



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:10 PM UTC

PDB ID : 8H3F / pdb_00008h3f
EMDB ID : EMD-34467
Title : Cryo-EM Structure of the KBTBD2-CRL3-CSN complex
Authors : Hu, Y.; Mao, Q.; Chen, Z.; Sun, L.
Deposited on : 2022-10-08
Resolution : 6.73 Å (reported)

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

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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
MolProbity : 4-5-2 with Phenix2.0
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

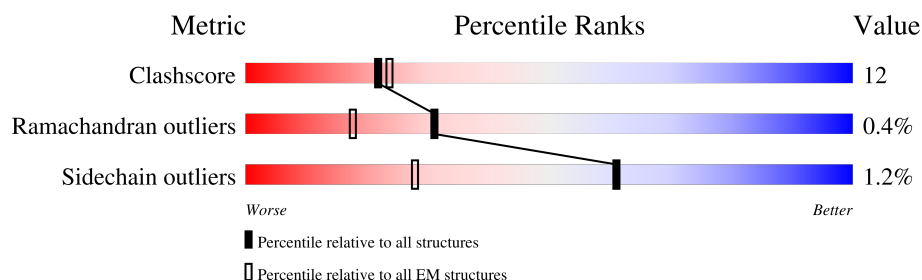
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.73 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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

Mol	Chain	Length	Quality of chain
1	E	334	
2	A	527	
3	B	443	
4	C	441	
5	D	406	
6	F	327	
7	G	220	
8	H	209	

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Mol	Chain	Length	Quality of chain
9	I	636	25% 65% 23% 12%
9	M	636	43% 64% 25% 11%
10	R	121	38% 35% 26%
11	L	768	15% 64% 28% 7%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 36711 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 COP9 signalosome complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	309	Total	C	N	O	S	0	0
			2457	1566	410	467	14		

- Molecule 2 is a protein called COP9 signalosome complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	412	Total	C	N	O	S	0	0
			3296	2088	574	612	22		

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q13098
A	2	ARG	-	expression tag	UNP Q13098
A	3	ASP	-	expression tag	UNP Q13098
A	4	SER	-	expression tag	UNP Q13098
A	5	SER	-	expression tag	UNP Q13098
A	6	ALA	-	expression tag	UNP Q13098
A	7	PRO	-	expression tag	UNP Q13098
A	8	SER	-	expression tag	UNP Q13098
A	9	SER	-	expression tag	UNP Q13098
A	10	ALA	-	expression tag	UNP Q13098
A	11	SER	-	expression tag	UNP Q13098
A	12	SER	-	expression tag	UNP Q13098
A	13	SER	-	expression tag	UNP Q13098
A	14	VAL	-	expression tag	UNP Q13098
A	15	THR	-	expression tag	UNP Q13098
A	16	ASP	-	expression tag	UNP Q13098
A	17	LEU	-	expression tag	UNP Q13098
A	18	TYR	-	expression tag	UNP Q13098
A	19	CYS	-	expression tag	UNP Q13098
A	20	THR	-	expression tag	UNP Q13098
A	21	PRO	-	expression tag	UNP Q13098

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	HIS	-	expression tag	UNP Q13098
A	23	SER	-	expression tag	UNP Q13098
A	24	SER	-	expression tag	UNP Q13098
A	25	ARG	-	expression tag	UNP Q13098
A	26	SER	-	expression tag	UNP Q13098
A	27	ASP	-	expression tag	UNP Q13098
A	28	LEU	-	expression tag	UNP Q13098
A	29	VAL	-	expression tag	UNP Q13098
A	30	LEU	-	expression tag	UNP Q13098
A	31	PRO	-	expression tag	UNP Q13098
A	32	GLY	-	expression tag	UNP Q13098
A	33	THR	-	expression tag	UNP Q13098
A	34	ALA	-	expression tag	UNP Q13098
A	35	GLY	-	expression tag	UNP Q13098
A	36	ASP	-	expression tag	UNP Q13098
A	37	PHE	-	expression tag	UNP Q13098
A	38	SER	-	expression tag	UNP Q13098
A	39	LEU	-	expression tag	UNP Q13098
A	40	SER	-	expression tag	UNP Q13098
A	41	ALA	-	expression tag	UNP Q13098
A	42	SER	-	expression tag	UNP Q13098
A	43	LEU	-	expression tag	UNP Q13098
A	44	SER	-	expression tag	UNP Q13098
A	45	ALA	-	expression tag	UNP Q13098
A	46	CYS	-	expression tag	UNP Q13098
A	47	THR	-	expression tag	UNP Q13098
A	48	LEU	-	expression tag	UNP Q13098
A	49	LEU	-	expression tag	UNP Q13098
A	50	TYR	-	expression tag	UNP Q13098
A	51	GLU	-	expression tag	UNP Q13098
A	?	-	ARG	deletion	UNP Q13098
A	?	-	SER	deletion	UNP Q13098
A	?	-	SER	deletion	UNP Q13098
A	?	-	LEU	deletion	UNP Q13098

- Molecule 3 is a protein called COP9 signalosome complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	420	Total	C	N	O	S	0	0
			3430	2173	587	655	15		

- Molecule 4 is a protein called COP9 signalosome complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	407	Total	C	N	O	S	0	0
			3235	2059	543	606	27		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	TRP	-	expression tag	UNP Q9UNS2
C	-16	SER	-	expression tag	UNP Q9UNS2
C	-15	HIS	-	expression tag	UNP Q9UNS2
C	-14	PRO	-	expression tag	UNP Q9UNS2
C	-13	GLN	-	expression tag	UNP Q9UNS2
C	-12	PHE	-	expression tag	UNP Q9UNS2
C	-11	GLU	-	expression tag	UNP Q9UNS2
C	-10	LYS	-	expression tag	UNP Q9UNS2
C	-9	LEU	-	expression tag	UNP Q9UNS2
C	-8	GLU	-	expression tag	UNP Q9UNS2
C	-7	VAL	-	expression tag	UNP Q9UNS2
C	-6	LEU	-	expression tag	UNP Q9UNS2
C	-5	PHE	-	expression tag	UNP Q9UNS2
C	-4	GLN	-	expression tag	UNP Q9UNS2
C	-3	GLY	-	expression tag	UNP Q9UNS2
C	-2	PRO	-	expression tag	UNP Q9UNS2
C	-1	GLY	-	expression tag	UNP Q9UNS2
C	0	SER	-	expression tag	UNP Q9UNS2

- Molecule 5 is a protein called COP9 signalosome complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	406	Total	C	N	O	S	0	0
			3251	2047	566	622	16		

- Molecule 6 is a protein called COP9 signalosome complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	288	Total	C	N	O	S	0	0
			2279	1452	379	433	15		

- Molecule 7 is a protein called COP9 signalosome complex subunit 7b.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	214	Total	C	N	O	S	0	0
			1692	1072	287	327	6		

- Molecule 8 is a protein called COP9 signalosome complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	177	Total	C	N	O	S	0	0
			1411	903	245	259	4		

- Molecule 9 is a protein called Kelch repeat and BTB domain-containing protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	557	Total	C	N	O	S	0	0
			4507	2880	746	843	38		
9	M	564	Total	C	N	O	S	0	0
			4559	2912	758	851	38		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	252	ASP	SER	engineered mutation	UNP Q8IY47
I	624	GLU	-	expression tag	UNP Q8IY47
I	625	ASN	-	expression tag	UNP Q8IY47
I	626	LEU	-	expression tag	UNP Q8IY47
I	627	TYR	-	expression tag	UNP Q8IY47
I	628	PHE	-	expression tag	UNP Q8IY47
I	629	GLN	-	expression tag	UNP Q8IY47
I	630	GLY	-	expression tag	UNP Q8IY47
I	631	HIS	-	expression tag	UNP Q8IY47
I	632	HIS	-	expression tag	UNP Q8IY47
I	633	HIS	-	expression tag	UNP Q8IY47
I	634	HIS	-	expression tag	UNP Q8IY47
I	635	HIS	-	expression tag	UNP Q8IY47
I	636	HIS	-	expression tag	UNP Q8IY47
M	252	ASP	SER	engineered mutation	UNP Q8IY47
M	624	GLU	-	expression tag	UNP Q8IY47
M	625	ASN	-	expression tag	UNP Q8IY47
M	626	LEU	-	expression tag	UNP Q8IY47
M	627	TYR	-	expression tag	UNP Q8IY47
M	628	PHE	-	expression tag	UNP Q8IY47
M	629	GLN	-	expression tag	UNP Q8IY47
M	630	GLY	-	expression tag	UNP Q8IY47
M	631	HIS	-	expression tag	UNP Q8IY47
M	632	HIS	-	expression tag	UNP Q8IY47
M	633	HIS	-	expression tag	UNP Q8IY47
M	634	HIS	-	expression tag	UNP Q8IY47
M	635	HIS	-	expression tag	UNP Q8IY47
M	636	HIS	-	expression tag	UNP Q8IY47

- Molecule 10 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	R	89	Total	C	N	O	S	0	0
			737	466	135	127	9		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-12	HIS	-	expression tag	UNP P62877
R	-11	HIS	-	expression tag	UNP P62877
R	-10	HIS	-	expression tag	UNP P62877
R	-9	HIS	-	expression tag	UNP P62877
R	-8	HIS	-	expression tag	UNP P62877
R	-7	HIS	-	expression tag	UNP P62877
R	-6	GLU	-	expression tag	UNP P62877
R	-5	ASN	-	expression tag	UNP P62877
R	-4	LEU	-	expression tag	UNP P62877
R	-3	TYR	-	expression tag	UNP P62877
R	-2	PHE	-	expression tag	UNP P62877
R	-1	GLN	-	expression tag	UNP P62877
R	0	GLY	-	expression tag	UNP P62877

- Molecule 11 is a protein called Cullin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	718	Total	C	N	O	S	0	0
			5853	3681	1035	1098	39		

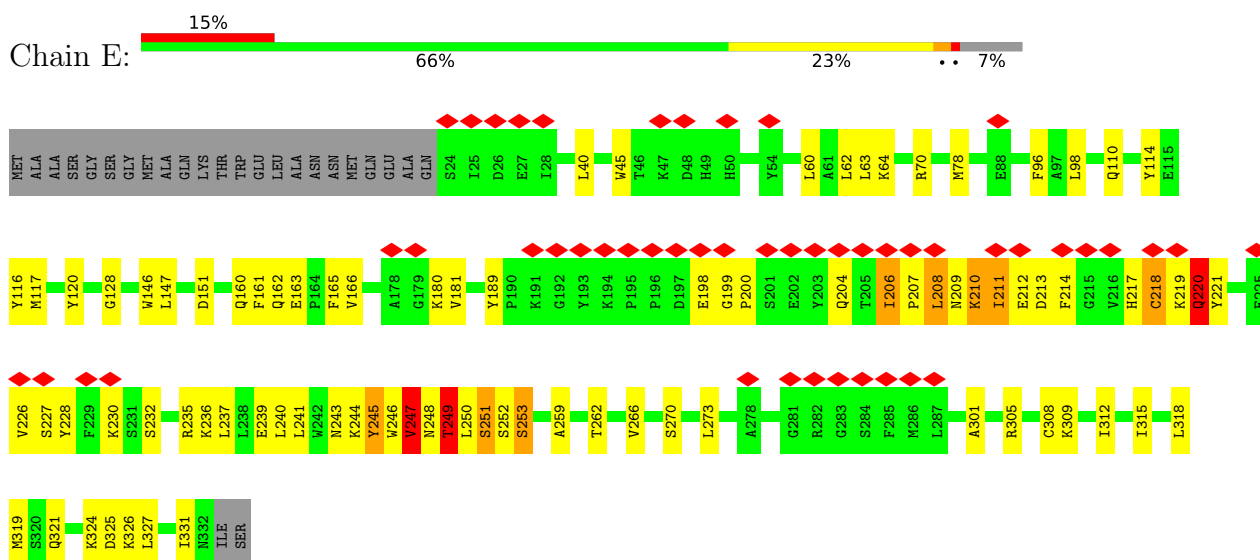
- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
12	E	1	Total	Zn	0
			1	1	
12	R	3	Total	Zn	0
			3	3	

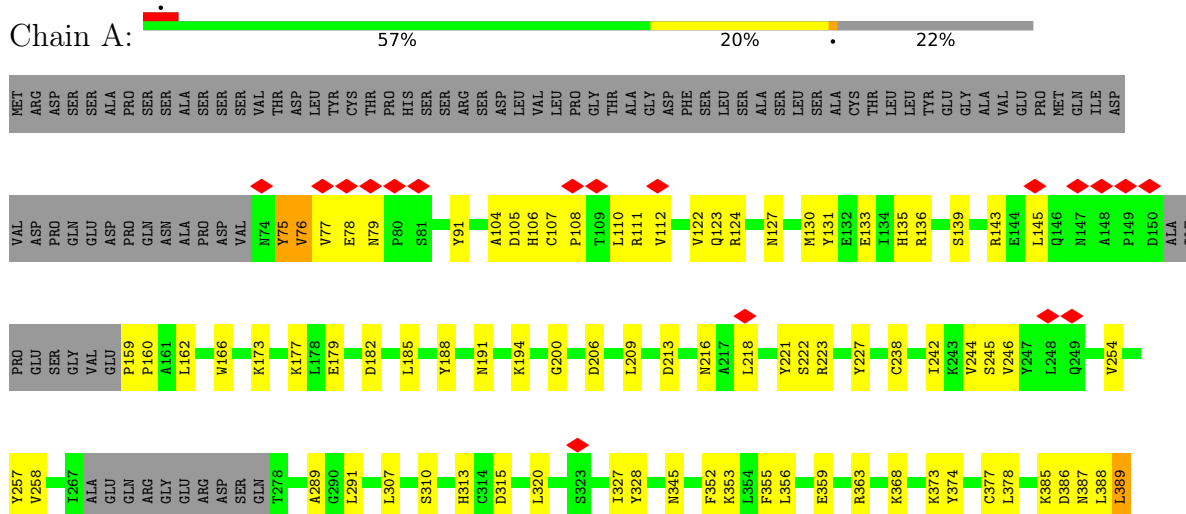
3 Residue-property plots

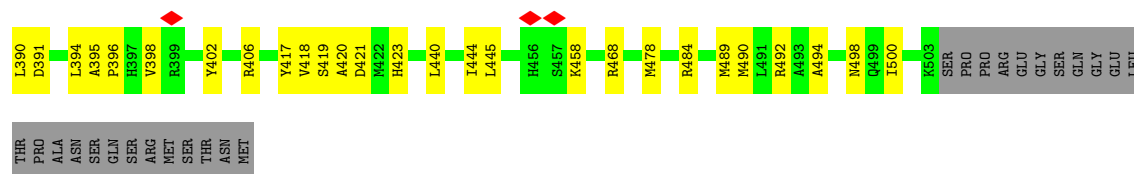
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: COP9 signalosome complex subunit 5

