SER:N	2.31	0.63
1:B:3556:ASN:OD1	1:B:3557:ASN:N	2.31	0.63
1:B:4908:GLU:O	1:B:4912:VAL:HG13	1.98	0.63
1:D:870:ARG:O	1:D:874:LYS:NZ	2.24	0.63
1:C:901:ASN:OD1	1:C:902:LYS:N	2.30	0.63
1:D:4908:GLU:O	1:D:4912:VAL:HG13	1.98	0.63
1:A:3235:ASN:OD1	1:A:3236:SER:N	2.30	0.63
1:C:3962:LYS:NZ	1:C:4025:ASP:OD2	2.21	0.63
1:C:4908:GLU:O	1:C:4912:VAL:HG13	1.98	0.63
1:A:2752:LEU:HD11	1:A:2824:VAL:HG23	1.80	0.63
1:A:3556:ASN:OD1	1:A:3557:ASN:N	2.31	0.63
1:B:2872:LEU:HD22	1:B:2932:GLN:NE2	2.14	0.62
1:B:2596:LEU:HD21	1:B:2604:ILE:HD12	1.82	0.62
1:D:2872:LEU:HD22	1:D:2932:GLN:NE2	2.15	0.62
1:D:3556:ASN:OD1	1:D:3557:ASN:N	2.31	0.62
1:B:3505:SER:OG	1:B:3508:THR:HG23	2.00	0.62
1:D:3505:SER:OG	1:D:3508:THR:HG23	2.00	0.62
1:A:922:ASN:HA	1:A:925:MET:HE2	1.82	0.62
1:A:2215:VAL:HG21	1:A:2229:MET:CE	2.30	0.62
1:A:2872:LEU:HD22	1:A:2932:GLN:NE2	2.14	0.62
1:B:922:ASN:HA	1:B:925:MET:HE2	1.82	0.62
1:C:922:ASN:HA	1:C:925:MET:HE2	1.82	0.62
1:D:922:ASN:HA	1:D:925:MET:HE2	1.82	0.62
2:G:80:ASP:OD1	2:G:81:TYR:N	2.33	0.62
1:C:2596:LEU:HD21	1:C:2604:ILE:HD12	1.82	0.62
1:A:3505:SER:OG	1:A:3508:THR:HG23	2.00	0.61
1:A:918:GLU:N	1:A:918:GLU:OE1	2.33	0.61
1:A:2596:LEU:HD21	1:A:2604:ILE:HD12	1.82	0.61
1:B:918:GLU:OE1	1:B:918:GLU:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2215:VAL:HG21	1:B:2229:MET:CE	2.30	0.61
1:C:2872:LEU:HD22	1:C:2932:GLN:NE2	2.14	0.61
1:C:4656:ILE:HD11	1:C:4794:MET:HB2	1.83	0.61
1:C:3505:SER:OG	1:C:3508:THR:HG23	2.00	0.61
1:C:729:ARG:NH2	1:C:1490:CYS:SG	2.74	0.61
1:D:2596:LEU:HD21	1:D:2604:ILE:HD12	1.82	0.61
1:D:868:LEU:HD12	1:D:930:LEU:HD23	1.83	0.61
1:B:2752:LEU:HD22	1:B:2814:LEU:HD11	1.82	0.61
1:D:2215:VAL:HG21	1:D:2229:MET:CE	2.30	0.61
1:B:4319:ARG:NH2	1:D:4906:GLU:HA	2.16	0.60
1:C:868:LEU:HD12	1:C:930:LEU:HD23	1.83	0.60
1:C:3243:ASP:OD1	1:C:3244:ILE:N	2.34	0.60
1:A:729:ARG:NH2	1:A:1490:CYS:SG	2.74	0.60
1:D:4656:ILE:HD11	1:D:4794:MET:HB2	1.83	0.60
1:A:2752:LEU:HD22	1:A:2814:LEU:HD11	1.82	0.60
1:D:2752:LEU:HD22	1:D:2814:LEU:HD11	1.82	0.60
1:D:4745:SER:O	1:D:4749:THR:HG23	2.02	0.60
1:A:4745:SER:O	1:A:4749:THR:HG23	2.02	0.60
1:B:729:ARG:NH2	1:B:1490:CYS:SG	2.74	0.60
1:C:918:GLU:OE1	1:C:918:GLU:N	2.33	0.60
1:D:729:ARG:NH2	1:D:1490:CYS:SG	2.74	0.60
1:D:918:GLU:N	1:D:918:GLU:OE1	2.33	0.60
1:A:4656:ILE:HD11	1:A:4794:MET:HB2	1.83	0.60
1:B:4656:ILE:HD11	1:B:4794:MET:HB2	1.82	0.60
1:C:2215:VAL:HG21	1:C:2229:MET:CE	2.30	0.60
1:A:2383:GLU:OE1	1:A:2386:ARG:NH2	2.35	0.60
1:A:870:ARG:O	1:A:874:LYS:NZ	2.24	0.60
1:B:868:LEU:HD12	1:B:930:LEU:HD23	1.83	0.60
1:B:3243:ASP:OD1	1:B:3244:ILE:N	2.34	0.60
1:B:4906:GLU:HA	1:D:4319:ARG:NH2	2.16	0.60
1:D:3243:ASP:OD1	1:D:3244:ILE:N	2.34	0.60
1:A:868:LEU:HD12	1:A:930:LEU:HD23	1.83	0.60
1:B:870:ARG:O	1:B:874:LYS:NZ	2.24	0.60
1:C:2752:LEU:HD22	1:C:2814:LEU:HD11	1.82	0.60
1:A:381:GLN:OE1	1:A:381:GLN:N	2.35	0.59
1:B:4745:SER:O	1:B:4749:THR:HG23	2.02	0.59
1:C:2759:PHE:CD2	1:C:2810:ILE:HG12	2.38	0.59
1:A:3243:ASP:OD1	1:A:3244:ILE:N	2.34	0.59
1:C:994:HIS:CE1	1:C:1028:LEU:HD11	2.37	0.59
1:A:1066:SER:OG	1:A:1067:GLN:OE1	2.14	0.59
2:H:26:HIS:ND1	2:H:105:LEU:HD11	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2383:GLU:OE1	1:C:2386:ARG:NH2	2.35	0.59
1:C:2774:ASN:O	1:C:2787:LYS:NZ	2.21	0.59
1:D:70:LEU:HD21	1:D:203:MET:HE1	1.84	0.59
1:D:994:HIS:CE1	1:D:1028:LEU:HD11	2.37	0.59
1:A:3373:VAL:HG12	1:A:3399:PHE:CZ	2.38	0.59
1:B:381:GLN:OE1	1:B:381:GLN:N	2.36	0.59
2:F:26:HIS:ND1	2:F:105:LEU:HD11	2.18	0.59
2:G:26:HIS:ND1	2:G:105:LEU:HD11	2.18	0.59
1:C:4745:SER:O	1:C:4749:THR:HG23	2.02	0.59
1:B:2759:PHE:CD2	1:B:2810:ILE:HG12	2.38	0.59
1:C:70:LEU:HD21	1:C:203:MET:HE1	1.84	0.59
1:C:3373:VAL:HG12	1:C:3399:PHE:CZ	2.38	0.59
1:C:4893:GLY:N	1:C:4897:ASP:OD2	2.35	0.59
1:A:3972:ILE:HG21	1:A:3983:LEU:HD12	1.84	0.59
1:B:994:HIS:CE1	1:B:1028:LEU:HD11	2.37	0.59
1:D:2383:GLU:OE1	1:D:2386:ARG:NH2	2.35	0.59
1:A:4319:ARG:NH2	1:C:4906:GLU:HA	2.18	0.59
1:C:870:ARG:O	1:C:874:LYS:NZ	2.24	0.59
1:D:2759:PHE:CD2	1:D:2810:ILE:HG12	2.38	0.59
1:B:3167:TYR:HD2	1:B:3240:MET:HE2	1.68	0.58
1:B:2383:GLU:OE1	1:B:2386:ARG:NH2	2.35	0.58
1:C:381:GLN:N	1:C:381:GLN:OE1	2.35	0.58
1:A:2759:PHE:CD2	1:A:2810:ILE:HG12	2.38	0.58
1:B:1521:VAL:HG12	1:B:1528:MET:HG2	1.86	0.58
1:A:3167:TYR:HD2	1:A:3240:MET:HE2	1.68	0.58
1:C:3506:VAL:O	1:C:3509:SER:OG	2.16	0.58
1:A:881:GLU:OE1	1:A:969:ALA:N	2.36	0.58
1:C:3167:TYR:HD2	1:C:3240:MET:HE2	1.68	0.58
1:B:457:SER:OG	1:B:459:GLU:OE1	2.21	0.58
1:B:3373:VAL:HG12	1:B:3399:PHE:CZ	2.38	0.58
1:C:3972:ILE:HG21	1:C:3983:LEU:HD12	1.84	0.58
1:D:457:SER:OG	1:D:459:GLU:OE1	2.21	0.58
1:A:994:HIS:CE1	1:A:1028:LEU:HD11	2.37	0.58
1:A:4893:GLY:N	1:A:4897:ASP:OD2	2.35	0.58
1:B:70:LEU:HD21	1:B:203:MET:HE1	1.84	0.58
1:B:3972:ILE:HG21	1:B:3983:LEU:HD12	1.84	0.58
1:A:951:LEU:HD11	1:A:1049:GLY:C	2.29	0.58
1:A:4730:PHE:HB2	1:A:4735:ILE:HD11	1.86	0.58
1:A:4906:GLU:HA	1:C:4319:ARG:NH2	2.18	0.58
2:E:26:HIS:ND1	2:E:105:LEU:HD11	2.18	0.58
1:D:381:GLN:OE1	1:D:381:GLN:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3373:VAL:HG12	1:D:3399:PHE:CZ	2.38	0.58
1:B:3107:MET:SD	1:B:3133:THR:OG1	2.58	0.58
1:D:881:GLU:OE1	1:D:969:ALA:N	2.36	0.58
1:B:4319:ARG:CZ	1:D:4906:GLU:HA	2.34	0.58
1:C:881:GLU:OE1	1:C:969:ALA:N	2.36	0.58
1:D:951:LEU:HD11	1:D:1049:GLY:C	2.29	0.58
1:D:2774:ASN:O	1:D:2787:LYS:NZ	2.21	0.57
1:D:3972:ILE:HG21	1:D:3983:LEU:HD12	1.84	0.57
1:A:1521:VAL:HG12	1:A:1528:MET:HG2	1.86	0.57
1:B:881:GLU:OE1	1:B:969:ALA:N	2.36	0.57
1:D:1066:SER:OG	1:D:1067:GLN:OE1	2.14	0.57
1:A:70:LEU:HD21	1:A:203:MET:HE1	1.84	0.57
1:A:457:SER:OG	1:A:459:GLU:OE1	2.21	0.57
1:A:3158:ILE:C	1:A:3159:LEU:HD12	2.30	0.57
1:B:4906:GLU:HA	1:D:4319:ARG:CZ	2.34	0.57
1:C:1521:VAL:HG12	1:C:1528:MET:HG2	1.86	0.57
1:D:3167:TYR:HD2	1:D:3240:MET:HE2	1.68	0.57
1:B:3158:ILE:C	1:B:3159:LEU:HD12	2.30	0.57
1:C:457:SER:OG	1:C:459:GLU:OE1	2.21	0.57
1:C:3158:ILE:C	1:C:3159:LEU:HD12	2.30	0.57
1:C:3294:PRO:CB	1:C:3297:LEU:HD13	2.34	0.57
1:B:2822:TRP:O	1:B:2824:VAL:HG13	2.05	0.57
1:B:3294:PRO:CB	1:B:3297:LEU:HD13	2.34	0.57
1:D:3158:ILE:C	1:D:3159:LEU:HD12	2.30	0.57
1:A:668:MET:SD	1:A:791:ARG:NH2	2.78	0.57
1:C:3366:LEU:HD21	1:C:3406:LEU:CD2	2.35	0.57
1:A:2822:TRP:O	1:A:2824:VAL:HG13	2.05	0.57
1:A:3294:PRO:CB	1:A:3297:LEU:HD13	2.34	0.57
1:B:951:LEU:HD11	1:B:1049:GLY:C	2.29	0.57
1:C:980:PRO:O	1:C:984:THR:HG23	2.05	0.57
1:C:2910:ASP:OD1	1:C:2911:THR:N	2.38	0.57
1:D:658:THR:HG22	1:D:1002:VAL:HG21	1.87	0.57
1:D:980:PRO:O	1:D:984:THR:HG23	2.05	0.57
1:D:3294:PRO:CB	1:D:3297:LEU:HD13	2.34	0.57
1:C:951:LEU:HD11	1:C:1049:GLY:C	2.29	0.57
1:D:668:MET:SD	1:D:791:ARG:NH2	2.78	0.57
1:D:1521:VAL:HG12	1:D:1528:MET:HG2	1.86	0.57
1:D:2268:MET:HE2	1:D:2272:THR:HG22	1.87	0.57
1:A:2789:HIS:HB3	1:A:2792:LEU:HD13	1.87	0.56
1:A:2910:ASP:OD1	1:A:2911:THR:N	2.38	0.56
1:C:4730:PHE:HB2	1:C:4735:ILE:HD11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3366:LEU:HD21	1:D:3406:LEU:CD2	2.35	0.56
1:D:4730:PHE:HB2	1:D:4735:ILE:HD11	1.86	0.56
1:A:47:LEU:HD12	1:A:126:ARG:NH1	2.21	0.56
1:B:3366:LEU:HD21	1:B:3406:LEU:CD2	2.35	0.56
1:B:4104:LYS:HG3	1:B:4104:LYS:O	2.05	0.56
1:C:668:MET:SD	1:C:791:ARG:NH2	2.78	0.56
1:C:4104:LYS:O	1:C:4104:LYS:HG3	2.05	0.56
1:D:4893:GLY:N	1:D:4897:ASP:OD2	2.35	0.56
1:B:980:PRO:O	1:B:984:THR:HG23	2.05	0.56
1:B:4730:PHE:HB2	1:B:4735:ILE:HD11	1.86	0.56
1:B:4893:GLY:N	1:B:4897:ASP:OD2	2.35	0.56
1:C:2822:TRP:O	1:C:2824:VAL:HG13	2.05	0.56
1:C:2981:VAL:O	1:C:2986:ARG:NH2	2.38	0.56
1:D:2789:HIS:HB3	1:D:2792:LEU:HD13	1.87	0.56
1:A:2268:MET:HE2	1:A:2272:THR:HG22	1.87	0.56
1:B:2748:ILE:HD12	1:B:2814:LEU:HD22	1.87	0.56
1:B:2789:HIS:HB3	1:B:2792:LEU:HD13	1.87	0.56
1:A:2981:VAL:O	1:A:2986:ARG:NH2	2.38	0.56
1:A:4104:LYS:HG3	1:A:4104:LYS:O	2.05	0.56
1:B:658:THR:HG22	1:B:1002:VAL:HG21	1.87	0.56
1:B:668:MET:SD	1:B:791:ARG:NH2	2.78	0.56
1:B:2892:LYS:O	1:B:2896:GLU:OE1	2.24	0.56
1:C:2824:VAL:HB	1:C:2936:TYR:HB3	1.88	0.56
1:D:2822:TRP:O	1:D:2824:VAL:HG13	2.05	0.56
1:D:4104:LYS:HG3	1:D:4104:LYS:O	2.05	0.56
1:A:976:VAL:O	1:A:1045:ARG:NH1	2.38	0.56
1:A:2824:VAL:HB	1:A:2936:TYR:HB3	1.88	0.56
1:A:3754:VAL:O	1:A:3759:LYS:NZ	2.39	0.56
1:A:4319:ARG:CZ	1:C:4906:GLU:HA	2.36	0.56
1:A:4906:GLU:HA	1:C:4319:ARG:CZ	2.36	0.56
1:D:4067:MET:HE2	1:D:4110:GLU:HG2	1.87	0.56
1:A:658:THR:HG22	1:A:1002:VAL:HG21	1.87	0.56
1:B:4686:ILE:HD12	1:B:4735:ILE:HD12	1.88	0.56
1:C:1562:VAL:HG12	1:C:1563:VAL:HG13	1.88	0.56
1:C:2756:ILE:HG22	1:C:2807:ARG:HG3	1.88	0.56
1:C:3754:VAL:O	1:C:3759:LYS:NZ	2.39	0.56
1:D:2748:ILE:HD12	1:D:2814:LEU:HD22	1.87	0.56
1:D:3754:VAL:O	1:D:3759:LYS:NZ	2.39	0.56
1:B:2268:MET:HE2	1:B:2272:THR:HG22	1.87	0.56
1:C:47:LEU:HD12	1:C:126:ARG:NH1	2.21	0.56
1:A:4067:MET:HE2	1:A:4110:GLU:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4686:ILE:HD12	1:A:4735:ILE:HD12	1.88	0.56
1:B:3754:VAL:O	1:B:3759:LYS:NZ	2.39	0.56
1:C:2007:ILE:HD11	1:C:3642:LEU:HD21	1.88	0.56
1:C:2268:MET:HE2	1:C:2272:THR:HG22	1.87	0.56
1:C:2789:HIS:HB3	1:C:2792:LEU:HD13	1.87	0.56
1:C:2892:LYS:O	1:C:2896:GLU:OE1	2.23	0.56
1:D:2910:ASP:OD1	1:D:2911:THR:N	2.38	0.56
1:A:980:PRO:O	1:A:984:THR:HG23	2.05	0.55
1:A:2892:LYS:O	1:A:2896:GLU:OE1	2.23	0.55
1:C:4067:MET:HE2	1:C:4110:GLU:HG2	1.87	0.55
1:D:2007:ILE:HD11	1:D:3642:LEU:HD21	1.88	0.55
1:C:658:THR:HG22	1:C:1002:VAL:HG21	1.87	0.55
1:D:47:LEU:HD12	1:D:126:ARG:NH1	2.21	0.55
1:D:976:VAL:O	1:D:1045:ARG:NH1	2.38	0.55
1:D:2892:LYS:O	1:D:2896:GLU:OE1	2.23	0.55
1:A:2748:ILE:HD12	1:A:2814:LEU:HD22	1.87	0.55
1:A:2756:ILE:HG22	1:A:2807:ARG:HG3	1.88	0.55
1:C:4686:ILE:HD12	1:C:4735:ILE:HD12	1.88	0.55
1:B:47:LEU:HD12	1:B:126:ARG:NH1	2.21	0.55
1:B:4067:MET:HE2	1:B:4110:GLU:HG2	1.87	0.55
1:C:2748:ILE:HD12	1:C:2814:LEU:HD22	1.87	0.55
1:C:3868:VAL:HG12	1:C:3869:ILE:N	2.22	0.55
1:A:1562:VAL:HG12	1:A:1563:VAL:HG13	1.88	0.55
2:H:12:ASP:OD2	2:H:13:GLY:N	2.40	0.55
1:B:2910:ASP:OD1	1:B:2911:THR:N	2.38	0.55
1:C:976:VAL:O	1:C:1045:ARG:NH1	2.38	0.55
1:D:2981:VAL:O	1:D:2986:ARG:NH2	2.38	0.55
1:D:2756:ILE:HG22	1:D:2807:ARG:HG3	1.88	0.55
1:D:3868:VAL:HG12	1:D:3869:ILE:N	2.22	0.55
1:A:3366:LEU:HD21	1:A:3406:LEU:CD2	2.35	0.55
1:B:2756:ILE:HG22	1:B:2807:ARG:HG3	1.88	0.55
1:D:1562:VAL:HG12	1:D:1563:VAL:HG13	1.88	0.55
1:B:2007:ILE:HD11	1:B:3642:LEU:HD21	1.88	0.55
1:D:4686:ILE:HD12	1:D:4735:ILE:HD12	1.88	0.55
2:G:12:ASP:OD1	2:G:13:GLY:N	2.41	0.54
1:B:3868:VAL:HG12	1:B:3869:ILE:N	2.22	0.54
1:D:941:GLY:N	1:D:1053:ASN:OD1	2.41	0.54
1:A:2007:ILE:HD11	1:A:3642:LEU:HD21	1.88	0.54
1:A:3343:ALA:O	1:A:3346:ILE:HG22	2.07	0.54
1:B:1562:VAL:HG12	1:B:1563:VAL:HG13	1.88	0.54
1:B:2824:VAL:HB	1:B:2936:TYR:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:941:GLY:N	1:C:1053:ASN:OD1	2.41	0.54
1:D:2477:ILE:CG2	1:D:2537:LEU:HD21	2.38	0.54
1:D:2816:ALA:HB1	1:D:2882:ASN:HD21	1.73	0.54
1:D:2877:GLU:OE2	1:D:2921:ARG:NE	2.41	0.54
1:C:4886:TYR:HA	1:D:4916:ILE:HD11	1.90	0.54
1:D:2824:VAL:HB	1:D:2936:TYR:HB3	1.88	0.54
1:A:185:THR:HG22	1:A:190:LEU:CD2	2.38	0.54
1:B:185:THR:HG22	1:B:190:LEU:CD2	2.38	0.54
1:B:941:GLY:N	1:B:1053:ASN:OD1	2.41	0.54
1:C:185:THR:HG22	1:C:190:LEU:CD2	2.38	0.54
1:A:2477:ILE:CG2	1:A:2537:LEU:HD21	2.38	0.54
1:A:2816:ALA:HB1	1:A:2882:ASN:HD21	1.73	0.54
1:A:3868:VAL:HG12	1:A:3869:ILE:N	2.22	0.54
2:F:12:ASP:OD2	2:F:13:GLY:N	2.40	0.54
1:B:2816:ALA:HB1	1:B:2882:ASN:HD21	1.73	0.54
1:D:185:THR:HG22	1:D:190:LEU:CD2	2.38	0.54
1:A:797:ARG:O	1:A:1620:ARG:NH2	2.41	0.54
1:A:3605:TYR:O	1:A:3609:GLN:NE2	2.41	0.54
1:B:976:VAL:O	1:B:1045:ARG:NH1	2.38	0.54
1:C:2477:ILE:CG2	1:C:2537:LEU:HD21	2.38	0.54
1:A:2816:ALA:HB1	1:A:2882:ASN:ND2	2.23	0.54
1:B:71:GLU:OE1	1:B:111:ARG:NE	2.40	0.54
1:B:2816:ALA:HB1	1:B:2882:ASN:ND2	2.23	0.54
1:C:71:GLU:OE1	1:C:111:ARG:NE	2.41	0.54
1:C:3605:TYR:O	1:C:3609:GLN:NE2	2.41	0.54
1:A:2872:LEU:HD22	1:A:2932:GLN:HE21	1.73	0.54
1:C:2816:ALA:HB1	1:C:2882:ASN:HD21	1.73	0.54
1:C:3343:ALA:O	1:C:3346:ILE:HG22	2.07	0.54
1:C:3683:GLU:O	1:C:3686:GLU:HG3	2.08	0.54
1:A:3683:GLU:O	1:A:3686:GLU:HG3	2.08	0.53
1:B:3683:GLU:O	1:B:3686:GLU:HG3	2.08	0.53
1:C:2793:ARG:NE	1:C:2797:THR:O	2.41	0.53
1:C:3414:ILE:HG23	1:C:3517:LYS:HD2	1.91	0.53
2:E:12:ASP:OD2	2:E:13:GLY:N	2.41	0.53
1:B:2793:ARG:NE	1:B:2797:THR:O	2.41	0.53
1:B:3343:ALA:O	1:B:3346:ILE:HG22	2.07	0.53
1:B:3605:TYR:O	1:B:3609:GLN:NE2	2.41	0.53
1:C:2872:LEU:HD22	1:C:2932:GLN:HE21	1.73	0.53
1:D:2816:ALA:HB1	1:D:2882:ASN:ND2	2.23	0.53
1:D:3605:TYR:O	1:D:3609:GLN:NE2	2.41	0.53
1:A:614:ALA:HB2	1:A:1677:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3343:ALA:O	1:D:3346:ILE:HG22	2.07	0.53
1:D:3414:ILE:HG23	1:D:3517:LYS:HD2	1.91	0.53
1:A:4706:THR:HG23	1:A:4708:SER:H	1.74	0.53
1:B:2477:ILE:CG2	1:B:2537:LEU:HD21	2.38	0.53
1:C:2877:GLU:OE2	1:C:2921:ARG:NE	2.41	0.53
1:D:2209:MET:HE1	1:D:2254:HIS:CG	2.44	0.53
1:A:941:GLY:N	1:A:1053:ASN:OD1	2.41	0.53
1:B:2167:LEU:HD11	1:B:2207:THR:HG23	1.91	0.53
1:D:2872:LEU:HD22	1:D:2932:GLN:HE21	1.73	0.53
1:D:3683:GLU:O	1:D:3686:GLU:HG3	2.08	0.53
1:A:71:GLU:OE1	1:A:111:ARG:NE	2.40	0.53
1:A:2166:LEU:HD21	1:A:2178:LEU:HD23	1.90	0.53
1:A:2209:MET:HE1	1:A:2254:HIS:CG	2.44	0.53
1:A:2793:ARG:NE	1:A:2797:THR:O	2.41	0.53
1:A:3414:ILE:HG23	1:A:3517:LYS:HD2	1.91	0.53
1:B:2981:VAL:O	1:B:2986:ARG:NH2	2.38	0.53
1:D:2167:LEU:HD11	1:D:2207:THR:HG23	1.91	0.53
1:D:2740:PRO:HG3	1:D:2886:THR:HG22	1.91	0.53
1:A:893:THR:O	1:A:905:HIS:N	2.42	0.53
1:C:4706:THR:HG23	1:C:4708:SER:H	1.74	0.53
1:C:4723:LEU:HA	1:C:4735:ILE:HG21	1.91	0.53
1:A:932:THR:O	1:A:936:LEU:HD23	2.09	0.53
1:A:4886:TYR:HA	1:B:4916:ILE:HD11	1.90	0.53
1:B:2166:LEU:HD21	1:B:2178:LEU:HD23	1.90	0.53
1:B:2209:MET:HE1	1:B:2254:HIS:CG	2.44	0.53
1:B:3414:ILE:HG23	1:B:3517:LYS:HD2	1.91	0.53
1:B:3672:ASP:OD2	1:B:3735:HIS:NE2	2.42	0.53
1:C:2166:LEU:HD21	1:C:2178:LEU:HD23	1.90	0.53
1:D:932:THR:O	1:D:936:LEU:HD23	2.09	0.53
1:D:2793:ARG:NE	1:D:2797:THR:O	2.41	0.53
1:A:2740:PRO:HG3	1:A:2886:THR:HG22	1.91	0.53
1:C:2209:MET:HE1	1:C:2254:HIS:CG	2.44	0.53
1:A:3672:ASP:OD2	1:A:3735:HIS:NE2	2.42	0.53
1:D:893:THR:O	1:D:905:HIS:N	2.42	0.53
1:D:2166:LEU:HD21	1:D:2178:LEU:HD23	1.90	0.53
1:D:3236:SER:OG	1:D:3238:GLU:OE1	2.27	0.53
1:A:2167:LEU:HD11	1:A:2207:THR:HG23	1.91	0.52
2:E:86:THR:HG23	2:E:87:GLY:N	2.24	0.52
1:B:4723:LEU:HA	1:B:4735:ILE:HG21	1.91	0.52
1:C:893:THR:O	1:C:905:HIS:N	2.42	0.52
1:C:2771:LYS:CE	1:C:2792:LEU:HD11	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:797:ARG:O	1:B:1620:ARG:NH2	2.41	0.52
1:C:2948:ASP:O	1:C:2954:LYS:NZ	2.41	0.52
1:C:3236:SER:OG	1:C:3238:GLU:OE1	2.27	0.52
1:D:3591:GLU:O	1:D:3595:ARG:HG2	2.10	0.52
1:D:4244:THR:HG22	1:D:4248:MET:HE3	1.90	0.52
1:A:2877:GLU:OE2	1:A:2921:ARG:NE	2.41	0.52
2:G:86:THR:HG23	2:G:87:GLY:N	2.24	0.52
1:B:924:GLN:O	1:B:925:MET:C	2.52	0.52
1:B:2774:ASN:O	1:B:2787:LYS:NZ	2.21	0.52
1:B:2877:GLU:OE2	1:B:2921:ARG:NE	2.41	0.52
1:C:921:TYR:CE1	1:C:925:MET:SD	3.03	0.52
1:C:2167:LEU:HD11	1:C:2207:THR:HG23	1.91	0.52
1:C:3591:GLU:O	1:C:3595:ARG:HG2	2.10	0.52
1:D:797:ARG:O	1:D:1620:ARG:NH2	2.41	0.52
1:D:3082:MET:HE1	1:D:3090:LYS:HA	1.92	0.52
1:B:614:ALA:HB2	1:B:1677:LEU:HD12	1.90	0.52
1:B:921:TYR:CE1	1:B:925:MET:SD	3.03	0.52
1:B:2771:LYS:CE	1:B:2792:LEU:HD11	2.39	0.52
1:B:4886:TYR:HA	1:C:4916:ILE:HD11	1.90	0.52
1:C:614:ALA:HB2	1:C:1677:LEU:HD12	1.90	0.52
1:C:2816:ALA:HB1	1:C:2882:ASN:ND2	2.23	0.52
1:C:3082:MET:HE1	1:C:3090:LYS:HA	1.92	0.52
1:D:3672:ASP:OD2	1:D:3735:HIS:NE2	2.42	0.52
1:A:249:GLU:HB3	1:A:253:VAL:HG11	1.92	0.52
1:A:2771:LYS:CE	1:A:2792:LEU:HD11	2.39	0.52
1:B:893:THR:O	1:B:905:HIS:N	2.42	0.52
1:B:2872:LEU:HD22	1:B:2932:GLN:HE21	1.73	0.52
1:B:3294:PRO:HB2	1:B:3297:LEU:HD22	1.92	0.52
1:B:4244:THR:HG22	1:B:4248:MET:HE3	1.90	0.52
1:D:921:TYR:CE1	1:D:925:MET:SD	3.03	0.52
1:D:4706:THR:HG23	1:D:4708:SER:H	1.74	0.52
1:D:4723:LEU:HA	1:D:4735:ILE:HG21	1.91	0.52
1:A:921:TYR:CE1	1:A:925:MET:SD	3.03	0.52
1:A:4244:THR:HG22	1:A:4248:MET:HE3	1.90	0.52
1:B:249:GLU:HB3	1:B:253:VAL:HG11	1.92	0.52
1:B:932:THR:O	1:B:936:LEU:HD23	2.09	0.52
1:B:2740:PRO:HG3	1:B:2886:THR:HG22	1.91	0.52
1:B:4706:THR:HG23	1:B:4708:SER:H	1.74	0.52
1:C:249:GLU:HB3	1:C:253:VAL:HG11	1.92	0.52
1:C:3294:PRO:HB2	1:C:3297:LEU:HD22	1.92	0.52
1:D:614:ALA:HB2	1:D:1677:LEU:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:924:GLN:O	1:D:925:MET:C	2.52	0.52
1:A:924:GLN:O	1:A:925:MET:C	2.52	0.52
1:C:932:THR:O	1:C:936:LEU:HD23	2.09	0.52
1:C:3672:ASP:OD2	1:C:3735:HIS:NE2	2.42	0.52
1:D:3294:PRO:HB2	1:D:3297:LEU:HD22	1.92	0.52
1:A:4916:ILE:HD11	1:D:4886:TYR:HA	1.90	0.52
1:B:3457:GLN:NE2	1:B:3461:VAL:HG11	2.25	0.52
1:D:249:GLU:HB3	1:D:253:VAL:HG11	1.92	0.52
1:A:3082:MET:HE1	1:A:3090:LYS:HA	1.92	0.52
1:B:2743:THR:HG22	1:B:2816:ALA:HB2	1.92	0.52
1:C:1423:ASP:OD1	1:C:1569:LYS:NZ	2.40	0.52
1:B:3532:ASP:OD1	1:B:3533:LEU:N	2.43	0.52
1:C:2740:PRO:HG3	1:C:2886:THR:HG22	1.91	0.52
1:C:3457:GLN:NE2	1:C:3461:VAL:HG11	2.25	0.52
1:D:2737:ASP:OD1	1:D:2892:LYS:NZ	2.37	0.52
1:C:3532:ASP:OD1	1:C:3533:LEU:N	2.43	0.51
1:D:2948:ASP:O	1:D:2954:LYS:NZ	2.42	0.51
1:A:3457:GLN:NE2	1:A:3461:VAL:HG11	2.25	0.51
2:F:86:THR:HG23	2:F:87:GLY:N	2.25	0.51
1:B:3591:GLU:O	1:B:3595:ARG:HG2	2.10	0.51
1:C:4244:THR:HG22	1:C:4248:MET:HE3	1.90	0.51
1:D:2695:GLU:OE1	1:D:2698:ARG:NH2	2.43	0.51
1:A:2267:GLY:O	1:A:2269:GLN:NE2	2.44	0.51
1:A:3294:PRO:HB2	1:A:3297:LEU:HD22	1.92	0.51
1:A:4723:LEU:HA	1:A:4735:ILE:HG21	1.91	0.51
1:B:2737:ASP:OD1	1:B:2892:LYS:NZ	2.37	0.51
1:B:2974:PHE:CD2	1:B:2996:ILE:HG13	2.46	0.51
1:B:3082:MET:HE1	1:B:3090:LYS:HA	1.92	0.51
1:C:2267:GLY:O	1:C:2269:GLN:NE2	2.44	0.51
1:A:321:LYS:NZ	1:A:382:GLU:O	2.42	0.51
1:B:620:ASP:OD1	1:B:1681:ARG:NH2	2.43	0.51
1:B:2267:GLY:O	1:B:2269:GLN:NE2	2.44	0.51
1:B:3506:VAL:O	1:B:3509:SER:OG	2.16	0.51
1:C:620:ASP:OD1	1:C:1681:ARG:NH2	2.43	0.51
1:D:71:GLU:OE1	1:D:111:ARG:NE	2.40	0.51
1:D:2974:PHE:CD2	1:D:2996:ILE:HG13	2.46	0.51
1:A:2695:GLU:OE1	1:A:2698:ARG:NH2	2.43	0.51
1:A:3236:SER:OG	1:A:3238:GLU:OE1	2.27	0.51
1:B:3236:SER:OG	1:B:3238:GLU:OE1	2.27	0.51
1:C:2743:THR:HG22	1:C:2816:ALA:HB2	1.92	0.51
1:D:2771:LYS:CE	1:D:2792:LEU:HD11	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4965:TYR:OH	1:C:5031:GLU:OE2	2.28	0.51
1:D:1252:GLU:N	1:D:1252:GLU:OE1	2.44	0.51
1:A:4899:ILE:HG13	1:A:4911:ARG:NH2	2.26	0.51
1:B:228:MET:O	1:B:229:ASP:OD1	2.29	0.51
1:B:318:ARG:NH1	1:B:325:ASP:OD1	2.44	0.51
1:C:797:ARG:O	1:C:1620:ARG:NH2	2.41	0.51
1:D:620:ASP:OD1	1:D:1681:ARG:NH2	2.43	0.51
1:D:3457:GLN:NE2	1:D:3461:VAL:HG11	2.25	0.51
1:C:2757:ASN:OD1	1:C:2807:ARG:NE	2.44	0.51
1:D:318:ARG:NH1	1:D:325:ASP:OD1	2.44	0.51
1:D:4700:ASP:C	1:D:4702:LEU:H	2.19	0.51
1:A:2743:THR:HG22	1:A:2816:ALA:HB2	1.92	0.51
1:A:3591:GLU:O	1:A:3595:ARG:HG2	2.10	0.51
1:C:2943:LYS:O	1:C:2947:LEU:HD13	2.11	0.51
1:D:2267:GLY:O	1:D:2269:GLN:NE2	2.44	0.51
1:B:4694:ASP:OD1	1:B:4697:GLY:N	2.30	0.51
1:B:4700:ASP:C	1:B:4702:LEU:H	2.19	0.51
1:D:2943:LYS:O	1:D:2947:LEU:HD13	2.11	0.51
1:A:2570:PHE:CE1	1:A:2583:MET:HE1	2.46	0.50
1:A:2942:LEU:HD23	1:A:2942:LEU:H	1.77	0.50
1:A:2974:PHE:CD2	1:A:2996:ILE:HG13	2.46	0.50
1:B:1159:ASN:ND2	1:B:1183:ILE:O	2.44	0.50
1:B:2570:PHE:CE1	1:B:2583:MET:HE1	2.46	0.50
1:B:2695:GLU:OE1	1:B:2698:ARG:NH2	2.43	0.50
1:B:2942:LEU:HD23	1:B:2942:LEU:H	1.76	0.50
1:C:318:ARG:NH1	1:C:325:ASP:OD1	2.44	0.50
1:C:1252:GLU:OE1	1:C:1252:GLU:N	2.44	0.50
1:C:3972:ILE:CG2	1:C:3983:LEU:HD12	2.42	0.50
1:D:4899:ILE:HG13	1:D:4911:ARG:NH2	2.26	0.50
1:A:228:MET:O	1:A:229:ASP:OD1	2.29	0.50
1:B:2948:ASP:O	1:B:2954:LYS:NZ	2.41	0.50
1:C:2953:GLU:OE1	1:C:2953:GLU:N	2.44	0.50
1:D:2570:PHE:CE1	1:D:2583:MET:HE1	2.46	0.50
1:D:3532:ASP:OD1	1:D:3533:LEU:N	2.43	0.50
1:B:4230:GLU:N	1:B:4230:GLU:OE1	2.44	0.50
1:C:2226:PHE:N	1:C:2227:PRO:HD3	2.26	0.50
1:C:2570:PHE:CE1	1:C:2583:MET:HE1	2.46	0.50
1:C:2942:LEU:HD23	1:C:2942:LEU:H	1.77	0.50
1:D:2942:LEU:HD23	1:D:2942:LEU:H	1.76	0.50
1:A:620:ASP:OD1	1:A:1681:ARG:NH2	2.43	0.50
1:A:1252:GLU:N	1:A:1252:GLU:OE1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2226:PHE:N	1:A:2227:PRO:HD3	2.26	0.50
1:A:4700:ASP:C	1:A:4702:LEU:H	2.19	0.50
1:C:2907:VAL:HG22	1:C:2911:THR:OG1	2.12	0.50
1:C:4230:GLU:OE1	1:C:4230:GLU:N	2.44	0.50
1:C:4625:MET:HE1	1:C:4627:TYR:CZ	2.47	0.50
1:D:228:MET:O	1:D:229:ASP:OD1	2.29	0.50
1:D:2907:VAL:HG22	1:D:2911:THR:OG1	2.12	0.50
1:A:2795:TYR:HA	1:A:2798:PHE:HB2	1.94	0.50
1:B:4899:ILE:HG13	1:B:4911:ARG:NH2	2.26	0.50
1:C:2192:PHE:HA	1:C:2199:MET:HE3	1.94	0.50
1:C:4700:ASP:C	1:C:4702:LEU:H	2.19	0.50
1:C:4899:ILE:HG13	1:C:4911:ARG:NH2	2.26	0.50
1:D:2795:TYR:HA	1:D:2798:PHE:HB2	1.94	0.50
1:D:2802:ASP:HA	1:D:2805:ILE:HG12	1.94	0.50
1:A:2757:ASN:OD1	1:A:2807:ARG:NE	2.44	0.50
2:H:86:THR:HG23	2:H:87:GLY:N	2.26	0.50
1:B:2645:LEU:HD13	1:B:2679:LEU:HD21	1.93	0.50
1:B:2907:VAL:HG22	1:B:2911:THR:OG1	2.12	0.50
1:B:4625:MET:HE1	1:B:4627:TYR:CZ	2.47	0.50
1:C:2695:GLU:OE1	1:C:2698:ARG:NH2	2.43	0.50
1:C:2802:ASP:HA	1:C:2805:ILE:HG12	1.94	0.50
1:C:2974:PHE:CD2	1:C:2996:ILE:HG13	2.46	0.50
1:D:3972:ILE:CG2	1:D:3983:LEU:HD12	2.42	0.50
1:D:4625:MET:HE1	1:D:4627:TYR:CZ	2.47	0.50
1:A:318:ARG:NH1	1:A:325:ASP:OD1	2.44	0.50
1:B:2943:LYS:O	1:B:2947:LEU:HD13	2.11	0.50
1:C:321:LYS:NZ	1:C:382:GLU:O	2.42	0.50
1:D:2743:THR:HG22	1:D:2816:ALA:HB2	1.92	0.50
1:A:649:ILE:HG23	1:A:815:ALA:HB3	1.93	0.50
1:A:2802:ASP:HA	1:A:2805:ILE:HG12	1.94	0.50
1:A:3972:ILE:CG2	1:A:3983:LEU:HD12	2.41	0.50
1:A:4230:GLU:OE1	1:A:4230:GLU:N	2.44	0.50
1:B:1252:GLU:OE1	1:B:1252:GLU:N	2.44	0.50
1:C:4088:ARG:HB2	1:C:4090:LEU:HD12	1.93	0.50
1:D:4230:GLU:OE1	1:D:4230:GLU:N	2.44	0.50
1:A:3532:ASP:OD1	1:A:3533:LEU:N	2.43	0.50
1:B:2226:PHE:N	1:B:2227:PRO:HD3	2.26	0.50
1:B:2795:TYR:HA	1:B:2798:PHE:HB2	1.94	0.50
1:B:4163:LEU:O	1:B:4167:LEU:HD23	2.12	0.50
1:C:228:MET:O	1:C:229:ASP:OD1	2.29	0.50
1:D:2226:PHE:N	1:D:2227:PRO:HD3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:THR:HG22	1:A:190:LEU:HD22	1.94	0.49
1:A:2907:VAL:HG22	1:A:2911:THR:OG1	2.12	0.49
1:A:4332:LEU:O	1:A:4336:LEU:HG	2.12	0.49
1:C:2795:TYR:HA	1:C:2798:PHE:HB2	1.94	0.49
1:D:649:ILE:HG23	1:D:815:ALA:HB3	1.93	0.49
1:D:2757:ASN:OD1	1:D:2807:ARG:NE	2.44	0.49
1:D:4846:VAL:HG11	1:D:4885:MET:HG2	1.94	0.49
1:B:2192:PHE:HA	1:B:2199:MET:HE3	1.94	0.49
1:B:4320:LEU:HD22	1:B:4325:ALA:HB2	1.95	0.49
1:B:4332:LEU:O	1:B:4336:LEU:HG	2.12	0.49
1:D:1064:VAL:O	1:D:1065:ASP:OD1	2.30	0.49
1:D:2953:GLU:OE1	1:D:2953:GLU:N	2.44	0.49
1:A:36:LEU:HD23	1:A:52:PRO:HA	1.94	0.49
1:A:215:VAL:HG21	1:A:391:LEU:HD12	1.94	0.49
1:A:1159:ASN:ND2	1:A:1183:ILE:O	2.44	0.49
1:A:4163:LEU:O	1:A:4167:LEU:HD23	2.12	0.49
1:B:1064:VAL:O	1:B:1065:ASP:OD1	2.30	0.49
1:C:924:GLN:O	1:C:925:MET:C	2.52	0.49
1:C:2645:LEU:HD13	1:C:2679:LEU:HD21	1.93	0.49
1:C:4846:VAL:HG11	1:C:4885:MET:HG2	1.94	0.49
1:D:4163:LEU:O	1:D:4167:LEU:HD23	2.12	0.49
1:D:4332:LEU:O	1:D:4336:LEU:HG	2.12	0.49
1:A:2645:LEU:HD13	1:A:2679:LEU:HD21	1.93	0.49
1:A:2943:LYS:O	1:A:2947:LEU:HD13	2.11	0.49
1:B:2757:ASN:OD1	1:B:2807:ARG:NE	2.44	0.49
1:B:3972:ILE:CG2	1:B:3983:LEU:HD12	2.41	0.49
1:C:4320:LEU:HD22	1:C:4325:ALA:HB2	1.95	0.49
1:D:185:THR:HG22	1:D:190:LEU:HD22	1.94	0.49
1:A:2192:PHE:HA	1:A:2199:MET:HE3	1.94	0.49
1:B:185:THR:HG22	1:B:190:LEU:HD22	1.94	0.49
1:D:4088:ARG:HB2	1:D:4090:LEU:HD12	1.93	0.49
1:D:4753:GLU:O	1:D:4754:ARG:CZ	2.61	0.49
1:A:156:LYS:HB2	1:D:228:MET:SD	2.52	0.49
1:A:1695:LEU:O	1:A:1699:LEU:HD13	2.13	0.49
1:A:3313:LEU:HD23	1:A:3346:ILE:HG13	1.94	0.49
1:B:2802:ASP:HA	1:B:2805:ILE:HG12	1.94	0.49
1:B:3041:THR:OG1	1:B:3081:VAL:HG21	2.13	0.49
1:B:3553:PHE:O	1:B:3556:ASN:OD1	2.31	0.49
1:C:36:LEU:HD23	1:C:52:PRO:HA	1.94	0.49
1:C:228:MET:SD	1:D:156:LYS:HB2	2.52	0.49
1:C:1159:ASN:ND2	1:C:1183:ILE:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3107:MET:SD	1:C:3133:THR:OG1	2.58	0.49
1:D:2645:LEU:HD13	1:D:2679:LEU:HD21	1.93	0.49
1:A:228:MET:SD	1:B:156:LYS:HB2	2.53	0.49
1:A:3553:PHE:O	1:A:3556:ASN:OD1	2.31	0.49
1:A:4088:ARG:HB2	1:A:4090:LEU:HD12	1.93	0.49
1:D:215:VAL:HG21	1:D:391:LEU:HD12	1.94	0.49
1:A:4625:MET:HE1	1:A:4627:TYR:CZ	2.47	0.49
1:B:1695:LEU:O	1:B:1699:LEU:HD13	2.13	0.49
1:C:1479:ASP:OD2	1:C:1483:ASN:ND2	2.46	0.49
1:C:1695:LEU:O	1:C:1699:LEU:HD13	2.13	0.49
1:C:4753:GLU:O	1:C:4754:ARG:CZ	2.61	0.49
1:A:3506:VAL:O	1:A:3509:SER:OG	2.16	0.49
1:A:3687:GLU:OE2	1:A:3695:LYS:NZ	2.46	0.49
1:B:1420:ASP:O	1:B:1421:ASN:OD1	2.31	0.49
1:B:2953:GLU:OE1	1:B:2953:GLU:N	2.44	0.49
1:C:649:ILE:HG23	1:C:815:ALA:HB3	1.93	0.49
1:C:2234:CYS:O	1:C:2237:LEU:N	2.46	0.49
1:C:4694:ASP:OD1	1:C:4697:GLY:N	2.30	0.49
1:D:2192:PHE:HA	1:D:2199:MET:HE3	1.94	0.49
1:A:1064:VAL:O	1:A:1065:ASP:OD1	2.30	0.49
1:A:4753:GLU:O	1:A:4754:ARG:CZ	2.61	0.49
1:B:228:MET:SD	1:C:156:LYS:HB2	2.52	0.49
1:B:4753:GLU:O	1:B:4754:ARG:CZ	2.61	0.49
1:A:1420:ASP:O	1:A:1421:ASN:OD1	2.31	0.48
1:A:4846:VAL:HG11	1:A:4885:MET:HG2	1.94	0.48
1:B:649:ILE:HG23	1:B:815:ALA:HB3	1.93	0.48
1:B:3313:LEU:HD23	1:B:3346:ILE:HG13	1.94	0.48
1:C:3041:THR:OG1	1:C:3081:VAL:HG21	2.13	0.48
1:C:3869:ILE:HG22	1:C:3872:GLN:H	1.78	0.48
1:C:4332:LEU:O	1:C:4336:LEU:HG	2.12	0.48
1:D:36:LEU:HD23	1:D:52:PRO:HA	1.94	0.48
1:D:1420:ASP:O	1:D:1421:ASN:OD1	2.31	0.48
1:D:3553:PHE:O	1:D:3556:ASN:OD1	2.31	0.48
1:A:2234:CYS:O	1:A:2237:LEU:N	2.46	0.48
1:A:4320:LEU:HD22	1:A:4325:ALA:HB2	1.95	0.48
1:B:2234:CYS:O	1:B:2237:LEU:N	2.46	0.48
1:C:1064:VAL:O	1:C:1065:ASP:OD1	2.30	0.48
1:C:3553:PHE:O	1:C:3556:ASN:OD1	2.31	0.48
1:C:4163:LEU:O	1:C:4167:LEU:HD23	2.12	0.48
1:D:3313:LEU:HD23	1:D:3346:ILE:HG13	1.94	0.48
1:D:4320:LEU:HD22	1:D:4325:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:THR:HG22	1:C:190:LEU:HD22	1.94	0.48
1:D:3687:GLU:OE2	1:D:3695:LYS:NZ	2.46	0.48
1:A:369:ARG:NH1	1:A:2308:LEU:HD11	2.28	0.48
1:A:4628:TYR:OH	1:B:4858:ARG:NH1	2.43	0.48
1:B:36:LEU:HD23	1:B:52:PRO:HA	1.94	0.48
1:B:369:ARG:NH1	1:B:2308:LEU:HD11	2.28	0.48
1:B:1479:ASP:OD2	1:B:1483:ASN:ND2	2.46	0.48
1:B:3025:VAL:HG23	1:B:3025:VAL:O	2.13	0.48
1:B:4685:TYR:CE2	1:B:4701:ARG:HG2	2.49	0.48
1:C:215:VAL:HG21	1:C:391:LEU:HD12	1.94	0.48
1:C:369:ARG:NH1	1:C:2308:LEU:HD11	2.28	0.48
1:D:1159:ASN:ND2	1:D:1183:ILE:O	2.44	0.48
1:A:723:TRP:CZ2	1:A:728:ALA:HB2	2.49	0.48
1:A:3025:VAL:HG23	1:A:3025:VAL:O	2.13	0.48
1:A:4072:LYS:HA	1:A:4132:ALA:HB1	1.95	0.48
1:B:723:TRP:CZ2	1:B:728:ALA:HB2	2.49	0.48
1:B:1066:SER:OG	1:B:1067:GLN:OE1	2.14	0.48
1:B:3380:LEU:HD21	1:B:3391:GLY:C	2.38	0.48
1:B:4846:VAL:HG11	1:B:4885:MET:HG2	1.94	0.48
1:D:2356:ARG:NH2	1:D:2450:GLU:OE2	2.47	0.48
1:D:3025:VAL:HG23	1:D:3025:VAL:O	2.13	0.48
1:D:3730:MET:O	1:D:3733:SER:OG	2.30	0.48
1:A:2948:ASP:O	1:A:2954:LYS:NZ	2.41	0.48
1:A:5011:MET:HE1	1:A:5018:ASP:HB2	1.96	0.48
1:B:2515:ASN:OD1	1:B:2517:ASP:N	2.45	0.48
1:B:4088:ARG:HB2	1:B:4090:LEU:HD12	1.93	0.48
1:C:2891:LYS:O	1:C:2895:LEU:HG	2.14	0.48
1:C:3313:LEU:HD23	1:C:3346:ILE:HG13	1.94	0.48
1:D:321:LYS:NZ	1:D:382:GLU:O	2.42	0.48
1:A:3730:MET:O	1:A:3733:SER:OG	2.30	0.48
1:A:3869:ILE:HG22	1:A:3872:GLN:H	1.78	0.48
1:B:321:LYS:NZ	1:B:382:GLU:O	2.42	0.48
1:B:658:THR:HG22	1:B:1002:VAL:CG2	2.44	0.48
1:C:723:TRP:CZ2	1:C:728:ALA:HB2	2.49	0.48
1:C:3687:GLU:OE2	1:C:3695:LYS:NZ	2.46	0.48
1:C:4179:PRO:O	1:C:4205:ARG:NH2	2.47	0.48
1:D:723:TRP:CZ2	1:D:728:ALA:HB2	2.49	0.48
1:D:1695:LEU:O	1:D:1699:LEU:HD13	2.13	0.48
1:B:1273:LEU:HD22	1:B:1290:LEU:HD11	1.96	0.48
1:B:3869:ILE:HG22	1:B:3872:GLN:H	1.78	0.48
1:B:4072:LYS:HA	1:B:4132:ALA:HB1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5011:MET:HE1	1:B:5018:ASP:HB2	1.96	0.48
1:C:2356:ARG:NH2	1:C:2450:GLU:OE2	2.47	0.48
1:C:3025:VAL:HG23	1:C:3025:VAL:O	2.13	0.48
1:C:4225:VAL:HG11	1:C:4948:VAL:HA	1.95	0.48
1:D:2234:CYS:O	1:D:2237:LEU:N	2.46	0.48
1:D:4179:PRO:O	1:D:4205:ARG:NH2	2.47	0.48
1:A:2737:ASP:OD1	1:A:2892:LYS:NZ	2.37	0.48
1:B:4860:PHE:CB	1:B:4911:ARG:HH12	2.27	0.48
1:C:1420:ASP:O	1:C:1421:ASN:OD1	2.31	0.48
1:D:369:ARG:NH1	1:D:2308:LEU:HD11	2.28	0.48
1:D:1273:LEU:HD22	1:D:1290:LEU:HD11	1.96	0.48
1:D:1479:ASP:OD2	1:D:1483:ASN:ND2	2.46	0.48
1:A:1281:GLN:O	1:A:1282:ASN:OD1	2.32	0.48
1:A:1479:ASP:OD2	1:A:1483:ASN:ND2	2.46	0.48
1:B:215:VAL:HG21	1:B:391:LEU:HD12	1.94	0.48
1:B:2891:LYS:O	1:B:2895:LEU:HG	2.14	0.48
1:B:4927:LEU:O	1:B:4931:GLN:OE1	2.32	0.48
1:C:2866:VAL:O	1:C:2929:LYS:NZ	2.40	0.48
1:C:2887:TRP:CG	1:C:2891:LYS:HZ1	2.32	0.48
1:C:4860:PHE:CB	1:C:4911:ARG:HH12	2.27	0.48
1:D:3282:LEU:HD12	1:D:3316:LEU:HD22	1.96	0.48
1:D:3380:LEU:HD21	1:D:3391:GLY:C	2.38	0.48
1:D:4685:TYR:CE2	1:D:4701:ARG:HG2	2.49	0.48
1:D:4927:LEU:O	1:D:4931:GLN:OE1	2.32	0.48
1:A:658:THR:HG22	1:A:1002:VAL:CG2	2.44	0.47
1:A:4860:PHE:CB	1:A:4911:ARG:HH12	2.27	0.47
1:B:2356:ARG:NH2	1:B:2450:GLU:OE2	2.47	0.47
1:B:3227:GLU:O	1:B:3228:ARG:HB3	2.14	0.47
1:C:876:ALA:O	1:C:879:ILE:HG22	2.14	0.47
1:C:3380:LEU:HD21	1:C:3391:GLY:C	2.38	0.47
1:D:4694:ASP:OD1	1:D:4697:GLY:N	2.30	0.47
1:A:1273:LEU:HD22	1:A:1290:LEU:HD11	1.96	0.47
1:A:3282:LEU:HD12	1:A:3316:LEU:HD22	1.96	0.47
1:A:3667:ASP:O	1:A:3667:ASP:OD1	2.32	0.47
1:A:4179:PRO:O	1:A:4205:ARG:NH2	2.47	0.47
1:B:864:LEU:HD13	1:B:869:GLU:HB2	1.96	0.47
1:C:1281:GLN:O	1:C:1282:ASN:OD1	2.32	0.47
1:A:581:GLU:HG3	1:A:621:LEU:HD22	1.96	0.47
1:A:3004:LEU:HB2	1:A:3005:PRO:HD3	1.96	0.47
1:A:3380:LEU:HD21	1:A:3391:GLY:C	2.38	0.47
1:B:3667:ASP:OD1	1:B:3667:ASP:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4225:VAL:HG11	1:B:4948:VAL:HA	1.95	0.47
1:C:1273:LEU:HD22	1:C:1290:LEU:HD11	1.96	0.47
1:C:3667:ASP:OD1	1:C:3667:ASP:O	2.32	0.47
1:D:876:ALA:O	1:D:879:ILE:HG22	2.14	0.47
1:D:3667:ASP:O	1:D:3667:ASP:OD1	2.32	0.47
1:D:3869:ILE:HG22	1:D:3872:GLN:H	1.78	0.47
1:A:876:ALA:O	1:A:879:ILE:HG22	2.14	0.47
1:A:2356:ARG:NH2	1:A:2450:GLU:OE2	2.47	0.47
1:A:2887:TRP:CG	1:A:2891:LYS:HZ1	2.32	0.47
1:A:3041:THR:OG1	1:A:3081:VAL:HG21	2.13	0.47
1:A:3227:GLU:O	1:A:3228:ARG:HB3	2.14	0.47
1:B:876:ALA:O	1:B:879:ILE:HG22	2.14	0.47
1:B:3687:GLU:OE2	1:B:3695:LYS:NZ	2.46	0.47
1:C:658:THR:HG22	1:C:1002:VAL:CG2	2.44	0.47
1:C:924:GLN:O	1:C:927:GLY:N	2.47	0.47
1:C:2525:VAL:HG23	1:C:2526:GLY:N	2.30	0.47
1:C:4685:TYR:CE2	1:C:4701:ARG:HG2	2.49	0.47
1:C:5032:ASP:OD1	1:C:5033:GLN:OE1	2.33	0.47
1:D:4225:VAL:HG11	1:D:4948:VAL:HA	1.95	0.47
1:A:1810:ARG:HG3	1:A:1856:PHE:CE1	2.50	0.47
1:A:4225:VAL:HG11	1:A:4948:VAL:HA	1.95	0.47
1:A:4235:GLU:OE2	1:A:5015:ARG:NH2	2.48	0.47
1:B:1281:GLN:O	1:B:1282:ASN:OD1	2.32	0.47
1:B:2887:TRP:CG	1:B:2891:LYS:HZ1	2.32	0.47
1:B:4235:GLU:OE2	1:B:5015:ARG:NH2	2.48	0.47
1:C:864:LEU:HD13	1:C:869:GLU:HB2	1.96	0.47
1:C:2771:LYS:HE2	1:C:2792:LEU:HD11	1.96	0.47
1:D:924:GLN:O	1:D:927:GLY:N	2.47	0.47
1:D:3041:THR:OG1	1:D:3081:VAL:HG21	2.13	0.47
1:A:4685:TYR:CE2	1:A:4701:ARG:HG2	2.49	0.47
1:B:2942:LEU:HA	1:B:2945:MET:SD	2.55	0.47
1:B:3282:LEU:HD12	1:B:3316:LEU:HD22	1.96	0.47
1:C:1810:ARG:HG3	1:C:1856:PHE:CE1	2.50	0.47
1:C:3951:LYS:NZ	1:C:4012:GLN:HB3	2.30	0.47
1:C:4235:GLU:OE2	1:C:5015:ARG:NH2	2.48	0.47
1:D:897:VAL:HG22	1:D:898:ARG:N	2.30	0.47
1:A:490:ASN:O	1:A:494:ARG:HG2	2.15	0.47
1:A:2953:GLU:N	1:A:2953:GLU:OE1	2.44	0.47
1:A:2996:ILE:HD12	1:A:2996:ILE:H	1.80	0.47
1:B:151:MET:HB3	1:B:170:LEU:HD12	1.97	0.47
1:B:897:VAL:HG22	1:B:898:ARG:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1810:ARG:HG3	1:B:1856:PHE:CE1	2.50	0.47
1:B:2771:LYS:HE2	1:B:2792:LEU:HD11	1.96	0.47
1:B:2887:TRP:CZ2	1:B:2905:LEU:HD23	2.50	0.47
1:B:2996:ILE:HD12	1:B:2996:ILE:H	1.80	0.47
1:B:3951:LYS:NZ	1:B:4012:GLN:HB3	2.30	0.47
1:B:4179:PRO:O	1:B:4205:ARG:NH2	2.47	0.47
1:D:658:THR:HG22	1:D:1002:VAL:CG2	2.44	0.47
1:D:1281:GLN:O	1:D:1282:ASN:OD1	2.32	0.47
1:D:2525:VAL:HG23	1:D:2526:GLY:N	2.30	0.47
1:D:2752:LEU:HD11	1:D:2824:VAL:CG2	2.43	0.47
1:D:2891:LYS:O	1:D:2895:LEU:HG	2.14	0.47
1:D:4072:LYS:HA	1:D:4132:ALA:HB1	1.95	0.47
1:A:897:VAL:HG22	1:A:898:ARG:N	2.30	0.47
1:A:3107:MET:SD	1:A:3133:THR:OG1	2.58	0.47
1:A:4926:LEU:HA	1:A:4929:ILE:HD12	1.97	0.47
1:A:5032:ASP:OD1	1:A:5033:GLN:OE1	2.33	0.47
2:F:26:HIS:HD1	2:F:105:LEU:HD11	1.80	0.47
1:C:151:MET:HB3	1:C:170:LEU:HD12	1.97	0.47
1:C:500:THR:HG23	1:C:503:HIS:H	1.80	0.47
1:C:2942:LEU:HA	1:C:2945:MET:SD	2.55	0.47
1:C:5011:MET:HE1	1:C:5018:ASP:HB2	1.96	0.47
1:D:151:MET:HB3	1:D:170:LEU:HD12	1.97	0.47
1:D:1810:ARG:HG3	1:D:1856:PHE:CE1	2.50	0.47
1:D:5011:MET:HE1	1:D:5018:ASP:HB2	1.96	0.47
1:A:3184:VAL:O	1:A:3188:ARG:HG3	2.15	0.47
1:B:490:ASN:O	1:B:494:ARG:HG2	2.15	0.47
1:B:500:THR:HG23	1:B:503:HIS:H	1.80	0.47
1:B:569:LEU:HD12	1:B:603:VAL:HG13	1.97	0.47
1:B:581:GLU:HG3	1:B:621:LEU:HD22	1.96	0.47
1:B:3004:LEU:HB2	1:B:3005:PRO:HD3	1.96	0.47
1:C:3004:LEU:HB2	1:C:3005:PRO:HD3	1.96	0.47
1:C:4072:LYS:HA	1:C:4132:ALA:HB1	1.95	0.47
1:C:4927:LEU:O	1:C:4931:GLN:OE1	2.32	0.47
1:D:2771:LYS:HE2	1:D:2792:LEU:HD11	1.96	0.47
1:D:2887:TRP:CZ2	1:D:2905:LEU:HD23	2.50	0.47
1:A:924:GLN:O	1:A:927:GLY:N	2.47	0.47
1:A:2891:LYS:O	1:A:2895:LEU:HG	2.14	0.47
1:B:924:GLN:O	1:B:927:GLY:N	2.47	0.47
1:C:3282:LEU:HD12	1:C:3316:LEU:HD22	1.96	0.47
1:C:3958:MET:HE3	1:C:4018:GLU:HG2	1.97	0.47
1:D:3548:GLU:OE1	1:D:3551:ARG:NH2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5032:ASP:OD1	1:D:5033:GLN:OE1	2.33	0.47
1:A:151:MET:HB3	1:A:170:LEU:HD12	1.97	0.46
1:A:3820:LEU:HD21	1:A:3901:ASP:HB3	1.98	0.46
1:B:4628:TYR:OH	1:C:4858:ARG:NH1	2.42	0.46
1:C:490:ASN:O	1:C:494:ARG:HG2	2.15	0.46
1:C:581:GLU:HG3	1:C:621:LEU:HD22	1.96	0.46
1:C:3227:GLU:O	1:C:3228:ARG:HB3	2.14	0.46
1:C:3820:LEU:HD21	1:C:3901:ASP:HB3	1.98	0.46
1:D:3004:LEU:HB2	1:D:3005:PRO:HD3	1.96	0.46
1:D:3951:LYS:NZ	1:D:4012:GLN:HB3	2.30	0.46
1:D:4965:TYR:OH	1:D:5031:GLU:OE2	2.28	0.46
1:A:2752:LEU:HD11	1:A:2824:VAL:CG2	2.43	0.46
1:A:2771:LYS:HE2	1:A:2792:LEU:HD11	1.96	0.46
1:B:1053:ASN:OD1	1:B:1053:ASN:O	2.34	0.46
1:D:500:THR:HG23	1:D:503:HIS:H	1.80	0.46
1:D:4860:PHE:CB	1:D:4911:ARG:HH12	2.27	0.46
1:A:1053:ASN:OD1	1:A:1053:ASN:O	2.34	0.46
1:A:1494:TYR:CB	1:A:1528:MET:HE1	2.46	0.46
1:C:1132:ARG:NH1	1:C:1138:GLU:OE1	2.49	0.46
1:D:938:CYS:HA	1:D:1057:PRO:HD3	1.98	0.46
1:D:3227:GLU:O	1:D:3228:ARG:HB3	2.14	0.46
1:A:864:LEU:HD13	1:A:869:GLU:HB2	1.96	0.46
1:A:2866:VAL:O	1:A:2929:LYS:NZ	2.40	0.46
1:A:3951:LYS:NZ	1:A:4012:GLN:HB3	2.30	0.46
2:G:26:HIS:HD1	2:G:105:LEU:HD11	1.80	0.46
1:B:1494:TYR:CB	1:B:1528:MET:HE1	2.46	0.46
1:B:2525:VAL:HG23	1:B:2526:GLY:N	2.30	0.46
1:B:3958:MET:HE3	1:B:4018:GLU:HG2	1.97	0.46
1:B:5032:ASP:OD1	1:B:5033:GLN:OE1	2.33	0.46
1:C:2737:ASP:OD1	1:C:2892:LYS:NZ	2.37	0.46
1:D:490:ASN:O	1:D:494:ARG:HG2	2.15	0.46
1:D:864:LEU:HD13	1:D:869:GLU:HB2	1.96	0.46
1:A:2525:VAL:HG23	1:A:2526:GLY:N	2.30	0.46
1:A:2942:LEU:HA	1:A:2945:MET:SD	2.55	0.46
1:C:70:LEU:HD13	1:C:102:LEU:HD11	1.97	0.46
1:C:3184:VAL:O	1:C:3188:ARG:HG3	2.15	0.46
1:C:4628:TYR:OH	1:D:4858:ARG:NH1	2.42	0.46
1:C:4814:ILE:HD12	1:C:4821:LEU:CD1	2.46	0.46
1:D:569:LEU:HD12	1:D:603:VAL:HG13	1.97	0.46
1:D:1053:ASN:OD1	1:D:1053:ASN:O	2.34	0.46
1:D:1494:TYR:CB	1:D:1528:MET:HE1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2391:PRO:O	1:D:2392:ALA:HB3	2.16	0.46
1:D:3184:VAL:O	1:D:3188:ARG:HG3	2.15	0.46
1:D:4235:GLU:OE2	1:D:5015:ARG:NH2	2.48	0.46
1:A:873:GLU:O	1:A:877:GLU:OE1	2.34	0.46
1:A:2391:PRO:O	1:A:2392:ALA:HB3	2.16	0.46
