



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:33 AM UTC

PDB ID : 9L2D / pdb_00009l2d
EMDB ID : EMD-62772
Title : Structure of SARM1 bound to M1 in the intermediate state 1
Authors : Huang, Y.; Zhang, J.; Zheng, S.; Wang, X.
Deposited on : 2024-12-17
Resolution : 2.83 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

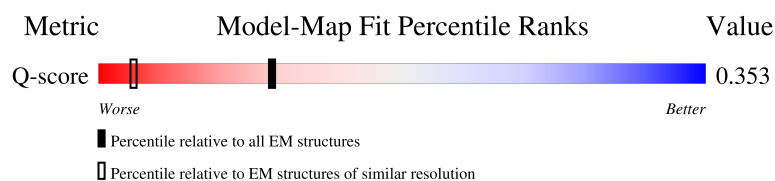
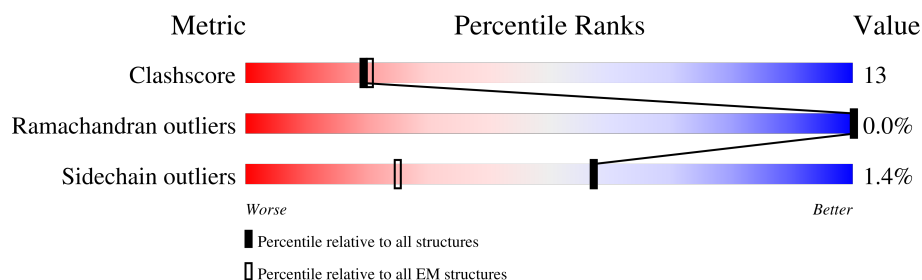
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 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	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11847 (2.33 - 3.33)

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 37836 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 NAD(+) hydrolase SARM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	600	Total	C	N	O	S	0	0
			4710	2978	847	862	23		
1	B	600	Total	C	N	O	S	0	0
			4710	2978	847	862	23		
1	C	600	Total	C	N	O	S	0	0
			4710	2978	847	862	23		
1	D	600	Total	C	N	O	S	0	0
			4710	2978	847	862	23		
1	E	600	Total	C	N	O	S	0	0
			4708	2977	847	862	22		
1	F	599	Total	C	N	O	S	0	0
			4704	2975	846	861	22		
1	G	600	Total	C	N	O	S	0	0
			4710	2978	847	862	23		
1	H	601	Total	C	N	O	S	0	0
			4714	2980	848	863	23		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	725	ASP	-	expression tag	UNP Q6SZW1
A	726	TYR	-	expression tag	UNP Q6SZW1
A	727	LYS	-	expression tag	UNP Q6SZW1
A	728	ASP	-	expression tag	UNP Q6SZW1
A	729	ASP	-	expression tag	UNP Q6SZW1
A	730	ASP	-	expression tag	UNP Q6SZW1
A	731	ASP	-	expression tag	UNP Q6SZW1
A	732	LYS	-	expression tag	UNP Q6SZW1
B	725	ASP	-	expression tag	UNP Q6SZW1
B	726	TYR	-	expression tag	UNP Q6SZW1
B	727	LYS	-	expression tag	UNP Q6SZW1
B	728	ASP	-	expression tag	UNP Q6SZW1
B	729	ASP	-	expression tag	UNP Q6SZW1
B	730	ASP	-	expression tag	UNP Q6SZW1

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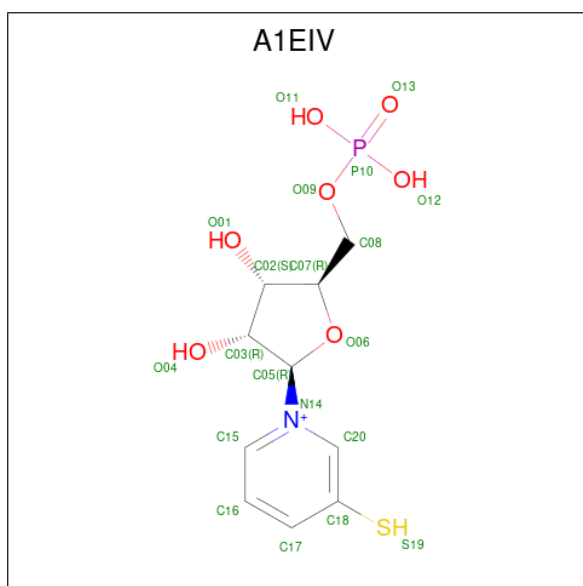
Chain	Residue	Modelled	Actual	Comment	Reference
B	731	ASP	-	expression tag	UNP Q6SZW1
B	732	LYS	-	expression tag	UNP Q6SZW1
C	725	ASP	-	expression tag	UNP Q6SZW1
C	726	TYR	-	expression tag	UNP Q6SZW1
C	727	LYS	-	expression tag	UNP Q6SZW1
C	728	ASP	-	expression tag	UNP Q6SZW1
C	729	ASP	-	expression tag	UNP Q6SZW1
C	730	ASP	-	expression tag	UNP Q6SZW1
C	731	ASP	-	expression tag	UNP Q6SZW1
C	732	LYS	-	expression tag	UNP Q6SZW1
D	725	ASP	-	expression tag	UNP Q6SZW1
D	726	TYR	-	expression tag	UNP Q6SZW1
D	727	LYS	-	expression tag	UNP Q6SZW1
D	728	ASP	-	expression tag	UNP Q6SZW1
D	729	ASP	-	expression tag	UNP Q6SZW1
D	730	ASP	-	expression tag	UNP Q6SZW1
D	731	ASP	-	expression tag	UNP Q6SZW1
D	732	LYS	-	expression tag	UNP Q6SZW1
E	725	ASP	-	expression tag	UNP Q6SZW1
E	726	TYR	-	expression tag	UNP Q6SZW1
E	727	LYS	-	expression tag	UNP Q6SZW1
E	728	ASP	-	expression tag	UNP Q6SZW1
E	729	ASP	-	expression tag	UNP Q6SZW1
E	730	ASP	-	expression tag	UNP Q6SZW1
E	731	ASP	-	expression tag	UNP Q6SZW1
E	732	LYS	-	expression tag	UNP Q6SZW1
F	725	ASP	-	expression tag	UNP Q6SZW1
F	726	TYR	-	expression tag	UNP Q6SZW1
F	727	LYS	-	expression tag	UNP Q6SZW1
F	728	ASP	-	expression tag	UNP Q6SZW1
F	729	ASP	-	expression tag	UNP Q6SZW1
F	730	ASP	-	expression tag	UNP Q6SZW1
F	731	ASP	-	expression tag	UNP Q6SZW1
F	732	LYS	-	expression tag	UNP Q6SZW1
G	725	ASP	-	expression tag	UNP Q6SZW1
G	726	TYR	-	expression tag	UNP Q6SZW1
G	727	LYS	-	expression tag	UNP Q6SZW1
G	728	ASP	-	expression tag	UNP Q6SZW1
G	729	ASP	-	expression tag	UNP Q6SZW1
G	730	ASP	-	expression tag	UNP Q6SZW1
G	731	ASP	-	expression tag	UNP Q6SZW1
G	732	LYS	-	expression tag	UNP Q6SZW1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	725	ASP	-	expression tag	UNP Q6SZW1
H	726	TYR	-	expression tag	UNP Q6SZW1
H	727	LYS	-	expression tag	UNP Q6SZW1
H	728	ASP	-	expression tag	UNP Q6SZW1
H	729	ASP	-	expression tag	UNP Q6SZW1
H	730	ASP	-	expression tag	UNP Q6SZW1
H	731	ASP	-	expression tag	UNP Q6SZW1
H	732	LYS	-	expression tag	UNP Q6SZW1

- Molecule 2 is [(2 {R},3 {S},4 {R},5 {R})-3,4-bis(oxidanyl)-5-(3-sulfanylpiperidin-1-yl)oxolan-2-yl]methyl dihydrogen phosphate (CCD ID: A1EIV) (formula: C₁₀H₁₅NO₇PS) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms						AltConf
2	G	1	Total	C	N	O	P	S	0
			20	10	1	7	1	1	
2	H	1	Total	C	N	O	P	S	0
			20	10	1	7	1	1	

SEQUENCE-PLOTS INFOmissingINFO

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42713	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 ($e^-/\text{\AA}^2$)	52.73	Depositor
Minimum defocus (nm)	710	Depositor
Maximum defocus (nm)	2240	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.128	Depositor
Minimum map value	-2.341	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.365	Depositor
Map size (Å)	323.2, 323.2, 323.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.808, 0.808, 0.808	Depositor

4 Model quality

4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1EIV

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	0.25	0/4786	0.50	3/6466 (0.0%)
1	B	0.18	0/4786	0.41	0/6466
1	C	0.24	0/4786	0.50	3/6466 (0.0%)
1	D	0.26	0/4786	0.51	2/6466 (0.0%)
1	E	0.24	0/4784	0.49	2/6464 (0.0%)
1	F	0.22	0/4780	0.46	0/6458
1	G	0.24	0/4786	0.46	0/6466
1	H	0.23	0/4790	0.44	2/6472 (0.0%)
All	All	0.23	0/38284	0.47	12/51724 (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	3
1	C	0	1
1	D	0	4
1	E	0	3
1	F	0	1
1	G	0	2
1	H	0	1
All	All	0	15

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	155	GLU	CA-CB-CG	6.09	126.28	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	143	GLN	CB-CA-C	-6.00	100.83	110.79
1	D	145	ALA	N-CA-C	-5.78	104.99	111.28
1	C	145	ALA	N-CA-C	-5.69	105.08	111.28
1	A	145	ALA	N-CA-C	-5.57	105.20	111.28
1	D	141	ARG	N-CA-C	-5.46	105.33	111.28
1	A	149	GLU	N-CA-C	-5.32	105.49	111.28
1	E	149	GLU	N-CA-C	-5.26	105.66	111.71
1	E	145	ALA	N-CA-C	-5.22	105.59	111.28
1	A	141	ARG	N-CA-C	-5.17	105.64	111.28
1	C	141	ARG	N-CA-C	-5.10	105.16	111.33
1	H	145	ALA	N-CA-C	-5.10	105.72	111.28

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ARG	Sidechain
1	A	141	ARG	Sidechain
1	A	146	ARG	Sidechain
1	C	110	ARG	Sidechain
1	D	110	ARG	Sidechain
1	D	146	ARG	Sidechain
1	D	159	ARG	Sidechain
1	D	162	ARG	Sidechain
1	E	110	ARG	Sidechain
1	E	141	ARG	Sidechain
1	E	146	ARG	Sidechain
1	F	146	ARG	Sidechain
1	G	110	ARG	Sidechain
1	G	146	ARG	Sidechain
1	H	146	ARG	Sidechain

4.2 Too-close contacts [i](#)

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	4710	0	4791	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4710	0	4791	119	0
1	C	4710	0	4791	130	0
1	D	4710	0	4791	123	0
1	E	4708	0	4788	125	0
1	F	4704	0	4786	126	0
1	G	4710	0	4791	129	0
1	H	4714	0	4793	119	0
2	A	20	0	0	0	0
2	B	20	0	0	3	0
2	C	20	0	0	1	0
2	D	20	0	0	0	0
2	E	20	0	0	1	0
2	F	20	0	0	0	0
2	G	20	0	0	1	0
2	H	20	0	0	3	0
All	All	37836	0	38322	959	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 13.