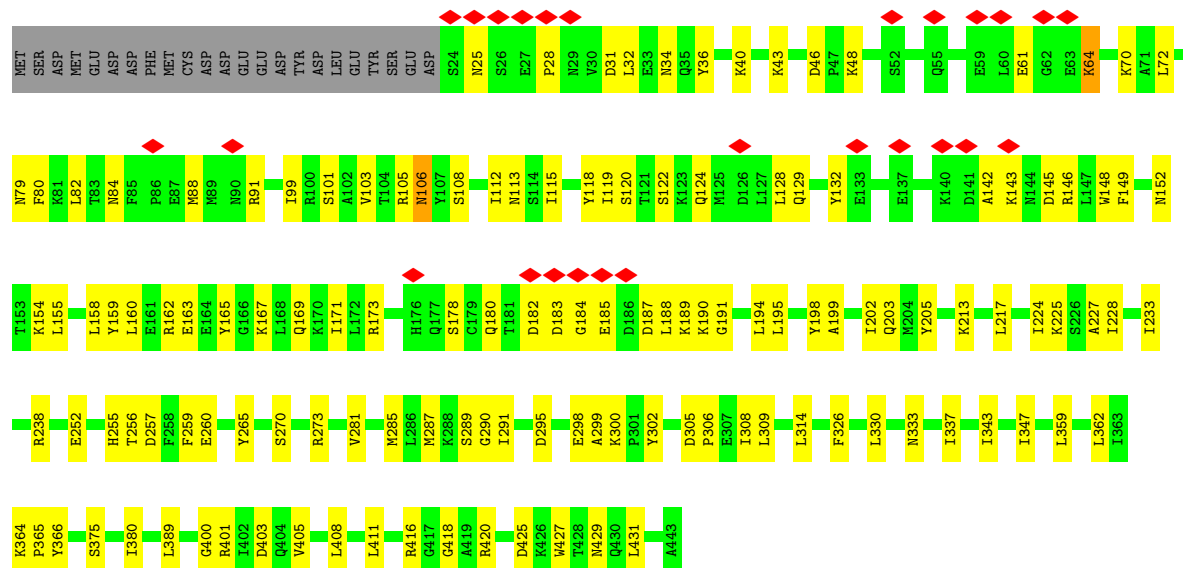


• Molecule 2: COP9 signalosome complex subunit 1

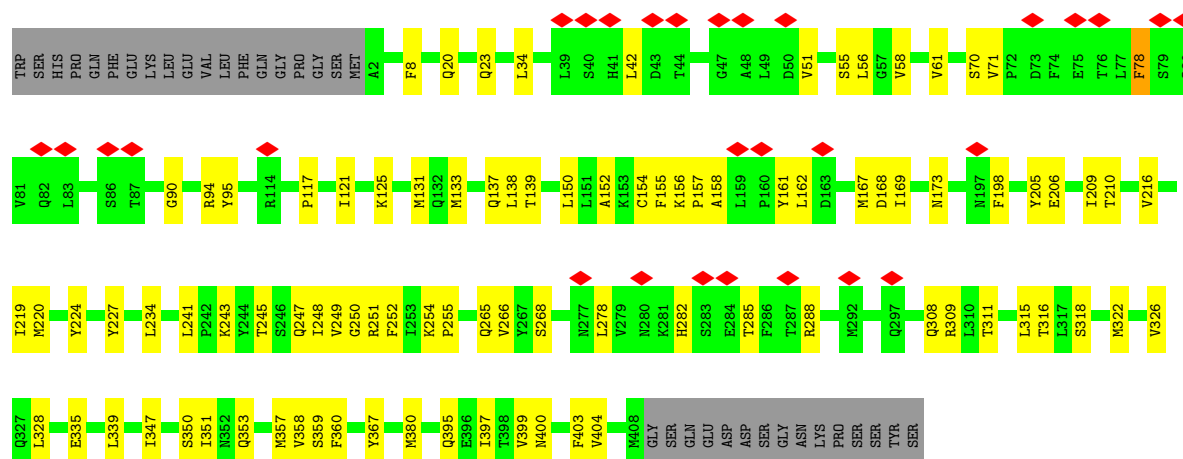




• Molecule 3: COP9 signalosome complex subunit 2

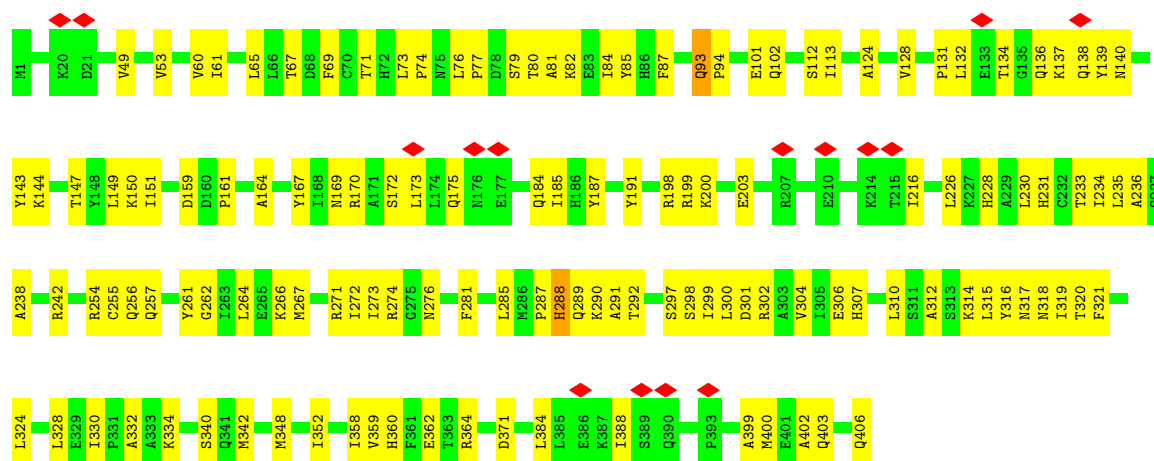


• Molecule 4: COP9 signalosome complex subunit 3

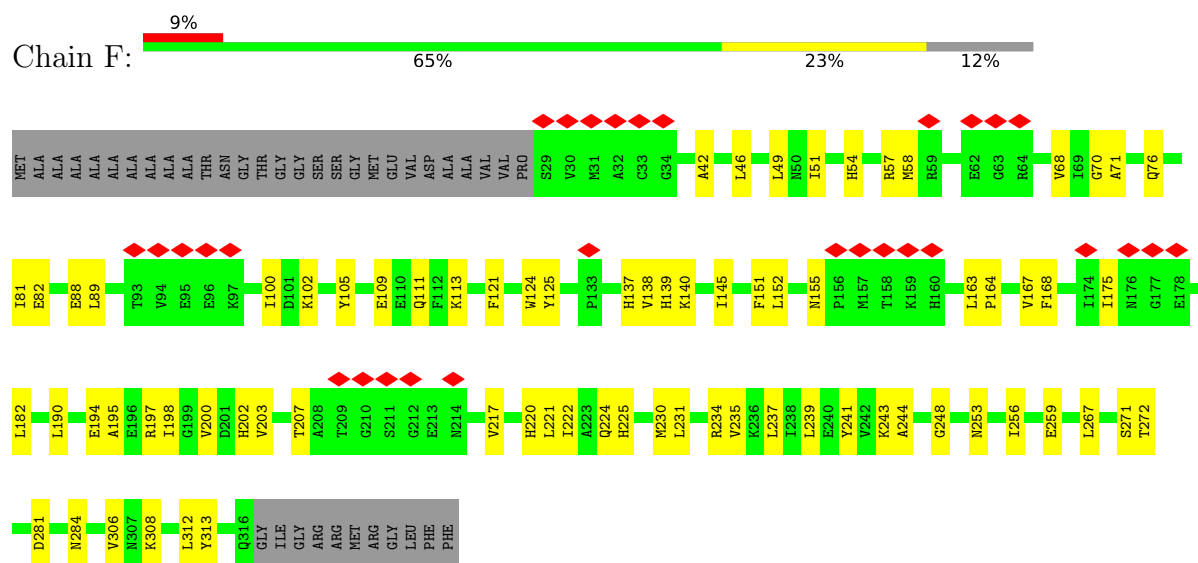


• Molecule 5: COP9 signalosome complex subunit 4

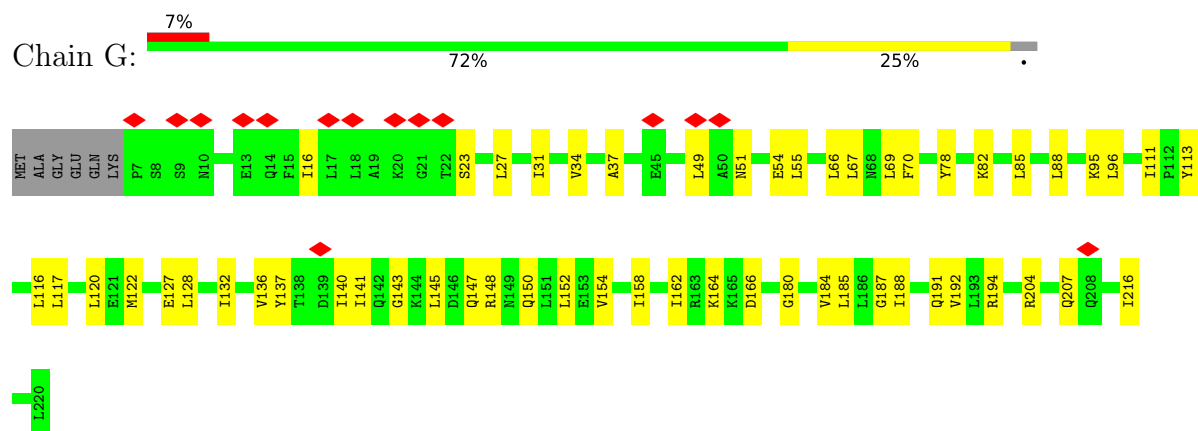




• Molecule 6: COP9 signalosome complex subunit 6

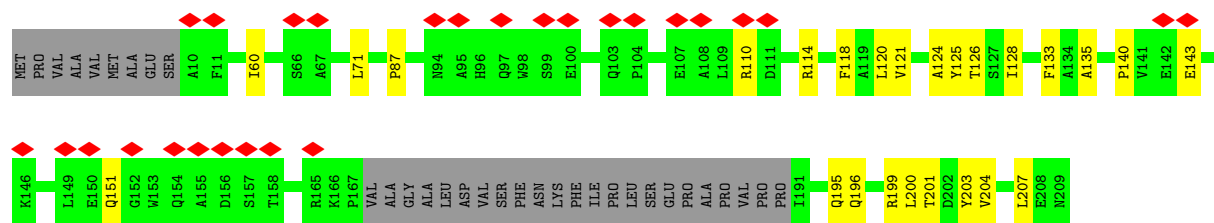


• Molecule 7: COP9 signalosome complex subunit 7b

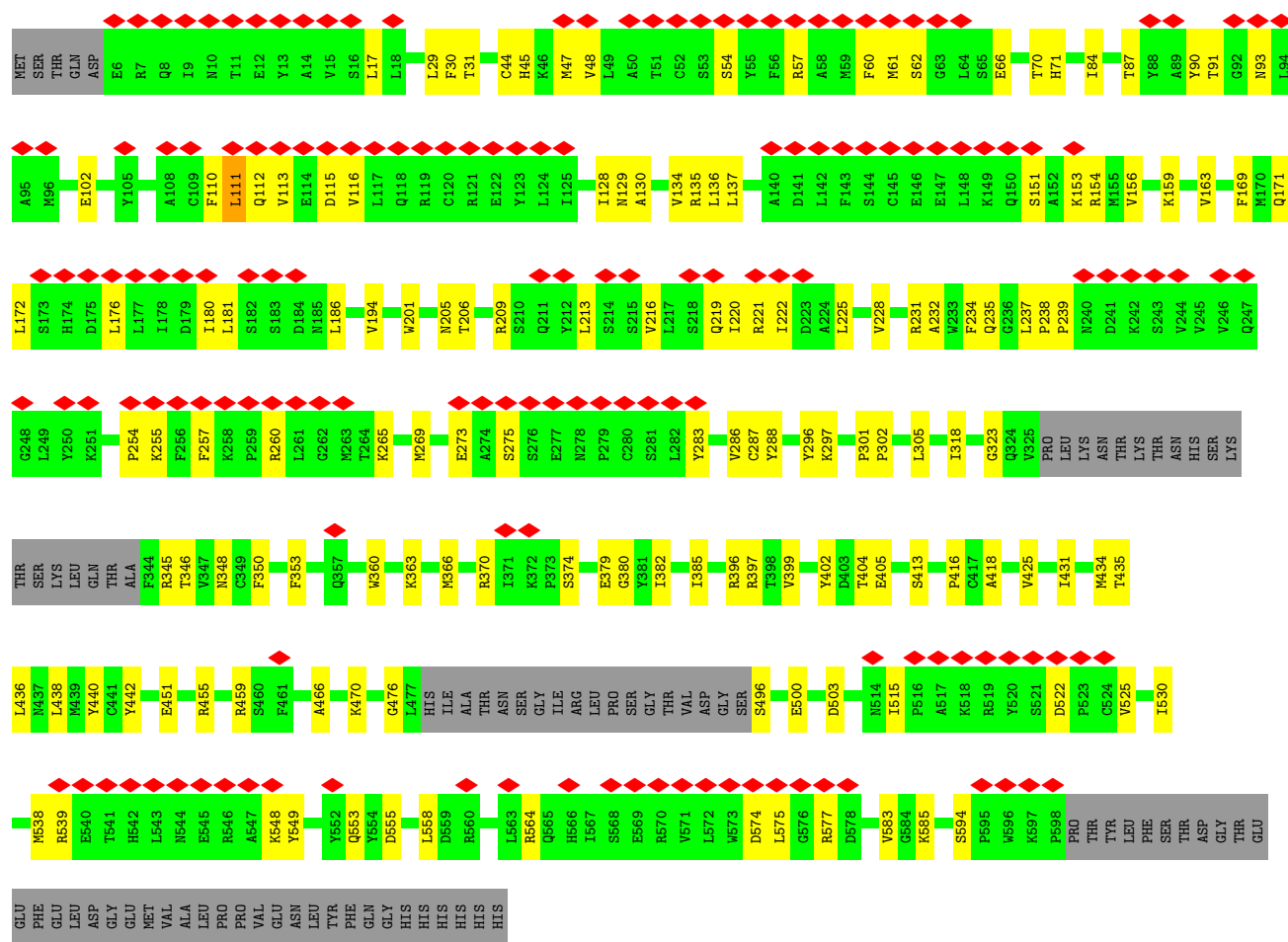


• Molecule 8: COP9 signalosome complex subunit 8

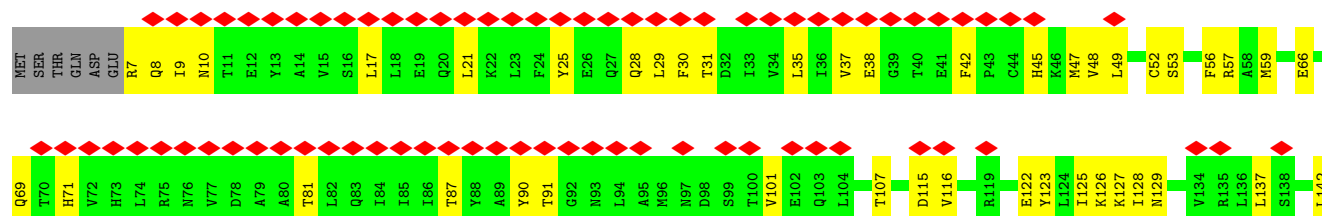
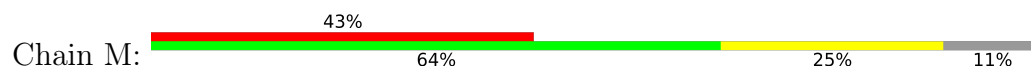


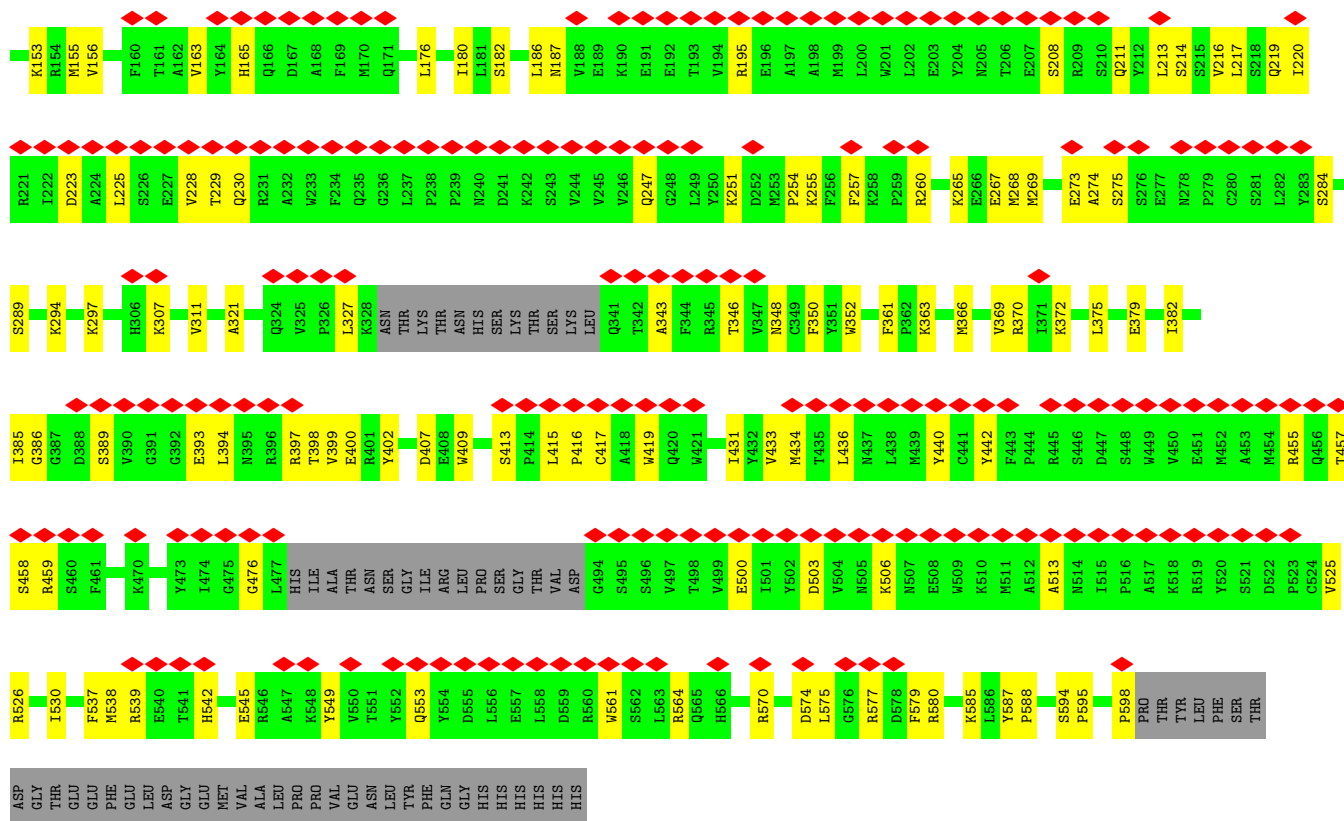


• Molecule 9: Kelch repeat and BTB domain-containing protein 2

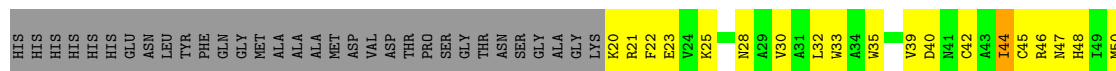


• Molecule 9: Kelch repeat and BTB domain-containing protein 2

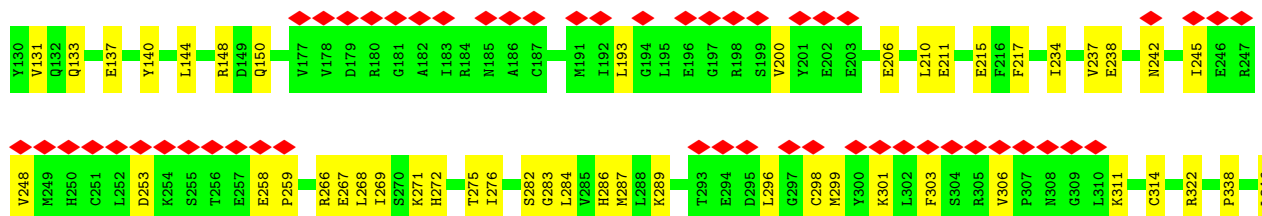
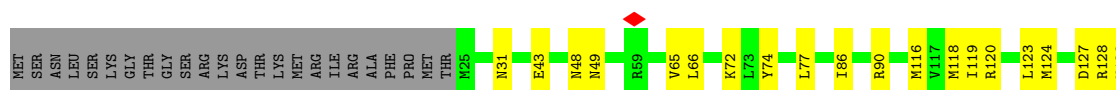