1:A:3761:MET:SD	1:A:4753:GLU:OE1	2.74	0.46
2:H:26:HIS:HD1	2:H:105:LEU:HD11	1.80	0.46
1:B:3184:VAL:O	1:B:3188:ARG:HG3	2.15	0.46
1:B:3761:MET:SD	1:B:4753:GLU:OE1	2.74	0.46
1:C:2996:ILE:HD12	1:C:2996:ILE:H	1.80	0.46
1:D:581:GLU:HG3	1:D:621:LEU:HD22	1.96	0.46
1:D:2942:LEU:HA	1:D:2945:MET:SD	2.55	0.46
1:D:3761:MET:SD	1:D:4753:GLU:OE1	2.74	0.46
1:D:3820:LEU:HD21	1:D:3901:ASP:HB3	1.98	0.46
1:A:1685:ALA:HA	2:E:91:ILE:HD11	1.97	0.46
1:A:2156:LEU:HD13	1:A:2199:MET:HE1	1.98	0.46
1:B:2752:LEU:HD11	1:B:2824:VAL:CG2	2.43	0.46
1:B:3820:LEU:HD21	1:B:3901:ASP:HB3	1.97	0.46
1:B:4318:ARG:NH1	1:D:4910:TYR:OH	2.49	0.46
1:C:569:LEU:HD12	1:C:603:VAL:HG13	1.97	0.46
1:C:1494:TYR:CB	1:C:1528:MET:HE1	2.46	0.46
1:D:2482:LYS:O	1:D:2483:ASP:OD2	2.34	0.46
1:D:4066:ASP:OD1	1:D:4066:ASP:C	2.59	0.46
1:D:4814:ILE:HD12	1:D:4821:LEU:CD1	2.46	0.46
1:A:70:LEU:HD13	1:A:102:LEU:HD11	1.97	0.46
1:A:2887:TRP:CZ2	1:A:2905:LEU:HD23	2.50	0.46
1:A:3082:MET:HE3	1:A:3093:LEU:CD2	2.43	0.46
1:A:4814:ILE:HD12	1:A:4821:LEU:CD1	2.46	0.46
1:B:4926:LEU:HA	1:B:4929:ILE:HD12	1.97	0.46
1:C:897:VAL:HG22	1:C:898:ARG:N	2.30	0.46
1:C:2752:LEU:HD11	1:C:2824:VAL:CG2	2.43	0.46
1:C:4186:ILE:CD1	1:C:4196:ILE:HD11	2.46	0.46
1:D:871:ILE:HD12	1:D:1050:TYR:HD2	1.81	0.46
1:D:873:GLU:O	1:D:877:GLU:OE1	2.34	0.46
1:D:2996:ILE:HD12	1:D:2996:ILE:H	1.80	0.46
1:A:4927:LEU:O	1:A:4931:GLN:OE1	2.32	0.46
1:C:1053:ASN:OD1	1:C:1053:ASN:O	2.34	0.46
1:C:1066:SER:OG	1:C:1067:GLN:OE1	2.14	0.46
1:C:2887:TRP:CZ2	1:C:2905:LEU:HD23	2.50	0.46
1:C:3761:MET:SD	1:C:4753:GLU:OE1	2.74	0.46
1:D:4926:LEU:HA	1:D:4929:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2482:LYS:O	1:B:2483:ASP:OD2	2.34	0.46
1:C:3051:VAL:CG2	1:C:3065:VAL:HG11	2.46	0.46
1:D:397:GLU:OE2	1:D:471:SER:OG	2.29	0.46
1:A:938:CYS:HA	1:A:1057:PRO:HD3	1.98	0.45
1:A:4720:ARG:HH11	1:A:4720:ARG:H	1.64	0.45
1:B:873:GLU:O	1:B:877:GLU:OE1	2.34	0.45
1:B:4814:ILE:HD12	1:B:4821:LEU:CD1	2.46	0.45
1:C:4926:LEU:HA	1:C:4929:ILE:HD12	1.97	0.45
1:A:3541:TYR:OH	1:A:3598:GLN:NE2	2.49	0.45
1:A:3958:MET:HE3	1:A:4018:GLU:HG2	1.97	0.45
1:B:2830:GLY:HA2	1:B:2934:ASN:HA	1.99	0.45
1:B:4720:ARG:HH11	1:B:4720:ARG:H	1.64	0.45
1:C:871:ILE:HD12	1:C:1050:TYR:HD2	1.81	0.45
1:C:2482:LYS:O	1:C:2483:ASP:OD2	2.34	0.45
1:D:2798:PHE:CZ	1:D:2802:ASP:HB3	2.51	0.45
1:D:2887:TRP:CG	1:D:2891:LYS:HZ1	2.33	0.45
1:D:3541:TYR:HB3	1:D:3605:TYR:CD2	2.52	0.45
1:A:2482:LYS:O	1:A:2483:ASP:OD2	2.34	0.45
1:A:2978:LEU:HD22	1:A:3057:LEU:HD23	1.98	0.45
1:A:3006:LEU:O	1:A:3007:ILE:C	2.60	0.45
1:B:2798:PHE:CZ	1:B:2802:ASP:HB3	2.51	0.45
1:B:4186:ILE:CD1	1:B:4196:ILE:HD11	2.46	0.45
1:C:2156:LEU:HD13	1:C:2199:MET:HE1	1.98	0.45
1:C:3591:GLU:O	1:C:3594:VAL:HG22	2.17	0.45
1:A:216:THR:OG1	1:A:219:HIS:CE1	2.70	0.45
1:A:500:THR:HG23	1:A:503:HIS:H	1.80	0.45
1:A:569:LEU:HD12	1:A:603:VAL:HG13	1.97	0.45
1:A:2007:ILE:CD1	1:A:3642:LEU:HD21	2.47	0.45
1:B:978:LEU:HD12	1:B:982:GLN:HB3	1.99	0.45
1:B:3006:LEU:O	1:B:3007:ILE:C	2.60	0.45
1:C:873:GLU:O	1:C:877:GLU:OE1	2.34	0.45
1:C:3548:GLU:OE1	1:C:3551:ARG:NH2	2.40	0.45
1:D:70:LEU:HD13	1:D:102:LEU:HD11	1.97	0.45
1:D:1132:ARG:NH1	1:D:1138:GLU:OE1	2.49	0.45
1:D:2978:LEU:HD22	1:D:3057:LEU:HD23	1.98	0.45
1:D:3591:GLU:O	1:D:3594:VAL:HG22	2.17	0.45
2:H:91:ILE:HD11	1:D:1685:ALA:HA	1.98	0.45
1:B:938:CYS:HA	1:B:1057:PRO:HD3	1.98	0.45
1:B:1793:ALA:C	1:B:1794:THR:HG1	2.15	0.45
1:B:3541:TYR:HB3	1:B:3605:TYR:CD2	2.52	0.45
1:B:3591:GLU:O	1:B:3594:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:THR:OG1	1:C:219:HIS:CE1	2.70	0.45
1:D:2830:GLY:HA2	1:D:2934:ASN:HA	1.99	0.45
1:D:3051:VAL:CG2	1:D:3065:VAL:HG11	2.46	0.45
1:D:3509:SER:OG	1:D:3512:VAL:HG12	2.17	0.45
1:A:871:ILE:HD12	1:A:1050:TYR:HD2	1.81	0.45
1:A:2798:PHE:CZ	1:A:2802:ASP:HB3	2.51	0.45
2:G:91:ILE:HD11	1:C:1685:ALA:HA	1.97	0.45
1:B:70:LEU:HD13	1:B:102:LEU:HD11	1.97	0.45
1:B:216:THR:OG1	1:B:219:HIS:CE1	2.70	0.45
1:B:2156:LEU:HD13	1:B:2199:MET:HE1	1.98	0.45
1:C:1041:CYS:SG	1:C:1042:GLN:NE2	2.87	0.45
1:C:2798:PHE:CZ	1:C:2802:ASP:HB3	2.51	0.45
1:D:216:THR:OG1	1:D:219:HIS:CE1	2.70	0.45
1:D:3958:MET:HE3	1:D:4018:GLU:HG2	1.97	0.45
1:D:4186:ILE:CD1	1:D:4196:ILE:HD11	2.46	0.45
1:A:3541:TYR:HB3	1:A:3605:TYR:CD2	2.52	0.45
1:B:2007:ILE:CD1	1:B:3642:LEU:HD21	2.47	0.45
1:B:3399:PHE:HB2	1:B:3455:GLU:HG3	1.99	0.45
1:B:3440:GLY:HA2	1:B:3515:LEU:HD12	1.99	0.45
1:C:2391:PRO:O	1:C:2392:ALA:HB3	2.16	0.45
1:C:3399:PHE:HB2	1:C:3455:GLU:HG3	1.99	0.45
1:C:3515:LEU:HD11	1:C:3603:VAL:HG13	1.99	0.45
1:C:4075:VAL:HG21	1:C:4132:ALA:HB2	1.99	0.45
1:D:3006:LEU:O	1:D:3007:ILE:C	2.60	0.45
1:A:978:LEU:HD12	1:A:982:GLN:HB3	1.99	0.45
1:A:2515:ASN:OD1	1:A:2517:ASP:N	2.45	0.45
1:B:1132:ARG:NH1	1:B:1138:GLU:OE1	2.49	0.45
1:B:2391:PRO:O	1:B:2392:ALA:HB3	2.16	0.45
1:C:938:CYS:HA	1:C:1057:PRO:HD3	1.98	0.45
1:C:4062:LEU:HD13	1:C:4170:ALA:HB2	1.99	0.45
1:D:877:GLU:O	1:D:881:GLU:HG2	2.17	0.45
1:D:4062:LEU:HD13	1:D:4170:ALA:HB2	1.99	0.45
1:A:877:GLU:O	1:A:881:GLU:HG2	2.17	0.45
1:A:1555:VAL:HG21	1:A:1562:VAL:CG1	2.47	0.45
1:A:3051:VAL:CG2	1:A:3065:VAL:HG11	2.46	0.45
1:A:4066:ASP:OD1	1:A:4066:ASP:C	2.59	0.45
1:A:4577:PHE:HB2	1:A:4630:LEU:HD11	1.99	0.45
1:B:2160:LEU:HD13	1:B:2204:MET:HG2	1.99	0.45
1:C:2160:LEU:HD13	1:C:2204:MET:HG2	1.99	0.45
1:C:2830:GLY:HA2	1:C:2934:ASN:HA	1.99	0.45
1:C:4577:PHE:HB2	1:C:4630:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3082:MET:HE3	1:D:3093:LEU:CD2	2.43	0.45
1:A:3130:LEU:O	1:A:3134:THR:HG22	2.17	0.45
1:A:3509:SER:OG	1:A:3512:VAL:HG12	2.17	0.45
1:A:4186:ILE:CD1	1:A:4196:ILE:HD11	2.46	0.45
2:F:91:ILE:HD11	1:B:1685:ALA:HA	1.97	0.45
1:B:877:GLU:O	1:B:881:GLU:HG2	2.17	0.45
1:B:1555:VAL:HG21	1:B:1562:VAL:CG1	2.47	0.45
1:B:1967:VAL:HG21	1:B:3650:ALA:HB1	1.99	0.45
1:B:2216:LEU:HD23	1:B:2224:ILE:HG21	1.99	0.45
1:B:4075:VAL:HG21	1:B:4132:ALA:HB2	1.99	0.45
1:C:978:LEU:HD12	1:C:982:GLN:HB3	1.99	0.45
1:C:3440:GLY:HA2	1:C:3515:LEU:HD12	1.99	0.45
1:D:2866:VAL:O	1:D:2929:LYS:NZ	2.40	0.45
1:D:3515:LEU:HD11	1:D:3603:VAL:HG13	1.99	0.45
2:E:26:HIS:HD1	2:E:105:LEU:HD11	1.81	0.44
1:B:2978:LEU:HD22	1:B:3057:LEU:HD23	1.98	0.44
1:B:3082:MET:HE3	1:B:3093:LEU:CD2	2.43	0.44
1:B:3674:MET:HE2	1:B:3726:TYR:HE1	1.83	0.44
1:C:446:LEU:HD23	1:C:526:LEU:HD22	2.00	0.44
1:C:4066:ASP:OD1	1:C:4066:ASP:C	2.59	0.44
1:C:4720:ARG:HH11	1:C:4720:ARG:H	1.64	0.44
1:D:1967:VAL:HG21	1:D:3650:ALA:HB1	1.99	0.44
1:D:2007:ILE:CD1	1:D:3642:LEU:HD21	2.47	0.44
1:D:2160:LEU:HD13	1:D:2204:MET:HG2	1.99	0.44
1:D:2771:LYS:HE3	1:D:2792:LEU:HD11	1.99	0.44
1:A:3399:PHE:HB2	1:A:3455:GLU:HG3	1.99	0.44
1:A:3683:GLU:OE1	1:A:3686:GLU:HG2	2.18	0.44
1:A:3999:PHE:HD1	1:A:4019:LEU:HD11	1.83	0.44
1:B:3999:PHE:HD1	1:B:4019:LEU:HD11	1.83	0.44
1:C:923:LEU:O	1:C:926:SER:OG	2.34	0.44
1:C:2892:LYS:HA	1:C:2895:LEU:HD12	2.00	0.44
1:C:4638:GLU:HB3	1:C:4639:PRO:HD3	2.00	0.44
1:D:3399:PHE:HB2	1:D:3455:GLU:HG3	1.99	0.44
1:D:3674:MET:HE2	1:D:3726:TYR:HE1	1.83	0.44
1:B:871:ILE:HD12	1:B:1050:TYR:HD2	1.81	0.44
1:B:3051:VAL:CG2	1:B:3065:VAL:HG11	2.47	0.44
1:C:2883:TYR:OH	1:C:2927:LEU:HD13	2.18	0.44
1:C:3170:LEU:CD1	1:C:3195:LEU:HD11	2.40	0.44
1:D:2883:TYR:OH	1:D:2927:LEU:HD13	2.18	0.44
1:D:4577:PHE:HB2	1:D:4630:LEU:HD11	1.99	0.44
1:D:4720:ARG:HH11	1:D:4720:ARG:H	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:TRP:CE2	1:A:728:ALA:HB2	2.53	0.44
1:A:2160:LEU:HD13	1:A:2204:MET:HG2	1.99	0.44
1:A:2432:ASP:OD2	1:A:2436:ARG:NE	2.50	0.44
1:A:3421:ARG:NH2	1:A:3517:LYS:O	2.51	0.44
1:A:4858:ARG:NH1	1:D:4628:TYR:OH	2.42	0.44
1:B:3130:LEU:O	1:B:3134:THR:HG22	2.17	0.44
1:B:3421:ARG:NH2	1:B:3517:LYS:O	2.51	0.44
1:B:4066:ASP:OD1	1:B:4066:ASP:C	2.59	0.44
1:B:4093:LYS:HE2	1:B:4093:LYS:HB2	1.30	0.44
1:C:4043:ILE:H	1:C:4043:ILE:HD12	1.83	0.44
1:D:2859:GLN:OE1	1:D:2859:GLN:N	2.51	0.44
1:D:4075:VAL:HG21	1:D:4132:ALA:HB2	1.99	0.44
1:A:2859:GLN:OE1	1:A:2859:GLN:N	2.51	0.44
1:A:2883:TYR:OH	1:A:2927:LEU:HD13	2.18	0.44
1:A:3674:MET:HE2	1:A:3726:TYR:HE1	1.83	0.44
1:A:4107:THR:HG22	1:A:4108:GLY:N	2.33	0.44
1:A:4965:TYR:OH	1:A:5031:GLU:OE2	2.28	0.44
1:B:3683:GLU:OE1	1:B:3686:GLU:HG2	2.18	0.44
1:B:4043:ILE:H	1:B:4043:ILE:HD12	1.83	0.44
1:B:4910:TYR:OH	1:D:4318:ARG:NH1	2.49	0.44
1:C:2859:GLN:OE1	1:C:2859:GLN:N	2.51	0.44
1:C:3541:TYR:HB3	1:C:3605:TYR:CD2	2.52	0.44
1:C:3674:MET:HE2	1:C:3726:TYR:HE1	1.83	0.44
1:D:3293:PRO:O	1:D:3295:PRO:CD	2.66	0.44
1:D:3440:GLY:HA2	1:D:3515:LEU:HD12	1.99	0.44
1:D:3683:GLU:OE1	1:D:3686:GLU:HG2	2.18	0.44
1:A:3591:GLU:O	1:A:3594:VAL:HG22	2.17	0.44
1:B:2859:GLN:N	1:B:2859:GLN:OE1	2.51	0.44
1:B:2928:LEU:HA	1:B:2931:LEU:HD12	1.99	0.44
1:B:3548:GLU:OE1	1:B:3551:ARG:NH2	2.40	0.44
1:B:4094:LYS:HD2	1:B:4094:LYS:HA	1.36	0.44
1:C:2216:LEU:HD23	1:C:2224:ILE:HG21	1.99	0.44
1:C:2759:PHE:HD1	1:C:2930:PHE:CG	2.36	0.44
1:C:2771:LYS:HE3	1:C:2792:LEU:HD11	1.99	0.44
1:A:1967:VAL:HG21	1:A:3650:ALA:HB1	1.99	0.44
1:A:2216:LEU:HD23	1:A:2224:ILE:HG21	1.99	0.44
1:A:2830:GLY:HA2	1:A:2934:ASN:HA	1.99	0.44
1:A:3106:LYS:O	1:A:3109:GLU:HG3	2.18	0.44
1:A:3515:LEU:HD11	1:A:3603:VAL:HG13	1.99	0.44
1:B:2266:LEU:HD13	1:B:2331:ARG:HE	1.83	0.44
1:B:3360:ILE:HB	1:B:3361:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4062:LEU:HD13	1:B:4170:ALA:HB2	1.99	0.44
1:B:4577:PHE:HB2	1:B:4630:LEU:HD11	1.99	0.44
1:C:1555:VAL:HG21	1:C:1562:VAL:CG1	2.47	0.44
1:C:2978:LEU:HD22	1:C:3057:LEU:HD23	1.99	0.44
1:C:3683:GLU:OE1	1:C:3686:GLU:HG2	2.18	0.44
1:C:4935:ILE:HG12	1:D:4932:GLY:HA2	1.99	0.44
1:D:1294:LEU:O	1:D:1580:MET:HE2	2.18	0.44
1:D:2266:LEU:HD21	1:D:2327:CYS:SG	2.58	0.44
1:D:2892:LYS:HA	1:D:2895:LEU:HD12	2.00	0.44
1:A:2887:TRP:O	1:A:2891:LYS:HE2	2.18	0.44
1:A:3591:GLU:HA	1:A:3594:VAL:HG22	2.00	0.44
1:B:2782:ILE:HG23	1:B:2782:ILE:O	2.18	0.44
1:B:3509:SER:OG	1:B:3512:VAL:HG12	2.17	0.44
1:B:4107:THR:HG22	1:B:4108:GLY:N	2.33	0.44
1:C:3509:SER:OG	1:C:3512:VAL:HG12	2.17	0.44
1:C:3999:PHE:HD1	1:C:4019:LEU:HD11	1.83	0.44
1:C:4828:VAL:HG21	1:D:4929:ILE:HD11	2.00	0.44
1:D:1555:VAL:HG21	1:D:1562:VAL:CG1	2.47	0.44
1:D:2156:LEU:HD13	1:D:2199:MET:HE1	1.98	0.44
1:D:3541:TYR:OH	1:D:3598:GLN:NE2	2.49	0.44
1:D:3591:GLU:HA	1:D:3594:VAL:HG22	2.00	0.44
1:A:3176:LEU:O	1:A:3176:LEU:HD23	2.18	0.44
1:A:4075:VAL:HG21	1:A:4132:ALA:HB2	1.99	0.44
1:A:4700:ASP:C	1:A:4702:LEU:N	2.76	0.44
1:B:1041:CYS:SG	1:B:1042:GLN:NE2	2.87	0.44
1:B:2759:PHE:HD1	1:B:2930:PHE:CG	2.36	0.44
1:B:4334:TRP:HA	1:B:4334:TRP:CE3	2.53	0.44
1:C:877:GLU:O	1:C:881:GLU:HG2	2.17	0.44
1:C:2007:ILE:CD1	1:C:3642:LEU:HD21	2.47	0.44
1:C:2782:ILE:HG23	1:C:2782:ILE:O	2.18	0.44
1:D:938:CYS:HA	1:D:1057:PRO:CD	2.48	0.44
1:D:978:LEU:HD12	1:D:982:GLN:HB3	1.99	0.44
1:D:3360:ILE:HB	1:D:3361:PRO:HD3	2.00	0.44
1:A:938:CYS:HA	1:A:1057:PRO:CD	2.48	0.43
1:A:3410:TYR:N	1:A:3411:PRO:HD2	2.33	0.43
1:A:4062:LEU:HD13	1:A:4170:ALA:HB2	1.99	0.43
1:B:2266:LEU:HD21	1:B:2327:CYS:SG	2.58	0.43
1:B:2887:TRP:O	1:B:2891:LYS:HE2	2.18	0.43
1:B:3515:LEU:HD11	1:B:3603:VAL:HG13	1.99	0.43
1:B:4965:TYR:OH	1:B:5031:GLU:OE2	2.28	0.43
1:C:1793:ALA:C	1:C:1794:THR:HG1	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3293:PRO:O	1:C:3295:PRO:CD	2.66	0.43
1:C:3421:ARG:NH2	1:C:3517:LYS:O	2.51	0.43
1:D:914:LEU:HD12	1:D:915:PRO:HD2	1.99	0.43
1:D:1793:ALA:C	1:D:1794:THR:HG1	2.14	0.43
1:D:3999:PHE:HD1	1:D:4019:LEU:HD11	1.83	0.43
1:A:3515:LEU:HD23	1:A:3515:LEU:C	2.43	0.43
1:A:4009:ASP:OD1	1:A:4010:SER:N	2.51	0.43
1:A:4706:THR:HA	1:A:4707:PRO:HD3	1.91	0.43
1:B:723:TRP:CE2	1:B:728:ALA:HB2	2.53	0.43
1:B:843:PRO:O	1:B:1197:PRO:HA	2.19	0.43
1:B:938:CYS:HA	1:B:1057:PRO:CD	2.48	0.43
1:B:2883:TYR:OH	1:B:2927:LEU:HD13	2.18	0.43
1:B:3170:LEU:CD1	1:B:3195:LEU:HD11	2.40	0.43
1:B:3293:PRO:O	1:B:3295:PRO:CD	2.66	0.43
1:B:4638:GLU:HB3	1:B:4639:PRO:HD3	2.00	0.43
1:C:938:CYS:HA	1:C:1057:PRO:CD	2.48	0.43
1:C:2187:MET:HE2	1:C:2236:PHE:HA	2.01	0.43
1:C:2928:LEU:HA	1:C:2931:LEU:HD12	1.99	0.43
1:D:723:TRP:CE2	1:D:728:ALA:HB2	2.53	0.43
1:D:864:LEU:HD12	1:D:864:LEU:O	2.19	0.43
1:D:2887:TRP:O	1:D:2891:LYS:HE2	2.18	0.43
1:D:2928:LEU:HA	1:D:2931:LEU:HD12	1.99	0.43
1:D:4090:LEU:HD22	1:D:4125:MET:HB3	2.00	0.43
1:A:923:LEU:O	1:A:926:SER:OG	2.34	0.43
1:A:3293:PRO:O	1:A:3295:PRO:CD	2.66	0.43
1:A:4694:ASP:OD1	1:A:4697:GLY:N	2.30	0.43
1:A:4935:ILE:HG12	1:B:4932:GLY:HA2	2.00	0.43
1:B:446:LEU:HD23	1:B:526:LEU:HD22	2.00	0.43
1:B:914:LEU:HD12	1:B:915:PRO:HD2	1.99	0.43
1:B:951:LEU:HD11	1:B:1049:GLY:O	2.18	0.43
1:B:3410:TYR:N	1:B:3411:PRO:HD2	2.33	0.43
1:B:3515:LEU:HD23	1:B:3515:LEU:C	2.43	0.43
1:C:1967:VAL:HG21	1:C:3650:ALA:HB1	1.99	0.43
1:C:3410:TYR:N	1:C:3411:PRO:HD2	2.33	0.43
1:D:2627:LEU:HD22	1:D:2641:PRO:HB3	2.00	0.43
1:D:3130:LEU:O	1:D:3134:THR:HG22	2.17	0.43
1:D:3506:VAL:O	1:D:3509:SER:OG	2.16	0.43
1:D:3515:LEU:HD23	1:D:3515:LEU:C	2.43	0.43
1:D:4638:GLU:HB3	1:D:4639:PRO:HD3	2.00	0.43
1:A:2266:LEU:HD21	1:A:2327:CYS:SG	2.58	0.43
1:A:2782:ILE:O	1:A:2782:ILE:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3440:GLY:HA2	1:A:3515:LEU:HD12	1.99	0.43
1:A:3638:ARG:HH11	1:A:3640:THR:HG23	1.84	0.43
1:A:4828:VAL:HG21	1:B:4929:ILE:HD11	2.01	0.43
1:B:2771:LYS:HE3	1:B:2792:LEU:HD11	1.99	0.43
1:B:2892:LYS:HA	1:B:2895:LEU:HD12	2.00	0.43
1:B:3541:TYR:OH	1:B:3598:GLN:NE2	2.49	0.43
1:C:47:LEU:HD12	1:C:126:ARG:HH12	1.84	0.43
1:C:2266:LEU:HD21	1:C:2327:CYS:SG	2.58	0.43
1:C:2887:TRP:O	1:C:2891:LYS:HE2	2.18	0.43
1:C:3006:LEU:O	1:C:3007:ILE:C	2.60	0.43
1:C:3082:MET:HE3	1:C:3093:LEU:CD2	2.43	0.43
1:C:3130:LEU:O	1:C:3134:THR:HG22	2.17	0.43
1:C:4107:THR:HG22	1:C:4108:GLY:N	2.33	0.43
1:D:2432:ASP:OD2	1:D:2436:ARG:NE	2.50	0.43
1:D:2515:ASN:OD1	1:D:2517:ASP:N	2.45	0.43
1:D:3410:TYR:N	1:D:3411:PRO:HD2	2.33	0.43
1:D:4043:ILE:H	1:D:4043:ILE:HD12	1.83	0.43
1:A:1132:ARG:NH1	1:A:1138:GLU:OE1	2.49	0.43
1:A:4090:LEU:HD22	1:A:4125:MET:HB3	2.00	0.43
1:B:3106:LYS:O	1:B:3109:GLU:HG3	2.18	0.43
1:B:4700:ASP:C	1:B:4702:LEU:N	2.76	0.43
1:C:461:GLN:HB2	1:C:464:GLU:OE1	2.19	0.43
1:C:951:LEU:HD11	1:C:1049:GLY:O	2.18	0.43
1:C:2438:ALA:HB2	1:C:2510:VAL:HG22	2.01	0.43
1:C:3106:LYS:O	1:C:3109:GLU:HG3	2.18	0.43
1:D:446:LEU:HD23	1:D:526:LEU:HD22	2.00	0.43
1:D:951:LEU:HD11	1:D:1049:GLY:O	2.18	0.43
1:D:1038:ASP:O	1:D:1042:GLN:HG2	2.19	0.43
1:D:2266:LEU:HD13	1:D:2331:ARG:HE	1.83	0.43
1:D:2782:ILE:O	1:D:2782:ILE:HG23	2.18	0.43
1:A:843:PRO:O	1:A:1197:PRO:HA	2.19	0.43
1:A:2438:ALA:HB2	1:A:2510:VAL:HG22	2.01	0.43
1:A:3360:ILE:HB	1:A:3361:PRO:HD3	2.00	0.43
1:B:670:ASP:OD2	1:B:789:LYS:NZ	2.33	0.43
1:B:1294:LEU:O	1:B:1580:MET:HE2	2.18	0.43
1:B:3176:LEU:O	1:B:3176:LEU:HD23	2.18	0.43
1:B:3591:GLU:HA	1:B:3594:VAL:HG22	2.00	0.43
1:B:4902:PRO:HB3	1:B:4911:ARG:HG2	2.01	0.43
1:C:3176:LEU:HD23	1:C:3176:LEU:O	2.18	0.43
1:D:858:ASP:OD1	1:D:859:THR:N	2.52	0.43
1:D:2216:LEU:HD23	1:D:2224:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3106:LYS:O	1:D:3109:GLU:HG3	2.18	0.43
1:D:3176:LEU:O	1:D:3176:LEU:HD23	2.18	0.43
1:A:446:LEU:HD23	1:A:526:LEU:HD22	2.00	0.43
1:A:1038:ASP:O	1:A:1042:GLN:HG2	2.19	0.43
1:A:1713:TYR:OH	1:A:1816:MET:SD	2.77	0.43
1:A:2627:LEU:HD22	1:A:2641:PRO:HB3	2.00	0.43
1:A:2928:LEU:HA	1:A:2931:LEU:HD12	1.99	0.43
1:A:4334:TRP:CE3	1:A:4334:TRP:HA	2.53	0.43
1:B:47:LEU:HD12	1:B:126:ARG:HH12	1.84	0.43
1:B:554:ARG:NE	1:B:556:GLU:OE2	2.51	0.43
1:B:4828:VAL:HG21	1:C:4929:ILE:HD11	2.01	0.43
1:C:546:ASP:OD1	1:C:583:HIS:NE2	2.38	0.43
1:C:723:TRP:CE2	1:C:728:ALA:HB2	2.53	0.43
1:C:1294:LEU:O	1:C:1580:MET:HE2	2.18	0.43
1:C:3228:ARG:HG2	1:C:3228:ARG:O	2.19	0.43
1:C:3360:ILE:HB	1:C:3361:PRO:HD3	2.00	0.43
1:C:3638:ARG:HH11	1:C:3640:THR:HG23	1.84	0.43
1:C:4334:TRP:HA	1:C:4334:TRP:CE3	2.53	0.43
1:C:4902:PRO:HB3	1:C:4911:ARG:HG2	2.01	0.43
1:D:47:LEU:HD12	1:D:126:ARG:HH12	1.84	0.43
1:D:2234:CYS:SG	1:D:2271:SER:HB3	2.59	0.43
1:D:3421:ARG:NH2	1:D:3517:LYS:O	2.51	0.43
1:A:858:ASP:OD1	1:A:859:THR:N	2.52	0.43
1:A:1294:LEU:O	1:A:1580:MET:HE2	2.18	0.43
1:A:3170:LEU:CD1	1:A:3195:LEU:HD11	2.40	0.43
1:B:422:PHE:O	1:B:423:SER:C	2.62	0.43
1:B:3638:ARG:HH11	1:B:3640:THR:HG23	1.84	0.43
1:B:4730:PHE:CB	1:B:4735:ILE:HD11	2.49	0.43
1:C:2234:CYS:SG	1:C:2271:SER:HB3	2.59	0.43
1:C:3591:GLU:HA	1:C:3594:VAL:HG22	2.00	0.43
1:C:4730:PHE:CB	1:C:4735:ILE:HD11	2.49	0.43
1:D:843:PRO:O	1:D:1197:PRO:HA	2.19	0.43
1:D:2759:PHE:HD1	1:D:2930:PHE:CG	2.36	0.43
1:A:864:LEU:HD12	1:A:864:LEU:O	2.19	0.43
1:A:2771:LYS:HE3	1:A:2792:LEU:HD11	1.99	0.43
1:A:2892:LYS:HA	1:A:2895:LEU:HD12	2.00	0.43
1:A:3551:ARG:HD2	1:A:3595:ARG:NH2	2.34	0.43
1:A:4318:ARG:NH1	1:C:4910:TYR:OH	2.50	0.43
1:A:4932:GLY:HA2	1:D:4935:ILE:HG12	2.00	0.43
1:B:910:ASN:O	1:B:914:LEU:N	2.52	0.43
1:B:1420:ASP:O	1:B:1422:ARG:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3253:GLU:O	1:B:3257:LEU:HD23	2.19	0.43
1:C:864:LEU:O	1:C:864:LEU:HD12	2.19	0.43
1:C:3515:LEU:C	1:C:3515:LEU:HD23	2.43	0.43
1:D:2187:MET:HE2	1:D:2236:PHE:HA	2.01	0.43
1:A:871:ILE:O	1:A:872:ARG:C	2.62	0.43
1:B:2234:CYS:SG	1:B:2271:SER:HB3	2.59	0.43
1:B:4706:THR:HA	1:B:4707:PRO:HD3	1.91	0.43
1:C:871:ILE:O	1:C:872:ARG:C	2.62	0.43
1:C:916:GLU:O	1:C:919:ARG:HG2	2.19	0.43
1:C:2213:VAL:HG21	1:C:2257:TYR:HE2	1.82	0.43
1:C:3730:MET:O	1:C:3733:SER:OG	2.30	0.43
1:D:422:PHE:O	1:D:423:SER:C	2.62	0.43
1:D:1420:ASP:O	1:D:1422:ARG:HD3	2.19	0.43
1:D:2481:GLY:O	1:D:2485:ALA:N	2.51	0.43
1:D:3208:GLU:OE2	1:D:3307:ALA:N	2.49	0.43
1:D:3228:ARG:O	1:D:3228:ARG:HG2	2.19	0.43
1:D:4334:TRP:CE3	1:D:4334:TRP:HA	2.53	0.43
1:D:4700:ASP:C	1:D:4702:LEU:N	2.76	0.43
1:A:397:GLU:OE2	1:A:471:SER:OG	2.29	0.42
1:A:916:GLU:O	1:A:919:ARG:HG2	2.19	0.42
1:A:1041:CYS:SG	1:A:1042:GLN:NE2	2.87	0.42
1:A:1420:ASP:O	1:A:1422:ARG:HD3	2.19	0.42
1:A:4043:ILE:H	1:A:4043:ILE:HD12	1.83	0.42
1:A:4638:GLU:HB3	1:A:4639:PRO:HD3	2.00	0.42
1:A:4929:ILE:HD11	1:D:4828:VAL:HG21	2.01	0.42
1:B:858:ASP:OD1	1:B:859:THR:N	2.52	0.42
1:B:3551:ARG:HD2	1:B:3595:ARG:NH2	2.34	0.42
1:B:4935:ILE:HG12	1:C:4932:GLY:HA2	2.00	0.42
1:C:843:PRO:O	1:C:1197:PRO:HA	2.19	0.42
1:C:871:ILE:HG13	1:C:1052:TYR:CE2	2.54	0.42
1:D:871:ILE:HG13	1:D:1052:TYR:CE2	2.54	0.42
1:D:4730:PHE:CB	1:D:4735:ILE:HD11	2.49	0.42
1:A:871:ILE:HG13	1:A:1052:TYR:CE2	2.54	0.42
1:A:910:ASN:O	1:A:914:LEU:N	2.52	0.42
1:B:461:GLN:HB2	1:B:464:GLU:OE1	2.19	0.42
1:B:864:LEU:HD12	1:B:864:LEU:O	2.19	0.42
1:B:2124:LEU:O	1:B:2128:GLN:HG2	2.20	0.42
1:B:4090:LEU:HD22	1:B:4125:MET:HB3	2.00	0.42
1:C:910:ASN:O	1:C:914:LEU:N	2.52	0.42
1:C:2265:GLY:O	1:C:2266:LEU:HB3	2.20	0.42
1:D:2265:GLY:O	1:D:2266:LEU:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3228:ARG:O	1:A:3228:ARG:HG2	2.19	0.42
1:B:1266:ASP:OD1	1:B:1267:THR:HG23	2.19	0.42
1:B:1713:TYR:OH	1:B:1816:MET:SD	2.77	0.42
1:B:3088:ILE:HD12	1:B:3088:ILE:H	1.85	0.42
1:C:397:GLU:OE2	1:C:471:SER:OG	2.29	0.42
1:C:1038:ASP:O	1:C:1042:GLN:HG2	2.19	0.42
1:C:4093:LYS:HB2	1:C:4093:LYS:HE2	1.30	0.42
1:D:3551:ARG:HD2	1:D:3595:ARG:NH2	2.34	0.42
1:D:3638:ARG:HH11	1:D:3640:THR:HG23	1.84	0.42
1:D:3974:GLY:N	1:D:3975:PRO:HA	2.34	0.42
1:A:914:LEU:HD12	1:A:915:PRO:HD2	1.99	0.42
1:A:2187:MET:HE2	1:A:2236:PHE:HA	2.01	0.42
1:A:2266:LEU:HD13	1:A:2331:ARG:HE	1.83	0.42
1:A:3088:ILE:H	1:A:3088:ILE:HD12	1.85	0.42
1:A:3428:PRO:HG2	1:A:3583:ARG:HD3	2.02	0.42
1:A:4902:PRO:HB3	1:A:4911:ARG:HG2	2.01	0.42
1:B:3282:LEU:HB2	1:B:3283:PRO:HD3	2.01	0.42
1:C:914:LEU:HD12	1:C:915:PRO:HD2	1.99	0.42
1:C:2266:LEU:HD13	1:C:2331:ARG:HE	1.83	0.42
1:C:2432:ASP:OD2	1:C:2436:ARG:NE	2.50	0.42
1:C:2515:ASN:OD1	1:C:2517:ASP:N	2.45	0.42
1:C:4072:LYS:HE3	1:C:4136:GLN:HG3	2.02	0.42
1:A:422:PHE:O	1:A:423:SER:C	2.62	0.42
1:A:1793:ALA:C	1:A:1794:THR:HG1	2.16	0.42
1:A:4685:TYR:HE2	1:A:4701:ARG:HG2	1.84	0.42
1:A:4730:PHE:CB	1:A:4735:ILE:HD11	2.49	0.42
1:A:4910:TYR:OH	1:C:4318:ARG:NH1	2.51	0.42
1:B:1038:ASP:O	1:B:1042:GLN:HG2	2.19	0.42
1:B:1437:SER:OG	1:B:1566:GLU:HB2	2.20	0.42
1:B:2866:VAL:O	1:B:2929:LYS:NZ	2.40	0.42
1:B:3228:ARG:HG2	1:B:3228:ARG:O	2.19	0.42
1:B:3428:PRO:HG2	1:B:3583:ARG:HD3	2.02	0.42
1:C:2124:LEU:O	1:C:2128:GLN:HG2	2.20	0.42
1:C:2627:LEU:HD22	1:C:2641:PRO:HB3	2.00	0.42
1:C:3037:LYS:O	1:C:3040:ILE:HG22	2.19	0.42
1:C:3551:ARG:HD2	1:C:3595:ARG:NH2	2.34	0.42
1:C:3974:GLY:N	1:C:3975:PRO:HA	2.34	0.42
1:D:461:GLN:HB2	1:D:464:GLU:OE1	2.19	0.42
1:D:4173:ILE:HD12	1:D:4173:ILE:H	1.85	0.42
1:D:4736:ALA:HB2	1:D:4743:LEU:CD1	2.50	0.42
1:A:2152:ASP:HB3	1:A:2191:VAL:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3037:LYS:O	1:A:3040:ILE:HG22	2.19	0.42
2:E:89:PRO:O	2:E:91:ILE:HD12	2.20	0.42
2:H:89:PRO:O	2:H:91:ILE:HD12	2.20	0.42
1:B:2810:ILE:H	1:B:2810:ILE:HD12	1.85	0.42
1:C:1420:ASP:O	1:C:1422:ARG:HD3	2.19	0.42
1:C:4675:LEU:HD23	1:C:4709:PHE:CE1	2.55	0.42
1:D:871:ILE:O	1:D:872:ARG:C	2.62	0.42
1:D:2152:ASP:HB3	1:D:2191:VAL:HG23	2.02	0.42
1:D:2810:ILE:HD12	1:D:2810:ILE:H	1.85	0.42
1:A:670:ASP:OD2	1:A:789:LYS:NZ	2.33	0.42
1:A:1437:SER:OG	1:A:1566:GLU:HB2	2.20	0.42
1:A:2124:LEU:O	1:A:2128:GLN:HG2	2.20	0.42
1:A:2234:CYS:SG	1:A:2271:SER:HB3	2.59	0.42
1:A:2759:PHE:HD1	1:A:2930:PHE:CG	2.36	0.42
1:A:2810:ILE:H	1:A:2810:ILE:HD12	1.85	0.42
1:A:4736:ALA:HB2	1:A:4743:LEU:CD1	2.50	0.42
2:H:12:ASP:OD2	2:H:12:ASP:C	2.63	0.42
1:B:627:LEU:N	1:B:628:PRO:HD2	2.34	0.42
1:B:871:ILE:O	1:B:872:ARG:C	2.62	0.42
1:B:4009:ASP:OD1	1:B:4010:SER:N	2.51	0.42
1:B:4072:LYS:HE3	1:B:4136:GLN:HG3	2.02	0.42
1:C:753:VAL:HB	1:C:754:PRO:C	2.45	0.42
1:C:1266:ASP:OD1	1:C:1267:THR:HG23	2.19	0.42
1:C:2810:ILE:H	1:C:2810:ILE:HD12	1.85	0.42
1:C:3253:GLU:O	1:C:3257:LEU:HD23	2.19	0.42
1:C:3428:PRO:HG2	1:C:3583:ARG:HD3	2.02	0.42
1:C:4090:LEU:HD22	1:C:4125:MET:HB3	2.00	0.42
1:D:753:VAL:HB	1:D:754:PRO:C	2.45	0.42
1:D:3282:LEU:HB2	1:D:3283:PRO:HD3	2.01	0.42
1:D:4107:THR:HG22	1:D:4108:GLY:N	2.33	0.42
1:A:103:LEU:HD12	1:A:161:GLY:O	2.20	0.42
1:A:461:GLN:HB2	1:A:464:GLU:OE1	2.19	0.42
1:A:951:LEU:HD11	1:A:1049:GLY:O	2.18	0.42
1:A:2265:GLY:O	1:A:2266:LEU:HB3	2.20	0.42
1:A:3195:LEU:HD12	1:A:3195:LEU:HA	1.93	0.42
1:A:3559:ASN:O	1:A:3560:LEU:HB2	2.20	0.42
1:B:103:LEU:HD12	1:B:161:GLY:O	2.20	0.42
1:B:871:ILE:HG13	1:B:1052:TYR:CE2	2.54	0.42
1:B:1758:GLY:O	1:B:1759:PRO:C	2.63	0.42
1:B:2627:LEU:HD22	1:B:2641:PRO:HB3	2.00	0.42
1:B:3227:GLU:C	1:B:3229:ALA:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3559:ASN:O	1:B:3560:LEU:HB2	2.20	0.42
1:C:1758:GLY:O	1:C:1759:PRO:C	2.63	0.42
1:C:2481:GLY:O	1:C:2485:ALA:N	2.51	0.42
1:D:916:GLU:O	1:D:919:ARG:HG2	2.19	0.42
1:D:2872:LEU:HD11	1:D:2940:ARG:NH1	2.35	0.42
1:D:4902:PRO:HB3	1:D:4911:ARG:HG2	2.01	0.42
1:A:554:ARG:NE	1:A:556:GLU:OE2	2.51	0.42
1:A:2752:LEU:HD23	1:A:2752:LEU:HA	1.93	0.42
1:A:3974:GLY:N	1:A:3975:PRO:HA	2.34	0.42
1:B:2438:ALA:HB2	1:B:2510:VAL:HG22	2.01	0.42
1:C:627:LEU:N	1:C:628:PRO:HD2	2.34	0.42
1:C:858:ASP:OD1	1:C:859:THR:N	2.52	0.42
1:C:3176:LEU:HD21	1:C:3184:VAL:HG13	2.02	0.42
1:D:1423:ASP:OD1	1:D:1569:LYS:NZ	2.40	0.42
1:D:2948:ASP:O	1:D:2949:THR:C	2.63	0.42
1:D:3088:ILE:H	1:D:3088:ILE:HD12	1.85	0.42
1:D:3428:PRO:HG2	1:D:3583:ARG:HD3	2.02	0.42
1:D:3559:ASN:O	1:D:3560:LEU:HB2	2.20	0.42
1:D:4072:LYS:HE3	1:D:4136:GLN:HG3	2.02	0.42
1:A:2814:LEU:HD23	1:A:2814:LEU:O	2.20	0.42
1:A:2925:GLN:O	1:A:2929:LYS:HG3	2.20	0.42
1:B:2925:GLN:O	1:B:2929:LYS:HG3	2.20	0.42
1:B:4685:TYR:HE2	1:B:4701:ARG:HG2	1.84	0.42
1:B:4736:ALA:HB2	1:B:4743:LEU:CD1	2.50	0.42
1:C:2925:GLN:O	1:C:2929:LYS:HG3	2.20	0.42
1:C:4736:ALA:HB2	1:C:4743:LEU:CD1	2.50	0.42
1:D:103:LEU:HD12	1:D:161:GLY:O	2.20	0.42
1:D:910:ASN:O	1:D:914:LEU:N	2.52	0.42
1:D:2183:ILE:HG23	1:D:2236:PHE:HB2	2.02	0.42
1:D:2234:CYS:C	1:D:2236:PHE:N	2.78	0.42
1:A:2872:LEU:HD11	1:A:2940:ARG:NH1	2.35	0.41
1:A:3548:GLU:OE1	1:A:3551:ARG:NH2	2.40	0.41
1:A:4094:LYS:HA	1:A:4094:LYS:HD2	1.35	0.41
2:F:8:ILE:HA	1:B:720:LEU:HD11	2.02	0.41
2:F:89:PRO:O	2:F:91:ILE:HD12	2.20	0.41
1:B:2183:ILE:HG23	1:B:2236:PHE:HB2	2.02	0.41
1:B:3176:LEU:HD21	1:B:3184:VAL:HG13	2.02	0.41
1:C:3457:GLN:O	1:C:3460:VAL:HG12	2.20	0.41
1:D:627:LEU:N	1:D:628:PRO:HD2	2.34	0.41
1:D:1266:ASP:OD1	1:D:1267:THR:HG23	2.19	0.41
1:A:627:LEU:N	1:A:628:PRO:HD2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1266:ASP:OD1	1:A:1267:THR:HG23	2.19	0.41
1:A:3253:GLU:O	1:A:3257:LEU:HD23	2.19	0.41
1:A:4093:LYS:HB2	1:A:4093:LYS:HE2	1.30	0.41
2:G:89:PRO:O	2:G:91:ILE:HD12	2.20	0.41
1:B:882:LEU:HD21	1:B:1042:GLN:HG3	2.03	0.41
1:B:3457:GLN:O	1:B:3460:VAL:HG12	2.20	0.41
1:C:103:LEU:HD12	1:C:161:GLY:O	2.20	0.41
1:C:938:CYS:SG	1:C:1054:ILE:HG23	2.60	0.41
1:C:2268:MET:CE	1:C:2272:THR:HG22	2.50	0.41
1:C:3088:ILE:H	1:C:3088:ILE:HD12	1.85	0.41
1:D:2438:ALA:HB2	1:D:2510:VAL:HG22	2.01	0.41
1:D:2581:ASP:OD2	1:D:2581:ASP:C	2.63	0.41
1:D:3176:LEU:HD21	1:D:3184:VAL:HG13	2.02	0.41
1:D:4074:ILE:HD12	1:D:4103:GLN:HE21	1.86	0.41
1:D:4323:ARG:O	1:D:4327:THR:HG23	2.21	0.41
1:A:47:LEU:HD12	1:A:126:ARG:HH12	1.84	0.41
1:B:916:GLU:O	1:B:919:ARG:HG2	2.19	0.41
1:B:2265:GLY:O	1:B:2266:LEU:HB3	2.20	0.41
1:B:2268:MET:CE	1:B:2272:THR:HG22	2.50	0.41
1:B:2948:ASP:O	1:B:2949:THR:C	2.63	0.41
1:B:4063:LYS:O	1:B:4067:MET:HG3	2.20	0.41
1:C:1964:GLU:HA	1:C:3651:CYS:SG	2.61	0.41
1:C:2152:ASP:HB3	1:C:2191:VAL:HG23	2.02	0.41
1:C:4323:ARG:O	1:C:4327:THR:HG23	2.21	0.41
1:C:4332:LEU:HD12	1:C:4332:LEU:C	2.46	0.41
1:D:883:TRP:O	1:D:887:ARG:HG2	2.20	0.41
1:D:4063:LYS:O	1:D:4067:MET:HG3	2.20	0.41
1:A:938:CYS:SG	1:A:1054:ILE:HG23	2.60	0.41
1:A:2179:MET:HE3	1:A:2183:ILE:HD11	2.02	0.41
1:A:2581:ASP:OD2	1:A:2585:HIS:ND1	2.54	0.41
1:A:3294:PRO:CB	1:A:3297:LEU:HD22	2.50	0.41
1:A:4063:LYS:O	1:A:4067:MET:HG3	2.20	0.41
1:A:4072:LYS:HE3	1:A:4136:GLN:HG3	2.02	0.41
1:B:753:VAL:HB	1:B:754:PRO:C	2.45	0.41
1:B:2814:LEU:O	1:B:2814:LEU:HD23	2.20	0.41
1:B:3037:LYS:O	1:B:3040:ILE:HG22	2.19	0.41
1:B:3294:PRO:CB	1:B:3297:LEU:HD22	2.50	0.41
1:B:4173:ILE:H	1:B:4173:ILE:HD12	1.85	0.41
1:C:2581:ASP:OD2	1:C:2585:HIS:ND1	2.54	0.41
1:C:3282:LEU:HB2	1:C:3283:PRO:HD3	2.01	0.41
1:C:3541:TYR:OH	1:C:3598:GLN:NE2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4173:ILE:H	1:C:4173:ILE:HD12	1.85	0.41
1:D:938:CYS:SG	1:D:1054:ILE:HG23	2.60	0.41
1:D:1964:GLU:HA	1:D:3651:CYS:SG	2.61	0.41
1:D:4009:ASP:OD1	1:D:4010:SER:N	2.51	0.41
1:A:3377:GLU:O	1:A:3381:ARG:HG2	2.21	0.41
1:A:4173:ILE:H	1:A:4173:ILE:HD12	1.85	0.41
2:H:8:ILE:HA	1:D:720:LEU:HD11	2.03	0.41
1:B:938:CYS:SG	1:B:1054:ILE:HG23	2.60	0.41
1:B:3974:GLY:N	1:B:3975:PRO:HA	2.34	0.41
1:B:4675:LEU:HD23	1:B:4709:PHE:CE1	2.55	0.41
1:C:883:TRP:O	1:C:887:ARG:HG2	2.20	0.41
1:D:892:TRP:HA	1:D:903:ARG:HB3	2.03	0.41
1:D:1437:SER:OG	1:D:1566:GLU:HB2	2.20	0.41
1:D:1750:PRO:O	1:D:1752:GLY:N	2.54	0.41
1:D:2179:MET:HE3	1:D:2183:ILE:HD11	2.02	0.41
1:D:4093:LYS:HE2	1:D:4093:LYS:HB2	1.30	0.41
1:D:4332:LEU:HD12	1:D:4332:LEU:C	2.46	0.41
1:A:3176:LEU:HD21	1:A:3184:VAL:HG13	2.02	0.41
1:B:365:PRO:O	1:B:366:LYS:HB3	2.21	0.41
1:B:546:ASP:OD1	1:B:583:HIS:NE2	2.38	0.41
1:B:554:ARG:NH2	1:B:556:GLU:OE2	2.51	0.41
1:B:1964:GLU:HA	1:B:3651:CYS:SG	2.61	0.41
1:B:2000:ARG:HG2	1:B:3639:MET:HE1	2.03	0.41
1:B:2581:ASP:OD2	1:B:2585:HIS:ND1	2.54	0.41
1:B:2872:LEU:HD11	1:B:2940:ARG:NH1	2.35	0.41
1:B:4074:ILE:HD12	1:B:4103:GLN:HE21	1.86	0.41
1:B:4332:LEU:C	1:B:4332:LEU:HD12	2.46	0.41
1:C:422:PHE:O	1:C:423:SER:C	2.62	0.41
1:C:1437:SER:OG	1:C:1566:GLU:HB2	2.20	0.41
1:C:3294:PRO:CB	1:C:3297:LEU:HD22	2.50	0.41
1:C:4700:ASP:C	1:C:4702:LEU:N	2.76	0.41
1:D:2814:LEU:O	1:D:2814:LEU:HD23	2.20	0.41
1:D:3294:PRO:HB2	1:D:3297:LEU:HD13	2.03	0.41
1:A:753:VAL:HB	1:A:754:PRO:C	2.45	0.41
1:A:883:TRP:O	1:A:887:ARG:HG2	2.20	0.41
1:A:2183:ILE:HG23	1:A:2236:PHE:HB2	2.02	0.41
1:A:3077:ASP:O	1:A:3081:VAL:HG23	2.21	0.41
1:A:4323:ARG:O	1:A:4327:THR:HG23	2.21	0.41
1:B:2187:MET:HE2	1:B:2236:PHE:HA	2.01	0.41
1:B:2563:ILE:HG22	1:B:2611:LEU:HD21	2.03	0.41
1:C:36:LEU:HD11	1:C:190:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:892:TRP:HA	1:C:903:ARG:HB3	2.03	0.41
1:C:2183:ILE:HG23	1:C:2236:PHE:HB2	2.02	0.41
1:C:4094:LYS:HD2	1:C:4094:LYS:HA	1.36	0.41
1:D:2213:VAL:HG21	1:D:2257:TYR:HE2	1.82	0.41
1:D:2581:ASP:OD2	1:D:2585:HIS:ND1	2.54	0.41
1:D:3077:ASP:O	1:D:3081:VAL:HG23	2.21	0.41
1:D:3170:LEU:CD1	1:D:3195:LEU:HD11	2.40	0.41
1:D:3227:GLU:C	1:D:3229:ALA:H	2.28	0.41
1:A:882:LEU:HD21	1:A:1042:GLN:HG3	2.03	0.41
1:A:1830:ASP:N	1:A:1830:ASP:OD1	2.54	0.41
1:A:1964:GLU:HA	1:A:3651:CYS:SG	2.61	0.41
1:A:2213:VAL:HG21	1:A:2257:TYR:HE2	1.82	0.41
1:A:4332:LEU:HD12	1:A:4332:LEU:C	2.46	0.41
1:B:623:THR:HG23	1:B:627:LEU:HD12	2.03	0.41
1:B:892:TRP:HA	1:B:903:ARG:HB3	2.03	0.41
1:B:2152:ASP:HB3	1:B:2191:VAL:HG23	2.02	0.41
1:B:3377:GLU:O	1:B:3381:ARG:HG2	2.21	0.41
1:C:365:PRO:O	1:C:366:LYS:HB3	2.21	0.41
1:C:623:THR:HG23	1:C:627:LEU:HD12	2.03	0.41
1:C:2563:ILE:HG22	1:C:2611:LEU:HD21	2.03	0.41
1:C:3250:LEU:HD23	1:C:3278:LEU:HD21	2.03	0.41
1:C:4009:ASP:OD1	1:C:4010:SER:N	2.51	0.41
1:C:4074:ILE:HD12	1:C:4103:GLN:HE21	1.86	0.41
1:D:2124:LEU:O	1:D:2128:GLN:HG2	2.20	0.41
1:D:3250:LEU:HD23	1:D:3278:LEU:HD21	2.03	0.41
1:D:3253:GLU:O	1:D:3257:LEU:HD23	2.19	0.41
1:D:3377:GLU:O	1:D:3381:ARG:HG2	2.21	0.41
1:D:4707:PRO:HD2	1:D:4770:ASP:OD2	2.21	0.41
1:A:1043:ALA:O	1:A:1047:LEU:HD23	2.21	0.41
1:A:2000:ARG:HG2	1:A:3639:MET:HE1	2.03	0.41
1:A:2337:ARG:HG2	1:A:2436:ARG:HD2	2.03	0.41
1:A:2563:ILE:HG22	1:A:2611:LEU:HD21	2.03	0.41
1:A:3208:GLU:OE2	1:A:3307:ALA:N	2.49	0.41
1:A:3534:ILE:HG13	1:A:3597:VAL:HG13	2.02	0.41
1:A:4707:PRO:HD2	1:A:4770:ASP:OD2	2.21	0.41
1:B:1830:ASP:N	1:B:1830:ASP:OD1	2.54	0.41
1:B:2179:MET:HE3	1:B:2183:ILE:HD11	2.02	0.41
1:B:3124:LYS:HG3	1:B:3125:GLY:H	1.86	0.41
1:B:4707:PRO:HD2	1:B:4770:ASP:OD2	2.21	0.41
1:B:4763:LEU:O	1:B:4767:MET:CE	2.69	0.41
1:C:2234:CYS:C	1:C:2236:PHE:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2581:ASP:OD2	1:C:2581:ASP:C	2.63	0.41
1:C:2814:LEU:HD23	1:C:2814:LEU:O	2.20	0.41
1:C:2872:LEU:HD11	1:C:2940:ARG:NH1	2.35	0.41
1:C:3227:GLU:C	1:C:3229:ALA:H	2.28	0.41
1:C:3534:ILE:HG13	1:C:3597:VAL:HG13	2.02	0.41
1:D:1758:GLY:O	1:D:1759:PRO:C	2.63	0.41
1:D:2000:ARG:HG2	1:D:3639:MET:HE1	2.03	0.41
1:D:2268:MET:CE	1:D:2272:THR:HG22	2.50	0.41
1:D:2337:ARG:HG2	1:D:2436:ARG:HD2	2.03	0.41
1:D:3124:LYS:HG3	1:D:3125:GLY:H	1.86	0.41
1:D:4675:LEU:HD23	1:D:4709:PHE:CE1	2.55	0.41
1:D:4763:LEU:O	1:D:4767:MET:CE	2.69	0.41
1:A:365:PRO:O	1:A:366:LYS:HB3	2.21	0.41
1:A:2748:ILE:O	1:A:2748:ILE:HG23	2.21	0.41
1:A:2948:ASP:O	1:A:2949:THR:C	2.63	0.41
1:A:3536:LEU:O	1:A:3540:ARG:HG2	2.21	0.41
2:G:12:ASP:OD1	2:G:12:ASP:C	2.64	0.41
1:B:923:LEU:O	1:B:926:SER:OG	2.34	0.41
1:B:2234:CYS:HB3	1:B:2238:CYS:HB3	1.88	0.41
1:B:3230:ILE:HD12	1:B:3230:ILE:H	1.86	0.41
1:C:2000:ARG:HG2	1:C:3639:MET:HE1	2.03	0.41
1:C:3077:ASP:O	1:C:3081:VAL:HG23	2.21	0.41
1:C:4576:LEU:HD23	1:C:4576:LEU:HA	1.74	0.41
1:D:2563:ILE:HG22	1:D:2611:LEU:HD21	2.03	0.41
1:A:546:ASP:OD1	1:A:583:HIS:NE2	2.38	0.40
1:A:720:LEU:HD11	2:E:8:ILE:HA	2.03	0.40
1:A:1750:PRO:O	1:A:1752:GLY:N	2.54	0.40
1:A:2581:ASP:OD2	1:A:2581:ASP:C	2.63	0.40
1:A:2869:SER:O	1:A:2870:ARG:C	2.64	0.40
1:A:3282:LEU:HB2	1:A:3283:PRO:HD3	2.01	0.40
1:A:3294:PRO:HB2	1:A:3297:LEU:HD13	2.03	0.40
1:A:4675:LEU:HD23	1:A:4709:PHE:CE1	2.55	0.40
1:A:4728:ASP:HB3	1:D:4104:LYS:HG2	2.03	0.40
1:A:4763:LEU:O	1:A:4767:MET:CE	2.69	0.40
1:B:863:VAL:O	1:B:863:VAL:HG13	2.21	0.40
1:B:883:TRP:O	1:B:887:ARG:HG2	2.20	0.40
1:B:2869:SER:O	1:B:2870:ARG:C	2.64	0.40
1:B:3534:ILE:HG13	1:B:3597:VAL:HG13	2.02	0.40
1:B:3536:LEU:O	1:B:3540:ARG:HG2	2.21	0.40
1:B:4323:ARG:O	1:B:4327:THR:HG23	2.21	0.40
1:C:55:ASN:OD1	1:C:58:ASN:ND2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:882:LEU:HD21	1:C:1042:GLN:HG3	2.03	0.40
1:C:2948:ASP:O	1:C:2949:THR:C	2.63	0.40
1:D:684:ARG:NH1	1:D:708:VAL:O	2.48	0.40
1:D:2925:GLN:O	1:D:2929:LYS:HG3	2.20	0.40
1:D:3536:LEU:O	1:D:3540:ARG:HG2	2.21	0.40
1:B:55:ASN:OD1	1:B:58:ASN:ND2	2.54	0.40
1:B:1750:PRO:HA	1:B:1751:PRO:HD3	1.99	0.40
1:B:3730:MET:O	1:B:3733:SER:OG	2.30	0.40
1:C:2179:MET:HE3	1:C:2183:ILE:HD11	2.02	0.40
1:C:3124:LYS:HG3	1:C:3125:GLY:H	1.86	0.40
1:C:4744:ALA:O	1:C:4748:ILE:HG22	2.21	0.40
1:D:3457:GLN:O	1:D:3460:VAL:HG12	2.20	0.40
1:D:4538:PHE:O	1:D:4542:LEU:HD23	2.21	0.40
1:D:4685:TYR:HE2	1:D:4701:ARG:HG2	1.84	0.40
1:A:55:ASN:OD1	1:A:58:ASN:ND2	2.54	0.40
1:A:1041:CYS:HA	1:A:1044:VAL:HG12	2.03	0.40
1:A:2701:MET:HB3	1:A:2702:PRO:HD3	2.04	0.40
1:A:2738:PRO:HB2	1:A:2885:ASN:HA	2.04	0.40
1:A:2865:VAL:HG13	1:A:2866:VAL:N	2.37	0.40
2:F:12:ASP:OD2	2:F:12:ASP:C	2.64	0.40
1:B:1043:ALA:O	1:B:1047:LEU:HD23	2.21	0.40
1:B:2978:LEU:O	1:B:2982:VAL:HG23	2.21	0.40
1:C:1750:PRO:O	1:C:1752:GLY:N	2.54	0.40
1:C:2473:LEU:O	1:C:2500:LYS:NZ	2.54	0.40
1:C:2869:SER:O	1:C:2870:ARG:C	2.64	0.40
1:C:4685:TYR:HE2	1:C:4701:ARG:HG2	1.84	0.40
1:D:36:LEU:HD11	1:D:190:LEU:HD13	2.03	0.40
1:D:55:ASN:OD1	1:D:58:ASN:ND2	2.54	0.40
1:D:775:ASP:OD1	1:D:775:ASP:N	2.53	0.40
1:D:3037:LYS:O	1:D:3040:ILE:HG22	2.19	0.40
1:D:4016:LEU:HD23	1:D:4135:PHE:CE1	2.57	0.40
1:A:892:TRP:HA	1:A:903:ARG:HB3	2.03	0.40
1:A:1064:VAL:O	1:A:1065:ASP:C	2.65	0.40
1:A:2268:MET:CE	1:A:2272:THR:HG22	2.50	0.40
1:A:2625:ARG:CD	1:A:2907:VAL:HG11	2.52	0.40
1:A:2997:LYS:HA	1:A:2997:LYS:HD2	1.95	0.40
1:A:4744:ALA:O	1:A:4748:ILE:HG22	2.21	0.40
2:F:5:VAL:HG22	2:F:75:LEU:HD22	2.03	0.40
1:B:2701:MET:HB3	1:B:2702:PRO:HD3	2.04	0.40
1:B:3077:ASP:O	1:B:3081:VAL:HG23	2.21	0.40
1:B:3158:ILE:O	1:B:3159:LEU:HD12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4016:LEU:HD23	1:B:4135:PHE:CE1	2.57	0.40
1:B:4538:PHE:O	1:B:4542:LEU:HD23	2.21	0.40
1:C:218:GLY:N	1:C:263:LEU:O	2.50	0.40
1:C:1713:TYR:OH	1:C:1816:MET:SD	2.77	0.40
1:C:3373:VAL:HG12	1:C:3399:PHE:CE2	2.57	0.40
1:C:3559:ASN:O	1:C:3560:LEU:HB2	2.20	0.40
1:C:4063:LYS:O	1:C:4067:MET:HG3	2.20	0.40
1:C:4538:PHE:O	1:C:4542:LEU:HD23	2.21	0.40
1:D:2473:LEU:O	1:D:2500:LYS:NZ	2.54	0.40
1:D:3837:ALA:O	1:D:3841:THR:HG23	2.22	0.40
1:D:4006:LEU:HA	1:D:4012:GLN:HE21	1.87	0.40
1:A:2892:LYS:O	1:A:2895:LEU:N	2.55	0.40
1:A:3158:ILE:O	1:A:3159:LEU:HD12	2.21	0.40
1:A:3250:LEU:HD23	1:A:3278:LEU:HD21	2.03	0.40
1:A:4538:PHE:O	1:A:4542:LEU:HD23	2.21	0.40
1:B:1064:VAL:O	1:B:1065:ASP:C	2.65	0.40
1:C:308:ALA:HB1	1:C:313:THR:HG21	2.04	0.40
1:C:1928:LEU:O	1:C:2105:ARG:NH2	2.55	0.40
1:C:3158:ILE:O	1:C:3159:LEU:HD12	2.21	0.40
1:C:4006:LEU:HA	1:C:4012:GLN:HE21	1.87	0.40
1:D:2738:PRO:HB2	1:D:2885:ASN:HA	2.04	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	4368/5035 (87%)	4233 (97%)	135 (3%)	0	100	100
1	B	4368/5035 (87%)	4233 (97%)	135 (3%)	0	100	100
1	C	4368/5035 (87%)	4233 (97%)	135 (3%)	0	100	100
1	D	4368/5035 (87%)	4234 (97%)	134 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	F	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	G	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
All	All	17892/20572 (87%)	17337 (97%)	555 (3%)	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	3823/4296 (89%)	3801 (99%)	22 (1%)	84	94
1	B	3823/4296 (89%)	3801 (99%)	22 (1%)	84	94
1	C	3823/4296 (89%)	3801 (99%)	22 (1%)	84	94
1	D	3823/4296 (89%)	3801 (99%)	22 (1%)	84	94
2	E	89/90 (99%)	89 (100%)	0	100	100
2	F	89/90 (99%)	89 (100%)	0	100	100
2	G	89/90 (99%)	89 (100%)	0	100	100
2	H	89/90 (99%)	89 (100%)	0	100	100
All	All	15648/17544 (89%)	15560 (99%)	88 (1%)	82	94