All (959) 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:H:155:GLU:OE1	1:H:155:GLU:N	2.03	0.92
1:A:121:ARG:HA	1:A:126:LEU:HD22	1.56	0.88
1:H:121:ARG:HA	1:H:126:LEU:HD22	1.56	0.88
1:B:121:ARG:HA	1:B:126:LEU:HD22	1.56	0.87
1:C:121:ARG:HA	1:C:126:LEU:HD22	1.56	0.87
1:E:121:ARG:HA	1:E:126:LEU:HD22	1.56	0.86
1:F:121:ARG:HA	1:F:126:LEU:HD22	1.56	0.85
1:G:121:ARG:HA	1:G:126:LEU:HD22	1.56	0.85
1:D:121:ARG:HA	1:D:126:LEU:HD22	1.56	0.85
1:A:196:GLU:HG2	1:A:200:GLN:HE22	1.42	0.84
1:C:196:GLU:HG2	1:C:200:GLN:HE22	1.43	0.84
1:G:196:GLU:HG2	1:G:200:GLN:HE22	1.43	0.84
1:E:196:GLU:HG2	1:E:200:GLN:HE22	1.42	0.84
1:H:196:GLU:HG2	1:H:200:GLN:HE22	1.43	0.83
1:G:208:LEU:HD23	1:G:248:LYS:HD3	1.61	0.83
1:F:142:VAL:HG22	1:F:180:LEU:HB2	1.60	0.83
1:D:196:GLU:HG2	1:D:200:GLN:HE22	1.42	0.82
1:F:196:GLU:HG2	1:F:200:GLN:HE22	1.42	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:GLU:HG2	1:B:200:GLN:HE22	1.43	0.82
1:E:208:LEU:HD23	1:E:248:LYS:HD3	1.61	0.82
1:F:208:LEU:HD23	1:F:248:LYS:HD3	1.61	0.82
1:D:208:LEU:HD23	1:D:248:LYS:HD3	1.61	0.81
1:C:208:LEU:HD23	1:C:248:LYS:HD3	1.61	0.81
1:H:208:LEU:HD23	1:H:248:LYS:HD3	1.61	0.81
1:A:208:LEU:HD23	1:A:248:LYS:HD3	1.61	0.81
1:B:208:LEU:HD23	1:B:248:LYS:HD3	1.61	0.80
1:B:142:VAL:HG22	1:B:180:LEU:HB2	1.60	0.80
1:G:103:TRP:HD1	1:G:150:GLN:HE22	1.28	0.80
1:H:151:ILE:O	1:H:153:VAL:N	2.15	0.80
1:B:403:ARG:O	1:B:423:GLN:NE2	2.17	0.77
1:G:403:ARG:O	1:G:423:GLN:NE2	2.17	0.77
1:A:403:ARG:O	1:A:423:GLN:NE2	2.17	0.77
1:E:328:GLN:HG2	1:E:368:ILE:HD11	1.67	0.77
1:G:328:GLN:HG2	1:G:368:ILE:HD11	1.67	0.77
1:F:328:GLN:HG2	1:F:368:ILE:HD11	1.66	0.77
1:B:79:LEU:HD11	1:B:92:LEU:HD23	1.67	0.76
1:B:328:GLN:HG2	1:B:368:ILE:HD11	1.66	0.76
1:D:403:ARG:O	1:D:423:GLN:NE2	2.17	0.76
1:A:79:LEU:HD11	1:A:92:LEU:HD23	1.67	0.76
1:D:328:GLN:HG2	1:D:368:ILE:HD11	1.67	0.76
1:H:328:GLN:HG2	1:H:368:ILE:HD11	1.67	0.76
1:C:79:LEU:HD11	1:C:92:LEU:HD23	1.67	0.76
1:E:79:LEU:HD11	1:E:92:LEU:HD23	1.67	0.75
1:C:264:GLU:OE1	1:C:307:ARG:NH2	2.20	0.75
1:B:264:GLU:OE1	1:B:307:ARG:NH2	2.20	0.75
1:H:79:LEU:HD11	1:H:92:LEU:HD23	1.67	0.75
1:G:264:GLU:OE1	1:G:307:ARG:NH2	2.20	0.75
1:A:103:TRP:CZ3	1:A:110:ARG:HA	2.21	0.75
1:D:264:GLU:OE1	1:D:307:ARG:NH2	2.20	0.75
1:E:264:GLU:OE1	1:E:307:ARG:NH2	2.20	0.75
1:H:264:GLU:OE1	1:H:307:ARG:NH2	2.20	0.75
1:A:264:GLU:OE1	1:A:307:ARG:NH2	2.20	0.74
1:A:328:GLN:HG2	1:A:368:ILE:HD11	1.67	0.74
1:C:328:GLN:HG2	1:C:368:ILE:HD11	1.67	0.74
1:F:403:ARG:O	1:F:423:GLN:NE2	2.17	0.74
1:F:103:TRP:CZ3	1:F:110:ARG:HA	2.21	0.74
1:H:403:ARG:O	1:H:423:GLN:NE2	2.17	0.74
1:D:79:LEU:HD11	1:D:92:LEU:HD23	1.67	0.74
1:H:152:LEU:HD11	1:H:187:ILE:HG23	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:79:LEU:HD11	1:F:92:LEU:HD23	1.67	0.74
1:F:264:GLU:OE1	1:F:307:ARG:NH2	2.20	0.74
1:G:79:LEU:HD11	1:G:92:LEU:HD23	1.67	0.74
1:C:403:ARG:O	1:C:423:GLN:NE2	2.17	0.73
1:E:103:TRP:HD1	1:E:150:GLN:HE22	1.37	0.73
1:G:103:TRP:CZ3	1:G:110:ARG:HA	2.23	0.73
1:G:117:CYS:HB3	1:G:156:ASN:HD21	1.54	0.73
1:A:216:ARG:HH21	1:H:688:GLN:HB2	1.54	0.72
1:B:688:GLN:HB2	1:C:216:ARG:HH21	1.53	0.72
1:D:219:ASP:HB3	1:D:222:LEU:HB3	1.72	0.72
1:E:103:TRP:CZ3	1:E:110:ARG:HA	2.24	0.72
1:E:403:ARG:O	1:E:423:GLN:NE2	2.17	0.72
1:A:103:TRP:HD1	1:A:150:GLN:HE22	1.38	0.72
1:B:219:ASP:HB3	1:B:222:LEU:HB3	1.72	0.72
1:D:160:VAL:HG13	1:D:164:GLY:HA3	1.72	0.72
1:F:219:ASP:HB3	1:F:222:LEU:HB3	1.72	0.71
1:H:219:ASP:HB3	1:H:222:LEU:HB3	1.72	0.71
1:A:219:ASP:HB3	1:A:222:LEU:HB3	1.72	0.71
1:E:688:GLN:HB2	1:F:216:ARG:HH21	1.56	0.71
1:F:688:GLN:HB2	1:G:216:ARG:HH21	1.55	0.71
1:C:219:ASP:HB3	1:C:222:LEU:HB3	1.72	0.70
1:D:103:TRP:CZ3	1:D:110:ARG:HA	2.26	0.70
1:E:219:ASP:HB3	1:E:222:LEU:HB3	1.72	0.70
1:G:688:GLN:HB2	1:H:216:ARG:HH21	1.56	0.70
1:E:103:TRP:HZ3	1:E:110:ARG:HA	1.55	0.69
1:G:219:ASP:HB3	1:G:222:LEU:HB3	1.72	0.69
1:B:257:LEU:HD23	1:B:266:LEU:HD11	1.74	0.69
1:G:257:LEU:HD23	1:G:266:LEU:HD11	1.74	0.69
1:D:103:TRP:HZ3	1:D:110:ARG:HA	1.57	0.69
1:F:257:LEU:HD23	1:F:266:LEU:HD11	1.74	0.69
1:A:688:GLN:HB2	1:B:216:ARG:HH21	1.56	0.69
1:A:257:LEU:HD23	1:A:266:LEU:HD11	1.74	0.69
1:H:257:LEU:HD23	1:H:266:LEU:HD11	1.74	0.68
1:C:257:LEU:HD23	1:C:266:LEU:HD11	1.74	0.68
1:E:257:LEU:HD23	1:E:266:LEU:HD11	1.74	0.68
1:A:103:TRP:HZ3	1:A:110:ARG:HA	1.59	0.68
1:C:147:LEU:O	1:C:151:ILE:HG12	1.94	0.68
1:D:257:LEU:HD23	1:D:266:LEU:HD11	1.74	0.68
1:H:157:ARG:HD2	1:H:194:HIS:HB2	1.77	0.67
1:C:103:TRP:HZ3	1:C:110:ARG:HA	1.60	0.67
1:G:103:TRP:HD1	1:G:150:GLN:NE2	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:688:GLN:HB2	1:E:216:ARG:HH21	1.59	0.66
1:G:103:TRP:CD1	1:G:150:GLN:HE22	2.13	0.66
1:C:688:GLN:HB2	1:D:216:ARG:HH21	1.58	0.66
1:D:117:CYS:HB3	1:D:156:ASN:HD21	1.61	0.66
1:F:103:TRP:HZ3	1:F:110:ARG:HA	1.59	0.65
1:C:103:TRP:CZ3	1:C:110:ARG:HA	2.31	0.65
1:E:117:CYS:HB3	1:E:156:ASN:HD21	1.61	0.65
1:E:103:TRP:HD1	1:E:150:GLN:NE2	1.94	0.65
1:C:117:CYS:HB3	1:C:156:ASN:HD21	1.61	0.64
1:B:152:LEU:HD11	1:B:187:ILE:HG23	1.79	0.63
1:D:196:GLU:HG2	1:D:200:GLN:NE2	2.13	0.63
1:G:196:GLU:HG2	1:G:200:GLN:NE2	2.13	0.63
1:C:103:TRP:HD1	1:C:150:GLN:HE22	1.44	0.63
1:G:375:LYS:HA	1:G:402:PRO:HG3	1.81	0.63
1:H:375:LYS:HA	1:H:402:PRO:HG3	1.81	0.63
1:F:375:LYS:HA	1:F:402:PRO:HG3	1.81	0.63
1:C:375:LYS:HA	1:C:402:PRO:HG3	1.81	0.63
1:E:375:LYS:HA	1:E:402:PRO:HG3	1.81	0.63
1:B:375:LYS:HA	1:B:402:PRO:HG3	1.81	0.63
1:D:375:LYS:HA	1:D:402:PRO:HG3	1.81	0.63
1:B:196:GLU:HG2	1:B:200:GLN:NE2	2.13	0.63
1:A:103:TRP:HD1	1:A:150:GLN:NE2	1.97	0.63
1:A:375:LYS:HA	1:A:402:PRO:HG3	1.80	0.63
1:G:159:ARG:HH12	1:G:163:ILE:HB	1.65	0.62
1:B:159:ARG:HH12	1:B:163:ILE:HB	1.64	0.62
1:F:159:ARG:HH12	1:F:163:ILE:HB	1.64	0.62
1:A:542:ALA:O	1:A:546:LEU:HB2	2.00	0.62
1:C:542:ALA:O	1:C:546:LEU:HB2	1.99	0.62
1:E:159:ARG:HH12	1:E:163:ILE:HB	1.64	0.62
1:F:196:GLU:HG2	1:F:200:GLN:NE2	2.13	0.62
1:B:542:ALA:O	1:B:546:LEU:HB2	2.00	0.62
1:C:159:ARG:HH12	1:C:163:ILE:HB	1.64	0.61
1:H:157:ARG:NH2	2:H:801:A1EIV:O13	2.33	0.61
1:H:159:ARG:HH12	1:H:163:ILE:HB	1.64	0.61
1:H:542:ALA:O	1:H:546:LEU:HB2	2.00	0.61
1:D:542:ALA:O	1:D:546:LEU:HB2	2.00	0.61
1:H:196:GLU:HG2	1:H:200:GLN:NE2	2.13	0.61
1:F:542:ALA:O	1:F:546:LEU:HB2	2.00	0.61
1:A:159:ARG:HH12	1:A:163:ILE:HB	1.64	0.61
1:C:146:ARG:O	1:C:149:GLU:HG2	2.01	0.61
1:C:196:GLU:HG2	1:C:200:GLN:NE2	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:ARG:HB2	1:C:214:TRP:HE1	1.66	0.61
1:F:175:ARG:HB2	1:F:214:TRP:HE1	1.66	0.61
1:G:542:ALA:O	1:G:546:LEU:HB2	2.00	0.61
1:C:152:LEU:HD11	1:C:187:ILE:HG23	1.82	0.60
1:H:175:ARG:HB2	1:H:214:TRP:HE1	1.66	0.60
1:F:286:GLU:OE1	1:F:286:GLU:HA	2.01	0.60
1:H:146:ARG:O	1:H:149:GLU:HG2	2.01	0.60
1:B:175:ARG:HB2	1:B:214:TRP:HE1	1.66	0.60
1:G:103:TRP:HZ3	1:G:110:ARG:HA	1.67	0.60
1:H:126:LEU:HD11	1:H:159:ARG:HG2	1.84	0.60
1:A:196:GLU:HG2	1:A:200:GLN:NE2	2.13	0.60
1:E:542:ALA:O	1:E:546:LEU:HB2	1.99	0.60
1:A:146:ARG:O	1:A:149:GLU:HG3	2.01	0.60
1:D:175:ARG:HB2	1:D:214:TRP:HE1	1.66	0.60
1:F:126:LEU:HD11	1:F:159:ARG:HG2	1.84	0.60
1:G:286:GLU:HA	1:G:286:GLU:OE1	2.01	0.60
1:A:175:ARG:HB2	1:A:214:TRP:HE1	1.66	0.60
1:B:286:GLU:HA	1:B:286:GLU:OE1	2.01	0.60
1:B:153:VAL:HG22	1:B:156:ASN:HD22	1.66	0.60
1:C:103:TRP:HD1	1:C:150:GLN:NE2	1.99	0.60
1:B:126:LEU:HD11	1:B:159:ARG:HG2	1.84	0.60
1:E:286:GLU:HA	1:E:286:GLU:OE1	2.01	0.60
1:G:175:ARG:HB2	1:G:214:TRP:HE1	1.66	0.60
1:E:175:ARG:HB2	1:E:214:TRP:HE1	1.66	0.60
1:D:258:ALA:HA	1:D:267:ARG:HA	1.84	0.60
1:A:117:CYS:HB3	1:A:156:ASN:HD21	1.66	0.59
1:C:258:ALA:HA	1:C:267:ARG:HA	1.85	0.59
1:A:286:GLU:OE1	1:A:286:GLU:HA	2.01	0.59
1:E:258:ALA:HA	1:E:267:ARG:HA	1.84	0.59
1:C:286:GLU:OE1	1:C:286:GLU:HA	2.01	0.59
1:D:286:GLU:OE1	1:D:286:GLU:HA	2.01	0.59
1:E:126:LEU:HD11	1:E:159:ARG:HG2	1.84	0.59
1:H:258:ALA:HA	1:H:267:ARG:HA	1.84	0.59
1:A:281:LYS:HB3	1:H:484:ARG:HG2	1.85	0.59
1:G:484:ARG:HG2	1:H:281:LYS:HB3	1.84	0.59
1:F:258:ALA:HA	1:F:267:ARG:HA	1.84	0.59
1:E:196:GLU:HG2	1:E:200:GLN:NE2	2.13	0.59
1:F:635:CYS:O	1:F:641:LYS:NZ	2.31	0.59
1:A:126:LEU:HD11	1:A:159:ARG:HG2	1.84	0.58
1:B:568:TYR:OH	1:B:594:ASP:OD1	2.19	0.58
1:C:126:LEU:HD11	1:C:159:ARG:HG2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:484:ARG:HG2	1:E:281:LYS:HB3	1.85	0.58
1:F:568:TYR:OH	1:F:594:ASP:OD1	2.19	0.58
1:H:286:GLU:OE1	1:H:286:GLU:HA	2.01	0.58
1:C:103:TRP:CD1	1:C:150:GLN:HE22	2.20	0.58
1:G:126:LEU:HD11	1:G:159:ARG:HG2	1.84	0.58
1:A:258:ALA:HA	1:A:267:ARG:HA	1.84	0.58
1:A:376:ARG:NH1	1:A:472:GLU:OE2	2.37	0.58
1:B:258:ALA:HA	1:B:267:ARG:HA	1.84	0.58
1:C:568:TYR:OH	1:C:594:ASP:OD1	2.19	0.58
1:E:158:ASP:OD1	1:E:194:HIS:NE2	2.35	0.58
1:E:626:LEU:HD12	1:E:663:PRO:HG3	1.86	0.58
1:F:484:ARG:HG2	1:G:281:LYS:HB3	1.85	0.58
1:D:626:LEU:HD12	1:D:663:PRO:HG3	1.86	0.58
1:F:376:ARG:NH1	1:F:472:GLU:OE2	2.37	0.58
1:G:376:ARG:NH1	1:G:472:GLU:OE2	2.37	0.58
1:B:376:ARG:NH1	1:B:472:GLU:OE2	2.37	0.58
1:E:376:ARG:NH1	1:E:472:GLU:OE2	2.37	0.58
1:A:626:LEU:HD12	1:A:663:PRO:HG3	1.86	0.58
1:B:272:LEU:HA	1:B:344:ILE:HG21	1.86	0.58
1:G:258:ALA:HA	1:G:267:ARG:HA	1.84	0.58
1:G:272:LEU:HA	1:G:344:ILE:HG21	1.86	0.58
1:A:272:LEU:HA	1:A:344:ILE:HG21	1.86	0.58
1:C:626:LEU:HD12	1:C:663:PRO:HG3	1.86	0.58
1:B:626:LEU:HD12	1:B:663:PRO:HG3	1.86	0.57
1:F:272:LEU:HA	1:F:344:ILE:HG21	1.86	0.57
1:F:563:ASP:HA	1:F:615:ARG:HB3	1.86	0.57
1:F:626:LEU:HD12	1:F:663:PRO:HG3	1.86	0.57
1:H:376:ARG:NH1	1:H:472:GLU:OE2	2.37	0.57
1:A:563:ASP:HA	1:A:615:ARG:HB3	1.86	0.57
1:A:568:TYR:OH	1:A:594:ASP:OD1	2.19	0.57
1:C:272:LEU:HA	1:C:344:ILE:HG21	1.86	0.57
1:E:563:ASP:HA	1:E:615:ARG:HB3	1.86	0.57
1:G:563:ASP:HA	1:G:615:ARG:HB3	1.86	0.57
1:B:563:ASP:HA	1:B:615:ARG:HB3	1.86	0.57
1:D:272:LEU:HA	1:D:344:ILE:HG21	1.86	0.57
1:D:563:ASP:HA	1:D:615:ARG:HB3	1.86	0.57
1:E:272:LEU:HA	1:E:344:ILE:HG21	1.86	0.57
1:H:626:LEU:HD12	1:H:663:PRO:HG3	1.86	0.57
1:D:376:ARG:NH1	1:D:472:GLU:OE2	2.37	0.57
1:H:154:ALA:HA	1:H:157:ARG:HB2	1.87	0.57
1:C:484:ARG:HG2	1:D:281:LYS:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:272:LEU:HA	1:H:344:ILE:HG21	1.86	0.57
1:D:303:LEU:HD12	1:D:308:PHE:CE2	2.40	0.57
1:G:626:LEU:HD12	1:G:663:PRO:HG3	1.86	0.57
1:A:484:ARG:HG2	1:B:281:LYS:HB3	1.87	0.57
1:B:103:TRP:CE3	2:B:801:A1EIV:S19	2.98	0.57
1:D:146:ARG:O	1:D:149:GLU:HG2	2.04	0.57
1:A:103:TRP:CD1	1:A:150:GLN:HE22	2.19	0.57
1:C:303:LEU:HD12	1:C:308:PHE:CE2	2.40	0.57
1:G:303:LEU:HD12	1:G:308:PHE:CE2	2.40	0.57
1:C:563:ASP:HA	1:C:615:ARG:HB3	1.86	0.56
1:A:303:LEU:HD12	1:A:308:PHE:CE2	2.40	0.56
1:H:303:LEU:HD12	1:H:308:PHE:CE2	2.40	0.56
1:C:376:ARG:NH1	1:C:472:GLU:OE2	2.37	0.56
1:D:568:TYR:OH	1:D:594:ASP:OD1	2.19	0.56
1:E:568:TYR:OH	1:E:594:ASP:OD1	2.19	0.56
1:H:563:ASP:HA	1:H:615:ARG:HB3	1.86	0.56
1:E:170:ASN:HA	1:E:173:LYS:HD2	1.88	0.56
1:E:303:LEU:HD12	1:E:308:PHE:CE2	2.40	0.56
1:E:484:ARG:HG2	1:F:281:LYS:HB3	1.87	0.56
1:B:303:LEU:HD12	1:B:308:PHE:CE2	2.40	0.56
1:D:137:GLU:HB2	1:D:140:THR:HG22	1.86	0.56
1:G:158:ASP:OD1	1:G:194:HIS:NE2	2.35	0.56
1:F:117:CYS:SG	1:F:151:ILE:HA	2.45	0.56
1:F:303:LEU:HD12	1:F:308:PHE:CE2	2.40	0.56
1:G:170:ASN:HA	1:G:173:LYS:HD2	1.88	0.56
1:H:170:ASN:HA	1:H:173:LYS:HD2	1.88	0.56
1:B:695:ILE:O	1:B:699:LEU:N	2.39	0.56
1:E:695:ILE:O	1:E:699:LEU:N	2.39	0.55
1:G:486:ASN:O	1:G:512:ARG:NH2	2.38	0.55
1:B:484:ARG:HG2	1:C:281:LYS:HB3	1.88	0.55
1:H:568:TYR:OH	1:H:594:ASP:OD1	2.19	0.55
1:E:417:VAL:HG22	1:E:443:LEU:HD22	1.89	0.55
1:F:417:VAL:HG22	1:F:443:LEU:HD22	1.89	0.55
1:D:417:VAL:HG22	1:D:443:LEU:HD22	1.89	0.55
1:D:170:ASN:HA	1:D:173:LYS:HD2	1.88	0.55
1:F:170:ASN:HA	1:F:173:LYS:HD2	1.88	0.55
1:G:417:VAL:HG22	1:G:443:LEU:HD22	1.89	0.55
1:A:170:ASN:HA	1:A:173:LYS:HD2	1.88	0.55
1:B:117:CYS:HB3	1:B:156:ASN:HD21	1.72	0.55
1:C:146:ARG:HG2	1:C:183:SER:OG	2.06	0.55
1:C:170:ASN:HA	1:C:173:LYS:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:VAL:HG22	1:C:443:LEU:HD22	1.89	0.55
1:C:695:ILE:O	1:C:699:LEU:N	2.39	0.55
1:G:377:LEU:HD23	1:G:390:ALA:HB2	1.89	0.55
1:H:417:VAL:HG22	1:H:443:LEU:HD22	1.89	0.55
1:H:158:ASP:OD1	1:H:194:HIS:NE2	2.35	0.55
1:A:417:VAL:HG22	1:A:443:LEU:HD22	1.89	0.54
1:D:159:ARG:HA	1:D:162:ARG:HE	1.72	0.54
1:A:351:ALA:O	1:A:355:ILE:HG12	2.08	0.54
1:B:170:ASN:HA	1:B:173:LYS:HD2	1.88	0.54
1:C:351:ALA:O	1:C:355:ILE:HG12	2.08	0.54
1:D:486:ASN:O	1:D:512:ARG:NH2	2.38	0.54
1:H:351:ALA:O	1:H:355:ILE:HG12	2.08	0.54
1:B:351:ALA:O	1:B:355:ILE:HG12	2.08	0.54
1:B:417:VAL:HG22	1:B:443:LEU:HD22	1.89	0.54
1:D:351:ALA:O	1:D:355:ILE:HG12	2.08	0.54
1:E:146:ARG:O	1:E:149:GLU:HG2	2.07	0.54
1:E:152:LEU:HD11	1:E:187:ILE:HG23	1.89	0.54
1:G:351:ALA:O	1:G:355:ILE:HG12	2.08	0.54
1:E:377:LEU:HD23	1:E:390:ALA:HB2	1.89	0.54
1:F:695:ILE:O	1:F:699:LEU:N	2.39	0.54
1:E:486:ASN:O	1:E:512:ARG:NH2	2.38	0.54
1:F:377:LEU:HD23	1:F:390:ALA:HB2	1.89	0.54
1:G:441:ASP:OD1	1:G:503:TYR:OH	2.22	0.54
1:H:695:ILE:O	1:H:699:LEU:N	2.39	0.54
1:C:441:ASP:OD1	1:C:503:TYR:OH	2.22	0.54
1:F:148:LEU:HA	1:F:151:ILE:HG12	1.89	0.54
1:G:575:GLN:HE22	1:G:579:LEU:HD11	1.73	0.54
1:H:441:ASP:OD1	1:H:503:TYR:OH	2.22	0.54
1:A:486:ASN:O	1:A:512:ARG:NH2	2.38	0.54
1:C:377:LEU:HD23	1:C:390:ALA:HB2	1.89	0.54
1:D:377:LEU:HD23	1:D:390:ALA:HB2	1.89	0.54
1:H:377:LEU:HD23	1:H:390:ALA:HB2	1.89	0.54
1:B:377:LEU:HD23	1:B:390:ALA:HB2	1.89	0.53
1:D:575:GLN:HE22	1:D:579:LEU:HD11	1.73	0.53
1:F:351:ALA:O	1:F:355:ILE:HG12	2.08	0.53
1:G:568:TYR:OH	1:G:594:ASP:OD1	2.19	0.53
1:B:153:VAL:HG22	1:B:156:ASN:ND2	2.23	0.53
1:E:575:GLN:HE22	1:E:579:LEU:HD11	1.73	0.53
1:A:695:ILE:O	1:A:699:LEU:N	2.39	0.53
1:E:351:ALA:O	1:E:355:ILE:HG12	2.08	0.53
1:G:635:CYS:SG	1:G:640:HIS:ND1	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:441:ASP:OD1	1:F:503:TYR:OH	2.22	0.53
1:A:377:LEU:HD23	1:A:390:ALA:HB2	1.89	0.53
1:D:635:CYS:O	1:D:641:LYS:NZ	2.31	0.53
1:E:287:VAL:O	1:E:290:SER:OG	2.25	0.53
1:G:234:ALA:O	1:G:242:GLN:NE2	2.42	0.53
1:G:695:ILE:O	1:G:699:LEU:N	2.39	0.53
1:H:696:ILE:HA	1:H:699:LEU:HB2	1.91	0.53
1:G:99:VAL:HG12	1:G:150:GLN:HE21	1.73	0.53
1:H:234:ALA:O	1:H:242:GLN:NE2	2.42	0.53
1:B:234:ALA:O	1:B:242:GLN:NE2	2.42	0.53
1:B:635:CYS:SG	1:B:640:HIS:ND1	2.72	0.53
1:C:431:GLU:OE2	1:C:434:ARG:NH2	2.42	0.53