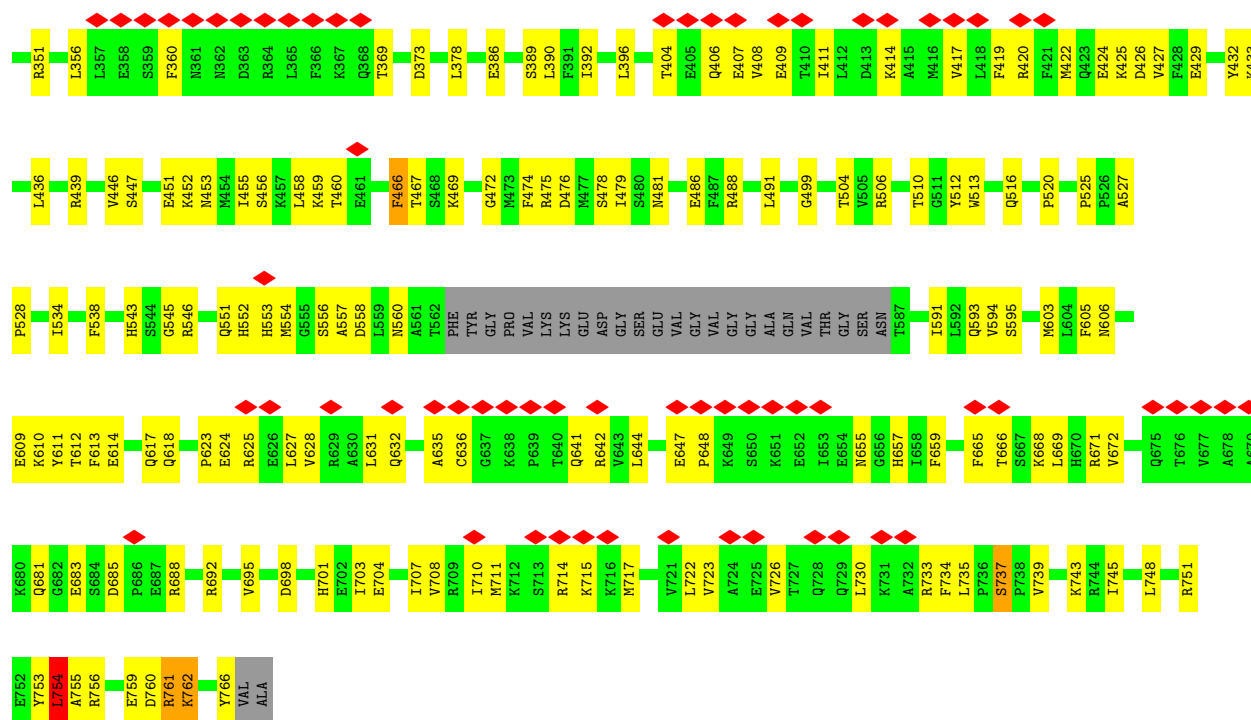


• Molecule 10: E3 ubiquitin-protein ligase RBX1



• Molecule 11: Cullin-3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	202164	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.579	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.001	Depositor
Map size (Å)	451.00803, 451.00803, 451.00803	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.088, 2.088, 2.088	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	E	0.66	1/2511 (0.0%)	0.91	8/3392 (0.2%)
2	A	0.19	0/3352	0.40	0/4520
3	B	0.20	0/3489	0.47	0/4696
4	C	0.18	0/3294	0.37	0/4448
5	D	0.13	0/3303	0.40	0/4460
6	F	0.32	0/2326	0.49	0/3153
7	G	0.10	0/1713	0.29	0/2318
8	H	0.10	0/1445	0.31	0/1965
9	I	0.17	0/4613	0.37	1/6256 (0.0%)
9	M	0.11	0/4666	0.31	0/6327
10	R	0.29	0/759	0.57	0/1029
11	L	0.29	0/5946	0.44	1/7989 (0.0%)
All	All	0.26	1/37417 (0.0%)	0.45	10/50553 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	212	GLU	C-O	5.70	1.30	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	247	VAL	N-CA-C	-10.47	100.37	110.42
1	E	218	CYS	N-CA-C	-6.24	104.37	112.23
1	E	220	GLN	CA-C-O	-5.57	114.97	120.70
1	E	249	THR	N-CA-C	-5.54	106.22	112.87
1	E	251	SER	N-CA-C	-5.47	103.46	111.17
1	E	220	GLN	N-CA-C	5.40	116.98	111.14
9	I	113	VAL	CA-C-O	-5.34	117.98	122.63
1	E	245	TYR	N-CA-C	-5.30	106.65	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	210	LYS	CA-C-O	-5.19	115.37	120.82
11	L	737	SER	O-C-N	-5.18	119.14	121.53

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	E	2457	0	2428	73	0
2	A	3296	0	3336	79	0
3	B	3430	0	3459	99	0
4	C	3235	0	3257	67	0
5	D	3251	0	3253	102	0
6	F	2279	0	2263	67	0
7	G	1692	0	1730	44	0
8	H	1411	0	1395	23	0
9	I	4507	0	4408	100	0
9	M	4559	0	4472	106	0
10	R	737	0	688	40	0
11	L	5853	0	5890	173	0
12	E	1	0	0	0	0
12	R	3	0	0	0	0
All	All	36711	0	36579	851	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 12.