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4082	ASP
1	A	4083	TYR
1	A	4090	LEU
1	A	4092	SER
1	A	4093	LYS
1	A	4094	LYS

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Mol	Chain	Res	Type
1	A	4097	GLN
1	A	4098	LYS
1	A	4100	MET
1	A	4129	GLU
1	A	4319	ARG
1	A	4320	LEU
1	A	4323	ARG
1	A	4332	LEU
1	A	4333	LEU
1	A	4576	LEU
1	A	4702	LEU
1	A	4706	THR
1	A	4718	VAL
1	A	4720	ARG
1	A	4771	VAL
1	A	4772	LYS
1	B	4082	ASP
1	B	4083	TYR
1	B	4090	LEU
1	B	4092	SER
1	B	4093	LYS
1	B	4094	LYS
1	B	4097	GLN
1	B	4098	LYS
1	B	4100	MET
1	B	4129	GLU
1	B	4319	ARG
1	B	4320	LEU
1	B	4323	ARG
1	B	4332	LEU
1	B	4333	LEU
1	B	4576	LEU
1	B	4702	LEU
1	B	4706	THR
1	B	4718	VAL
1	B	4720	ARG
1	B	4771	VAL
1	B	4772	LYS
1	C	4082	ASP
1	C	4083	TYR
1	C	4090	LEU
1	C	4092	SER

