Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 07:43 AM UTC

PDB ID	:	8H3A / pdb_00008h3a
EMDB ID	:	EMD-34462
Title	:	Cryo-EM Structure of the KBTBD2-CRL3 N8(removed)-CSN complex
Authors	:	Hu, Y.; Mao, Q.; Chen, Z.; Sun, L.
Deposited on	:	2022-10-08
Resolution	:	7.51 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

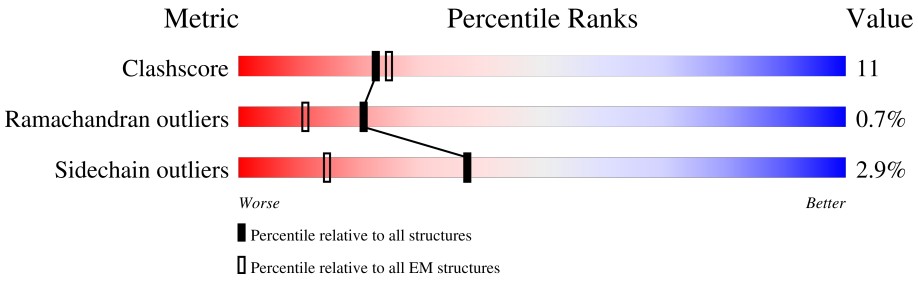
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.51 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 <=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	33% 69% 19% · 7%
2	A	527	· 58% 20% 22%
3	B	443	· 63% 31% 5%
4	C	423	7% 76% 18% · ·
5	D	406	73% 26% ·
6	F	327	17% 63% 25% 12%
7	G	264	· 68% 13% 19%
8	H	209	5% 69% 16% 15%

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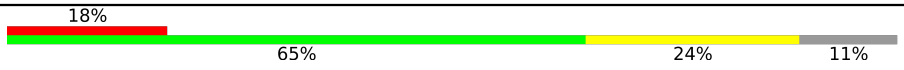
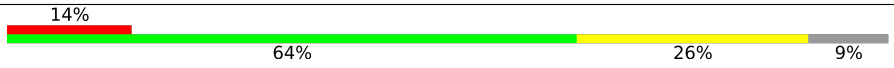
Mol	Chain	Length	Quality of chain
9	I	623	
9	M	623	
10	L	768	
11	R	108	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 36704 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		

- 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	556	Total	C	N	O	S	0	0
			4500	2875	745	842	38		
9	M	564	Total	C	N	O	S	0	0
			4559	2912	758	851	38		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	252	ASP	SER	engineered mutation	UNP Q8IY47
M	252	ASP	SER	engineered mutation	UNP Q8IY47

- Molecule 10 is a protein called Cullin-3.

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

- Molecule 11 is a protein called E3 ubiquitin-protein ligase RBX1.

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

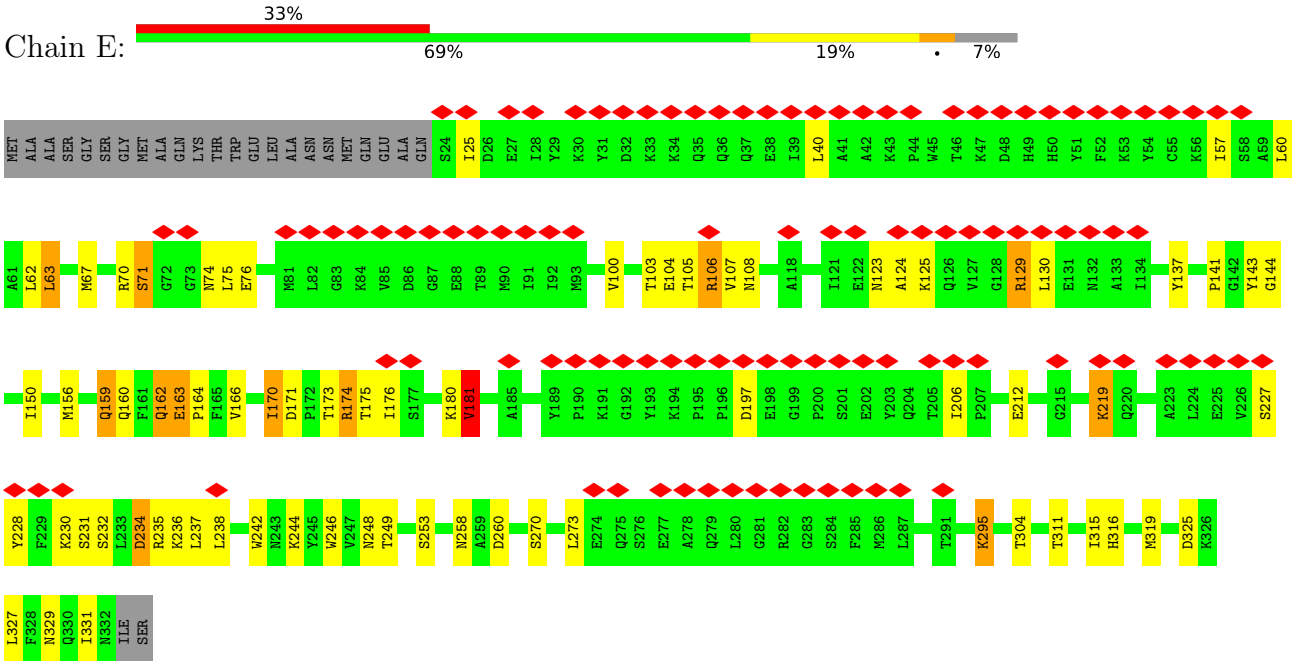
- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

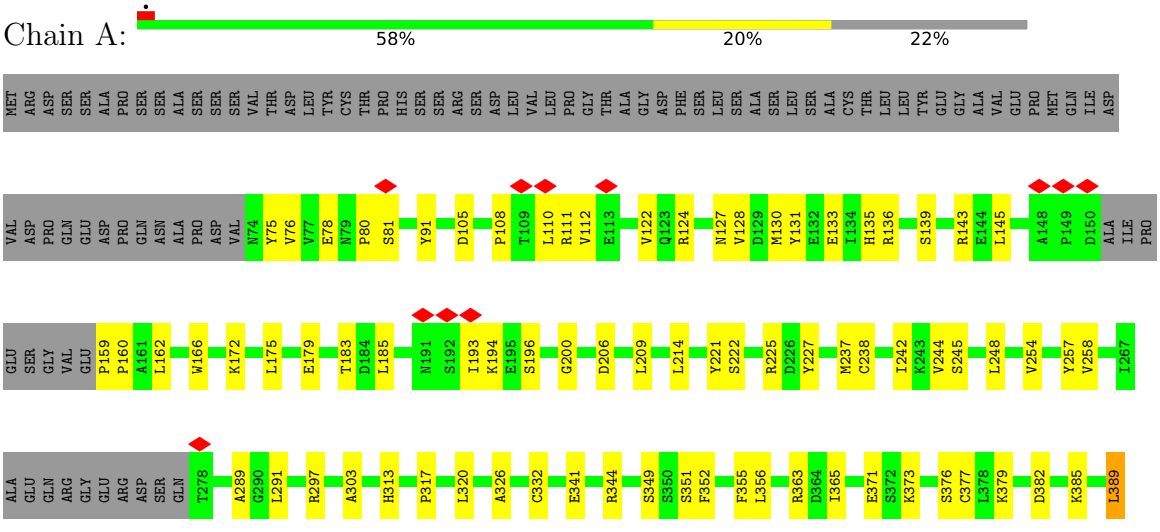
3 Residue-property plots (i)

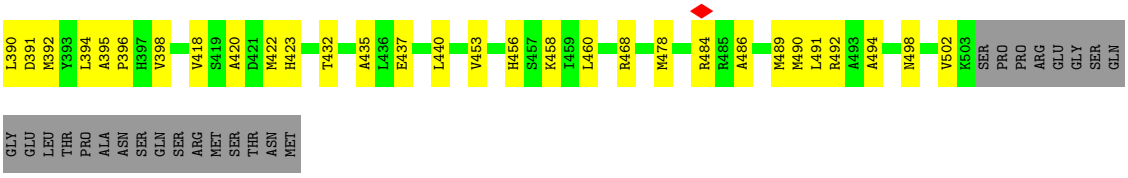
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: COP9 signalosome complex subunit 5



• Molecule 2: COP9 signalosome complex subunit 1

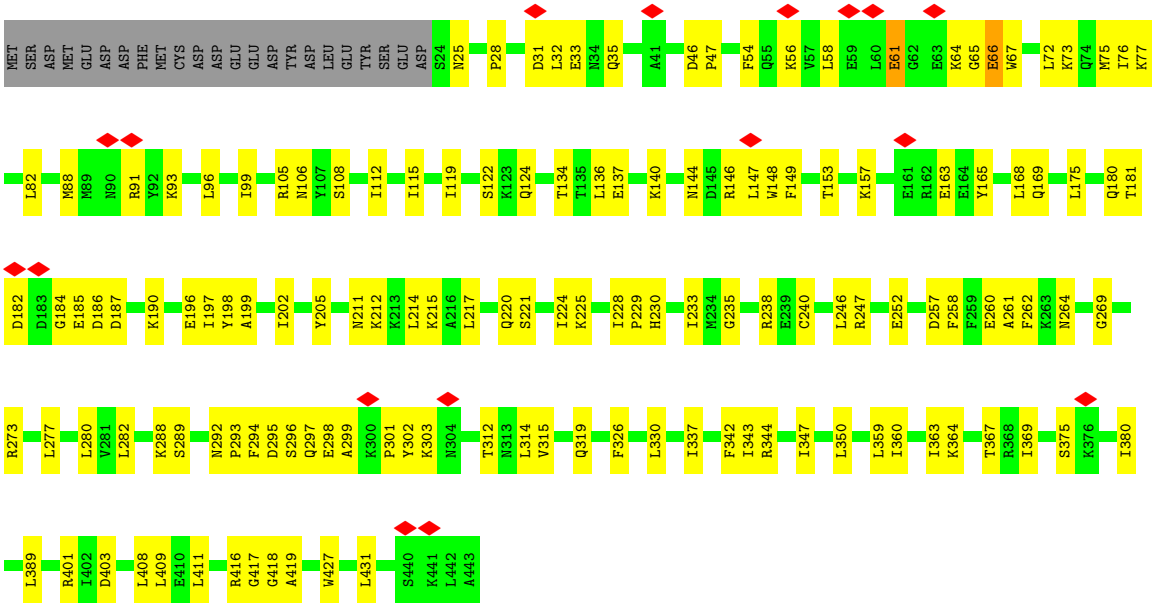




• Molecule 3: COP9 signalosome complex subunit 2

Chain B:

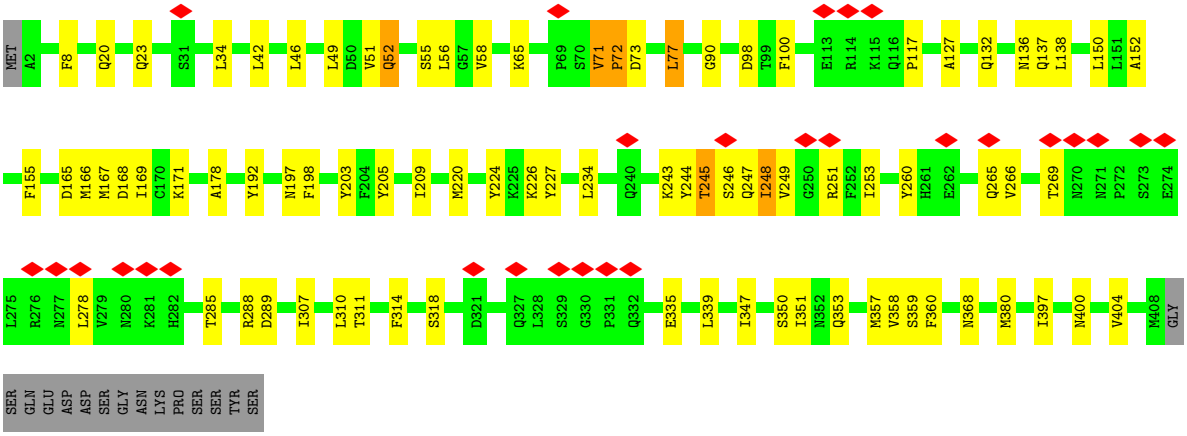




• Molecule 4: COP9 signalosome complex subunit 3

Chain C:

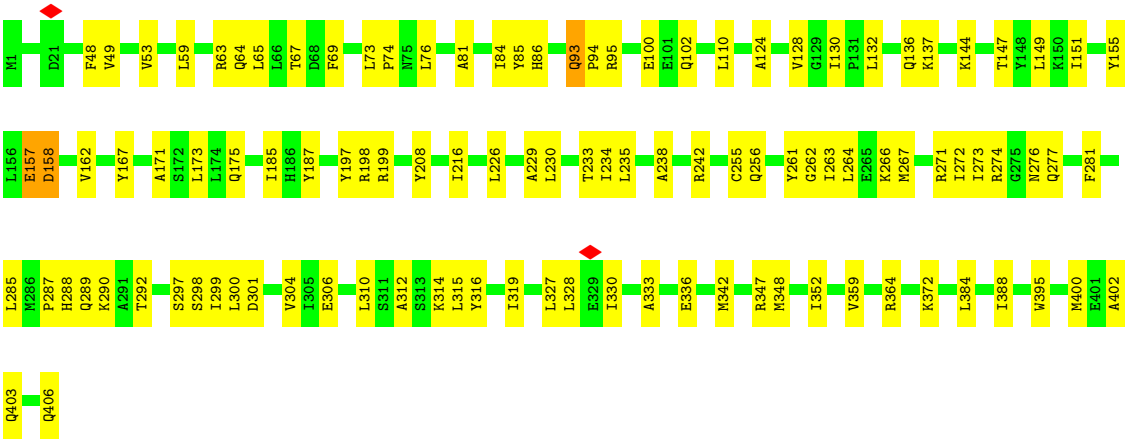




• Molecule 5: COP9 signalosome complex subunit 4

Chain D:

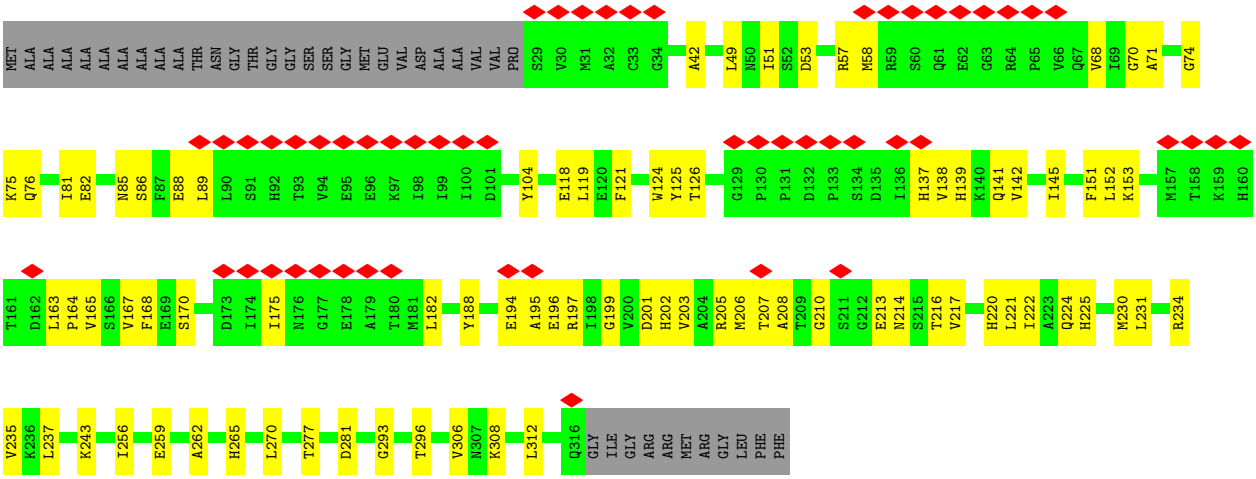




• Molecule 6: COP9 signalosome complex subunit 6

Chain F:

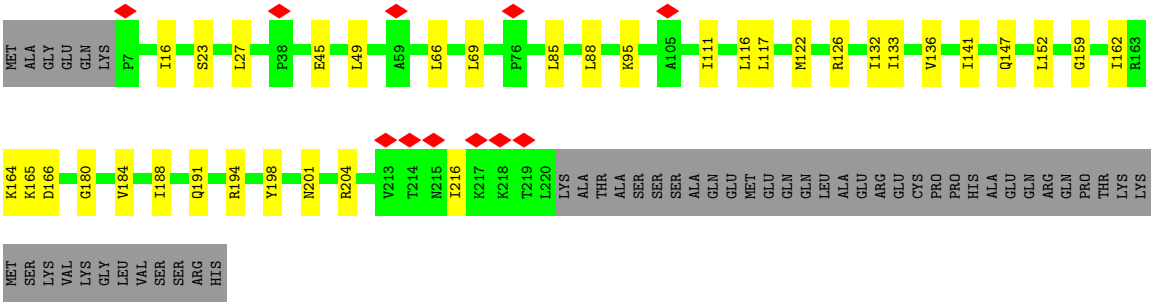




• Molecule 7: COP9 signalosome complex subunit 7b

Chain G:

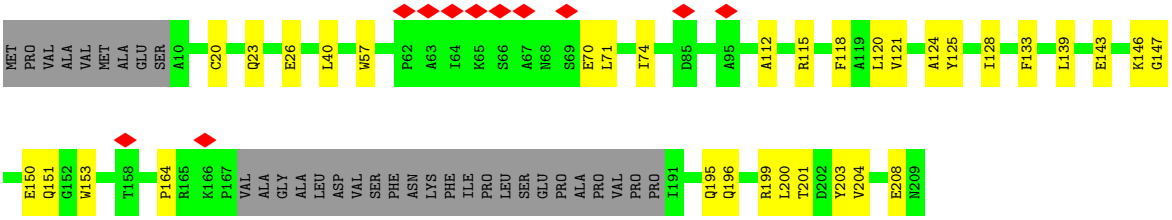




• Molecule 8: COP9 signalosome complex subunit 8

Chain H:

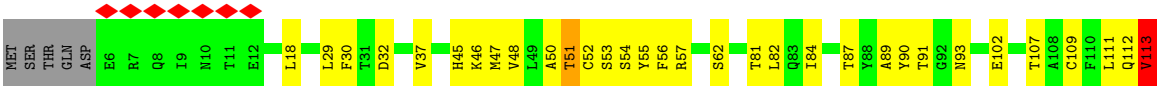


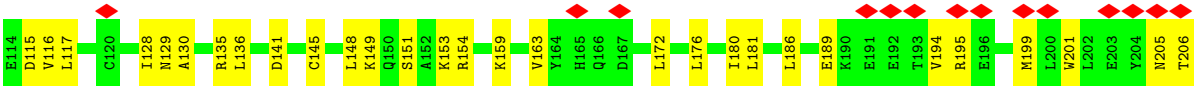


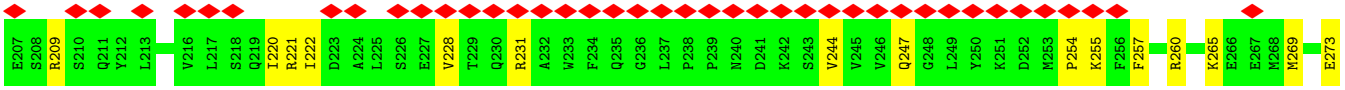
• Molecule 9: Kelch repeat and BTB domain-containing protein 2

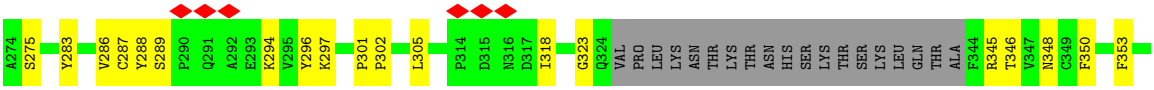
Chain I:

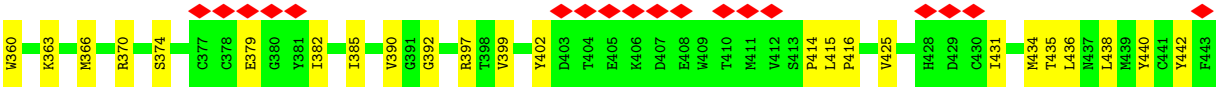


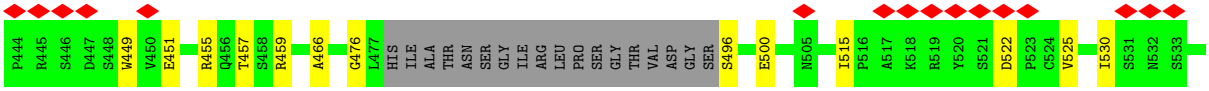


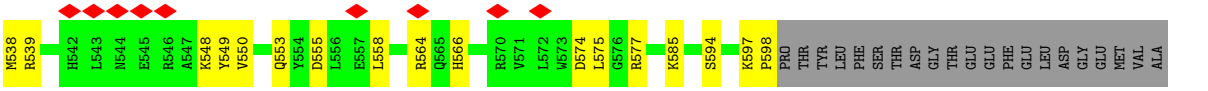






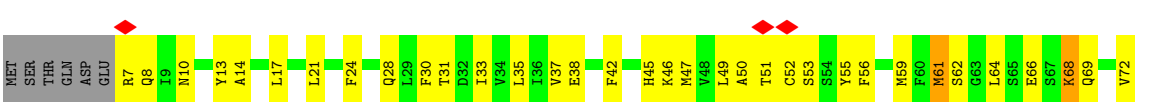


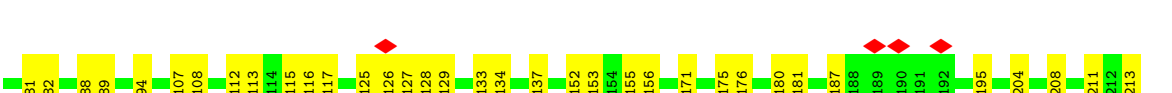








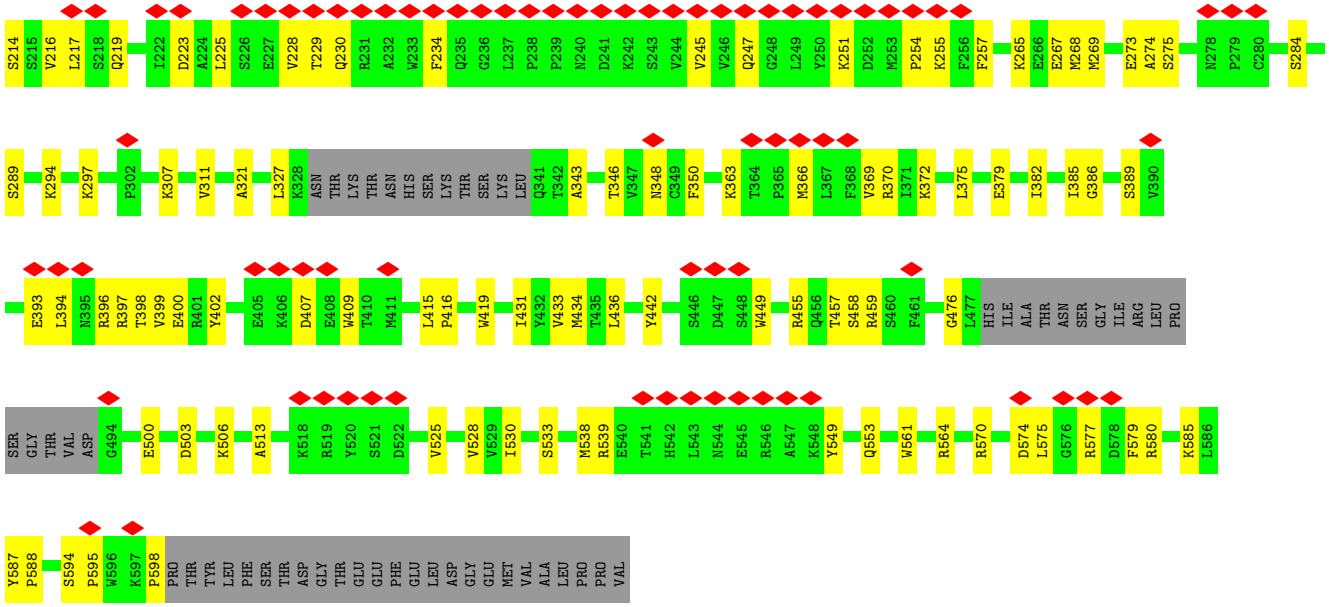






• Molecule 9: Kelch repeat and BTB domain-containing protein 2

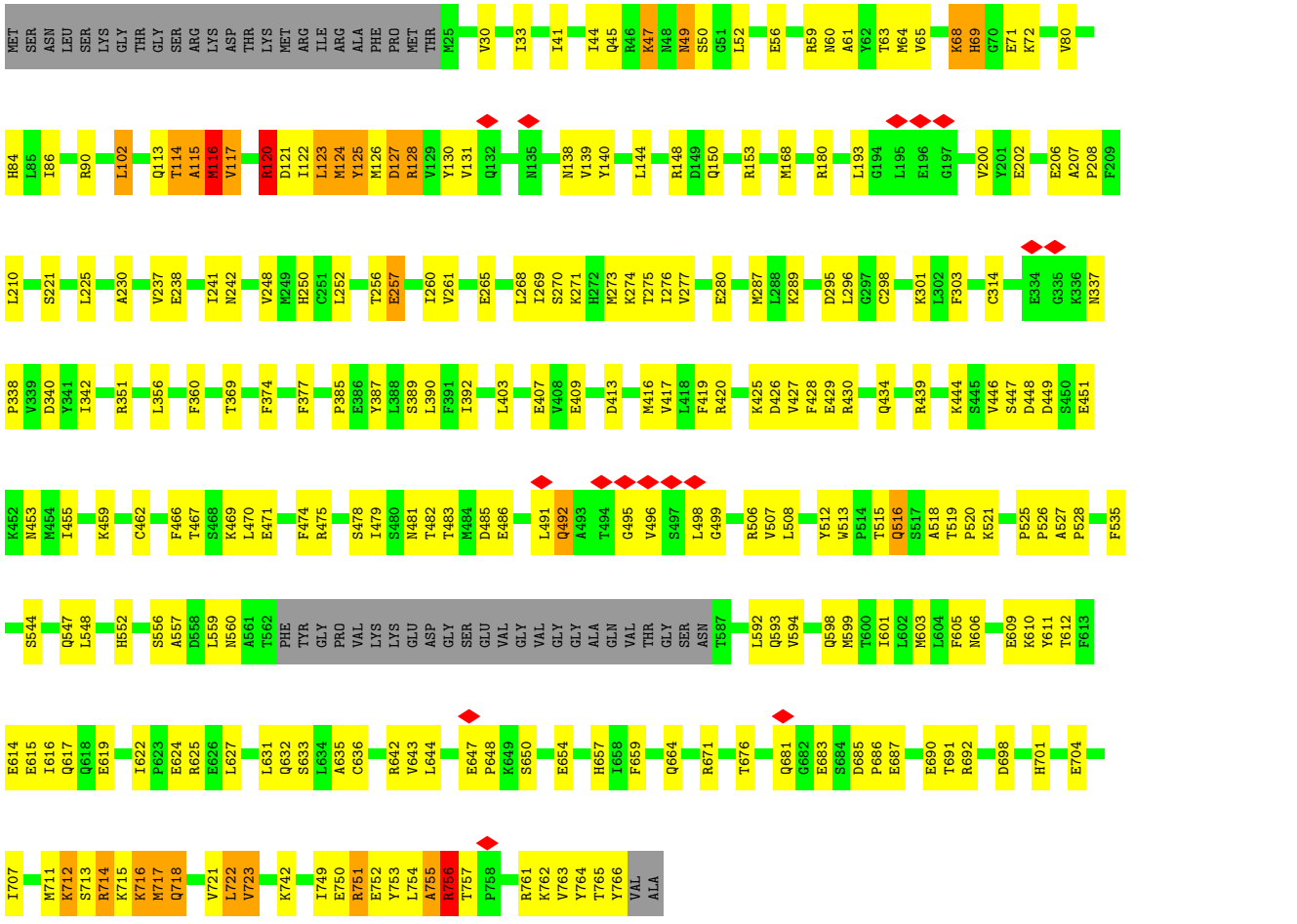
Chain M:



• Molecule 10: Cullin-3

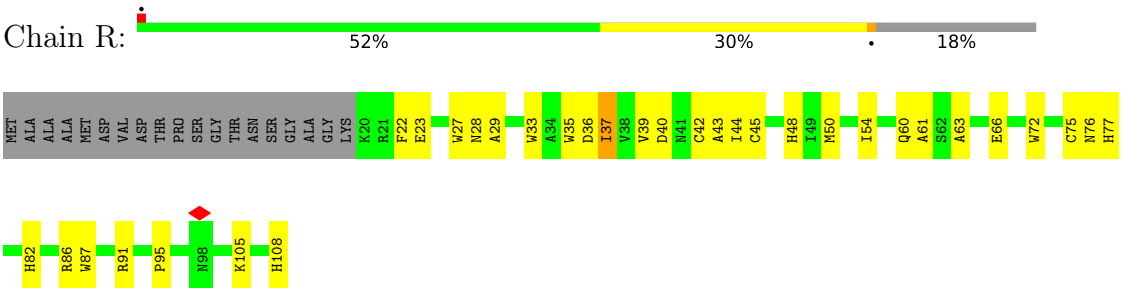
Chain L:





• Molecule 11: E3 ubiquitin-protein ligase RBX1

Chain R:


52%
30%
18%
MET ALA ALA ALA MET ASP VAL ASP THR PRO SER GLY THR ASN SER GLY ALA GLY LYS K20 R21 F22 E23 W27 N28 A29 W33 A34 W35 D36 I37 V38 V39 D40 N41 C42 A43 I44 C45 H48 I49 M50 I54 Q60 A61 S62 A63 E66 W72 C75 N76 H77
H82 R86 W87 R91 P95 N98 K105 H108

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	55391	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 ($e^-/Å^2$)	53	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	1.725	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	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	0.76	0/2511	0.94	4/3392 (0.1%)
2	A	0.22	0/3352	0.40	0/4520
3	B	0.22	0/3489	0.48	0/4696
4	C	0.16	0/3294	0.39	1/4448 (0.0%)
5	D	0.23	0/3303	0.47	1/4460 (0.0%)
6	F	0.22	0/2326	0.38	0/3153
7	G	0.11	0/1713	0.30	0/2318
8	H	0.10	0/1445	0.30	0/1965
9	I	0.22	0/4606	0.42	1/6246 (0.0%)
9	M	0.17	0/4666	0.38	0/6327
10	L	0.42	3/5946 (0.1%)	0.59	5/7989 (0.1%)
11	R	0.15	0/759	0.47	0/1029
All	All	0.31	3/37410 (0.0%)	0.49	12/50543 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	116	MET	C-O	-6.13	1.16	1.24
10	L	122	ILE	C-O	5.32	1.30	1.24
10	L	120	ARG	C-O	-5.13	1.17	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	390	VAL	N-CA-C	-6.81	107.24	113.71
4	C	245	THR	CB-CA-C	-6.52	107.29	115.89
1	E	144	GLY	CA-C-O	-5.97	118.11	122.23
10	L	131	VAL	N-CA-C	-5.71	107.21	113.43
5	D	158	ASP	N-CA-C	-5.69	106.18	113.23
10	L	125	TYR	N-CA-C	-5.42	105.93	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	175	THR	N-CA-C	-5.36	106.00	112.54
10	L	718	GLN	N-CA-C	-5.14	106.35	113.18
1	E	159	GLN	N-CA-C	-5.12	107.20	113.50
10	L	115	ALA	N-CA-C	-5.11	104.97	111.11
10	L	492	GLN	N-CA-C	-5.02	105.89	111.36
1	E	143	TYR	CB-CA-C	5.01	118.36	109.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2457	0	2428	48	0
2	A	3296	0	3336	77	0
3	B	3430	0	3459	99	0
4	C	3235	0	3257	68	0
5	D	3251	0	3253	78	0
6	F	2279	0	2263	78	0
7	G	1692	0	1730	25	0
8	H	1411	0	1395	25	0
9	I	4500	0	4399	116	0
9	M	4559	0	4472	122	0
10	L	5853	0	5890	175	0
11	R	737	0	693	33	0
12	E	1	0	0	0	0
12	R	3	0	0	0	0
All	All	36704	0	36575	826	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 11.