All (851) 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:E:241:LEU:HD13	6:F:200:VAL:HB	1.37	1.04
1:E:128:GLY:O	6:F:57:ARG:HD2	1.60	1.02
11:L:711:MET:SD	11:L:722:LEU:HB3	1.99	1.02
3:B:260:GLU:HB2	10:R:98:ASN:HD22	1.26	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:717:MET:HG2	11:L:717:MET:O	1.62	0.97
11:L:717:MET:O	11:L:717:MET:CG	2.15	0.95
11:L:751:ARG:HB3	11:L:753:TYR:CE1	2.01	0.93
1:E:96:PHE:CD2	1:E:120:TYR:CE2	2.57	0.92
1:E:273:LEU:HD12	3:B:431:LEU:HD13	1.58	0.84
10:R:94:CYS:HB2	10:R:101:TRP:HB2	1.61	0.83
6:F:200:VAL:O	6:F:203:VAL:HG12	1.80	0.82
1:E:63:LEU:HD13	6:F:49:LEU:HD22	1.60	0.81
6:F:194:GLU:O	6:F:198:ILE:HD12	1.82	0.80
11:L:745:ILE:O	11:L:748:LEU:CD1	2.30	0.79
2:A:127:ASN:HD21	2:A:130:MET:HB2	1.49	0.77
3:B:145:ASP:HA	3:B:148:TRP:HB3	1.67	0.76
11:L:269:ILE:HD11	11:L:303:PHE:HA	1.67	0.76
11:L:735:LEU:HD12	11:L:737:SER:H	1.50	0.75
11:L:735:LEU:HD12	11:L:737:SER:N	2.02	0.75
1:E:240:LEU:HD21	6:F:163:LEU:HD13	1.68	0.74
9:I:30:PHE:HZ	9:M:57:ARG:HA	1.51	0.74
2:A:386:ASP:HA	2:A:389:LEU:HD23	1.68	0.73
11:L:237:VAL:HG23	11:L:268:LEU:HD13	1.71	0.73
11:L:129:VAL:O	11:L:133:GLN:NE2	2.22	0.73
9:I:205:ASN:HB3	9:I:209:ARG:HG3	1.70	0.71
7:G:162:ILE:HG22	7:G:164:LYS:H	1.56	0.71
2:A:418:VAL:HG13	3:B:401:ARG:HB2	1.73	0.71
4:C:339:LEU:HD11	8:H:120:LEU:HB3	1.73	0.71
11:L:433:LYS:HA	11:L:436:LEU:HD12	1.73	0.71
2:A:468:ARG:HH12	6:F:281:ASP:HB3	1.54	0.71
9:I:348:ASN:ND2	9:I:366:MET:O	2.24	0.70
11:L:556:SER:HA	11:L:595:SER:HA	1.73	0.70
11:L:624:GLU:HG3	11:L:625:ARG:H	1.56	0.70
1:E:63:LEU:HD13	6:F:49:LEU:CD2	2.21	0.70
8:H:110:ARG:HE	8:H:114:ARG:HH12	1.37	0.70
4:C:154:CYS:SG	4:C:156:LYS:NZ	2.61	0.70
11:L:745:ILE:O	11:L:748:LEU:HD11	1.91	0.70
11:L:681:GLN:NE2	11:L:683:GLU:OE2	2.25	0.69
1:E:63:LEU:HD23	1:E:64:LYS:N	2.06	0.69
11:L:751:ARG:HB3	11:L:753:TYR:HE1	1.56	0.69
5:D:199:ARG:O	5:D:199:ARG:NH1	2.26	0.69
1:E:128:GLY:O	6:F:57:ARG:CD	2.40	0.69
9:I:434:MET:HE2	9:I:455:ARG:HE	1.58	0.69
3:B:403:ASP:HB3	3:B:408:LEU:HB3	1.75	0.69
5:D:271:ARG:HG3	7:G:137:TYR:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:217:HIS:HA	1:E:220:GLN:HB3	1.75	0.68
2:A:394:LEU:HG	2:A:398:VAL:HB	1.76	0.68
2:A:490:MET:HB3	4:C:167:MET:HG2	1.75	0.68
9:M:187:ASN:ND2	9:M:587:TYR:OH	2.27	0.68
3:B:160:LEU:HD21	3:B:203:GLN:HB2	1.74	0.67
4:C:397:ILE:HG23	6:F:312:LEU:HD12	1.75	0.67
11:L:451:GLU:HB3	11:L:474:PHE:CZ	2.29	0.67
2:A:468:ARG:HH22	6:F:281:ASP:HA	1.58	0.67
3:B:187:ASP:HB3	3:B:190:LYS:HB2	1.76	0.67
4:C:137:GLN:HG2	4:C:168:ASP:HB3	1.76	0.66
2:A:78:GLU:HG3	2:A:108:PRO:HG2	1.78	0.66
2:A:489:MET:HE2	6:F:306:VAL:HG22	1.77	0.66
2:A:494:ALA:O	2:A:498:ASN:ND2	2.29	0.66
2:A:500:ILE:HG13	4:C:169:ILE:HG21	1.78	0.66
4:C:380:MET:HG3	8:H:203:TYR:HE1	1.59	0.65
2:A:258:VAL:HG11	2:A:289:ALA:HB2	1.77	0.65
9:M:297:LYS:HZ1	9:M:595:PRO:HD3	1.60	0.65
11:L:593:GLN:HB2	11:L:671:ARG:HH12	1.61	0.65
5:D:76:LEU:HD22	5:D:81:ALA:HB2	1.78	0.65
9:I:128:ILE:HG12	9:I:136:LEU:HD21	1.79	0.65
9:I:436:LEU:O	9:I:455:ARG:NH2	2.30	0.65
2:A:79:ASN:HD22	2:A:386:ASP:HB2	1.61	0.64
10:R:67:GLU:OE2	11:L:753:TYR:CD1	2.50	0.64
11:L:488:ARG:HD2	11:L:491:LEU:HD21	1.79	0.64
11:L:753:TYR:HD1	11:L:754:LEU:N	1.95	0.64
11:L:632:GLN:HB2	11:L:636:CYS:HB3	1.79	0.64
11:L:704:GLU:HA	11:L:707:ILE:HG22	1.78	0.64
3:B:113:ASN:OD1	3:B:154:LYS:NZ	2.31	0.64
3:B:291:ILE:HG12	10:R:44:ILE:HA	1.80	0.64
9:M:217:LEU:HD13	9:M:225:LEU:HD11	1.77	0.64
2:A:139:SER:HA	2:A:160:PRO:HD2	1.80	0.64
2:A:352:PHE:HA	2:A:355:PHE:HB2	1.78	0.64
5:D:317:ASN:N	7:G:145:LEU:O	2.31	0.63
9:I:151:SER:HA	9:I:154:ARG:HE	1.64	0.63
1:E:308:CYS:O	1:E:312:ILE:HD12	1.99	0.63
2:A:123:GLN:HB3	2:A:131:TYR:HE2	1.64	0.63
5:D:328:LEU:HB2	5:D:330:ILE:HG12	1.81	0.63
5:D:384:LEU:HD21	6:F:259:GLU:HB3	1.79	0.63
1:E:96:PHE:CE2	1:E:120:TYR:CE2	2.87	0.63
3:B:105:ARG:NH2	11:L:396:LEU:O	2.31	0.62
5:D:352:ILE:HG12	5:D:359:VAL:HG13	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:445:LEU:HD22	4:C:309:ARG:HH21	1.65	0.62
1:E:319:MET:HG2	8:H:200:LEU:HD13	1.82	0.62
1:E:270:SER:HA	3:B:431:LEU:HD11	1.81	0.62
5:D:93:GLN:HG3	5:D:94:PRO:HD3	1.81	0.62
5:D:315:LEU:HD21	7:G:136:VAL:HG11	1.80	0.62
9:I:273:GLU:HA	9:I:283:TYR:HB3	1.81	0.62
11:L:446:VAL:HG23	11:L:447:SER:H	1.64	0.62
1:E:120:TYR:HA	6:F:111:GLN:HE22	1.64	0.62
5:D:320:THR:HG22	5:D:358:ILE:HG12	1.82	0.62
9:M:254:PRO:O	9:M:255:LYS:HG2	1.99	0.62
5:D:288:HIS:ND1	5:D:289:GLN:OE1	2.33	0.62
9:I:305:LEU:HD21	9:I:323:GLY:HA3	1.82	0.61
9:M:126:LYS:NZ	9:M:407:ASP:OD2	2.33	0.61
1:E:331:ILE:HD11	7:G:180:GLY:HA3	1.82	0.61
3:B:290:GLY:O	10:R:46:ARG:NH1	2.28	0.61
5:D:358:ILE:HG21	7:G:148:ARG:HB2	1.81	0.61
11:L:715:LYS:H	11:L:722:LEU:HD11	1.66	0.61
9:I:525:VAL:HA	9:I:538:MET:HG2	1.83	0.61
2:A:307:LEU:HD13	2:A:345:ASN:HB3	1.83	0.61
9:M:393:GLU:HG3	9:M:394:LEU:H	1.65	0.61
11:L:717:MET:HB2	11:L:722:LEU:HB2	1.81	0.61
4:C:397:ILE:HG21	6:F:308:LYS:HB3	1.81	0.61
5:D:132:LEU:HD22	5:D:144:LYS:HG2	1.82	0.61
9:M:350:PHE:HD2	9:M:363:LYS:HB2	1.66	0.61
11:L:525:PRO:HB2	11:L:528:PRO:HD2	1.83	0.60
11:L:753:TYR:HD1	11:L:754:LEU:H	1.49	0.60
5:D:384:LEU:O	5:D:388:ILE:HG13	2.02	0.60
7:G:16:ILE:HG12	7:G:49:LEU:HD11	1.83	0.60
11:L:90:ARG:NH2	11:L:150:GLN:OE1	2.35	0.60
9:M:127:LYS:O	9:M:129:ASN:ND2	2.35	0.60
9:M:225:LEU:O	9:M:230:GLN:NE2	2.35	0.60
9:M:397:ARG:HD3	9:M:415:LEU:HB3	1.83	0.60
5:D:235:LEU:HD22	5:D:299:ILE:HG23	1.83	0.60
1:E:315:ILE:HD13	8:H:203:TYR:HB3	1.83	0.60
4:C:350:SER:O	4:C:359:SER:N	2.33	0.60
7:G:117:LEU:HA	7:G:122:MET:HB3	1.84	0.60
9:I:47:MET:HE1	9:M:90:TYR:HE1	1.66	0.60
9:M:214:SER:O	9:M:251:LYS:NZ	2.35	0.59
3:B:195:LEU:HB3	3:B:225:LYS:HG3	1.83	0.59
5:D:82:LYS:HE3	5:D:113:ILE:HD13	1.83	0.59
6:F:220:HIS:O	6:F:224:GLN:NE2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:352:ILE:HG23	5:D:359:VAL:HG22	1.82	0.59
1:E:78:MET:HE1	1:E:110:GLN:HB3	1.84	0.59
9:I:62:SER:OG	9:I:66:GLU:OE2	2.20	0.59
9:I:431:ILE:HB	9:I:442:TYR:HB3	1.83	0.59
11:L:520:PRO:HG2	11:L:552:HIS:HB2	1.84	0.59
1:E:96:PHE:CD2	1:E:120:TYR:HE2	2.17	0.59
1:E:248:ASN:C	1:E:250:LEU:H	2.10	0.59
8:H:140:PRO:HG2	8:H:143:GLU:OE2	2.03	0.59
9:I:201:TRP:O	9:I:209:ARG:NH2	2.36	0.59
4:C:125:LYS:NZ	4:C:157:PRO:O	2.36	0.59
9:M:455:ARG:NH1	9:M:500:GLU:OE2	2.36	0.59
11:L:745:ILE:O	11:L:748:LEU:HG	2.01	0.59
2:A:484:ARG:NH1	4:C:206:GLU:OE1	2.35	0.58
3:B:314:LEU:HD11	3:B:337:ILE:HD12	1.83	0.58
2:A:386:ASP:OD1	2:A:387:ASN:N	2.37	0.58
9:M:269:MET:HE3	9:M:530:ILE:HD12	1.85	0.58
9:M:539:ARG:HH22	9:M:577:ARG:HD3	1.66	0.58
10:R:45:CYS:SG	10:R:47:ASN:ND2	2.76	0.58
6:F:163:LEU:HD12	6:F:164:PRO:HD2	1.86	0.58
1:E:321:GLN:NE2	1:E:325:ASP:OD2	2.36	0.58
3:B:36:TYR:CZ	3:B:40:LYS:HD2	2.39	0.58
3:B:163:GLU:OE1	3:B:165:TYR:OH	2.20	0.58
9:M:37:VAL:HG12	9:M:38:GLU:HG2	1.85	0.58
9:M:370:ARG:NH1	9:M:386:GLY:O	2.36	0.58
9:M:434:MET:HE2	9:M:455:ARG:HE	1.68	0.58
2:A:245:SER:HB2	2:A:254:VAL:HG23	1.86	0.58
9:I:181:LEU:HD21	9:I:220:ILE:HG23	1.85	0.58
11:L:525:PRO:HB3	11:L:603:MET:HG3	1.86	0.58
1:E:198:GLU:OE1	1:E:200:PRO:HD3	2.03	0.58
7:G:78:TYR:OH	7:G:82:LYS:NZ	2.37	0.58
2:A:162:LEU:HD12	2:A:166:TRP:HE1	1.69	0.58
2:A:417:TYR:HB3	2:A:420:ALA:HB2	1.86	0.58
2:A:418:VAL:HG23	2:A:419:SER:H	1.68	0.58
9:I:555:ASP:HB3	9:I:558:LEU:HB2	1.84	0.58
3:B:375:SER:OG	3:B:380:ILE:O	2.22	0.57
9:M:28:GLN:NE2	9:M:31:THR:OG1	2.33	0.57
6:F:194:GLU:CD	6:F:195:ALA:N	2.62	0.57
10:R:21:ARG:NH1	11:L:609:GLU:OE2	2.37	0.57
11:L:708:VAL:HA	11:L:762:LYS:HD3	1.85	0.57
5:D:233:THR:O	5:D:242:ARG:NE	2.35	0.57
1:E:244:LYS:HA	1:E:247:VAL:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:234:ILE:O	5:D:242:ARG:NH2	2.36	0.57
9:M:459:ARG:HB3	9:M:476:GLY:HA3	1.86	0.57
5:D:84:ILE:HA	5:D:87:PHE:HB3	1.87	0.57
5:D:342:MET:HE2	5:D:348:MET:HB2	1.85	0.57
5:D:254:ARG:HA	5:D:257:GLN:HG2	1.86	0.57
9:M:153:LYS:HE2	9:M:180:ILE:HA	1.86	0.57
1:E:318:LEU:HD11	8:H:200:LEU:HD22	1.86	0.57
5:D:169:ASN:ND2	10:R:40:ASP:HA	2.20	0.57
5:D:256:GLN:HA	5:D:261:TYR:CG	2.40	0.57
9:M:436:LEU:O	9:M:455:ARG:NH2	2.37	0.57
1:E:147:LEU:H	1:E:221:TYR:HE2	1.53	0.57
1:E:305:ARG:O	1:E:309:LYS:HG2	2.04	0.57
2:A:291:LEU:HD13	2:A:320:LEU:HD22	1.87	0.57
3:B:191:GLY:HA2	3:B:194:LEU:HD12	1.87	0.56
4:C:198:PHE:HB2	4:C:234:LEU:HD13	1.86	0.56
5:D:318:ASN:OD1	7:G:147:GLN:N	2.38	0.56
7:G:66:LEU:HD11	7:G:88:LEU:HD21	1.87	0.56
10:R:63:ALA:HB1	10:R:66:GLU:HA	1.87	0.56
9:M:553:GLN:HB2	9:M:564:ARG:HB2	1.87	0.56
5:D:169:ASN:HD21	10:R:40:ASP:HA	1.68	0.56
9:I:459:ARG:HB3	9:I:476:GLY:HA3	1.87	0.56
3:B:146:ARG:HH21	11:L:452:LYS:HB2	1.71	0.56
6:F:100:ILE:HD11	6:F:138:VAL:HG13	1.86	0.56
9:I:382:ILE:HB	9:I:402:TYR:HB3	1.87	0.56
9:I:302:PRO:HG2	9:I:305:LEU:HB3	1.86	0.56
1:E:63:LEU:HD23	1:E:63:LEU:C	2.30	0.56
2:A:218:LEU:O	2:A:222:SER:N	2.35	0.56
4:C:318:SER:HA	4:C:357:MET:HA	1.88	0.56
5:D:400:MET:SD	5:D:403:GLN:NE2	2.79	0.56
11:L:43:GLU:OE2	11:L:48:ASN:ND2	2.32	0.56
4:C:8:PHE:HB2	4:C:34:LEU:HD11	1.87	0.56
9:M:35:LEU:HB2	9:M:42:PHE:HB2	1.88	0.56
9:M:115:ASP:OD1	9:M:116:VAL:N	2.39	0.56
3:B:122:SER:OG	3:B:124:GLN:OE1	2.22	0.56
3:B:158:LEU:HD11	3:B:162:ARG:HH21	1.71	0.56
11:L:120:ARG:O	11:L:124:MET:N	2.36	0.56
11:L:287:MET:HE3	11:L:296:LEU:HD22	1.87	0.56
11:L:356:LEU:HD12	11:L:360:PHE:HB2	1.87	0.56
11:L:458:LEU:HB3	11:L:467:THR:HG22	1.87	0.56
9:I:129:ASN:OD1	9:I:130:ALA:N	2.38	0.55
1:E:259:ALA:HB1	3:B:420:ARG:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:179:GLU:O	9:M:7:ARG:NH1	2.38	0.55
3:B:425:ASP:OD1	3:B:429:ASN:ND2	2.39	0.55
6:F:137:HIS:HA	6:F:140:LYS:HE3	1.87	0.55
9:I:29:LEU:HB3	9:I:30:PHE:HD1	1.72	0.55
11:L:49:ASN:HD22	11:L:118:MET:HE1	1.71	0.55
1:E:327:LEU:HD12	7:G:184:VAL:HG21	1.89	0.55
11:L:707:ILE:HD13	11:L:726:VAL:HG11	1.87	0.55
1:E:237:LEU:HB3	6:F:200:VAL:HG13	1.88	0.55
5:D:185:ILE:HG13	5:D:216:ILE:HD11	1.89	0.55
9:I:57:ARG:HA	9:M:30:PHE:HZ	1.72	0.55
9:M:223:ASP:HB3	9:M:257:PHE:CE1	2.41	0.55
11:L:298:CYS:HA	11:L:301:LYS:HE3	1.88	0.55
11:L:417:VAL:HG13	11:L:420:ARG:HH21	1.72	0.55
10:R:28:ASN:ND2	11:L:556:SER:OG	2.39	0.55
4:C:250:GLY:O	4:C:254:LYS:NZ	2.37	0.55
2:A:213:ASP:HB3	2:A:216:ASN:HB2	1.88	0.55
9:M:213:LEU:HA	9:M:216:VAL:HG12	1.89	0.55
11:L:745:ILE:O	11:L:748:LEU:CG	2.54	0.55
2:A:374:TYR:HA	2:A:377:CYS:HB3	1.89	0.55
4:C:326:VAL:HG23	4:C:328:LEU:HG	1.89	0.55
9:I:366:MET:HE1	9:I:370:ARG:HE	1.72	0.55
11:L:644:LEU:HD11	11:L:659:PHE:HB3	1.89	0.55
11:L:282:SER:H	11:L:286:HIS:CD2	2.24	0.54
1:E:248:ASN:C	1:E:250:LEU:N	2.63	0.54
9:I:186:LEU:HD13	9:I:194:VAL:HG11	1.88	0.54
3:B:155:LEU:HD23	3:B:171:ILE:HD11	1.89	0.54
9:I:254:PRO:O	9:I:255:LYS:HG2	2.08	0.54
9:M:9:ILE:HG13	9:M:10:ASN:H	1.71	0.54
3:B:146:ARG:HH22	11:L:453:ASN:N	2.05	0.54
5:D:161:PRO:HG2	5:D:198:ARG:CZ	2.38	0.54
5:D:170:ARG:HA	5:D:173:LEU:HG	1.88	0.54
1:E:270:SER:HB2	3:B:427:TRP:HD1	1.73	0.54
2:A:112:VAL:HG21	2:A:145:LEU:HD11	1.88	0.54
2:A:206:ASP:OD1	2:A:221:TYR:OH	2.26	0.54
2:A:209:LEU:HD11	2:A:244:VAL:HG22	1.90	0.54
3:B:112:ILE:HA	3:B:115:ILE:HB	1.90	0.54
5:D:301:ASP:HA	5:D:304:VAL:HB	1.89	0.54
5:D:319:ILE:HG12	5:D:324:LEU:HB2	1.89	0.54
11:L:472:GLY:HA2	11:L:475:ARG:HE	1.72	0.54
11:L:753:TYR:CD1	11:L:754:LEU:N	2.76	0.54
1:E:252:SER:O	1:E:253:SER:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:228:ILE:HB	11:L:455:ILE:HD12	1.88	0.54
4:C:56:LEU:HD21	4:C:90:GLY:HA2	1.89	0.54
3:B:305:ASP:OD1	3:B:306:PRO:HD2	2.08	0.54
9:I:553:GLN:HB2	9:I:564:ARG:HB2	1.90	0.54
3:B:146:ARG:HH22	11:L:453:ASN:HB2	1.72	0.54
3:B:146:ARG:HA	3:B:149:PHE:CE2	2.43	0.54
5:D:388:ILE:HG12	6:F:256:ILE:HG21	1.89	0.53
9:I:374:SER:OG	9:I:385:ILE:O	2.25	0.53
9:I:60:PHE:HB2	9:M:30:PHE:CE2	2.43	0.53
9:I:91:THR:HG23	9:I:93:ASN:H	1.74	0.53
1:E:40:LEU:HD23	1:E:45:TRP:HH2	1.73	0.53
3:B:169:GLN:NE2	9:I:451:GLU:O	2.42	0.53
6:F:312:LEU:HD23	6:F:313:TYR:CD1	2.43	0.53
11:L:641:GLN:OE1	11:L:666:THR:OG1	2.26	0.53
1:E:245:TYR:OH	6:F:190:LEU:HG	2.07	0.53
5:D:93:GLN:H	5:D:94:PRO:CD	2.21	0.53
9:M:195:ARG:HD3	9:M:229:THR:HG21	1.90	0.53
9:M:208:SER:O	9:M:211:GLN:NE2	2.41	0.53
4:C:55:SER:HA	4:C:58:VAL:HB	1.89	0.53
6:F:109:GLU:HG2	6:F:113:LYS:HZ1	1.72	0.53
1:E:325:ASP:OD1	1:E:326:LYS:N	2.42	0.53
9:I:54:SER:HB3	9:I:112:GLN:HB2	1.90	0.53
4:C:209:ILE:HA	4:C:220:MET:HE1	1.90	0.53
9:M:52:CYS:SG	9:M:53:SER:N	2.81	0.53
11:L:476:ASP:OD2	11:L:513:TRP:NE1	2.40	0.53
3:B:183:ASP:OD1	3:B:184:GLY:N	2.42	0.53
7:G:136:VAL:HG22	7:G:141:ILE:HG13	1.90	0.53
9:M:228:VAL:O	9:M:229:THR:OG1	2.24	0.53
3:B:255:HIS:O	3:B:259:PHE:HB2	2.09	0.53
5:D:69:PHE:O	5:D:73:LEU:HD23	2.09	0.53
5:D:161:PRO:HG2	5:D:198:ARG:NH2	2.24	0.53
5:D:267:MET:HE1	5:D:307:HIS:HB2	1.91	0.53
3:B:105:ARG:HG3	3:B:106:ASN:H	1.73	0.53
5:D:238:ALA:HB1	5:D:310:LEU:HD11	1.91	0.53
7:G:31:ILE:HD13	7:G:67:LEU:HD22	1.90	0.53
7:G:51:ASN:HA	7:G:54:GLU:HG2	1.90	0.53
9:I:45:HIS:ND1	9:I:90:TYR:OH	2.33	0.52
9:I:476:GLY:O	9:I:496:SER:N	2.42	0.52
10:R:77:HIS:HB2	10:R:101:TRP:HZ3	1.73	0.52
9:M:297:LYS:HB3	9:M:594:SER:HB2	1.90	0.52
5:D:271:ARG:O	5:D:307:HIS:NE2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:17:LEU:HD21	9:M:21:LEU:HD12	1.91	0.52
9:M:275:SER:OG	9:M:574:ASP:O	2.28	0.52
1:E:60:LEU:HA	6:F:49:LEU:HD21	1.90	0.52
7:G:143:GLY:HA3	7:G:154:VAL:HA	1.91	0.52
8:H:195:GLN:HB3	8:H:199:ARG:HH21	1.75	0.52
1:E:181:VAL:HG23	6:F:202:HIS:HB3	1.92	0.52
6:F:217:VAL:HB	8:H:204:VAL:HG11	1.92	0.52
9:I:269:MET:HE3	9:I:530:ILE:HG22	1.92	0.52
4:C:400:ASN:HD22	6:F:312:LEU:HG	1.75	0.52
4:C:95:TYR:O	4:C:173:ASN:ND2	2.35	0.52
4:C:248:ILE:HG22	4:C:251:ARG:HD2	1.92	0.52
4:C:380:MET:HG3	8:H:203:TYR:CE1	2.42	0.52
5:D:362:GLU:HB3	5:D:364:ARG:NH1	2.25	0.52
11:L:120:ARG:HG3	11:L:140:TYR:HB2	1.92	0.52
11:L:269:ILE:HD13	11:L:306:VAL:HB	1.91	0.52
6:F:71:ALA:HB1	6:F:121:PHE:HE1	1.75	0.52
11:L:124:MET:HA	11:L:127:ASP:HB2	1.92	0.52
1:E:114:TYR:HA	1:E:117:MET:HE3	1.92	0.52
3:B:40:LYS:O	3:B:43:LYS:HG2	2.10	0.52
6:F:225:HIS:HB2	7:G:188:ILE:HG21	1.91	0.52
6:F:239:LEU:HG	6:F:243:LYS:HE2	1.92	0.51
7:G:188:ILE:O	7:G:192:VAL:HG23	2.10	0.51
9:I:228:VAL:HA	9:I:231:ARG:HD3	1.92	0.51
5:D:138:GLN:NE2	5:D:139:TYR:O	2.43	0.51
11:L:127:ASP:O	11:L:131:VAL:HG22	2.09	0.51
11:L:451:GLU:HB3	11:L:474:PHE:HZ	1.75	0.51
9:M:273:GLU:OE2	9:M:307:LYS:N	2.44	0.51
11:L:605:PHE:HZ	11:L:659:PHE:HD2	1.56	0.51
11:L:635:ALA:O	11:L:642:ARG:NH1	2.44	0.51
3:B:194:LEU:HD13	3:B:224:ILE:HG23	1.92	0.51
3:B:259:PHE:CZ	10:R:95:PRO:HA	2.45	0.51
3:B:298:GLU:HA	3:B:302:TYR:HB2	1.93	0.51
5:D:79:SER:O	5:D:81:ALA:N	2.44	0.51
6:F:231:LEU:O	6:F:235:VAL:HG23	2.10	0.51
3:B:99:ILE:HG12	3:B:108:SER:HB2	1.91	0.51
6:F:151:PHE:HD2	6:F:168:PHE:HB2	1.74	0.51
7:G:111:ILE:O	7:G:152:LEU:N	2.43	0.51
9:I:455:ARG:HD2	9:I:500:GLU:OE1	2.10	0.51
11:L:148:ARG:HH11	11:L:200:VAL:HG21	1.75	0.51
3:B:287:MET:HE2	3:B:289:SER:HB2	1.92	0.51
3:B:291:ILE:HD13	10:R:95:PRO:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:102:LYS:HA	6:F:105:TYR:HB3	1.91	0.51
9:I:366:MET:HE1	9:I:370:ARG:NE	2.26	0.51
9:M:389:SER:OG	9:M:398:THR:OG1	2.20	0.51
9:M:570:ARG:HA	9:M:598:PRO:HB3	1.91	0.51
11:L:217:PHE:HB3	11:L:267:GLU:OE2	2.11	0.51
4:C:351:ILE:HG23	4:C:358:VAL:HG22	1.91	0.51
9:I:287:CYS:N	9:I:296:TYR:O	2.37	0.51
3:B:132:TYR:CD2	3:B:155:LEU:HD13	2.45	0.51
5:D:236:ALA:HB3	5:D:242:ARG:HD2	1.93	0.51
7:G:122:MET:HG2	7:G:128:LEU:HB2	1.91	0.51
11:L:144:LEU:HD12	11:L:193:LEU:HA	1.92	0.51
11:L:429:GLU:HA	11:L:432:TYR:HB3	1.93	0.51
11:L:623:PRO:O	11:L:627:LEU:HD23	2.09	0.51
3:B:195:LEU:HD13	3:B:233:ILE:HG21	1.93	0.50
4:C:367:TYR:O	6:F:284:ASN:ND2	2.44	0.50
5:D:362:GLU:HB3	5:D:364:ARG:HH12	1.77	0.50
9:I:301:PRO:HG3	9:I:360:TRP:CE2	2.46	0.50
3:B:295:ASP:HB3	10:R:96:LEU:HD21	1.93	0.50
8:H:196:GLN:O	8:H:200:LEU:HG	2.12	0.50
10:R:87:TRP:NE1	10:R:95:PRO:HD3	2.27	0.50
9:M:348:ASN:ND2	9:M:366:MET:O	2.44	0.50
2:A:104:ALA:HB1	2:A:111:ARG:HG3	1.93	0.50
2:A:123:GLN:HG3	9:I:345:ARG:HB3	1.94	0.50
4:C:395:GLN:O	4:C:399:VAL:HG23	2.12	0.50
9:M:455:ARG:NH1	9:M:457:THR:O	2.45	0.50
11:L:429:GLU:HG2	11:L:466:PHE:HB3	1.93	0.50
4:C:209:ILE:HG12	4:C:220:MET:HE1	1.93	0.50
5:D:321:PHE:HB3	5:D:332:ALA:HB1	1.94	0.50
7:G:23:SER:HA	7:G:27:LEU:HB2	1.92	0.50
3:B:205:TYR:HD2	3:B:217:LEU:HD11	1.76	0.50
3:B:238:ARG:O	3:B:257:ASP:HB3	2.12	0.50
5:D:67:THR:OG1	5:D:102:GLN:NE2	2.34	0.50
9:I:232:ALA:O	9:I:235:GLN:NE2	2.45	0.50
9:M:163:VAL:HG12	9:M:165:HIS:H	1.77	0.50
11:L:520:PRO:HG3	11:L:553:HIS:CE1	2.47	0.50
11:L:711:MET:HB2	11:L:762:LYS:HD2	1.93	0.50
1:E:116:TYR:CD1	1:E:116:TYR:C	2.89	0.50
2:A:133:GLU:OE2	2:A:136:ARG:NH2	2.44	0.50
9:M:137:LEU:HD22	9:M:156:VAL:HG11	1.94	0.50
9:M:458:SER:O	9:M:459:ARG:NH1	2.41	0.50
4:C:243:LYS:HA	4:C:245:THR:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:264:LEU:HA	5:D:267:MET:HB3	1.94	0.50
11:L:386:GLU:OE2	11:L:692:ARG:NH2	2.45	0.50
9:I:30:PHE:CZ	9:M:57:ARG:HA	2.40	0.50
11:L:346:LEU:HD11	11:L:414:LYS:HB3	1.94	0.50
1:E:78:MET:HE2	1:E:98:LEU:HD12	1.92	0.49
1:E:315:ILE:O	1:E:318:LEU:HG	2.12	0.49
2:A:421:ASP:HB2	3:B:405:VAL:HG22	1.94	0.49
9:I:129:ASN:ND2	9:I:405:GLU:O	2.45	0.49
11:L:276:ILE:HG13	11:L:284:LEU:HB2	1.93	0.49
1:E:180:LYS:HG3	6:F:202:HIS:NE2	2.26	0.49
2:A:173:LYS:O	2:A:177:LYS:HG2	2.12	0.49
3:B:105:ARG:NE	11:L:446:VAL:O	2.45	0.49
5:D:147:THR:O	5:D:151:ILE:HG13	2.12	0.49
6:F:217:VAL:O	6:F:221:LEU:HG	2.12	0.49
10:R:72:TRP:HZ2	10:R:108:HIS:CE1	2.30	0.49
9:M:289:SER:HG	9:M:294:LYS:H	1.56	0.49
5:D:124:ALA:O	5:D:128:VAL:HG23	2.12	0.49
9:M:431:ILE:HB	9:M:442:TYR:HB3	1.93	0.49
9:I:172:LEU:HD22	9:I:176:LEU:HD23	1.93	0.49
4:C:266:VAL:HG21	4:C:278:LEU:HD22	1.95	0.49
5:D:262:GLY:O	5:D:266:LYS:HG2	2.11	0.49
7:G:113:TYR:HB2	7:G:150:GLN:HB3	1.95	0.49
9:M:419:TRP:HZ3	9:M:433:VAL:HG13	1.76	0.49
11:L:77:LEU:HD22	11:L:123:LEU:HD13	1.95	0.49
11:L:234:ILE:HD12	11:L:272:HIS:HE1	1.78	0.49
2:A:368:LYS:HG2	2:A:373:LYS:HE2	1.95	0.49
9:I:61:MET:HE3	9:M:29:LEU:HG	1.95	0.49
10:R:30:VAL:HG22	11:L:506:ARG:HB2	1.94	0.49
1:E:312:ILE:HD11	8:H:207:LEU:HB3	1.94	0.49
4:C:216:VAL:HG22	4:C:249:VAL:HA	1.94	0.49
5:D:132:LEU:HD11	5:D:147:THR:HB	1.95	0.49
9:I:297:LYS:HB3	9:I:594:SER:HB2	1.94	0.49
9:M:321:ALA:HB3	9:M:375:LEU:HD11	1.93	0.49
11:L:404:THR:OG1	11:L:407:GLU:OE1	2.29	0.49
1:E:146:TRP:CE3	1:E:214:PHE:HA	2.47	0.49
2:A:143:ARG:HB2	2:A:159:PRO:HG3	1.94	0.49
3:B:149:PHE:HA	3:B:152:ASN:HB2	1.94	0.49
5:D:76:LEU:HD22	5:D:81:ALA:CB	2.43	0.49
8:H:125:TYR:CD2	8:H:128:ILE:HD12	2.48	0.49
9:I:548:LYS:NZ	9:I:549:TYR:O	2.43	0.49
10:R:47:ASN:HD21	10:R:54:ILE:HG23	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:427:VAL:HG12	11:L:695:VAL:HG11	1.95	0.49
2:A:182:ASP:HB2	9:M:7:ARG:HH11	1.78	0.49
3:B:199:ALA:HB2	3:B:233:ILE:HG23	1.94	0.49
5:D:131:PRO:HB2	5:D:134:THR:HG23	1.94	0.49
5:D:200:LYS:HB3	5:D:203:GLU:HB2	1.95	0.49
9:I:137:LEU:HD22	9:I:156:VAL:HG21	1.94	0.48
3:B:31:ASP:OD1	3:B:32:LEU:N	2.45	0.48
3:B:195:LEU:HB3	3:B:225:LYS:CG	2.43	0.48
1:E:301:ALA:O	1:E:305:ARG:NE	2.44	0.48
2:A:492:ARG:NH1	4:C:210:THR:O	2.46	0.48
4:C:315:LEU:O	4:C:360:PHE:N	2.45	0.48
11:L:710:ILE:O	11:L:714:ARG:HG2	2.12	0.48
1:E:146:TRP:CH2	1:E:213:ASP:HB3	2.47	0.48
6:F:225:HIS:CE1	7:G:185:LEU:HD22	2.49	0.48
11:L:378:LEU:HD22	11:L:422:MET:HG2	1.96	0.48
11:L:478:SER:HA	11:L:481:ASN:HD21	1.78	0.48
9:I:350:PHE:HD2	9:I:363:LYS:HB2	1.77	0.48