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Mol	Chain	Res	Type
1	C	4093	LYS
1	C	4094	LYS
1	C	4097	GLN
1	C	4098	LYS
1	C	4100	MET
1	C	4129	GLU
1	C	4319	ARG
1	C	4320	LEU
1	C	4323	ARG
1	C	4332	LEU
1	C	4333	LEU
1	C	4576	LEU
1	C	4702	LEU
1	C	4706	THR
1	C	4718	VAL
1	C	4720	ARG
1	C	4771	VAL
1	C	4772	LYS
1	D	4082	ASP
1	D	4083	TYR
1	D	4090	LEU
1	D	4092	SER
1	D	4093	LYS
1	D	4094	LYS
1	D	4097	GLN
1	D	4098	LYS
1	D	4100	MET
1	D	4129	GLU
1	D	4319	ARG
1	D	4320	LEU
1	D	4323	ARG
1	D	4332	LEU
1	D	4333	LEU
1	D	4576	LEU
1	D	4702	LEU
1	D	4706	THR
1	D	4718	VAL
1	D	4720	ARG
1	D	4771	VAL
1	D	4772	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (169) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	57	GLN
1	A	58	ASN
1	A	106	HIS
1	A	242	GLN
1	A	413	ASN
1	A	462	HIS
1	A	534	ASN
1	A	766	GLN
1	A	924	GLN
1	A	1004	GLN
1	A	1126	ASN
1	A	1232	GLN
1	A	1461	HIS
1	A	1546	ASN
1	A	1587	ASN
1	A	1591	GLN
1	A	1939	GLN
1	A	1973	ASN
1	A	2030	GLN
1	A	2101	HIS
1	A	2128	GLN
1	A	2162	GLN
1	A	2188	ASN
1	A	2418	HIS
1	A	2488	GLN
1	A	2689	HIS
1	A	2878	GLN
1	A	2977	HIS
1	A	2992	HIS
1	A	3009	GLN
1	A	3555	GLN
1	A	3598	GLN
1	A	3609	GLN
1	A	3817	GLN
1	A	3917	ASN
1	A	4103	GLN
1	A	4159	HIS
1	A	4204	ASN
1	A	4219	GLN
1	A	4774	GLN
1	A	4855	ASN
1	A	4945	GLN

