Full wwPDB EM Validation Report

May 15, 2025 – 10:38 AM EDT

PDB ID	:	9E2J / pdb_00009e2j
EMDB ID	:	EMD-47454
Title	:	Variediene synthase with five cyclases
Authors	:	Wenger, E.S.; Christianson, D.W.
Deposited on	:	2024-10-22
Resolution	:	3.59 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 (i) 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 (i)) were used in the production of this report:

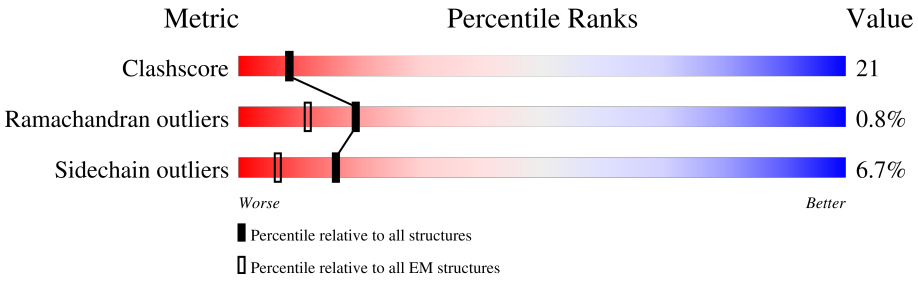
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.59 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	725	8% 44% 36% • 17%
1	B	725	12% 42% 32% • 24%
1	C	725	13% 45% 33% • 19%
1	D	725	10% 44% 35% • 18%
1	E	725	14% 44% 30% • 25%
1	F	725	• 27% 12% • 60%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25560 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 Variediene synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	605	Total	C	N	O	S	0	0
			4891	3104	843	915	29		
1	B	553	Total	C	N	O	S	0	0
			4448	2829	761	831	27		
1	C	584	Total	C	N	O	S	0	0
			4705	2989	807	880	29		
1	D	596	Total	C	N	O	S	0	0
			4814	3056	826	902	30		
1	E	546	Total	C	N	O	S	0	0
			4387	2782	757	821	27		
1	F	290	Total	C	N	O	S	0	0
			2315	1457	402	443	13		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A0P0ZD79
A	2	GLY	-	expression tag	UNP A0A0P0ZD79
A	3	SER	-	expression tag	UNP A0A0P0ZD79
A	4	SER	-	expression tag	UNP A0A0P0ZD79
A	5	HIS	-	expression tag	UNP A0A0P0ZD79
A	6	HIS	-	expression tag	UNP A0A0P0ZD79
A	7	HIS	-	expression tag	UNP A0A0P0ZD79
A	8	HIS	-	expression tag	UNP A0A0P0ZD79
A	9	HIS	-	expression tag	UNP A0A0P0ZD79
A	10	HIS	-	expression tag	UNP A0A0P0ZD79
A	11	SER	-	expression tag	UNP A0A0P0ZD79
A	12	SER	-	expression tag	UNP A0A0P0ZD79
A	13	GLY	-	expression tag	UNP A0A0P0ZD79
A	14	LEU	-	expression tag	UNP A0A0P0ZD79
A	15	VAL	-	expression tag	UNP A0A0P0ZD79
A	16	PRO	-	expression tag	UNP A0A0P0ZD79
A	17	ARG	-	expression tag	UNP A0A0P0ZD79
A	18	GLY	-	expression tag	UNP A0A0P0ZD79

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Chain	Residue	Modelled	Actual	Comment	Reference
A	19	SER	-	expression tag	UNP A0A0P0ZD79
A	20	HIS	-	expression tag	UNP A0A0P0ZD79
B	1	MET	-	initiating methionine	UNP A0A0P0ZD79
B	2	GLY	-	expression tag	UNP A0A0P0ZD79
B	3	SER	-	expression tag	UNP A0A0P0ZD79
B	4	SER	-	expression tag	UNP A0A0P0ZD79
B	5	HIS	-	expression tag	UNP A0A0P0ZD79
B	6	HIS	-	expression tag	UNP A0A0P0ZD79
B	7	HIS	-	expression tag	UNP A0A0P0ZD79
B	8	HIS	-	expression tag	UNP A0A0P0ZD79
B	9	HIS	-	expression tag	UNP A0A0P0ZD79
B	10	HIS	-	expression tag	UNP A0A0P0ZD79
B	11	SER	-	expression tag	UNP A0A0P0ZD79
B	12	SER	-	expression tag	UNP A0A0P0ZD79
B	13	GLY	-	expression tag	UNP A0A0P0ZD79
B	14	LEU	-	expression tag	UNP A0A0P0ZD79
B	15	VAL	-	expression tag	UNP A0A0P0ZD79
B	16	PRO	-	expression tag	UNP A0A0P0ZD79
B	17	ARG	-	expression tag	UNP A0A0P0ZD79
B	18	GLY	-	expression tag	UNP A0A0P0ZD79
B	19	SER	-	expression tag	UNP A0A0P0ZD79
B	20	HIS	-	expression tag	UNP A0A0P0ZD79
C	1	MET	-	initiating methionine	UNP A0A0P0ZD79
C	2	GLY	-	expression tag	UNP A0A0P0ZD79
C	3	SER	-	expression tag	UNP A0A0P0ZD79
C	4	SER	-	expression tag	UNP A0A0P0ZD79
C	5	HIS	-	expression tag	UNP A0A0P0ZD79
C	6	HIS	-	expression tag	UNP A0A0P0ZD79
C	7	HIS	-	expression tag	UNP A0A0P0ZD79
C	8	HIS	-	expression tag	UNP A0A0P0ZD79
C	9	HIS	-	expression tag	UNP A0A0P0ZD79
C	10	HIS	-	expression tag	UNP A0A0P0ZD79
C	11	SER	-	expression tag	UNP A0A0P0ZD79
C	12	SER	-	expression tag	UNP A0A0P0ZD79
C	13	GLY	-	expression tag	UNP A0A0P0ZD79
C	14	LEU	-	expression tag	UNP A0A0P0ZD79
C	15	VAL	-	expression tag	UNP A0A0P0ZD79
C	16	PRO	-	expression tag	UNP A0A0P0ZD79
C	17	ARG	-	expression tag	UNP A0A0P0ZD79
C	18	GLY	-	expression tag	UNP A0A0P0ZD79
C	19	SER	-	expression tag	UNP A0A0P0ZD79
C	20	HIS	-	expression tag	UNP A0A0P0ZD79

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP A0A0P0ZD79
D	2	GLY	-	expression tag	UNP A0A0P0ZD79
D	3	SER	-	expression tag	UNP A0A0P0ZD79
D	4	SER	-	expression tag	UNP A0A0P0ZD79
D	5	HIS	-	expression tag	UNP A0A0P0ZD79
D	6	HIS	-	expression tag	UNP A0A0P0ZD79
D	7	HIS	-	expression tag	UNP A0A0P0ZD79
D	8	HIS	-	expression tag	UNP A0A0P0ZD79
D	9	HIS	-	expression tag	UNP A0A0P0ZD79
D	10	HIS	-	expression tag	UNP A0A0P0ZD79
D	11	SER	-	expression tag	UNP A0A0P0ZD79
D	12	SER	-	expression tag	UNP A0A0P0ZD79
D	13	GLY	-	expression tag	UNP A0A0P0ZD79
D	14	LEU	-	expression tag	UNP A0A0P0ZD79
D	15	VAL	-	expression tag	UNP A0A0P0ZD79
D	16	PRO	-	expression tag	UNP A0A0P0ZD79
D	17	ARG	-	expression tag	UNP A0A0P0ZD79
D	18	GLY	-	expression tag	UNP A0A0P0ZD79
D	19	SER	-	expression tag	UNP A0A0P0ZD79
D	20	HIS	-	expression tag	UNP A0A0P0ZD79
E	1	MET	-	initiating methionine	UNP A0A0P0ZD79
E	2	GLY	-	expression tag	UNP A0A0P0ZD79
E	3	SER	-	expression tag	UNP A0A0P0ZD79
E	4	SER	-	expression tag	UNP A0A0P0ZD79
E	5	HIS	-	expression tag	UNP A0A0P0ZD79
E	6	HIS	-	expression tag	UNP A0A0P0ZD79
E	7	HIS	-	expression tag	UNP A0A0P0ZD79
E	8	HIS	-	expression tag	UNP A0A0P0ZD79
E	9	HIS	-	expression tag	UNP A0A0P0ZD79
E	10	HIS	-	expression tag	UNP A0A0P0ZD79
E	11	SER	-	expression tag	UNP A0A0P0ZD79
E	12	SER	-	expression tag	UNP A0A0P0ZD79
E	13	GLY	-	expression tag	UNP A0A0P0ZD79
E	14	LEU	-	expression tag	UNP A0A0P0ZD79
E	15	VAL	-	expression tag	UNP A0A0P0ZD79
E	16	PRO	-	expression tag	UNP A0A0P0ZD79
E	17	ARG	-	expression tag	UNP A0A0P0ZD79
E	18	GLY	-	expression tag	UNP A0A0P0ZD79
E	19	SER	-	expression tag	UNP A0A0P0ZD79
E	20	HIS	-	expression tag	UNP A0A0P0ZD79
F	1	MET	-	initiating methionine	UNP A0A0P0ZD79
F	2	GLY	-	expression tag	UNP A0A0P0ZD79

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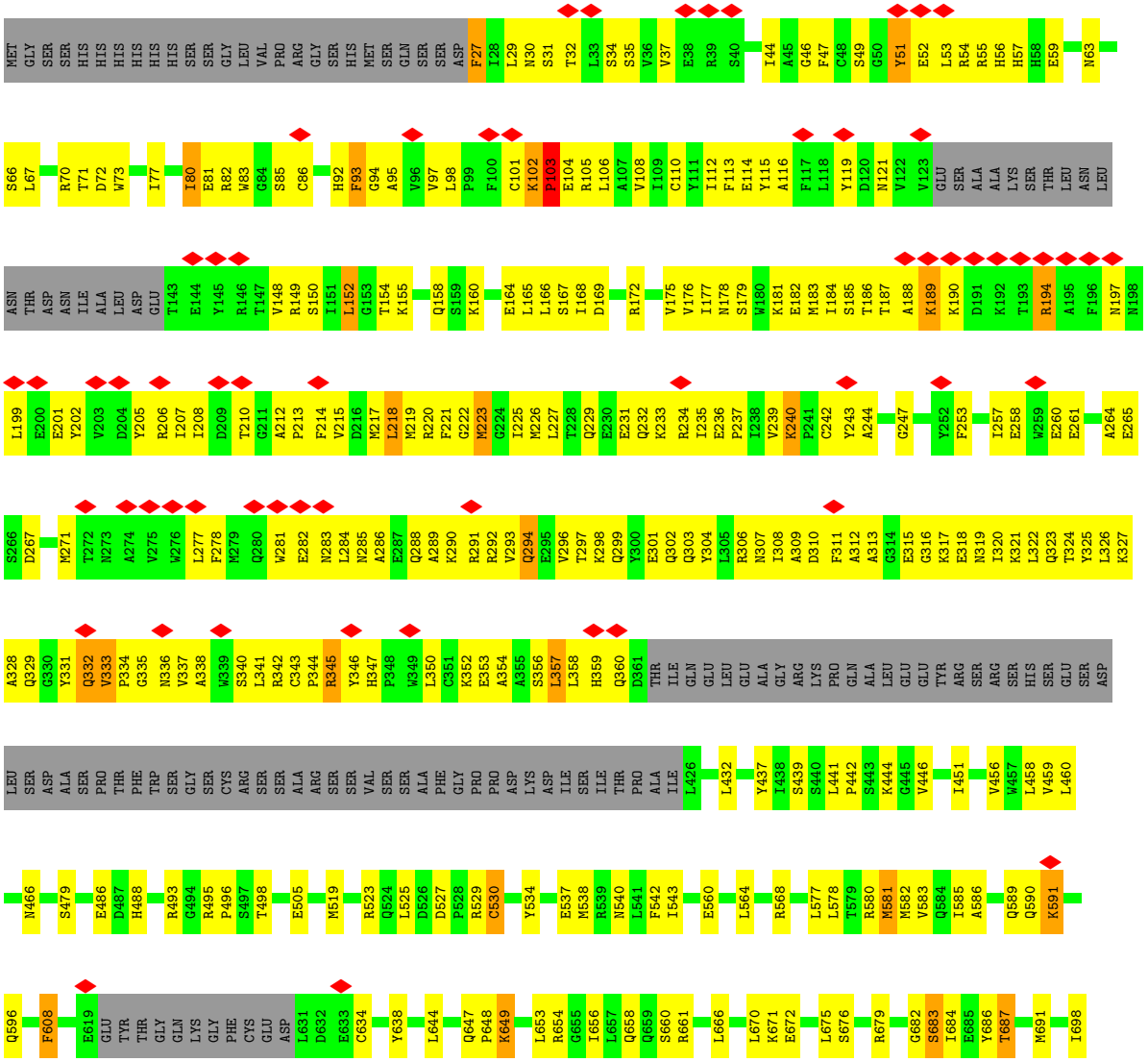
Chain	Residue	Modelled	Actual	Comment	Reference
F	3	SER	-	expression tag	UNP A0A0P0ZD79
F	4	SER	-	expression tag	UNP A0A0P0ZD79
F	5	HIS	-	expression tag	UNP A0A0P0ZD79
F	6	HIS	-	expression tag	UNP A0A0P0ZD79
F	7	HIS	-	expression tag	UNP A0A0P0ZD79
F	8	HIS	-	expression tag	UNP A0A0P0ZD79
F	9	HIS	-	expression tag	UNP A0A0P0ZD79
F	10	HIS	-	expression tag	UNP A0A0P0ZD79
F	11	SER	-	expression tag	UNP A0A0P0ZD79
F	12	SER	-	expression tag	UNP A0A0P0ZD79
F	13	GLY	-	expression tag	UNP A0A0P0ZD79
F	14	LEU	-	expression tag	UNP A0A0P0ZD79
F	15	VAL	-	expression tag	UNP A0A0P0ZD79
F	16	PRO	-	expression tag	UNP A0A0P0ZD79
F	17	ARG	-	expression tag	UNP A0A0P0ZD79
F	18	GLY	-	expression tag	UNP A0A0P0ZD79
F	19	SER	-	expression tag	UNP A0A0P0ZD79
F	20	HIS	-	expression tag	UNP A0A0P0ZD79

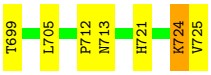
3 Residue-property plots (i)

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: Variediene synthase

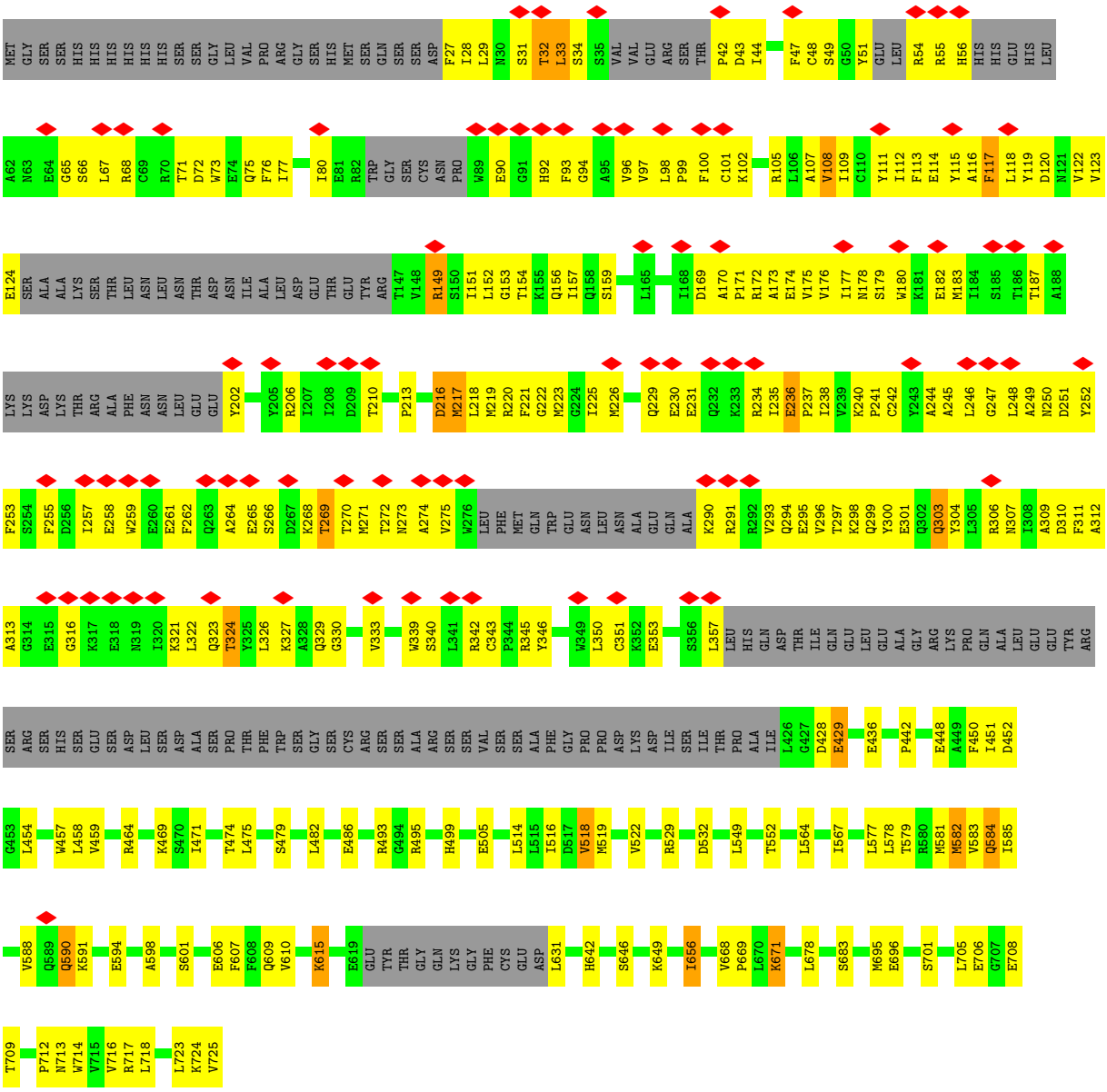
Chain A:





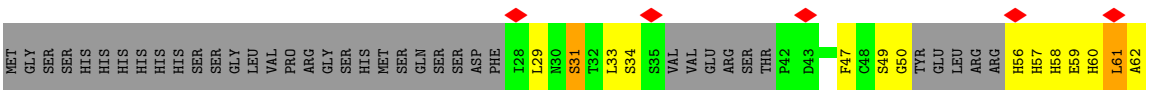
• Molecule 1: Variediene synthase

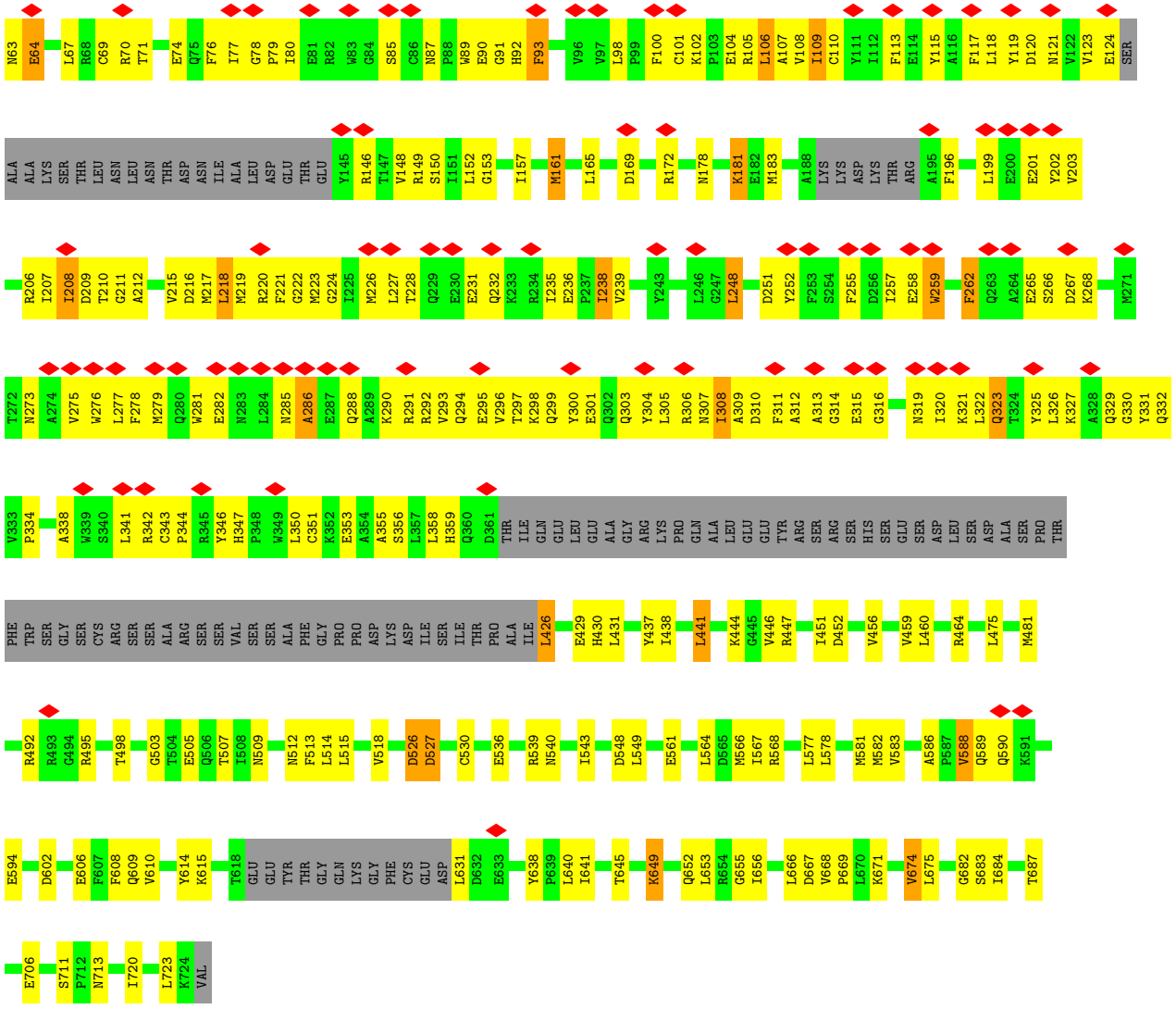
Chain B:



• Molecule 1: Variediene synthase

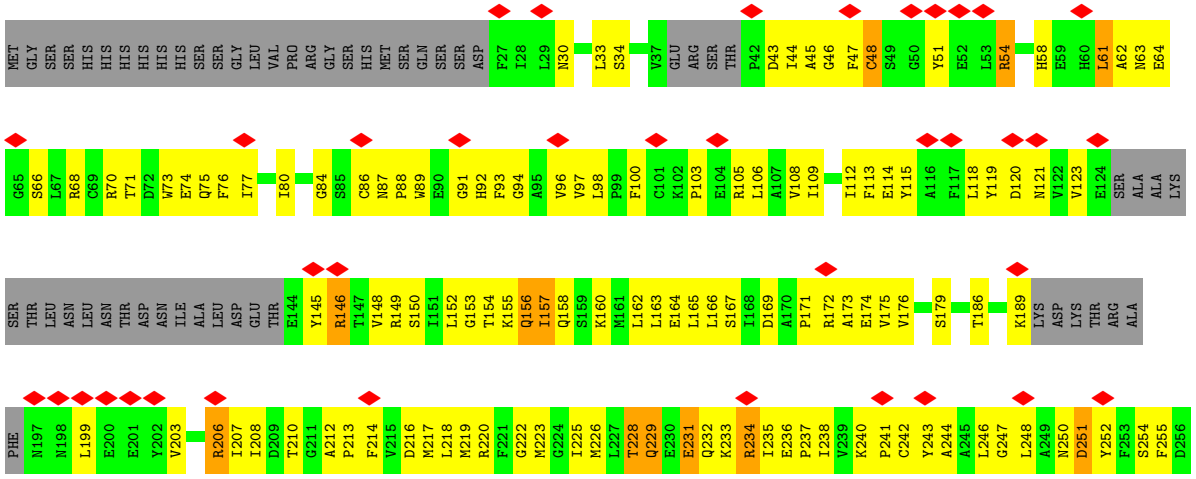
Chain C:

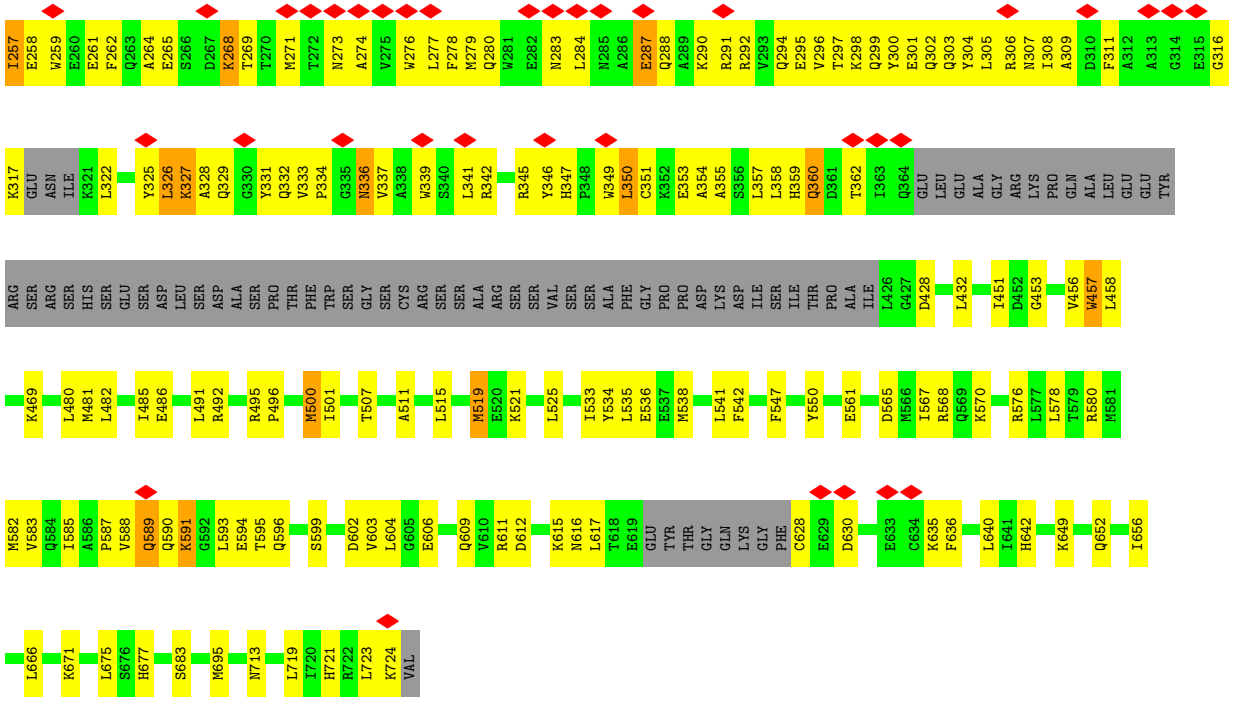




• Molecule 1: Variediene synthase

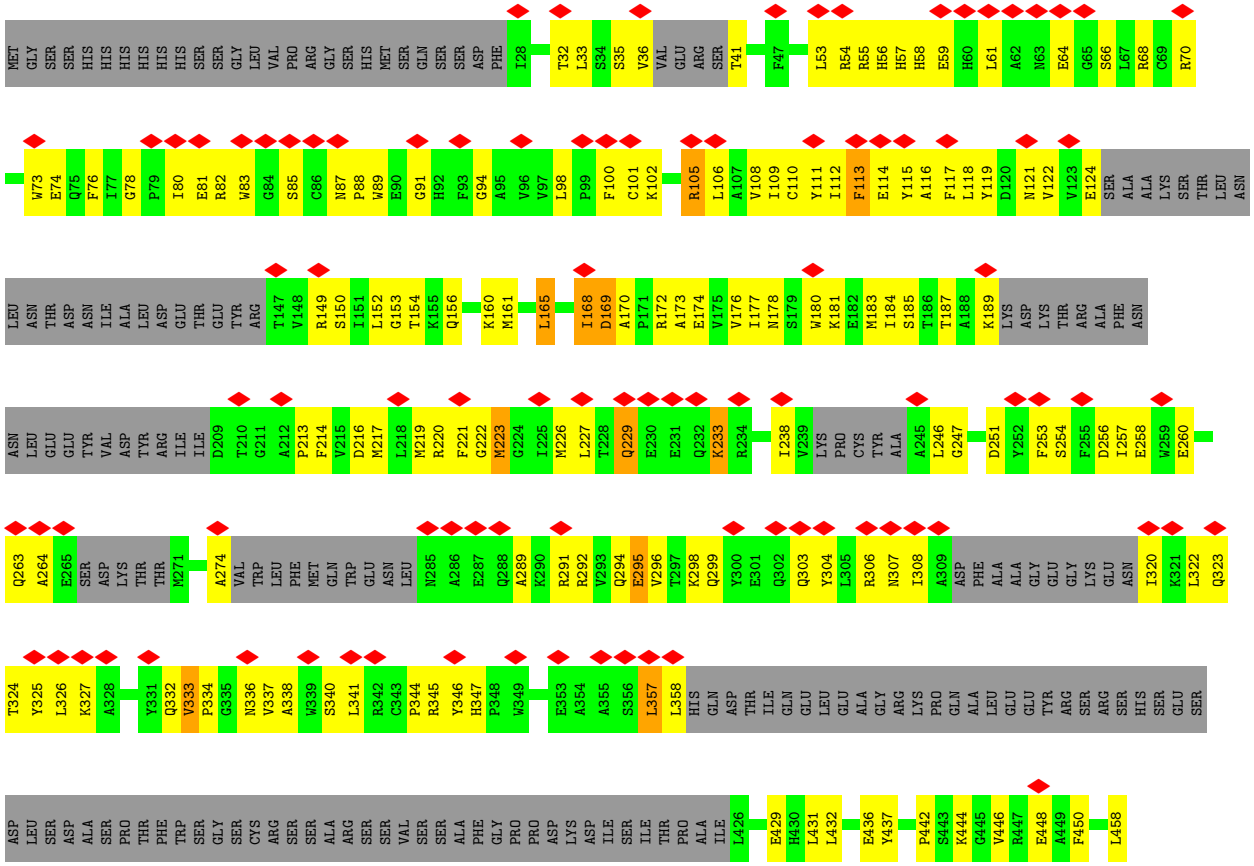
Chain D:

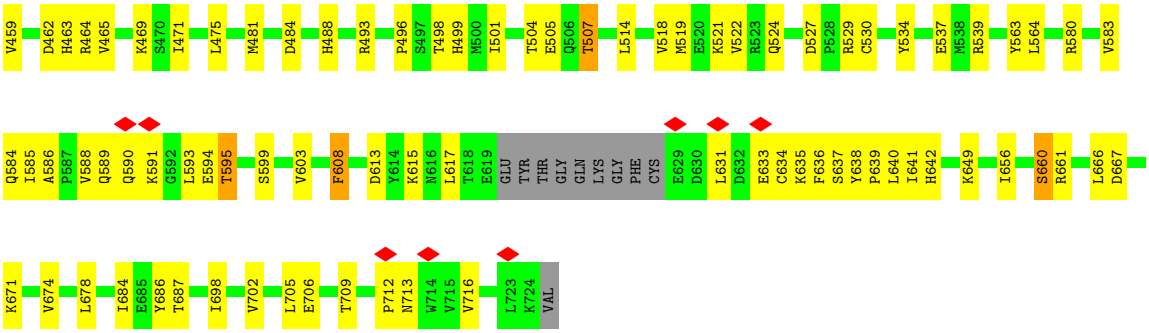




• Molecule 1: Variediene synthase

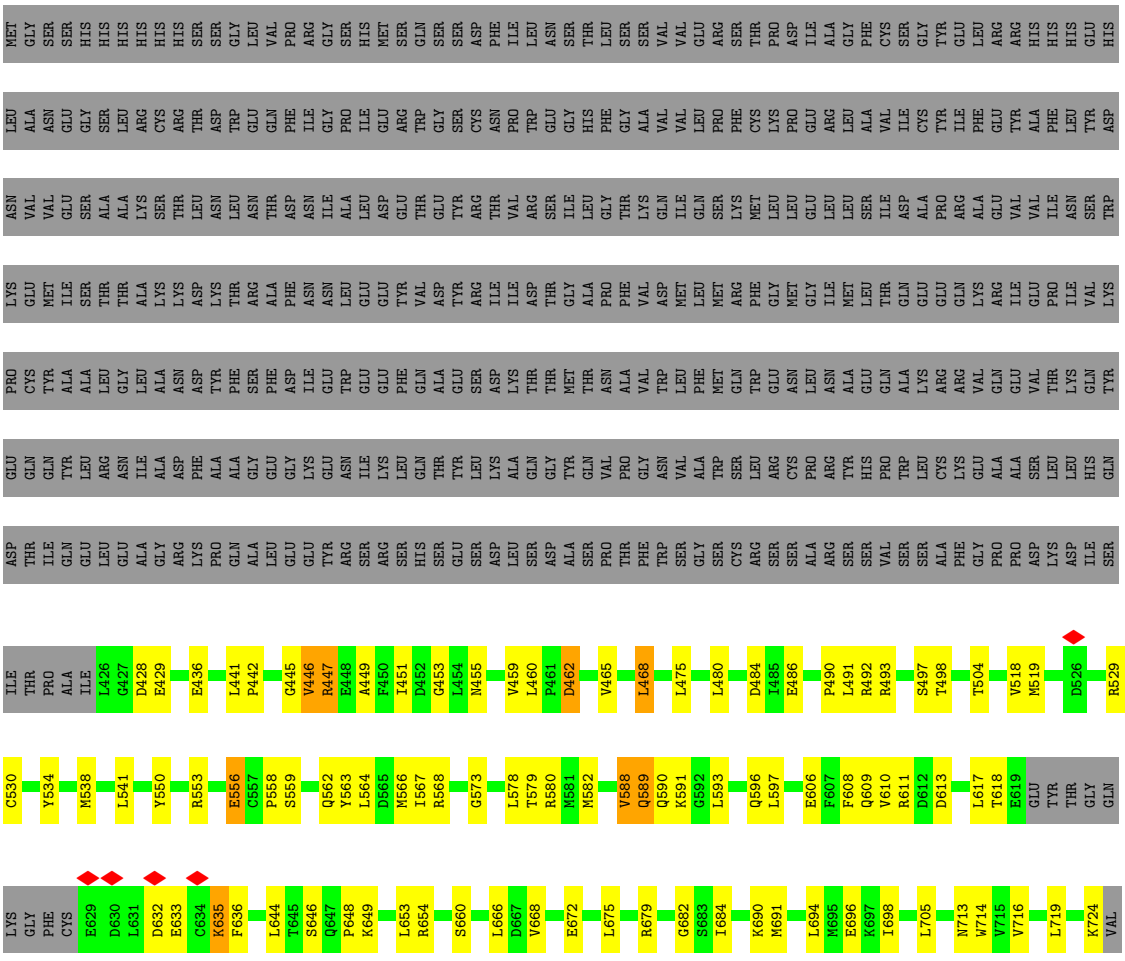
Chain E:





• Molecule 1: Variediene synthase

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51215	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 ($e^-/Å^2$)	43	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.048	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	414.72003, 414.72003, 414.72003	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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	0.22	0/4995	0.56	3/6755 (0.0%)
1	B	0.22	0/4534	0.53	0/6120
1	C	0.22	0/4804	0.52	0/6496
1	D	0.22	0/4914	0.60	3/6643 (0.0%)
1	E	0.22	0/4471	0.53	2/6038 (0.0%)
1	F	0.22	0/2355	0.46	0/3181
All	All	0.22	0/26073	0.54	8/35233 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	327	LYS	N-CA-C	-9.15	101.21	111.82
1	E	583	VAL	N-CA-C	-5.73	107.26	111.90
1	D	457	TRP	N-CA-C	-5.70	105.73	114.16
1	E	585	ILE	N-CA-C	-5.47	107.46	113.43
1	D	536	GLU	N-CA-C	-5.37	107.98	114.75
1	A	332	GLN	CA-C-N	5.16	123.49	120.24
1	A	332	GLN	C-N-CA	5.16	123.49	120.24
1	A	103	PRO	N-CA-CB	-5.09	97.90	103.25

There are no chirality outliers.

There are no planarity outliers.

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	4891	0	4826	229	0
1	B	4448	0	4410	201	0
1	C	4705	0	4629	197	0
1	D	4814	0	4737	254	0
1	E	4387	0	4342	175	0
1	F	2315	0	2312	60	0
All	All	25560	0	25256	1084	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 21.