11:L:751:ARG:CB	11:L:753:TYR:CE1	2.89	0.48
4:C:121:ILE:HG21	4:C:157:PRO:HG2	1.95	0.48
4:C:351:ILE:N	8:H:124:ALA:O	2.22	0.48
4:C:404:VAL:HG11	7:G:216:ILE:HG21	1.95	0.48
11:L:446:VAL:HG23	11:L:447:SER:N	2.29	0.48
11:L:475:ARG:O	11:L:479:ILE:HG12	2.13	0.48
3:B:259:PHE:HZ	10:R:95:PRO:HA	1.78	0.48
7:G:132:ILE:HG21	7:G:145:LEU:HD21	1.95	0.48
11:L:527:ALA:HB3	11:L:528:PRO:HD3	1.95	0.48
11:L:723:VAL:O	11:L:726:VAL:CG1	2.62	0.48
2:A:391:ASP:HB3	2:A:394:LEU:HB3	1.96	0.48
3:B:142:ALA:O	3:B:143:LYS:HG2	2.13	0.48
7:G:145:LEU:HG	7:G:152:LEU:HD13	1.96	0.48
9:M:122:GLU:O	9:M:125:ILE:HG22	2.14	0.48
9:M:385:ILE:HA	9:M:399:VAL:HG12	1.94	0.48
2:A:423:HIS:CE1	2:A:458:LYS:HB2	2.49	0.48
1:E:146:TRP:HH2	1:E:213:ASP:HB3	1.78	0.48
3:B:146:ARG:HH12	11:L:453:ASN:HB2	1.78	0.48
5:D:330:ILE:HB	5:D:334:LYS:HD3	1.96	0.48
6:F:105:TYR:HE2	6:F:145:ILE:HG21	1.79	0.48
10:R:22:PHE:HB2	11:L:606:ASN:HD21	1.79	0.48
10:R:45:CYS:HB2	10:R:54:ILE:HG23	1.95	0.48
9:M:49:LEU:HB3	9:M:56:PHE:CD2	2.48	0.48
3:B:72:LEU:HD22	3:B:91:ARG:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:118:PHE:HZ	8:H:151:GLN:HG2	1.78	0.47
9:I:275:SER:OG	9:I:574:ASP:O	2.21	0.47
2:A:105:ASP:O	2:A:111:ARG:NH2	2.47	0.47
2:A:194:LYS:HG2	2:A:227:TYR:HD2	1.79	0.47
6:F:124:TRP:HE1	6:F:139:HIS:HD1	1.63	0.47
9:M:415:LEU:HD23	9:M:417:CYS:H	1.79	0.47
11:L:338:PRO:HB2	11:L:390:LEU:HD11	1.95	0.47
4:C:51:VAL:HA	4:C:55:SER:HB3	1.95	0.47
5:D:285:LEU:HB3	5:D:290:LYS:N	2.29	0.47
9:I:220:ILE:HG13	9:I:225:LEU:HD11	1.96	0.47
10:R:33:TRP:CE3	11:L:546:ARG:HG2	2.48	0.47
9:M:17:LEU:O	9:M:21:LEU:HG	2.13	0.47
11:L:612:THR:OG1	11:L:655:ASN:O	2.32	0.47
3:B:188:LEU:HB3	11:L:460:THR:HG21	1.96	0.47
3:B:400:GLY:HA3	3:B:411:LEU:HA	1.96	0.47
5:D:226:LEU:HD21	5:D:255:CYS:SG	2.53	0.47
9:I:87:THR:O	9:I:91:THR:HG22	2.15	0.47
11:L:314:CYS:HB3	11:L:369:THR:HG21	1.97	0.47
11:L:419:PHE:HZ	11:L:425:LYS:HG3	1.79	0.47
1:E:96:PHE:CE2	1:E:120:TYR:CD2	3.02	0.47
2:A:112:VAL:HG11	2:A:145:LEU:HD11	1.97	0.47
5:D:112:SER:OG	5:D:150:LYS:NZ	2.45	0.47
4:C:131:MET:SD	4:C:139:THR:HG21	2.54	0.47
4:C:311:THR:HG21	4:C:347:ILE:HD12	1.95	0.47
7:G:70:PHE:CE1	7:G:96:LEU:HB2	2.50	0.47
11:L:557:ALA:HB3	11:L:594:VAL:HG23	1.96	0.47
3:B:270:SER:O	3:B:273:ARG:HG3	2.14	0.47
4:C:150:LEU:HA	4:C:155:PHE:HE1	1.79	0.47
9:I:265:LYS:HE3	9:I:585:LYS:HB2	1.97	0.47
9:I:385:ILE:HA	9:I:399:VAL:HG12	1.97	0.47
9:M:397:ARG:NH2	9:M:416:PRO:O	2.48	0.47
4:C:400:ASN:OD1	4:C:403:PHE:HB3	2.15	0.47
6:F:58:MET:HG3	6:F:68:VAL:HG12	1.96	0.47
9:M:382:ILE:HB	9:M:402:TYR:HB3	1.97	0.47
11:L:469:LYS:HA	11:L:512:TYR:HD2	1.80	0.47
1:E:63:LEU:HD22	6:F:49:LEU:HD23	1.97	0.47
2:A:468:ARG:HH12	6:F:281:ASP:CB	2.22	0.47
4:C:350:SER:OG	8:H:126:THR:OG1	2.31	0.47
9:M:182:SER:HB3	9:M:219:GLN:HB3	1.97	0.47
3:B:343:ILE:O	3:B:347:ILE:HG12	2.14	0.47
4:C:205:TYR:HB3	4:C:227:TYR:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:274:ARG:HE	5:D:276:ASN:ND2	2.13	0.47
6:F:54:HIS:CE1	6:F:68:VAL:HB	2.49	0.47
11:L:609:GLU:HG3	11:L:610:LYS:H	1.80	0.47
3:B:305:ASP:O	3:B:309:LEU:N	2.32	0.46
10:R:32:LEU:HD21	11:L:510:THR:HB	1.97	0.46
4:C:117:PRO:HG2	4:C:152:ALA:HB2	1.96	0.46
5:D:272:ILE:HB	7:G:137:TYR:HE2	1.79	0.46
10:R:20:LYS:HE3	10:R:23:GLU:HG2	1.96	0.46
1:E:180:LYS:HG3	6:F:202:HIS:CE1	2.50	0.46
2:A:291:LEU:HD22	2:A:320:LEU:HB2	1.97	0.46
3:B:79:ASN:HB3	3:B:84:ASN:HB3	1.96	0.46
4:C:254:LYS:HB2	4:C:255:PRO:HD3	1.97	0.46
9:I:515:ILE:HG12	9:I:538:MET:HE1	1.96	0.46
9:M:352:TRP:O	9:M:361:PHE:N	2.43	0.46
11:L:289:LYS:O	11:L:351:ARG:NH2	2.47	0.46
11:L:543:HIS:CE1	11:L:546:ARG:HH21	2.33	0.46
2:A:310:SER:O	2:A:313:HIS:ND1	2.35	0.46
4:C:265:GLN:O	4:C:268:SER:OG	2.26	0.46
4:C:288:ARG:O	4:C:288:ARG:HG2	2.15	0.46
4:C:308:GLN:HG2	4:C:347:ILE:HD11	1.97	0.46
5:D:191:TYR:OH	10:R:51:ASP:OD1	2.34	0.46
7:G:187:GLY:O	7:G:191:GLN:HG2	2.16	0.46
9:I:379:GLU:HG3	9:I:379:GLU:O	2.15	0.46
9:M:416:PRO:HG2	9:M:440:TYR:CE1	2.51	0.46
2:A:185:LEU:HD13	2:A:200:GLY:HA3	1.98	0.46
3:B:115:ILE:O	3:B:119:ILE:HG12	2.15	0.46
7:G:120:LEU:HD23	7:G:120:LEU:O	2.16	0.46
11:L:266:ARG:HH21	11:L:267:GLU:HB3	1.80	0.46
3:B:252:GLU:HG2	10:R:91:ARG:HH21	1.81	0.46
4:C:94:ARG:HD3	4:C:133:MET:HE1	1.98	0.46
5:D:266:LYS:HA	5:D:271:ARG:HD3	1.97	0.46
2:A:124:ARG:HG2	9:I:346:THR:H	1.80	0.46
2:A:223:ARG:HD2	2:A:223:ARG:HA	1.69	0.46
7:G:122:MET:HE2	7:G:127:GLU:HB2	1.97	0.46
6:F:203:VAL:O	6:F:207:THR:HG23	2.16	0.46
10:R:94:CYS:O	10:R:96:LEU:N	2.49	0.46
9:M:30:PHE:O	9:M:45:HIS:NE2	2.49	0.46
11:L:486:GLU:HG2	11:L:538:PHE:HZ	1.80	0.46
1:E:207:PRO:HB2	1:E:210:LYS:HG3	1.97	0.46
3:B:238:ARG:NH1	3:B:260:GLU:OE1	2.49	0.46
5:D:101:GLU:HB2	5:D:137:LYS:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:76:GLN:HG3	6:F:81:ILE:HG12	1.96	0.46
9:I:353:PHE:HB2	9:I:360:TRP:CH2	2.51	0.46
9:M:503:ASP:HB3	9:M:506:LYS:HB2	1.98	0.46
11:L:271:LYS:O	11:L:275:THR:OG1	2.29	0.46
6:F:241:TYR:OH	6:F:253:ASN:ND2	2.49	0.46
9:I:171:GLN:O	9:I:171:GLN:HG2	2.16	0.46
9:I:382:ILE:O	9:I:402:TYR:N	2.42	0.46
9:M:370:ARG:NH2	9:M:398:THR:O	2.46	0.46
5:D:230:LEU:HD13	5:D:264:LEU:HD13	1.98	0.45
5:D:273:ILE:HG12	5:D:307:HIS:HD2	1.81	0.45
6:F:152:LEU:HD12	6:F:167:VAL:HG22	1.98	0.45
9:I:425:VAL:HB	9:I:466:ALA:HB2	1.97	0.45
2:A:242:ILE:HA	2:A:254:VAL:HG22	1.98	0.45
3:B:129:GLN:HA	3:B:132:TYR:HB2	1.98	0.45
3:B:189:LYS:HA	11:L:456:SER:HB2	1.97	0.45
4:C:322:MET:O	4:C:326:VAL:HG22	2.17	0.45
5:D:310:LEU:O	5:D:314:LYS:HG2	2.16	0.45
6:F:244:ALA:O	6:F:248:GLY:N	2.34	0.45
9:I:522:ASP:OD1	9:I:522:ASP:N	2.49	0.45
11:L:267:GLU:OE2	11:L:268:LEU:HG	2.16	0.45
2:A:122:VAL:HG13	2:A:127:ASN:HD22	1.80	0.45
5:D:302:ARG:NH1	5:D:306:GLU:OE1	2.47	0.45
6:F:70:GLY:HA3	6:F:125:TYR:CZ	2.52	0.45
6:F:71:ALA:HB2	6:F:89:LEU:HD11	1.98	0.45
11:L:258:GLU:HB3	11:L:259:PRO:HD3	1.98	0.45
3:B:80:PHE:HB3	3:B:118:TYR:HE2	1.82	0.45
3:B:88:MET:HE3	3:B:88:MET:HB3	1.83	0.45
3:B:366:TYR:HA	5:D:352:ILE:HB	1.98	0.45
4:C:20:GLN:HB3	4:C:23:GLN:HB2	1.98	0.45
7:G:162:ILE:HG23	7:G:166:ASP:HB2	1.98	0.45
1:E:206:ILE:HG22	1:E:210:LYS:HB2	1.98	0.45
1:E:250:LEU:O	1:E:251:SER:C	2.60	0.45
2:A:242:ILE:O	2:A:246:VAL:HG23	2.17	0.45
6:F:89:LEU:HD22	6:F:105:TYR:HB2	1.99	0.45
7:G:69:LEU:HD13	7:G:85:LEU:HD11	1.99	0.45
9:M:247:GLN:O	9:M:251:LYS:HB2	2.17	0.45
9:M:415:LEU:HD11	9:M:433:VAL:HG11	1.99	0.45
9:M:526:ARG:HB2	9:M:537:PHE:HB3	1.97	0.45
11:L:754:LEU:HB3	11:L:755:ALA:H	1.62	0.45
3:B:265:TYR:HB3	3:B:273:ARG:HG2	1.99	0.45
8:H:60:ILE:HD13	8:H:71:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:268:MET:HE1	9:M:588:PRO:HG3	1.97	0.45
9:M:311:VAL:HB	9:M:375:LEU:HB3	1.98	0.45
8:H:121:VAL:HG11	8:H:133:PHE:CD1	2.52	0.45
9:M:48:VAL:HG21	9:M:90:TYR:CE1	2.51	0.45
11:L:685:ASP:HA	11:L:688:ARG:HB3	1.99	0.45
1:E:180:LYS:HE3	6:F:202:HIS:NE2	2.32	0.45
9:I:413:SER:HB3	9:I:442:TYR:HE1	1.82	0.45
11:L:560:ASN:HA	11:L:591:ILE:HG13	1.97	0.45
3:B:228:ILE:HB	11:L:455:ILE:CD1	2.47	0.44
4:C:247:GLN:O	4:C:249:VAL:N	2.51	0.44
5:D:60:VAL:HG21	11:L:618:GLN:HG3	2.00	0.44
11:L:74:TYR:OH	11:L:137:GLU:OE2	2.34	0.44
1:E:70:ARG:HD2	1:E:70:ARG:HA	1.58	0.44
3:B:169:GLN:O	3:B:173:ARG:HG3	2.18	0.44
3:B:326:PHE:O	3:B:330:LEU:HG	2.17	0.44
5:D:67:THR:O	5:D:71:THR:HG23	2.17	0.44
5:D:140:ASN:O	5:D:143:TYR:N	2.48	0.44
5:D:319:ILE:HD13	5:D:324:LEU:HD13	1.98	0.44
10:R:28:ASN:OD1	11:L:556:SER:N	2.35	0.44
1:E:327:LEU:O	1:E:331:ILE:HB	2.17	0.44
1:E:147:LEU:HD22	1:E:151:ASP:HB3	1.98	0.44
2:A:478:MET:HE3	2:A:478:MET:HB3	1.88	0.44
3:B:103:VAL:O	3:B:103:VAL:HG13	2.16	0.44
9:I:84:ILE:HA	9:I:87:THR:HG22	1.99	0.44
10:R:48:HIS:HB3	10:R:50:MET:O	2.18	0.44
1:E:208:LEU:HD13	1:E:208:LEU:HA	1.79	0.44
3:B:178:SER:O	3:B:190:LYS:NZ	2.34	0.44
5:D:360:HIS:CE1	7:G:148:ARG:HH11	2.35	0.44
6:F:42:ALA:HB3	6:F:82:GLU:HA	1.99	0.44
6:F:51:ILE:HG12	6:F:125:TYR:CD1	2.52	0.44
6:F:57:ARG:NH2	6:F:88:GLU:OE2	2.42	0.44
7:G:194:ARG:HD3	8:H:201:THR:HG21	2.00	0.44
9:I:181:LEU:HD22	9:I:219:GLN:HB2	2.00	0.44
9:M:274:ALA:N	9:M:284:SER:O	2.48	0.44
2:A:315:ASP:OD2	9:I:396:ARG:HB2	2.18	0.44
2:A:327:ILE:HD13	2:A:388:LEU:HD11	2.00	0.44
5:D:149:LEU:HD21	5:D:187:TYR:HA	1.98	0.44
7:G:34:VAL:O	7:G:95:LYS:NZ	2.50	0.44
10:R:86:ARG:O	10:R:89:LYS:HG2	2.18	0.44
9:M:87:THR:O	9:M:91:THR:HG22	2.18	0.44
11:L:409:GLU:OE2	11:L:453:ASN:ND2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:180:GLN:HG2	3:B:185:GLU:HA	1.99	0.44
4:C:311:THR:HG22	4:C:360:PHE:CD1	2.53	0.44
9:I:45:HIS:CD2	9:M:47:MET:HG2	2.52	0.44
9:I:70:THR:HG23	9:I:71:HIS:CD2	2.53	0.44
11:L:723:VAL:O	11:L:726:VAL:HG12	2.18	0.44
2:A:254:VAL:O	2:A:258:VAL:HG23	2.18	0.44
3:B:64:LYS:HD3	3:B:101:SER:HB3	1.99	0.44
7:G:116:LEU:HD13	7:G:132:ILE:HD11	2.00	0.44
9:I:301:PRO:HB2	9:I:302:PRO:HD3	2.00	0.44
9:M:379:GLU:O	9:M:379:GLU:HG3	2.18	0.44
4:C:316:THR:HA	4:C:359:SER:HA	1.99	0.44
5:D:76:LEU:HG	5:D:77:PRO:HD2	2.00	0.44
1:E:189:TYR:HD2	1:E:220:GLN:O	2.00	0.43
6:F:175:ILE:HD11	6:F:182:LEU:HD11	2.00	0.43
11:L:116:MET:HA	11:L:119:ILE:HB	2.00	0.43
2:A:77:VAL:HG21	2:A:389:LEU:HD21	1.99	0.43
3:B:256:THR:HA	3:B:259:PHE:HB3	1.99	0.43
10:R:70:VAL:O	10:R:107:GLY:N	2.49	0.43
11:L:238:GLU:O	11:L:242:ASN:ND2	2.35	0.43
11:L:735:LEU:HD11	11:L:737:SER:HB3	2.00	0.43
10:R:35:TRP:CE3	11:L:546:ARG:HD2	2.54	0.43
10:R:52:LEU:HD12	10:R:56:CYS:HB3	1.99	0.43
11:L:31:ASN:OD1	11:L:72:LYS:NZ	2.50	0.43
11:L:211:GLU:O	11:L:215:GLU:HG2	2.18	0.43
4:C:351:ILE:HA	4:C:358:VAL:HA	1.99	0.43
5:D:172:SER:HB2	5:D:187:TYR:OH	2.17	0.43
9:I:286:VAL:HA	9:I:297:LYS:HA	1.99	0.43
9:I:416:PRO:HG2	9:I:440:TYR:CD1	2.53	0.43
9:M:513:ALA:HB3	9:M:561:TRP:HZ3	1.82	0.43
11:L:516:GLN:HE22	11:L:553:HIS:HB3	1.83	0.43
1:E:262:THR:O	1:E:266:VAL:HG23	2.18	0.43
2:A:327:ILE:HG13	2:A:359:GLU:HG3	2.00	0.43
4:C:224:TYR:HE2	4:C:241:LEU:HD11	1.83	0.43
5:D:164:ALA:HA	5:D:167:TYR:HB2	2.01	0.43
5:D:274:ARG:HE	5:D:276:ASN:HD21	1.65	0.43
7:G:140:ILE:O	7:G:158:ILE:HG13	2.18	0.43
9:I:287:CYS:SG	9:I:288:TYR:N	2.92	0.43
10:R:47:ASN:HD22	10:R:53:CYS:HA	1.83	0.43
9:M:267:GLU:HG2	9:M:530:ILE:HG13	1.99	0.43
11:L:276:ILE:HD12	11:L:283:GLY:HA2	1.99	0.43
1:E:40:LEU:HD23	1:E:45:TRP:CH2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:78:PHE:HD1	4:C:78:PHE:HA	1.70	0.43
9:I:60:PHE:HB2	9:M:30:PHE:HE2	1.83	0.43
9:I:435:THR:HG22	9:I:438:LEU:O	2.18	0.43
11:L:124:MET:O	11:L:128:ARG:HG2	2.16	0.43
11:L:426:ASP:HA	11:L:466:PHE:CE2	2.53	0.43
3:B:34:ASN:ND2	11:L:668:LYS:HG3	2.34	0.43
9:I:549:TYR:OH	9:I:575:LEU:N	2.44	0.43
9:M:101:VAL:HG11	9:M:123:TYR:CD2	2.53	0.43
2:A:402:TYR:O	2:A:406:ARG:HD3	2.19	0.43
9:I:222:ILE:HG12	9:I:257:PHE:HB2	2.01	0.43
9:I:434:MET:HE2	9:I:455:ARG:NE	2.29	0.43
11:L:424:GLU:H	11:L:734:PHE:HA	1.84	0.43
11:L:657:HIS:HD2	11:L:659:PHE:CE1	2.37	0.43
11:L:761:ARG:HD3	11:L:761:ARG:HA	1.81	0.43
2:A:238:CYS:HA	2:A:257:TYR:HD2	1.82	0.43
3:B:46:ASP:O	3:B:48:LYS:N	2.52	0.43
6:F:109:GLU:HG2	6:F:113:LYS:NZ	2.33	0.43
9:I:470:LYS:NZ	9:I:503:ASP:OD2	2.46	0.43
9:M:265:LYS:HB2	9:M:585:LYS:HB3	2.01	0.43
11:L:669:LEU:HB2	11:L:672:VAL:HB	2.01	0.43
2:A:91:TYR:HE2	2:A:320:LEU:HA	1.84	0.43
4:C:380:MET:HE2	8:H:203:TYR:CE1	2.54	0.43
9:I:213:LEU:HA	9:I:216:VAL:HG12	2.01	0.43
11:L:282:SER:H	11:L:286:HIS:HD2	1.67	0.43
11:L:613:PHE:HE1	11:L:627:LEU:HD11	1.84	0.43
3:B:198:TYR:O	3:B:202:ILE:N	2.52	0.42
3:B:362:LEU:HG	3:B:366:TYR:OH	2.18	0.42
5:D:175:GLN:NE2	5:D:184:GLN:HG2	2.34	0.42
9:I:269:MET:HE1	9:I:583:VAL:HG23	2.01	0.42
2:A:108:PRO:C	2:A:110:LEU:H	2.26	0.42
3:B:120:SER:HA	3:B:128:LEU:HD11	2.02	0.42
3:B:330:LEU:HD22	3:B:337:ILE:HG21	2.01	0.42
4:C:138:LEU:HB3	4:C:169:ILE:HD13	2.01	0.42
4:C:335:GLU:OE2	4:C:353:GLN:NE2	2.52	0.42
5:D:175:GLN:HE22	5:D:184:GLN:HG2	1.84	0.42
9:I:318:ILE:HB	9:I:353:PHE:HB3	2.01	0.42
9:M:217:LEU:HA	9:M:220:ILE:HG22	2.02	0.42
11:L:625:ARG:NH1	11:L:628:VAL:HB	2.33	0.42
5:D:312:ALA:HA	5:D:316:TYR:HD2	1.83	0.42
9:M:400:GLU:HG2	9:M:409:TRP:HE3	1.84	0.42
11:L:762:LYS:H	11:L:762:LYS:HG2	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211:ILE:HA	1:E:214:PHE:HB3	2.02	0.42
2:A:135:HIS:NE2	2:A:162:LEU:HB3	2.35	0.42
9:I:31:THR:OG1	9:I:44:CYS:O	2.26	0.42
10:R:25:LYS:HE2	10:R:25:LYS:HB2	1.88	0.42
1:E:241:LEU:HG	1:E:245:TYR:HB2	2.01	0.42
1:E:241:LEU:HD11	6:F:197:ARG:HA	2.02	0.42
1:E:301:ALA:C	1:E:305:ARG:HE	2.26	0.42
3:B:365:PRO:HG2	5:D:340:SER:OG	2.19	0.42
3:B:416:ARG:HG2	3:B:418:GLY:H	1.84	0.42
7:G:204:ARG:O	7:G:207:GLN:HG2	2.19	0.42
9:I:111:LEU:H	9:I:111:LEU:HG	1.59	0.42
11:L:206:GLU:O	11:L:210:LEU:N	2.31	0.42
3:B:213:LYS:O	3:B:217:LEU:HG	2.20	0.42
3:B:227:ALA:HA	11:L:459:LYS:HG3	2.02	0.42
9:I:47:MET:SD	9:M:21:LEU:HD22	2.60	0.42
9:I:397:ARG:HG2	9:I:418:ALA:N	2.35	0.42
10:R:60:GLN:HG3	10:R:61:ALA:H	1.84	0.42
3:B:260:GLU:HB2	10:R:98:ASN:ND2	2.11	0.42
4:C:216:VAL:HG21	4:C:252:PHE:HB2	2.01	0.42
5:D:319:ILE:HG13	7:G:147:GLN:OE1	2.20	0.42
8:H:87:PRO:HG3	8:H:135:ALA:HB1	2.01	0.42
9:M:539:ARG:HD3	9:M:549:TYR:CZ	2.55	0.42
3:B:159:TYR:CE2	3:B:167:LYS:HB2	2.54	0.42
7:G:37:ALA:O	7:G:95:LYS:NZ	2.50	0.42
9:M:69:GLN:HG2	9:M:71:HIS:H	1.84	0.42
11:L:545:GLY:C	11:L:546:ARG:HD3	2.45	0.42
5:D:159:ASP:C	5:D:161:PRO:HD3	2.45	0.42
5:D:228:HIS:HA	5:D:290:LYS:NZ	2.35	0.42
9:I:153:LYS:HE2	9:I:180:ILE:HA	2.02	0.42
9:M:275:SER:N	9:M:575:LEU:O	2.51	0.42
11:L:631:LEU:HD11	11:L:659:PHE:CE2	2.54	0.42
1:E:250:LEU:HD21	5:D:371:ASP:HA	2.01	0.42
3:B:82:LEU:O	3:B:82:LEU:HD23	2.19	0.42
5:D:73:LEU:N	5:D:74:PRO:HD2	2.35	0.42
5:D:297:SER:O	5:D:301:ASP:HB2	2.20	0.42
9:M:525:VAL:HA	9:M:538:MET:HG2	2.02	0.42
11:L:605:PHE:HE1	11:L:611:TYR:HB2	1.84	0.42
11:L:703:ILE:HG22	11:L:730:LEU:HD13	2.01	0.42
2:A:353:LYS:HE3	2:A:353:LYS:HB3	1.81	0.41
2:A:356:LEU:HD13	2:A:363:ARG:HG3	2.02	0.41
5:D:136:GLN:HG2	5:D:137:LYS:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:121:VAL:HG11	8:H:133:PHE:HD1	1.84	0.41
9:I:130:ALA:HA	9:I:159:LYS:NZ	2.35	0.41
9:I:238:PRO:HA	9:I:239:PRO:HD3	1.95	0.41
11:L:558:ASP:OD1	11:L:671:ARG:NH2	2.53	0.41
2:A:75:TYR:HB2	2:A:76:VAL:H	1.62	0.41
2:A:395:ALA:HB3	2:A:396:PRO:HD3	2.02	0.41
4:C:158:ALA:O	4:C:162:LEU:N	2.53	0.41
5:D:288:HIS:HB3	5:D:289:GLN:H	1.68	0.41
9:M:372:LYS:NZ	9:M:580:ARG:HE	2.17	0.41
2:A:418:VAL:HG23	2:A:419:SER:N	2.33	0.41
4:C:219:ILE:HD12	4:C:219:ILE:H	1.85	0.41
4:C:351:ILE:HG12	4:C:358:VAL:HG13	2.03	0.41
9:I:380:GLY:O	9:I:404:THR:OG1	2.34	0.41
11:L:556:SER:HB2	11:L:593:GLN:HE21	1.84	0.41
3:B:115:ILE:HD13	3:B:115:ILE:HA	1.88	0.41
3:B:333:ASN:O	3:B:337:ILE:HG12	2.20	0.41
5:D:49:VAL:O	5:D:53:VAL:HG23	2.20	0.41
9:M:127:LYS:HA	9:M:127:LYS:HD2	1.84	0.41
9:M:142:LEU:HG	11:L:66:LEU:HD11	2.02	0.41
9:M:327:LEU:HG	9:M:343:ALA:HB1	2.02	0.41
11:L:86:ILE:HG23	11:L:90:ARG:HD2	2.02	0.41
11:L:322:ARG:NE	11:L:373:ASP:OD1	2.46	0.41
11:L:499:GLY:H	11:L:534:ILE:HD11	1.86	0.41
5:D:324:LEU:O	5:D:328:LEU:HG	2.21	0.41
1:E:62:LEU:HD22	1:E:228:TYR:HE2	1.85	0.41
3:B:359:LEU:HD21	3:B:389:LEU:HD23	2.02	0.41
9:I:159:LYS:O	9:I:163:VAL:HG22	2.20	0.41
9:I:234:PHE:HA	9:I:237:LEU:HD23	2.01	0.41
11:L:86:ILE:O	11:L:90:ARG:HB3	2.20	0.41
11:L:406:GLN:HG2	11:L:407:GLU:N	2.35	0.41
11:L:605:PHE:CZ	11:L:659:PHE:HD2	2.36	0.41
11:L:735:LEU:CD1	11:L:737:SER:HB3	2.50	0.41
2:A:79:ASN:OD1	2:A:79:ASN:N	2.54	0.41
3:B:281:VAL:HG12	3:B:285:MET:HE3	2.03	0.41
2:A:188:TYR:HA	2:A:191:ASN:HD22	1.86	0.41
5:D:134:THR:HB	5:D:136:GLN:OE1	2.20	0.41
5:D:399:ALA:HB1	6:F:237:LEU:HD22	2.03	0.41
9:I:221:ARG:NE	9:I:260:ARG:HG2	2.36	0.41
9:M:137:LEU:HG	9:M:176:LEU:HD21	2.03	0.41
9:M:346:THR:HG22	9:M:369:VAL:HB	2.01	0.41
1:E:249:THR:HG22	1:E:324:LYS:HZ2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:305:ASP:HB3	3:B:308:ILE:HB	2.03	0.41
4:C:282:HIS:HB3	4:C:285:THR:HB	2.03	0.41
5:D:159:ASP:OD2	5:D:292:THR:OG1	2.29	0.41
5:D:285:LEU:HD22	5:D:290:LYS:HB2	2.03	0.41
5:D:402:ALA:O	5:D:406:GLN:NE2	2.54	0.41
9:I:539:ARG:HH22	9:I:577:ARG:HD3	1.86	0.41
9:M:128:ILE:HG13	9:M:155:MET:HG2	2.02	0.41
9:M:225:LEU:HD12	9:M:225:LEU:HA	1.91	0.41
9:M:539:ARG:HH21	9:M:579:PHE:HE1	1.67	0.41
11:L:311:LYS:HE3	11:L:311:LYS:HB3	1.88	0.41
11:L:389:SER:O	11:L:392:ILE:HG22	2.20	0.41
11:L:408:VAL:O	11:L:411:ILE:HG22	2.21	0.41
11:L:436:LEU:HA	11:L:439:ARG:HG2	2.03	0.41
11:L:472:GLY:HA3	11:L:512:TYR:CD1	2.55	0.41
11:L:657:HIS:CD2	11:L:659:PHE:CE1	3.09	0.41
1:E:120:TYR:HA	6:F:111:GLN:NE2	2.34	0.41
2:A:378:LEU:HD22	2:A:406:ARG:HD2	2.03	0.41
2:A:385:LYS:O	2:A:389:LEU:HB3	2.21	0.41
5:D:281:PHE:HB3	5:D:300:LEU:HD11	2.03	0.41
9:I:539:ARG:HD3	9:I:549:TYR:CZ	2.56	0.41
9:M:81:THR:OG1	9:M:107:THR:HG21	2.21	0.41
2:A:328:TYR:HE1	2:A:394:LEU:HD22	1.86	0.40
2:A:440:LEU:O	2:A:444:ILE:HG13	2.21	0.40
4:C:125:LYS:HD2	4:C:161:TYR:CZ	2.56	0.40
5:D:73:LEU:HB3	5:D:85:TYR:OH	2.21	0.40
5:D:231:HIS:HB2	5:D:290:LYS:NZ	2.36	0.40
9:I:48:VAL:HG21	9:I:90:TYR:CZ	2.55	0.40
10:R:30:VAL:O	11:L:551:GLN:NE2	2.54	0.40
9:M:7:ARG:HG2	9:M:8:GLN:OE1	2.20	0.40
9:M:59:MET:HE3	9:M:66:GLU:HG3	2.03	0.40
9:M:542:HIS:HB2	9:M:545:GLU:HB2	2.03	0.40
11:L:543:HIS:ND1	11:L:543:HIS:O	2.54	0.40
6:F:155:ASN:HB3	6:F:164:PRO:HB2	2.04	0.40
6:F:222:ILE:HD13	6:F:222:ILE:HA	1.97	0.40
9:I:102:GLU:HG3	9:I:135:ARG:HH12	1.86	0.40
11:L:245:ILE:HA	11:L:248:VAL:HG12	2.03	0.40
11:L:614:GLU:HA	11:L:617:GLN:HG2	2.03	0.40
1:E:239:GLU:OE2	1:E:243:ASN:ND2	2.52	0.40
1:E:244:LYS:C	1:E:246:TRP:N	2.78	0.40
2:A:107:CYS:HB2	2:A:390:LEU:HD13	2.03	0.40
3:B:364:LYS:HD3	3:B:364:LYS:HA	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:319:ILE:HG13	7:G:147:GLN:CD	2.46	0.40
6:F:230:MET:O	6:F:234:ARG:HG2	2.22	0.40
10:R:28:ASN:HA	11:L:504:THR:O	2.22	0.40
11:L:429:GLU:HG2	11:L:466:PHE:CB	2.52	0.40
11:L:647:GLU:HB2	11:L:648:PRO:HD3	2.02	0.40
11:L:698:ASP:HA	11:L:701:HIS:NE2	2.35	0.40
11:L:722:LEU:HA	11:L:722:LEU:HD23	1.81	0.40
4:C:42:LEU:HD23	4:C:61:VAL:HG13	2.03	0.40
5:D:61:ILE:O	5:D:65:LEU:HB2	2.22	0.40
9:I:265:LYS:HG3	9:I:585:LYS:HB3	2.04	0.40
11:L:613:PHE:HB2	11:L:657:HIS:CE1	2.57	0.40
11:L:711:MET:SD	11:L:722:LEU:HD13	2.60	0.40
1:E:63:LEU:HD21	6:F:46:LEU:HD13	2.03	0.40
2:A:76:VAL:HG13	2:A:106:HIS:HA	2.04	0.40
7:G:55:LEU:HD23	7:G:55:LEU:HA	1.95	0.40
7:G:70:PHE:HE1	7:G:96:LEU:HB2	1.86	0.40
8:H:60:ILE:HG21	8:H:71:LEU:HD21	2.02	0.40
9:I:134:VAL:HG21	9:I:169:PHE:HA	2.03	0.40
9:I:205:ASN:ND2	9:I:206:THR:H	2.19	0.40
9:M:25:TYR:HB2	9:M:90:TYR:CE1	2.57	0.40
9:M:186:LEU:HD21	9:M:260:ARG:HB3	2.04	0.40
9:M:352:TRP:HE3	9:M:361:PHE:HB2	1.86	0.40
9:M:413:SER:HB3	9:M:442:TYR:HE1	1.87	0.40
11:L:65:VAL:HG11	11:L:129:VAL:HG21	2.04	0.40
11:L:276:ILE:HD13	11:L:299:MET:HE1	2.04	0.40
11:L:553:HIS:O	11:L:554:MET:HE2	2.22	0.40
11:L:665:PHE:HE1	11:L:668:LYS:HD3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	E	307/334 (92%)	287 (94%)	18 (6%)	2 (1%)	18	56
2	A	406/527 (77%)	381 (94%)	25 (6%)	0	100	100
3	B	418/443 (94%)	382 (91%)	30 (7%)	6 (1%)	9	40
4	C	405/441 (92%)	383 (95%)	22 (5%)	0	100	100
5	D	404/406 (100%)	371 (92%)	27 (7%)	6 (2%)	8	40
6	F	286/327 (88%)	274 (96%)	12 (4%)	0	100	100
7	G	212/220 (96%)	209 (99%)	3 (1%)	0	100	100
8	H	173/209 (83%)	172 (99%)	1 (1%)	0	100	100
9	I	551/636 (87%)	512 (93%)	38 (7%)	1 (0%)	43	78
9	M	558/636 (88%)	526 (94%)	32 (6%)	0	100	100
10	R	87/121 (72%)	64 (74%)	23 (26%)	0	100	100
11	L	714/768 (93%)	655 (92%)	55 (8%)	4 (1%)	21	59
All	All	4521/5068 (89%)	4216 (93%)	286 (6%)	19 (0%)	31	67