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Mol	Chain	Res	Type
2	E	26	HIS
2	G	26	HIS
2	H	26	HIS
1	B	57	GLN
1	B	106	HIS
1	B	242	GLN
1	B	413	ASN
1	B	462	HIS
1	B	534	ASN
1	B	766	GLN
1	B	924	GLN
1	B	1004	GLN
1	B	1085	GLN
1	B	1126	ASN
1	B	1232	GLN
1	B	1546	ASN
1	B	1591	GLN
1	B	1632	GLN
1	B	1939	GLN
1	B	1973	ASN
1	B	2030	GLN
1	B	2128	GLN
1	B	2162	GLN
1	B	2188	ASN
1	B	2488	GLN
1	B	2689	HIS
1	B	2789	HIS
1	B	2878	GLN
1	B	2977	HIS
1	B	2992	HIS
1	B	3009	GLN
1	B	3555	GLN
1	B	3598	GLN
1	B	3609	GLN
1	B	3817	GLN
1	B	3917	ASN
1	B	4097	GLN
1	B	4103	GLN
1	B	4159	HIS
1	B	4204	ASN
1	B	4219	GLN
1	B	4774	GLN

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Mol	Chain	Res	Type
1	B	4855	ASN
1	B	4945	GLN
1	C	57	GLN
1	C	106	HIS
1	C	242	GLN
1	C	413	ASN
1	C	462	HIS
1	C	534	ASN
1	C	766	GLN
1	C	924	GLN
1	C	1004	GLN
1	C	1085	GLN
1	C	1126	ASN
1	C	1232	GLN
1	C	1461	HIS
1	C	1546	ASN
1	C	1587	ASN
1	C	1591	GLN
1	C	1778	HIS
1	C	1939	GLN
1	C	1973	ASN
1	C	2030	GLN
1	C	2101	HIS
1	C	2162	GLN
1	C	2188	ASN
1	C	2488	GLN
1	C	2689	HIS
1	C	2789	HIS
1	C	2878	GLN
1	C	2977	HIS
1	C	2992	HIS
1	C	3009	GLN
1	C	3419	ASN
1	C	3555	GLN
1	C	3598	GLN
1	C	3609	GLN
1	C	3817	GLN
1	C	3917	ASN
1	C	3963	GLN
1	C	4103	GLN
1	C	4204	ASN
1	C	4219	GLN

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Mol	Chain	Res	Type
1	C	4945	GLN
1	D	57	GLN
1	D	106	HIS
1	D	242	GLN
1	D	413	ASN
1	D	462	HIS
1	D	534	ASN
1	D	766	GLN
1	D	924	GLN
1	D	1004	GLN
1	D	1085	GLN
1	D	1126	ASN
1	D	1232	GLN
1	D	1546	ASN
1	D	1587	ASN
1	D	1591	GLN
1	D	1939	GLN
1	D	1973	ASN
1	D	2030	GLN
1	D	2162	GLN
1	D	2188	ASN
1	D	2415	ASN
1	D	2488	GLN
1	D	2499	HIS
1	D	2689	HIS
1	D	2878	GLN
1	D	2977	HIS
1	D	2992	HIS
1	D	3009	GLN
1	D	3555	GLN
1	D	3598	GLN
1	D	3609	GLN
1	D	3817	GLN
1	D	3917	ASN
1	D	4097	GLN
1	D	4103	GLN
1	D	4159	HIS
1	D	4204	ASN
1	D	4219	GLN
1	D	4774	GLN
1	D	4855	ASN
1	D	4945	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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	A	8003	-	53,53,53	1.24	7 (13%)	59,61,61	1.03	3 (5%)
4	PCW	D	5101	-	53,53,53	1.24	7 (13%)	59,61,61	1.03	3 (5%)
4	PCW	B	8002	-	53,53,53	1.25	7 (13%)	59,61,61	1.04	3 (5%)
4	PCW	C	8003	-	53,53,53	1.24	7 (13%)	59,61,61	1.03	3 (5%)
4	PCW	B	8003	-	53,53,53	1.24	7 (13%)	59,61,61	1.03	3 (5%)
4	PCW	D	5103	-	53,53,53	1.25	7 (13%)	59,61,61	1.04	3 (5%)
4	PCW	A	8002	-	53,53,53	1.25	7 (13%)	59,61,61	1.04	3 (5%)
4	PCW	C	8002	-	53,53,53	1.25	7 (13%)	59,61,61	1.04	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCW	A	8003	-	-	25/57/57/57	-
4	PCW	D	5101	-	-	25/57/57/57	-
4	PCW	B	8002	-	-	33/57/57/57	-
4	PCW	C	8003	-	-	25/57/57/57	-
4	PCW	B	8003	-	-	25/57/57/57	-
4	PCW	D	5103	-	-	33/57/57/57	-
4	PCW	A	8002	-	-	33/57/57/57	-
4	PCW	C	8002	-	-	33/57/57/57	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	8003	PCW	O3-C11	3.02	1.42	1.33
4	C	8003	PCW	O3-C11	3.02	1.42	1.33
4	D	5101	PCW	O3-C11	3.02	1.42	1.33
4	A	8003	PCW	O3-C11	2.99	1.42	1.33
4	A	8002	PCW	O3-C11	2.96	1.42	1.33
4	B	8002	PCW	O3-C11	2.96	1.42	1.33
4	C	8002	PCW	O3-C11	2.96	1.42	1.33
4	D	5103	PCW	O3-C11	2.94	1.41	1.33
4	D	5103	PCW	O2-C31	2.88	1.42	1.34
4	A	8002	PCW	O2-C31	2.87	1.42	1.34
4	B	8002	PCW	O2-C31	2.87	1.42	1.34
4	C	8002	PCW	O2-C31	2.87	1.42	1.34
4	B	8003	PCW	O2-C31	2.80	1.42	1.34
4	A	8003	PCW	O2-C31	2.80	1.42	1.34
4	C	8003	PCW	O2-C31	2.80	1.42	1.34
4	D	5101	PCW	O2-C31	2.80	1.42	1.34
4	A	8002	PCW	P-O4P	2.62	1.69	1.59
4	B	8002	PCW	P-O4P	2.62	1.69	1.59
4	C	8002	PCW	P-O4P	2.62	1.69	1.59
4	D	5103	PCW	P-O4P	2.62	1.69	1.59
4	B	8003	PCW	P-O4P	2.58	1.69	1.59
4	C	8003	PCW	P-O4P	2.58	1.69	1.59
4	D	5101	PCW	P-O4P	2.58	1.69	1.59
4	A	8003	PCW	P-O4P	2.57	1.69	1.59
4	A	8003	PCW	O2-C2	-2.35	1.41	1.46
4	B	8003	PCW	O2-C2	-2.35	1.41	1.46
4	C	8003	PCW	O2-C2	-2.35	1.41	1.46
4	D	5101	PCW	O2-C2	-2.35	1.41	1.46
4	A	8002	PCW	O2-C2	-2.29	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	8002	PCW	O2-C2	-2.29	1.41	1.46
4	C	8002	PCW	O2-C2	-2.29	1.41	1.46
4	D	5103	PCW	O2-C2	-2.29	1.41	1.46
4	A	8002	PCW	C5-C4	2.29	1.58	1.51
4	B	8002	PCW	C5-C4	2.29	1.58	1.51
4	D	5103	PCW	C5-C4	2.29	1.58	1.51
4	C	8002	PCW	C5-C4	2.29	1.58	1.51
4	A	8003	PCW	C5-C4	2.26	1.58	1.51
4	B	8003	PCW	C5-C4	2.26	1.58	1.51
4	C	8003	PCW	C5-C4	2.26	1.58	1.51
4	D	5101	PCW	C5-C4	2.26	1.58	1.51
4	D	5103	PCW	P-O3P	2.22	1.68	1.59
4	A	8002	PCW	C32-C31	2.21	1.57	1.50
4	B	8002	PCW	C32-C31	2.21	1.57	1.50
4	C	8002	PCW	C32-C31	2.21	1.57	1.50
4	D	5103	PCW	C32-C31	2.21	1.57	1.50
4	A	8002	PCW	P-O3P	2.21	1.68	1.59
4	B	8002	PCW	P-O3P	2.21	1.68	1.59
4	C	8002	PCW	P-O3P	2.21	1.68	1.59
4	C	8003	PCW	P-O3P	2.20	1.68	1.59
4	A	8003	PCW	C32-C31	2.19	1.57	1.50
4	B	8003	PCW	C32-C31	2.19	1.57	1.50
4	C	8003	PCW	C32-C31	2.19	1.57	1.50
4	D	5101	PCW	C32-C31	2.19	1.57	1.50
4	A	8003	PCW	P-O3P	2.18	1.67	1.59
4	B	8003	PCW	P-O3P	2.18	1.67	1.59
4	D	5101	PCW	P-O3P	2.18	1.67	1.59

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	8002	PCW	C21-C20-C19	3.88	153.88	124.83
4	B	8002	PCW	C21-C20-C19	3.88	153.88	124.83
4	C	8002	PCW	C21-C20-C19	3.88	153.88	124.83
4	D	5103	PCW	C21-C20-C19	3.88	153.88	124.83
4	A	8003	PCW	C21-C20-C19	3.81	153.38	124.83
4	D	5101	PCW	C21-C20-C19	3.81	153.38	124.83
4	B	8003	PCW	C21-C20-C19	3.81	153.37	124.83
4	C	8003	PCW	C21-C20-C19	3.81	153.35	124.83
4	A	8002	PCW	O2-C31-C32	3.64	119.35	111.48
4	B	8002	PCW	O2-C31-C32	3.64	119.35	111.48
4	C	8002	PCW	O2-C31-C32	3.64	119.35	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	5103	PCW	O2-C31-C32	3.61	119.30	111.48
4	A	8003	PCW	O2-C31-C32	3.38	118.80	111.48
4	C	8003	PCW	O2-C31-C32	3.38	118.80	111.48
4	D	5101	PCW	O2-C31-C32	3.38	118.80	111.48
4	B	8003	PCW	O2-C31-C32	3.37	118.77	111.48
4	A	8003	PCW	O3-C11-C12	2.58	119.71	111.83
4	D	5103	PCW	O3-C11-C12	2.58	119.71	111.83
4	A	8002	PCW	O3-C11-C12	2.58	119.70	111.83
4	B	8002	PCW	O3-C11-C12	2.58	119.70	111.83
4	B	8003	PCW	O3-C11-C12	2.58	119.70	111.83
4	C	8003	PCW	O3-C11-C12	2.58	119.70	111.83
4	D	5101	PCW	O3-C11-C12	2.58	119.70	111.83
4	C	8002	PCW	O3-C11-C12	2.56	119.65	111.83

There are no chirality outliers.