All (1084) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:GLN:HA	1:D:291:ARG:HB2	1.49	0.91
1:B:304:TYR:HA	1:B:307:ASN:HB2	1.54	0.87
1:A:341:LEU:HD13	1:A:342:ARG:HG3	1.58	0.85
1:D:297:THR:O	1:D:301:GLU:N	2.10	0.85
1:D:292:ARG:O	1:D:296:VAL:N	2.09	0.85
1:C:259:TRP:HA	1:C:262:PHE:HB3	1.57	0.84
1:A:181:LYS:HA	1:A:184:ILE:HG22	1.61	0.83
1:A:51:TYR:HB3	1:A:334:PRO:HG3	1.60	0.83
1:A:258:GLU:HA	1:A:261:GLU:HG2	1.61	0.82
1:B:300:TYR:O	1:B:304:TYR:N	2.13	0.81
1:E:115:TYR:O	1:E:119:TYR:N	2.12	0.81
1:E:112:ILE:O	1:E:116:ALA:N	2.12	0.81
1:C:299:GLN:O	1:C:303:GLN:N	2.12	0.80
1:A:656:ILE:HD11	1:A:670:LEU:HD22	1.63	0.80
1:B:33:LEU:HB2	1:B:56:HIS:HA	1.63	0.80
1:D:300:TYR:HA	1:D:303:GLN:HB2	1.63	0.80
1:B:297:THR:HA	1:B:300:TYR:HB2	1.63	0.79
1:A:357:LEU:HA	1:A:360:GLN:HB2	1.62	0.79
1:D:257:ILE:HD11	1:D:346:TYR:HA	1.65	0.79
1:E:55:ARG:HG2	1:E:56:HIS:H	1.48	0.79
1:E:183:MET:HG3	1:E:214:PHE:HB2	1.63	0.79
1:E:471:ILE:HD11	1:E:522:VAL:HG22	1.64	0.78
1:B:303:GLN:O	1:B:307:ASN:N	2.17	0.78
1:C:481:MET:HG3	1:C:498:THR:HG21	1.64	0.78
1:A:46:GLY:O	1:A:298:LYS:NZ	2.17	0.77
1:D:257:ILE:O	1:D:261:GLU:N	2.15	0.77
1:B:306:ARG:O	1:B:310:ASP:N	2.13	0.76
1:B:268:LYS:HE3	1:B:271:MET:HB2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:GLU:O	1:D:299:GLN:N	2.18	0.76
1:E:481:MET:HG2	1:E:498:THR:HG21	1.67	0.75
1:B:102:LYS:HD2	1:B:105:ARG:HE	1.50	0.75
1:A:261:GLU:O	1:A:265:GLU:N	2.18	0.75
1:A:194:ARG:NH1	1:A:201:GLU:OE1	2.18	0.75
1:A:527:ASP:HB3	1:A:530:CYS:HB2	1.68	0.75
1:F:480:LEU:HD22	1:F:492:ARG:HH12	1.49	0.74
1:E:35:SER:HA	1:E:57:HIS:CE1	2.23	0.74
1:A:495:ARG:HG3	1:A:496:PRO:HD2	1.67	0.74
1:A:231:GLU:HA	1:A:234:ARG:HB3	1.69	0.74
1:D:583:VAL:HG21	1:D:594:GLU:HG3	1.69	0.74
1:A:179:SER:HA	1:A:182:GLU:HB3	1.69	0.73
1:D:298:LYS:HA	1:D:301:GLU:HB3	1.69	0.73
1:A:315:GLU:HB2	1:A:318:GLU:HB2	1.71	0.73
1:B:248:LEU:HA	1:B:251:ASP:HB2	1.71	0.73
1:B:229:GLN:NE2	1:B:230:GLU:OE1	2.22	0.73
1:B:464:ARG:HD3	1:B:585:ILE:HD11	1.71	0.73
1:C:98:LEU:HD21	1:C:219:MET:HG3	1.70	0.72
1:C:536:GLU:HG2	1:C:539:ARG:HH22	1.54	0.72
1:B:172:ARG:HG2	1:B:221:PHE:HD1	1.55	0.72
1:F:475:LEU:HD13	1:F:518:VAL:HG21	1.72	0.72
1:A:441:LEU:HB3	1:A:493:ARG:HD3	1.72	0.71
1:F:442:PRO:O	1:F:493:ARG:NH1	2.22	0.71
1:C:106:LEU:O	1:C:110:CYS:N	2.19	0.71
1:D:329:GLN:OE1	1:D:332:GLN:NE2	2.24	0.71
1:A:232:GLN:HA	1:A:235:ILE:HG22	1.72	0.71
1:B:448:GLU:HG2	1:B:469:LYS:HD3	1.71	0.71
1:C:76:PHE:O	1:C:149:ARG:NH1	2.23	0.71
1:C:291:ARG:O	1:C:295:GLU:N	2.22	0.71
1:E:33:LEU:HB2	1:E:56:HIS:CE1	2.25	0.71
1:E:176:VAL:O	1:E:180:TRP:N	2.23	0.71
1:B:258:GLU:HA	1:B:261:GLU:HB2	1.73	0.70
1:C:583:VAL:HG11	1:C:594:GLU:HG3	1.73	0.70
1:D:300:TYR:O	1:D:304:TYR:N	2.24	0.70
1:A:296:VAL:HA	1:A:299:GLN:HG3	1.72	0.70
1:D:298:LYS:O	1:D:302:GLN:N	2.17	0.70
1:E:101:CYS:HA	1:E:223:MET:HE2	1.74	0.70
1:E:98:LEU:HD21	1:E:219:MET:HB2	1.73	0.70
1:B:116:ALA:O	1:B:120:ASP:N	2.23	0.70
1:B:114:GLU:HA	1:B:117:PHE:HB2	1.74	0.69
1:A:101:CYS:HB2	1:A:106:LEU:HD13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:MET:HE1	1:A:329:GLN:HG2	1.74	0.69
1:B:269:THR:OG1	1:B:270:THR:N	2.25	0.69
1:D:279:MET:O	1:D:283:ASN:ND2	2.25	0.69
1:B:235:ILE:HD13	1:B:322:LEU:HD21	1.74	0.69
1:A:206:ARG:NH1	1:A:247:GLY:O	2.25	0.69
1:A:223:MET:SD	1:A:225:ILE:HG13	2.33	0.69
1:A:350:LEU:O	1:A:354:ALA:N	2.19	0.69
1:B:34:SER:HB2	1:B:54:ARG:HB3	1.74	0.69
1:D:354:ALA:O	1:D:358:LEU:N	2.25	0.69
1:B:252:TYR:OH	1:B:291:ARG:NH1	2.26	0.68
1:D:115:TYR:O	1:D:119:TYR:N	2.18	0.68
1:E:121:ASN:HA	1:E:124:GLU:HB2	1.74	0.68
1:D:311:PHE:O	1:D:316:GLY:N	2.27	0.68
1:B:451:ILE:HD13	1:B:582:MET:HE2	1.73	0.68
1:D:311:PHE:CE2	1:D:326:LEU:HD11	2.29	0.68
1:E:76:PHE:O	1:E:149:ARG:NH2	2.26	0.68
1:C:212:ALA:HA	1:C:215:VAL:HB	1.74	0.68
1:C:667:ASP:OD2	1:C:668:VAL:N	2.27	0.68
1:D:87:ASN:ND2	1:D:342:ARG:O	2.27	0.68
1:A:458:LEU:HD22	1:A:590:GLN:HB3	1.76	0.67
1:A:303:GLN:O	1:A:307:ASN:N	2.25	0.67
1:C:178:ASN:HA	1:C:181:LYS:HE3	1.77	0.67
1:D:357:LEU:HA	1:D:360:GLN:HB2	1.75	0.67
1:D:54:ARG:NH1	1:D:331:TYR:OH	2.27	0.67
1:D:259:TRP:HA	1:D:271:MET:HE2	1.76	0.67
1:D:642:HIS:HD2	1:D:683:SER:HA	1.59	0.67
1:D:451:ILE:HD11	1:D:578:LEU:HD13	1.75	0.67
1:A:257:ILE:HB	1:A:346:TYR:HB3	1.76	0.67
1:B:105:ARG:HD2	1:B:222:GLY:HA2	1.76	0.67
1:B:567:ILE:HD12	1:B:609:GLN:HG2	1.76	0.67
1:C:110:CYS:HA	1:C:113:PHE:HB2	1.75	0.67
1:C:217:MET:SD	1:C:220:ARG:NH1	2.68	0.67
1:C:316:GLY:HA2	1:C:319:ASN:HB2	1.76	0.67
1:B:115:TYR:O	1:B:119:TYR:N	2.25	0.66
1:D:156:GLN:O	1:D:158:GLN:N	2.27	0.66
1:A:34:SER:HA	1:A:56:HIS:HA	1.77	0.66
1:B:178:ASN:O	1:B:182:GLU:N	2.20	0.66
1:D:257:ILE:HG22	1:D:261:GLU:HB2	1.76	0.66
1:E:149:ARG:O	1:E:153:GLY:N	2.25	0.66
1:A:181:LYS:O	1:A:185:SER:N	2.17	0.66
1:A:85:SER:OG	1:A:86:CYS:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:GLU:O	1:B:268:LYS:NZ	2.28	0.66
1:A:184:ILE:O	1:A:188:ALA:N	2.29	0.66
1:D:287:GLU:HB2	1:D:291:ARG:HH21	1.60	0.66
1:B:324:THR:HA	1:B:327:LYS:HB3	1.78	0.66
1:A:229:GLN:HA	1:A:232:GLN:HB3	1.77	0.66
1:A:284:LEU:HB3	1:A:288:GLN:HB3	1.75	0.66
1:C:326:LEU:HA	1:C:329:GLN:HB3	1.77	0.66
1:E:89:TRP:HE1	1:E:357:LEU:HG	1.60	0.66
1:B:42:PRO:HB2	1:B:51:TYR:H	1.60	0.66
1:D:305:LEU:O	1:D:309:ALA:N	2.17	0.65
1:A:116:ALA:HA	1:A:119:TYR:HB3	1.77	0.65
1:E:588:VAL:HA	1:E:591:LYS:HG3	1.77	0.65
1:C:235:ILE:HA	1:C:238:ILE:HB	1.78	0.65
1:D:73:TRP:CD1	1:D:77:ILE:HB	2.32	0.65
1:E:73:TRP:O	1:E:78:GLY:N	2.29	0.65
1:E:631:LEU:HD12	1:E:671:LYS:HG2	1.78	0.65
1:C:216:ASP:O	1:C:220:ARG:N	2.27	0.65
1:D:328:ALA:HA	1:D:331:TYR:HD2	1.61	0.65
1:D:354:ALA:HA	1:D:357:LEU:HB3	1.77	0.65
1:B:55:ARG:NH1	1:B:56:HIS:O	2.30	0.65
1:B:519:MET:HA	1:B:522:VAL:HG22	1.79	0.65
1:C:322:LEU:HD12	1:C:322:LEU:H	1.61	0.65
1:C:118:LEU:HA	1:C:121:ASN:HB2	1.79	0.64
1:A:34:SER:HB2	1:A:54:ARG:HD2	1.80	0.64
1:A:183:MET:O	1:A:187:THR:N	2.30	0.64
1:C:308:ILE:HA	1:C:311:PHE:HB3	1.79	0.64
1:B:261:GLU:O	1:B:265:GLU:N	2.23	0.64
1:D:251:ASP:OD2	1:D:274:ALA:N	2.26	0.64
1:E:172:ARG:HH21	1:E:226:MET:HB2	1.62	0.64
1:A:240:LYS:HA	1:A:243:TYR:HB2	1.79	0.64
1:A:340:SER:HB2	1:A:346:TYR:OH	1.97	0.64
1:F:568:ARG:NH1	1:F:606:GLU:OE2	2.31	0.64
1:C:503:GLY:O	1:C:507:THR:OG1	2.16	0.64
1:B:262:PHE:HA	1:B:268:LYS:HD3	1.78	0.64
1:D:214:PHE:HA	1:D:217:MET:HB3	1.79	0.63
1:C:109:ILE:O	1:C:113:PHE:N	2.27	0.63
1:E:173:ALA:O	1:E:177:ILE:N	2.27	0.63
1:D:290:LYS:O	1:D:294:GLN:N	2.30	0.63
1:C:172:ARG:HA	1:C:226:MET:HE1	1.80	0.63
1:B:213:PRO:O	1:B:217:MET:N	2.29	0.63
1:A:596:GLN:HB3	1:A:705:LEU:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:539:ARG:NH2	1:F:428:ASP:OD2	2.32	0.63
1:C:69:CYS:HB3	1:C:118:LEU:HD12	1.81	0.62
1:C:87:ASN:HD21	1:C:90:GLU:HB2	1.62	0.62
1:E:177:ILE:O	1:E:181:LYS:N	2.23	0.62
1:F:559:SER:HB3	1:F:562:GLN:HG3	1.80	0.62
1:B:94:GLY:HA2	1:B:97:VAL:HB	1.82	0.62
1:D:248:LEU:HA	1:D:251:ASP:HB3	1.81	0.62
1:D:274:ALA:HA	1:D:277:LEU:HB2	1.81	0.62
1:D:303:GLN:HG3	1:D:306:ARG:HH21	1.65	0.62
1:D:305:LEU:HA	1:D:308:ILE:HB	1.81	0.62
1:D:628:CYS:SG	1:D:671:LYS:NZ	2.72	0.62
1:D:105:ARG:HD2	1:D:109:ILE:HD11	1.81	0.62
1:B:65:GLY:HA2	1:B:68:ARG:HE	1.64	0.62
1:C:85:SER:HB2	1:C:93:PHE:HB2	1.81	0.62
1:C:608:PHE:HE2	1:C:723:LEU:HD21	1.64	0.62
1:E:168:ILE:O	1:E:170:ALA:N	2.32	0.62
1:B:33:LEU:HD13	1:B:56:HIS:CD2	2.35	0.62
1:E:617:LEU:HD12	1:E:639:PRO:HB2	1.82	0.62
1:C:49:SER:HB2	1:C:298:LYS:HG3	1.80	0.62
1:A:291:ARG:HA	1:A:294:GLN:HB2	1.82	0.62
1:A:335:GLY:HA2	1:A:338:ALA:HB3	1.82	0.61
1:C:149:ARG:O	1:C:153:GLY:N	2.28	0.61
1:C:308:ILE:O	1:C:312:ALA:N	2.25	0.61
1:D:47:PHE:HA	1:D:298:LYS:HE3	1.82	0.61
1:D:304:TYR:O	1:D:308:ILE:N	2.32	0.61
1:B:293:VAL:O	1:B:297:THR:N	2.27	0.61
1:C:47:PHE:HB3	1:C:294:GLN:HG2	1.82	0.61
1:A:456:VAL:HA	1:B:152:LEU:HD11	1.83	0.61
1:B:151:ILE:O	1:B:154:THR:OG1	2.19	0.61
1:C:58:HIS:HB3	1:C:61:LEU:HB3	1.82	0.61
1:A:215:VAL:HA	1:A:218:LEU:HB2	1.82	0.61
1:B:631:LEU:HB2	1:B:671:LYS:HD2	1.81	0.61
1:D:61:LEU:HA	1:D:64:GLU:HB3	1.82	0.61
1:D:226:MET:HE3	1:D:226:MET:O	2.01	0.61
1:B:474:THR:HG23	1:B:514:LEU:HD22	1.83	0.61
1:D:146:ARG:O	1:D:150:SER:N	2.29	0.61
1:D:351:CYS:O	1:D:355:ALA:N	2.31	0.60
1:A:35:SER:O	1:A:55:ARG:N	2.33	0.60
1:A:315:GLU:OE2	1:A:315:GLU:N	2.35	0.60
1:C:303:GLN:HA	1:C:306:ARG:HB2	1.84	0.60
1:C:588:VAL:HG12	1:C:589:GLN:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:LEU:O	1:A:654:ARG:NH2	2.35	0.60
1:C:105:ARG:HH21	1:C:221:PHE:HE1	1.49	0.60
1:A:534:TYR:HA	1:A:577:LEU:HD11	1.83	0.60
1:B:170:ALA:HA	1:B:173:ALA:HB3	1.84	0.60
1:A:207:ILE:HB	1:A:213:PRO:HD3	1.84	0.60
1:A:282:GLU:OE1	1:A:292:ARG:NH1	2.35	0.60
1:B:307:ASN:HA	1:B:310:ASP:HB2	1.83	0.60
1:D:243:TYR:O	1:D:247:GLY:N	2.33	0.60
1:A:278:PHE:HA	1:A:281:TRP:HB2	1.84	0.60
1:C:56:HIS:CE1	1:C:106:LEU:HD22	2.36	0.60
1:B:96:VAL:HG23	1:B:339:TRP:HD1	1.67	0.60
1:C:326:LEU:O	1:C:330:GLY:N	2.35	0.60
1:D:453:GLY:O	1:D:713:ASN:ND2	2.35	0.60
1:A:47:PHE:HE1	1:A:337:VAL:HG11	1.65	0.60
1:A:184:ILE:HA	1:A:187:THR:HB	1.83	0.59
1:A:299:GLN:OE1	1:A:303:GLN:NE2	2.35	0.59
1:C:87:ASN:HB3	1:C:91:GLY:O	2.02	0.59
1:C:505:GLU:CD	1:D:486:GLU:HB2	2.27	0.59
1:E:177:ILE:HA	1:E:180:TRP:HB3	1.83	0.59
1:E:588:VAL:HG12	1:E:591:LYS:HE3	1.84	0.59
1:D:206:ARG:O	1:D:210:THR:N	2.35	0.59
1:D:149:ARG:O	1:D:153:GLY:N	2.32	0.59
1:A:218:LEU:O	1:A:222:GLY:N	2.35	0.59
1:A:304:TYR:O	1:A:308:ILE:N	2.24	0.59
1:D:120:ASP:HA	1:D:123:VAL:HG12	1.83	0.59
1:A:70:ARG:HH21	1:A:80:ILE:HG23	1.68	0.59
1:C:464:ARG:HH12	1:C:526:ASP:H	1.48	0.59
1:D:246:LEU:O	1:D:250:ASN:N	2.31	0.59
1:A:164:GLU:O	1:A:167:SER:OG	2.19	0.58
1:C:217:MET:HA	1:C:220:ARG:HB2	1.85	0.58
1:D:203:VAL:O	1:D:207:ILE:HG13	2.04	0.58
1:A:235:ILE:HG13	1:A:239:VAL:HG23	1.84	0.58
1:C:117:PHE:O	1:C:121:ASN:N	2.37	0.58
1:C:152:LEU:HD13	1:D:456:VAL:HG12	1.85	0.58
1:C:305:LEU:O	1:C:309:ALA:N	2.30	0.58
1:C:682:GLY:O	1:C:684:ILE:N	2.36	0.58
1:A:207:ILE:O	1:A:212:ALA:N	2.33	0.58
1:B:253:PHE:CD1	1:B:340:SER:HB3	2.39	0.58
1:C:276:TRP:O	1:C:279:MET:HG2	2.04	0.58
1:C:105:ARG:NH2	1:C:169:ASP:OD2	2.36	0.58
1:D:213:PRO:O	1:D:217:MET:N	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:PHE:HB3	1:D:292:ARG:HH21	1.68	0.58
1:A:583:VAL:O	1:A:591:LYS:NZ	2.36	0.58
1:D:451:ILE:HD12	1:D:582:MET:HE1	1.85	0.58
1:A:239:VAL:O	1:A:243:TYR:N	2.30	0.58
1:D:71:THR:HA	1:D:74:GLU:HB2	1.86	0.58
1:A:258:GLU:OE2	1:A:271:MET:HE3	2.03	0.58
1:A:220:ARG:HH22	1:A:227:LEU:HB2	1.69	0.58
1:D:64:GLU:O	1:D:68:ARG:NH1	2.35	0.58
1:D:298:LYS:HD3	1:D:298:LYS:N	2.19	0.58
1:E:481:MET:HE3	1:E:507:THR:HG22	1.85	0.58
1:B:111:TYR:O	1:B:115:TYR:N	2.27	0.57
1:B:255:PHE:HA	1:B:271:MET:HE1	1.86	0.57
1:D:88:PRO:HG2	1:D:357:LEU:HG	1.85	0.57
1:A:166:LEU:HD21	1:A:177:ILE:HD11	1.85	0.57
1:A:352:LYS:O	1:A:352:LYS:NZ	2.33	0.57
1:B:291:ARG:O	1:B:295:GLU:N	2.36	0.57
1:A:187:THR:HA	1:A:190:LYS:HB2	1.86	0.57
1:B:309:ALA:HA	1:B:312:ALA:HB3	1.86	0.57
1:D:46:GLY:O	1:D:294:GLN:HG2	2.03	0.57
1:F:682:GLY:O	1:F:684:ILE:N	2.36	0.57
1:C:513:PHE:HB2	1:D:542:PHE:HD2	1.69	0.57
1:D:354:ALA:HB1	1:D:358:LEU:HD23	1.86	0.57
1:D:588:VAL:O	1:D:590:GLN:N	2.37	0.57
1:B:206:ARG:HD2	1:B:210:THR:HG23	1.86	0.57
1:D:326:LEU:HA	1:D:329:GLN:HB2	1.86	0.57
1:A:277:LEU:O	1:A:281:TRP:N	2.22	0.57
1:C:102:LYS:HD3	1:C:105:ARG:HD2	1.87	0.57
1:D:64:GLU:HG2	1:D:68:ARG:HH22	1.69	0.57
1:E:475:LEU:HD13	1:E:518:VAL:HG21	1.87	0.57
1:B:175:VAL:O	1:B:179:SER:N	2.34	0.57
1:D:342:ARG:HA	1:D:347:HIS:CE1	2.40	0.57
1:E:53:LEU:HA	1:E:334:PRO:HB2	1.87	0.57
1:A:37:VAL:HB	1:A:55:ARG:HB2	1.87	0.57
1:C:321:LYS:O	1:C:325:TYR:N	2.35	0.57
1:D:109:ILE:HG22	1:D:113:PHE:CE2	2.40	0.57
1:F:596:GLN:HB2	1:F:705:LEU:HD11	1.87	0.56
1:A:53:LEU:HD13	1:A:334:PRO:HB2	1.87	0.56
1:B:112:ILE:HA	1:B:115:TYR:HB3	1.86	0.56
1:E:213:PRO:O	1:E:217:MET:N	2.27	0.56
1:B:179:SER:HA	1:B:182:GLU:HB3	1.87	0.56
1:C:77:ILE:HD11	1:C:157:ILE:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:PHE:HB3	1:C:292:ARG:HD2	1.87	0.56
1:E:247:GLY:O	1:E:251:ASP:N	2.34	0.56
1:A:29:LEU:O	1:A:54:ARG:NH2	2.38	0.56
1:B:464:ARG:HG2	1:B:464:ARG:HH11	1.71	0.56
1:B:588:VAL:HA	1:B:591:LYS:HE2	1.87	0.56
1:D:220:ARG:HA	1:D:225:ILE:HB	1.86	0.56
1:C:527:ASP:HB3	1:C:530:CYS:HB2	1.87	0.56
1:D:208:ILE:H	1:D:208:ILE:HD12	1.71	0.56
1:A:437:TYR:HD2	1:A:498:THR:HG23	1.69	0.56
1:C:215:VAL:O	1:C:219:MET:N	2.34	0.56
1:E:256:ASP:O	1:E:260:GLU:HG2	2.06	0.56
1:E:183:MET:CG	1:E:214:PHE:HB2	2.33	0.56
1:E:119:TYR:HA	1:E:122:VAL:HB	1.87	0.56
1:B:295:GLU:OE1	1:B:299:GLN:NE2	2.39	0.56
1:E:640:LEU:HA	1:E:678:LEU:HD21	1.88	0.56
1:A:92:HIS:O	1:A:94:GLY:N	2.39	0.56
1:A:253:PHE:HE1	1:A:337:VAL:HG22	1.71	0.56
1:D:231:GLU:HA	1:D:234:ARG:HB3	1.88	0.56
1:D:278:PHE:O	1:D:283:ASN:N	2.38	0.55
1:C:62:ALA:HB2	1:C:106:LEU:HD21	1.87	0.55
1:C:288:GLN:HA	1:C:291:ARG:HB2	1.87	0.55
1:E:519:MET:HE1	1:F:519:MET:HG2	1.88	0.55
1:A:27:PHE:CZ	1:A:321:LYS:HA	2.41	0.55
1:A:319:ASN:O	1:A:323:GLN:NE2	2.40	0.55
1:D:534:TYR:CE1	1:D:538:MET:HG3	2.41	0.55
1:E:458:LEU:HD22	1:E:590:GLN:HG3	1.87	0.55
1:A:278:PHE:O	1:A:283:ASN:N	2.40	0.55
1:A:294:GLN:O	1:A:298:LYS:HG3	2.06	0.55
1:B:66:SER:HA	1:B:114:GLU:OE1	2.07	0.55
1:C:307:ASN:O	1:C:311:PHE:N	2.29	0.55
1:B:176:VAL:O	1:B:180:TRP:N	2.36	0.55
1:C:206:ARG:HE	1:C:210:THR:HG23	1.71	0.55
1:E:35:SER:N	1:E:55:ARG:O	2.29	0.55
1:F:558:PRO:HD3	1:F:636:PHE:CD2	2.42	0.55
1:A:217:MET:HA	1:A:220:ARG:HG2	1.88	0.55
1:D:71:THR:O	1:D:75:GLN:N	2.40	0.55
1:D:649:LYS:H	1:D:649:LYS:HD3	1.72	0.55
1:E:74:GLU:HA	1:E:78:GLY:HA2	1.89	0.55
1:E:220:ARG:NH2	1:E:227:LEU:O	2.39	0.55
1:A:298:LYS:O	1:A:302:GLN:HG2	2.07	0.55
1:B:119:TYR:HA	1:B:122:VAL:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:GLU:OE2	1:D:265:GLU:HG3	2.07	0.55
1:D:311:PHE:CZ	1:D:326:LEU:HD21	2.42	0.55
1:E:160:LYS:HE3	1:F:714:TRP:CE2	2.42	0.55
1:B:172:ARG:NH2	1:B:226:MET:HE2	2.22	0.54
1:B:242:CYS:O	1:B:246:LEU:N	2.26	0.54
1:B:326:LEU:O	1:B:330:GLY:N	2.36	0.54
1:D:262:PHE:CD2	1:D:271:MET:HE3	2.43	0.54
1:B:105:ARG:HH12	1:B:169:ASP:HB2	1.72	0.54
1:C:106:LEU:HA	1:C:109:ILE:HB	1.90	0.54
1:D:458:LEU:HD11	1:D:583:VAL:HG12	1.89	0.54
1:E:323:GLN:O	1:E:327:LYS:N	2.39	0.54
1:D:220:ARG:O	1:D:225:ILE:N	2.41	0.54
1:D:561:GLU:OE2	1:D:561:GLU:N	2.31	0.54
1:E:499:HIS:HB2	1:E:504:THR:HG22	1.89	0.54
1:F:484:ASP:CG	1:F:492:ARG:HH21	2.16	0.54
1:A:82:ARG:HG3	1:A:82:ARG:O	2.07	0.54
1:A:322:LEU:HA	1:A:325:TYR:HB3	1.90	0.54
1:C:656:ILE:HG12	1:E:501:ILE:HG23	1.90	0.54
1:D:157:ILE:HA	1:D:160:LYS:HB2	1.89	0.54
1:E:345:ARG:HH11	1:E:346:TYR:HE1	1.56	0.54
1:A:342:ARG:HA	1:A:347:HIS:CE1	2.43	0.54
1:B:724:LYS:HD3	1:B:725:VAL:H	1.73	0.54
1:D:86:CYS:HA	1:D:92:HIS:HA	1.90	0.54
1:E:153:GLY:HA2	1:E:156:GLN:HB3	1.88	0.54
1:E:219:MET:HG3	1:E:223:MET:SD	2.46	0.54
1:E:320:ILE:HG22	1:E:324:THR:HG23	1.90	0.54
1:A:442:PRO:HD3	1:A:495:ARG:HH12	1.72	0.54
1:B:244:ALA:O	1:B:248:LEU:N	2.29	0.54
1:B:294:GLN:O	1:B:298:LYS:N	2.41	0.54
1:E:36:VAL:HG22	1:E:54:ARG:HH21	1.73	0.54
1:A:98:LEU:HD13	1:A:106:LEU:HD11	1.89	0.54
1:B:183:MET:O	1:B:187:THR:OG1	2.23	0.54
1:E:291:ARG:HA	1:E:294:GLN:HG3	1.90	0.54
1:B:66:SER:HG	1:B:92:HIS:CD2	2.25	0.53
1:C:304:TYR:O	1:C:308:ILE:N	2.32	0.53
1:C:543:ILE:HD11	1:D:428:ASP:HB2	1.90	0.53
1:E:304:TYR:O	1:E:308:ILE:HG12	2.08	0.53
1:A:82:ARG:NH2	1:A:121:ASN:OD1	2.38	0.53
1:C:258:GLU:O	1:C:262:PHE:N	2.34	0.53
1:A:519:MET:HG3	1:A:534:TYR:HE1	1.74	0.53
1:B:457:TRP:CD1	1:B:709:THR:HG21	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:GLN:HG3	1:D:76:PHE:CD1	2.43	0.53
1:E:108:VAL:O	1:E:112:ILE:HG13	2.09	0.53
1:E:462:ASP:OD2	1:E:463:HIS:N	2.40	0.53
1:B:442:PRO:O	1:B:493:ARG:NH1	2.42	0.53
1:E:292:ARG:O	1:E:296:VAL:HG12	2.08	0.53
1:B:33:LEU:HD22	1:B:56:HIS:NE2	2.23	0.53
1:B:247:GLY:O	1:B:251:ASP:N	2.32	0.53
1:B:297:THR:O	1:B:301:GLU:HB2	2.09	0.53
1:E:599:SER:O	1:E:603:VAL:HG12	2.08	0.53