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	253	SER
3	B	106	ASN
5	D	80	THR
5	D	93	GLN
5	D	287	PRO
5	D	288	HIS
5	D	291	ALA
11	L	253	ASP
3	B	300	LYS
3	B	182	ASP
9	I	110	PHE
11	L	466	PHE
3	B	299	ALA
5	D	298	SER
11	L	754	LEU
3	B	28	PRO
3	B	25	ASN
11	L	733	ARG
1	E	199	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	265/283 (94%)	243 (92%)	22 (8%)	10	30
2	A	360/458 (79%)	357 (99%)	3 (1%)	73	80
3	B	382/405 (94%)	379 (99%)	3 (1%)	73	80
4	C	363/393 (92%)	360 (99%)	3 (1%)	73	80
5	D	347/347 (100%)	347 (100%)	0	100	100
6	F	255/276 (92%)	252 (99%)	3 (1%)	63	75
7	G	187/191 (98%)	187 (100%)	0	100	100
8	H	147/173 (85%)	147 (100%)	0	100	100
9	I	501/572 (88%)	498 (99%)	3 (1%)	78	83
9	M	507/572 (89%)	507 (100%)	0	100	100
10	R	78/102 (76%)	75 (96%)	3 (4%)	29	50
11	L	651/693 (94%)	642 (99%)	9 (1%)	59	72
All	All	4043/4465 (90%)	3994 (99%)	49 (1%)	61	75