1:E:103:TRP:CD1	1:E:150:GLN:HE22	2.21	0.53
1:G:146:ARG:O	1:G:149:GLU:HG2	2.09	0.53
1:H:575:GLN:HE22	1:H:579:LEU:HD11	1.73	0.53
1:E:103:TRP:HA	1:E:103:TRP:CE3	2.44	0.52
1:E:234:ALA:O	1:E:242:GLN:NE2	2.42	0.52
1:F:465:ARG:HG3	1:F:468:ARG:HH21	1.74	0.52
1:E:465:ARG:HG3	1:E:468:ARG:HH21	1.74	0.52
1:G:465:ARG:HG3	1:G:468:ARG:HH21	1.74	0.52
1:A:696:ILE:HA	1:A:699:LEU:HB2	1.91	0.52
1:B:696:ILE:HA	1:B:699:LEU:HB2	1.91	0.52
1:C:575:GLN:HE22	1:C:579:LEU:HD11	1.73	0.52
1:D:350:CYS:SG	1:D:392:ARG:HG3	2.50	0.52
1:E:431:GLU:OE2	1:E:434:ARG:NH2	2.42	0.52
1:F:575:GLN:HE22	1:F:579:LEU:HD11	1.73	0.52
1:F:696:ILE:HA	1:F:699:LEU:HB2	1.91	0.52
1:B:378:VAL:HB	1:B:402:PRO:HG2	1.92	0.52
1:B:431:GLU:OE2	1:B:434:ARG:NH2	2.42	0.52
1:E:350:CYS:SG	1:E:392:ARG:HG3	2.50	0.52
1:E:635:CYS:O	1:E:641:LYS:NZ	2.31	0.52
1:A:378:VAL:HB	1:A:402:PRO:HG2	1.92	0.52
1:A:465:ARG:HG3	1:A:468:ARG:HH21	1.74	0.52
1:C:234:ALA:O	1:C:242:GLN:NE2	2.42	0.52
1:D:465:ARG:HG3	1:D:468:ARG:HH21	1.74	0.52
1:G:350:CYS:SG	1:G:392:ARG:HG3	2.50	0.52
1:G:635:CYS:O	1:G:641:LYS:NZ	2.31	0.52
1:A:575:GLN:HE22	1:A:579:LEU:HD11	1.73	0.52
1:C:486:ASN:O	1:C:512:ARG:NH2	2.38	0.52
1:D:234:ALA:O	1:D:242:GLN:NE2	2.42	0.52
1:F:234:ALA:O	1:F:242:GLN:NE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:486:ASN:O	1:F:512:ARG:NH2	2.38	0.52
1:H:465:ARG:HG3	1:H:468:ARG:HH21	1.74	0.52
1:A:234:ALA:O	1:A:242:GLN:NE2	2.42	0.52
1:B:575:GLN:HE22	1:B:579:LEU:HD11	1.73	0.52
1:C:153:VAL:HG22	1:C:156:ASN:ND2	2.24	0.52
1:D:695:ILE:O	1:D:699:LEU:N	2.39	0.52
1:F:350:CYS:SG	1:F:392:ARG:HG3	2.50	0.52
1:A:350:CYS:SG	1:A:392:ARG:HG3	2.50	0.52
1:C:465:ARG:HG3	1:C:468:ARG:HH21	1.74	0.52
1:H:378:VAL:HB	1:H:402:PRO:HG2	1.92	0.52
1:A:103:TRP:HA	1:A:103:TRP:CE3	2.45	0.52
1:B:350:CYS:SG	1:B:392:ARG:HG3	2.50	0.52
1:C:350:CYS:SG	1:C:392:ARG:HG3	2.50	0.52
1:E:378:VAL:HB	1:E:402:PRO:HG2	1.92	0.52
1:G:696:ILE:HA	1:G:699:LEU:HB2	1.91	0.52
1:G:431:GLU:OE2	1:G:434:ARG:NH2	2.42	0.52
1:C:339:LEU:HD11	1:C:383:ASN:HD22	1.76	0.51
1:C:696:ILE:HA	1:C:699:LEU:HB2	1.91	0.51
1:G:378:VAL:HB	1:G:402:PRO:HG2	1.92	0.51
1:H:339:LEU:HD11	1:H:383:ASN:HD22	1.76	0.51
1:B:465:ARG:HG3	1:B:468:ARG:HH21	1.74	0.51
1:E:441:ASP:OD1	1:E:503:TYR:OH	2.22	0.51
1:G:339:LEU:HD11	1:G:383:ASN:HD22	1.75	0.51
1:D:696:ILE:HA	1:D:699:LEU:HB2	1.91	0.51
1:E:137:GLU:O	1:E:140:THR:HG22	2.11	0.51
1:E:339:LEU:HD11	1:E:383:ASN:HD22	1.75	0.51
1:E:566:ILE:HG21	1:E:577:ALA:HB1	1.93	0.51
1:B:143:GLN:HG2	1:B:146:ARG:HH21	1.76	0.51
1:B:566:ILE:HG21	1:B:577:ALA:HB1	1.93	0.51
1:D:117:CYS:HB3	1:D:156:ASN:ND2	2.25	0.51
1:F:339:LEU:HD11	1:F:383:ASN:HD22	1.76	0.51
1:F:663:PRO:HB2	1:F:668:LEU:HD11	1.93	0.51
1:A:431:GLU:OE2	1:A:434:ARG:NH2	2.42	0.51
1:A:441:ASP:OD1	1:A:503:TYR:OH	2.22	0.51
1:A:663:PRO:HB2	1:A:668:LEU:HD11	1.93	0.51
1:C:566:ILE:HG21	1:C:577:ALA:HB1	1.93	0.51
1:D:103:TRP:HA	1:D:103:TRP:CE3	2.45	0.51
1:D:339:LEU:HD11	1:D:383:ASN:HD22	1.76	0.51
1:G:275:ALA:HB1	1:G:341:ALA:HA	1.93	0.51
1:G:663:PRO:HB2	1:G:668:LEU:HD11	1.93	0.51
1:H:663:PRO:HB2	1:H:668:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:CYS:HB3	1:A:156:ASN:ND2	2.25	0.51
1:A:275:ALA:HB1	1:A:341:ALA:HA	1.93	0.51
1:D:157:ARG:HG2	1:D:191:MET:SD	2.51	0.51
1:D:378:VAL:HB	1:D:402:PRO:HG2	1.92	0.51
1:D:431:GLU:OE2	1:D:434:ARG:NH2	2.42	0.51
1:F:566:ILE:HG21	1:F:577:ALA:HB1	1.93	0.51
1:H:350:CYS:SG	1:H:392:ARG:HG3	2.50	0.51
1:B:663:PRO:HB2	1:B:668:LEU:HD11	1.93	0.51
1:C:663:PRO:HB2	1:C:668:LEU:HD11	1.93	0.51
1:E:663:PRO:HB2	1:E:668:LEU:HD11	1.93	0.51
1:F:287:VAL:O	1:F:290:SER:OG	2.25	0.51
1:G:271:CYS:HA	1:G:274:VAL:HG12	1.93	0.51
1:B:339:LEU:HD11	1:B:383:ASN:HD22	1.76	0.51
1:C:275:ALA:HB1	1:C:341:ALA:HA	1.93	0.51
1:D:663:PRO:HB2	1:D:668:LEU:HD11	1.93	0.51
1:G:152:LEU:HD11	1:G:187:ILE:HG23	1.93	0.51
1:A:339:LEU:HD11	1:A:383:ASN:HD22	1.76	0.51
1:A:566:ILE:HG21	1:A:577:ALA:HB1	1.93	0.51
1:C:378:VAL:HB	1:C:402:PRO:HG2	1.92	0.51
1:D:566:ILE:HG21	1:D:577:ALA:HB1	1.93	0.51
1:E:696:ILE:HA	1:E:699:LEU:HB2	1.91	0.51
1:F:103:TRP:CE3	1:F:103:TRP:HA	2.46	0.51
1:F:271:CYS:HA	1:F:274:VAL:HG12	1.93	0.51
1:G:564:VAL:HB	1:G:591:VAL:HG22	1.93	0.51
1:H:271:CYS:HA	1:H:274:VAL:HG12	1.93	0.51
1:E:275:ALA:HB1	1:E:341:ALA:HA	1.93	0.50
1:F:378:VAL:HB	1:F:402:PRO:HG2	1.92	0.50
1:H:635:CYS:SG	1:H:640:HIS:ND1	2.72	0.50
1:A:152:LEU:HD11	1:A:187:ILE:HG23	1.91	0.50
1:B:531:LEU:HD12	1:B:534:HIS:CE1	2.46	0.50
1:D:564:VAL:HB	1:D:591:VAL:HG22	1.93	0.50
1:G:566:ILE:HG21	1:G:577:ALA:HB1	1.93	0.50
1:H:566:ILE:HG21	1:H:577:ALA:HB1	1.93	0.50
1:C:103:TRP:HA	1:C:103:TRP:CE3	2.45	0.50
1:E:564:VAL:HB	1:E:591:VAL:HG22	1.93	0.50
1:H:486:ASN:O	1:H:512:ARG:NH2	2.38	0.50
1:B:157:ARG:HD3	1:B:190:HIS:O	2.11	0.50
1:B:275:ALA:HB1	1:B:341:ALA:HA	1.93	0.50
1:C:271:CYS:HA	1:C:274:VAL:HG12	1.93	0.50
1:E:444:LEU:HD22	1:E:474:LYS:HG2	1.93	0.50
1:H:564:VAL:HB	1:H:591:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:LEU:HD22	1:A:474:LYS:HG2	1.93	0.50
1:F:431:GLU:OE2	1:F:434:ARG:NH2	2.42	0.50
1:F:444:LEU:HD22	1:F:474:LYS:HG2	1.93	0.50
1:F:564:VAL:HB	1:F:591:VAL:HG22	1.94	0.50
1:G:531:LEU:HD12	1:G:534:HIS:CE1	2.46	0.50
1:D:531:LEU:HD12	1:D:534:HIS:CE1	2.46	0.50
1:A:564:VAL:HB	1:A:591:VAL:HG22	1.94	0.50
1:B:105:LEU:HB2	1:B:109:GLY:HA2	1.94	0.50
1:B:564:VAL:HB	1:B:591:VAL:HG22	1.93	0.50
1:C:531:LEU:HD12	1:C:534:HIS:CE1	2.46	0.50
1:C:564:VAL:HB	1:C:591:VAL:HG22	1.94	0.50
1:D:159:ARG:NH1	1:D:163:ILE:HB	2.26	0.50
1:F:531:LEU:HD12	1:F:534:HIS:CE1	2.46	0.50
1:H:155:GLU:H	1:H:155:GLU:CD	2.07	0.50
1:B:444:LEU:HD22	1:B:474:LYS:HG2	1.93	0.50
1:C:105:LEU:HB2	1:C:109:GLY:HA2	1.94	0.50
1:D:444:LEU:HD22	1:D:474:LYS:HG2	1.93	0.50
1:E:271:CYS:HA	1:E:274:VAL:HG12	1.93	0.50
1:F:169:LEU:O	1:F:173:LYS:HG3	2.12	0.50
1:C:169:LEU:O	1:C:173:LYS:HG3	2.12	0.50
1:D:105:LEU:HB2	1:D:109:GLY:HA2	1.94	0.50
1:D:271:CYS:HA	1:D:274:VAL:HG12	1.93	0.50
1:E:531:LEU:HD12	1:E:534:HIS:CE1	2.46	0.50
1:G:241:VAL:O	1:G:245:MET:HG3	2.12	0.50
1:H:635:CYS:O	1:H:641:LYS:NZ	2.31	0.50
1:A:271:CYS:HA	1:A:274:VAL:HG12	1.93	0.49
1:A:287:VAL:O	1:A:290:SER:OG	2.25	0.49
1:B:271:CYS:HA	1:B:274:VAL:HG12	1.93	0.49
1:C:117:CYS:HB3	1:C:156:ASN:ND2	2.27	0.49
1:D:275:ALA:HB1	1:D:341:ALA:HA	1.93	0.49
1:E:105:LEU:HB2	1:E:109:GLY:HA2	1.94	0.49
1:F:105:LEU:HB2	1:F:109:GLY:HA2	1.94	0.49
1:F:241:VAL:O	1:F:245:MET:HG3	2.12	0.49
1:H:275:ALA:HB1	1:H:341:ALA:HA	1.93	0.49
1:A:105:LEU:HB2	1:A:109:GLY:HA2	1.94	0.49
1:B:103:TRP:CZ3	2:B:801:A1EIV:S19	3.05	0.49
1:D:93:ALA:O	1:D:97:GLN:HG2	2.12	0.49
1:G:143:GLN:HE21	1:G:146:ARG:HH21	1.59	0.49
1:G:444:LEU:HD22	1:G:474:LYS:HG2	1.93	0.49
1:H:531:LEU:HD12	1:H:534:HIS:CE1	2.46	0.49
1:A:531:LEU:HD12	1:A:534:HIS:CE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:LEU:HD22	1:C:474:LYS:HG2	1.93	0.49
1:H:444:LEU:HD22	1:H:474:LYS:HG2	1.93	0.49
1:A:241:VAL:O	1:A:245:MET:HG3	2.12	0.49
1:D:169:LEU:O	1:D:173:LYS:HG3	2.12	0.49
1:E:93:ALA:O	1:E:97:GLN:HG2	2.12	0.49
1:F:117:CYS:HB3	1:F:156:ASN:HD21	1.77	0.49
1:F:275:ALA:HB1	1:F:341:ALA:HA	1.93	0.49
1:G:105:LEU:HB2	1:G:109:GLY:HA2	1.94	0.49
1:H:169:LEU:O	1:H:173:LYS:HG3	2.12	0.49
1:A:153:VAL:HG22	1:A:156:ASN:ND2	2.27	0.49
1:C:93:ALA:O	1:C:97:GLN:HG2	2.12	0.49
1:C:635:CYS:SG	1:C:640:HIS:ND1	2.72	0.49
1:B:93:ALA:O	1:B:97:GLN:HG2	2.12	0.49
1:C:241:VAL:O	1:C:245:MET:HG3	2.12	0.49
1:E:635:CYS:SG	1:E:640:HIS:ND1	2.72	0.49
1:H:105:LEU:HB2	1:H:109:GLY:HA2	1.94	0.49
1:A:93:ALA:O	1:A:97:GLN:HG2	2.13	0.49
1:A:169:LEU:O	1:A:173:LYS:HG3	2.12	0.49
1:E:169:LEU:O	1:E:173:LYS:HG3	2.12	0.49
1:H:241:VAL:O	1:H:245:MET:HG3	2.12	0.49
1:A:146:ARG:HG2	1:A:183:SER:OG	2.13	0.49
1:B:339:LEU:HD12	1:B:386:LYS:HD3	1.95	0.49
1:C:216:ARG:HG2	1:C:253:TRP:CZ3	2.48	0.49
1:D:241:VAL:O	1:D:245:MET:HG3	2.12	0.49
1:B:169:LEU:O	1:B:173:LYS:HG3	2.12	0.48
1:F:93:ALA:O	1:F:97:GLN:HG2	2.12	0.48
1:H:93:ALA:O	1:H:97:GLN:HG2	2.12	0.48
1:H:431:GLU:OE2	1:H:434:ARG:NH2	2.42	0.48
1:A:216:ARG:HG2	1:A:253:TRP:CZ3	2.48	0.48
1:D:216:ARG:HG2	1:D:253:TRP:CZ3	2.48	0.48
1:D:339:LEU:HD12	1:D:386:LYS:HD3	1.95	0.48
1:G:93:ALA:O	1:G:97:GLN:HG2	2.12	0.48
1:H:137:GLU:O	1:H:140:THR:HG22	2.13	0.48
1:A:137:GLU:O	1:A:140:THR:HG22	2.13	0.48
1:B:241:VAL:O	1:B:245:MET:HG3	2.12	0.48
1:F:635:CYS:SG	1:F:640:HIS:ND1	2.72	0.48
1:E:339:LEU:HD12	1:E:386:LYS:HD3	1.96	0.48
1:G:137:GLU:HB2	1:G:140:THR:HG22	1.95	0.48
1:G:169:LEU:O	1:G:173:LYS:HG3	2.12	0.48
1:B:216:ARG:HG2	1:B:253:TRP:CZ3	2.48	0.48
1:G:148:LEU:O	1:G:152:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:LEU:HB3	1:B:589:PHE:HB2	1.96	0.48
1:D:287:VAL:O	1:D:290:SER:OG	2.25	0.48
1:E:216:ARG:HG2	1:E:253:TRP:CZ3	2.48	0.48
1:E:241:VAL:O	1:E:245:MET:HG3	2.12	0.48
1:F:129:LEU:HD23	1:F:148:LEU:HD13	1.96	0.48
1:H:61:VAL:HG23	1:H:63:ASP:H	1.79	0.48
1:B:61:VAL:HG23	1:B:63:ASP:H	1.79	0.48
1:C:420:TRP:CE2	1:C:473:LEU:HD22	2.49	0.48
1:H:420:TRP:CE2	1:H:473:LEU:HD22	2.49	0.48
1:A:339:LEU:HD12	1:A:386:LYS:HD3	1.95	0.48
1:B:137:GLU:HB2	1:B:140:THR:HG22	1.95	0.48
1:B:388:ALA:O	1:B:392:ARG:HG2	2.14	0.48
1:C:142:VAL:O	1:C:146:ARG:HG3	2.13	0.48
1:C:157:ARG:NH1	1:C:193:LYS:HE2	2.29	0.48
1:D:584:LEU:HB3	1:D:589:PHE:HB2	1.96	0.48
1:G:130:LEU:HD23	1:G:133:LEU:HD22	1.96	0.48
1:G:216:ARG:HG2	1:G:253:TRP:CZ3	2.48	0.48
1:G:388:ALA:O	1:G:392:ARG:HG2	2.14	0.48
1:A:420:TRP:CE2	1:A:473:LEU:HD22	2.49	0.47
1:C:137:GLU:HB2	1:C:140:THR:HG22	1.95	0.47
1:F:216:ARG:HG2	1:F:253:TRP:CZ3	2.48	0.47
1:F:388:ALA:O	1:F:392:ARG:HG2	2.14	0.47
1:H:271:CYS:SG	1:H:299:LEU:HD13	2.54	0.47
1:A:584:LEU:HB3	1:A:589:PHE:HB2	1.96	0.47
1:B:635:CYS:O	1:B:641:LYS:NZ	2.31	0.47
1:C:584:LEU:HB3	1:C:589:PHE:HB2	1.96	0.47
1:D:420:TRP:CE2	1:D:473:LEU:HD22	2.49	0.47
1:H:130:LEU:HD23	1:H:133:LEU:HD22	1.96	0.47
1:A:635:CYS:O	1:A:641:LYS:NZ	2.31	0.47
1:C:339:LEU:HD12	1:C:386:LYS:HD3	1.96	0.47
1:F:271:CYS:SG	1:F:299:LEU:HD13	2.55	0.47
1:F:339:LEU:HD12	1:F:386:LYS:HD3	1.95	0.47
1:B:420:TRP:CE2	1:B:473:LEU:HD22	2.49	0.47
1:B:486:ASN:O	1:B:512:ARG:NH2	2.38	0.47
1:C:388:ALA:O	1:C:392:ARG:HG2	2.14	0.47
1:D:271:CYS:SG	1:D:299:LEU:HD13	2.54	0.47
1:E:584:LEU:HB3	1:E:589:PHE:HB2	1.96	0.47
1:F:137:GLU:HB2	1:F:140:THR:HG22	1.95	0.47
1:H:216:ARG:HG2	1:H:253:TRP:CZ3	2.48	0.47
1:A:388:ALA:O	1:A:392:ARG:HG2	2.14	0.47
1:E:271:CYS:SG	1:E:299:LEU:HD13	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:93:ALA:N	1:G:143:GLN:OE1	2.47	0.47
1:G:146:ARG:HG2	1:G:183:SER:OG	2.13	0.47
1:G:420:TRP:CE2	1:G:473:LEU:HD22	2.49	0.47
1:H:151:ILE:C	1:H:153:VAL:H	2.17	0.47
1:H:339:LEU:HD12	1:H:386:LYS:HD3	1.96	0.47
1:H:388:ALA:O	1:H:392:ARG:HG2	2.14	0.47
1:B:271:CYS:SG	1:B:299:LEU:HD13	2.55	0.47
1:F:130:LEU:HD23	1:F:133:LEU:HD22	1.96	0.47
1:G:103:TRP:HA	1:G:103:TRP:CE3	2.49	0.47
1:G:271:CYS:SG	1:G:299:LEU:HD13	2.55	0.47
1:G:582:VAL:HG11	1:H:256:PRO:HD3	1.96	0.47
1:H:584:LEU:HB3	1:H:589:PHE:HB2	1.96	0.47
1:A:157:ARG:NH1	1:A:193:LYS:HE2	2.30	0.47
1:A:635:CYS:SG	1:A:640:HIS:ND1	2.72	0.47
1:B:408:SER:HA	1:B:478:ASN:HB3	1.97	0.47
1:D:61:VAL:HG23	1:D:63:ASP:H	1.79	0.47
1:E:388:ALA:O	1:E:392:ARG:HG2	2.14	0.47
1:E:408:SER:HA	1:E:478:ASN:HB3	1.97	0.47
1:E:420:TRP:CE2	1:E:473:LEU:HD22	2.49	0.47
1:F:61:VAL:HG23	1:F:63:ASP:H	1.79	0.47
1:G:339:LEU:HD12	1:G:386:LYS:HD3	1.95	0.47
1:H:157:ARG:HH22	2:H:801:A1EIV:P10	2.38	0.47
1:D:635:CYS:SG	1:D:640:HIS:ND1	2.72	0.47
1:G:117:CYS:HB3	1:G:156:ASN:ND2	2.26	0.47
1:A:408:SER:HA	1:A:478:ASN:HB3	1.97	0.47
1:C:129:LEU:HD23	1:C:148:LEU:HD13	1.96	0.47
1:D:130:LEU:HD23	1:D:133:LEU:HD22	1.96	0.47
1:D:408:SER:HA	1:D:478:ASN:HB3	1.97	0.47
1:F:584:LEU:HB3	1:F:589:PHE:HB2	1.96	0.47
1:G:584:LEU:HB3	1:G:589:PHE:HB2	1.96	0.47
1:A:61:VAL:HG23	1:A:63:ASP:H	1.79	0.47
1:A:239:GLN:HG2	1:H:480:SER:HB3	1.97	0.47
1:A:271:CYS:SG	1:A:299:LEU:HD13	2.54	0.47
1:C:130:LEU:HD23	1:C:133:LEU:HD22	1.96	0.47
1:C:271:CYS:SG	1:C:299:LEU:HD13	2.55	0.47
1:C:408:SER:HA	1:C:478:ASN:HB3	1.97	0.47
1:F:408:SER:HA	1:F:478:ASN:HB3	1.97	0.47
1:G:153:VAL:HG22	1:G:156:ASN:ND2	2.30	0.47
1:C:61:VAL:HG23	1:C:63:ASP:H	1.79	0.46
1:D:388:ALA:O	1:D:392:ARG:HG2	2.14	0.46
1:F:420:TRP:CE2	1:F:473:LEU:HD22	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:408:SER:HA	1:G:478:ASN:HB3	1.97	0.46
1:H:297:GLU:HB3	1:H:298:PRO:HD3	1.97	0.46
1:A:130:LEU:HD23	1:A:133:LEU:HD22	1.96	0.46
1:H:408:SER:HA	1:H:478:ASN:HB3	1.97	0.46
1:B:134:GLN:HE21	1:B:167:VAL:HG21	1.81	0.46
1:G:403:ARG:NH2	1:G:419:THR:OG1	2.49	0.46
1:E:130:LEU:HD23	1:E:133:LEU:HD22	1.96	0.46
1:A:134:GLN:HE21	1:A:167:VAL:HG21	1.81	0.46
1:C:297:GLU:HB3	1:C:298:PRO:HD3	1.97	0.46
1:F:134:GLN:HE21	1:F:167:VAL:HG21	1.81	0.46
1:F:297:GLU:HB3	1:F:298:PRO:HD3	1.97	0.46
1:G:149:GLU:OE1	1:G:183:SER:HA	2.15	0.46
1:G:297:GLU:HB3	1:G:298:PRO:HD3	1.97	0.46
1:A:403:ARG:NH2	1:A:419:THR:OG1	2.49	0.46
1:B:403:ARG:NH2	1:B:419:THR:OG1	2.49	0.46
1:E:403:ARG:NH2	1:E:419:THR:OG1	2.49	0.46
1:H:403:ARG:NH2	1:H:419:THR:OG1	2.49	0.46
1:C:134:GLN:HE21	1:C:167:VAL:HG21	1.81	0.46
1:E:146:ARG:HG2	1:E:183:SER:OG	2.15	0.46
1:A:297:GLU:HB3	1:A:298:PRO:HD3	1.97	0.46
1:C:153:VAL:HG22	1:C:156:ASN:HD22	1.80	0.46
1:C:299:LEU:HD23	1:C:303:LEU:HD22	1.98	0.46
1:C:403:ARG:NH2	1:C:419:THR:OG1	2.49	0.46
1:D:403:ARG:NH2	1:D:419:THR:OG1	2.49	0.46
1:F:403:ARG:NH2	1:F:419:THR:OG1	2.49	0.46
1:B:130:LEU:HD23	1:B:133:LEU:HD22	1.96	0.46
1:B:299:LEU:HD23	1:B:303:LEU:HD22	1.98	0.46
1:C:208:LEU:O	1:C:212:LEU:HG	2.16	0.46
1:D:208:LEU:O	1:D:212:LEU:HG	2.16	0.46
1:F:649:CYS:HB3	1:F:651:LYS:HE2	1.98	0.46
1:G:61:VAL:HG23	1:G:63:ASP:H	1.79	0.46
1:C:263:ASP:O	1:C:267:ARG:HG3	2.17	0.45
1:D:103:TRP:HD1	1:D:150:GLN:HE21	1.64	0.45
1:D:134:GLN:HE21	1:D:167:VAL:HG21	1.81	0.45
1:E:649:CYS:HB3	1:E:651:LYS:HE2	1.98	0.45
1:H:134:GLN:HE21	1:H:167:VAL:HG21	1.81	0.45
1:B:208:LEU:O	1:B:212:LEU:HG	2.16	0.45
1:D:263:ASP:O	1:D:267:ARG:HG3	2.17	0.45
1:E:61:VAL:HG23	1:E:63:ASP:H	1.79	0.45
1:E:263:ASP:O	1:E:267:ARG:HG3	2.17	0.45
1:E:297:GLU:HB3	1:E:298:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:134:GLN:HE21	1:G:167:VAL:HG21	1.81	0.45
1:A:299:LEU:HD23	1:A:303:LEU:HD22	1.98	0.45
1:D:297:GLU:HB3	1:D:298:PRO:HD3	1.97	0.45
1:D:299:LEU:HD23	1:D:303:LEU:HD22	1.98	0.45
1:E:208:LEU:O	1:E:212:LEU:HG	2.16	0.45