1:D:54:ARG:HD2	1:D:331:TYR:CZ	2.44	0.53
1:E:115:TYR:CE2	1:E:161:MET:HG2	2.43	0.53
1:E:229:GLN:O	1:E:233:LYS:NZ	2.42	0.53
1:B:98:LEU:HD21	1:B:219:MET:HA	1.90	0.53
1:C:293:VAL:O	1:C:297:THR:N	2.23	0.53
1:D:495:ARG:HD2	1:D:496:PRO:HD2	1.90	0.53
1:A:150:SER:O	1:A:154:THR:OG1	2.25	0.53
1:C:102:LYS:HD3	1:C:105:ARG:HH11	1.74	0.53
1:C:202:TYR:OH	1:C:251:ASP:OD1	2.25	0.53
1:C:294:GLN:O	1:C:298:LYS:HB3	2.09	0.53
1:D:66:SER:HA	1:D:114:GLU:HG2	1.91	0.53
1:E:631:LEU:O	1:E:660:SER:OG	2.22	0.53
1:D:186:THR:HA	1:D:189:LYS:HG3	1.91	0.53
1:E:586:ALA:HB1	1:E:590:GLN:HE21	1.74	0.53
1:A:172:ARG:HH12	1:A:226:MET:HG3	1.73	0.53
1:B:296:VAL:O	1:B:300:TYR:N	2.40	0.53
1:A:82:ARG:O	1:A:345:ARG:NH1	2.41	0.52
1:E:706:GLU:HG2	1:E:712:PRO:HA	1.90	0.52
1:A:306:ARG:O	1:A:310:ASP:N	2.41	0.52
1:D:617:LEU:HB3	1:D:675:LEU:HD21	1.91	0.52
1:E:88:PRO:HG3	1:E:358:LEU:HG	1.92	0.52
1:E:174:GLU:O	1:E:178:ASN:N	2.31	0.52
1:D:496:PRO:HB2	1:D:501:ILE:HD11	1.90	0.52
1:A:233:LYS:O	1:A:236:GLU:HG3	2.09	0.52
1:A:286:ALA:O	1:A:290:LYS:HG2	2.10	0.52
1:D:591:LYS:O	1:D:593:LEU:N	2.37	0.52
1:A:92:HIS:O	1:A:95:ALA:N	2.41	0.52
1:A:236:GLU:O	1:A:240:LYS:HG2	2.08	0.52
1:A:47:PHE:HD2	1:A:294:GLN:HG3	1.74	0.52
1:B:206:ARG:NH2	1:B:250:ASN:OD1	2.43	0.52
1:D:262:PHE:CE1	1:D:269:THR:HA	2.45	0.52
1:E:100:PHE:HB2	1:E:223:MET:SD	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:463:HIS:CE1	1:E:464:ARG:HG2	2.45	0.52
1:F:451:ILE:HD11	1:F:578:LEU:HD13	1.90	0.52
1:A:451:ILE:HD11	1:A:578:LEU:HD13	1.92	0.52
1:B:55:ARG:HD2	1:B:99:PRO:HB3	1.92	0.52
1:C:265:GLU:O	1:C:267:ASP:N	2.42	0.52
1:D:176:VAL:HG22	1:D:217:MET:HG3	1.91	0.52
1:E:73:TRP:HH2	1:E:122:VAL:HG23	1.75	0.52
1:E:521:LYS:HA	1:E:524:GLN:OE1	2.10	0.52
1:A:194:ARG:HH21	1:A:205:TYR:HB3	1.74	0.51
1:C:290:LYS:O	1:C:294:GLN:N	2.33	0.51
1:D:241:PRO:HA	1:D:300:TYR:OH	2.10	0.51
1:C:641:ILE:O	1:C:645:THR:OG1	2.16	0.51
1:D:30:ASN:HB3	1:D:33:LEU:HD12	1.91	0.51
1:D:695:MET:HE2	1:D:724:LYS:HE3	1.92	0.51
1:A:94:GLY:O	1:A:98:LEU:N	2.26	0.51
1:B:173:ALA:O	1:B:177:ILE:N	2.27	0.51
1:C:282:GLU:HB2	1:C:292:ARG:HH22	1.75	0.51
1:F:445:GLY:O	1:F:447:ARG:N	2.44	0.51
1:A:115:TYR:O	1:A:119:TYR:N	2.44	0.51
1:B:245:ALA:O	1:B:249:ALA:N	2.41	0.51
1:B:252:TYR:HH	1:B:291:ARG:NH1	2.09	0.51
1:D:328:ALA:HA	1:D:331:TYR:CD2	2.41	0.51
1:E:634:CYS:SG	1:E:661:ARG:NH1	2.83	0.51
1:C:207:ILE:HG13	1:C:208:ILE:HG13	1.92	0.51
1:C:456:VAL:HG23	1:D:152:LEU:HD22	1.93	0.51
1:D:565:ASP:OD1	1:D:568:ARG:NH2	2.43	0.51
1:E:152:LEU:O	1:E:156:GLN:N	2.39	0.51
1:A:666:LEU:HD12	1:A:671:LYS:HE3	1.93	0.51
1:B:43:ASP:HB3	1:B:49:SER:HA	1.92	0.51
1:E:254:SER:O	1:E:258:GLU:HG3	2.11	0.51
1:B:29:LEU:HG	1:B:324:THR:OG1	2.11	0.51
1:D:48:CYS:SG	1:D:51:TYR:HB2	2.50	0.51
1:D:485:ILE:HD11	1:D:507:THR:HG23	1.91	0.51
1:A:253:PHE:HB2	1:A:346:TYR:CZ	2.46	0.51
1:C:172:ARG:HG2	1:C:224:GLY:HA2	1.93	0.51
1:D:719:LEU:O	1:D:723:LEU:HD12	2.11	0.51
1:E:66:SER:O	1:E:70:ARG:HD3	2.11	0.51
1:E:251:ASP:HB3	1:E:274:ALA:H	1.76	0.51
1:B:107:ALA:O	1:B:111:TYR:N	2.38	0.51
1:D:164:GLU:O	1:D:167:SER:OG	2.26	0.51
1:F:497:SER:OG	1:F:498:THR:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ILE:HA	1:B:238:ILE:HB	1.93	0.50
1:C:102:LYS:HD2	1:C:223:MET:HA	1.92	0.50
1:D:278:PHE:HZ	1:D:296:VAL:HG11	1.76	0.50
1:A:257:ILE:HB	1:A:346:TYR:CB	2.42	0.50
1:B:55:ARG:HH21	1:B:94:GLY:C	2.19	0.50
1:C:206:ARG:HG3	1:C:210:THR:HG23	1.93	0.50
1:C:561:GLU:CD	1:C:561:GLU:H	2.18	0.50
1:E:295:GLU:O	1:E:299:GLN:N	2.29	0.50
1:A:102:LYS:HG3	1:A:105:ARG:HD3	1.92	0.50
1:A:285:ASN:O	1:A:289:ALA:N	2.40	0.50
1:B:323:GLN:O	1:B:327:LYS:N	2.42	0.50
1:D:46:GLY:C	1:D:47:PHE:HD1	2.20	0.50
1:E:105:ARG:HG3	1:E:222:GLY:HA2	1.92	0.50
1:E:105:ARG:HH12	1:E:169:ASP:HB2	1.76	0.50
1:F:618:THR:HG22	1:F:618:THR:O	2.11	0.50
1:A:328:ALA:HA	1:A:331:TYR:HB2	1.94	0.50
1:B:173:ALA:HA	1:B:176:VAL:HB	1.94	0.50
1:E:332:GLN:HG3	1:E:333:VAL:HG22	1.93	0.50
1:B:98:LEU:HD23	1:B:100:PHE:H	1.75	0.50
1:B:241:PRO:O	1:B:245:ALA:N	2.34	0.50
1:C:288:GLN:HG3	1:C:291:ARG:HH21	1.77	0.50
1:D:244:ALA:HB3	1:D:300:TYR:OH	2.12	0.50
1:C:212:ALA:O	1:C:216:ASP:N	2.35	0.50
1:D:231:GLU:O	1:D:235:ILE:HG12	2.12	0.50
1:D:358:LEU:O	1:D:362:THR:N	2.43	0.50
1:C:89:TRP:HZ3	1:C:344:PRO:HG3	1.77	0.50
1:D:92:HIS:O	1:D:96:VAL:HG23	2.12	0.50
1:D:118:LEU:HD23	1:D:121:ASN:HD22	1.77	0.50
1:E:55:ARG:HH21	1:E:91:GLY:HA3	1.76	0.50
1:F:541:LEU:HD21	1:F:573:GLY:HA3	1.92	0.50
1:A:31:SER:HA	1:A:54:ARG:HH12	1.76	0.50
1:B:202:TYR:OH	1:B:272:THR:HG23	2.12	0.50
1:B:303:GLN:HA	1:B:306:ARG:HE	1.77	0.50
1:A:486:GLU:OE2	1:B:505:GLU:HG2	2.11	0.50
1:E:115:TYR:HA	1:E:118:LEU:HB2	1.94	0.50
1:A:683:SER:O	1:A:687:THR:N	2.45	0.49
1:B:549:LEU:HA	1:B:552:THR:HG22	1.93	0.49
1:C:706:GLU:CD	1:C:713:ASN:H	2.20	0.49
1:D:44:ILE:HG12	1:D:47:PHE:HB2	1.94	0.49
1:C:120:ASP:HA	1:C:123:VAL:HB	1.94	0.49
1:C:311:PHE:O	1:C:316:GLY:N	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:LEU:HD11	1:E:338:ALA:HB2	1.94	0.49
1:E:519:MET:SD	1:F:519:MET:HE3	2.51	0.49
1:A:175:VAL:O	1:A:179:SER:N	2.44	0.49
1:B:105:ARG:HA	1:B:108:VAL:HG13	1.94	0.49
1:B:584:GLN:C	1:B:584:GLN:HE21	2.20	0.49
1:A:44:ILE:N	1:A:47:PHE:O	2.39	0.49
1:A:81:GLU:N	1:A:81:GLU:OE2	2.45	0.49
1:C:61:LEU:HD13	1:C:107:ALA:HB2	1.94	0.49
1:C:70:ARG:HB3	1:C:80:ILE:HD12	1.94	0.49
1:C:252:TYR:HA	1:C:275:VAL:HG21	1.94	0.49
1:D:322:LEU:HD12	1:D:322:LEU:H	1.76	0.49
1:A:101:CYS:O	1:A:102:LYS:C	2.54	0.49
1:A:199:LEU:HD12	1:A:199:LEU:H	1.78	0.49
1:E:448:GLU:HG3	1:E:469:LYS:HE3	1.94	0.49
1:A:242:CYS:SG	1:A:329:GLN:HB3	2.53	0.49
1:A:458:LEU:HD12	1:A:582:MET:HG2	1.94	0.49
1:C:638:TYR:HD2	1:C:687:THR:HG22	1.77	0.49
1:D:255:PHE:CE1	1:D:259:TRP:HB2	2.47	0.49
1:A:149:ARG:HG2	1:A:149:ARG:HH11	1.78	0.49
1:A:534:TYR:CE2	1:A:538:MET:HE3	2.47	0.49
1:B:101:CYS:SG	1:B:222:GLY:HA3	2.53	0.49
1:D:252:TYR:OH	1:D:290:LYS:HD3	2.13	0.49
1:B:223:MET:HB2	1:B:225:ILE:HG12	1.95	0.49
1:C:309:ALA:O	1:C:313:ALA:N	2.37	0.49
1:E:81:GLU:OE1	1:E:82:ARG:N	2.46	0.49
1:B:72:ASP:HB3	1:B:157:ILE:HD11	1.95	0.49
1:B:705:LEU:O	1:B:708:GLU:HG3	2.13	0.49
1:F:567:ILE:HD12	1:F:609:GLN:HB3	1.95	0.49
1:A:523:ARG:NH2	1:B:532:ASP:OD2	2.46	0.49
1:C:115:TYR:HE2	1:C:157:ILE:HG13	1.78	0.49
1:E:636:PHE:HB3	1:E:641:ILE:HD11	1.95	0.49
1:D:254:SER:O	1:D:258:GLU:HB2	2.13	0.48
1:E:61:LEU:HB2	1:E:106:LEU:HD23	1.94	0.48
1:E:633:GLU:HB2	1:E:635:LYS:HG2	1.94	0.48
1:A:121:ASN:HD21	1:A:345:ARG:HH22	1.60	0.48
1:A:311:PHE:CD2	1:A:323:GLN:HG3	2.48	0.48
1:B:482:LEU:O	1:B:486:GLU:HG2	2.13	0.48
1:D:89:TRP:CH2	1:D:350:LEU:HB3	2.48	0.48
1:D:94:GLY:O	1:D:98:LEU:N	2.34	0.48
1:D:162:LEU:HD12	1:D:166:LEU:HD11	1.95	0.48
1:E:613:ASP:CG	1:E:637:SER:HB2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ARG:HH11	1:B:56:HIS:N	2.11	0.48
1:D:611:ARG:NH1	1:D:723:LEU:HD23	2.28	0.48
1:E:61:LEU:HA	1:E:64:GLU:OE2	2.13	0.48
1:E:303:GLN:HA	1:E:306:ARG:HE	1.77	0.48
1:A:451:ILE:HG23	1:A:582:MET:HE1	1.94	0.48
1:B:47:PHE:HD1	1:B:48:CYS:N	2.11	0.48
1:C:226:MET:O	1:C:321:LYS:NZ	2.45	0.48
1:B:73:TRP:HE3	1:B:118:LEU:HD13	1.78	0.48
1:C:232:GLN:O	1:C:236:GLU:N	2.46	0.48
1:C:512:ASN:ND2	1:D:482:LEU:HD11	2.28	0.48
1:D:44:ILE:H	1:D:47:PHE:HB2	1.78	0.48
1:E:174:GLU:HA	1:E:177:ILE:HB	1.96	0.48
1:A:97:VAL:O	1:A:332:GLN:HG2	2.13	0.48
1:A:290:LYS:O	1:A:294:GLN:NE2	2.47	0.48
1:A:564:LEU:O	1:A:568:ARG:HG3	2.13	0.48
1:D:165:LEU:HD21	1:D:173:ALA:HB1	1.96	0.48
1:D:203:VAL:HG13	1:D:244:ALA:HB2	1.96	0.48
1:F:675:LEU:O	1:F:679:ARG:HG3	2.14	0.48
1:A:102:LYS:HB2	1:A:105:ARG:HG3	1.95	0.48
1:D:262:PHE:HA	1:D:268:LYS:HB3	1.95	0.48
1:D:616:ASN:HB3	1:D:630:ASP:HB2	1.96	0.48
1:E:432:LEU:O	1:E:436:GLU:HG2	2.13	0.48
1:A:97:VAL:HG13	1:A:332:GLN:HB3	1.95	0.48
1:A:108:VAL:O	1:A:112:ILE:N	2.44	0.48
1:B:598:ALA:O	1:B:601:SER:OG	2.31	0.48
1:C:262:PHE:HA	1:C:265:GLU:HB2	1.95	0.48
1:C:667:ASP:OD2	1:C:669:PRO:HD2	2.13	0.48
1:E:98:LEU:HD22	1:E:223:MET:HE1	1.95	0.48
1:A:326:LEU:HA	1:A:329:GLN:HB2	1.96	0.48
1:B:642:HIS:HD2	1:B:646:SER:HB3	1.79	0.48
1:C:291:ARG:HA	1:C:294:GLN:HB2	1.96	0.48
1:B:451:ILE:HD11	1:B:578:LEU:HB3	1.95	0.48
1:C:59:GLU:O	1:C:63:ASN:N	2.29	0.48
1:C:277:LEU:HD13	1:C:281:TRP:CZ2	2.49	0.48
1:C:329:GLN:HA	1:C:332:GLN:HG3	1.96	0.48
1:D:212:ALA:HB1	1:D:243:TYR:HB3	1.95	0.48
1:D:261:GLU:OE2	1:D:264:ALA:HB3	2.14	0.48
1:A:309:ALA:O	1:A:313:ALA:N	2.47	0.47
1:B:257:ILE:HB	1:B:345:ARG:O	2.13	0.47
1:C:311:PHE:CZ	1:C:316:GLY:HA3	2.49	0.47
1:B:218:LEU:HA	1:B:221:PHE:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:GLU:HB2	1:D:268:LYS:HB2	1.96	0.47
1:E:35:SER:HA	1:E:57:HIS:HE1	1.75	0.47
1:E:85:SER:HB3	1:E:117:PHE:CG	2.49	0.47
1:E:105:ARG:O	1:E:109:ILE:N	2.41	0.47
1:E:260:GLU:HA	1:E:263:GLN:HB2	1.96	0.47
1:A:67:LEU:O	1:A:71:THR:OG1	2.27	0.47
1:B:271:MET:HG2	1:B:273:ASN:HB2	1.95	0.47
1:D:326:LEU:HA	1:D:329:GLN:CB	2.45	0.47
1:F:611:ARG:HA	1:F:691:MET:HE3	1.95	0.47
1:A:148:VAL:HG12	1:A:152:LEU:HD23	1.96	0.47
1:D:89:TRP:CD2	1:D:350:LEU:HD13	2.49	0.47
1:B:251:ASP:HB3	1:B:274:ALA:H	1.80	0.47
1:E:102:LYS:N	1:E:223:MET:HA	2.30	0.47
1:F:713:ASN:HB3	1:F:716:VAL:HG22	1.97	0.47
1:A:186:THR:HG21	1:A:208:ILE:HG21	1.96	0.47
1:A:220:ARG:HH12	1:A:227:LEU:HB2	1.79	0.47
1:A:653:LEU:O	1:A:656:ILE:HG22	2.14	0.47
1:B:114:GLU:O	1:B:118:LEU:N	2.41	0.47
1:B:261:GLU:HA	1:B:264:ALA:HB3	1.95	0.47
1:B:309:ALA:O	1:B:313:ALA:N	2.29	0.47
1:C:206:ARG:HG3	1:C:206:ARG:O	2.15	0.47
1:D:45:ALA:O	1:D:294:GLN:NE2	2.45	0.47
1:E:106:LEU:HA	1:E:109:ILE:HB	1.96	0.47
1:E:178:ASN:HA	1:E:181:LYS:HD2	1.96	0.47
1:F:660:SER:HB2	1:F:666:LEU:HG	1.96	0.47
1:A:172:ARG:O	1:A:176:VAL:HG23	2.14	0.47
1:A:240:LYS:O	1:A:244:ALA:N	2.41	0.47
1:A:293:VAL:O	1:A:297:THR:OG1	2.17	0.47
1:A:437:TYR:OH	1:A:496:PRO:O	2.28	0.47
1:B:72:ASP:HA	1:B:75:GLN:HB2	1.97	0.47
1:C:568:ARG:HG3	1:C:602:ASP:OD1	2.14	0.47
1:D:219:MET:HG2	1:D:332:GLN:HE21	1.80	0.47
1:D:533:ILE:HG23	1:D:580:ARG:HH11	1.80	0.47
1:E:253:PHE:HB3	1:E:347:HIS:CE1	2.49	0.47
1:A:93:PHE:CG	1:A:94:GLY:N	2.82	0.47
1:A:342:ARG:NH2	1:A:353:GLU:OE2	2.48	0.47
1:B:275:VAL:HG22	1:B:290:LYS:HA	1.97	0.47
1:C:588:VAL:HG12	1:C:589:GLN:N	2.28	0.47
1:B:428:ASP:O	1:B:429:GLU:HG2	2.14	0.47
1:B:584:GLN:HA	1:B:584:GLN:NE2	2.29	0.47
1:C:248:LEU:HG	1:C:296:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:PHE:CE1	1:C:323:GLN:HG2	2.50	0.47
1:D:525:LEU:HD13	1:D:585:ILE:HD11	1.95	0.47
1:E:169:ASP:O	1:E:173:ALA:N	2.33	0.47
1:E:705:LEU:O	1:E:709:THR:OG1	2.23	0.47
1:F:449:ALA:O	1:F:453:GLY:N	2.37	0.47
1:A:691:MET:HE2	1:A:725:VAL:HB	1.97	0.47
1:B:67:LEU:O	1:B:71:THR:OG1	2.22	0.47
1:B:149:ARG:O	1:B:153:GLY:N	2.44	0.47
1:B:514:LEU:O	1:B:518:VAL:HG23	2.15	0.47
1:B:668:VAL:HB	1:B:669:PRO:HD3	1.97	0.47
1:C:172:ARG:NE	1:C:226:MET:SD	2.88	0.47
1:C:671:LYS:O	1:C:675:LEU:HG	2.15	0.47
1:D:80:ILE:HD12	1:D:80:ILE:HA	1.82	0.47
1:E:83:TRP:CD1	1:E:344:PRO:HB2	2.50	0.47
1:E:324:THR:HA	1:E:327:LYS:HD3	1.96	0.47
1:A:178:ASN:O	1:A:182:GLU:N	2.45	0.46
1:A:217:MET:SD	1:A:217:MET:N	2.88	0.46
1:A:721:HIS:O	1:A:724:LYS:HB2	2.15	0.46
1:B:312:ALA:HA	1:B:323:GLN:HG3	1.95	0.46
1:B:117:PHE:HA	1:B:120:ASP:HB3	1.97	0.46
1:B:311:PHE:O	1:B:316:GLY:N	2.49	0.46
1:D:594:GLU:OE2	1:D:594:GLU:N	2.33	0.46
1:A:658:GLN:O	1:A:658:GLN:NE2	2.48	0.46
1:D:594:GLU:H	1:D:594:GLU:CD	2.21	0.46
1:E:437:TYR:OH	1:E:496:PRO:O	2.29	0.46
1:E:501:ILE:O	1:F:553:ARG:NH2	2.49	0.46
1:A:35:SER:HB3	1:A:57:HIS:NE2	2.30	0.46
1:A:505:GLU:HB3	1:B:549:LEU:HD22	1.97	0.46
1:B:170:ALA:O	1:B:174:GLU:N	2.45	0.46
1:B:245:ALA:HA	1:B:248:LEU:HB2	1.97	0.46
1:C:148:VAL:O	1:C:152:LEU:HG	2.15	0.46
1:C:211:GLY:O	1:C:215:VAL:N	2.43	0.46
1:E:518:VAL:O	1:E:522:VAL:HG23	2.15	0.46
1:F:564:LEU:HD11	1:F:690:LYS:HE3	1.97	0.46
1:E:289:ALA:HA	1:E:292:ARG:HG3	1.97	0.46
1:A:30:ASN:OD1	1:A:32:THR:N	2.49	0.46
1:A:82:ARG:HE	1:A:121:ASN:ND2	2.13	0.46
1:A:176:VAL:HA	1:A:179:SER:OG	2.16	0.46
1:B:268:LYS:NZ	1:B:271:MET:SD	2.88	0.46
1:D:302:GLN:O	1:D:306:ARG:N	2.25	0.46
1:F:566:MET:HE3	1:F:566:MET:HB3	1.87	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:653:LEU:HD12	1:F:653:LEU:HA	1.79	0.46
1:A:34:SER:OG	1:A:54:ARG:NH1	2.48	0.46
1:A:214:PHE:O	1:A:218:LEU:N	2.43	0.46
1:B:656:ILE:H	1:B:656:ILE:HG13	1.58	0.46
1:C:444:LYS:HG3	1:C:446:VAL:HG23	1.96	0.46
1:D:199:LEU:O	1:D:203:VAL:HG23	2.16	0.46
1:C:31:SER:HA	1:C:34:SER:HB3	1.98	0.46
1:D:223:MET:SD	1:D:223:MET:N	2.89	0.46
1:D:240:LYS:HB3	1:D:241:PRO:HD3	1.98	0.46
1:D:333:VAL:O	1:D:336:ASN:ND2	2.45	0.46
1:E:299:GLN:O	1:E:303:GLN:N	2.29	0.46
1:D:355:ALA:O	1:D:359:HIS:ND1	2.49	0.46
1:D:666:LEU:HD12	1:D:666:LEU:H	1.80	0.46
1:E:519:MET:HA	1:E:522:VAL:HG23	1.97	0.46
1:E:713:ASN:HB3	1:E:716:VAL:HB	1.97	0.46
1:A:110:CYS:HA	1:A:113:PHE:CD2	2.50	0.46
1:B:90:GLU:HG2	1:B:342:ARG:HB2	1.98	0.46
1:B:96:VAL:HG23	1:B:339:TRP:CD1	2.48	0.46
1:C:311:PHE:HE1	1:C:323:GLN:HG2	1.81	0.46
1:C:322:LEU:HA	1:C:325:TYR:HB3	1.98	0.46
1:C:430:HIS:CE1	1:D:550:TYR:CE2	3.03	0.46
1:C:548:ASP:HB2	1:C:566:MET:SD	2.56	0.46
1:C:606:GLU:O	1:C:610:VAL:HG22	2.16	0.46
1:D:76:PHE:CD2	1:D:156:GLN:HG2	2.51	0.46
1:D:296:VAL:O	1:D:300:TYR:HB3	2.16	0.46
1:B:169:ASP:CG	1:B:172:ARG:HB3	2.41	0.45
1:C:219:MET:C	1:C:222:GLY:H	2.24	0.45
1:D:218:LEU:HA	1:D:218:LEU:HD23	1.77	0.45
1:D:567:ILE:CD1	1:D:609:GLN:HG2	2.46	0.45
1:D:602:ASP:OD2	1:D:602:ASP:N	2.49	0.45
1:E:118:LEU:O	1:E:122:VAL:N	2.44	0.45
1:E:253:PHE:HB3	1:E:347:HIS:HE1	1.79	0.45
1:A:108:VAL:O	1:A:112:ILE:HG13	2.16	0.45
1:A:292:ARG:O	1:A:296:VAL:HG22	2.16	0.45
1:A:318:GLU:OE2	1:A:318:GLU:N	2.46	0.45
1:C:206:ARG:HA	1:C:209:ASP:HB3	1.99	0.45
1:C:671:LYS:O	1:C:674:VAL:HG12	2.17	0.45
1:D:47:PHE:HZ	1:D:252:TYR:CD1	2.33	0.45
1:D:671:LYS:HE2	1:D:671:LYS:HB3	1.70	0.45
1:E:180:TRP:HE1	1:E:184:ILE:HD11	1.81	0.45
1:B:100:PHE:HB3	1:B:223:MET:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:CYS:O	1:C:355:ALA:N	2.34	0.45
1:D:568:ARG:HD3	1:D:602:ASP:HB3	1.98	0.45
1:F:534:TYR:CE1	1:F:538:MET:HG3	2.51	0.45
1:A:197:ASN:H	1:A:201:GLU:CD	2.25	0.45
1:A:560:GLU:OE1	1:A:686:TYR:OH	2.32	0.45
1:B:27:PHE:HA	1:B:321:LYS:HA	1.98	0.45
1:D:145:TYR:O	1:D:149:ARG:N	2.45	0.45
1:E:639:PRO:HG3	1:E:687:THR:HG21	1.99	0.45
1:A:324:THR:HA	1:A:327:LYS:HB3	1.97	0.45
1:A:519:MET:SD	1:B:519:MET:HG3	2.56	0.45
1:B:471:ILE:HD13	1:B:522:VAL:HG12	1.99	0.45
1:C:183:MET:HG3	1:C:211:GLY:HA2	1.98	0.45
1:C:297:THR:HA	1:C:300:TYR:HB2	1.98	0.45
1:D:238:ILE:O	1:D:241:PRO:HD2	2.17	0.45
1:E:87:ASN:HB3	1:E:91:GLY:O	2.17	0.45
1:E:484:ASP:O	1:E:488:HIS:N	2.50	0.45
1:F:468:LEU:HD23	1:F:582:MET:SD	2.56	0.45
1:D:73:TRP:HD1	1:D:77:ILE:HB	1.76	0.45
1:D:229:GLN:HA	1:D:232:GLN:HB3	1.97	0.45
1:F:445:GLY:O	1:F:446:VAL:C	2.60	0.45
1:A:542:PHE:HE2	1:B:516:ILE:HD12	1.82	0.45
1:A:580:ARG:HE	1:A:580:ARG:HB3	1.58	0.45
1:D:303:GLN:HG3	1:D:306:ARG:HE	1.81	0.45
1:D:599:SER:O	1:D:603:VAL:HG23	2.16	0.45
1:F:462:ASP:O	1:F:465:VAL:HG12	2.16	0.45
1:A:525:LEU:HG	1:A:585:ILE:HD12	1.99	0.45
1:A:682:GLY:O	1:A:684:ILE:N	2.50	0.45
1:B:577:LEU:HG	1:B:581:MET:HE3	1.99	0.45
1:A:55:ARG:HH22	1:A:59:GLU:HB3	1.82	0.45
1:B:713:ASN:C	1:B:713:ASN:OD1	2.59	0.45
1:C:577:LEU:O	1:C:581:MET:HG3	2.16	0.45
1:E:68:ARG:HH12	1:E:111:TYR:HB2	1.81	0.45
1:E:322:LEU:O	1:E:326:LEU:N	2.42	0.45
1:A:49:SER:N	1:A:301:GLU:HG2	2.32	0.45
1:A:294:GLN:O	1:A:297:THR:OG1	2.35	0.45
1:C:586:ALA:O	1:C:588:VAL:N	2.48	0.45
1:D:93:PHE:CE1	1:D:97:VAL:HG21	2.52	0.45
1:D:295:GLU:O	1:D:299:GLN:HG3	2.16	0.45
1:D:336:ASN:ND2	1:D:337:VAL:HG13	2.32	0.45
1:E:110:CYS:HA	1:E:113:PHE:HB2	1.98	0.45
1:E:152:LEU:HD21	1:F:455:ASN:HD22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:LEU:HD12	1:A:432:LEU:HA	1.84	0.44
1:B:454:LEU:HD12	1:B:582:MET:HE3	1.98	0.44
1:B:696:GLU:OE1	1:B:696:GLU:HA	2.17	0.44
1:D:262:PHE:HE1	1:D:269:THR:HA	1.82	0.44