All (826) 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:63:LEU:CD2	6:F:203:VAL:HG21	1.50	1.38
10:L:41:ILE:CG2	10:L:80:VAL:HG11	1.64	1.25
1:E:63:LEU:HD21	6:F:203:VAL:HG21	1.21	1.14
1:E:70:ARG:HG2	6:F:195:ALA:HB1	1.20	1.12
1:E:67:MET:HE1	6:F:196:GLU:HG2	1.11	1.07
1:E:63:LEU:HD22	6:F:203:VAL:HG21	1.32	1.06
10:L:41:ILE:HG21	10:L:80:VAL:CG1	1.86	1.04
1:E:124:ALA:HB1	1:E:129:ARG:HB2	1.43	1.00
1:E:70:ARG:CG	6:F:195:ALA:HB1	1.97	0.95
1:E:67:MET:HE1	6:F:196:GLU:CG	1.97	0.94
1:E:63:LEU:CD2	6:F:203:VAL:CG2	2.44	0.94
1:E:67:MET:CE	6:F:196:GLU:HG2	1.96	0.94
1:E:70:ARG:HG2	6:F:195:ALA:CB	2.00	0.92
10:L:41:ILE:HG21	10:L:80:VAL:HG11	0.91	0.86
1:E:63:LEU:HD21	6:F:203:VAL:CG2	2.07	0.83
10:L:123:LEU:HB3	10:L:139:VAL:HG11	1.60	0.82
10:L:127:ASP:HA	10:L:130:TYR:HB2	1.63	0.81
10:L:41:ILE:CG2	10:L:80:VAL:CG1	2.50	0.80
3:B:293:PRO:HD2	3:B:315:VAL:HG11	1.65	0.78
2:A:258:VAL:HG11	2:A:289:ALA:HB2	1.67	0.76
10:L:469:LYS:HE3	10:L:512:TYR:HA	1.66	0.76
11:R:60:GLN:CD	11:R:61:ALA:H	1.93	0.76
10:L:592:LEU:HD21	10:L:643:VAL:HG11	1.68	0.75
1:E:273:LEU:HD12	3:B:431:LEU:HD13	1.67	0.75
5:D:238:ALA:HA	5:D:242:ARG:HD3	1.69	0.74
9:I:205:ASN:HB3	9:I:209:ARG:HG3	1.70	0.74
2:A:127:ASN:HD21	2:A:130:MET:HB2	1.53	0.74
1:E:63:LEU:HD22	6:F:203:VAL:CG2	2.15	0.74
10:L:221:SER:HB3	10:L:268:LEU:HG	1.70	0.74
3:B:31:ASP:O	3:B:35:GLN:NE2	2.20	0.73
10:L:45:GLN:CD	10:L:84:HIS:HB2	2.14	0.73
2:A:124:ARG:HG2	9:I:346:THR:H	1.53	0.72
5:D:100:GLU:H	5:D:137:LYS:HE3	1.54	0.72
6:F:210:GLY:HA3	6:F:214:ASN:H	1.54	0.72
4:C:339:LEU:HD11	8:H:120:LEU:HB3	1.73	0.71
9:I:46:LYS:HB3	9:M:30:PHE:HD2	1.55	0.71
1:E:234:ASP:HB2	6:F:207:THR:HG22	1.72	0.71
9:I:29:LEU:HB3	9:I:30:PHE:HD1	1.53	0.71
10:L:385:PRO:HB3	10:L:428:PHE:HB2	1.72	0.70
9:I:47:MET:HG2	9:M:21:LEU:HD22	1.73	0.69
2:A:490:MET:HG2	4:C:167:MET:HE2	1.73	0.69
10:L:749:ILE:HA	10:L:755:ALA:HB1	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:714:ARG:HE	10:L:715:LYS:H	1.41	0.69
10:L:559:LEU:HB3	10:L:592:LEU:HB2	1.75	0.69
1:E:60:LEU:HD22	6:F:53:ASP:CG	2.18	0.69
5:D:132:LEU:HD22	5:D:144:LYS:HG2	1.75	0.69
9:M:187:ASN:ND2	9:M:587:TYR:OH	2.26	0.69
1:E:315:ILE:HD13	8:H:203:TYR:HB3	1.75	0.68
5:D:266:LYS:HB3	5:D:271:ARG:HD3	1.75	0.68
9:I:434:MET:HE2	9:I:455:ARG:HE	1.58	0.68
9:I:348:ASN:ND2	9:I:366:MET:O	2.27	0.67
1:E:325:ASP:OD1	1:E:329:ASN:ND2	2.27	0.67
5:D:136:GLN:HA	10:L:521:LYS:HD2	1.77	0.66
5:D:198:ARG:O	5:D:199:ARG:NH1	2.28	0.66
10:L:206:GLU:O	10:L:210:LEU:N	2.20	0.66
10:L:749:ILE:HG12	10:L:756:ARG:HB2	1.78	0.66
9:I:151:SER:HA	9:I:154:ARG:HE	1.60	0.66
2:A:394:LEU:HG	2:A:398:VAL:HB	1.78	0.65
10:L:624:GLU:HG3	10:L:625:ARG:H	1.62	0.65
9:M:297:LYS:HZ1	9:M:595:PRO:HD3	1.62	0.65
1:E:70:ARG:CG	6:F:195:ALA:CB	2.70	0.65
3:B:211:ASN:OD1	3:B:247:ARG:NH1	2.29	0.65
2:A:489:MET:HE2	6:F:306:VAL:HG22	1.79	0.65
9:I:91:THR:HG23	9:I:93:ASN:H	1.60	0.65
3:B:273:ARG:NH1	3:B:302:TYR:OH	2.29	0.65
1:E:331:ILE:HD11	7:G:180:GLY:HA3	1.79	0.64
4:C:205:TYR:HB3	4:C:227:TYR:HB2	1.80	0.64
5:D:76:LEU:HD22	5:D:81:ALA:HB2	1.79	0.64
2:A:356:LEU:HB3	2:A:363:ARG:HB2	1.77	0.64
9:I:47:MET:HE3	9:M:45:HIS:CE1	2.33	0.64
11:R:37:ILE:HG12	11:R:76:ASN:ND2	2.13	0.64
3:B:296:SER:HB2	11:R:77:HIS:HD2	1.62	0.64
10:L:225:LEU:HD22	10:L:275:THR:HG21	1.80	0.64
9:I:54:SER:HB2	9:I:113:VAL:HG13	1.80	0.64
9:M:17:LEU:O	9:M:21:LEU:HG	1.98	0.64
4:C:51:VAL:HA	4:C:55:SER:HB3	1.78	0.63
10:L:273:MET:O	10:L:277:VAL:HG22	1.98	0.63
9:M:153:LYS:HE2	9:M:180:ILE:HA	1.79	0.63
2:A:468:ARG:HH22	6:F:281:ASP:HA	1.63	0.63
9:I:436:LEU:O	9:I:455:ARG:NH2	2.32	0.63
4:C:226:LYS:NZ	4:C:289:ASP:OD1	2.32	0.63
10:L:144:LEU:HD12	10:L:193:LEU:HA	1.81	0.63
9:M:52:CYS:SG	9:M:53:SER:N	2.72	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:93:GLN:HG3	5:D:94:PRO:HD3	1.80	0.63
3:B:106:ASN:ND2	10:L:446:VAL:O	2.32	0.62
3:B:221:SER:O	3:B:225:LYS:HB3	1.99	0.62
9:I:89:ALA:HA	9:M:13:TYR:CE1	2.34	0.62
9:M:254:PRO:O	9:M:255:LYS:HG2	1.99	0.62
10:L:90:ARG:NH2	10:L:150:GLN:OE1	2.32	0.62
3:B:363:ILE:HD12	3:B:369:ILE:HG21	1.82	0.62
1:E:270:SER:HA	3:B:431:LEU:HD11	1.81	0.62
3:B:260:GLU:O	3:B:264:ASN:ND2	2.31	0.62
9:I:45:HIS:HB2	9:I:48:VAL:HG22	1.81	0.62
9:M:28:GLN:NE2	9:M:31:THR:OG1	2.30	0.62
9:I:128:ILE:HG12	9:I:136:LEU:HD21	1.82	0.62
9:I:129:ASN:OD1	9:I:130:ALA:N	2.28	0.62
10:L:125:TYR:HD1	9:M:112:GLN:HG3	1.64	0.61
2:A:139:SER:HA	2:A:160:PRO:HD2	1.82	0.61
2:A:162:LEU:HD12	2:A:166:TRP:HE1	1.65	0.61
3:B:282:LEU:HD22	3:B:343:ILE:HG12	1.82	0.61
10:L:455:ILE:HG22	10:L:470:LEU:HD23	1.83	0.61
9:M:217:LEU:HD13	9:M:225:LEU:HD11	1.83	0.61
5:D:173:LEU:HD11	11:R:108:HIS:HD2	1.64	0.61
9:I:273:GLU:HA	9:I:283:TYR:HB3	1.83	0.61
2:A:222:SER:O	2:A:225:ARG:HG2	2.01	0.61
9:M:214:SER:O	9:M:251:LYS:NZ	2.33	0.61
9:M:393:GLU:HG3	9:M:394:LEU:H	1.65	0.60
11:R:87:TRP:HA	11:R:91:ARG:HH21	1.65	0.60
2:A:371:GLU:OE1	2:A:373:LYS:NZ	2.34	0.60
11:R:75:CYS:SG	11:R:77:HIS:ND1	2.63	0.60
2:A:297:ARG:HH12	2:A:396:PRO:HB2	1.66	0.60
4:C:132:GLN:HB2	4:C:137:GLN:HB2	1.83	0.60
9:I:30:PHE:CG	9:M:50:ALA:HB2	2.37	0.60
10:L:498:LEU:HG	10:L:499:GLY:H	1.67	0.60
9:M:171:GLN:NE2	9:M:204:TYR:OH	2.34	0.60
9:M:269:MET:HE3	9:M:530:ILE:HD12	1.83	0.60
3:B:181:THR:OG1	3:B:187:ASP:OD1	2.20	0.60
6:F:194:GLU:OE2	6:F:197:ARG:NH2	2.22	0.60
10:L:622:ILE:HG12	10:L:627:LEU:HD13	1.81	0.60
9:I:201:TRP:O	9:I:209:ARG:NH2	2.35	0.60
10:L:409:GLU:OE2	10:L:453:ASN:ND2	2.34	0.60
9:M:37:VAL:HG12	9:M:38:GLU:HG2	1.83	0.60
9:I:431:ILE:HB	9:I:442:TYR:HB3	1.84	0.60
3:B:363:ILE:HG22	3:B:411:LEU:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:243:LYS:HA	4:C:245:THR:HG23	1.83	0.60
9:M:225:LEU:O	9:M:230:GLN:NE2	2.35	0.60
2:A:352:PHE:HA	2:A:355:PHE:HB2	1.83	0.60
9:M:47:MET:O	9:M:50:ALA:HB3	2.02	0.60
4:C:397:ILE:HG21	6:F:308:LYS:HB3	1.83	0.59
5:D:67:THR:OG1	5:D:102:GLN:NE2	2.34	0.59
5:D:230:LEU:HD13	5:D:264:LEU:HD13	1.83	0.59
3:B:199:ALA:HB2	3:B:233:ILE:HG23	1.83	0.59
9:I:265:LYS:HB3	9:I:585:LYS:HD3	1.84	0.59
10:L:356:LEU:HD12	10:L:360:PHE:HB2	1.84	0.59
9:M:350:PHE:HD2	9:M:363:LYS:HB2	1.67	0.59
2:A:494:ALA:HB1	4:C:169:ILE:H	1.66	0.59
9:I:46:LYS:HB3	9:M:30:PHE:CD2	2.37	0.59