1:F:157:ARG:O	1:F:191:MET:HE1	2.17	0.45
1:B:263:ASP:O	1:B:267:ARG:HG3	2.17	0.45
1:B:480:SER:HB3	1:C:239:GLN:HG2	1.98	0.45
1:D:649:CYS:HB3	1:D:651:LYS:HE2	1.98	0.45
1:E:134:GLN:HE21	1:E:167:VAL:HG21	1.81	0.45
1:F:146:ARG:HG2	1:F:183:SER:OG	2.17	0.45
1:A:208:LEU:O	1:A:212:LEU:HG	2.16	0.45
1:D:627:ASP:O	1:D:630:MET:HG2	2.17	0.45
1:E:627:ASP:O	1:E:630:MET:HG2	2.17	0.45
1:H:575:GLN:NE2	1:H:579:LEU:HD11	2.32	0.45
1:A:153:VAL:HG22	1:A:156:ASN:HD22	1.81	0.45
1:A:575:GLN:NE2	1:A:579:LEU:HD11	2.32	0.45
1:B:581:LYS:HG3	1:B:591:VAL:HB	1.99	0.45
1:B:627:ASP:O	1:B:630:MET:HG2	2.17	0.45
1:D:103:TRP:CD1	1:D:150:GLN:NE2	2.84	0.45
1:D:694:LYS:HE2	1:D:698:PHE:HE2	1.82	0.45
1:E:129:LEU:HD23	1:E:148:LEU:HD13	1.98	0.45
1:E:581:LYS:HG3	1:E:591:VAL:HB	1.99	0.45
1:F:146:ARG:O	1:F:149:GLU:HG2	2.16	0.45
1:F:208:LEU:O	1:F:212:LEU:HG	2.16	0.45
1:H:208:LEU:O	1:H:212:LEU:HG	2.16	0.45
1:A:627:ASP:O	1:A:630:MET:HG2	2.17	0.45
1:C:153:VAL:HA	2:C:801:A1EIV:C08	2.47	0.45
1:C:565:PHE:HE2	1:C:610:SER:HB3	1.82	0.45
1:G:649:CYS:HB3	1:G:651:LYS:HE2	1.98	0.45
1:A:649:CYS:HB3	1:A:651:LYS:HE2	1.98	0.45
1:F:263:ASP:O	1:F:267:ARG:HG3	2.17	0.45
1:H:224:ARG:NE	1:H:263:ASP:OD2	2.49	0.45
1:H:681:ILE:HG23	1:H:694:LYS:HD3	1.99	0.45
1:A:681:ILE:HG23	1:A:694:LYS:HD3	1.99	0.45
1:B:576:LEU:HD23	1:B:620:VAL:HG13	1.99	0.45
1:B:649:CYS:HB3	1:B:651:LYS:HE2	1.98	0.45
1:D:148:LEU:O	1:D:152:LEU:HG	2.17	0.45
1:D:581:LYS:HG3	1:D:591:VAL:HB	1.99	0.45
1:F:576:LEU:HD23	1:F:620:VAL:HG13	1.99	0.45
1:G:299:LEU:HD23	1:G:303:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:649:CYS:HB3	1:H:651:LYS:HE2	1.98	0.45
1:B:565:PHE:HE2	1:B:610:SER:HB3	1.82	0.44
1:F:627:ASP:O	1:F:630:MET:HG2	2.17	0.44
1:G:565:PHE:HE2	1:G:610:SER:HB3	1.82	0.44
1:H:299:LEU:HD23	1:H:303:LEU:HD22	1.98	0.44
1:A:263:ASP:O	1:A:267:ARG:HG3	2.17	0.44
1:B:297:GLU:HB3	1:B:298:PRO:HD3	1.97	0.44
1:C:157:ARG:O	1:C:191:MET:HE1	2.17	0.44
1:C:649:CYS:HB3	1:C:651:LYS:HE2	1.98	0.44
1:F:299:LEU:HD23	1:F:303:LEU:HD22	1.98	0.44
1:H:565:PHE:HE2	1:H:610:SER:HB3	1.82	0.44
1:H:576:LEU:HD23	1:H:620:VAL:HG13	2.00	0.44
1:B:147:LEU:O	1:B:151:ILE:HG12	2.18	0.44
1:B:155:GLU:O	1:B:158:ASP:HB2	2.17	0.44
1:B:681:ILE:HG23	1:B:694:LYS:HD3	1.99	0.44
1:B:694:LYS:HE2	1:B:698:PHE:HE2	1.82	0.44
1:C:575:GLN:NE2	1:C:579:LEU:HD11	2.32	0.44
1:D:575:GLN:NE2	1:D:579:LEU:HD11	2.32	0.44
1:E:575:GLN:NE2	1:E:579:LEU:HD11	2.32	0.44
1:G:208:LEU:O	1:G:212:LEU:HG	2.16	0.44
1:G:263:ASP:O	1:G:267:ARG:HG3	2.17	0.44
1:B:569:ARG:HD3	1:B:569:ARG:HA	1.80	0.44
1:C:627:ASP:O	1:C:630:MET:HG2	2.17	0.44
1:D:582:VAL:HG11	1:E:256:PRO:HD3	1.99	0.44
1:G:103:TRP:HH2	1:G:110:ARG:HD3	1.83	0.44
1:G:681:ILE:HG23	1:G:694:LYS:HD3	1.99	0.44
1:H:627:ASP:O	1:H:630:MET:HG2	2.17	0.44
1:B:575:GLN:NE2	1:B:579:LEU:HD11	2.32	0.44
1:E:299:LEU:HD23	1:E:303:LEU:HD22	1.98	0.44
1:E:565:PHE:HE2	1:E:610:SER:HB3	1.82	0.44
1:F:575:GLN:NE2	1:F:579:LEU:HD11	2.32	0.44
1:G:627:ASP:O	1:G:630:MET:HG2	2.17	0.44
1:A:565:PHE:HE2	1:A:610:SER:HB3	1.82	0.44
1:C:581:LYS:HG3	1:C:591:VAL:HB	1.99	0.44
1:D:576:LEU:HD23	1:D:620:VAL:HG13	1.99	0.44
1:E:153:VAL:HA	2:E:801:A1EIV:C08	2.47	0.44
1:E:578:SER:OG	1:F:259:PHE:HD2	2.01	0.44
1:G:581:LYS:HG3	1:G:591:VAL:HB	1.99	0.44
1:C:131:ARG:HA	1:C:134:GLN:OE1	2.18	0.44
1:C:681:ILE:HG23	1:C:694:LYS:HD3	1.99	0.44
1:F:101:GLU:O	1:F:105:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:ARG:HA	1:F:134:GLN:OE1	2.18	0.44
1:G:131:ARG:HA	1:G:134:GLN:OE1	2.18	0.44
1:G:688:GLN:OE1	1:H:216:ARG:HB3	2.18	0.44
1:H:263:ASP:O	1:H:267:ARG:HG3	2.17	0.44
1:A:131:ARG:HA	1:A:134:GLN:OE1	2.18	0.44
1:A:480:SER:HB3	1:B:239:GLN:HG2	1.99	0.44
1:F:681:ILE:HG23	1:F:694:LYS:HD3	1.99	0.44
1:H:131:ARG:HA	1:H:134:GLN:OE1	2.18	0.44
1:C:224:ARG:NE	1:C:263:ASP:OD2	2.49	0.44
1:E:480:SER:HB3	1:F:239:GLN:HG2	1.99	0.44
1:F:565:PHE:HE2	1:F:610:SER:HB3	1.82	0.44
1:F:694:LYS:HE2	1:F:698:PHE:HE2	1.82	0.44
1:H:581:LYS:HG3	1:H:591:VAL:HB	1.99	0.44
1:A:101:GLU:O	1:A:105:LEU:HG	2.18	0.43
1:D:578:SER:OG	1:E:259:PHE:HD2	2.01	0.43
1:B:117:CYS:HB3	1:B:156:ASN:ND2	2.32	0.43
1:B:131:ARG:HA	1:B:134:GLN:OE1	2.18	0.43
1:C:694:LYS:HE2	1:C:698:PHE:HE2	1.82	0.43
1:D:159:ARG:CZ	1:D:163:ILE:HB	2.47	0.43
1:D:565:PHE:HE2	1:D:610:SER:HB3	1.82	0.43
1:D:681:ILE:HG23	1:D:694:LYS:HD3	1.99	0.43
1:E:101:GLU:O	1:E:105:LEU:HG	2.18	0.43
1:E:681:ILE:HG23	1:E:694:LYS:HD3	1.99	0.43
1:F:581:LYS:HG3	1:F:591:VAL:HB	1.99	0.43
1:D:157:ARG:NH1	1:D:193:LYS:HE2	2.34	0.43
1:E:131:ARG:HA	1:E:134:GLN:OE1	2.18	0.43
1:G:575:GLN:NE2	1:G:579:LEU:HD11	2.32	0.43
1:A:576:LEU:HD23	1:A:620:VAL:HG13	1.99	0.43
1:E:117:CYS:HB3	1:E:156:ASN:ND2	2.30	0.43
1:F:582:VAL:HG11	1:G:256:PRO:HD3	2.01	0.43
1:H:694:LYS:HE2	1:H:698:PHE:HE2	1.82	0.43
1:A:694:LYS:HE2	1:A:698:PHE:HE2	1.82	0.43
1:G:101:GLU:O	1:G:105:LEU:HG	2.18	0.43
1:G:576:LEU:HD23	1:G:620:VAL:HG13	2.00	0.43
1:A:581:LYS:HG3	1:A:591:VAL:HB	1.99	0.43
1:B:101:GLU:O	1:B:105:LEU:HG	2.18	0.43
1:C:242:GLN:OE1	1:C:280:ASN:ND2	2.52	0.43
1:C:578:SER:OG	1:D:259:PHE:HD2	2.02	0.43
1:D:242:GLN:OE1	1:D:280:ASN:ND2	2.52	0.43
1:G:694:LYS:HE2	1:G:698:PHE:HE2	1.82	0.43
1:H:101:GLU:O	1:H:105:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:THR:O	1:A:695:ILE:HG13	2.19	0.43
1:B:157:ARG:HG2	1:B:191:MET:SD	2.59	0.43
1:C:488:ALA:HB2	1:C:502:THR:HG21	2.01	0.43
1:E:694:LYS:HE2	1:E:698:PHE:HE2	1.82	0.43
1:F:691:THR:O	1:F:695:ILE:HG13	2.19	0.43
1:H:146:ARG:HG2	1:H:183:SER:OG	2.19	0.43
1:H:242:GLN:OE1	1:H:280:ASN:ND2	2.52	0.43
1:C:576:LEU:HD23	1:C:620:VAL:HG13	1.99	0.43
1:D:101:GLU:O	1:D:105:LEU:HG	2.18	0.43
1:D:131:ARG:HA	1:D:134:GLN:OE1	2.18	0.43
1:E:576:LEU:HD23	1:E:620:VAL:HG13	2.00	0.43
1:F:446:LEU:HD12	1:F:446:LEU:HA	1.92	0.43
1:G:480:SER:HB3	1:H:239:GLN:HG2	2.01	0.43
1:H:287:VAL:O	1:H:290:SER:OG	2.25	0.43
1:C:446:LEU:HD12	1:C:446:LEU:HA	1.92	0.43
1:C:691:THR:O	1:C:695:ILE:HG13	2.19	0.43
1:D:157:ARG:HD3	1:D:190:HIS:O	2.18	0.43
1:F:480:SER:HB3	1:G:239:GLN:HG2	2.00	0.43
1:G:242:GLN:OE1	1:G:280:ASN:ND2	2.52	0.43
1:H:691:THR:O	1:H:695:ILE:HG13	2.19	0.43
1:A:242:GLN:OE1	1:A:280:ASN:ND2	2.52	0.43
1:B:190:HIS:NE2	2:B:801:A1EIV:O04	2.52	0.43
1:G:142:VAL:O	1:G:146:ARG:HG3	2.19	0.43
1:B:691:THR:O	1:B:695:ILE:HG13	2.19	0.42
1:E:488:ALA:HB2	1:E:502:THR:HG21	2.01	0.42
1:C:101:GLU:O	1:C:105:LEU:HG	2.18	0.42
1:D:129:LEU:HD23	1:D:148:LEU:HD13	2.01	0.42
1:F:569:ARG:HD3	1:F:569:ARG:HA	1.80	0.42
1:H:569:ARG:NH2	1:H:625:ALA:O	2.45	0.42
1:A:157:ARG:HH12	1:A:193:LYS:HE2	1.85	0.42
1:A:672:MET:O	1:A:675:VAL:HG12	2.20	0.42
1:C:480:SER:HB3	1:D:239:GLN:HG2	2.00	0.42
1:D:691:THR:O	1:D:695:ILE:HG13	2.19	0.42
1:E:529:ILE:O	1:E:535:ARG:NH1	2.44	0.42
1:G:578:SER:OG	1:H:259:PHE:HD2	2.02	0.42
1:E:691:THR:O	1:E:695:ILE:HG13	2.19	0.42
1:G:193:LYS:NZ	2:G:801:A1EIV:O11	2.52	0.42
1:G:691:THR:O	1:G:695:ILE:HG13	2.19	0.42
1:A:529:ILE:O	1:A:535:ARG:NH1	2.44	0.42
1:B:374:LEU:O	1:B:378:VAL:HG23	2.20	0.42
1:B:488:ALA:HB2	1:B:502:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:LEU:O	1:C:378:VAL:HG23	2.20	0.42
1:F:242:GLN:OE1	1:F:280:ASN:ND2	2.52	0.42
1:D:480:SER:HB3	1:E:239:GLN:HG2	2.01	0.42
1:D:488:ALA:HB2	1:D:502:THR:HG21	2.01	0.42
1:E:224:ARG:NE	1:E:263:ASP:OD2	2.49	0.42
1:E:242:GLN:OE1	1:E:280:ASN:ND2	2.52	0.42
1:H:267:ARG:HB2	1:H:299:LEU:HD11	2.02	0.42
1:H:672:MET:O	1:H:675:VAL:HG12	2.20	0.42
1:C:103:TRP:CD1	1:C:150:GLN:NE2	2.82	0.42
1:D:160:VAL:CG1	1:D:164:GLY:HA3	2.47	0.42
1:D:664:GLU:HB2	1:D:667:VAL:HG22	2.01	0.42
1:B:242:GLN:OE1	1:B:280:ASN:ND2	2.52	0.42
1:C:380:TYR:OH	1:C:420:TRP:NE1	2.51	0.42
1:C:664:GLU:HB2	1:C:667:VAL:HG22	2.02	0.42
1:D:328:GLN:HG2	1:D:368:ILE:CD1	2.45	0.42
1:F:224:ARG:NE	1:F:263:ASP:OD2	2.49	0.42
1:F:328:GLN:HG2	1:F:368:ILE:CD1	2.45	0.42
1:G:672:MET:O	1:G:675:VAL:HG12	2.20	0.42
1:A:267:ARG:HB2	1:A:299:LEU:HD11	2.02	0.42
1:C:328:GLN:HG2	1:C:368:ILE:CD1	2.45	0.42
1:E:157:ARG:NH1	1:E:193:LYS:HE2	2.35	0.42
1:F:151:ILE:O	1:F:153:VAL:N	2.49	0.42
1:G:267:ARG:HB2	1:G:299:LEU:HD11	2.02	0.42
1:G:488:ALA:HB2	1:G:502:THR:HG21	2.01	0.42
1:A:488:ALA:HB2	1:A:502:THR:HG21	2.01	0.42
1:A:619:LEU:HG	1:A:621:LEU:HD22	2.02	0.42
1:B:672:MET:O	1:B:675:VAL:HG12	2.20	0.42
1:D:146:ARG:HG2	1:D:183:SER:OG	2.20	0.42
1:E:672:MET:O	1:E:675:VAL:HG12	2.20	0.42
1:F:619:LEU:HG	1:F:621:LEU:HD22	2.02	0.42
1:G:224:ARG:NE	1:G:263:ASP:OD2	2.49	0.42
1:H:619:LEU:HG	1:H:621:LEU:HD22	2.02	0.42
1:A:664:GLU:HB2	1:A:667:VAL:HG22	2.01	0.41
1:C:569:ARG:HD3	1:C:569:ARG:HA	1.80	0.41
1:C:672:MET:O	1:C:675:VAL:HG12	2.20	0.41
1:E:664:GLU:HB2	1:E:667:VAL:HG22	2.01	0.41
1:G:619:LEU:HG	1:G:621:LEU:HD22	2.02	0.41
1:G:664:GLU:HB2	1:G:667:VAL:HG22	2.01	0.41
1:A:129:LEU:HD23	1:A:148:LEU:HD13	2.01	0.41
1:A:424:ILE:HD12	1:A:469:GLU:OE1	2.20	0.41
1:B:446:LEU:HD12	1:B:446:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:ILE:HD12	1:C:469:GLU:OE1	2.20	0.41
1:D:380:TYR:OH	1:D:420:TRP:NE1	2.51	0.41
1:E:328:GLN:HG2	1:E:368:ILE:CD1	2.45	0.41
1:H:374:LEU:O	1:H:378:VAL:HG23	2.20	0.41
1:C:451:LEU:HD22	1:C:457:MET:SD	2.61	0.41
1:D:374:LEU:O	1:D:378:VAL:HG23	2.20	0.41
1:E:103:TRP:CD1	1:E:150:GLN:NE2	2.83	0.41
1:E:374:LEU:O	1:E:378:VAL:HG23	2.20	0.41
1:E:380:TYR:OH	1:E:420:TRP:NE1	2.51	0.41
1:E:619:LEU:HG	1:E:621:LEU:HD22	2.02	0.41
1:H:488:ALA:HB2	1:H:502:THR:HG21	2.01	0.41
1:H:664:GLU:HB2	1:H:667:VAL:HG22	2.01	0.41
1:A:451:LEU:HD22	1:A:457:MET:SD	2.61	0.41
1:B:224:ARG:NE	1:B:263:ASP:OD2	2.49	0.41
1:C:293:LEU:HD22	1:C:340:GLU:CB	2.51	0.41
1:D:672:MET:O	1:D:675:VAL:HG12	2.20	0.41
1:H:110:ARG:HH22	2:H:801:A1EIV:P10	2.43	0.41
1:H:451:LEU:HD22	1:H:457:MET:SD	2.61	0.41
1:B:619:LEU:HG	1:B:621:LEU:HD22	2.02	0.41
1:C:140:THR:O	1:C:141:ARG:C	2.62	0.41
1:F:157:ARG:NH1	1:F:193:LYS:HE2	2.35	0.41
1:F:672:MET:O	1:F:675:VAL:HG12	2.20	0.41
1:G:424:ILE:HD12	1:G:469:GLU:OE1	2.20	0.41
1:G:451:LEU:HD22	1:G:457:MET:SD	2.61	0.41
1:H:424:ILE:HD12	1:H:469:GLU:OE1	2.21	0.41
1:B:180:LEU:O	1:B:184:VAL:HG12	2.21	0.41
1:B:267:ARG:HB2	1:B:299:LEU:HD11	2.02	0.41
1:B:293:LEU:HD22	1:B:340:GLU:CB	2.51	0.41
1:B:424:ILE:HD12	1:B:469:GLU:OE1	2.20	0.41
1:D:180:LEU:O	1:D:184:VAL:HG12	2.21	0.41
1:E:180:LEU:O	1:E:184:VAL:HG12	2.21	0.41
1:G:193:LYS:O	1:G:193:LYS:HG2	2.20	0.41
1:C:180:LEU:O	1:C:184:VAL:HG12	2.21	0.41
1:C:662:TRP:CZ3	1:C:676:LEU:HA	2.56	0.41
1:A:569:ARG:NH2	1:A:625:ALA:O	2.45	0.41
1:B:305:PRO:HG3	1:B:347:PHE:CE2	2.56	0.41
1:B:664:GLU:HB2	1:B:667:VAL:HG22	2.02	0.41
1:E:451:LEU:HD22	1:E:457:MET:SD	2.61	0.41
1:F:180:LEU:O	1:F:184:VAL:HG12	2.21	0.41
1:F:488:ALA:HB2	1:F:502:THR:HG21	2.01	0.41
1:G:374:LEU:O	1:G:378:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LEU:HD22	1:A:340:GLU:CB	2.51	0.41
1:A:569:ARG:HD3	1:A:569:ARG:HA	1.80	0.41
1:A:578:SER:OG	1:B:259:PHE:HD2	2.03	0.41
1:A:662:TRP:CZ3	1:A:676:LEU:HA	2.56	0.41
1:A:692:ILE:HD13	1:A:695:ILE:HD12	2.03	0.41
1:B:451:LEU:HD22	1:B:457:MET:SD	2.61	0.41
1:C:305:PRO:HG3	1:C:347:PHE:CE2	2.56	0.41
1:D:148:LEU:HD12	1:D:148:LEU:HA	1.93	0.41
1:D:267:ARG:HB2	1:D:299:LEU:HD11	2.02	0.41
1:D:293:LEU:HD22	1:D:340:GLU:CB	2.51	0.41
1:E:424:ILE:HD12	1:E:469:GLU:OE1	2.20	0.41
1:F:267:ARG:HB2	1:F:299:LEU:HD11	2.02	0.41
1:F:451:LEU:HD22	1:F:457:MET:SD	2.61	0.41
1:F:688:GLN:OE1	1:G:216:ARG:HB3	2.20	0.41
1:G:662:TRP:CZ3	1:G:676:LEU:HA	2.56	0.41
1:H:529:ILE:O	1:H:535:ARG:NH1	2.44	0.41
1:A:180:LEU:O	1:A:184:VAL:HG12	2.21	0.41
1:A:374:LEU:O	1:A:378:VAL:HG23	2.20	0.41
1:B:328:GLN:HG2	1:B:368:ILE:CD1	2.45	0.41
1:B:692:ILE:HD13	1:B:695:ILE:HD12	2.03	0.41
1:C:267:ARG:HB2	1:C:299:LEU:HD11	2.02	0.41
1:D:195:SER:O	1:D:198:THR:OG1	2.39	0.41
1:D:619:LEU:HG	1:D:621:LEU:HD22	2.02	0.41
1:E:195:SER:O	1:E:198:THR:OG1	2.39	0.41
1:E:267:ARG:HB2	1:E:299:LEU:HD11	2.02	0.41
1:F:116:LEU:O	1:F:120:ILE:HG13	2.21	0.41
1:F:424:ILE:HD12	1:F:469:GLU:OE1	2.20	0.41
1:F:578:SER:OG	1:G:259:PHE:HD2	2.04	0.41
1:F:664:GLU:HB2	1:F:667:VAL:HG22	2.02	0.41
1:F:681:ILE:HD11	1:F:698:PHE:HD2	1.86	0.41
1:B:681:ILE:HD11	1:B:698:PHE:HD2	1.87	0.40
1:C:116:LEU:O	1:C:120:ILE:HG13	2.21	0.40
1:C:635:CYS:O	1:C:641:LYS:NZ	2.31	0.40
1:C:681:ILE:HD11	1:C:698:PHE:HD2	1.86	0.40
1:E:446:LEU:HD12	1:E:446:LEU:HA	1.92	0.40
1:E:681:ILE:HD11	1:E:698:PHE:HD2	1.86	0.40
1:G:403:ARG:HA	1:G:404:PRO:HD3	1.97	0.40
1:G:533:VAL:O	1:G:537:ARG:HG3	2.22	0.40
1:H:293:LEU:HD22	1:H:340:GLU:CB	2.51	0.40
1:A:305:PRO:HG3	1:A:347:PHE:CE2	2.56	0.40
1:C:287:VAL:O	1:C:290:SER:OG	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:619:LEU:HG	1:C:621:LEU:HD22	2.02	0.40
1:D:305:PRO:HG3	1:D:347:PHE:CE2	2.56	0.40
1:F:371:ILE:HG13	1:F:372:GLN:N	2.37	0.40
1:F:374:LEU:O	1:F:378:VAL:HG23	2.20	0.40
1:F:662:TRP:CZ3	1:F:676:LEU:HA	2.56	0.40
1:G:293:LEU:HD22	1:G:340:GLU:CB	2.51	0.40
1:H:533:VAL:O	1:H:537:ARG:HG3	2.22	0.40
1:A:334:LEU:HD11	1:A:349:LEU:HD13	2.03	0.40
1:A:483:ASP:OD1	1:A:487:LEU:HB3	2.21	0.40
1:C:159:ARG:NH1	1:C:163:ILE:HB	2.35	0.40
1:C:533:VAL:O	1:C:537:ARG:HG3	2.22	0.40
1:D:424:ILE:HD12	1:D:469:GLU:OE1	2.20	0.40
1:E:305:PRO:HG3	1:E:347:PHE:CE2	2.56	0.40
1:E:371:ILE:HG13	1:E:372:GLN:N	2.37	0.40
1:F:533:VAL:O	1:F:537:ARG:HG3	2.22	0.40
1:G:371:ILE:HG13	1:G:372:GLN:N	2.37	0.40
1:A:255:PHE:HB3	1:A:256:PRO:HD3	2.04	0.40
1:A:325:ASP:O	1:A:329:ARG:HG2	2.22	0.40
1:B:483:ASP:OD1	1:B:487:LEU:HB3	2.22	0.40
1:C:245:MET:HE3	1:C:245:MET:HB3	1.96	0.40
1:D:116:LEU:O	1:D:120:ILE:HG13	2.22	0.40
1:D:451:LEU:HD22	1:D:457:MET:SD	2.61	0.40
1:D:662:TRP:CZ3	1:D:676:LEU:HA	2.56	0.40
1:D:681:ILE:HD11	1:D:698:PHE:HD2	1.87	0.40
1:E:293:LEU:HD22	1:E:340:GLU:CB	2.51	0.40
1:E:334:LEU:HD11	1:E:349:LEU:HD13	2.03	0.40
1:F:245:MET:HE3	1:F:245:MET:HB3	1.96	0.40
1:F:268:LEU:HG	1:F:348:TYR:OH	2.22	0.40
1:F:380:TYR:OH	1:F:420:TRP:NE1	2.51	0.40
1:G:116:LEU:O	1:G:120:ILE:HG13	2.21	0.40
1:H:103:TRP:HZ3	1:H:110:ARG:HD2	1.87	0.40
1:H:305:PRO:HG3	1:H:347:PHE:CE2	2.56	0.40
1:B:129:LEU:HD23	1:B:148:LEU:HD13	2.04	0.40
1:B:325:ASP:O	1:B:329:ARG:HG2	2.22	0.40
1:F:293:LEU:HD22	1:F:340:GLU:CB	2.51	0.40
1:F:305:PRO:HG3	1:F:347:PHE:CE2	2.56	0.40
1:G:692:ILE:HD13	1:G:695:ILE:HD12	2.03	0.40
1:H:255:PHE:HB3	1:H:256:PRO:HD3	2.04	0.40
1:H:334:LEU:HD11	1:H:349:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