1:D:276:TRP:O	1:D:280:GLN:NE2	2.50	0.44
1:E:150:SER:O	1:E:154:THR:N	2.41	0.44
1:A:187:THR:HA	1:A:190:LYS:HD3	2.00	0.44
1:A:540:ASN:HA	1:A:543:ILE:HG22	1.99	0.44
1:B:100:PHE:HB3	1:B:223:MET:CG	2.47	0.44
1:B:583:VAL:HG21	1:B:594:GLU:OE2	2.17	0.44
1:C:231:GLU:CD	1:C:322:LEU:HD21	2.42	0.44
1:E:337:VAL:HA	1:E:340:SER:HB2	2.00	0.44
1:E:450:PHE:CD1	1:E:450:PHE:C	2.95	0.44
1:A:286:ALA:O	1:A:290:LYS:N	2.40	0.44
1:C:101:CYS:HB3	1:C:106:LEU:HD12	2.00	0.44
1:D:154:THR:O	1:D:158:GLN:HB3	2.18	0.44
1:D:262:PHE:CG	1:D:271:MET:HE3	2.52	0.44
1:D:457:TRP:O	1:D:458:LEU:HD23	2.17	0.44
1:A:102:LYS:O	1:A:104:GLU:N	2.50	0.44
1:A:102:LYS:O	1:A:103:PRO:C	2.60	0.44
1:A:186:THR:HB	1:A:208:ILE:HD12	2.00	0.44
1:A:236:GLU:N	1:A:237:PRO:HD2	2.32	0.44
1:A:648:PRO:HG2	1:A:649:LYS:HD3	1.99	0.44
1:B:176:VAL:HG21	1:B:221:PHE:CD1	2.52	0.44
1:B:450:PHE:CZ	1:B:454:LEU:HD11	2.52	0.44
1:C:50:GLY:HA3	1:C:301:GLU:HG2	1.97	0.44
1:C:74:GLU:HA	1:C:78:GLY:O	2.18	0.44
1:E:529:ARG:HG2	1:E:584:GLN:OE1	2.17	0.44
1:B:113:PHE:O	1:B:117:PHE:N	2.50	0.44
1:C:74:GLU:HG2	1:C:79:PRO:HA	1.99	0.44
1:C:199:LEU:HD22	1:C:278:PHE:HE1	1.82	0.44
1:C:228:THR:HG23	1:C:231:GLU:H	1.83	0.44
1:C:652:GLN:O	1:C:656:ILE:HG13	2.17	0.44
1:D:61:LEU:HD12	1:D:62:ALA:N	2.32	0.44
1:D:172:ARG:H	1:D:172:ARG:HG3	1.59	0.44
1:D:287:GLU:O	1:D:291:ARG:N	2.49	0.44
1:D:295:GLU:O	1:D:298:LYS:N	2.49	0.44
1:E:256:ASP:OD2	1:E:257:ILE:N	2.51	0.44
1:A:352:LYS:HA	1:A:352:LYS:HD2	1.77	0.44
1:A:537:GLU:HB2	1:A:577:LEU:HD12	1.99	0.44
1:B:112:ILE:O	1:B:116:ALA:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:GLU:HG2	1:B:234:ARG:HH11	1.83	0.44
1:B:714:TRP:CZ3	1:B:717:ARG:HD3	2.52	0.44
1:D:576:ARG:HG2	1:D:580:ARG:HD2	2.00	0.44
1:A:320:ILE:HG13	1:A:321:LYS:HD2	1.99	0.44
1:A:353:GLU:O	1:A:356:SER:OG	2.24	0.44
1:B:299:GLN:O	1:B:303:GLN:HB3	2.17	0.44
1:D:109:ILE:HA	1:D:112:ILE:HD12	1.99	0.44
1:D:500:MET:HE3	1:D:500:MET:HB3	1.72	0.44
1:E:304:TYR:CZ	1:E:308:ILE:HD11	2.53	0.44
1:E:475:LEU:HD12	1:E:475:LEU:HA	1.77	0.44
1:A:261:GLU:O	1:A:264:ALA:N	2.51	0.44
1:B:27:PHE:HD1	1:B:321:LYS:HB2	1.83	0.44
1:B:607:PHE:HE1	1:B:723:LEU:HG	1.83	0.44
1:B:678:LEU:HB3	1:B:683:SER:OG	2.16	0.44
1:C:90:GLU:N	1:C:90:GLU:CD	2.76	0.44
1:A:289:ALA:O	1:A:293:VAL:HG23	2.17	0.44
1:B:220:ARG:H	1:B:220:ARG:HG2	1.51	0.44
1:B:458:LEU:HA	1:B:590:GLN:HG3	1.99	0.44
1:C:251:ASP:O	1:C:255:PHE:N	2.22	0.44
1:D:44:ILE:HB	1:D:341:LEU:HD11	1.99	0.44
1:D:93:PHE:HB2	1:D:339:TRP:CE2	2.53	0.44
1:D:233:LYS:HA	1:D:236:GLU:HB2	1.99	0.44
1:D:576:ARG:O	1:D:580:ARG:HG3	2.16	0.44
1:E:684:ILE:HD13	1:E:684:ILE:HA	1.87	0.44
1:F:480:LEU:HD13	1:F:492:ARG:NH1	2.32	0.44
1:A:336:ASN:O	1:A:340:SER:HB3	2.17	0.43
1:B:649:LYS:HB3	1:F:429:GLU:OE2	2.18	0.43
1:D:350:LEU:O	1:D:354:ALA:N	2.27	0.43
1:E:594:GLU:HB3	1:E:595:THR:H	1.59	0.43
1:F:589:GLN:HB2	1:F:590:GLN:OE1	2.18	0.43
1:A:160:LYS:HE2	1:B:714:TRP:CE2	2.53	0.43
1:B:311:PHE:HE2	1:B:322:LEU:HB3	1.83	0.43
1:B:458:LEU:O	1:B:590:GLN:NE2	2.51	0.43
1:C:33:LEU:HB2	1:C:57:HIS:HB2	1.99	0.43
1:C:292:ARG:O	1:C:296:VAL:N	2.49	0.43
1:C:429:GLU:C	1:C:431:LEU:H	2.27	0.43
1:C:614:TYR:CE1	1:C:684:ILE:HG23	2.53	0.43
1:D:353:GLU:O	1:D:357:LEU:N	2.50	0.43
1:F:588:VAL:O	1:F:589:GLN:C	2.61	0.43
1:A:713:ASN:OD1	1:A:713:ASN:C	2.61	0.43
1:B:120:ASP:O	1:B:124:GLU:N	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:GLU:HB3	1:B:237:PRO:HD3	2.00	0.43
1:D:169:ASP:OD1	1:D:171:PRO:HD2	2.19	0.43
1:D:636:PHE:HD1	1:D:640:LEU:HD23	1.83	0.43
1:F:519:MET:SD	1:F:519:MET:N	2.91	0.43
1:A:183:MET:O	1:A:187:THR:OG1	2.36	0.43
1:B:701:SER:O	1:B:705:LEU:HB2	2.18	0.43
1:C:60:HIS:O	1:C:64:GLU:HB3	2.18	0.43
1:C:67:LEU:O	1:C:71:THR:HG23	2.19	0.43
1:C:98:LEU:HD12	1:C:113:PHE:HZ	1.83	0.43
1:C:146:ARG:O	1:C:150:SER:N	2.45	0.43
1:C:262:PHE:CD1	1:C:268:LYS:HD2	2.52	0.43
1:C:331:TYR:HA	1:C:334:PRO:HG2	2.00	0.43
1:C:567:ILE:HB	1:C:609:GLN:HG3	2.00	0.43
1:E:111:TYR:O	1:E:115:TYR:HB3	2.18	0.43
1:F:490:PRO:C	1:F:491:LEU:HD23	2.42	0.43
1:B:591:LYS:HA	1:B:591:LYS:HD3	1.69	0.43
1:C:115:TYR:O	1:C:119:TYR:N	2.23	0.43
1:C:315:GLU:O	1:C:319:ASN:ND2	2.51	0.43
1:C:426:LEU:HG	1:D:547:PHE:CE2	2.53	0.43
1:D:247:GLY:O	1:D:251:ASP:N	2.33	0.43
1:D:606:GLU:HA	1:D:606:GLU:OE2	2.17	0.43
1:E:112:ILE:HD11	1:E:165:LEU:HG	1.99	0.43
1:A:66:SER:HA	1:A:114:GLU:HG2	1.99	0.43
1:B:251:ASP:HB3	1:B:274:ALA:N	2.33	0.43
1:C:655:GLY:HA2	1:F:553:ARG:HH21	1.83	0.43
1:D:284:LEU:HB2	1:D:292:ARG:CZ	2.47	0.43
1:F:644:LEU:HD22	1:F:654:ARG:HH11	1.83	0.43
1:A:155:LYS:NZ	1:B:452:ASP:OD1	2.51	0.43
1:A:713:ASN:HA	1:B:156:GLN:HE22	1.83	0.43
1:B:216:ASP:O	1:B:220:ARG:HG2	2.19	0.43
1:B:353:GLU:O	1:B:357:LEU:HG	2.19	0.43
1:B:529:ARG:NH1	1:B:529:ARG:HB3	2.33	0.43
1:D:51:TYR:HB3	1:D:334:PRO:HG3	2.00	0.43
1:E:152:LEU:HD21	1:F:455:ASN:ND2	2.34	0.43
1:E:161:MET:HE1	1:E:165:LEU:HD12	2.00	0.43
1:E:295:GLU:H	1:E:295:GLU:HG3	1.68	0.43
1:E:522:VAL:HG21	1:E:534:TYR:CD2	2.54	0.43
1:F:556:GLU:H	1:F:556:GLU:HG2	1.58	0.43
1:F:588:VAL:HG12	1:F:591:LYS:HE2	2.00	0.43
1:F:590:GLN:HB2	1:F:593:LEU:HD13	2.00	0.43
1:A:219:MET:O	1:A:223:MET:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:LEU:HD23	1:A:670:LEU:HA	1.82	0.43
1:D:43:ASP:HB2	1:D:47:PHE:H	1.84	0.43
1:E:537:GLU:OE2	1:E:580:ARG:NH2	2.52	0.43
1:F:579:THR:HG23	1:F:597:LEU:HD13	2.01	0.43
1:A:35:SER:N	1:A:55:ARG:O	2.52	0.43
1:A:63:ASN:HA	1:A:92:HIS:CE1	2.54	0.43
1:A:333:VAL:HA	1:A:336:ASN:OD1	2.18	0.43
1:B:120:ASP:HA	1:B:123:VAL:HB	2.01	0.43
1:C:262:PHE:O	1:C:268:LYS:HD3	2.19	0.43
1:E:227:LEU:HD11	1:E:325:TYR:CG	2.52	0.43
1:A:35:SER:OG	1:A:55:ARG:HB3	2.18	0.43
1:A:202:TYR:O	1:A:206:ARG:HB2	2.18	0.43
1:A:529:ARG:CZ	1:A:529:ARG:HB3	2.49	0.43
1:A:560:GLU:OE2	1:A:638:TYR:OH	2.33	0.43
1:A:672:GLU:O	1:A:676:SER:OG	2.34	0.43
1:B:259:TRP:O	1:B:262:PHE:HB3	2.19	0.43
1:B:326:LEU:O	1:B:329:GLN:HG2	2.19	0.43
1:C:29:LEU:HD13	1:C:327:LYS:HZ2	1.84	0.43
1:C:656:ILE:HG22	1:C:666:LEU:HD11	2.00	0.43
1:D:288:GLN:O	1:D:292:ARG:N	2.40	0.43
1:D:302:GLN:HA	1:D:305:LEU:HD12	2.00	0.43
1:A:194:ARG:NH2	1:A:205:TYR:HB3	2.33	0.42
1:A:312:ALA:HA	1:A:316:GLY:HA2	2.01	0.42
1:A:679:ARG:NH1	1:A:679:ARG:HB2	2.34	0.42
1:D:33:LEU:HD23	1:D:58:HIS:HE1	1.84	0.42
1:D:70:ARG:NH1	1:D:114:GLU:OE2	2.52	0.42
1:D:587:PRO:HB3	1:D:589:GLN:HE22	1.84	0.42
1:E:118:LEU:HA	1:E:121:ASN:HB2	2.00	0.42
1:A:27:PHE:CE2	1:A:321:LYS:HA	2.54	0.42
1:A:169:ASP:OD2	1:A:172:ARG:N	2.51	0.42
1:B:29:LEU:HD13	1:B:100:PHE:CZ	2.53	0.42
1:E:185:SER:HB2	1:E:189:LYS:NZ	2.34	0.42
1:E:442:PRO:HB2	1:E:493:ARG:HG2	2.01	0.42
1:A:199:LEU:HD11	1:A:292:ARG:HH22	1.84	0.42
1:A:712:PRO:O	1:B:156:GLN:NE2	2.52	0.42
1:B:31:SER:O	1:B:32:THR:C	2.62	0.42
1:B:495:ARG:H	1:B:495:ARG:HG2	1.63	0.42
1:B:584:GLN:NE2	1:B:584:GLN:CA	2.82	0.42
1:D:291:ARG:HA	1:D:294:GLN:OE1	2.19	0.42
1:E:101:CYS:SG	1:E:106:LEU:HD22	2.59	0.42
1:E:295:GLU:HA	1:E:298:LYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:303:GLN:HG3	1:E:306:ARG:HH21	1.83	0.42
1:E:563:TYR:CD1	1:E:563:TYR:C	2.97	0.42
1:E:589:GLN:HG3	1:E:590:GLN:OE1	2.19	0.42
1:F:484:ASP:OD2	1:F:492:ARG:NH2	2.52	0.42
1:A:70:ARG:HH22	1:A:83:TRP:HA	1.83	0.42
1:C:279:MET:HE3	1:C:286:ALA:H	1.84	0.42
1:C:505:GLU:OE1	1:D:485:ILE:HG22	2.19	0.42
1:C:649:LYS:HB3	1:C:649:LYS:HE3	1.72	0.42
1:D:44:ILE:HG13	1:D:341:LEU:HD21	2.01	0.42
1:E:238:ILE:HG23	1:E:307:ASN:HB3	2.01	0.42
1:E:698:ILE:O	1:E:702:VAL:HG23	2.20	0.42
1:A:343:CYS:HA	1:A:344:PRO:HD3	1.87	0.42
1:C:90:GLU:OE1	1:C:342:ARG:HB3	2.19	0.42
1:C:98:LEU:HD23	1:C:98:LEU:HA	1.73	0.42
1:D:206:ARG:HD3	1:D:206:ARG:HA	1.79	0.42
1:D:236:GLU:N	1:D:237:PRO:HD2	2.34	0.42
1:D:341:LEU:HD23	1:D:341:LEU:HA	1.79	0.42
1:E:180:TRP:O	1:E:184:ILE:HG12	2.19	0.42
1:F:582:MET:HB3	1:F:582:MET:HE3	1.76	0.42
1:A:165:LEU:HD11	1:A:176:VAL:HG11	2.00	0.42
1:A:257:ILE:O	1:A:260:GLU:HB3	2.19	0.42
1:A:519:MET:HG3	1:A:534:TYR:CE1	2.54	0.42
1:C:350:LEU:HA	1:C:353:GLU:OE1	2.20	0.42
1:C:437:TYR:O	1:C:441:LEU:HD23	2.19	0.42
1:C:514:LEU:HD23	1:C:514:LEU:HA	1.83	0.42
1:C:609:GLN:OE1	1:C:609:GLN:HA	2.19	0.42
1:D:103:PRO:HA	1:D:106:LEU:HD11	2.02	0.42
1:D:121:ASN:HD21	1:D:345:ARG:NH2	2.18	0.42
1:D:481:MET:HE2	1:D:511:ALA:HB2	2.02	0.42
1:D:604:LEU:HD23	1:D:604:LEU:HA	1.90	0.42
1:E:32:THR:O	1:E:57:HIS:HB2	2.20	0.42
1:E:638:TYR:HB3	1:E:639:PRO:HD3	2.01	0.42
1:F:635:LYS:HB3	1:F:635:LYS:HE2	1.80	0.42
1:A:53:LEU:HD12	1:A:53:LEU:HA	1.93	0.42
1:B:294:GLN:HA	1:B:297:THR:HB	2.01	0.42
1:C:120:ASP:O	1:C:124:GLU:N	2.40	0.42
1:C:235:ILE:O	1:C:239:VAL:HG22	2.19	0.42
1:D:567:ILE:HD12	1:D:609:GLN:HG2	2.01	0.42
1:E:590:GLN:O	1:E:593:LEU:HG	2.20	0.42
1:F:610:VAL:HA	1:F:613:ASP:HB2	2.02	0.42
1:B:92:HIS:O	1:B:94:GLY:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:GLU:H	1:C:104:GLU:CD	2.25	0.42
1:C:219:MET:HB3	1:C:219:MET:HE2	1.77	0.42
1:E:56:HIS:CE1	1:E:58:HIS:HB2	2.55	0.42
1:E:66:SER:HB3	1:E:114:GLU:HG2	2.01	0.42
1:E:337:VAL:O	1:E:341:LEU:HD12	2.20	0.42
1:F:694:LEU:O	1:F:698:ILE:HG22	2.20	0.42
1:B:464:ARG:HG2	1:B:464:ARG:NH1	2.33	0.42
1:B:581:MET:O	1:B:585:ILE:HG22	2.20	0.42
1:B:724:LYS:HA	1:B:724:LYS:HE2	2.02	0.42
1:E:446:VAL:HG11	1:E:608:PHE:HE2	1.85	0.42
1:F:475:LEU:HD12	1:F:475:LEU:HA	1.81	0.42
1:F:550:TYR:HE1	1:F:556:GLU:HG3	1.85	0.42
1:A:354:ALA:O	1:A:358:LEU:HB2	2.20	0.42
1:B:255:PHE:HD1	1:B:273:ASN:ND2	2.17	0.42
1:C:342:ARG:HA	1:C:347:HIS:CE1	2.55	0.42
1:C:451:ILE:HD11	1:C:578:LEU:HD22	2.01	0.42
1:C:631:LEU:HD23	1:C:631:LEU:O	2.19	0.42
1:D:252:TYR:O	1:D:255:PHE:HB3	2.19	0.42
1:D:328:ALA:O	1:D:331:TYR:HB2	2.19	0.42
1:E:94:GLY:O	1:E:98:LEU:HB2	2.20	0.42
1:A:660:SER:HB2	1:A:666:LEU:HD11	2.02	0.41
1:D:171:PRO:O	1:D:174:GLU:HG2	2.19	0.41
1:D:591:LYS:HE2	1:D:591:LYS:N	2.35	0.41
1:D:615:LYS:HB3	1:D:615:LYS:HE3	1.86	0.41
1:D:649:LYS:HD3	1:D:649:LYS:N	2.35	0.41
1:E:216:ASP:O	1:E:220:ARG:N	2.48	0.41
1:E:444:LYS:HE3	1:E:444:LYS:HB2	1.82	0.41
1:F:441:LEU:HD23	1:F:493:ARG:HD2	2.01	0.41
1:B:34:SER:CB	1:B:54:ARG:HB3	2.48	0.41
1:B:240:LYS:O	1:B:244:ALA:N	2.34	0.41
1:C:231:GLU:OE1	1:C:322:LEU:HD21	2.20	0.41
1:C:251:ASP:HB3	1:C:273:ASN:ND2	2.35	0.41
1:C:295:GLU:O	1:C:299:GLN:HB3	2.20	0.41
1:C:343:CYS:SG	1:C:346:TYR:HB2	2.60	0.41
1:D:218:LEU:O	1:D:222:GLY:N	2.53	0.41
1:D:251:ASP:O	1:D:273:ASN:ND2	2.47	0.41
1:D:308:ILE:HD13	1:D:308:ILE:HA	1.88	0.41
1:E:161:MET:O	1:E:165:LEU:N	2.46	0.41
1:A:577:LEU:O	1:A:581:MET:HB2	2.20	0.41
1:B:76:PHE:O	1:B:77:ILE:HD13	2.20	0.41
1:B:350:LEU:O	1:B:353:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:ARG:HB3	1:B:529:ARG:CZ	2.50	0.41
1:C:218:LEU:HD23	1:C:218:LEU:HA	1.84	0.41
1:C:666:LEU:HD23	1:C:666:LEU:HA	1.81	0.41
1:D:179:SER:HB3	1:D:217:MET:HE3	2.02	0.41
1:D:228:THR:O	1:D:231:GLU:HG3	2.20	0.41
1:D:311:PHE:C	1:D:316:GLY:H	2.27	0.41
1:D:469:LYS:HE3	1:D:469:LYS:HB2	1.78	0.41
1:D:480:LEU:HD22	1:D:492:ARG:NH1	2.35	0.41
1:A:298:LYS:O	1:A:301:GLU:N	2.53	0.41
1:A:306:ARG:HD2	1:A:310:ASP:OD2	2.20	0.41
1:A:525:LEU:HD12	1:A:525:LEU:HA	1.85	0.41
1:B:615:LYS:HB3	1:B:615:LYS:HE2	1.77	0.41
1:B:706:GLU:HG2	1:B:712:PRO:HA	2.02	0.41
1:D:515:LEU:C	1:D:519:MET:HE2	2.46	0.41
1:D:538:MET:HE3	1:D:538:MET:HB3	1.95	0.41
1:E:333:VAL:N	1:E:334:PRO:HD2	2.35	0.41
1:F:504:THR:O	1:F:504:THR:OG1	2.38	0.41
1:A:634:CYS:SG	1:A:661:ARG:NH1	2.93	0.41
1:B:105:ARG:O	1:B:109:ILE:N	2.38	0.41
1:B:257:ILE:HG23	1:B:258:GLU:HG3	2.03	0.41
1:B:343:CYS:HB2	1:B:346:TYR:CD2	2.55	0.41
1:C:29:LEU:HB3	1:C:100:PHE:CE1	2.55	0.41
1:C:310:ASP:O	1:C:314:GLY:N	2.53	0.41
1:D:46:GLY:O	1:D:47:PHE:HD1	2.03	0.41
1:D:61:LEU:H	1:D:61:LEU:HG	1.66	0.41
1:D:287:GLU:H	1:D:287:GLU:HG2	1.50	0.41
1:D:534:TYR:HE1	1:D:538:MET:HG3	1.83	0.41
1:E:219:MET:O	1:E:223:MET:HG2	2.21	0.41
1:E:429:GLU:C	1:E:431:LEU:H	2.28	0.41
1:E:505:GLU:HG3	1:F:486:GLU:HG2	2.01	0.41
1:A:186:THR:HA	1:A:189:LYS:HD2	2.03	0.41
1:A:589:GLN:OE1	1:A:590:GLN:NE2	2.54	0.41
1:B:206:ARG:HG2	1:B:251:ASP:OD2	2.21	0.41
1:D:432:LEU:HD23	1:D:432:LEU:HA	1.87	0.41
1:C:196:PHE:HA	1:C:201:GLU:OE1	2.21	0.41
1:C:196:PHE:HB3	1:C:281:TRP:HZ2	1.85	0.41
1:C:301:GLU:O	1:C:305:LEU:HG	2.20	0.41
1:C:514:LEU:O	1:C:518:VAL:HG23	2.21	0.41
1:C:582:MET:HE3	1:C:582:MET:HB3	1.80	0.41
1:D:89:TRP:CE2	1:D:350:LEU:HD22	2.56	0.41
1:D:255:PHE:HB2	1:D:273:ASN:CG	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:646:SER:O	1:F:648:PRO:HD3	2.21	0.41
1:A:240:LYS:HA	1:A:240:LYS:HD2	1.88	0.41
1:C:161:MET:O	1:C:165:LEU:N	2.33	0.41
1:C:203:VAL:O	1:C:207:ILE:N	2.52	0.41
1:C:441:LEU:HD11	1:C:495:ARG:HB2	2.02	0.41
1:C:653:LEU:HD12	1:C:653:LEU:HA	1.79	0.41
1:D:336:ASN:HD21	1:D:337:VAL:HG13	1.85	0.41
1:D:675:LEU:HA	1:D:675:LEU:HD23	1.75	0.41
1:E:223:MET:HG2	1:E:223:MET:H	1.75	0.41
1:E:527:ASP:CG	1:E:530:CYS:HB2	2.46	0.41
1:A:206:ARG:O	1:A:210:THR:HG22	2.21	0.41
1:B:73:TRP:CD1	1:B:80:ILE:HG13	2.56	0.41
1:B:220:ARG:HB2	1:B:225:ILE:O	2.21	0.41
1:C:285:ASN:OD1	1:C:285:ASN:N	2.54	0.41
1:C:549:LEU:HD23	1:C:549:LEU:HA	1.89	0.41
1:C:588:VAL:C	1:C:590:GLN:H	2.28	0.41
1:D:87:ASN:O	1:D:91:GLY:N	2.27	0.41
1:D:241:PRO:HB2	1:D:304:TYR:CD1	2.56	0.41
1:D:242:CYS:HB2	1:D:304:TYR:OH	2.20	0.41
1:D:294:GLN:O	1:D:297:THR:HB	2.21	0.41
1:D:595:THR:OG1	1:D:596:GLN:NE2	2.54	0.41
1:E:183:MET:O	1:E:187:THR:OG1	2.27	0.41
1:E:514:LEU:O	1:E:518:VAL:HG23	2.21	0.41
1:F:568:ARG:HG3	1:F:606:GLU:OE2	2.20	0.41
1:B:170:ALA:HB3	1:B:171:PRO:HD3	2.03	0.41
1:B:606:GLU:O	1:B:610:VAL:HG23	2.21	0.41
1:C:338:ALA:HA	1:C:341:LEU:HD12	2.02	0.41
1:C:452:ASP:OD2	1:D:155:LYS:NZ	2.54	0.41
1:D:103:PRO:HA	1:D:106:LEU:CD1	2.50	0.41
1:D:291:ARG:HA	1:D:294:GLN:HB2	2.02	0.41
1:E:656:ILE:HD13	1:E:674:VAL:HG23	2.03	0.41
1:A:73:TRP:NE1	1:A:77:ILE:HB	2.36	0.40
1:B:475:LEU:CD1	1:B:518:VAL:HG21	2.51	0.40
1:D:34:SER:HB2	1:D:54:ARG:HE	1.86	0.40
1:D:89:TRP:CZ3	1:D:357:LEU:HD23	2.56	0.40
1:D:98:LEU:HD11	1:D:113:PHE:CZ	2.55	0.40
1:A:219:MET:CE	1:A:329:GLN:HE21	2.34	0.40
1:A:311:PHE:HD2	1:A:323:GLN:HG3	1.84	0.40
1:C:564:LEU:HD22	1:C:606:GLU:OE1	2.21	0.40
1:D:84:GLY:HA3	1:D:345:ARG:CZ	2.51	0.40
1:D:485:ILE:HD11	1:D:507:THR:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:612:ASP:O	1:D:616:ASN:ND2	2.42	0.40
1:E:357:LEU:HD13	1:E:357:LEU:HA	1.93	0.40
1:A:176:VAL:HG21	1:A:221:PHE:CG	2.56	0.40
1:A:446:VAL:HG21	1:A:608:PHE:CZ	2.56	0.40
1:A:460:LEU:HD21	1:A:586:ALA:HA	2.02	0.40
1:B:322:LEU:O	1:B:326:LEU:HD12	2.21	0.40
1:D:93:PHE:HA	1:D:339:TRP:CD1	2.56	0.40
1:D:100:PHE:HD2	1:D:223:MET:HE3	1.85	0.40
1:E:615:LYS:HB3	1:E:615:LYS:HE2	1.83	0.40
1:F:563:TYR:O	1:F:567:ILE:HG23	2.21	0.40
1:A:181:LYS:HB2	1:A:181:LYS:HE3	1.81	0.40
1:C:290:LYS:O	1:C:294:GLN:HG3	2.22	0.40
1:C:353:GLU:HA	1:C:356:SER:HB2	2.02	0.40
1:C:429:GLU:O	1:C:430:HIS:HB2	2.21	0.40
1:D:307:ASN:O	1:D:307:ASN:ND2	2.53	0.40
1:D:332:GLN:O	1:D:336:ASN:N	2.50	0.40
1:E:56:HIS:O	1:E:59:GLU:HB2	2.22	0.40
1:E:260:GLU:O	1:E:264:ALA:N	2.44	0.40
1:E:519:MET:CE	1:F:519:MET:HG2	2.51	0.40
1:E:642:HIS:HD1	1:E:686:TYR:HD2	1.68	0.40
1:A:316:GLY:O	1:A:323:GLN:NE2	2.54	0.40
1:C:63:ASN:O	1:C:67:LEU:HG	2.21	0.40
1:C:464:ARG:NH1	1:C:526:ASP:H	2.15	0.40
1:C:540:ASN:O	1:C:543:ILE:HG22	2.21	0.40
1:D:73:TRP:CD1	1:D:73:TRP:O	2.75	0.40
1:D:86:CYS:HB2	1:D:358:LEU:HD11	2.04	0.40
1:D:89:TRP:HD1	1:D:342:ARG:CZ	2.34	0.40
1:D:157:ILE:C	1:D:160:LYS:H	2.29	0.40
1:D:570:LYS:HE2	1:D:570:LYS:HB3	1.91	0.40
1:E:291:ARG:O	1:E:295:GLU:HG3	2.21	0.40
1:E:324:THR:HA	1:E:327:LYS:HB2	2.03	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	597/725 (82%)	549 (92%)	44 (7%)	4 (1%)	19	53
1	B	533/725 (74%)	488 (92%)	39 (7%)	6 (1%)	12	45
1	C	570/725 (79%)	525 (92%)	38 (7%)	7 (1%)	11	43
1	D	582/725 (80%)	526 (90%)	53 (9%)	3 (0%)	25	59
1	E	526/725 (73%)	489 (93%)	35 (7%)	2 (0%)	30	63
1	F	286/725 (39%)	267 (93%)	16 (6%)	3 (1%)	13	46
All	All	3094/4350 (71%)	2844 (92%)	225 (7%)	25 (1%)	19	51