10:L:439:ARG:HD3	10:L:446:VAL:HG11	1.84	0.59
9:I:525:VAL:HA	9:I:538:MET:HG2	1.83	0.59
10:L:698:ASP:HA	10:L:701:HIS:CD2	2.38	0.59
10:L:180:ARG:HH22	10:L:250:HIS:HB3	1.68	0.59
5:D:238:ALA:HB3	5:D:306:GLU:HB3	1.83	0.58
9:I:555:ASP:HB3	9:I:558:LEU:HB2	1.85	0.58
3:B:292:ASN:HB2	3:B:319:GLN:HE21	1.68	0.58
3:B:165:TYR:HA	3:B:168:LEU:HB3	1.85	0.58
5:D:400:MET:SD	5:D:403:GLN:NE2	2.76	0.58
3:B:99:ILE:HG12	3:B:108:SER:HB2	1.84	0.58
10:L:269:ILE:O	10:L:273:MET:HB3	2.04	0.58
9:M:539:ARG:HH22	9:M:577:ARG:HD3	1.67	0.58
10:L:30:VAL:HB	10:L:64:MET:HE1	1.86	0.58
9:I:186:LEU:HD13	9:I:194:VAL:HG11	1.86	0.58
9:M:370:ARG:NH1	9:M:386:GLY:O	2.35	0.58
9:M:436:LEU:O	9:M:455:ARG:NH2	2.37	0.58
3:B:403:ASP:HB3	3:B:408:LEU:HB3	1.85	0.58
3:B:163:GLU:OE1	3:B:165:TYR:OH	2.22	0.57
3:B:292:ASN:H	11:R:43:ALA:HB1	1.69	0.57
10:L:252:LEU:HB3	10:L:256:THR:HG21	1.85	0.57
11:R:63:ALA:HB1	11:R:66:GLU:HA	1.85	0.57
3:B:180:GLN:HG2	3:B:185:GLU:HA	1.86	0.57
4:C:318:SER:HA	4:C:357:MET:HA	1.85	0.57
4:C:220:MET:HG2	4:C:253:ILE:HD11	1.86	0.57
4:C:248:ILE:HD12	4:C:251:ARG:HD2	1.85	0.57
2:A:418:VAL:HB	3:B:401:ARG:HD2	1.87	0.57
4:C:266:VAL:HG21	4:C:278:LEU:HD22	1.86	0.57
5:D:256:GLN:HA	5:D:261:TYR:CG	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:417:VAL:HG13	10:L:420:ARG:HH21	1.69	0.57
9:M:459:ARG:HB3	9:M:476:GLY:HA3	1.86	0.57
10:L:45:GLN:NE2	10:L:80:VAL:HG12	2.20	0.57
10:L:598:GLN:HA	10:L:601:ILE:HD12	1.87	0.57
5:D:149:LEU:HD21	5:D:187:TYR:HA	1.87	0.57
9:M:35:LEU:HB2	9:M:42:PHE:HB2	1.86	0.57
3:B:289:SER:OG	11:R:91:ARG:NH1	2.37	0.57
10:L:44:ILE:HG23	10:L:49:ASN:HB3	1.87	0.57
6:F:163:LEU:HD12	6:F:164:PRO:HD2	1.87	0.57
10:L:113:GLN:HA	10:L:116:MET:HE2	1.87	0.57
9:M:431:ILE:HB	9:M:442:TYR:HB3	1.87	0.57
3:B:299:ALA:O	3:B:303:LYS:N	2.31	0.57
10:L:711:MET:HG3	10:L:722:LEU:HD13	1.86	0.57
5:D:342:MET:HE2	5:D:348:MET:HB2	1.87	0.56
9:M:385:ILE:HA	9:M:399:VAL:HG12	1.85	0.56
9:I:382:ILE:HB	9:I:402:TYR:HB3	1.87	0.56
9:M:553:GLN:HB2	9:M:564:ARG:HB2	1.86	0.56
6:F:220:HIS:O	6:F:224:GLN:NE2	2.38	0.56
10:L:556:SER:OG	11:R:28:ASN:ND2	2.35	0.56
9:M:434:MET:HE2	9:M:455:ARG:HE	1.69	0.56
5:D:266:LYS:HD3	5:D:271:ARG:HH11	1.71	0.56
9:M:455:ARG:NH1	9:M:500:GLU:OE2	2.38	0.56
5:D:281:PHE:HB3	5:D:300:LEU:HD11	1.87	0.56
3:B:187:ASP:HB2	3:B:190:LYS:HB2	1.87	0.56
4:C:165:ASP:CG	4:C:167:MET:HE1	2.30	0.56
10:L:287:MET:HE3	10:L:295:ASP:HB3	1.88	0.56
10:L:444:LYS:HG2	10:L:506:ARG:HH22	1.70	0.56
2:A:313:HIS:HE1	2:A:355:PHE:HZ	1.54	0.56
4:C:46:LEU:HD22	4:C:58:VAL:HG13	1.87	0.56
4:C:397:ILE:HG23	6:F:312:LEU:HD12	1.87	0.56
9:M:52:CYS:HB3	9:M:89:ALA:HB2	1.87	0.56
1:E:258:ASN:ND2	1:E:260:ASP:OD2	2.39	0.56
5:D:48:PHE:HZ	5:D:65:LEU:HB3	1.70	0.56
10:L:273:MET:HG3	10:L:303:PHE:HE2	1.71	0.56
10:L:270:SER:HA	10:L:273:MET:HE2	1.88	0.55
10:L:632:GLN:HB2	10:L:636:CYS:HB3	1.88	0.55
5:D:384:LEU:HD21	6:F:259:GLU:HB3	1.88	0.55
9:I:32:ASP:HB3	9:M:46:LYS:HD2	1.87	0.55
3:B:72:LEU:HD22	3:B:91:ARG:HB3	1.88	0.55
3:B:96:LEU:HA	3:B:99:ILE:HD12	1.89	0.55
3:B:146:ARG:HA	3:B:149:PHE:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:475:ARG:O	10:L:479:ILE:HG12	2.06	0.55
3:B:360:ILE:O	3:B:364:LYS:HG3	2.06	0.55
8:H:195:GLN:HB3	8:H:199:ARG:HH21	1.71	0.55
3:B:416:ARG:HD2	3:B:418:GLY:H	1.71	0.55
3:B:359:LEU:O	3:B:363:ILE:HG12	2.07	0.55
9:I:48:VAL:HG21	9:I:90:TYR:CZ	2.42	0.55
9:M:137:LEU:HB2	9:M:156:VAL:HG21	1.88	0.55
2:A:206:ASP:OD1	2:A:221:TYR:OH	2.24	0.55
9:M:419:TRP:HZ3	9:M:433:VAL:HG13	1.72	0.55
10:L:116:MET:O	10:L:117:VAL:C	2.49	0.55
10:L:434:GLN:NE2	10:L:687:GLU:OE1	2.40	0.55
5:D:173:LEU:HD11	11:R:108:HIS:CD2	2.41	0.55
9:I:89:ALA:HA	9:M:13:TYR:HE1	1.72	0.55
10:L:45:GLN:NE2	10:L:84:HIS:HB2	2.22	0.55
2:A:185:LEU:HD13	2:A:200:GLY:HA3	1.88	0.54
6:F:57:ARG:NH2	6:F:88:GLU:OE2	2.37	0.54
6:F:75:LYS:HE2	6:F:118:GLU:HB3	1.89	0.54
5:D:197:TYR:HB3	5:D:198:ARG:NH2	2.22	0.54
9:I:459:ARG:HB3	9:I:476:GLY:HA3	1.89	0.54
9:M:195:ARG:HD3	9:M:229:THR:HG21	1.89	0.54
5:D:384:LEU:O	5:D:388:ILE:HG13	2.08	0.54
7:G:69:LEU:HD13	7:G:85:LEU:HD11	1.89	0.54
9:I:53:SER:HB2	9:I:111:LEU:HD13	1.88	0.54
9:I:228:VAL:HA	9:I:231:ARG:HD3	1.89	0.54
9:M:289:SER:HG	9:M:294:LYS:H	1.55	0.54
2:A:317:PRO:HG2	9:I:392:GLY:HA2	1.88	0.54
3:B:367:THR:HA	3:B:411:LEU:HD12	1.88	0.54
9:I:455:ARG:HD2	9:I:500:GLU:OE1	2.08	0.54
10:L:314:CYS:HB3	10:L:369:THR:HG21	1.90	0.54
9:M:273:GLU:OE2	9:M:307:LYS:N	2.41	0.54
9:M:213:LEU:HA	9:M:216:VAL:HG12	1.89	0.54
2:A:133:GLU:OE2	2:A:136:ARG:NH2	2.37	0.54
10:L:631:LEU:HD11	10:L:659:PHE:HE2	1.72	0.54
9:M:297:LYS:HB3	9:M:594:SER:HB2	1.89	0.54
1:E:327:LEU:HD12	7:G:184:VAL:HG21	1.89	0.54
7:G:23:SER:HA	7:G:27:LEU:HB2	1.89	0.54
9:M:126:LYS:NZ	9:M:407:ASP:OD2	2.41	0.54
2:A:183:THR:HA	9:M:8:GLN:HB2	1.89	0.54
4:C:65:LYS:HE3	4:C:72:PRO:HD3	1.90	0.54
9:I:181:LEU:HD21	9:I:220:ILE:HG13	1.90	0.54
9:M:370:ARG:NH2	9:M:398:THR:O	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:350:SER:O	4:C:359:SER:N	2.38	0.54
9:M:127:LYS:O	9:M:129:ASN:ND2	2.41	0.54
2:A:303:ALA:HB2	2:A:332:CYS:HB3	1.90	0.53
5:D:352:ILE:HG23	5:D:359:VAL:HG22	1.90	0.53
3:B:105:ARG:NH1	10:L:403:LEU:O	2.40	0.53
6:F:165:VAL:O	6:F:188:TYR:OH	2.26	0.53
9:I:476:GLY:O	9:I:496:SER:N	2.42	0.53
10:L:407:GLU:OE1	10:L:407:GLU:N	2.32	0.53
1:E:70:ARG:HE	6:F:195:ALA:HB2	1.73	0.53
2:A:242:ILE:HA	2:A:254:VAL:HG22	1.90	0.53
5:D:263:ILE:O	5:D:267:MET:HG2	2.09	0.53
6:F:71:ALA:HB1	6:F:121:PHE:HE1	1.74	0.53
9:I:30:PHE:HE2	9:M:56:PHE:HB2	1.73	0.53
9:I:45:HIS:ND1	9:I:90:TYR:OH	2.38	0.53
10:L:210:LEU:HD23	10:L:260:ILE:HD13	1.91	0.53
1:E:57:ILE:HB	1:E:228:TYR:CZ	2.44	0.53
9:I:141:ASP:HB2	9:I:149:LYS:HZ1	1.74	0.53
9:I:254:PRO:O	9:I:255:LYS:HG2	2.08	0.53
9:M:348:ASN:ND2	9:M:366:MET:O	2.42	0.53
2:A:194:LYS:HG2	2:A:227:TYR:HD2	1.74	0.53
3:B:122:SER:OG	3:B:124:GLN:NE2	2.41	0.53
3:B:198:TYR:O	3:B:202:ILE:HG12	2.09	0.53
10:L:337:ASN:HB3	10:L:340:ASP:HB2	1.90	0.53
1:E:270:SER:HB2	3:B:427:TRP:HD1	1.74	0.53
6:F:201:ASP:OD2	6:F:205:ARG:NH1	2.42	0.53
9:I:366:MET:HE1	9:I:370:ARG:HE	1.73	0.53
10:L:614:GLU:HA	10:L:617:GLN:HG2	1.90	0.53
4:C:198:PHE:HB2	4:C:234:LEU:HD13	1.91	0.53