4.3 Torsion angles

4.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	590/522 (113%)	582 (99%)	8 (1%)	0	100	100
1	B	590/522 (113%)	582 (99%)	8 (1%)	0	100	100
1	C	590/522 (113%)	582 (99%)	8 (1%)	0	100	100
1	D	590/522 (113%)	583 (99%)	7 (1%)	0	100	100
1	E	590/522 (113%)	582 (99%)	8 (1%)	0	100	100
1	F	589/522 (113%)	581 (99%)	8 (1%)	0	100	100
1	G	590/522 (113%)	582 (99%)	8 (1%)	0	100	100
1	H	591/522 (113%)	582 (98%)	8 (1%)	1 (0%)	43	62
All	All	4720/4176 (113%)	4656 (99%)	63 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	152	LEU

4.3.2 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	502/417 (120%)	493 (98%)	9 (2%)	51	74
1	B	502/417 (120%)	495 (99%)	7 (1%)	59	78
1	C	502/417 (120%)	495 (99%)	7 (1%)	59	78
1	D	502/417 (120%)	496 (99%)	6 (1%)	63	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	501/417 (120%)	493 (98%)	8 (2%)	55	76
1	F	501/417 (120%)	495 (99%)	6 (1%)	63	80
1	G	502/417 (120%)	494 (98%)	8 (2%)	55	76
1	H	502/417 (120%)	495 (99%)	7 (1%)	59	78
All	All	4014/3336 (120%)	3956 (99%)	58 (1%)	57	78

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	TRP
1	A	149	GLU
1	A	150	GLN
1	A	189	GLU
1	A	285	ARG
1	A	286	GLU
1	A	349	LEU
1	A	368	ILE
1	A	468	ARG
1	B	155	GLU
1	B	189	GLU
1	B	285	ARG
1	B	286	GLU
1	B	349	LEU
1	B	368	ILE
1	B	468	ARG
1	C	158	ASP
1	C	189	GLU
1	C	285	ARG
1	C	286	GLU
1	C	349	LEU
1	C	368	ILE
1	C	468	ARG
1	D	189	GLU
1	D	285	ARG
1	D	286	GLU
1	D	349	LEU
1	D	368	ILE
1	D	468	ARG
1	E	103	TRP
1	E	150	GLN
1	E	189	GLU

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Mol	Chain	Res	Type
1	E	285	ARG
1	E	286	GLU
1	E	349	LEU
1	E	368	ILE
1	E	468	ARG
1	F	189	GLU
1	F	285	ARG
1	F	286	GLU
1	F	349	LEU
1	F	368	ILE
1	F	468	ARG
1	G	143	GLN
1	G	153	VAL
1	G	189	GLU
1	G	285	ARG
1	G	286	GLU
1	G	349	LEU
1	G	368	ILE
1	G	468	ARG
1	H	155	GLU
1	H	189	GLU
1	H	285	ARG
1	H	286	GLU
1	H	349	LEU
1	H	368	ILE
1	H	468	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	156	ASN
1	A	269	HIS
1	A	280	ASN
1	A	516	HIS
1	A	575	GLN
1	B	156	ASN
1	B	269	HIS
1	B	280	ASN
1	B	516	HIS
1	B	575	GLN
1	B	673	GLN

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Mol	Chain	Res	Type
1	C	150	GLN
1	C	156	ASN
1	C	200	GLN
1	C	280	ASN
1	C	516	HIS
1	C	575	GLN
1	D	150	GLN
1	D	269	HIS
1	D	280	ASN
1	D	516	HIS
1	D	575	GLN
1	E	150	GLN
1	E	200	GLN
1	E	269	HIS
1	E	280	ASN
1	E	383	ASN
1	E	500	GLN
1	E	516	HIS
1	E	575	GLN
1	F	156	ASN
1	F	200	GLN
1	F	269	HIS
1	F	280	ASN
1	F	516	HIS
1	F	575	GLN
1	G	150	GLN
1	G	156	ASN
1	G	200	GLN
1	G	269	HIS
1	G	280	ASN
1	G	575	GLN
1	H	269	HIS
1	H	280	ASN
1	H	383	ASN
1	H	516	HIS
1	H	575	GLN

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

4.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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
2	A1EIV	B	801	-	19,21,21	2.23	5 (26%)	23,31,31	1.37	4 (17%)
2	A1EIV	D	801	-	19,21,21	2.18	4 (21%)	23,31,31	1.29	2 (8%)
2	A1EIV	H	801	-	19,21,21	2.12	4 (21%)	23,31,31	1.22	3 (13%)
2	A1EIV	A	801	-	19,21,21	2.21	4 (21%)	23,31,31	1.35	4 (17%)
2	A1EIV	F	801	-	19,21,21	1.92	5 (26%)	23,31,31	1.49	3 (13%)
2	A1EIV	G	801	-	19,21,21	2.13	4 (21%)	23,31,31	1.28	4 (17%)
2	A1EIV	C	801	-	19,21,21	2.21	4 (21%)	23,31,31	1.28	2 (8%)
2	A1EIV	E	801	-	19,21,21	2.16	3 (15%)	23,31,31	1.30	3 (13%)

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
2	A1EIV	B	801	-	-	3/10/26/26	0/2/2/2
2	A1EIV	D	801	-	-	5/10/26/26	0/2/2/2
2	A1EIV	H	801	-	-	3/10/26/26	0/2/2/2
2	A1EIV	A	801	-	-	4/10/26/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1EIV	F	801	-	-	4/10/26/26	0/2/2/2
2	A1EIV	G	801	-	-	5/10/26/26	0/2/2/2
2	A1EIV	C	801	-	-	5/10/26/26	0/2/2/2
2	A1EIV	E	801	-	-	3/10/26/26	0/2/2/2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	A1EIV	P10-O09	6.98	1.82	1.60
2	A	801	A1EIV	P10-O09	6.91	1.82	1.60
2	B	801	A1EIV	P10-O09	6.89	1.82	1.60
2	D	801	A1EIV	P10-O09	6.78	1.81	1.60
2	E	801	A1EIV	P10-O09	6.70	1.81	1.60
2	H	801	A1EIV	P10-O09	6.47	1.80	1.60
2	G	801	A1EIV	P10-O09	6.36	1.80	1.60
2	F	801	A1EIV	P10-O09	5.43	1.77	1.60
2	F	801	A1EIV	O09-C08	-3.53	1.31	1.44
2	G	801	A1EIV	O09-C08	-3.38	1.31	1.44
2	E	801	A1EIV	O09-C08	-3.28	1.32	1.44
2	B	801	A1EIV	C20-N14	3.27	1.38	1.35
2	A	801	A1EIV	C20-N14	3.20	1.38	1.35
2	A	801	A1EIV	O09-C08	-3.20	1.32	1.44
2	H	801	A1EIV	O09-C08	-3.20	1.32	1.44
2	D	801	A1EIV	O09-C08	-3.19	1.32	1.44
2	C	801	A1EIV	O09-C08	-3.18	1.32	1.44
2	C	801	A1EIV	C20-N14	3.14	1.38	1.35
2	B	801	A1EIV	O09-C08	-3.10	1.32	1.44
2	H	801	A1EIV	C20-N14	3.09	1.38	1.35
2	D	801	A1EIV	C20-N14	3.05	1.38	1.35
2	E	801	A1EIV	C20-N14	3.03	1.38	1.35
2	G	801	A1EIV	C20-N14	2.96	1.38	1.35
2	G	801	A1EIV	O06-C07	-2.85	1.38	1.45
2	F	801	A1EIV	O06-C07	-2.42	1.39	1.45
2	H	801	A1EIV	O06-C07	-2.25	1.40	1.45
2	F	801	A1EIV	C20-N14	2.20	1.37	1.35
2	B	801	A1EIV	O06-C07	-2.19	1.40	1.45
2	B	801	A1EIV	C08-C07	2.18	1.58	1.51
2	F	801	A1EIV	O01-C02	-2.08	1.37	1.43
2	D	801	A1EIV	C08-C07	2.07	1.57	1.51
2	A	801	A1EIV	C08-C07	2.05	1.57	1.51
2	C	801	A1EIV	O06-C07	-2.04	1.40	1.45

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	A1EIV	O12-P10-O09	-3.54	97.45	106.67
2	A	801	A1EIV	C15-N14-C20	-3.27	119.10	121.88
2	E	801	A1EIV	C15-N14-C20	-3.21	119.15	121.88
2	C	801	A1EIV	C15-N14-C20	-3.13	119.21	121.88
2	F	801	A1EIV	C07-O06-C05	3.12	112.78	109.92
2	D	801	A1EIV	C15-N14-C20	-3.11	119.23	121.88
2	G	801	A1EIV	C15-N14-C20	-3.05	119.28	121.88
2	F	801	A1EIV	C15-N14-C20	-3.00	119.33	121.88
2	F	801	A1EIV	O12-P10-O09	-2.81	99.35	106.67
2	H	801	A1EIV	C15-N14-C20	-2.78	119.51	121.88
2	D	801	A1EIV	O12-P10-O09	-2.76	99.47	106.67
2	C	801	A1EIV	O12-P10-O09	-2.75	99.50	106.67
2	B	801	A1EIV	C15-N14-C20	-2.70	119.58	121.88
2	E	801	A1EIV	O12-P10-O09	-2.67	99.70	106.67
2	G	801	A1EIV	O12-P10-O09	-2.64	99.79	106.67
2	B	801	A1EIV	C07-O06-C05	-2.55	107.59	109.92
2	H	801	A1EIV	O12-P10-O09	-2.54	100.05	106.67
2	A	801	A1EIV	O12-P10-O09	-2.45	100.29	106.67
2	G	801	A1EIV	O12-P10-O11	2.21	116.11	107.80
2	G	801	A1EIV	O11-P10-O09	-2.21	100.91	106.67
2	B	801	A1EIV	O12-P10-O11	2.15	115.88	107.80
2	A	801	A1EIV	C07-O06-C05	2.12	111.86	109.92
2	H	801	A1EIV	O12-P10-O11	2.07	115.56	107.80
2	E	801	A1EIV	O11-P10-O09	-2.06	101.31	106.67
2	A	801	A1EIV	O11-P10-O09	-2.06	101.31	106.67

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	A1EIV	C08-O09-P10-O11
2	A	801	A1EIV	C08-O09-P10-O12
2	B	801	A1EIV	C08-O09-P10-O11
2	B	801	A1EIV	C08-O09-P10-O12
2	C	801	A1EIV	C08-O09-P10-O11
2	E	801	A1EIV	C08-O09-P10-O11
2	E	801	A1EIV	C08-O09-P10-O12
2	E	801	A1EIV	C08-O09-P10-O13
2	F	801	A1EIV	C08-O09-P10-O11
2	F	801	A1EIV	C08-O09-P10-O12
2	G	801	A1EIV	C08-O09-P10-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	G	801	A1EIV	C08-O09-P10-O12
2	H	801	A1EIV	C08-O09-P10-O11
2	H	801	A1EIV	C08-O09-P10-O12
2	H	801	A1EIV	C08-O09-P10-O13
2	C	801	A1EIV	O06-C07-C08-O09
2	D	801	A1EIV	O06-C07-C08-O09
2	G	801	A1EIV	C02-C07-C08-O09
2	G	801	A1EIV	O06-C07-C08-O09
2	F	801	A1EIV	O06-C07-C08-O09
2	C	801	A1EIV	C02-C07-C08-O09
2	D	801	A1EIV	C02-C07-C08-O09
2	A	801	A1EIV	C08-O09-P10-O13
2	B	801	A1EIV	C08-O09-P10-O13
2	G	801	A1EIV	C08-O09-P10-O13
2	C	801	A1EIV	C08-O09-P10-O12
2	D	801	A1EIV	C08-O09-P10-O11
2	D	801	A1EIV	C08-O09-P10-O12
2	C	801	A1EIV	C08-O09-P10-O13
2	D	801	A1EIV	C08-O09-P10-O13
2	F	801	A1EIV	C08-O09-P10-O13
2	A	801	A1EIV	O06-C07-C08-O09