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	PHE
1	A	103	PRO
1	B	32	THR
1	B	93	PHE
1	B	269	THR
1	B	351	CYS
1	C	266	SER
1	C	286	ALA
1	C	588	VAL
1	D	157	ILE
1	D	589	GLN
1	E	169	ASP
1	F	446	VAL
1	F	589	GLN
1	C	320	ILE
1	A	683	SER
1	C	93	PHE
1	C	683	SER
1	A	459	VAL
1	B	266	SER
1	B	459	VAL
1	D	156	GLN
1	E	459	VAL
1	C	459	VAL
1	F	459	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	535/638 (84%)	497 (93%)	38 (7%)	12 39
1	B	487/638 (76%)	458 (94%)	29 (6%)	16 45
1	C	514/638 (81%)	476 (93%)	38 (7%)	11 37
1	D	527/638 (83%)	488 (93%)	39 (7%)	11 37
1	E	482/638 (76%)	458 (95%)	24 (5%)	20 49
1	F	260/638 (41%)	239 (92%)	21 (8%)	9 35
All	All	2805/3828 (73%)	2616 (93%)	189 (7%)	16 41

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	PHE
1	A	51	TYR
1	A	52	GLU
1	A	72	ASP
1	A	80	ILE
1	A	102	LYS
1	A	103	PRO
1	A	152	LEU
1	A	158	GLN
1	A	168	ILE
1	A	189	LYS
1	A	194	ARG
1	A	218	LEU
1	A	223	MET
1	A	240	LYS
1	A	267	ASP
1	A	294	GLN
1	A	317	LYS
1	A	333	VAL
1	A	345	ARG
1	A	357	LEU
1	A	359	HIS