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	160	GLN
1	E	161	PHE
1	E	162	GLN
1	E	163	GLU
1	E	165	PHE
1	E	166	VAL
1	E	204	GLN
1	E	206	ILE
1	E	208	LEU
1	E	209	ASN
1	E	211	ILE
1	E	218	CYS
1	E	219	LYS
1	E	220	GLN

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Mol	Chain	Res	Type
1	E	226	VAL
1	E	227	SER
1	E	230	LYS
1	E	232	SER
1	E	235	ARG
1	E	236	LYS
1	E	247	VAL
1	E	249	THR
2	A	75	TYR
2	A	76	VAL
2	A	389	LEU
3	B	61	GLU
3	B	64	LYS
3	B	70	LYS
4	C	70	SER
4	C	71	VAL
4	C	78	PHE
6	F	267	LEU
6	F	271	SER
6	F	272	THR
9	I	111	LEU
9	I	115	ASP
9	I	116	VAL
10	R	39	VAL
10	R	42	CYS
10	R	44	ILE
11	L	739	VAL
11	L	743	LYS
11	L	754	LEU
11	L	756	ARG
11	L	759	GLU
11	L	760	ASP
11	L	761	ARG
11	L	762	LYS
11	L	766	TYR

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

Mol	Chain	Res	Type
1	E	68	HIS
1	E	123	ASN
1	E	126	GLN

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Mol	Chain	Res	Type
1	E	132	ASN
1	E	204	GLN
1	E	209	ASN
1	E	316	HIS
2	A	101	GLN
2	A	135	HIS
2	A	191	ASN
2	A	387	ASN
2	A	397	HIS
2	A	423	HIS
2	A	501	HIS
3	B	90	ASN
3	B	169	GLN
3	B	180	GLN
3	B	193	GLN
3	B	284	ASN
3	B	297	GLN
3	B	320	ASN
3	B	346	HIS
4	C	29	ASN
4	C	261	HIS
4	C	340	HIS
5	D	72	HIS
5	D	86	HIS
5	D	125	GLN
5	D	406	GLN
6	F	92	HIS
6	F	111	GLN
6	F	224	GLN
6	F	253	ASN
7	G	53	GLN
7	G	98	HIS
7	G	208	GLN
8	H	23	GLN
8	H	103	GLN
9	I	69	GLN
9	I	93	ASN
9	I	150	GLN
9	I	205	ASN
9	I	356	GLN
9	I	357	GLN
10	R	47	ASN

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Mol	Chain	Res	Type
10	R	98	ASN
9	M	20	GLN
9	M	27	GLN
9	M	69	GLN
9	M	129	ASN
9	M	150	GLN
9	M	165	HIS
9	M	187	ASN
9	M	219	GLN
9	M	230	GLN
9	M	235	GLN
11	L	87	ASN
11	L	112	HIS
11	L	132	GLN
11	L	163	GLN
11	L	286	HIS
11	L	435	HIS
11	L	516	GLN
11	L	553	HIS
11	L	606	ASN
11	L	657	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

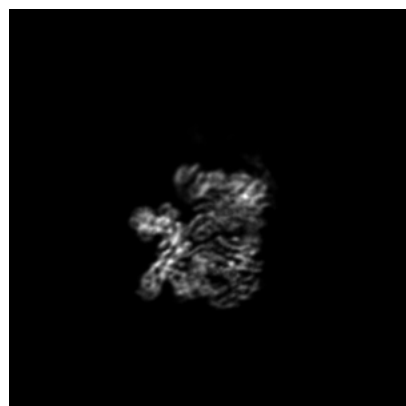
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34467. These allow visual inspection of the internal detail of the map and identification of artifacts.

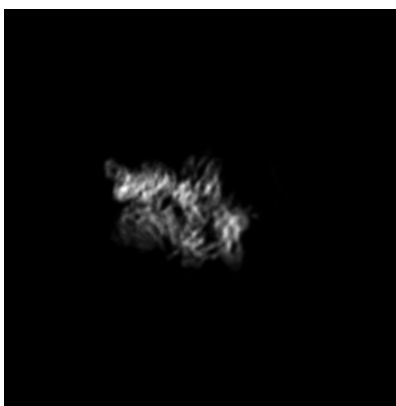
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

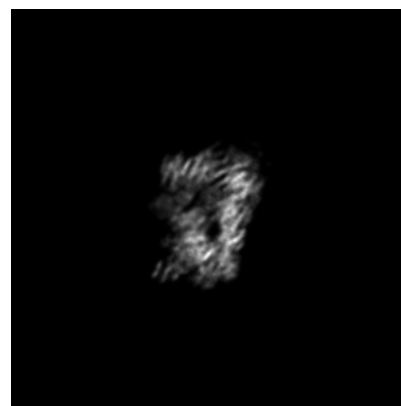
6.1.1 Primary map



X

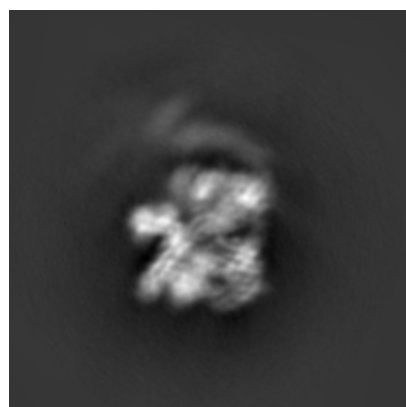


Y

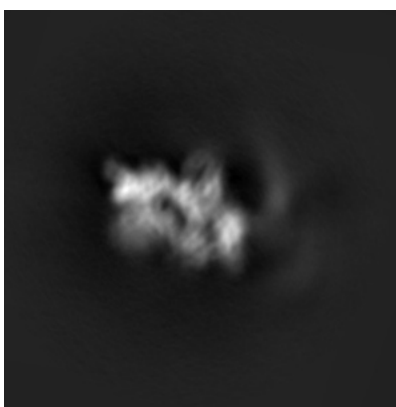


Z

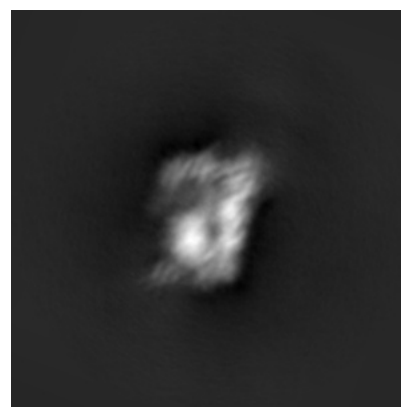
6.1.2 Raw map



X



Y

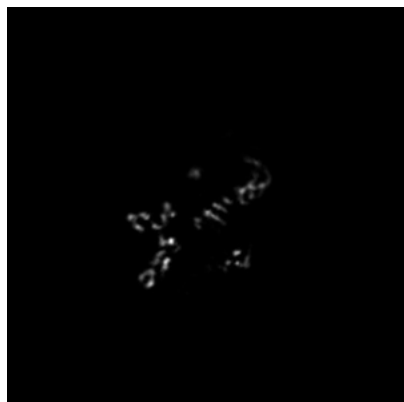


Z

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

6.2 Central slices [i](#)

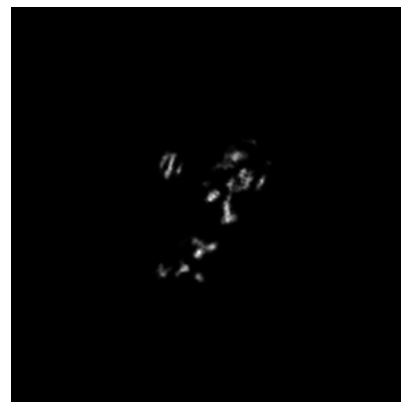
6.2.1 Primary map



X Index: 108

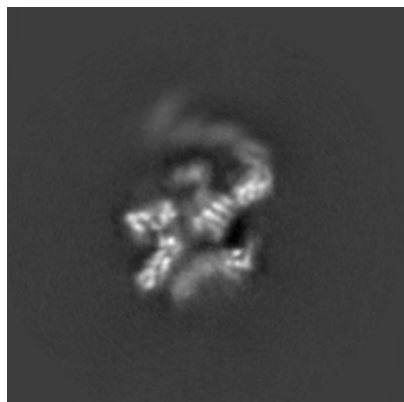


Y Index: 108

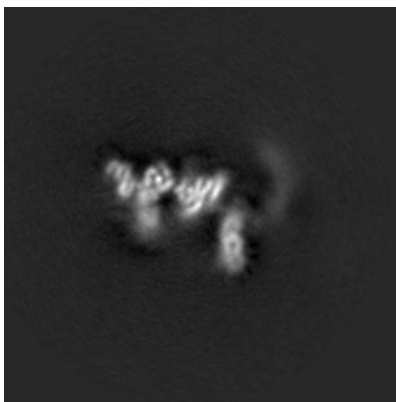


Z Index: 108

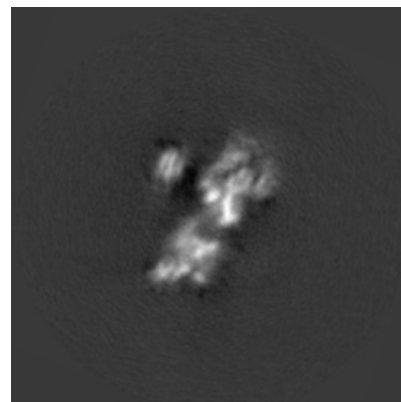
6.2.2 Raw map



X Index: 108



Y Index: 108



Z Index: 108

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: 116

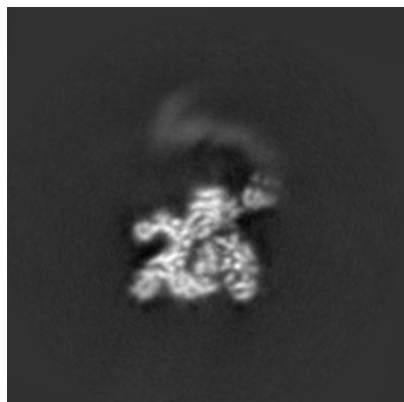


Y Index: 91

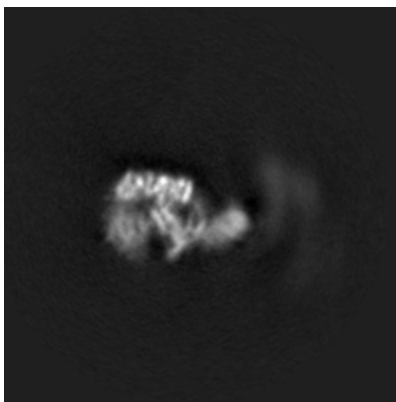


Z Index: 99

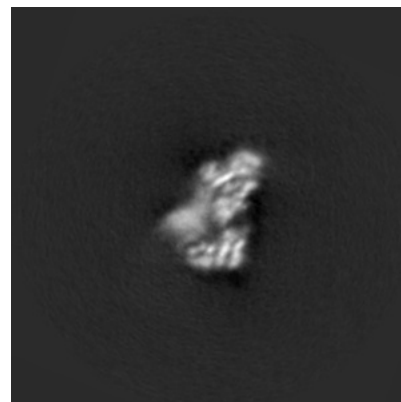
6.3.2 Raw map



X Index: 117



Y Index: 91

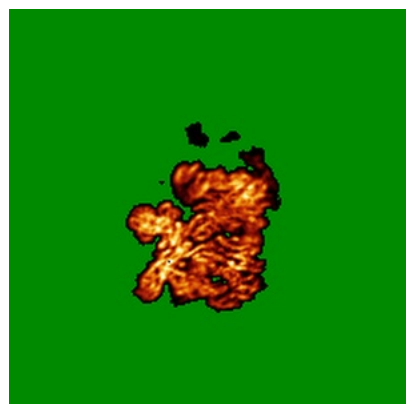


Z Index: 76

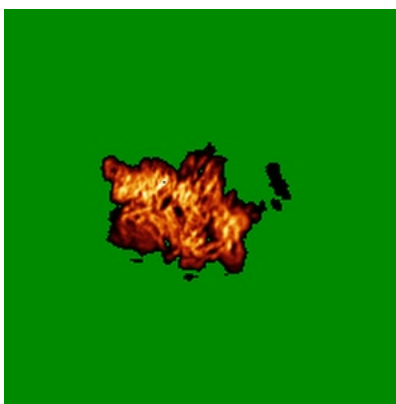
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

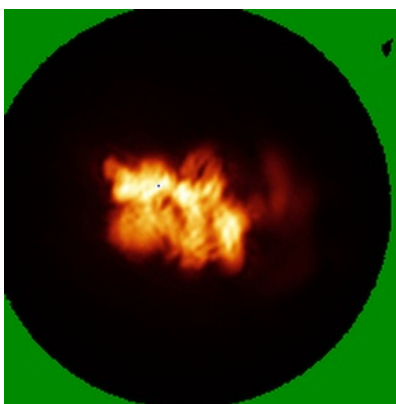


Z

6.4.2 Raw map



X



Y

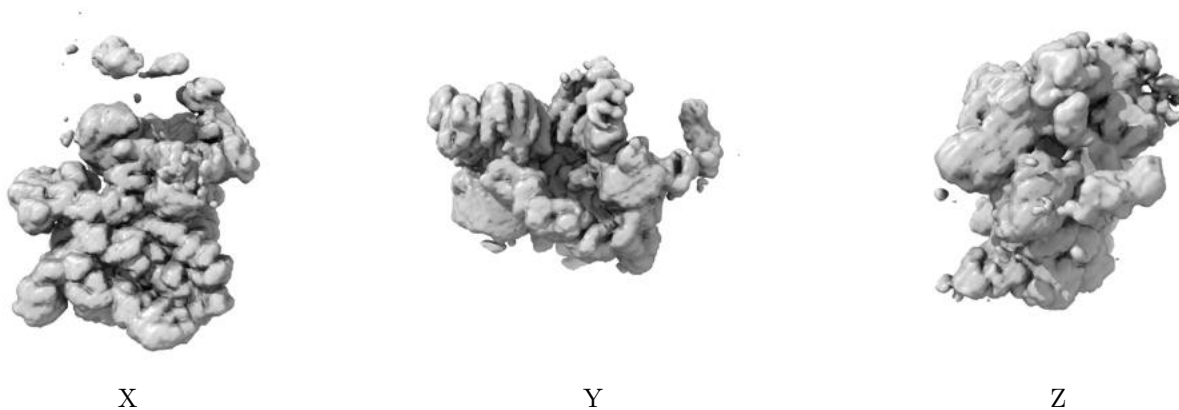


Z

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

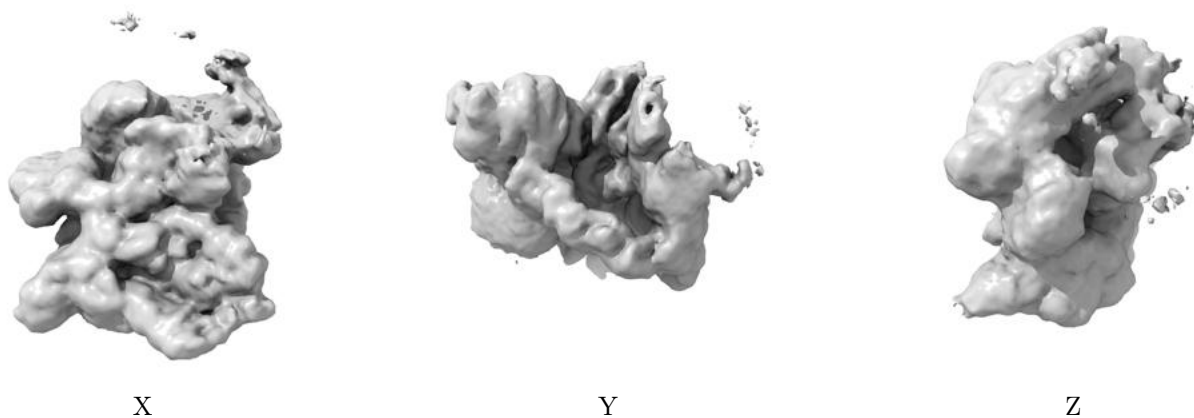
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.001. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

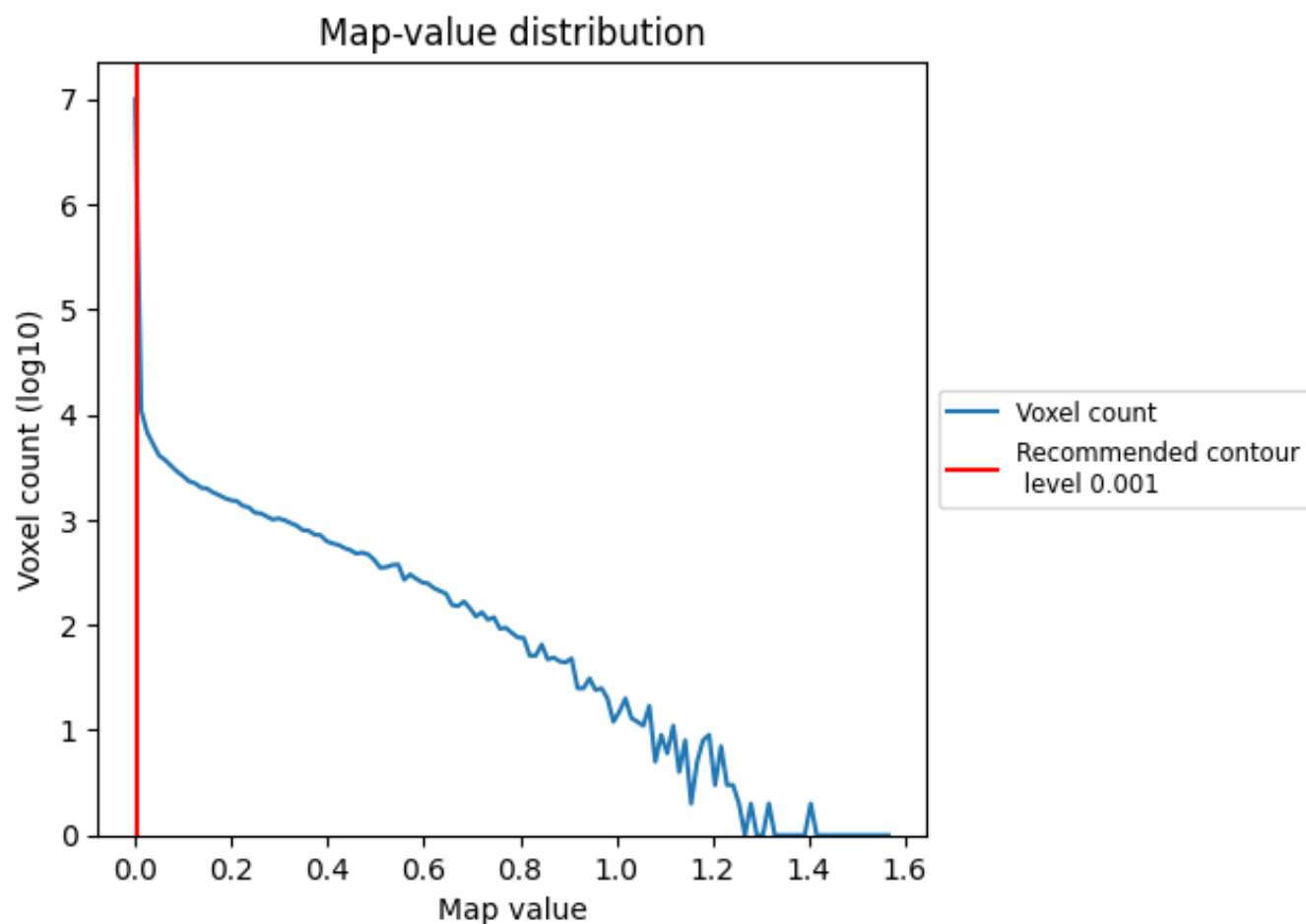
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