7:G:16:ILE:HG12	7:G:49:LEU:HD11	1.91	0.53
9:I:50:ALA:HB2	9:M:30:PHE:CZ	2.44	0.53
9:M:49:LEU:HB3	9:M:56:PHE:CD2	2.44	0.53
9:M:275:SER:OG	9:M:574:ASP:O	2.27	0.53
6:F:202:HIS:NE2	6:F:206:MET:SD	2.82	0.53
10:L:657:HIS:HD2	10:L:659:PHE:CE1	2.27	0.53
9:I:550:VAL:HG23	9:I:566:HIS:HA	1.91	0.52
3:B:238:ARG:O	3:B:257:ASP:HB3	2.09	0.52
5:D:147:THR:O	5:D:151:ILE:HG13	2.09	0.52
9:I:374:SER:OG	9:I:385:ILE:O	2.24	0.52
9:I:553:GLN:HB2	9:I:564:ARG:HB2	1.92	0.52
2:A:395:ALA:HB3	2:A:396:PRO:HD3	1.92	0.52
4:C:247:GLN:O	4:C:249:VAL:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:437:GLU:OE1	2:A:458:LYS:NZ	2.42	0.52
5:D:402:ALA:O	5:D:406:GLN:NE2	2.43	0.52
9:I:548:LYS:NZ	9:I:549:TYR:O	2.42	0.52
11:R:39:VAL:HG22	11:R:40:ASP:H	1.75	0.52
5:D:235:LEU:HD22	5:D:299:ILE:HG23	1.91	0.52
9:I:29:LEU:HB3	9:I:30:PHE:CD1	2.40	0.52
7:G:111:ILE:O	7:G:152:LEU:N	2.38	0.52
9:I:302:PRO:HG2	9:I:305:LEU:HB3	1.92	0.52
6:F:124:TRP:HE1	6:F:139:HIS:HD1	1.58	0.52
10:L:451:GLU:O	10:L:455:ILE:HG12	2.09	0.52
5:D:93:GLN:H	5:D:94:PRO:CD	2.22	0.52
5:D:388:ILE:HG12	6:F:256:ILE:HG21	1.91	0.52
10:L:478:SER:HA	10:L:481:ASN:HD21	1.74	0.52
2:A:225:ARG:HB2	2:A:237:MET:SD	2.49	0.51
10:L:606:ASN:HD21	11:R:22:PHE:HB2	1.74	0.51
9:M:128:ILE:HG13	9:M:155:MET:HG2	1.91	0.51
9:M:570:ARG:HA	9:M:598:PRO:HB3	1.92	0.51
10:L:650:SER:OG	10:L:654:GLU:OE2	2.22	0.51
4:C:42:LEU:O	4:C:46:LEU:HG	2.11	0.51
5:D:395:TRP:HZ2	6:F:237:LEU:HB3	1.76	0.51
6:F:141:GLN:O	6:F:145:ILE:HG13	2.10	0.51
9:M:208:SER:O	9:M:211:GLN:NE2	2.43	0.51
2:A:214:LEU:HB3	2:A:248:LEU:HD21	1.93	0.51
3:B:31:ASP:OD1	3:B:32:LEU:N	2.43	0.51
3:B:153:THR:O	3:B:157:LYS:HG2	2.10	0.51
10:L:609:GLU:HG2	10:L:610:LYS:H	1.76	0.51
11:R:48:HIS:CD2	11:R:50:MET:H	2.27	0.51
6:F:138:VAL:HA	6:F:141:GLN:HE21	1.75	0.51
10:L:241:ILE:HG12	10:L:265:GLU:CD	2.36	0.51
9:M:33:ILE:HD11	9:M:72:VAL:HG13	1.93	0.51
3:B:115:ILE:O	3:B:119:ILE:HG12	2.11	0.51
5:D:69:PHE:O	5:D:73:LEU:HD23	2.10	0.51
6:F:51:ILE:HG12	6:F:125:TYR:CD1	2.46	0.51
10:L:557:ALA:HB3	10:L:594:VAL:HG23	1.93	0.51
2:A:245:SER:HB2	2:A:254:VAL:HG23	1.92	0.51
4:C:8:PHE:HB2	4:C:34:LEU:HD11	1.93	0.51
8:H:139:LEU:HB3	8:H:143:GLU:OE2	2.11	0.50
4:C:307:ILE:O	4:C:311:THR:HG23	2.11	0.50
6:F:151:PHE:HD2	6:F:168:PHE:HB2	1.75	0.50
8:H:196:GLN:O	8:H:200:LEU:HG	2.12	0.50
5:D:328:LEU:HB2	5:D:330:ILE:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:321:ALA:HB3	9:M:375:LEU:HD11	1.94	0.50
5:D:171:ALA:O	5:D:175:GLN:HB2	2.10	0.50
7:G:66:LEU:HD11	7:G:88:LEU:HD21	1.92	0.50
9:I:397:ARG:O	9:I:397:ARG:HG2	2.10	0.50
10:L:520:PRO:HG2	10:L:552:HIS:H	1.77	0.50
10:L:125:TYR:CD1	9:M:112:GLN:HG3	2.46	0.50
10:L:635:ALA:O	10:L:642:ARG:NH1	2.43	0.50
6:F:208:ALA:O	6:F:216:THR:HA	2.11	0.50
9:I:51:THR:HG21	9:M:17:LEU:HD12	1.93	0.50
9:I:350:PHE:HD2	9:I:363:LYS:HB2	1.77	0.50
9:M:115:ASP:OD1	9:M:116:VAL:N	2.44	0.50
1:E:25:ILE:HG23	1:E:231:SER:HA	1.94	0.50
4:C:335:GLU:OE2	4:C:353:GLN:NE2	2.45	0.50
10:L:448:ASP:N	10:L:451:GLU:OE1	2.44	0.50
10:L:515:THR:O	10:L:516:GLN:HB2	2.12	0.50
2:A:423:HIS:CE1	2:A:458:LYS:HB2	2.47	0.49
4:C:310:LEU:O	4:C:314:PHE:N	2.43	0.49
6:F:58:MET:HG3	6:F:68:VAL:HG12	1.93	0.49
2:A:175:LEU:O	2:A:179:GLU:HG2	2.12	0.49
4:C:266:VAL:O	4:C:269:THR:OG1	2.23	0.49
9:I:305:LEU:HD21	9:I:323:GLY:HA3	1.93	0.49
10:L:238:GLU:O	10:L:242:ASN:ND2	2.40	0.49
10:L:559:LEU:HD23	10:L:592:LEU:HD12	1.95	0.49
9:M:389:SER:OG	9:M:398:THR:OG1	2.22	0.49
3:B:228:ILE:HG12	10:L:455:ILE:HD12	1.94	0.49
9:I:287:CYS:N	9:I:296:TYR:O	2.38	0.49
9:I:385:ILE:HA	9:I:399:VAL:HG12	1.94	0.49
9:M:175:ASP:OD1	9:M:176:LEU:N	2.46	0.49
11:R:35:TRP:HB2	11:R:76:ASN:ND2	2.27	0.49
5:D:266:LYS:NZ	5:D:277:GLN:OE1	2.45	0.49
9:I:109:CYS:C	9:I:111:LEU:H	2.19	0.49
9:I:301:PRO:HG3	9:I:360:TRP:CE2	2.46	0.49
6:F:76:GLN:HG3	6:F:81:ILE:HG12	1.93	0.49
10:L:120:ARG:HG3	10:L:140:TYR:HD1	1.76	0.49
11:R:82:HIS:O	11:R:86:ARG:HG2	2.13	0.49
4:C:380:MET:SD	8:H:203:TYR:HE1	2.35	0.49
5:D:197:TYR:HB3	5:D:198:ARG:HH22	1.76	0.49
9:I:159:LYS:O	9:I:163:VAL:HG22	2.13	0.49
10:L:614:GLU:OE1	10:L:617:GLN:NE2	2.44	0.49
2:A:78:GLU:HG3	2:A:108:PRO:HG2	1.95	0.49
10:L:45:GLN:NE2	10:L:80:VAL:CG1	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:605:PHE:HZ	10:L:659:PHE:HD2	1.61	0.49
10:L:120:ARG:HG3	10:L:140:TYR:CD1	2.47	0.49
9:M:53:SER:HA	9:M:113:VAL:HG22	1.95	0.49
9:M:228:VAL:O	9:M:229:THR:OG1	2.24	0.49
9:M:382:ILE:HB	9:M:402:TYR:HB3	1.94	0.49
4:C:351:ILE:HG23	4:C:358:VAL:HG22	1.95	0.48
6:F:221:LEU:HB3	7:G:188:ILE:HG23	1.95	0.48
10:L:698:ASP:HA	10:L:701:HIS:NE2	2.28	0.48
10:L:723:VAL:HG11	10:L:742:LYS:HE2	1.95	0.48
9:M:458:SER:O	9:M:459:ARG:NH1	2.42	0.48
11:R:72:TRP:HB2	11:R:105:LYS:HB3	1.95	0.48
8:H:121:VAL:HG11	8:H:133:PHE:CD1	2.48	0.48
5:D:59:LEU:HD13	5:D:95:ARG:HD3	1.95	0.48
9:I:366:MET:HE1	9:I:370:ARG:NE	2.28	0.48
10:L:429:GLU:HG2	10:L:466:PHE:HB2	1.96	0.48
10:L:642:ARG:O	10:L:664:GLN:HG3	2.13	0.48
3:B:149:PHE:HE2	3:B:196:GLU:OE2	1.97	0.48
1:E:60:LEU:HD22	6:F:53:ASP:CB	2.43	0.48
2:A:91:TYR:HE2	2:A:320:LEU:HA	1.79	0.48
5:D:124:ALA:O	5:D:128:VAL:HG23	2.14	0.48
9:I:297:LYS:HB3	9:I:594:SER:HB2	1.96	0.48
9:I:549:TYR:OH	9:I:575:LEU:N	2.43	0.48
2:A:422:MET:SD	2:A:453:VAL:HG13	2.54	0.48
4:C:100:PHE:HE2	4:C:127:ALA:HB1	1.79	0.48
5:D:281:PHE:O	5:D:285:LEU:HG	2.14	0.48
9:I:37:VAL:HG21	9:I:82:LEU:HD23	1.95	0.48
10:L:33:ILE:HG23	10:L:60:ASN:HB3	1.95	0.48
10:L:525:PRO:HB2	10:L:528:PRO:HD2	1.95	0.48
9:M:274:ALA:N	9:M:284:SER:O	2.46	0.48
9:I:47:MET:HE2	9:M:24:PHE:HB2	1.95	0.48
9:I:382:ILE:O	9:I:402:TYR:N	2.42	0.48
10:L:447:SER:C	10:L:449:ASP:H	2.20	0.48
1:E:62:LEU:HD22	1:E:228:TYR:CE1	2.49	0.48
10:L:289:LYS:O	10:L:351:ARG:NH2	2.47	0.48
10:L:605:PHE:HE1	10:L:611:TYR:HB2	1.79	0.48
9:M:265:LYS:HB2	9:M:585:LYS:HB3	1.95	0.48
8:H:57:TRP:HZ3	8:H:71:LEU:HG	1.79	0.47
5:D:185:ILE:HG13	5:D:216:ILE:HD11	1.96	0.47
10:L:631:LEU:HD11	10:L:659:PHE:CE2	2.49	0.47
2:A:105:ASP:O	2:A:111:ARG:NH2	2.47	0.47
2:A:394:LEU:O	2:A:398:VAL:N	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:137:GLN:HG2	4:C:168:ASP:HB3	1.96	0.47
4:C:368:ASN:ND2	6:F:277:THR:HG23	2.29	0.47
8:H:143:GLU:HA	8:H:146:LYS:HG2	1.94	0.47