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Mol	Chain	Res	Type
1	A	439	SER
1	A	444	LYS
1	A	466	ASN
1	A	479	SER
1	A	488	HIS
1	A	530	CYS
1	A	581	MET
1	A	591	LYS
1	A	608	PHE
1	A	647	GLN
1	A	649	LYS
1	A	675	LEU
1	A	687	THR
1	A	698	ILE
1	A	699	THR
1	A	724	LYS
1	B	28	ILE
1	B	33	LEU
1	B	44	ILE
1	B	108	VAL
1	B	117	PHE
1	B	149	ARG
1	B	159	SER
1	B	216	ASP
1	B	217	MET
1	B	236	GLU
1	B	303	GLN
1	B	324	THR
1	B	333	VAL
1	B	429	GLU
1	B	436	GLU
1	B	479	SER
1	B	499	HIS
1	B	518	VAL
1	B	564	LEU
1	B	579	THR
1	B	582	MET
1	B	584	GLN
1	B	590	GLN
1	B	615	LYS
1	B	656	ILE
1	B	671	LYS

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Mol	Chain	Res	Type
1	B	695	MET
1	B	716	VAL
1	B	718	LEU
1	C	31	SER
1	C	61	LEU
1	C	64	GLU
1	C	92	HIS
1	C	106	LEU
1	C	108	VAL
1	C	109	ILE
1	C	161	MET
1	C	181	LYS
1	C	208	ILE
1	C	218	LEU
1	C	227	LEU
1	C	238	ILE
1	C	248	LEU
1	C	257	ILE
1	C	259	TRP
1	C	262	PHE
1	C	308	ILE
1	C	323	GLN
1	C	358	LEU
1	C	359	HIS
1	C	426	LEU
1	C	438	ILE
1	C	441	LEU
1	C	447	ARG
1	C	460	LEU
1	C	475	LEU
1	C	492	ARG
1	C	509	ASN
1	C	515	LEU
1	C	526	ASP
1	C	527	ASP
1	C	615	LYS
1	C	640	LEU
1	C	649	LYS
1	C	674	VAL
1	C	711	SER
1	C	720	ILE
1	D	48	CYS

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Mol	Chain	Res	Type
1	D	54	ARG
1	D	61	LEU
1	D	63	ASN
1	D	108	VAL
1	D	146	ARG
1	D	148	VAL
1	D	163	LEU
1	D	175	VAL
1	D	206	ARG
1	D	216	ASP
1	D	228	THR
1	D	229	GLN
1	D	231	GLU
1	D	234	ARG
1	D	251	ASP
1	D	257	ILE
1	D	268	LYS
1	D	287	GLU
1	D	317	LYS
1	D	325	TYR
1	D	326	LEU
1	D	327	LYS
1	D	336	ASN
1	D	349	TRP
1	D	350	LEU
1	D	360	GLN
1	D	491	LEU
1	D	500	MET
1	D	519	MET
1	D	521	LYS
1	D	535	LEU
1	D	541	LEU
1	D	591	LYS
1	D	635	LYS
1	D	652	GLN
1	D	656	ILE
1	D	677	HIS
1	D	721	HIS
1	E	41	THR
1	E	80	ILE
1	E	105	ARG
1	E	113	PHE

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Mol	Chain	Res	Type
1	E	165	LEU
1	E	168	ILE
1	E	221	PHE
1	E	223	MET
1	E	229	GLN
1	E	233	LYS
1	E	246	LEU
1	E	295	GLU
1	E	333	VAL
1	E	336	ASN
1	E	357	LEU
1	E	465	VAL
1	E	507	THR
1	E	564	LEU
1	E	595	THR
1	E	608	PHE
1	E	649	LYS
1	E	660	SER
1	E	666	LEU
1	E	667	ASP
1	F	436	GLU
1	F	447	ARG
1	F	460	LEU
1	F	462	ASP
1	F	468	LEU
1	F	529	ARG
1	F	530	CYS
1	F	556	GLU
1	F	580	ARG
1	F	588	VAL
1	F	608	PHE
1	F	617	LEU
1	F	632	ASP
1	F	633	GLU
1	F	635	LYS
1	F	649	LYS
1	F	668	VAL
1	F	672	GLU
1	F	696	GLU
1	F	719	LEU
1	F	724	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	250	ASN
1	A	285	ASN
1	A	307	ASN
1	A	562	GLN
1	A	647	GLN
1	B	294	GLN
1	B	323	GLN
1	B	584	GLN
1	B	647	GLN
1	C	58	HIS
1	C	178	ASN
1	C	347	HIS
1	C	430	HIS
1	C	467	GLN
1	C	477	ASN
1	C	506	GLN
1	C	589	GLN
1	C	677	HIS
1	D	121	ASN
1	D	283	ASN
1	D	499	HIS
1	D	569	GLN
1	D	647	GLN
1	D	650	ASN
1	D	658	GLN
1	D	680	GLN
1	E	75	GLN
1	E	329	GLN
1	E	463	HIS
1	E	476	HIS
1	E	569	GLN
1	E	596	GLN
1	E	650	ASN
1	E	677	HIS
1	F	463	HIS
1	F	524	GLN
1	F	540	ASN
1	F	554	ASN
1	F	562	GLN
1	F	584	GLN
1	F	652	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

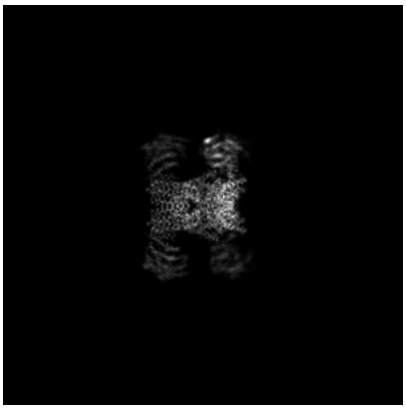
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-47454. These allow visual inspection of the internal detail of the map and identification of artifacts.

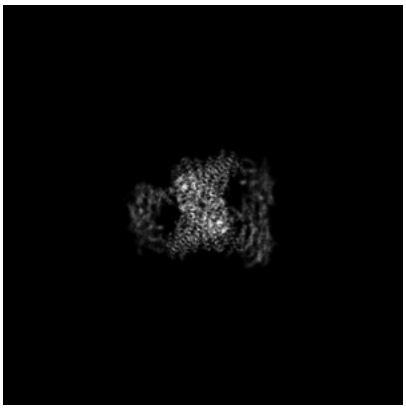
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

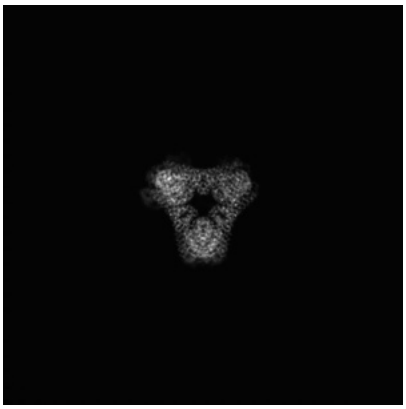
6.1.1 Primary map



X

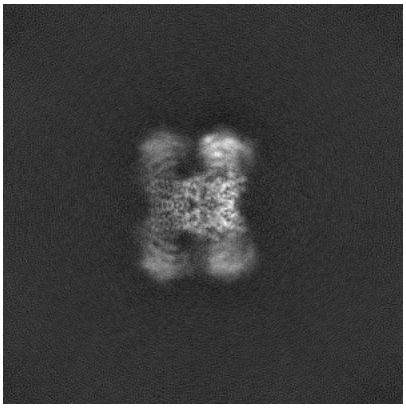


Y

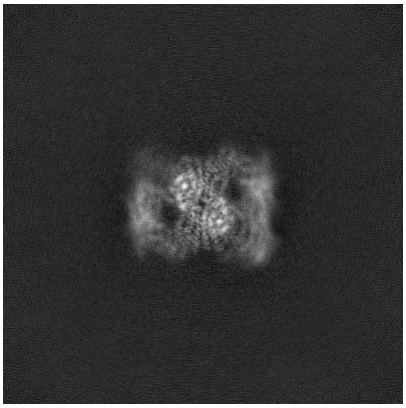


Z

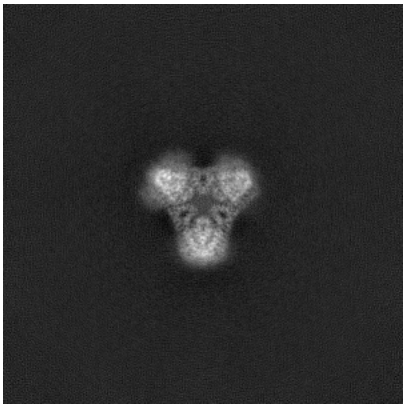
6.1.2 Raw map



X



Y

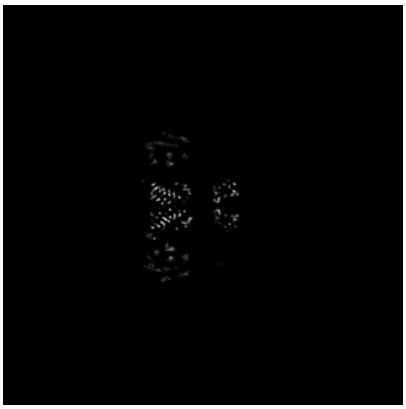


Z

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

6.2 Central slices (i)

6.2.1 Primary map

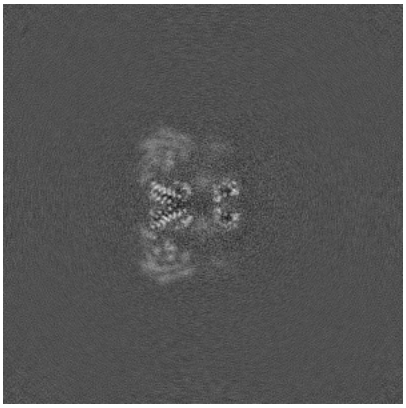


X Index: 192

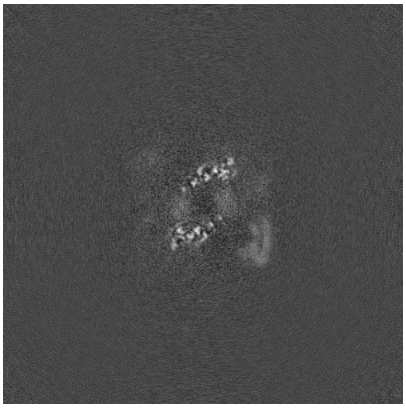
Y Index: 192

Z Index: 192

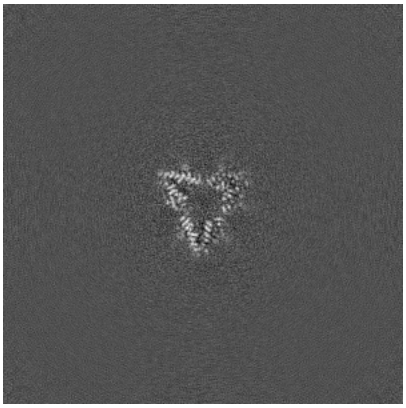
6.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

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

6.3 Largest variance slices (i)

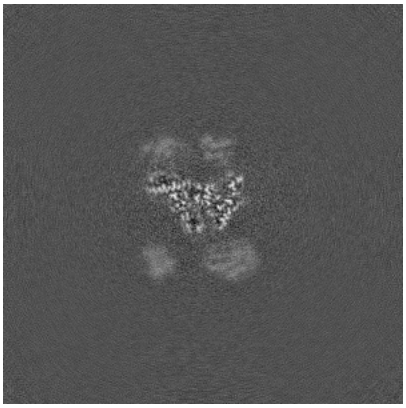
6.3.1 Primary map

X Index: 168

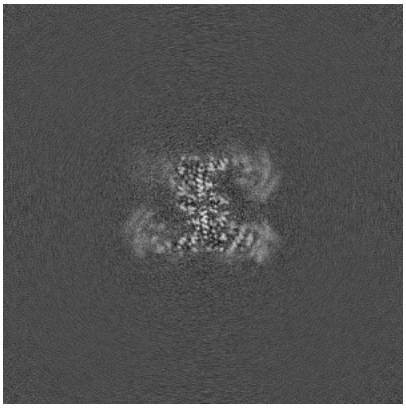
Y Index: 216

Z Index: 194

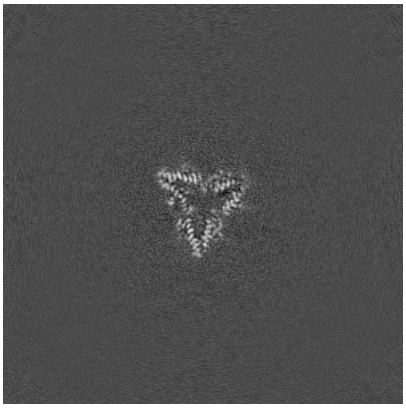
6.3.2 Raw map



X Index: 174



Y Index: 216

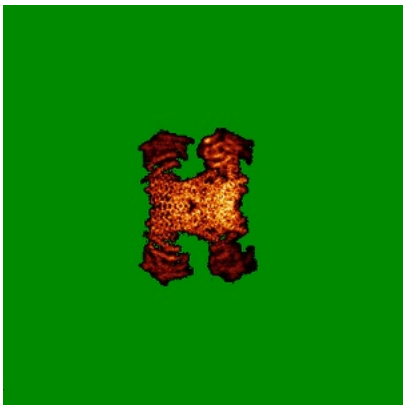


Z Index: 194

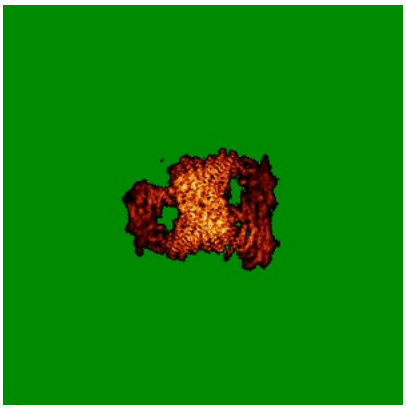
The images above show the largest variance slices of the map in three orthogonal directions.

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

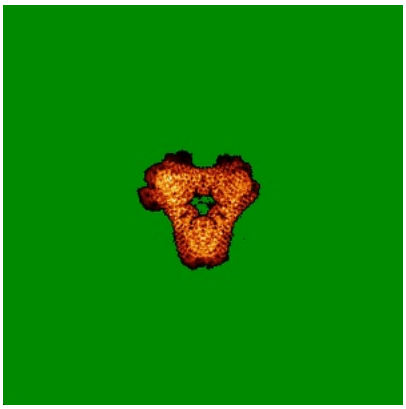
6.4.1 Primary map



X

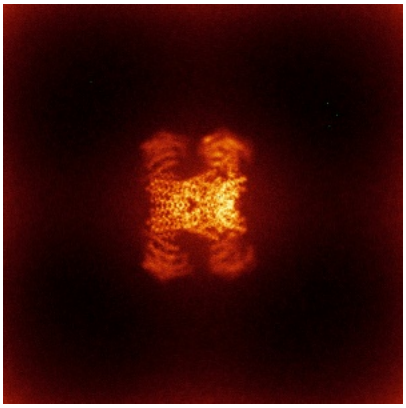


Y

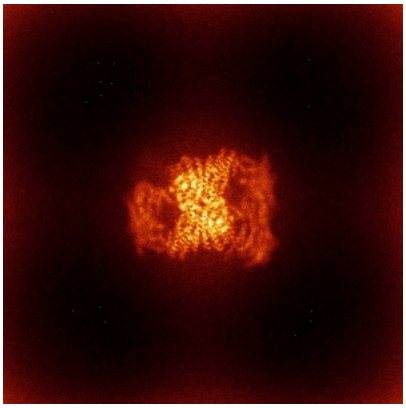


Z

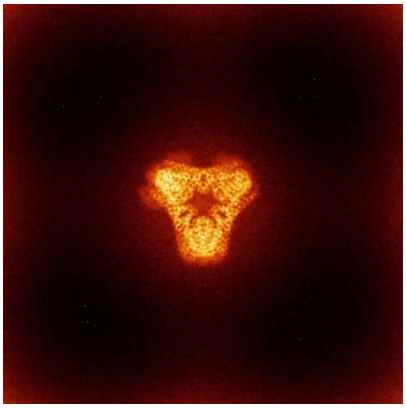
6.4.2 Raw map



X



Y

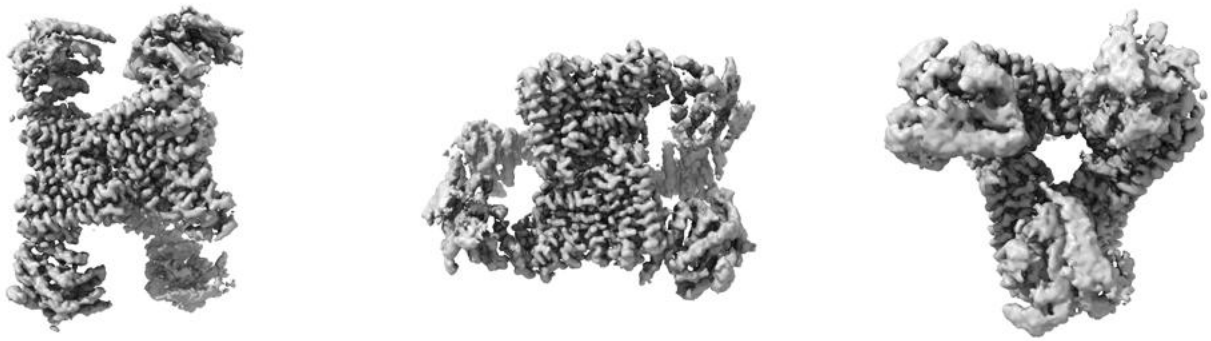


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. 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

X Y Z

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.