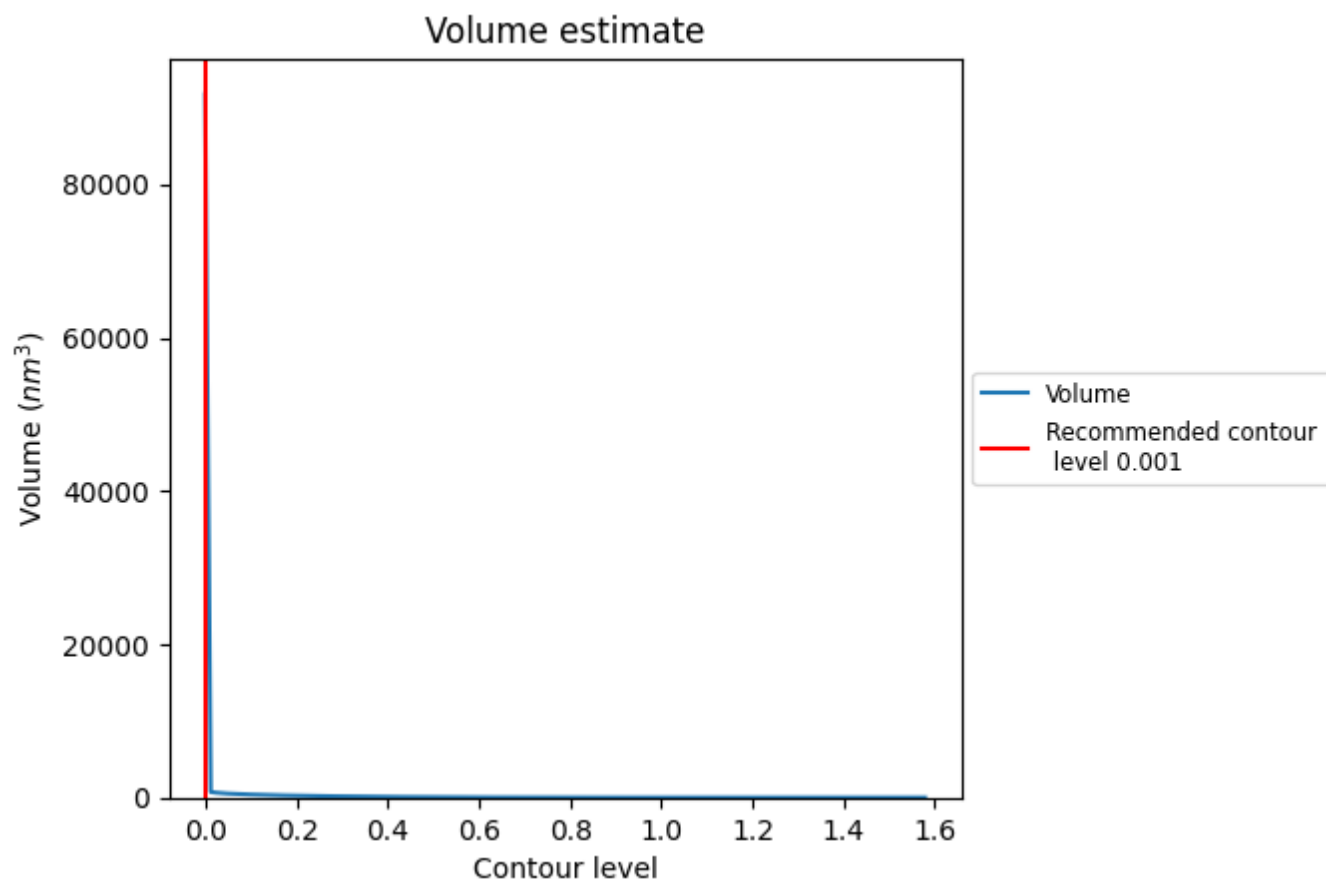
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

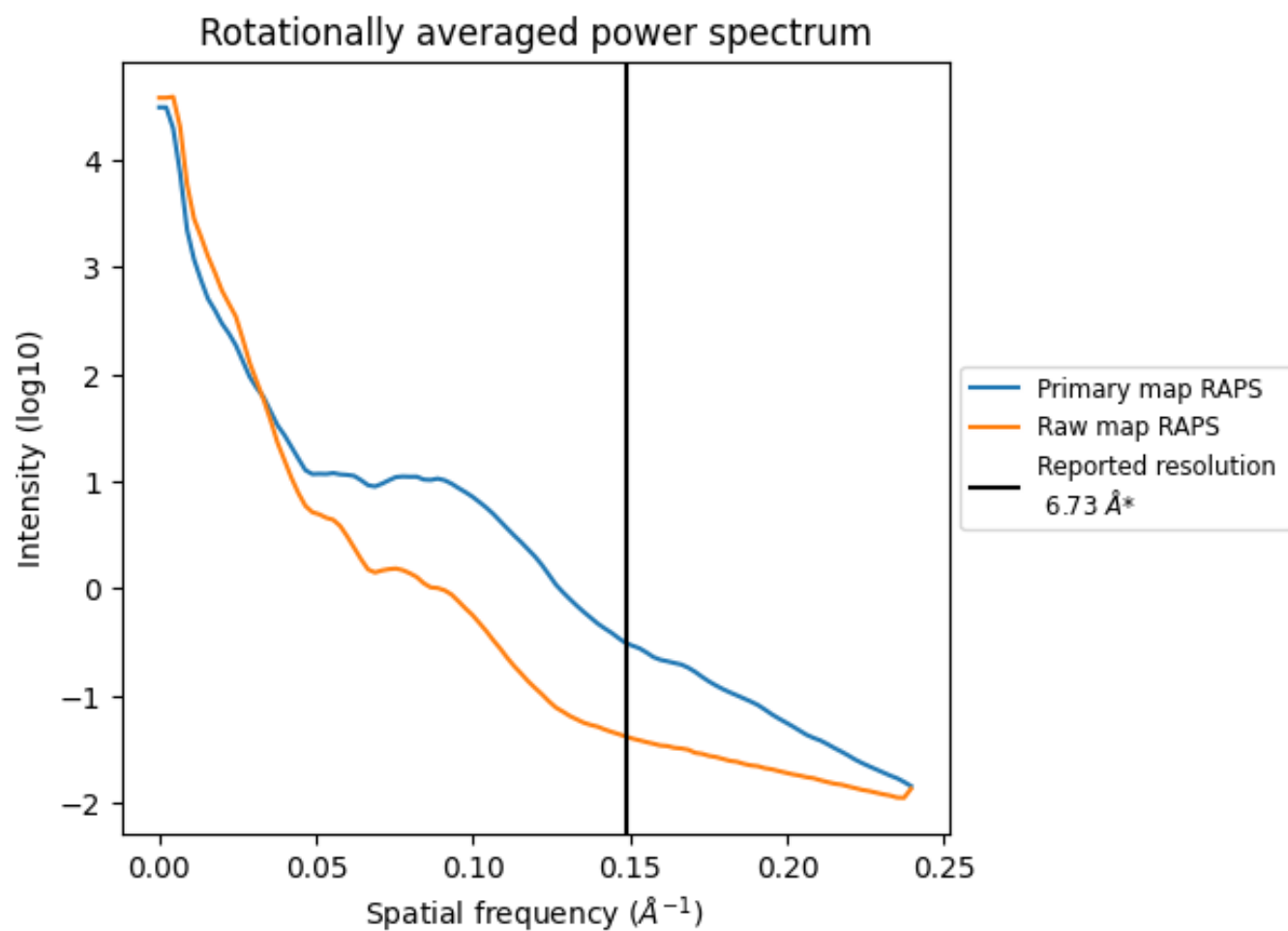
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 78258 nm^3 ; this corresponds to an approximate mass of 70692 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

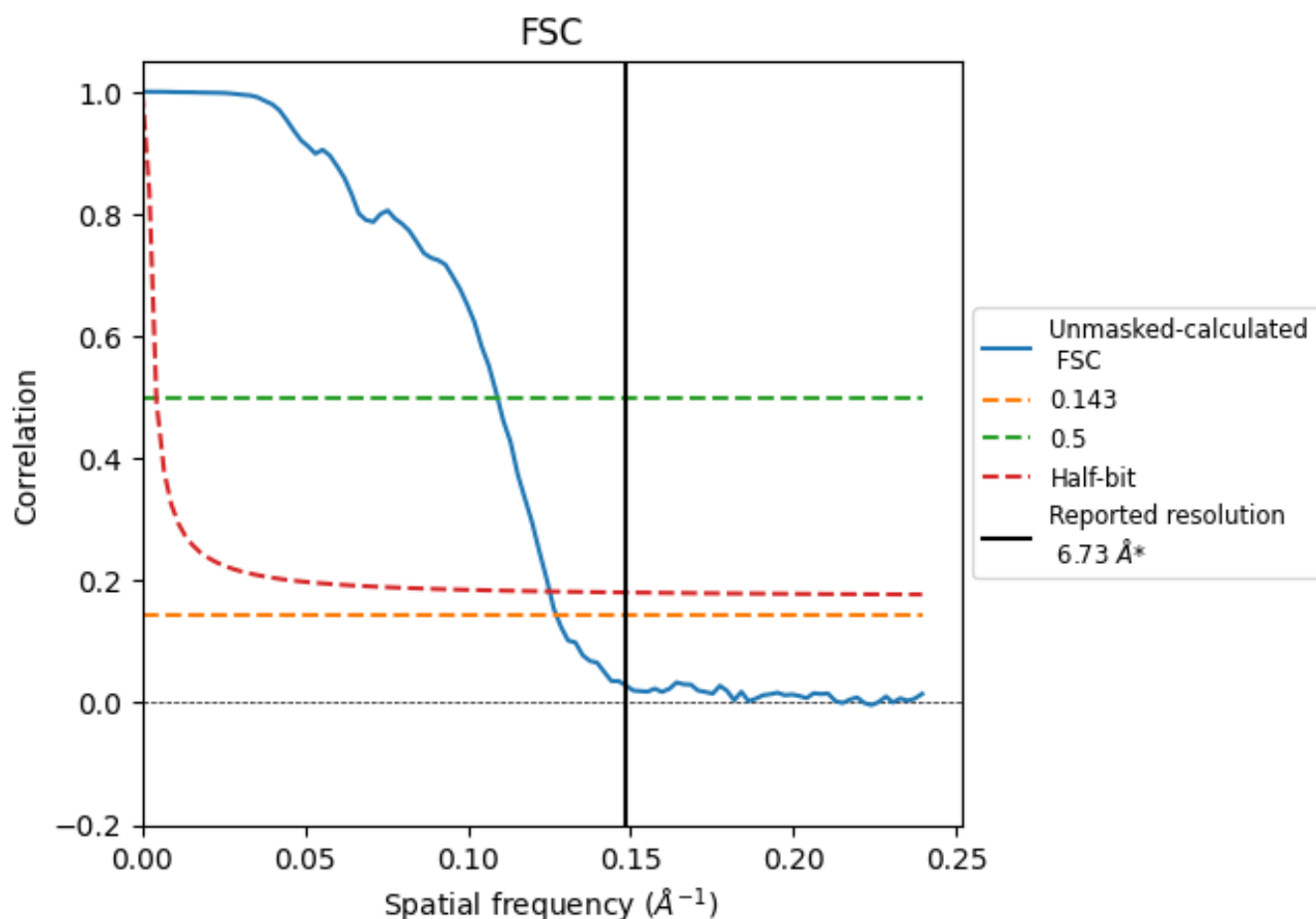


*Reported resolution corresponds to spatial frequency of 0.149 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.149 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.73	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.86	9.17	7.99

*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 7.86 differs from the reported value 6.73 by more than 10 %

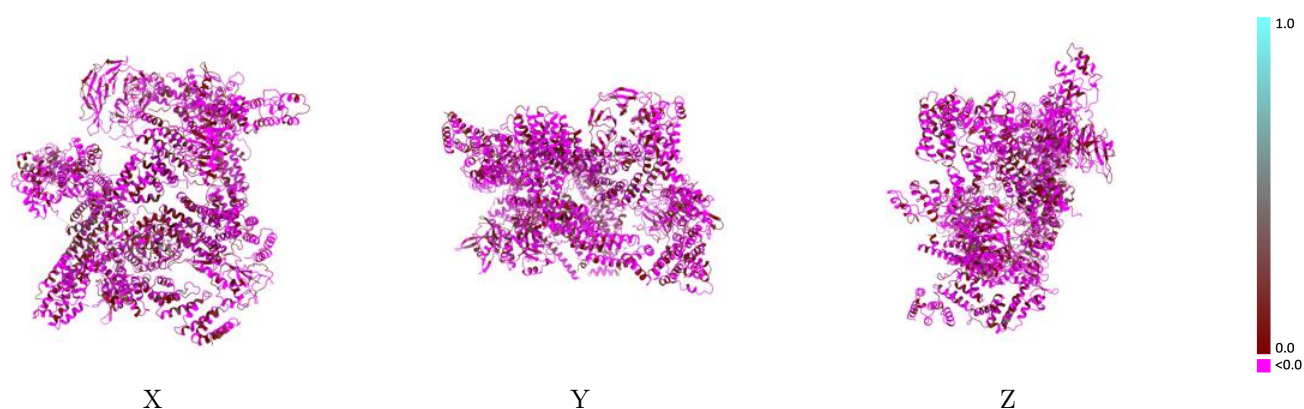
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-34467 and PDB model 8H3F. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

This section was not generated.

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

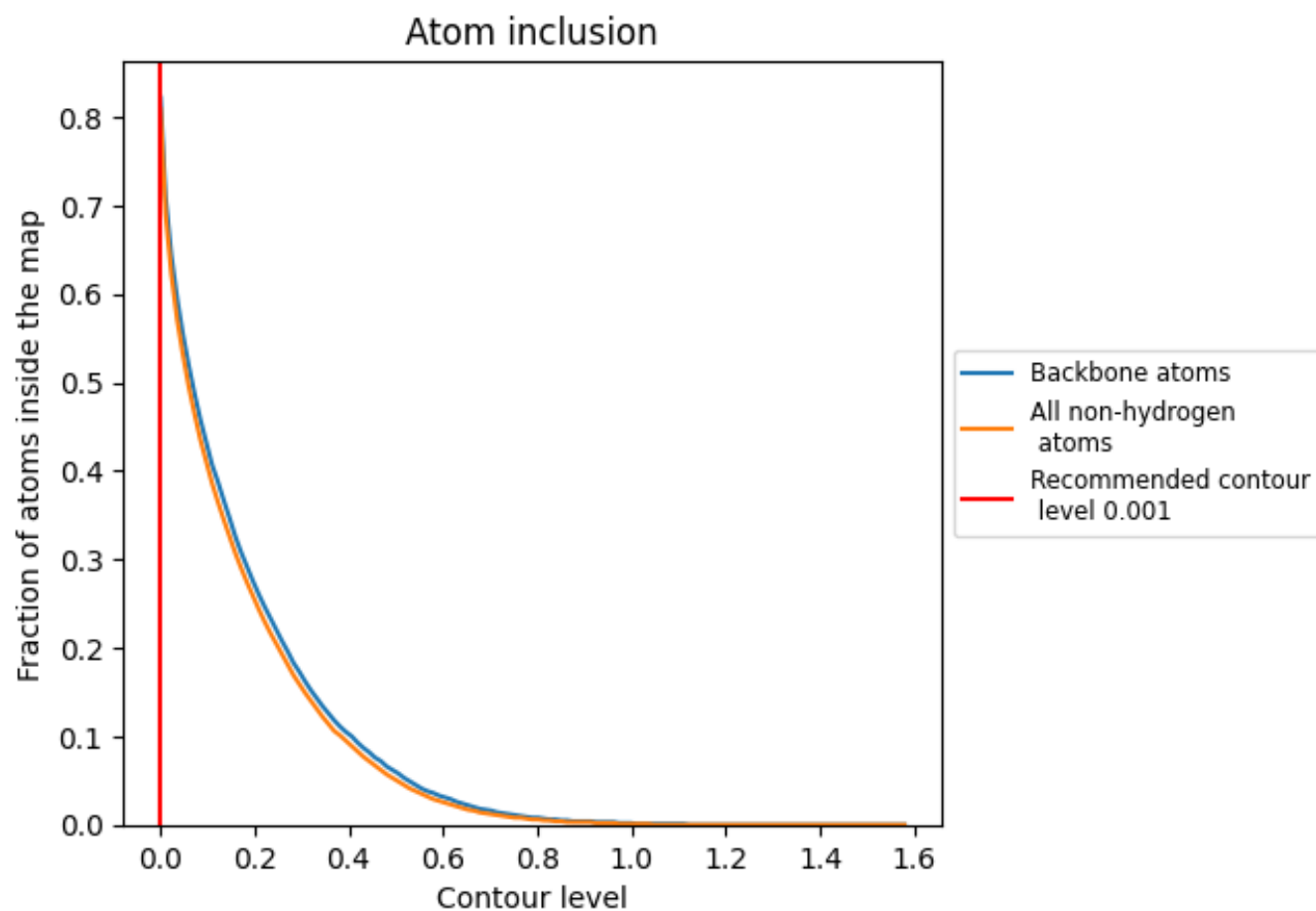


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 81% 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 (0.001) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8090	-0.0460
A	0.9260	-0.0310
B	0.9260	-0.0180
C	0.9060	-0.0630
D	0.9340	-0.0360
E	0.8300	-0.0350
F	0.8830	-0.0290
G	0.8990	-0.0550
H	0.8320	-0.0380
I	0.6900	-0.0510
L	0.8060	-0.0670
M	0.4850	-0.0560
R	0.9640	-0.0260

1.0
0.0
-0.0