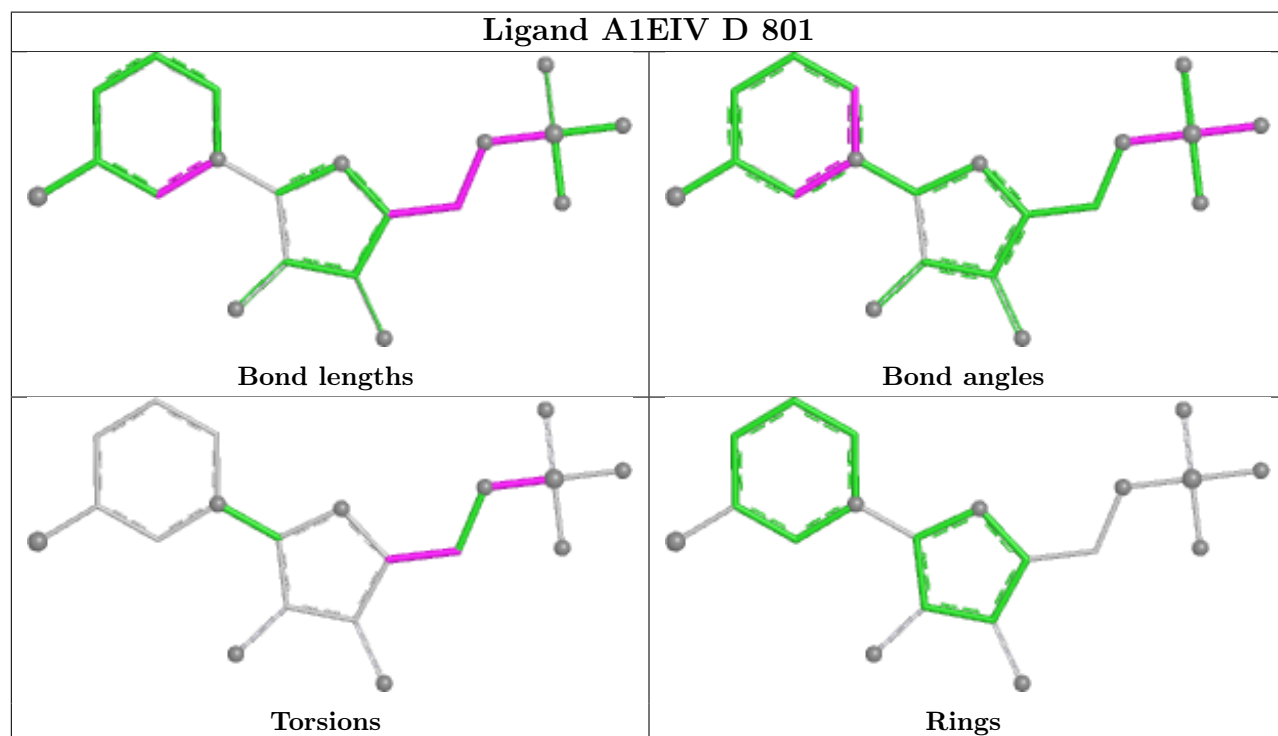
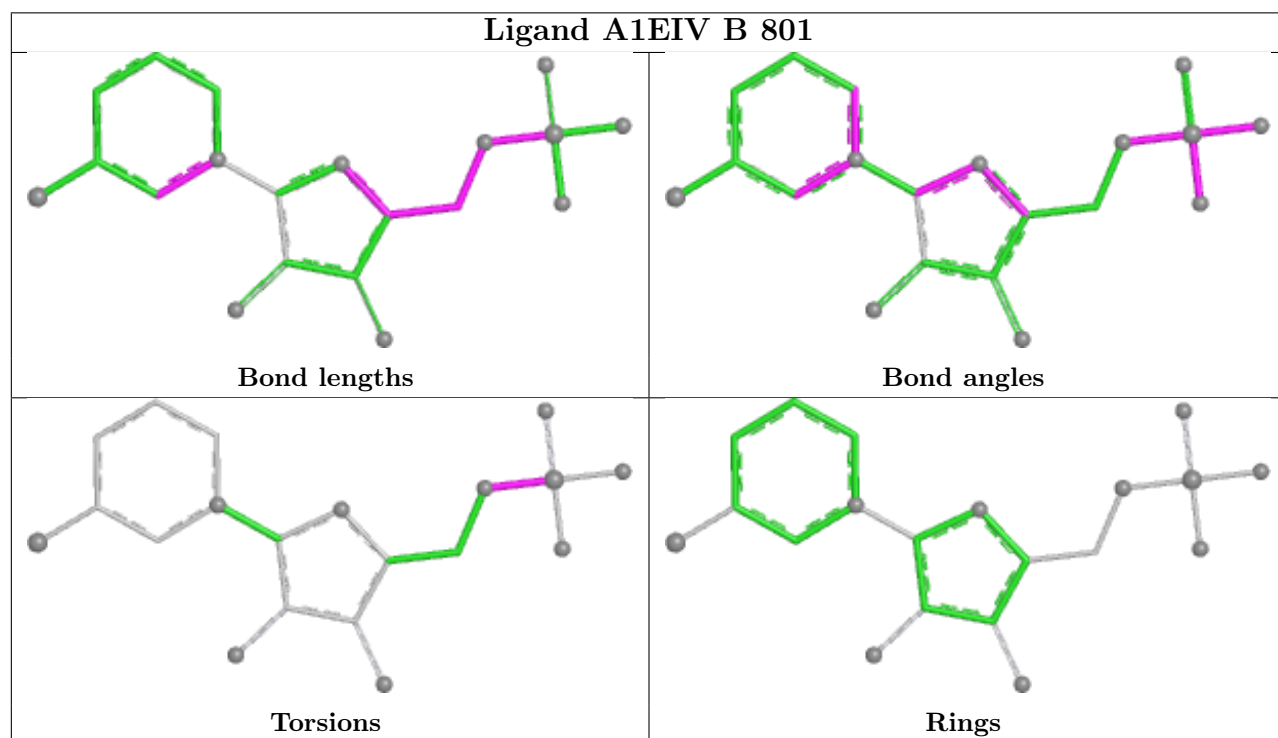
There are no ring outliers.

5 monomers are involved in 9 short contacts:

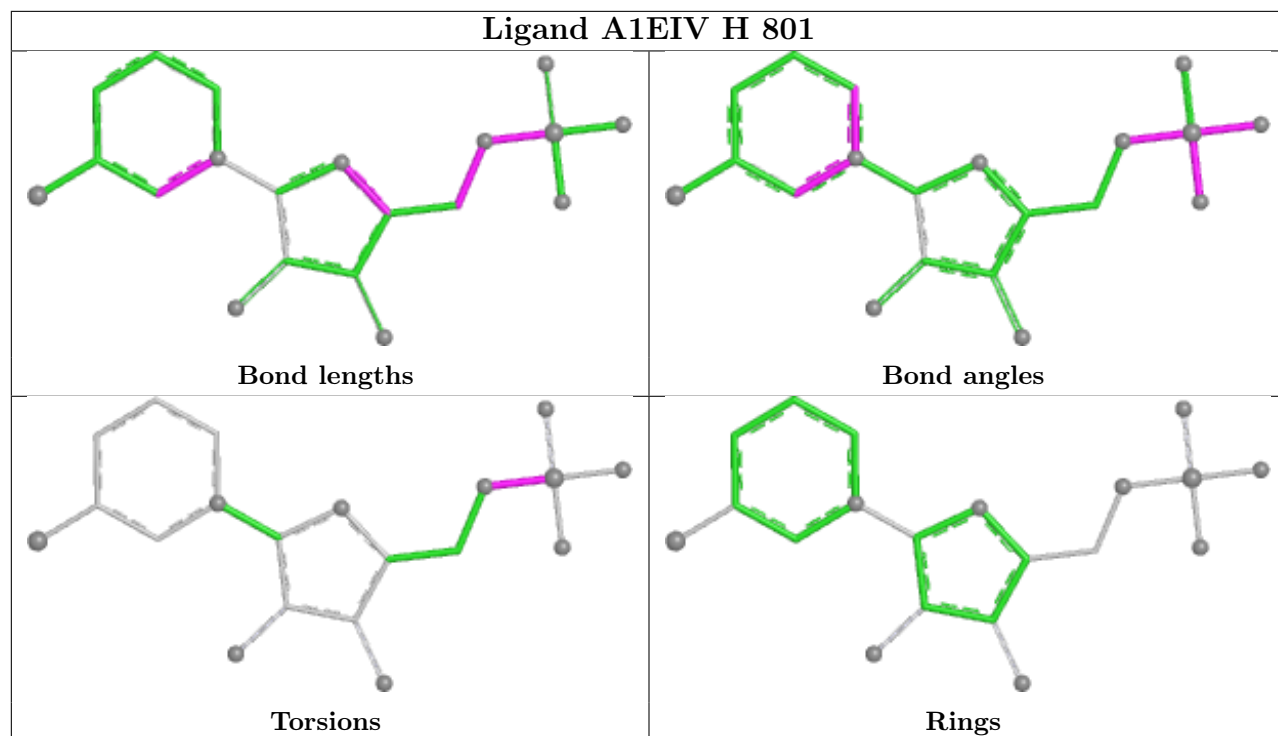
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	A1EIV	3	0
2	H	801	A1EIV	3	0
2	G	801	A1EIV	1	0
2	C	801	A1EIV	1	0
2	E	801	A1EIV	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

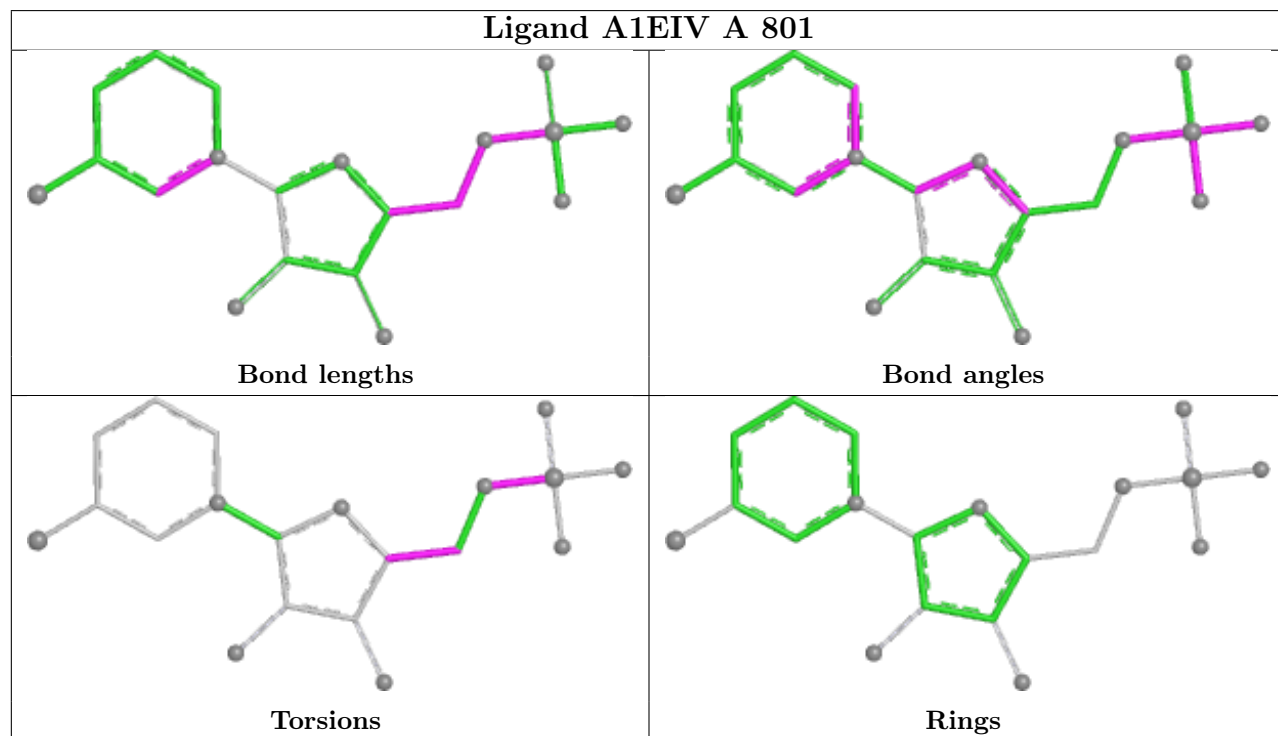
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



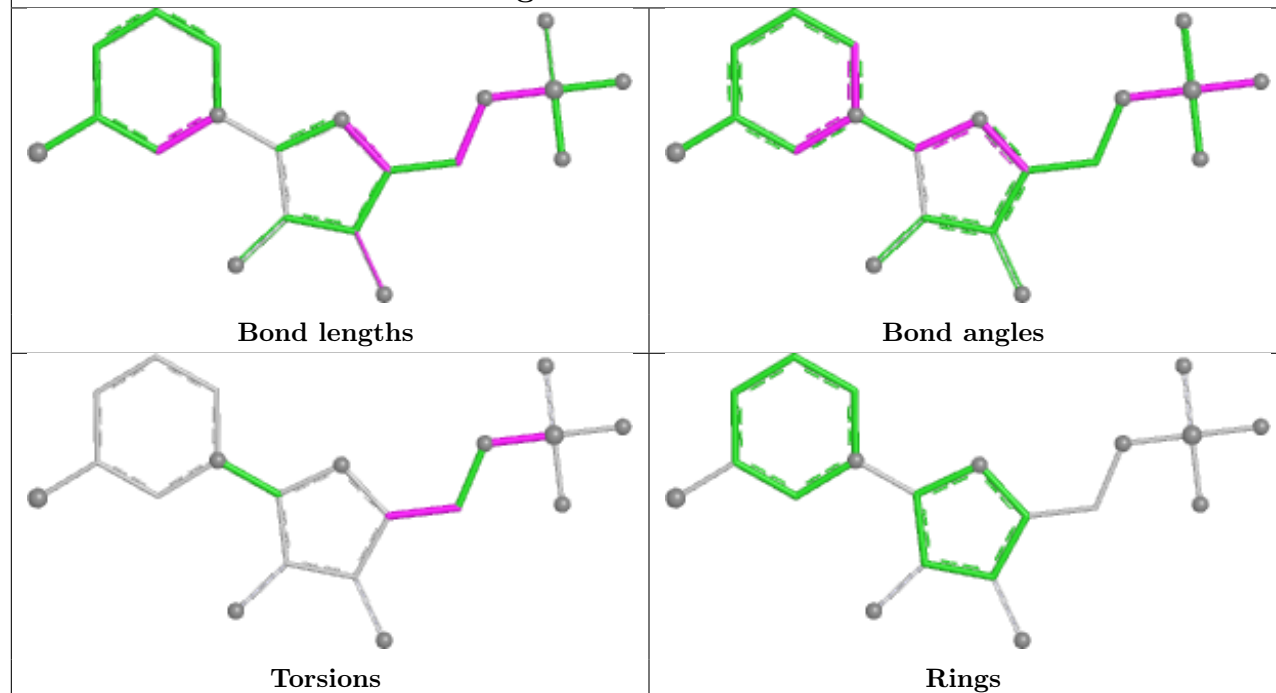
Ligand A1EIV H 801



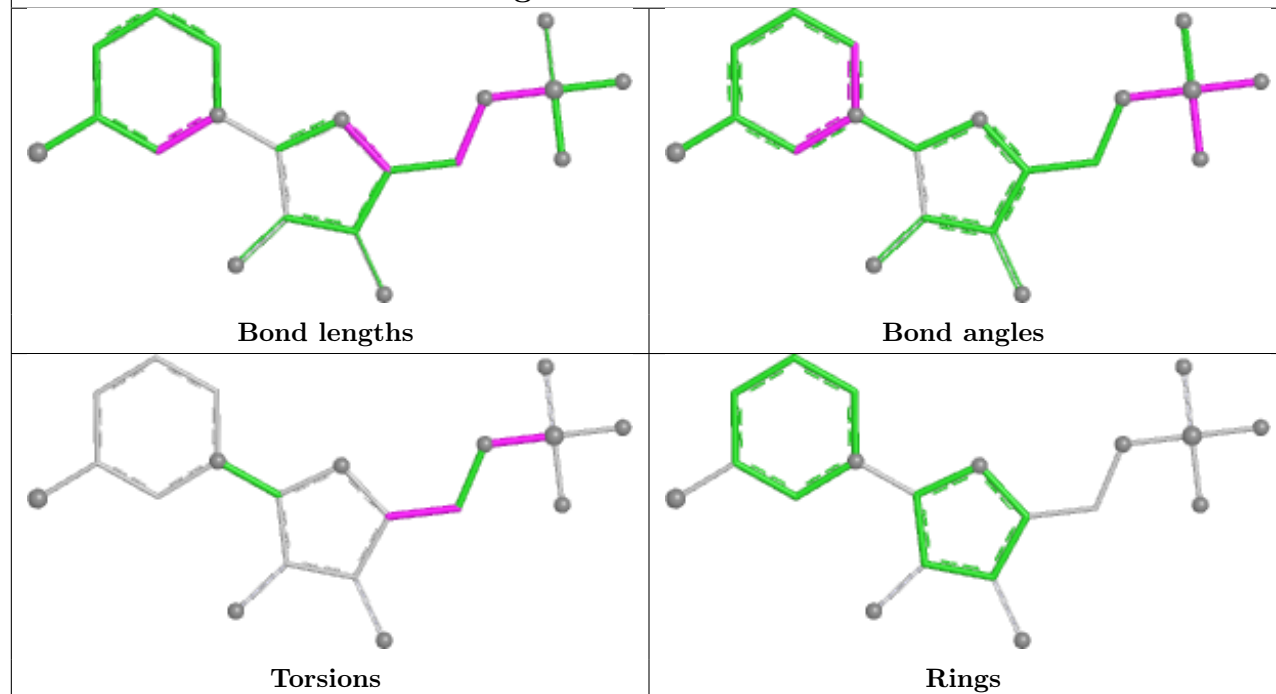
Ligand A1EIV A 801

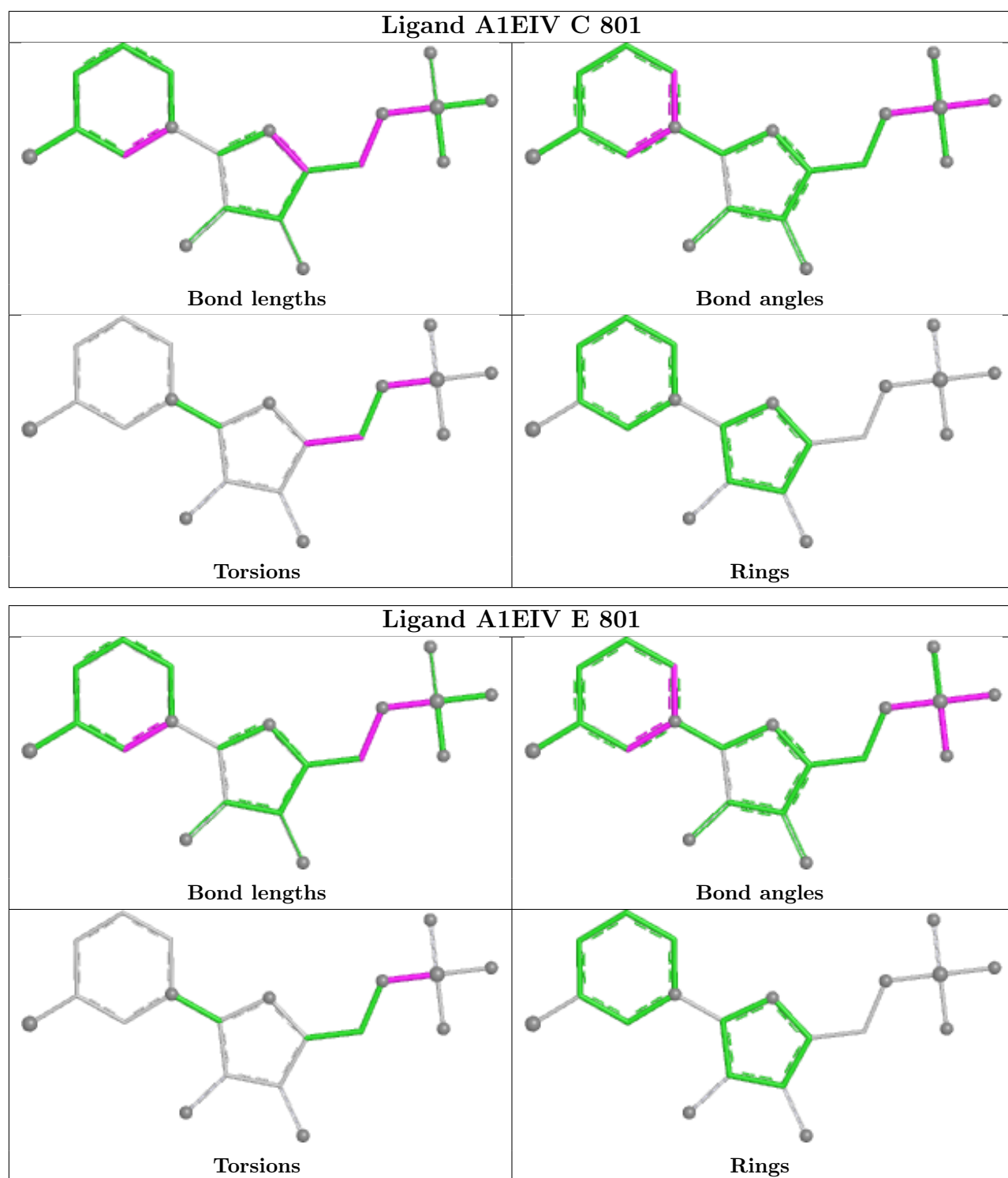


Ligand A1EIV F 801



Ligand A1EIV G 801





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

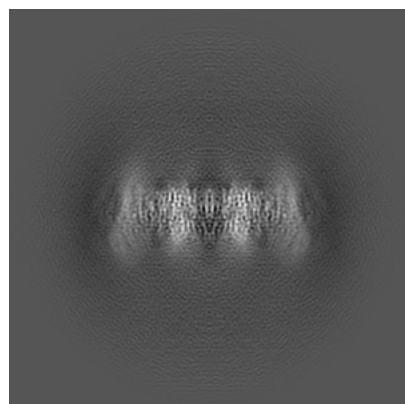
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62772. These allow visual inspection of the internal detail of the map and identification of artifacts.