All (232) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	8002	PCW	C32-C31-O2-C2
4	A	8002	PCW	C1-O3P-P-O1P
4	A	8002	PCW	C1-O3P-P-O2P
4	A	8002	PCW	C1-O3P-P-O4P
4	A	8002	PCW	C4-O4P-P-O1P
4	A	8002	PCW	C4-O4P-P-O3P
4	A	8003	PCW	O4P-C4-C5-N
4	A	8003	PCW	C32-C31-O2-C2
4	B	8002	PCW	C32-C31-O2-C2
4	B	8002	PCW	C1-O3P-P-O1P
4	B	8002	PCW	C1-O3P-P-O2P
4	B	8002	PCW	C1-O3P-P-O4P
4	B	8002	PCW	C4-O4P-P-O1P
4	B	8002	PCW	C4-O4P-P-O3P
4	B	8003	PCW	O4P-C4-C5-N
4	B	8003	PCW	C32-C31-O2-C2
4	C	8002	PCW	C32-C31-O2-C2
4	C	8002	PCW	C1-O3P-P-O1P
4	C	8002	PCW	C1-O3P-P-O2P
4	C	8002	PCW	C1-O3P-P-O4P
4	C	8002	PCW	C4-O4P-P-O1P
4	C	8002	PCW	C4-O4P-P-O3P
4	C	8003	PCW	O4P-C4-C5-N
4	C	8003	PCW	C32-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
4	D	5101	PCW	O4P-C4-C5-N
4	D	5101	PCW	C32-C31-O2-C2
4	D	5103	PCW	C32-C31-O2-C2
4	D	5103	PCW	C1-O3P-P-O1P
4	D	5103	PCW	C1-O3P-P-O2P
4	D	5103	PCW	C1-O3P-P-O4P
4	D	5103	PCW	C4-O4P-P-O1P
4	D	5103	PCW	C4-O4P-P-O3P
4	A	8002	PCW	O31-C31-O2-C2
4	A	8003	PCW	O31-C31-O2-C2
4	B	8002	PCW	O31-C31-O2-C2
4	B	8003	PCW	O31-C31-O2-C2
4	C	8002	PCW	O31-C31-O2-C2
4	C	8003	PCW	O31-C31-O2-C2
4	D	5101	PCW	O31-C31-O2-C2
4	D	5103	PCW	O31-C31-O2-C2
4	A	8002	PCW	C22-C23-C24-C25
4	B	8002	PCW	C22-C23-C24-C25
4	C	8002	PCW	C22-C23-C24-C25
4	D	5103	PCW	C22-C23-C24-C25
4	A	8002	PCW	C31-C32-C33-C34
4	B	8002	PCW	C31-C32-C33-C34
4	C	8002	PCW	C31-C32-C33-C34
4	D	5103	PCW	C31-C32-C33-C34
4	A	8002	PCW	C12-C11-O3-C3
4	B	8002	PCW	C12-C11-O3-C3
4	C	8002	PCW	C12-C11-O3-C3
4	D	5103	PCW	C12-C11-O3-C3
4	A	8003	PCW	C31-C32-C33-C34
4	B	8003	PCW	C31-C32-C33-C34
4	C	8003	PCW	C31-C32-C33-C34
4	D	5101	PCW	C31-C32-C33-C34
4	A	8003	PCW	C22-C23-C24-C25
4	B	8003	PCW	C22-C23-C24-C25
4	C	8003	PCW	C22-C23-C24-C25
4	D	5101	PCW	C22-C23-C24-C25
4	A	8002	PCW	O11-C11-O3-C3
4	B	8002	PCW	O11-C11-O3-C3
4	C	8002	PCW	O11-C11-O3-C3
4	D	5103	PCW	O11-C11-O3-C3
4	A	8003	PCW	C14-C15-C16-C17
4	B	8003	PCW	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
4	C	8003	PCW	C14-C15-C16-C17
4	D	5101	PCW	C14-C15-C16-C17
4	B	8003	PCW	C13-C14-C15-C16
4	A	8003	PCW	C13-C14-C15-C16
4	C	8003	PCW	C13-C14-C15-C16
4	D	5101	PCW	C13-C14-C15-C16
4	A	8003	PCW	O2-C2-C3-O3
4	B	8003	PCW	O2-C2-C3-O3
4	C	8003	PCW	O2-C2-C3-O3
4	D	5101	PCW	O2-C2-C3-O3
4	A	8003	PCW	O3P-C1-C2-C3
4	B	8003	PCW	O3P-C1-C2-C3
4	C	8003	PCW	O3P-C1-C2-C3
4	D	5101	PCW	O3P-C1-C2-C3
4	A	8002	PCW	C35-C36-C37-C38
4	B	8002	PCW	C35-C36-C37-C38
4	C	8002	PCW	C35-C36-C37-C38
4	D	5103	PCW	C35-C36-C37-C38
4	A	8003	PCW	C41-C42-C43-C44
4	B	8003	PCW	C41-C42-C43-C44
4	C	8003	PCW	C41-C42-C43-C44
4	D	5101	PCW	C41-C42-C43-C44
4	A	8002	PCW	C42-C43-C44-C45
4	B	8002	PCW	C42-C43-C44-C45
4	C	8002	PCW	C42-C43-C44-C45
4	D	5103	PCW	C42-C43-C44-C45
4	A	8002	PCW	C25-C26-C27-C28
4	B	8002	PCW	C25-C26-C27-C28
4	C	8002	PCW	C25-C26-C27-C28
4	D	5103	PCW	C25-C26-C27-C28
4	A	8003	PCW	C1-C2-C3-O3
4	B	8003	PCW	C1-C2-C3-O3
4	C	8003	PCW	C1-C2-C3-O3
4	D	5101	PCW	C1-C2-C3-O3
4	A	8003	PCW	O3P-C1-C2-O2
4	B	8003	PCW	O3P-C1-C2-O2
4	C	8003	PCW	O3P-C1-C2-O2
4	D	5101	PCW	O3P-C1-C2-O2
4	A	8003	PCW	C21-C22-C23-C24
4	C	8003	PCW	C21-C22-C23-C24
4	D	5101	PCW	C21-C22-C23-C24
4	B	8003	PCW	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
4	A	8003	PCW	C33-C34-C35-C36
4	B	8003	PCW	C33-C34-C35-C36
4	C	8003	PCW	C33-C34-C35-C36
4	D	5101	PCW	C33-C34-C35-C36
4	A	8002	PCW	C24-C25-C26-C27
4	A	8002	PCW	C43-C44-C45-C46
4	B	8002	PCW	C24-C25-C26-C27
4	B	8002	PCW	C43-C44-C45-C46
4	C	8002	PCW	C24-C25-C26-C27
4	C	8002	PCW	C43-C44-C45-C46
4	D	5103	PCW	C43-C44-C45-C46
4	D	5103	PCW	C24-C25-C26-C27
4	A	8002	PCW	O4P-C4-C5-N
4	B	8002	PCW	O4P-C4-C5-N
4	C	8002	PCW	O4P-C4-C5-N
4	D	5103	PCW	O4P-C4-C5-N
4	A	8002	PCW	O2-C2-C3-O3
4	B	8002	PCW	O2-C2-C3-O3
4	C	8002	PCW	O2-C2-C3-O3
4	D	5103	PCW	O2-C2-C3-O3
4	A	8002	PCW	C4-O4P-P-O2P
4	A	8003	PCW	C1-O3P-P-O2P
4	A	8003	PCW	C4-O4P-P-O2P
4	B	8002	PCW	C4-O4P-P-O2P
4	B	8003	PCW	C1-O3P-P-O2P
4	B	8003	PCW	C4-O4P-P-O2P
4	C	8002	PCW	C4-O4P-P-O2P
4	C	8003	PCW	C1-O3P-P-O2P
4	C	8003	PCW	C4-O4P-P-O2P
4	D	5101	PCW	C1-O3P-P-O2P
4	D	5101	PCW	C4-O4P-P-O2P
4	D	5103	PCW	C4-O4P-P-O2P
4	A	8003	PCW	C12-C13-C14-C15
4	B	8003	PCW	C12-C13-C14-C15
4	C	8003	PCW	C12-C13-C14-C15
4	D	5101	PCW	C12-C13-C14-C15
4	A	8002	PCW	C2-C1-O3P-P
4	B	8002	PCW	C2-C1-O3P-P
4	C	8002	PCW	C2-C1-O3P-P
4	D	5103	PCW	C2-C1-O3P-P
4	A	8002	PCW	C21-C22-C23-C24
4	B	8002	PCW	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
4	C	8002	PCW	C21-C22-C23-C24
4	D	5103	PCW	C21-C22-C23-C24
4	A	8002	PCW	C12-C13-C14-C15
4	B	8002	PCW	C12-C13-C14-C15
4	C	8002	PCW	C12-C13-C14-C15
4	D	5103	PCW	C12-C13-C14-C15
4	C	8002	PCW	C33-C34-C35-C36
4	A	8002	PCW	C33-C34-C35-C36
4	D	5103	PCW	C33-C34-C35-C36
4	B	8002	PCW	C33-C34-C35-C36
4	A	8002	PCW	C14-C15-C16-C17
4	B	8002	PCW	C14-C15-C16-C17
4	C	8002	PCW	C14-C15-C16-C17
4	D	5103	PCW	C14-C15-C16-C17
4	A	8003	PCW	C35-C36-C37-C38
4	B	8003	PCW	C35-C36-C37-C38
4	C	8003	PCW	C35-C36-C37-C38
4	D	5101	PCW	C35-C36-C37-C38
4	A	8003	PCW	C20-C21-C22-C23
4	B	8003	PCW	C20-C21-C22-C23
4	C	8003	PCW	C20-C21-C22-C23
4	D	5101	PCW	C20-C21-C22-C23
4	A	8002	PCW	C37-C38-C39-C40
4	B	8002	PCW	C37-C38-C39-C40
4	C	8002	PCW	C37-C38-C39-C40
4	D	5103	PCW	C37-C38-C39-C40
4	D	5103	PCW	C44-C45-C46-C47
4	A	8002	PCW	C44-C45-C46-C47
4	B	8002	PCW	C44-C45-C46-C47
4	C	8002	PCW	C44-C45-C46-C47
4	A	8002	PCW	C36-C37-C38-C39
4	A	8002	PCW	C40-C41-C42-C43
4	B	8002	PCW	C36-C37-C38-C39
4	B	8002	PCW	C40-C41-C42-C43
4	C	8002	PCW	C36-C37-C38-C39
4	C	8002	PCW	C40-C41-C42-C43
4	D	5103	PCW	C36-C37-C38-C39
4	D	5103	PCW	C40-C41-C42-C43
4	A	8003	PCW	C39-C40-C41-C42
4	B	8003	PCW	C39-C40-C41-C42
4	C	8003	PCW	C39-C40-C41-C42
4	D	5101	PCW	C39-C40-C41-C42

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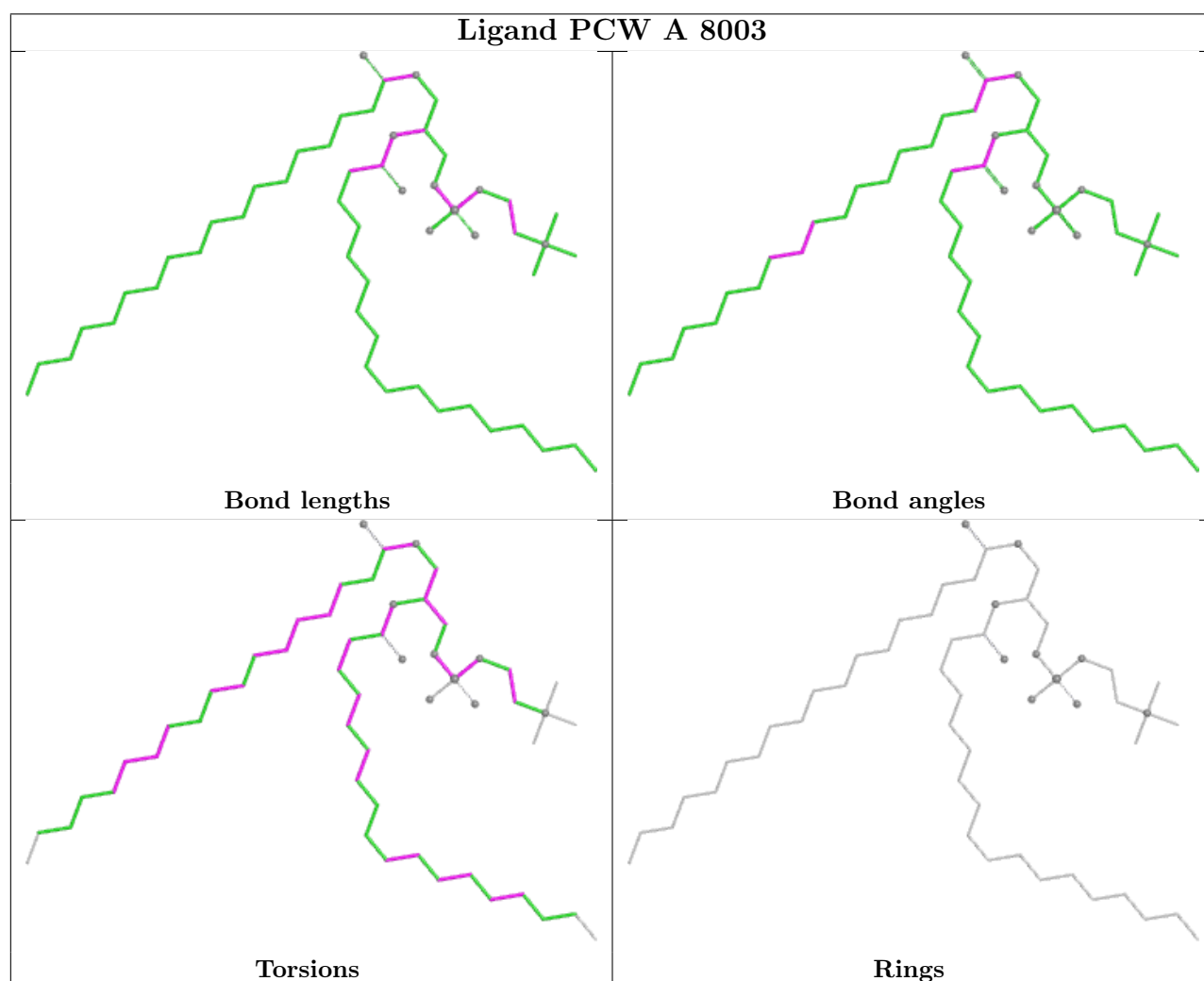
Continued from previous page...

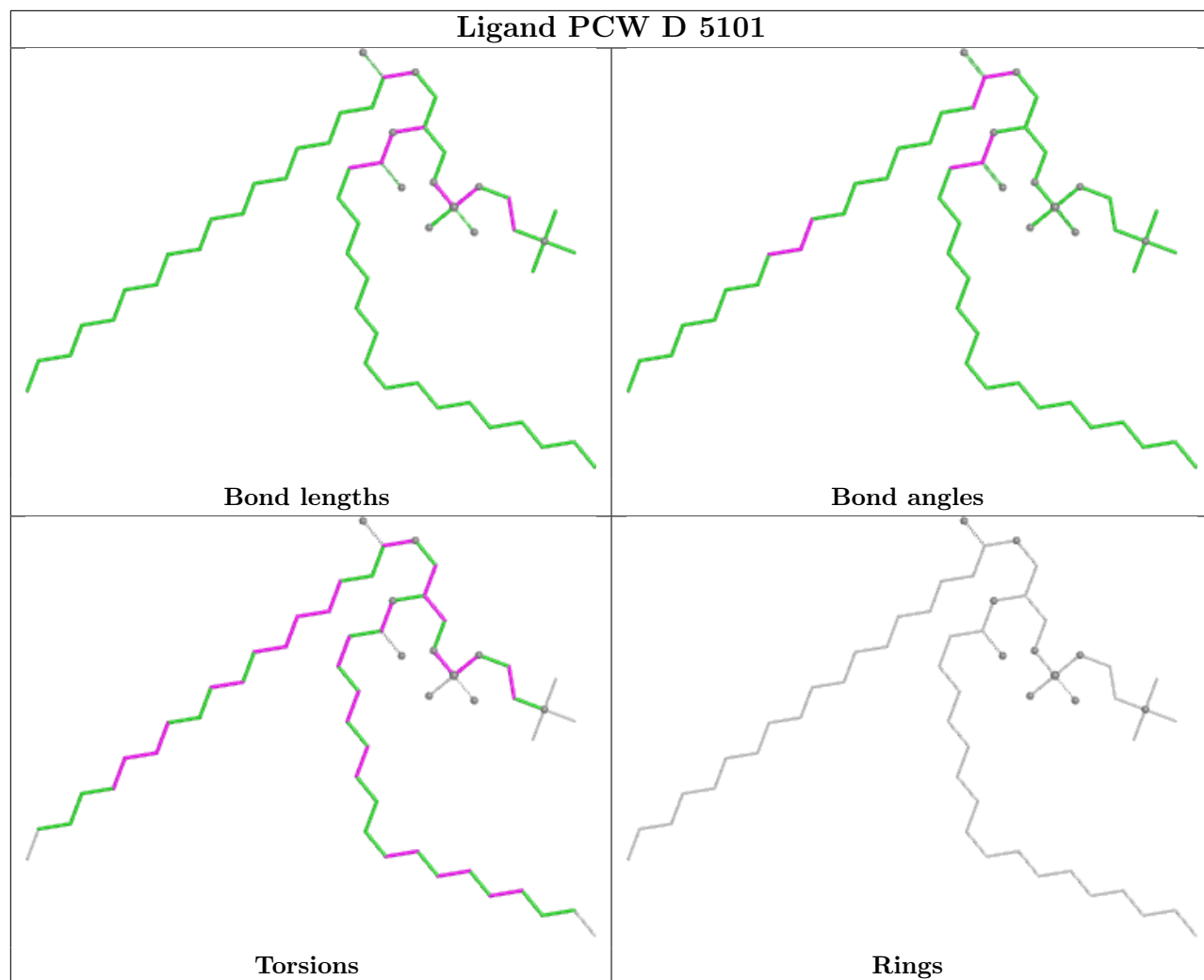
Mol	Chain	Res	Type	Atoms
4	A	8003	PCW	C17-C18-C19-C20
4	C	8003	PCW	C17-C18-C19-C20
4	D	5101	PCW	C17-C18-C19-C20
4	A	8002	PCW	C23-C24-C25-C26
4	B	8002	PCW	C23-C24-C25-C26
4	C	8002	PCW	C23-C24-C25-C26
4	D	5103	PCW	C23-C24-C25-C26
4	A	8002	PCW	C1-C2-C3-O3
4	B	8002	PCW	C1-C2-C3-O3
4	C	8002	PCW	C1-C2-C3-O3
4	D	5103	PCW	C1-C2-C3-O3
4	B	8003	PCW	O11-C11-O3-C3
4	C	8003	PCW	O11-C11-O3-C3
4	D	5101	PCW	O11-C11-O3-C3
4	B	8003	PCW	C17-C18-C19-C20
4	A	8003	PCW	O11-C11-O3-C3
4	A	8002	PCW	C19-C20-C21-C22
4	B	8002	PCW	C19-C20-C21-C22
4	C	8002	PCW	C19-C20-C21-C22
4	D	5103	PCW	C19-C20-C21-C22
4	A	8003	PCW	C15-C16-C17-C18
4	C	8003	PCW	C15-C16-C17-C18
4	D	5101	PCW	C15-C16-C17-C18
4	B	8003	PCW	C15-C16-C17-C18
4	B	8003	PCW	C43-C44-C45-C46
4	C	8003	PCW	C43-C44-C45-C46
4	A	8003	PCW	C43-C44-C45-C46
4	D	5101	PCW	C43-C44-C45-C46
4	A	8003	PCW	C12-C11-O3-C3
4	B	8003	PCW	C12-C11-O3-C3
4	C	8003	PCW	C12-C11-O3-C3
4	D	5101	PCW	C12-C11-O3-C3
4	A	8002	PCW	C17-C18-C19-C20
4	B	8002	PCW	C17-C18-C19-C20
4	C	8002	PCW	C17-C18-C19-C20
4	D	5103	PCW	C17-C18-C19-C20
4	A	8002	PCW	C39-C40-C41-C42
4	B	8002	PCW	C39-C40-C41-C42
4	C	8002	PCW	C39-C40-C41-C42
4	D	5103	PCW	C39-C40-C41-C42

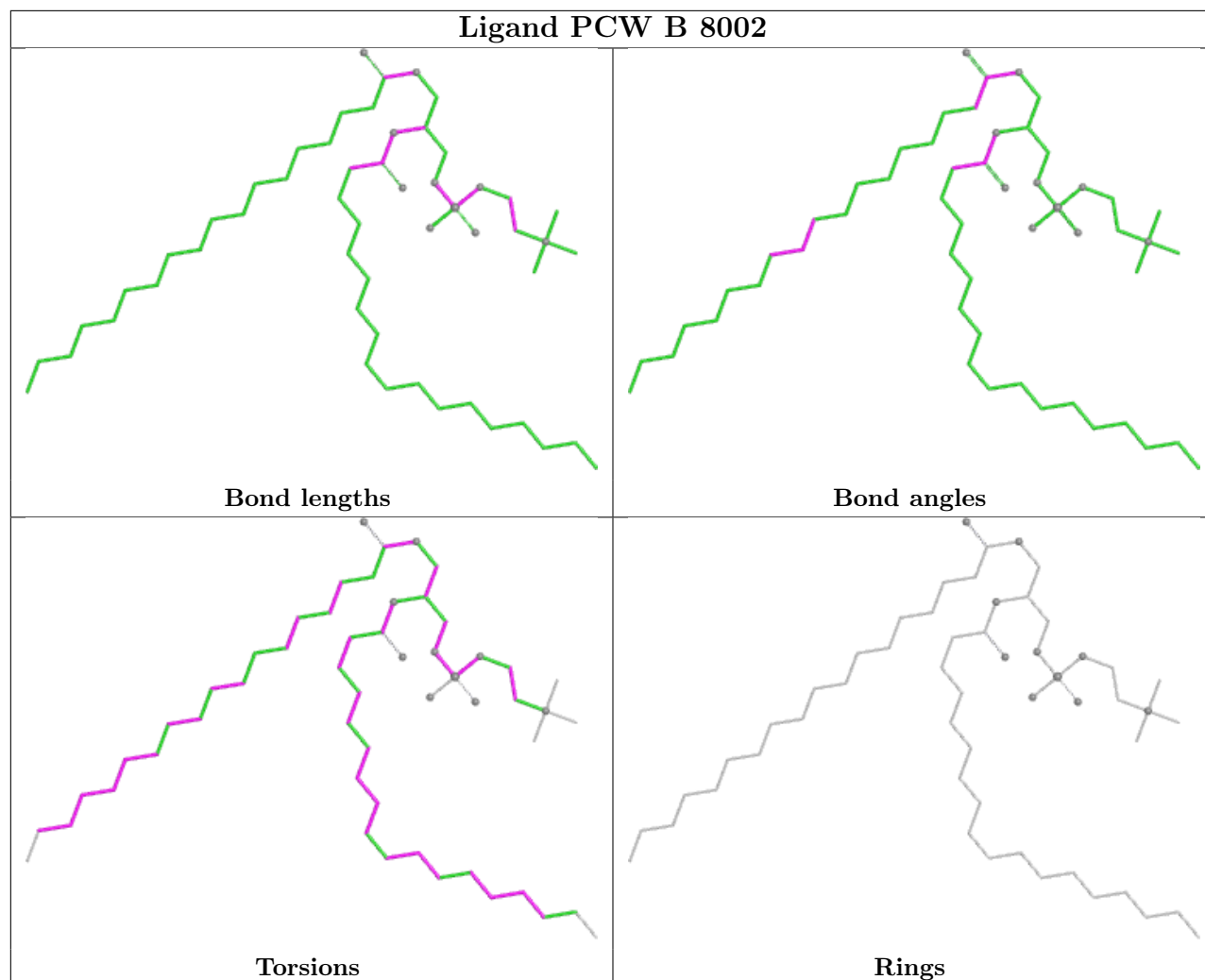
There are no ring outliers.

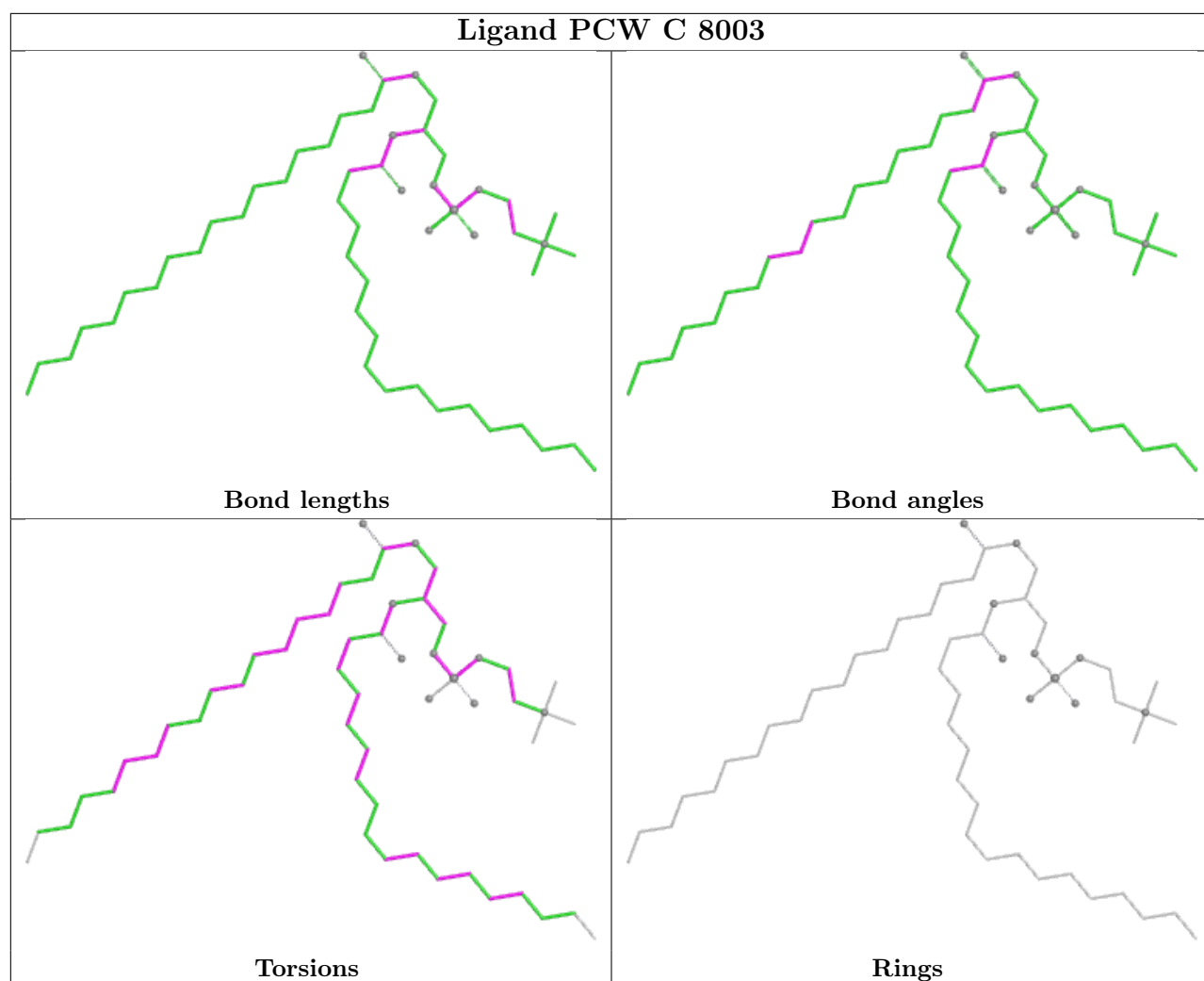
No monomer is involved in short contacts.