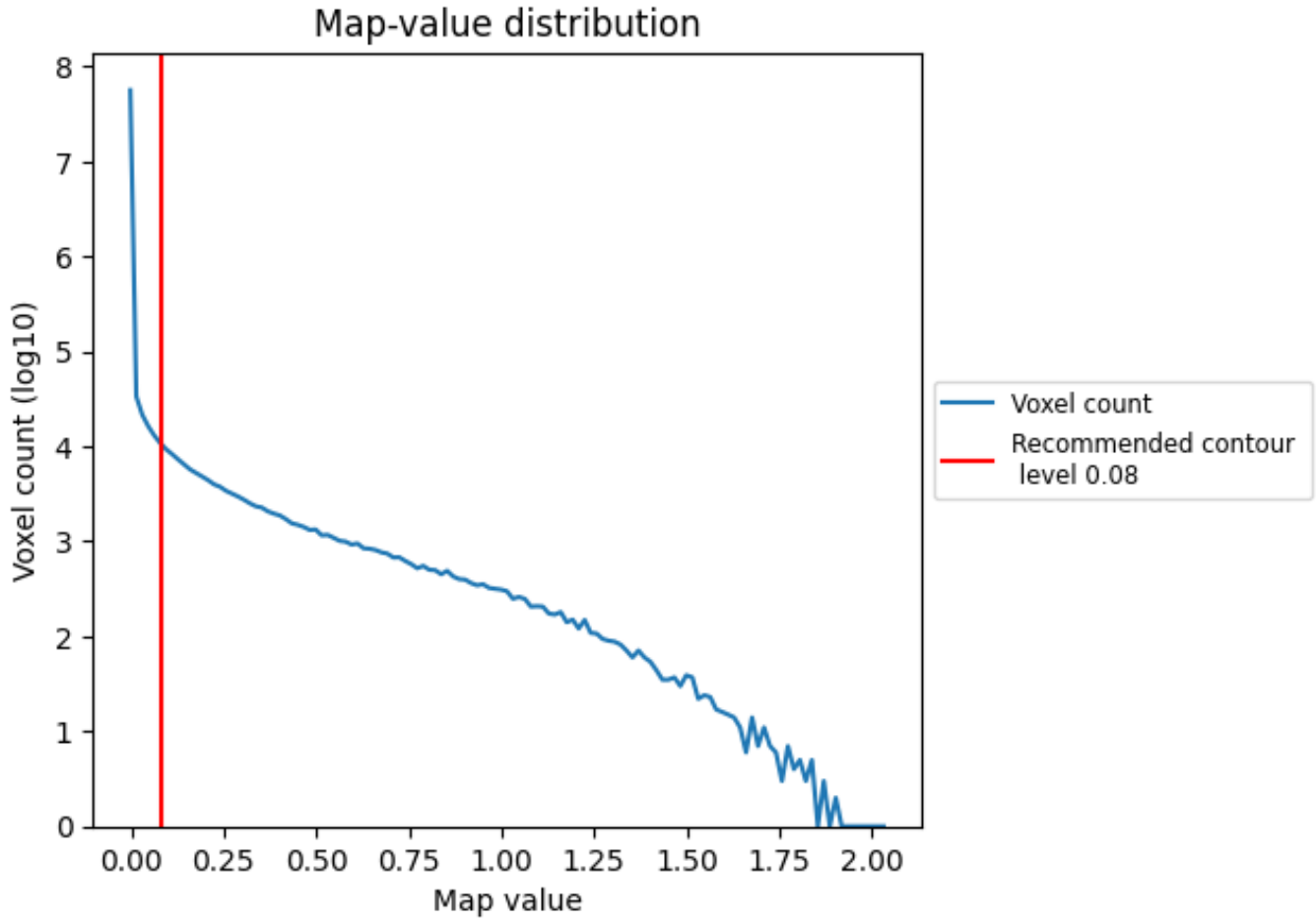
6.6 Mask visualisation (i)

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

7 Map analysis

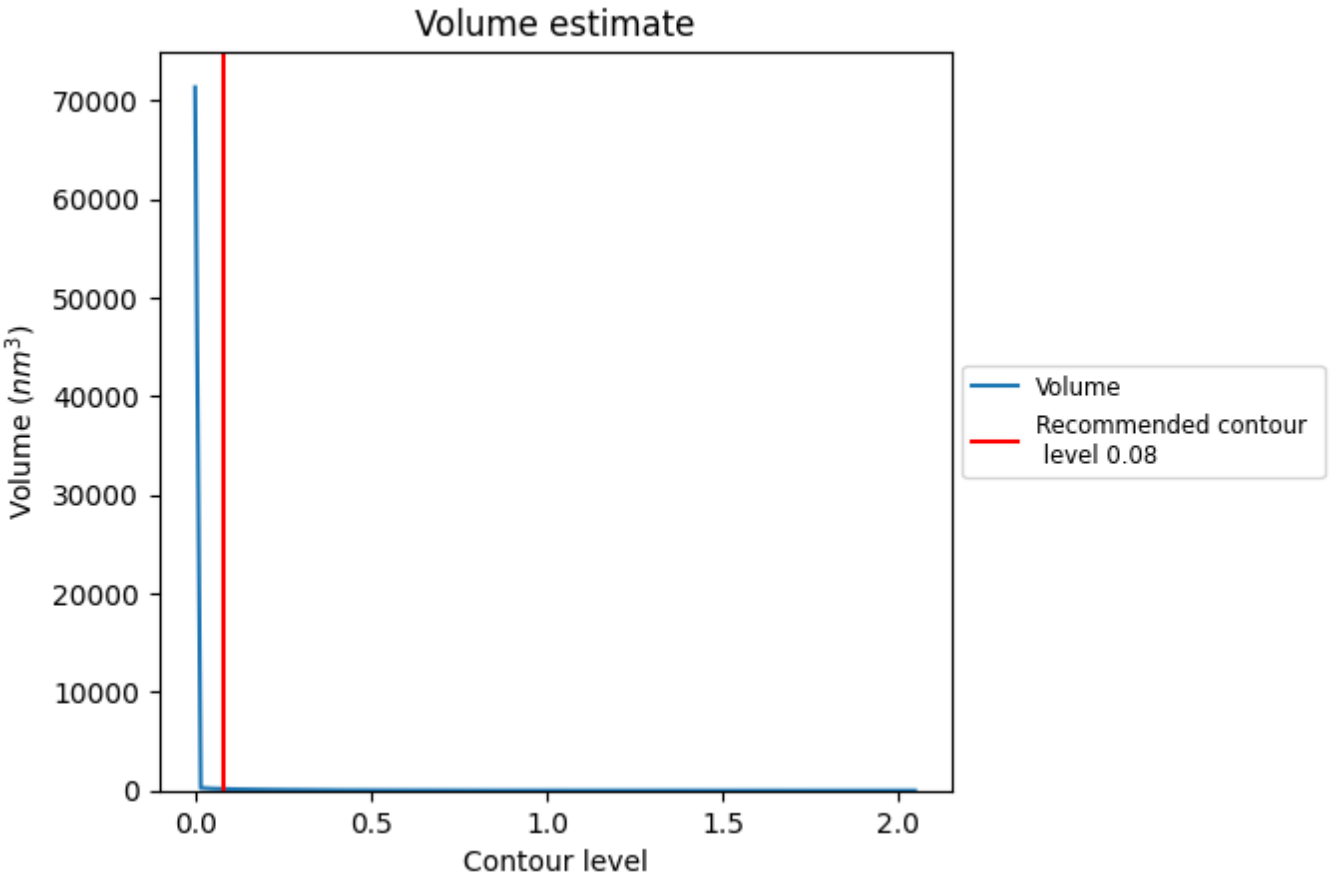
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

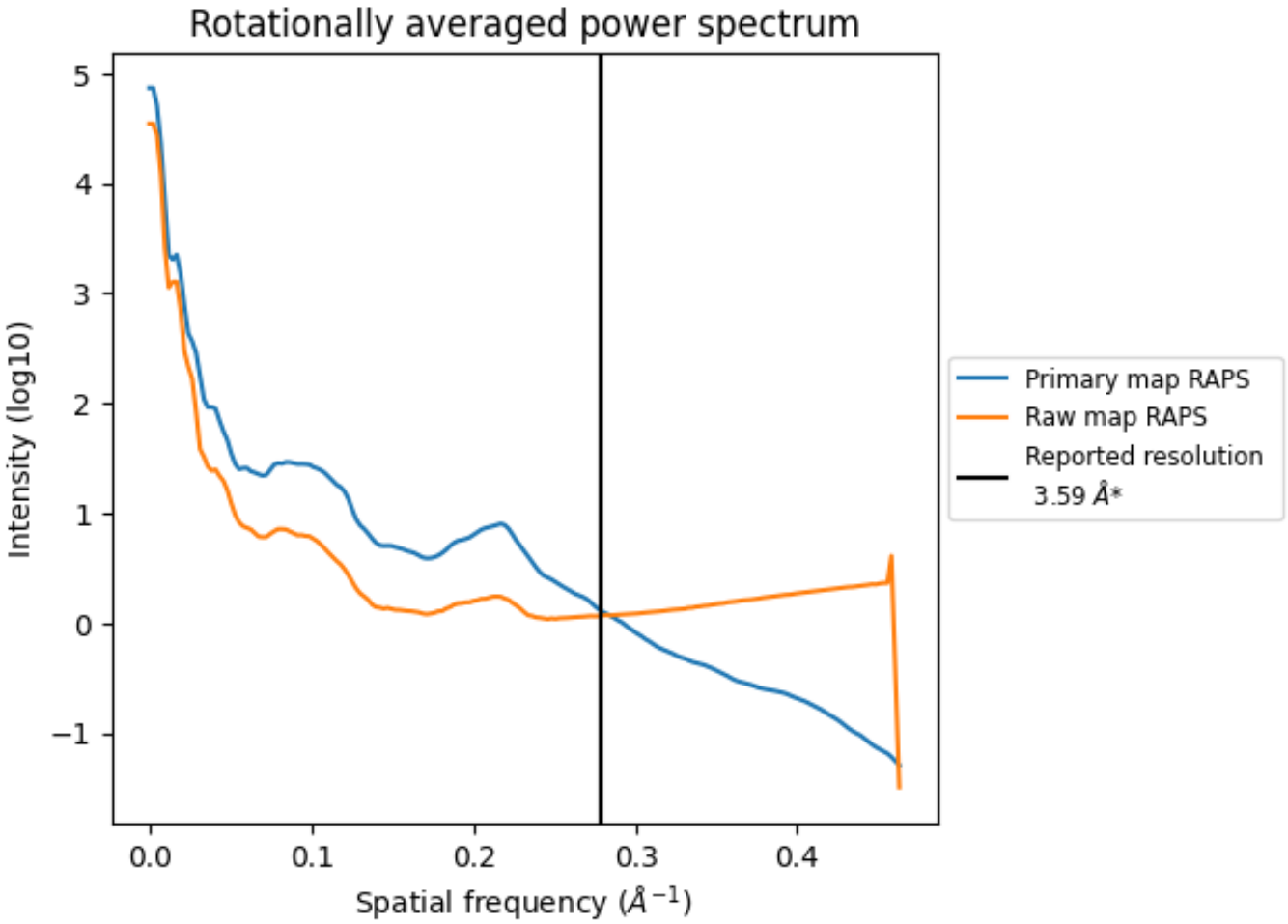
7.2 Volume estimate



The volume at the recommended contour level is 161 nm^3; this corresponds to an approximate mass of 146 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 (i)

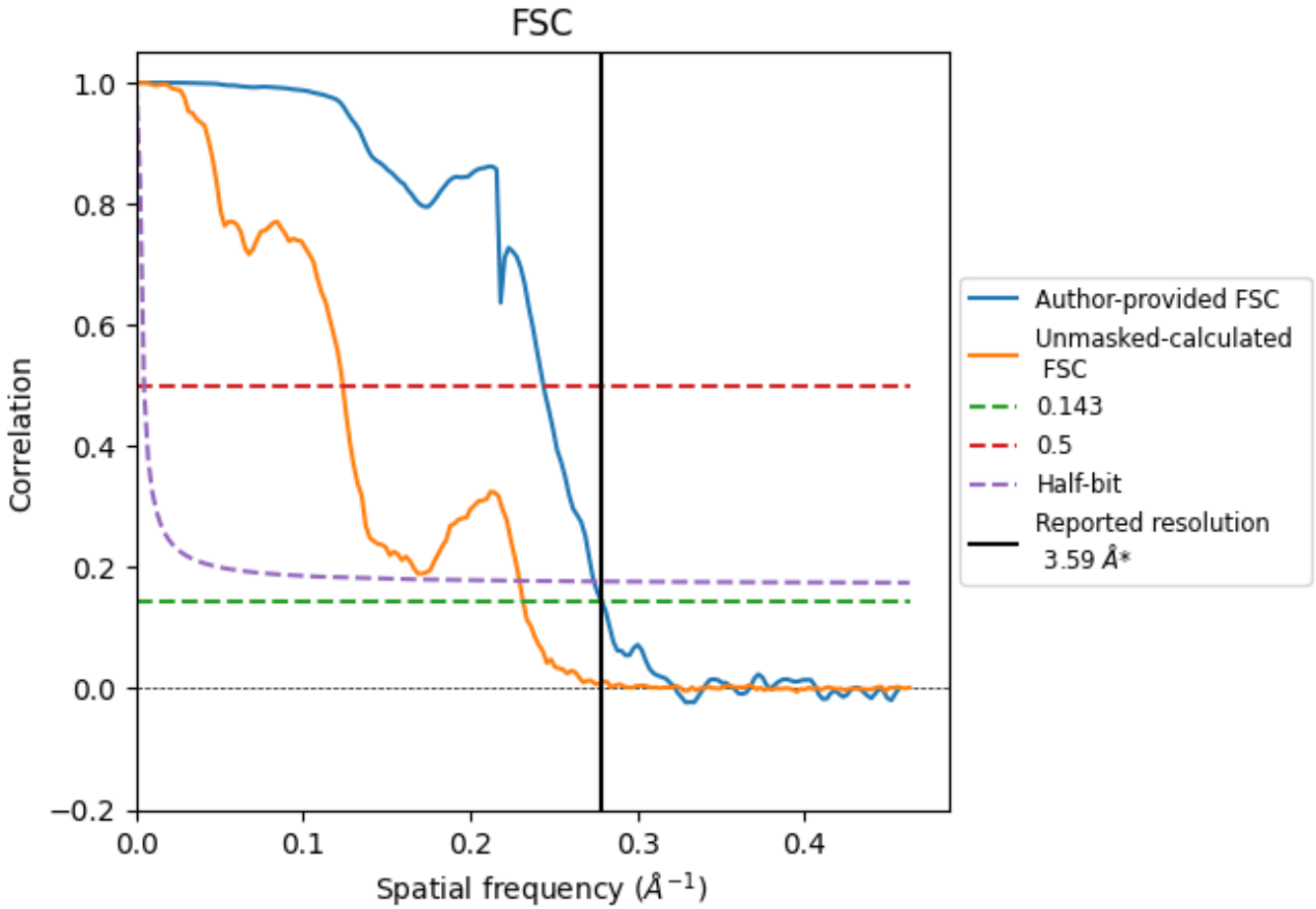


*Reported resolution corresponds to spatial frequency of 0.279 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.279 Å^{-1}

8.2 Resolution estimates (i)

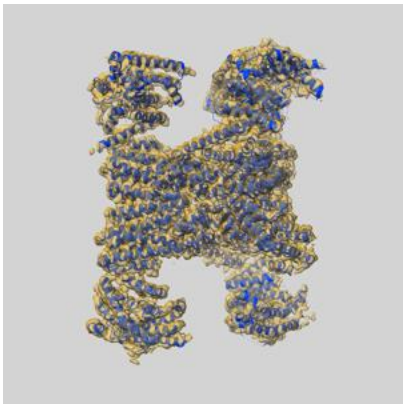
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.59	-	-
Author-provided FSC curve	3.59	4.10	3.65
Unmasked-calculated*	4.32	8.08	4.36

*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 4.32 differs from the reported value 3.59 by more than 10 %

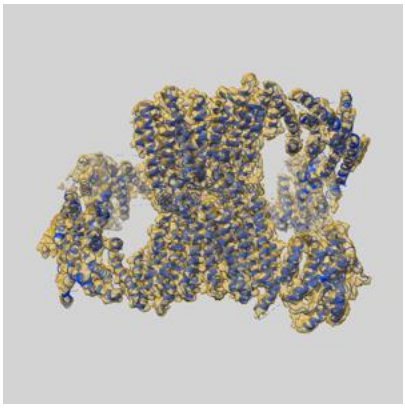
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-47454 and PDB model 9E2J. Per-residue inclusion information can be found in section 3 on page 7.

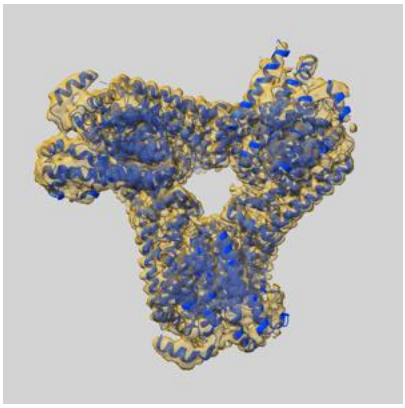
9.1 Map-model overlay



X



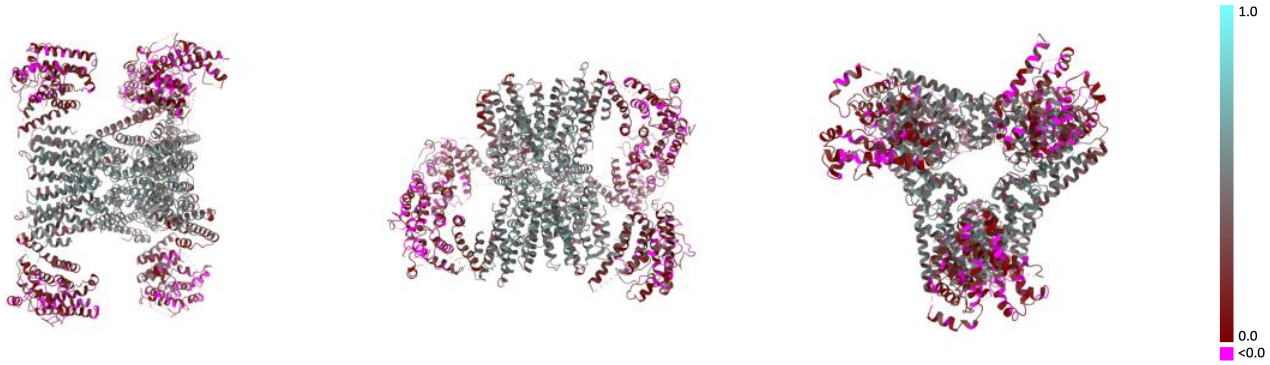
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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.

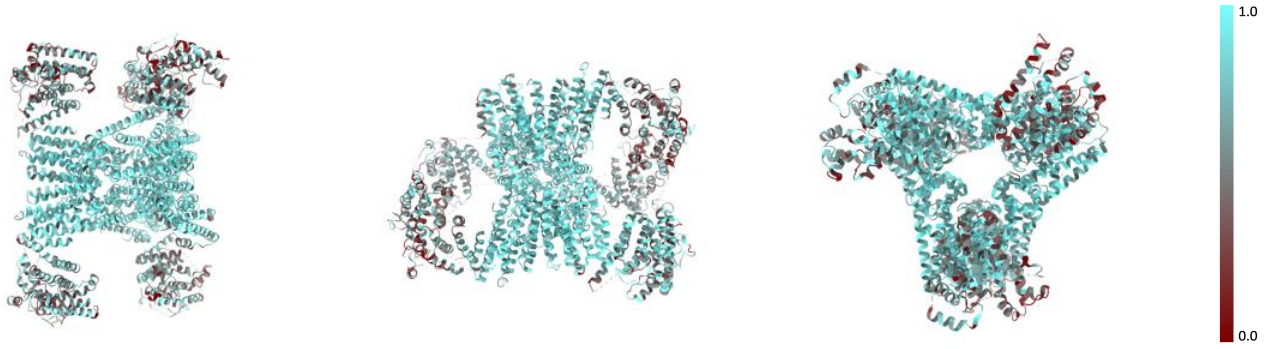
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

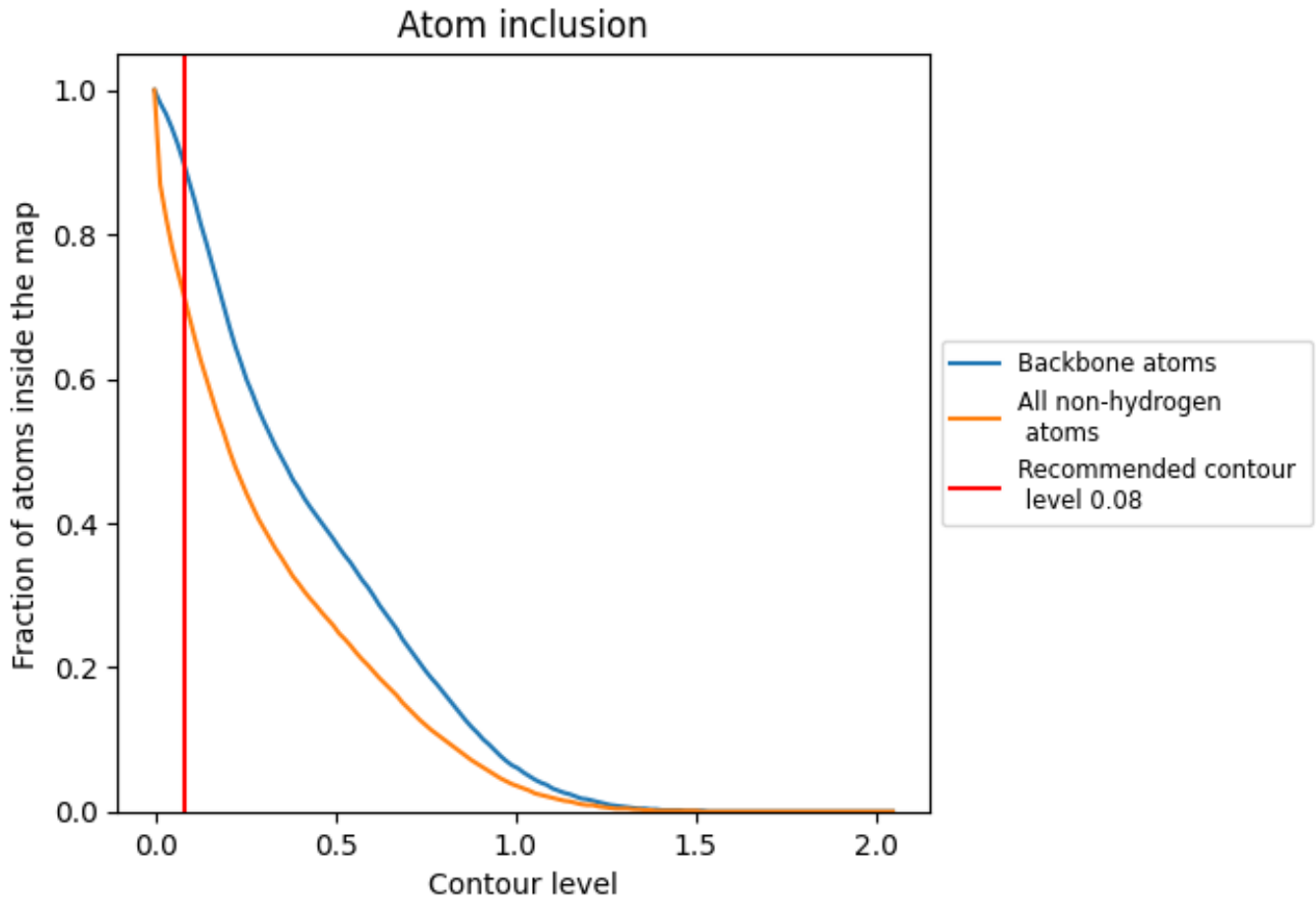
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 72% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7150	0.3120
A	0.7430	0.3100
B	0.7040	0.3070
C	0.6930	0.2950
D	0.7120	0.2980
E	0.6540	0.2770
F	0.8480	0.4600