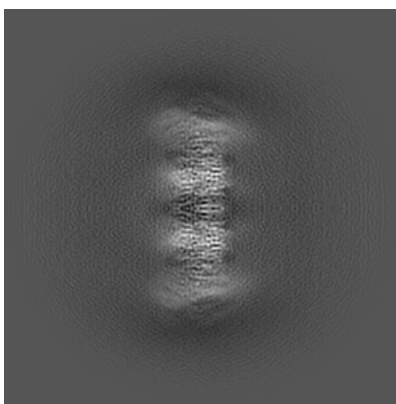
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

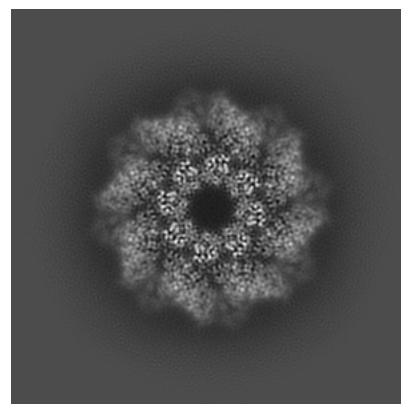
5.1.1 Primary map



X

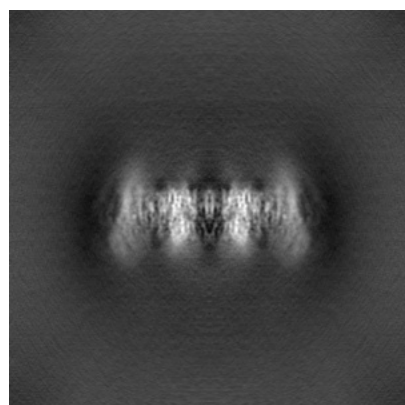


Y

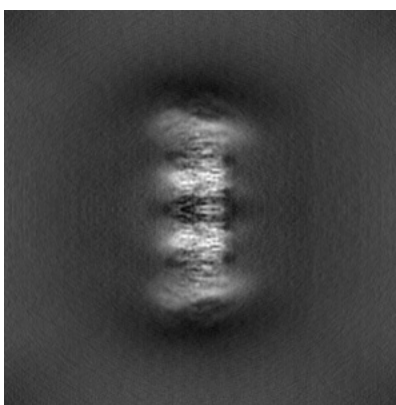


Z

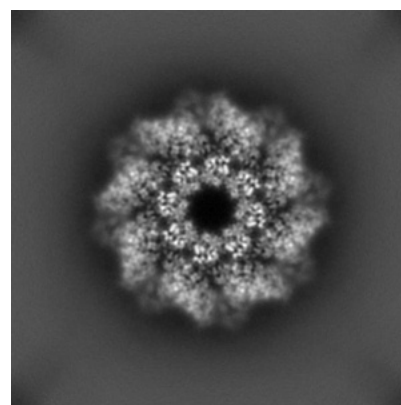
5.1.2 Raw map



X



Y

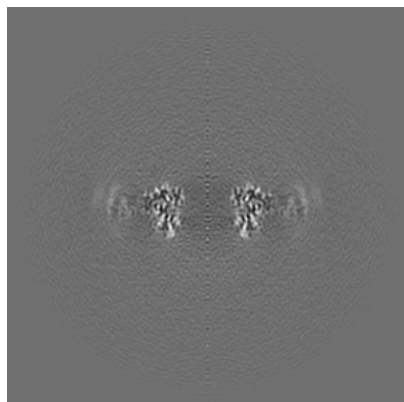


Z

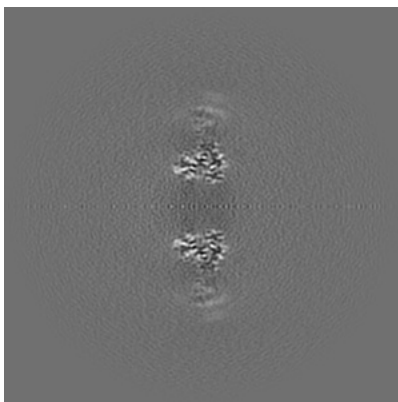
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

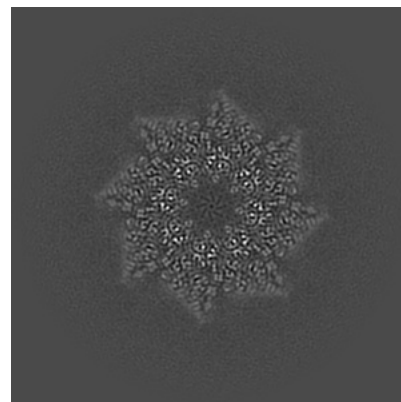
5.2.1 Primary map



X Index: 200

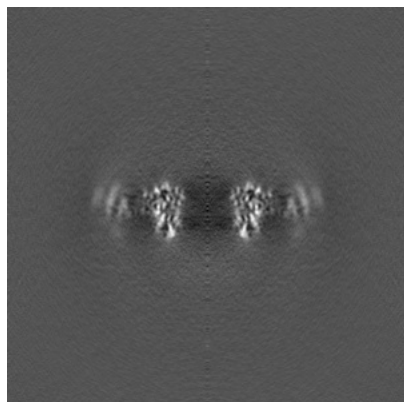


Y Index: 200

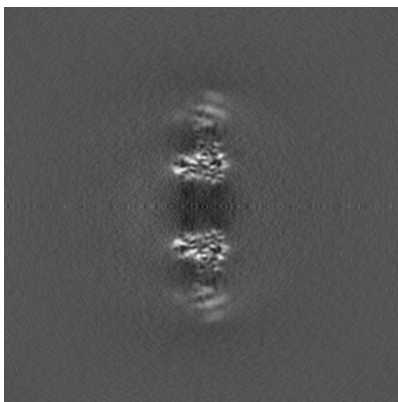


Z Index: 200

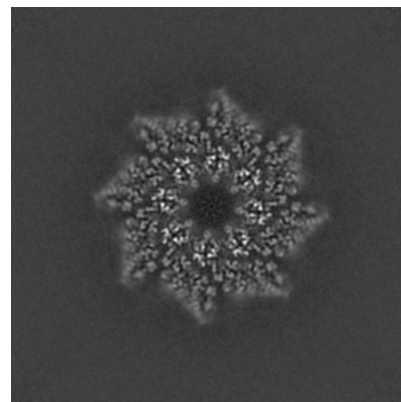
5.2.2 Raw map



X Index: 200



Y Index: 200

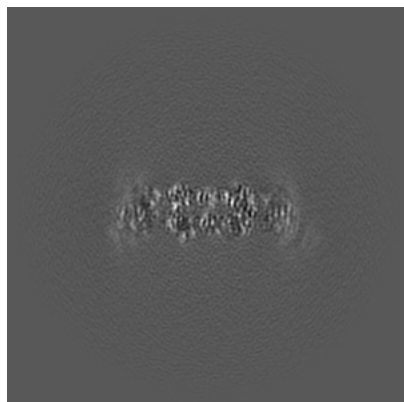


Z Index: 200

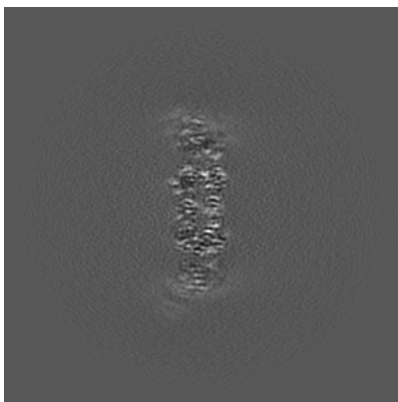
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

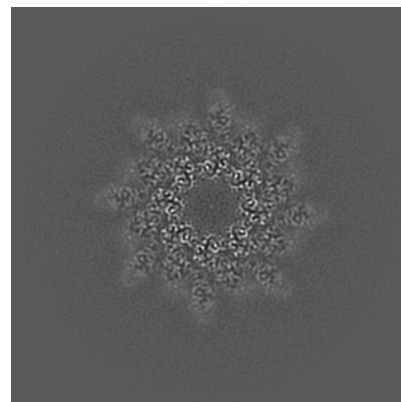
5.3.1 Primary map



X Index: 170

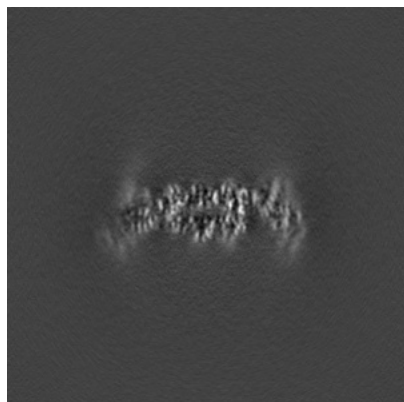


Y Index: 170

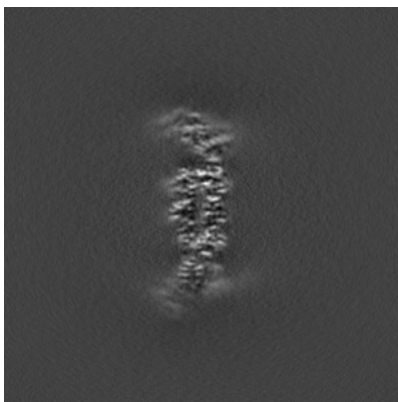


Z Index: 203

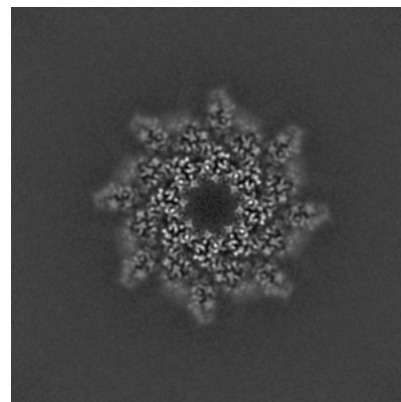
5.3.2 Raw map



X Index: 235



Y Index: 165

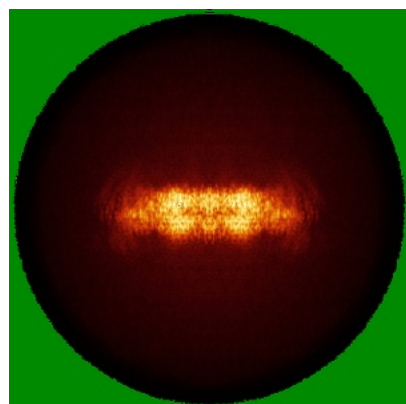


Z Index: 204

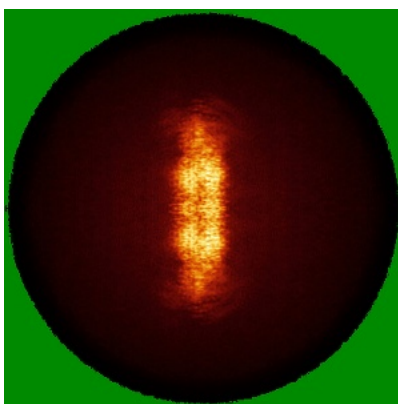
The images above show the largest variance slices of the map in three orthogonal directions.

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

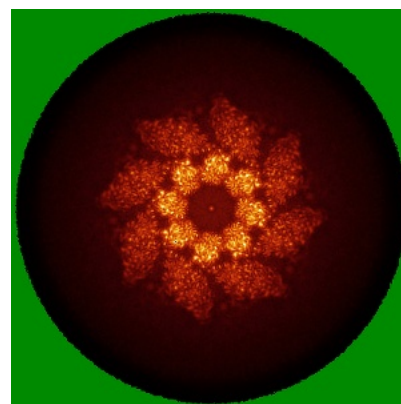
5.4.1 Primary map



X

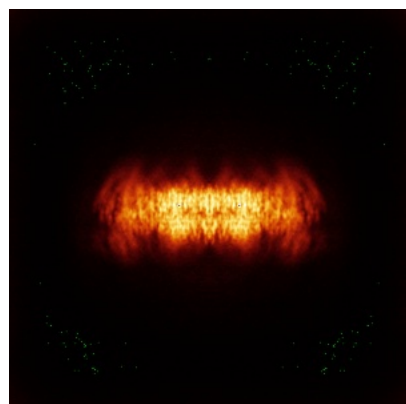


Y

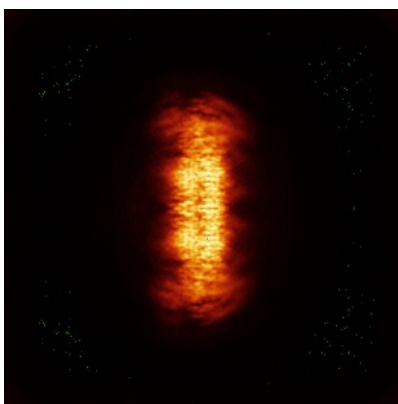


Z

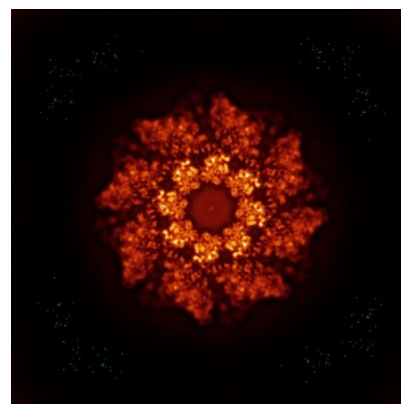
5.4.2 Raw map



X



Y

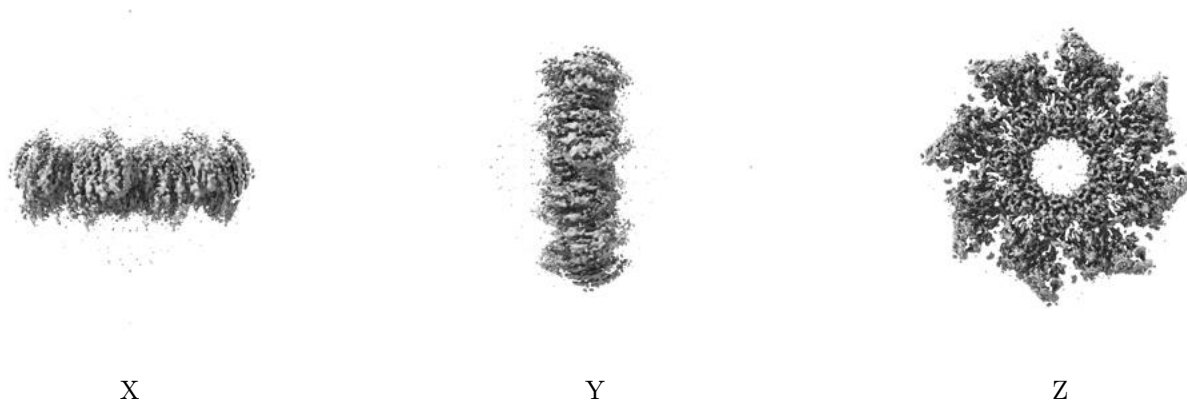


Z

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.

5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.365. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

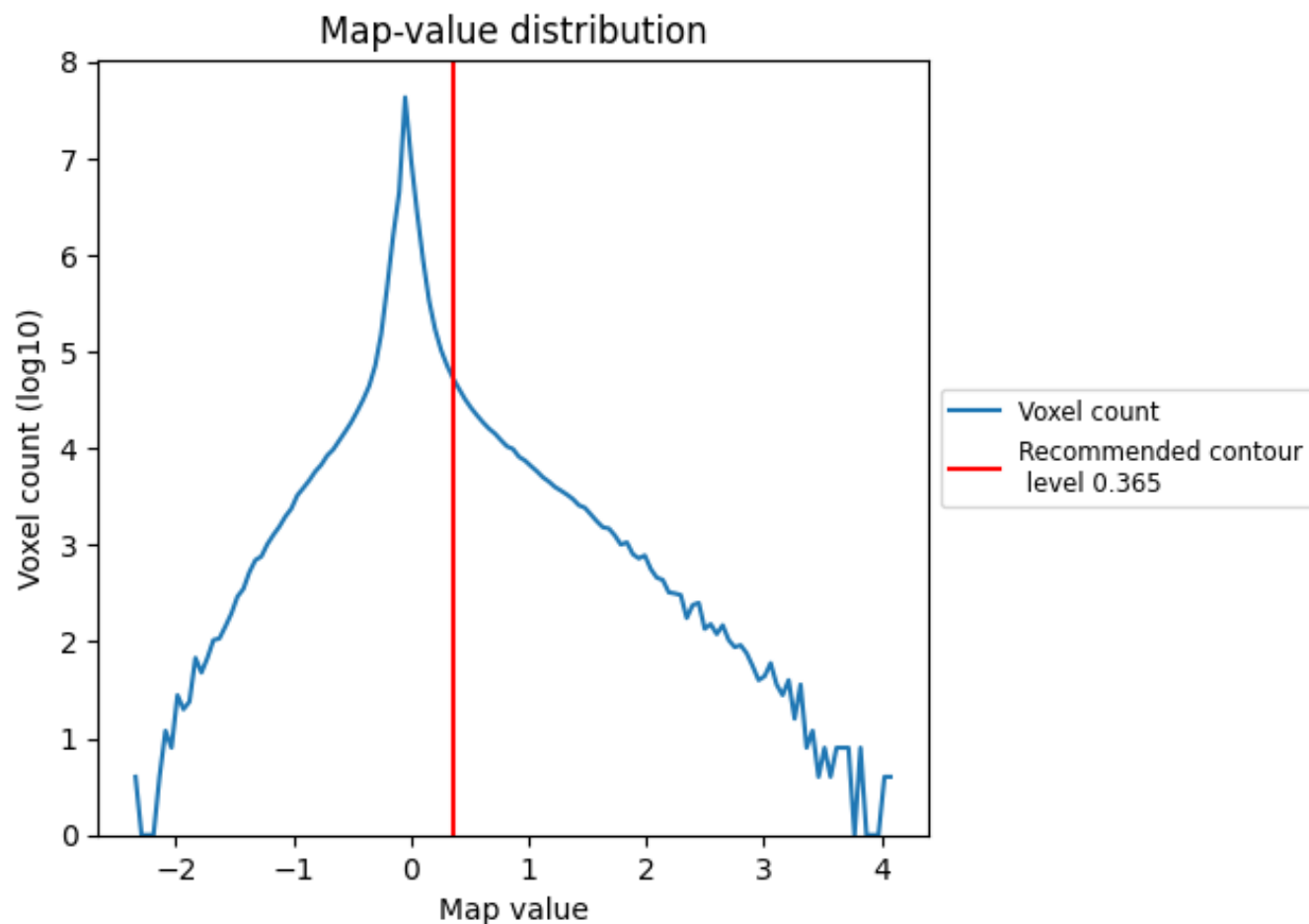
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