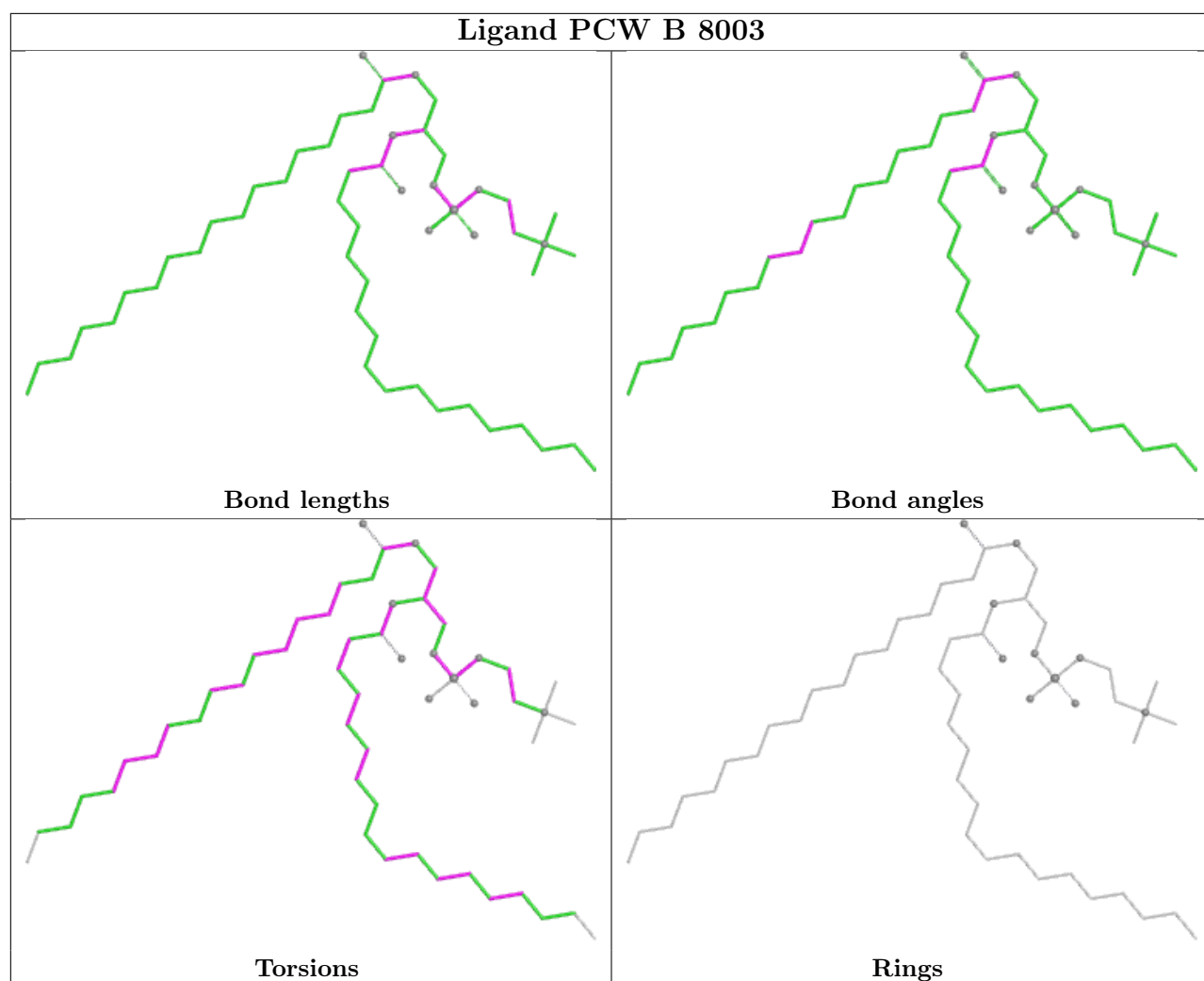
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

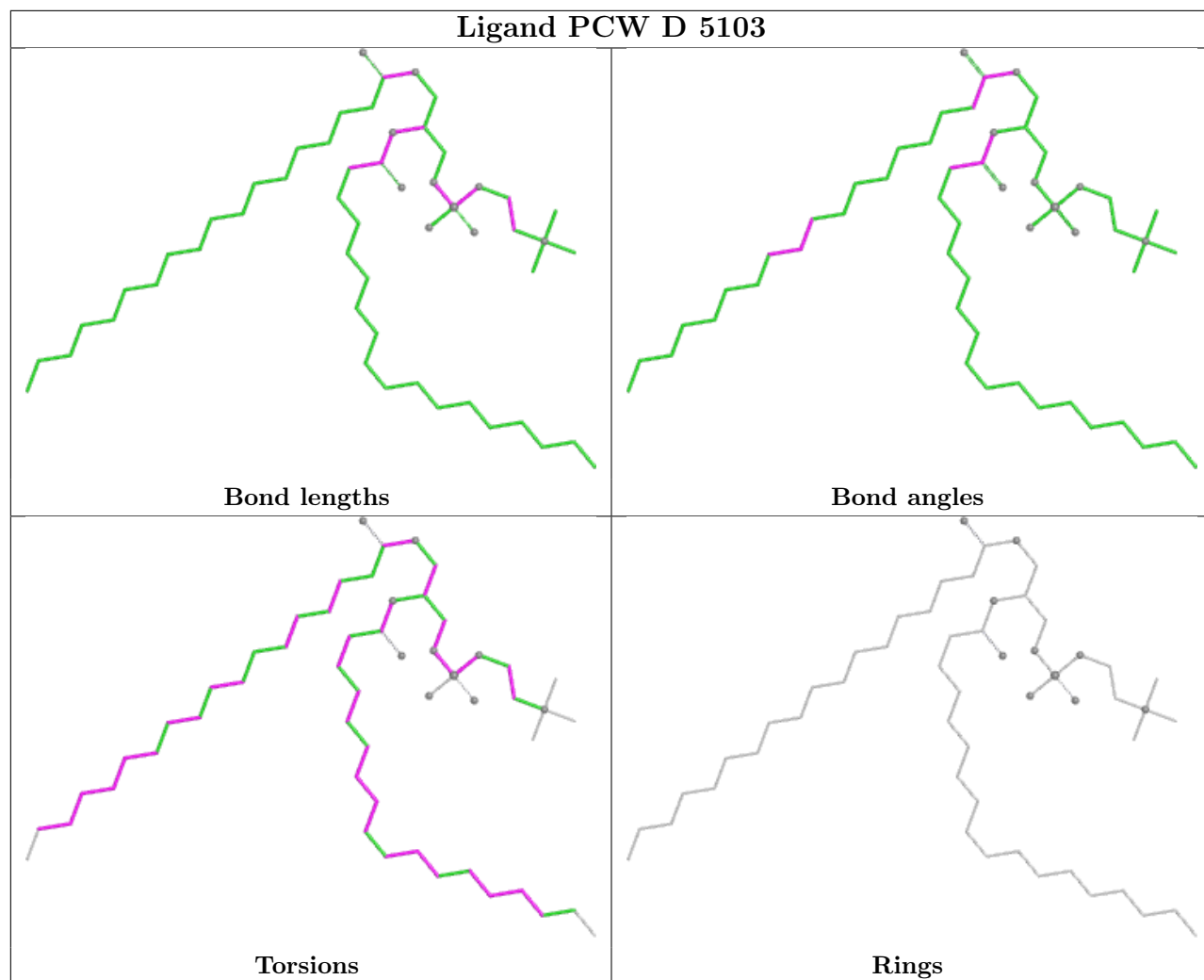


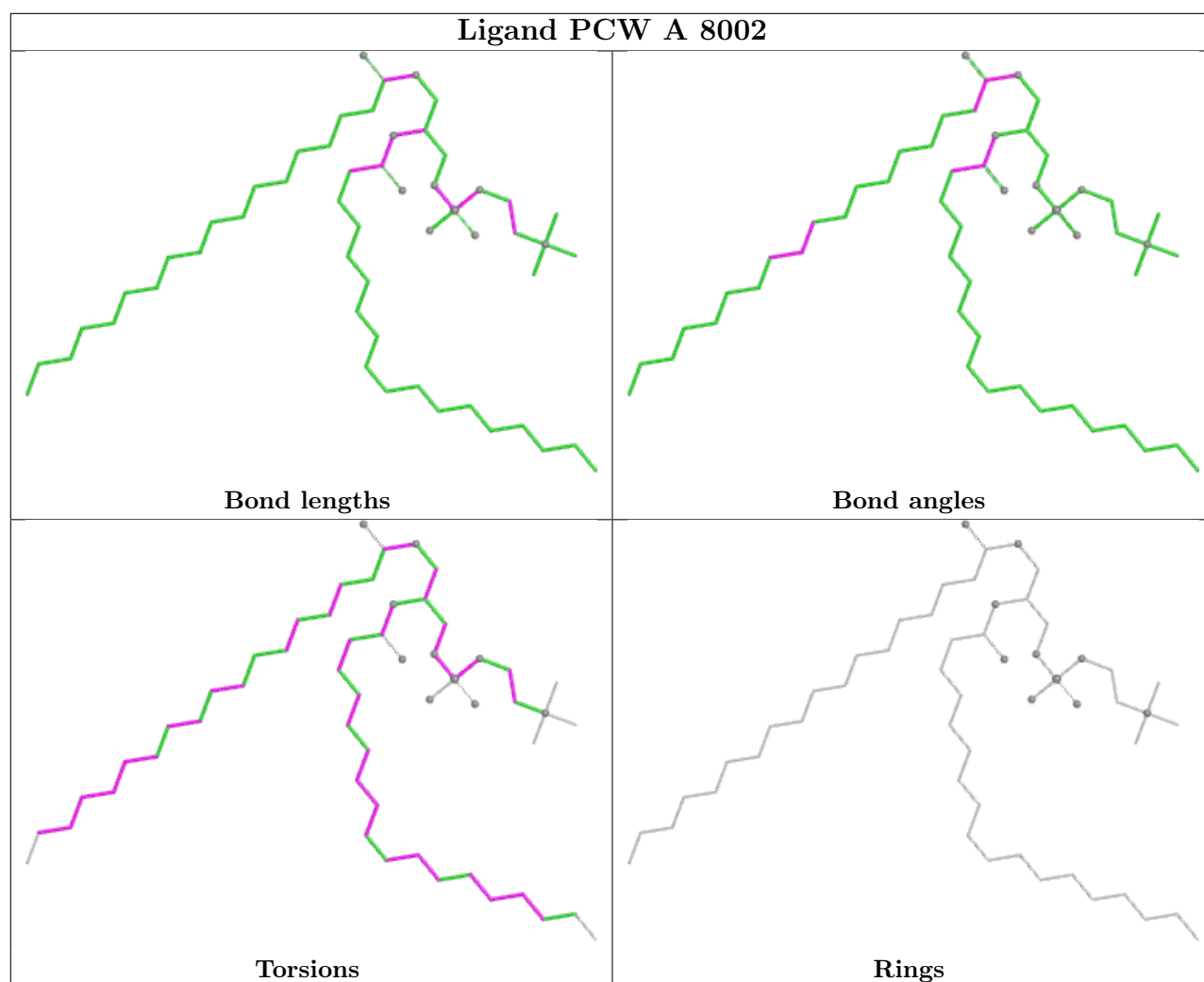


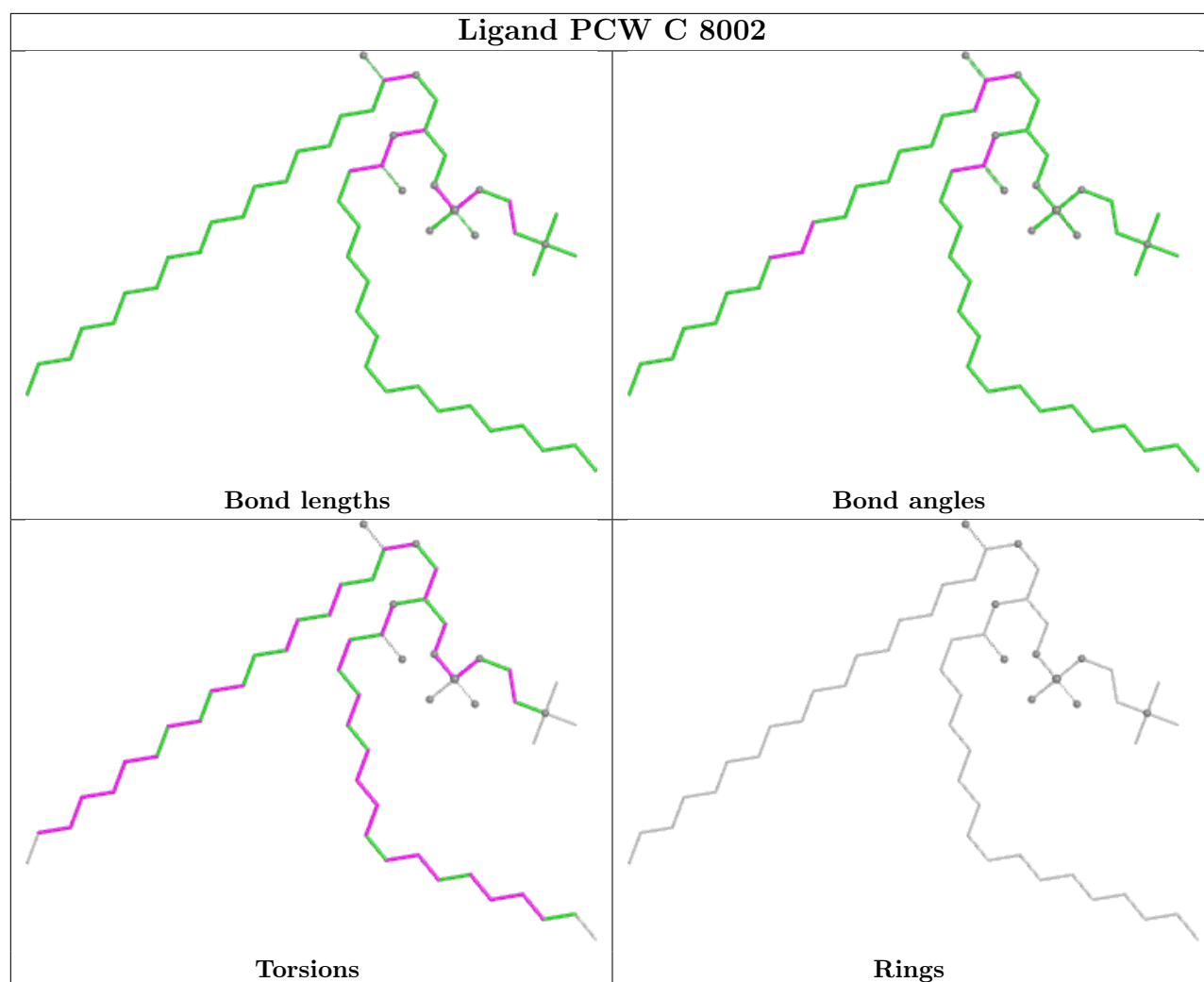












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

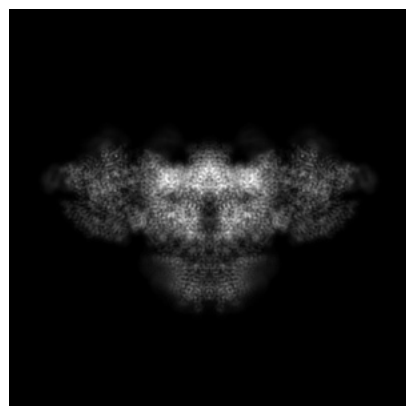
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49538. These allow visual inspection of the internal detail of the map and identification of artifacts.

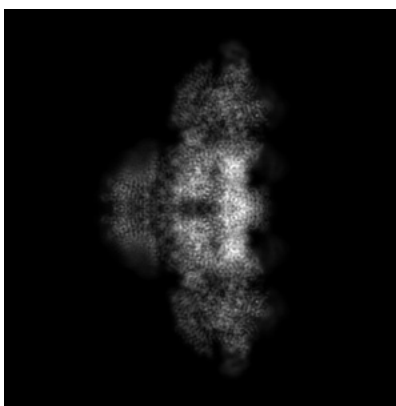
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

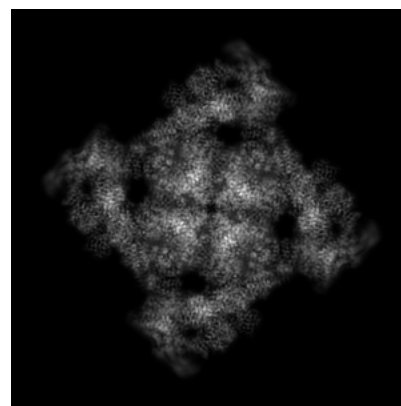
6.1.1 Primary map



X

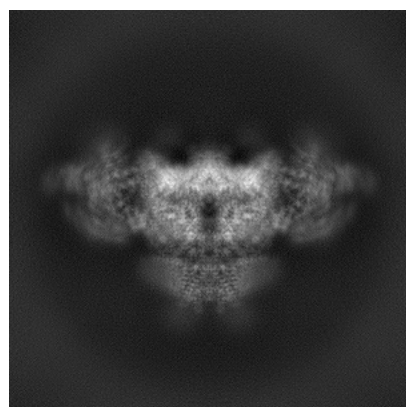


Y

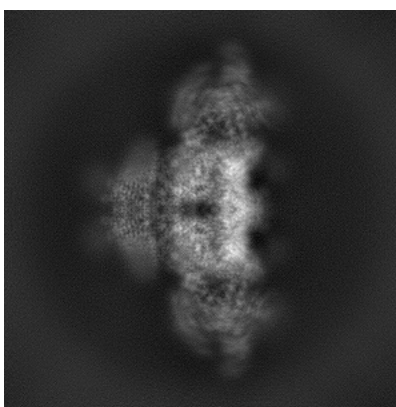


Z

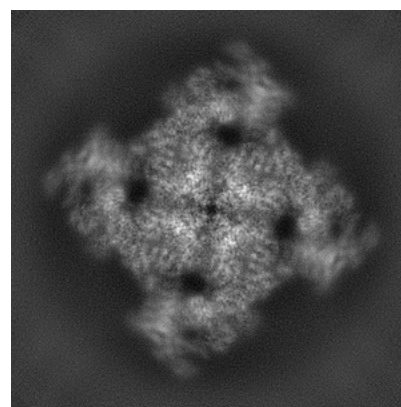
6.1.2 Raw map



X



Y



Z

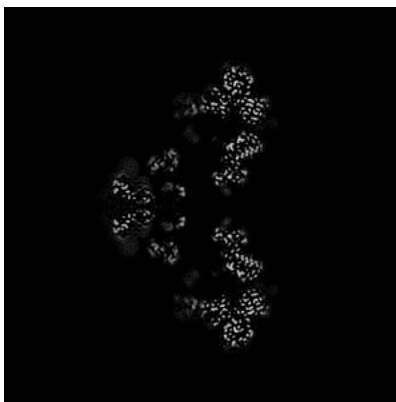
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

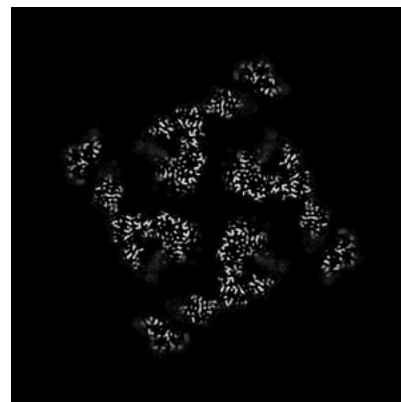
6.2.1 Primary map



X Index: 256

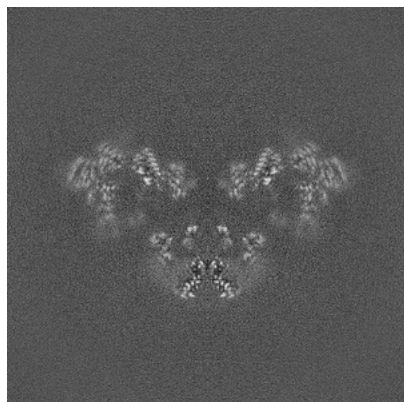


Y Index: 256

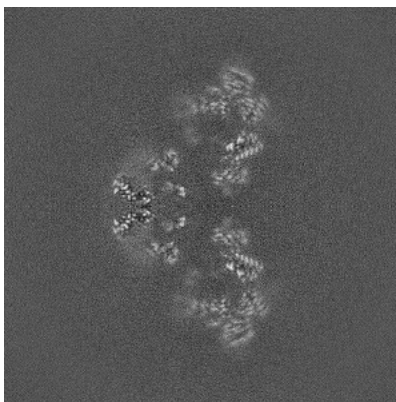


Z Index: 256

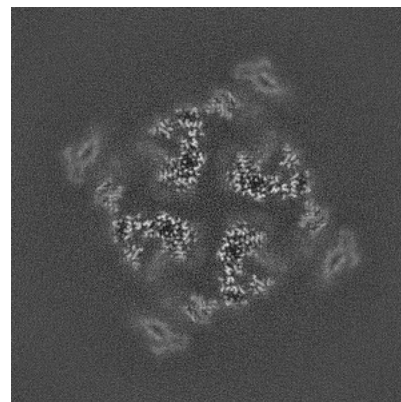
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

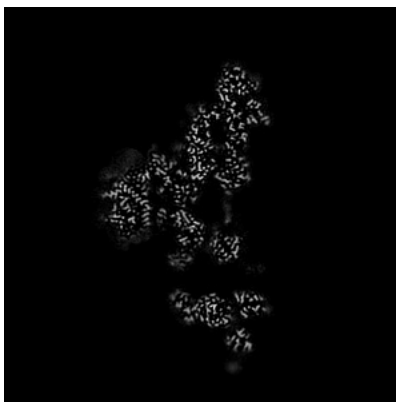
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

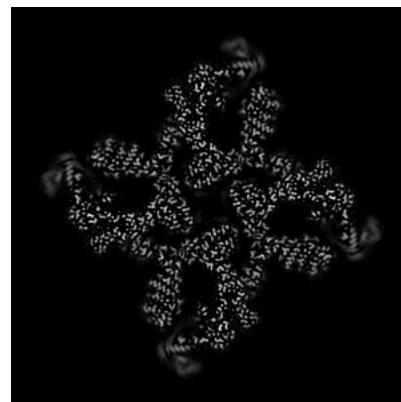
6.3.1 Primary map



X Index: 238

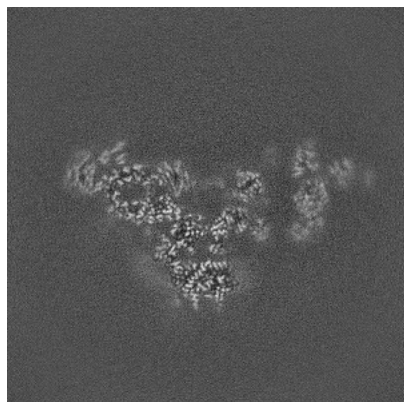


Y Index: 274

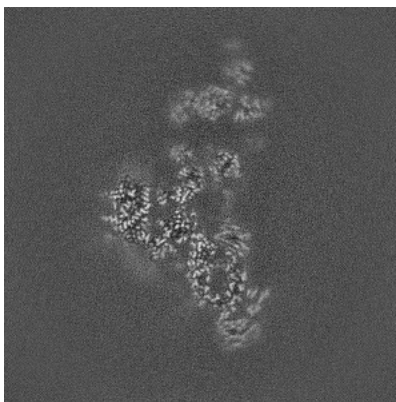


Z Index: 291

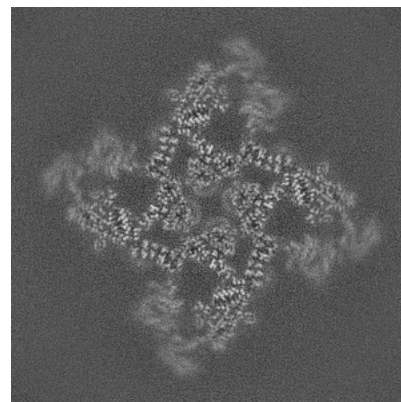
6.3.2 Raw map



X Index: 274



Y Index: 238

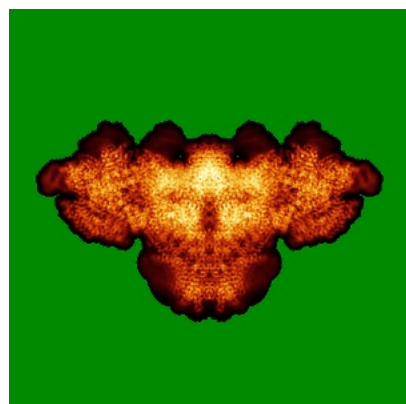


Z Index: 286

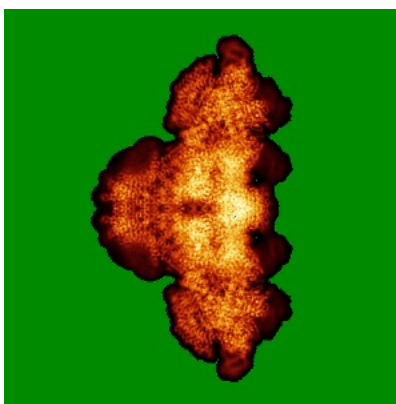
The images above show the largest variance slices of the map in three orthogonal directions.

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

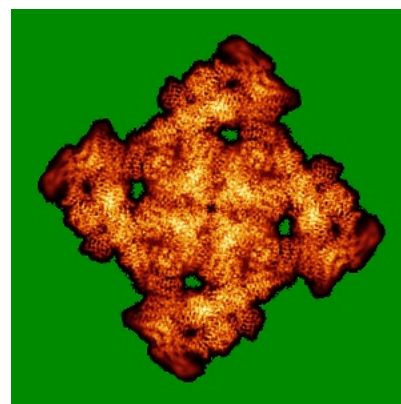
6.4.1 Primary map



X

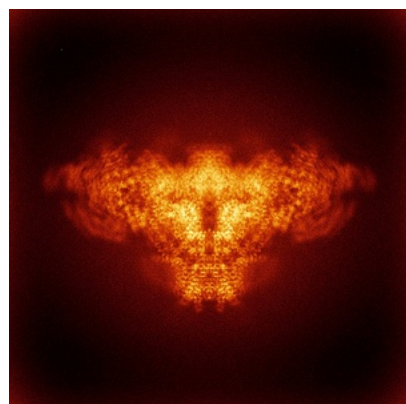


Y

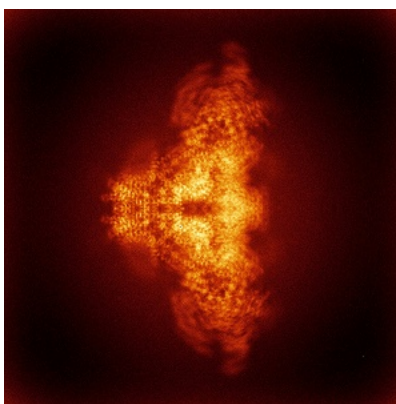


Z

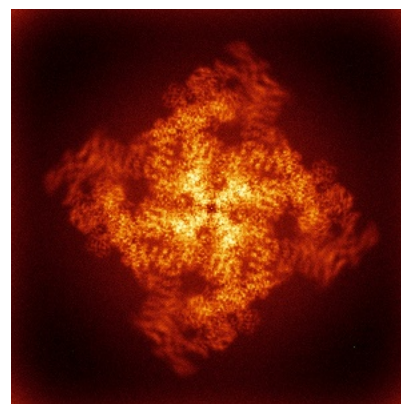
6.4.2 Raw map



X



Y

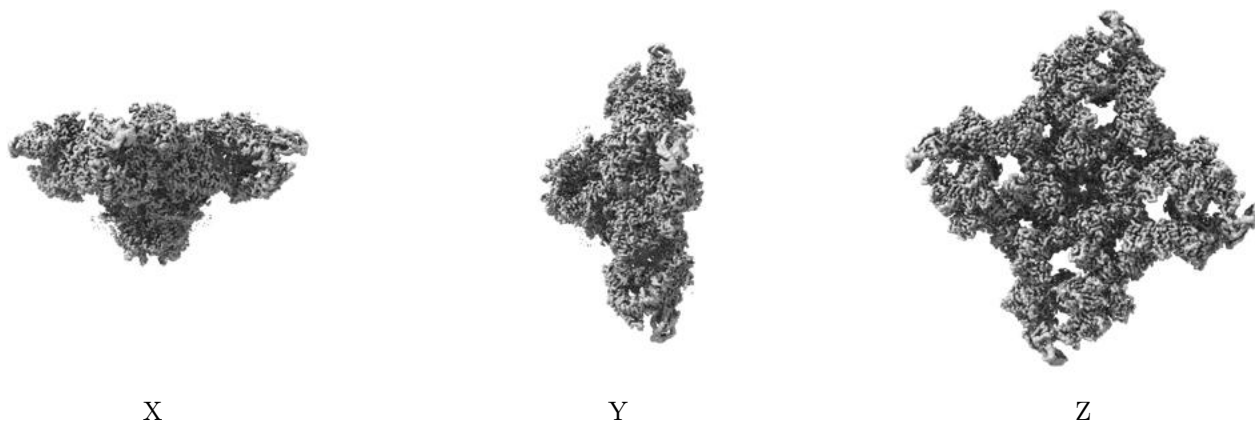


Z

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.