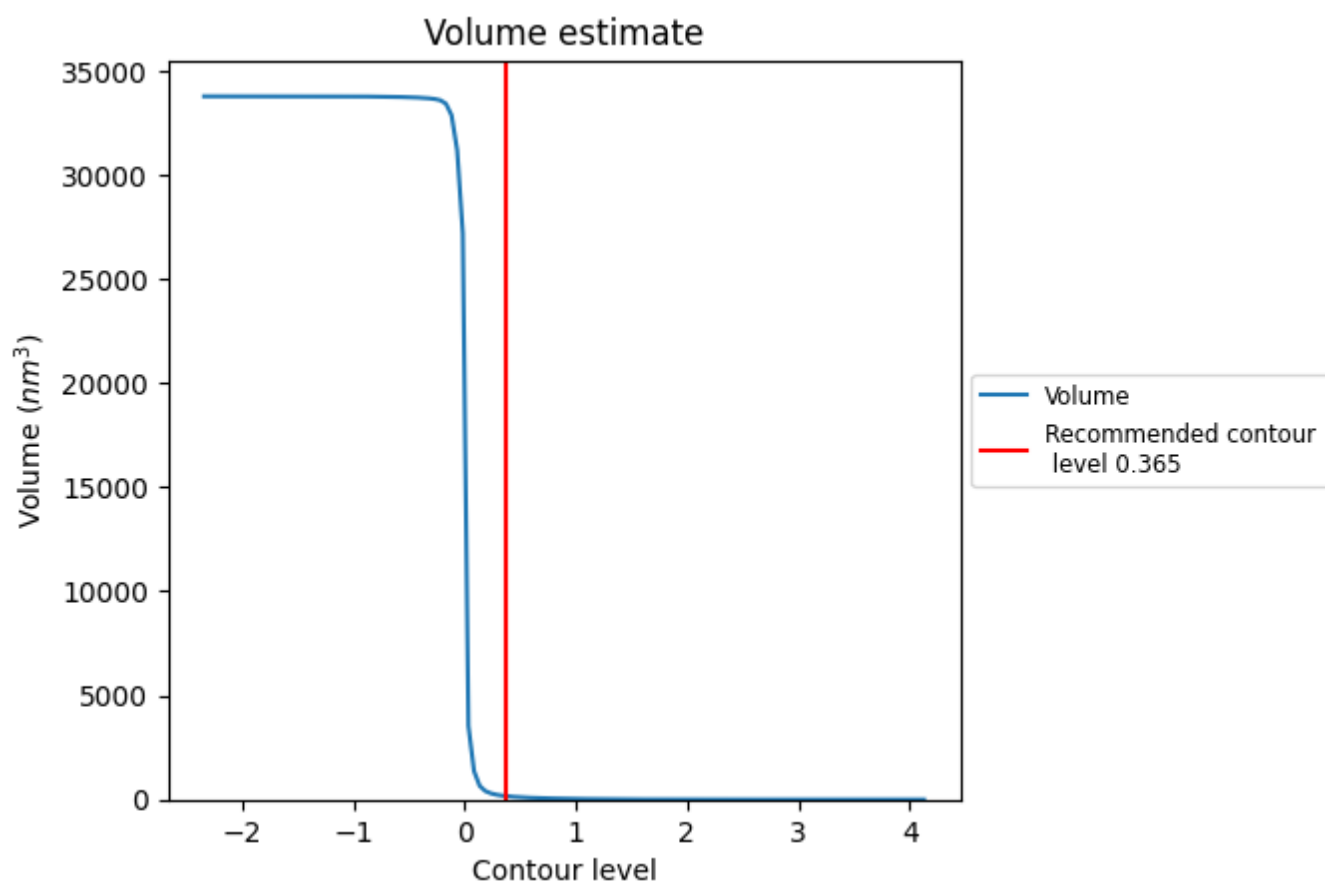
This section contains the results of statistical analysis of the map.

6.1 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.

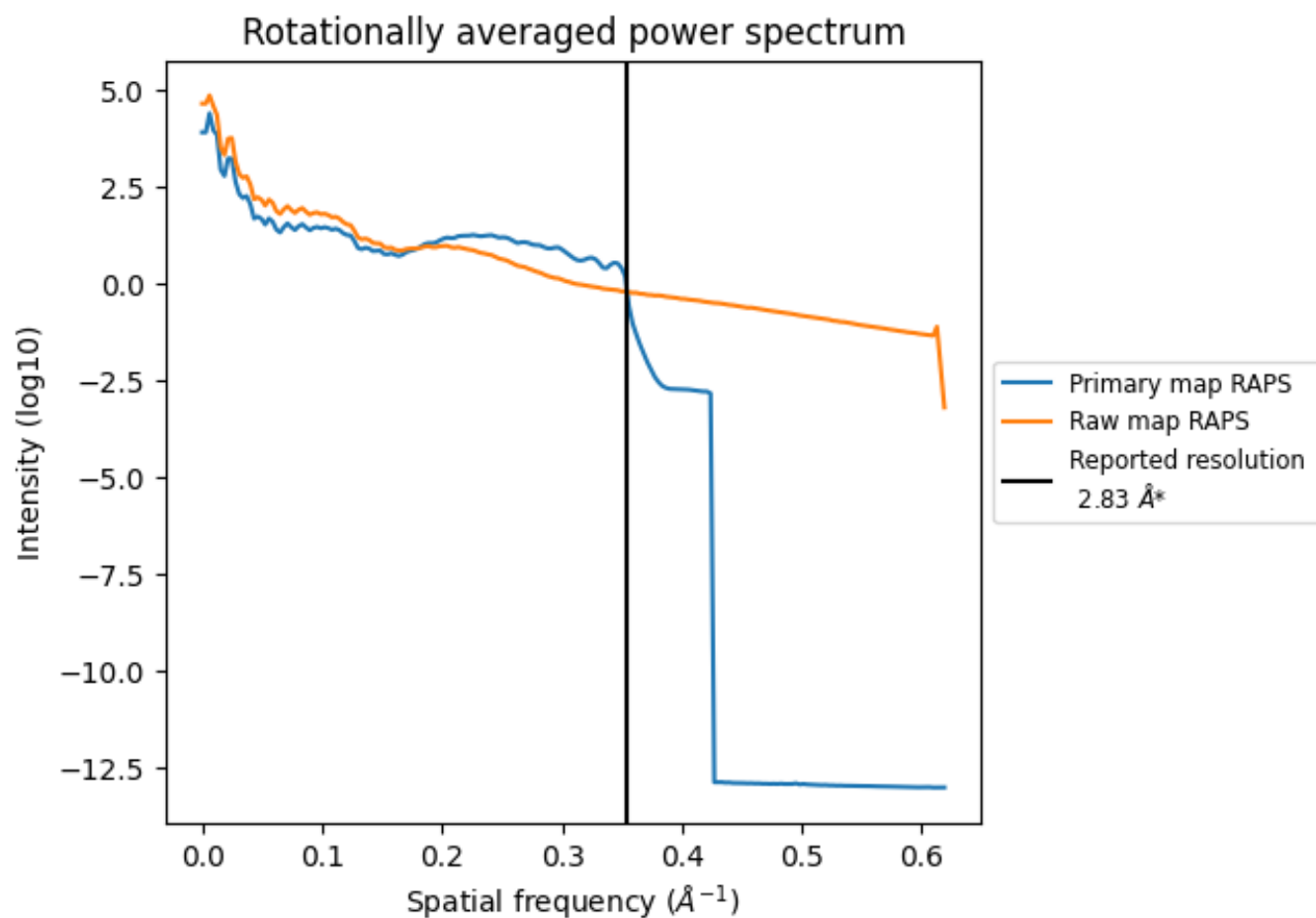
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 171 nm³; this corresponds to an approximate mass of 154 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.

6.3 Rotationally averaged power spectrum ⓘ

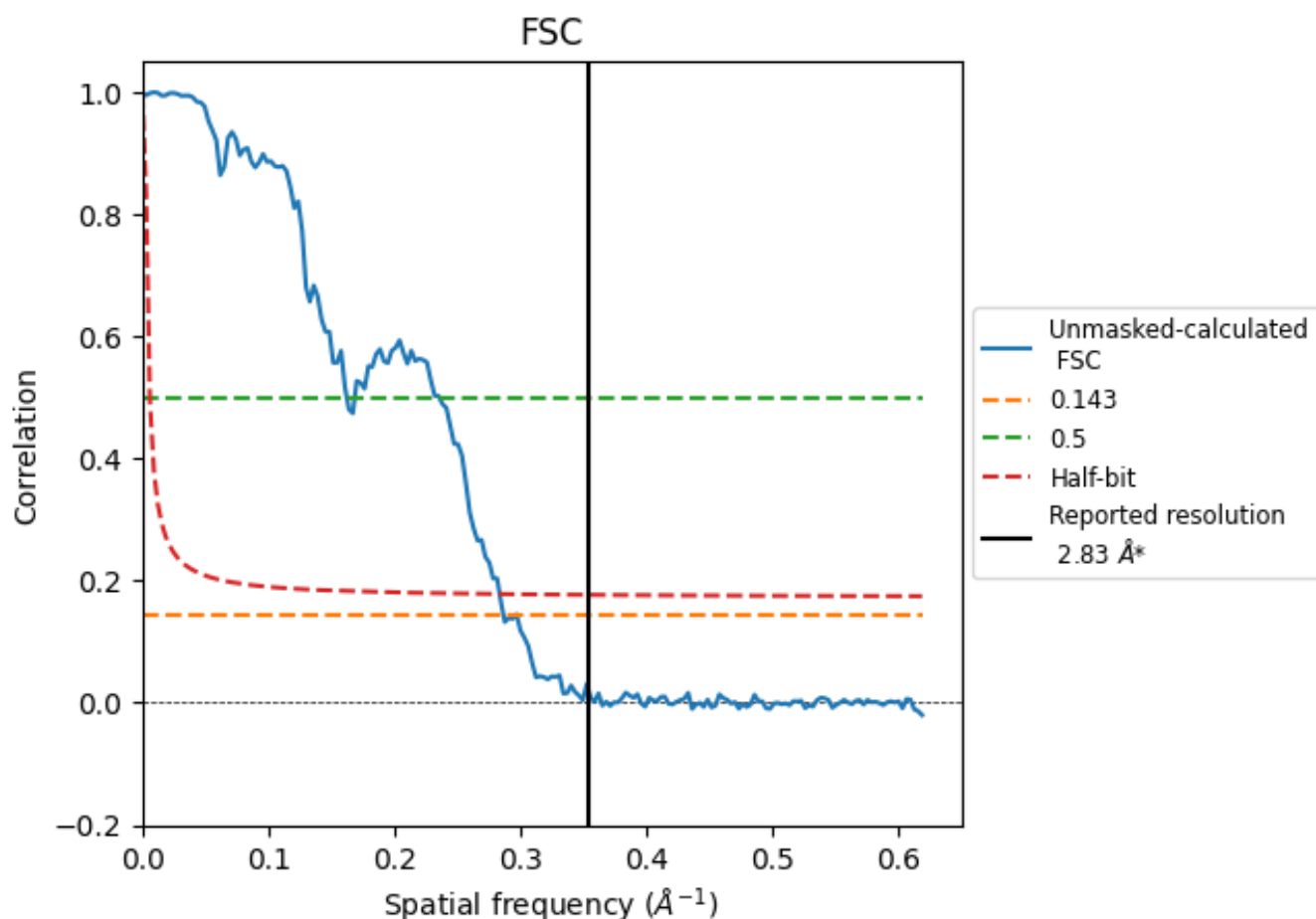


*Reported resolution corresponds to spatial frequency of $0.353 \text{ \AA}^{-1}$

7 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.

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.353 $\text{\AA}^{-1}$

7.2 Resolution estimates [i](#)

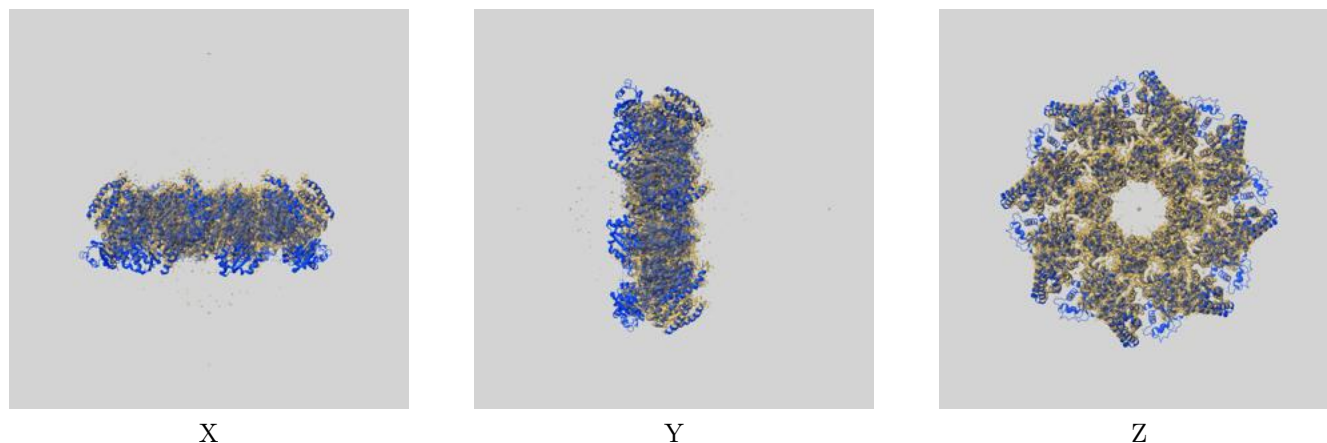
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.49	6.16	3.53

*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 3.49 differs from the reported value 2.83 by more than 10 %

8 Map-model fit [i](#)

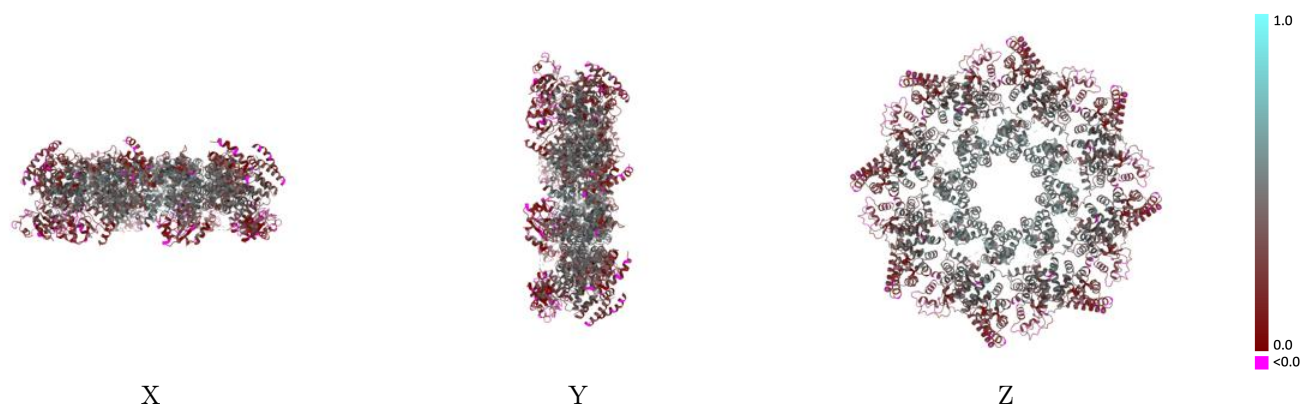
This section contains information regarding the fit between EMDB map EMD-62772 and PDB model 9L2D. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



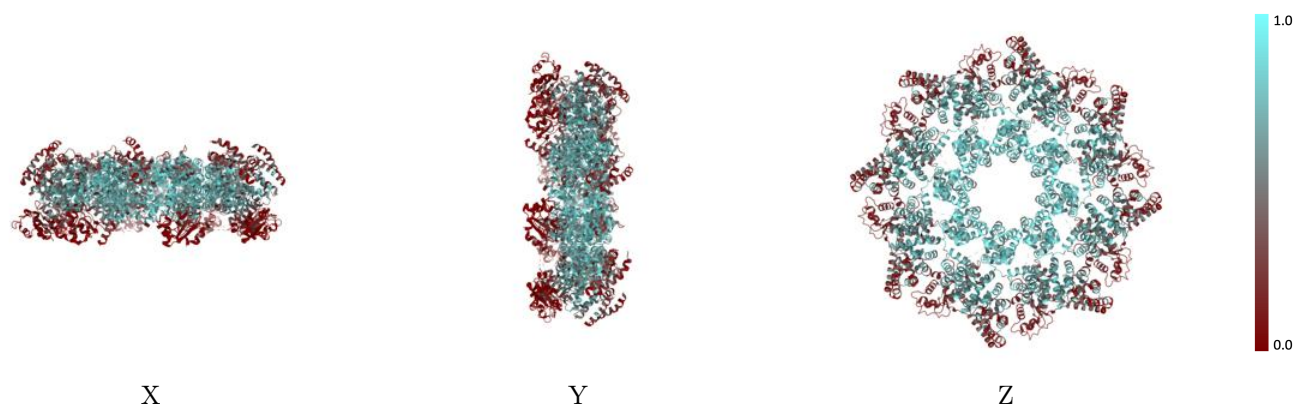
The images above show the 3D surface view of the map at the recommended contour level 0.365 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



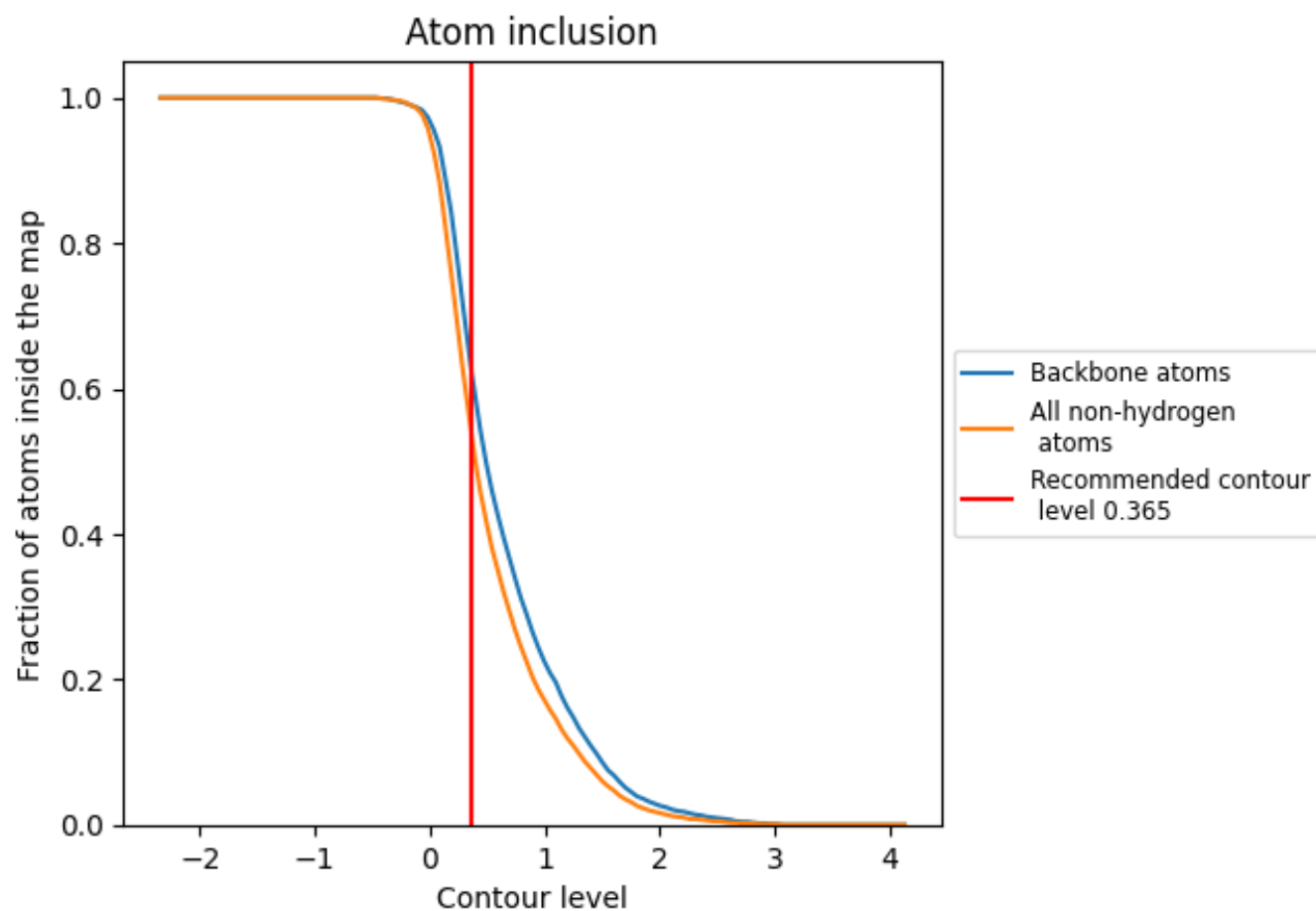
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 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 (0.365).

8.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.365) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5330	0.3530
A	0.5320	0.3530
B	0.5320	0.3510
C	0.5320	0.3530
D	0.5330	0.3540
E	0.5330	0.3530
F	0.5320	0.3530
G	0.5340	0.3530
H	0.5320	0.3520

1.0

0.0

<0.0