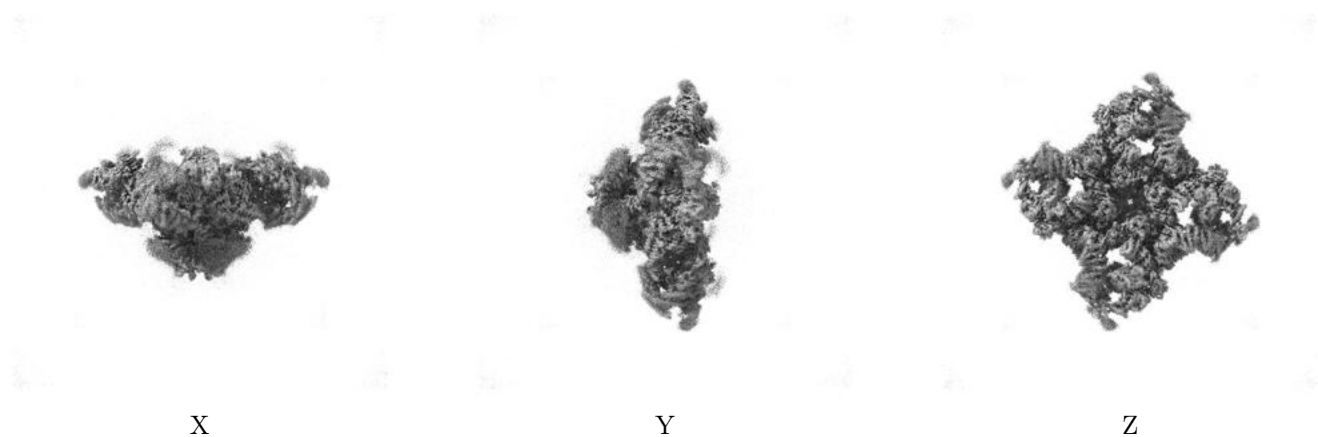
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

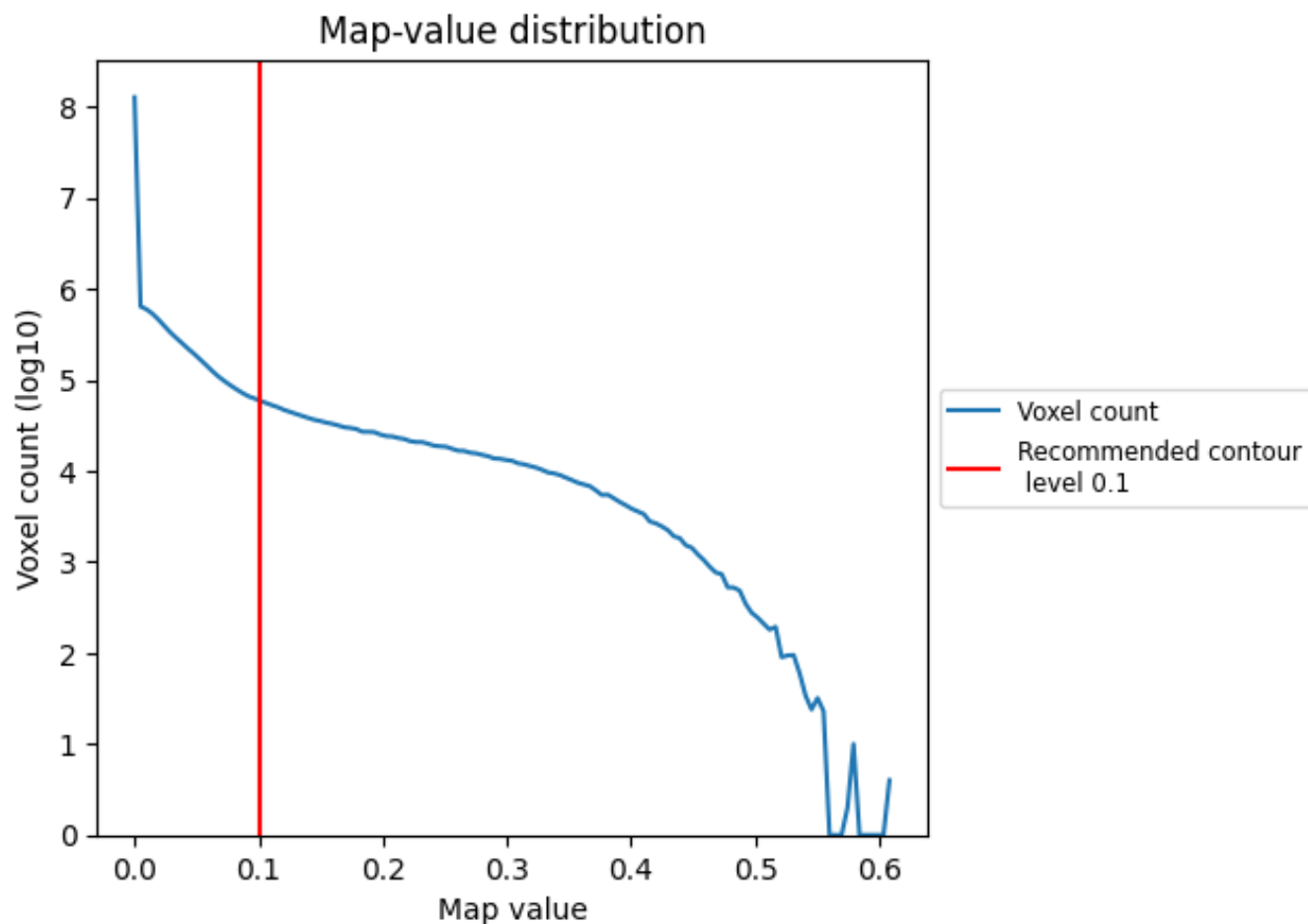
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

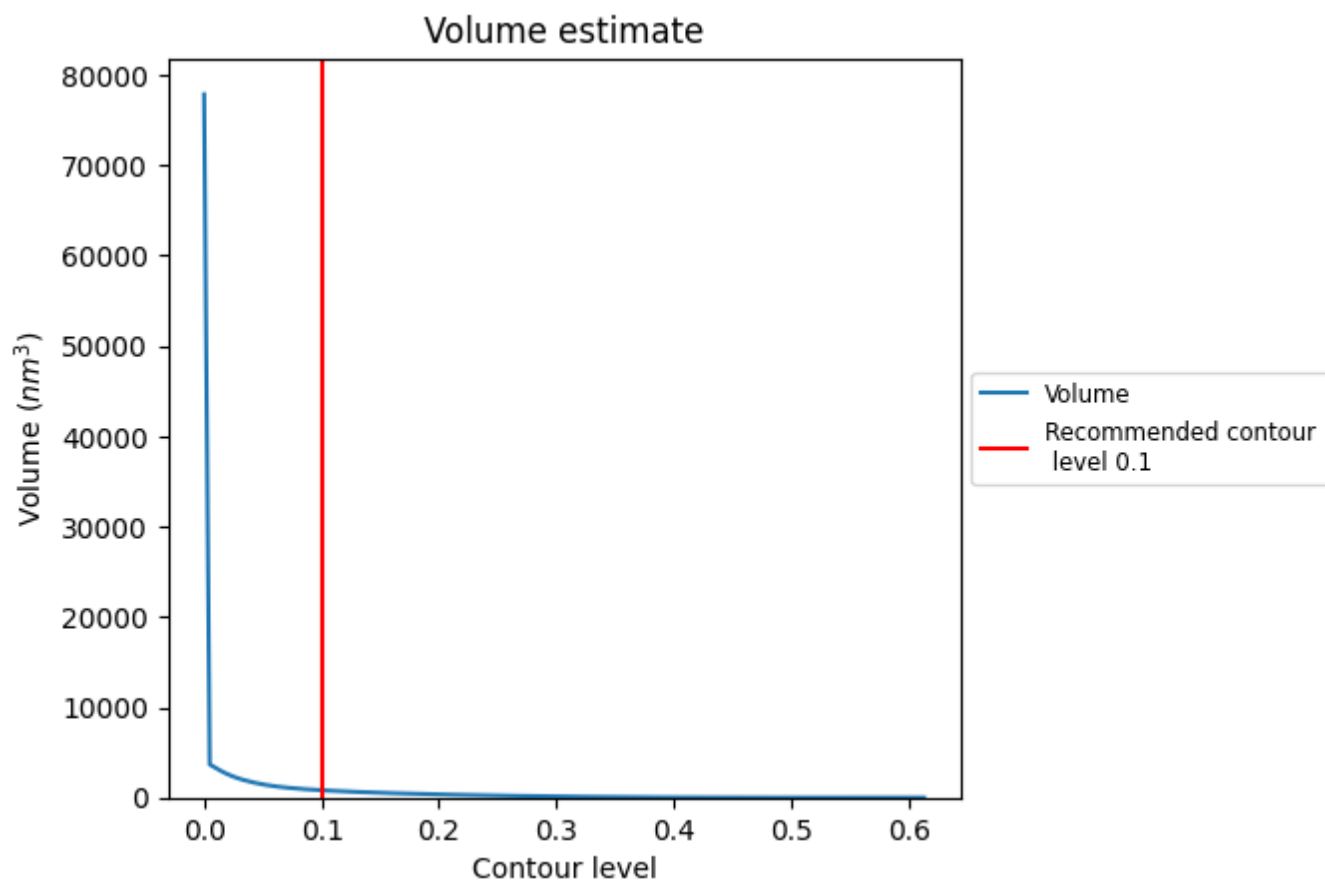
This section contains the results of statistical analysis of the map.

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.

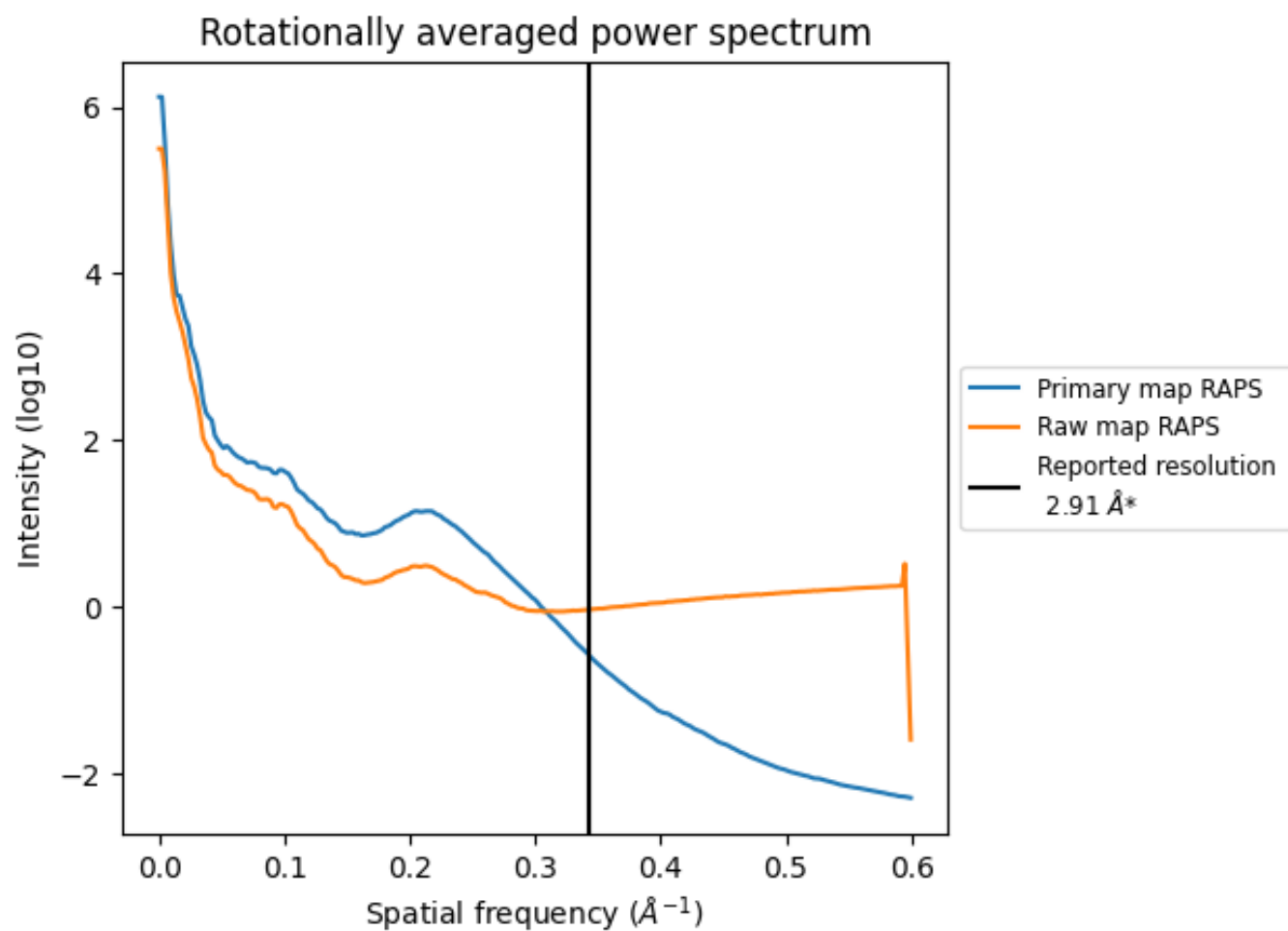
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 812 nm³; this corresponds to an approximate mass of 734 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 ⓘ

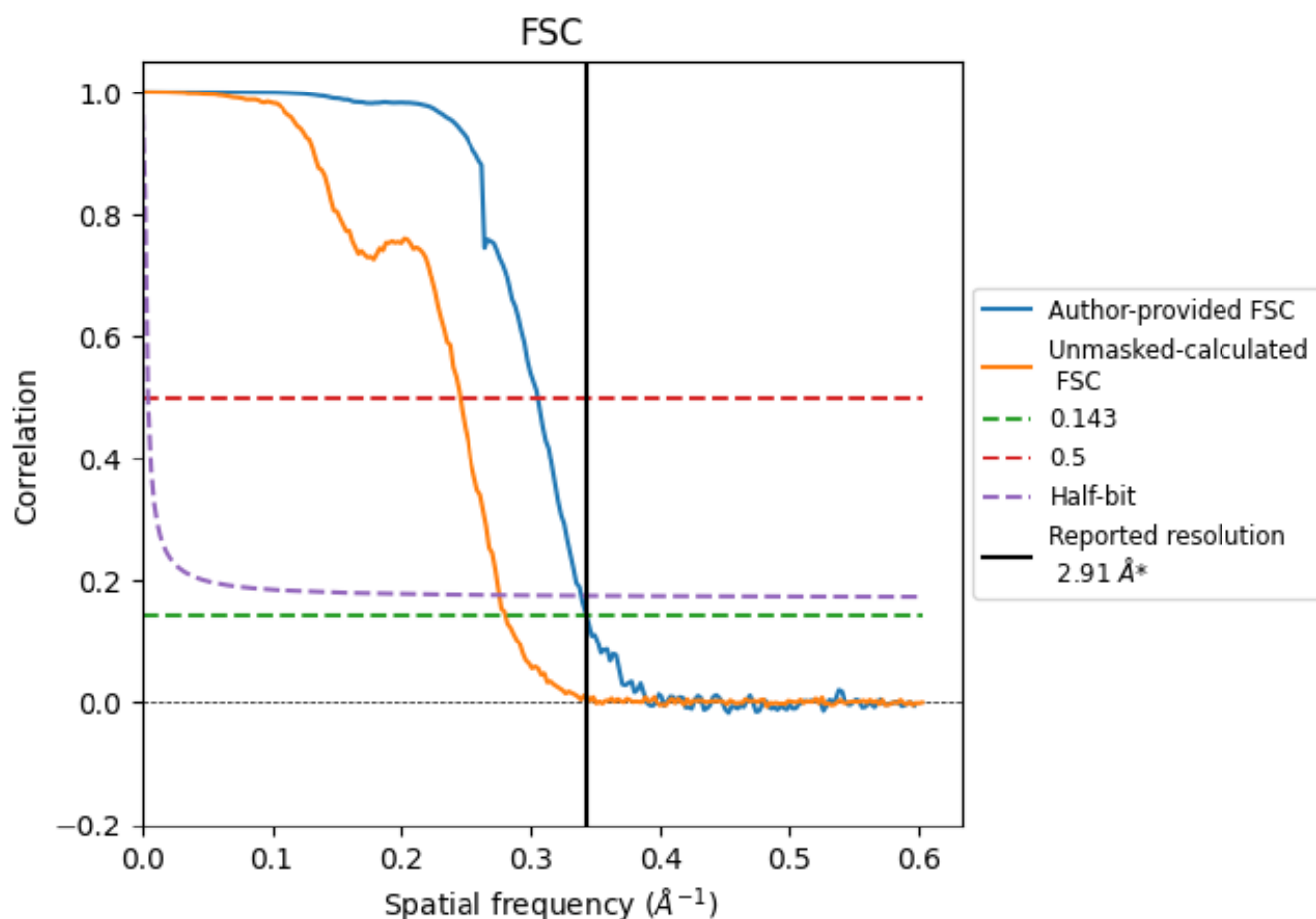


*Reported resolution corresponds to spatial frequency of 0.344 \AA^{-1}

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 0.344 \AA^{-1}

8.2 Resolution estimates [i](#)

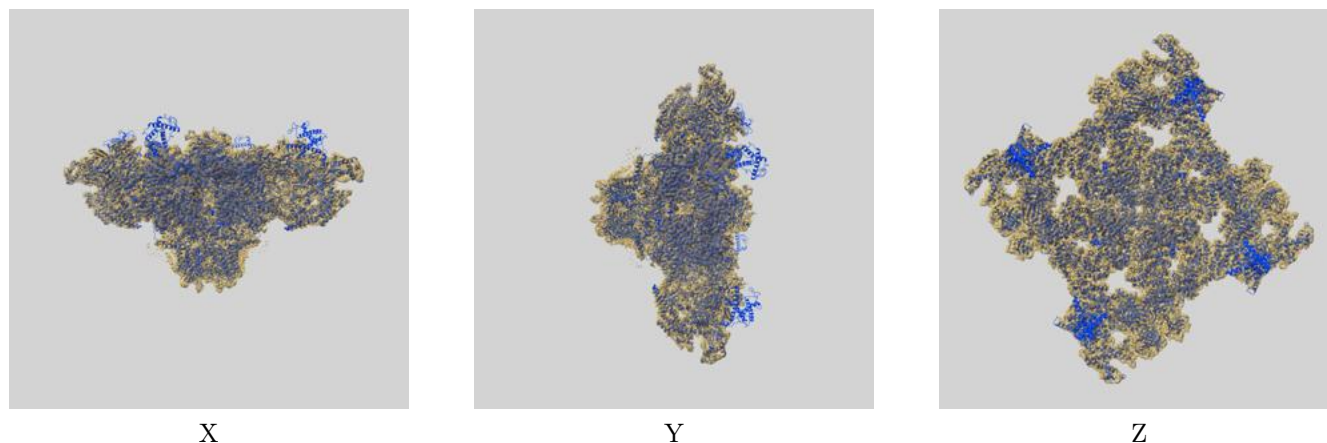
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	2.91	3.27	2.95
Unmasked-calculated*	3.56	4.07	3.62

*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 3.56 differs from the reported value 2.91 by more than 10 %

9 Map-model fit [i](#)

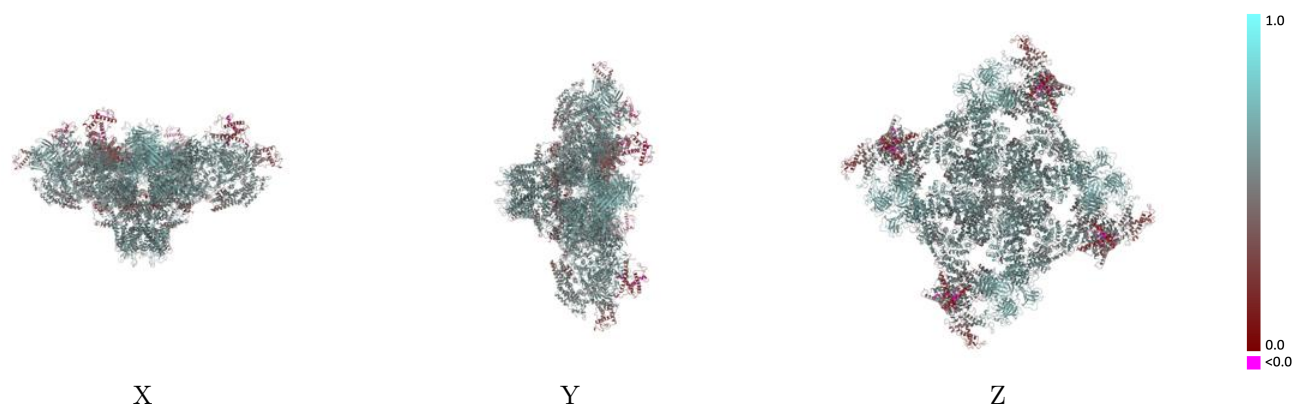
This section contains information regarding the fit between EMDB map EMD-49538 and PDB model 9NMR. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



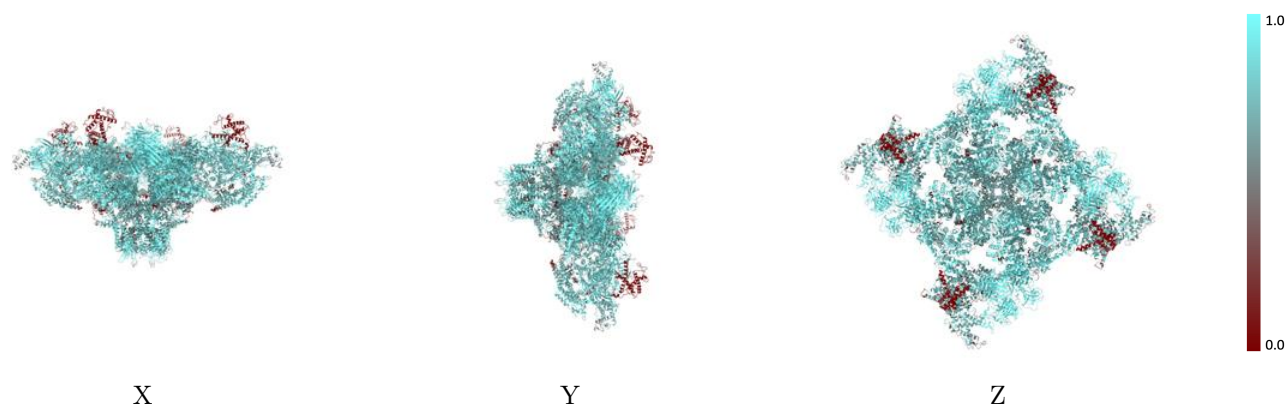
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



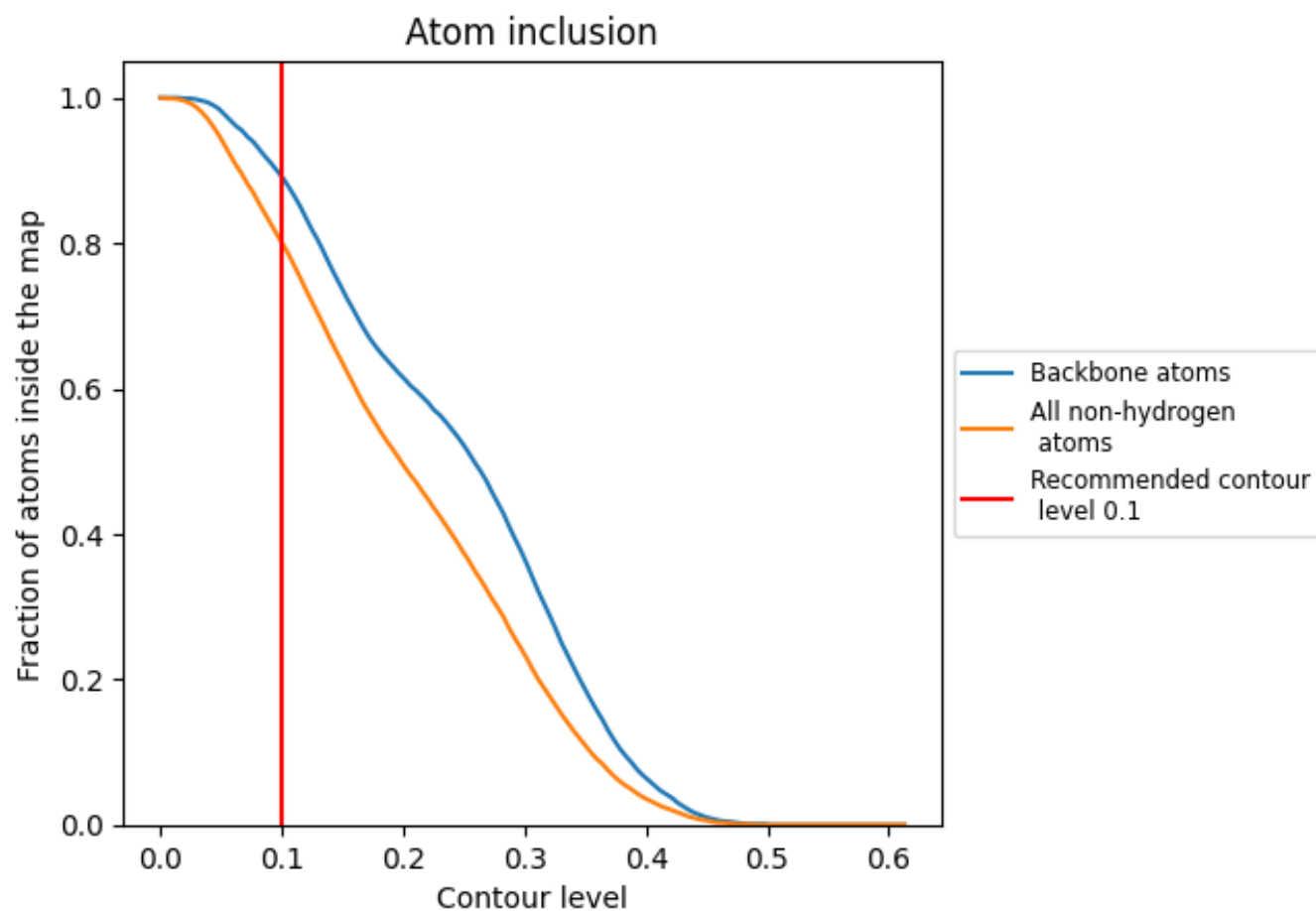
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 80% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8000	<div></div> 0.5360
A	<div></div> 0.7980	<div></div> 0.5340
B	<div></div> 0.7980	<div></div> 0.5340
C	<div></div> 0.7970	<div></div> 0.5340
D	<div></div> 0.7980	<div></div> 0.5350
E	<div></div> 0.9050	<div></div> 0.6020
F	<div></div> 0.9000	<div></div> 0.6000
G	<div></div> 0.9040	<div></div> 0.6040
H	<div></div> 0.9020	<div></div> 0.6040