10:L:68:LYS:HA	10:L:68:LYS:HD2	1.49	0.47
2:A:112:VAL:HG11	2:A:145:LEU:HD11	1.96	0.47
4:C:150:LEU:HA	4:C:155:PHE:HE1	1.79	0.47
5:D:130:ILE:HG21	5:D:147:THR:HG21	1.97	0.47
9:M:525:VAL:HA	9:M:538:MET:HG2	1.97	0.47
11:R:33:TRP:HZ3	11:R:35:TRP:HB3	1.80	0.47
4:C:351:ILE:N	8:H:124:ALA:O	2.31	0.47
10:L:127:ASP:CG	10:L:138:ASN:HA	2.40	0.47
10:L:756:ARG:HA	10:L:764:TYR:HD1	1.78	0.47
1:E:62:LEU:HD21	6:F:206:MET:SD	2.54	0.47
2:A:432:THR:HG23	2:A:435:ALA:H	1.78	0.47
4:C:136:ASN:HB3	4:C:167:MET:SD	2.54	0.47
10:L:120:ARG:O	10:L:121:ASP:C	2.57	0.47
2:A:238:CYS:HA	2:A:257:TYR:HD2	1.79	0.47
10:L:508:LEU:HD13	10:L:513:TRP:CE2	2.49	0.47
10:L:751:ARG:HD2	10:L:751:ARG:HA	1.59	0.47
4:C:220:MET:SD	4:C:249:VAL:HG13	2.55	0.47
10:L:478:SER:HA	10:L:481:ASN:ND2	2.29	0.47
6:F:70:GLY:HA3	6:F:125:TYR:CZ	2.49	0.47
9:I:318:ILE:HB	9:I:353:PHE:HB3	1.97	0.47
10:L:704:GLU:HA	10:L:707:ILE:HG22	1.96	0.47
5:D:233:THR:O	5:D:242:ARG:NE	2.43	0.47
10:L:525:PRO:HA	10:L:603:MET:SD	2.55	0.47
1:E:295:LYS:HD3	1:E:295:LYS:HA	1.41	0.46
4:C:98:ASP:OD1	4:C:98:ASP:N	2.48	0.46
10:L:612:THR:HG22	10:L:615:GLU:HG2	1.97	0.46
9:M:223:ASP:HB3	9:M:257:PHE:CE1	2.49	0.46
2:A:80:PRO:O	2:A:81:SER:OG	2.28	0.46
3:B:360:ILE:HG22	3:B:364:LYS:HE3	1.97	0.46
9:I:172:LEU:HD22	9:I:176:LEU:HD23	1.96	0.46
10:L:387:TYR:O	10:L:390:LEU:HG	2.15	0.46
1:E:70:ARG:O	1:E:71:SER:C	2.59	0.46
4:C:192:TYR:HD1	4:C:197:ASN:HB3	1.80	0.46
6:F:199:GLY:O	6:F:203:VAL:HG23	2.14	0.46
6:F:222:ILE:HA	6:F:225:HIS:HB3	1.96	0.46
9:I:414:PRO:O	9:I:449:TRP:NE1	2.48	0.46
10:L:287:MET:HE2	10:L:296:LEU:HD22	1.96	0.46
9:M:88:TYR:HD1	9:M:94:LEU:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:397:ARG:NH2	9:M:419:TRP:O	2.48	0.46
3:B:303:LYS:HG3	3:B:312:THR:HG21	1.97	0.46
7:G:201:ASN:OD1	7:G:204:ARG:NH1	2.48	0.46
9:I:30:PHE:H	9:M:61:MET:HG3	1.81	0.46
9:M:47:MET:O	9:M:51:THR:HG23	2.14	0.46
1:E:171:ASP:CG	1:E:174:ARG:HB2	2.40	0.46
3:B:262:PHE:HE2	3:B:297:GLN:HG2	1.80	0.46
4:C:138:LEU:HB3	4:C:169:ILE:HD13	1.98	0.46
4:C:285:THR:HG23	4:C:288:ARG:HH21	1.80	0.46
7:G:16:ILE:HD11	7:G:45:GLU:HB3	1.97	0.46
9:I:416:PRO:HG2	9:I:440:TYR:CG	2.51	0.46
9:I:425:VAL:HB	9:I:466:ALA:HB2	1.97	0.46
4:C:400:ASN:HD22	6:F:312:LEU:HG	1.81	0.46
5:D:271:ARG:NE	5:D:272:ILE:O	2.48	0.46
9:M:7:ARG:NH1	9:M:8:GLN:O	2.48	0.46
9:M:247:GLN:O	9:M:251:LYS:HB2	2.15	0.46
2:A:326:ALA:HB2	2:A:355:PHE:HD1	1.80	0.46
3:B:326:PHE:O	3:B:330:LEU:HG	2.16	0.46
8:H:125:TYR:CD2	8:H:128:ILE:HD12	2.50	0.46
9:I:397:ARG:HB2	9:I:415:LEU:HB3	1.97	0.46
10:L:248:VAL:HG13	10:L:257:GLU:OE1	2.15	0.46
9:M:52:CYS:O	9:M:113:VAL:HG13	2.16	0.46
1:E:137:TYR:HD2	1:E:170:ILE:HD11	1.81	0.46
2:A:242:ILE:HG23	2:A:254:VAL:HG13	1.98	0.46
4:C:260:TYR:OH	4:C:289:ASP:OD2	2.25	0.46
9:I:109:CYS:C	9:I:111:LEU:N	2.73	0.46
10:L:429:GLU:OE2	10:L:470:LEU:HD11	2.16	0.46
9:M:268:MET:HE1	9:M:588:PRO:HG3	1.97	0.46
9:M:533:SER:HG	9:M:553:GLN:HE21	1.64	0.46
3:B:106:ASN:CG	10:L:447:SER:HA	2.41	0.46
5:D:226:LEU:HD21	5:D:255:CYS:SG	2.55	0.46
9:I:286:VAL:HA	9:I:297:LYS:HA	1.98	0.46
9:I:515:ILE:HG12	9:I:538:MET:HE1	1.97	0.46
10:L:271:LYS:O	10:L:275:THR:HG23	2.15	0.46
10:L:413:ASP:O	10:L:416:MET:HG3	2.16	0.46
10:L:605:PHE:CZ	10:L:659:PHE:HD2	2.34	0.46
9:M:155:MET:HE2	9:M:155:MET:HB2	1.87	0.46
3:B:295:ASP:OD2	11:R:43:ALA:HB2	2.16	0.45
7:G:191:GLN:OE1	8:H:201:THR:OG1	2.22	0.45
8:H:121:VAL:HG11	8:H:133:PHE:HD1	1.81	0.45
10:L:237:VAL:O	10:L:241:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:311:VAL:HB	9:M:375:LEU:HB3	1.97	0.45
9:M:455:ARG:NH1	9:M:457:THR:O	2.49	0.45
2:A:143:ARG:HB2	2:A:159:PRO:HG3	1.99	0.45
2:A:440:LEU:HD13	2:A:460:LEU:HD22	1.99	0.45
3:B:202:ILE:HD12	3:B:240:CYS:SG	2.55	0.45
4:C:117:PRO:HG2	4:C:152:ALA:HB2	1.98	0.45
5:D:86:HIS:CE1	5:D:110:LEU:HD21	2.51	0.45
5:D:234:ILE:HA	5:D:242:ARG:HH21	1.81	0.45
5:D:364:ARG:HH12	5:D:372:LYS:HD2	1.80	0.45
9:M:55:TYR:OH	9:M:59:MET:SD	2.64	0.45
2:A:382:ASP:O	2:A:385:LYS:HB3	2.16	0.45
2:A:478:MET:HE3	2:A:478:MET:HB3	1.88	0.45
3:B:296:SER:HB2	11:R:77:HIS:CD2	2.48	0.45
5:D:276:ASN:OD1	5:D:277:GLN:NE2	2.37	0.45
5:D:315:LEU:HD21	7:G:136:VAL:HG11	1.98	0.45
9:I:87:THR:O	9:I:91:THR:HG22	2.16	0.45
10:L:120:ARG:HG3	10:L:140:TYR:HB2	1.98	0.45
11:R:45:CYS:HB2	11:R:54:ILE:HG23	1.98	0.45
2:A:75:TYR:HE1	2:A:396:PRO:HG3	1.82	0.45
2:A:209:LEU:HD11	2:A:244:VAL:HG22	1.98	0.45
2:A:484:ARG:HH11	4:C:203:TYR:HD1	1.62	0.45
4:C:56:LEU:HD21	4:C:90:GLY:HA2	1.98	0.45
5:D:149:LEU:HD11	5:D:187:TYR:HB2	1.98	0.45
2:A:254:VAL:O	2:A:258:VAL:HG23	2.16	0.45
10:L:274:LYS:HB3	10:L:274:LYS:HE2	1.77	0.45
10:L:426:ASP:OD1	10:L:426:ASP:N	2.49	0.45
2:A:166:TRP:HB2	9:I:345:ARG:HH12	1.81	0.45
5:D:73:LEU:HB3	5:D:85:TYR:OH	2.15	0.45
6:F:137:HIS:O	6:F:141:GLN:HG3	2.16	0.45
10:L:230:ALA:HB2	10:L:276:ILE:HG13	1.98	0.45
10:L:687:GLU:HA	10:L:690:GLU:HG3	1.99	0.45
9:M:61:MET:HB3	9:M:61:MET:HE3	1.72	0.45
1:E:174:ARG:HB3	1:E:181:VAL:HG21	1.98	0.45
2:A:124:ARG:HG2	9:I:346:THR:N	2.26	0.45
3:B:235:GLY:HA2	3:B:261:ALA:HA	1.97	0.45
5:D:310:LEU:O	5:D:314:LYS:HG2	2.16	0.45
10:L:114:THR:O	10:L:115:ALA:C	2.60	0.45
10:L:298:CYS:HA	10:L:301:LYS:HE3	1.98	0.45
1:E:319:MET:HG2	8:H:200:LEU:HD13	1.98	0.45
4:C:265:GLN:O	4:C:269:THR:HG23	2.17	0.45
10:L:338:PRO:HB3	10:L:387:TYR:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:547:GLN:OE1	10:L:547:GLN:N	2.50	0.45
10:L:644:LEU:HD11	10:L:659:PHE:HB3	1.98	0.45
11:R:36:ASP:OD1	11:R:37:ILE:N	2.49	0.45
3:B:134:THR:O	3:B:137:GLU:HG3	2.17	0.45
7:G:136:VAL:HG22	7:G:141:ILE:HG13	1.99	0.45
9:I:522:ASP:OD1	9:I:522:ASP:N	2.48	0.45
10:L:261:VAL:O	10:L:265:GLU:HG2	2.17	0.45
10:L:712:LYS:HA	10:L:712:LYS:HD3	1.52	0.45
9:M:267:GLU:HG2	9:M:530:ILE:HG13	1.99	0.45
1:E:316:HIS:HE1	6:F:216:THR:HB	1.82	0.45
9:I:113:VAL:H	9:I:117:LEU:HD12	1.82	0.45
9:M:396:ARG:O	9:M:396:ARG:HD3	2.17	0.45
2:A:122:VAL:HG12	2:A:131:TYR:HD2	1.82	0.44
2:A:456:HIS:CD2	4:C:357:MET:HE2	2.51	0.44
4:C:311:THR:HG22	4:C:360:PHE:CD1	2.52	0.44
6:F:152:LEU:HD12	6:F:167:VAL:HG22	1.98	0.44
9:I:84:ILE:HA	9:I:87:THR:HG22	1.98	0.44
9:I:102:GLU:HG3	9:I:135:ARG:HH12	1.82	0.44
10:L:148:ARG:HH11	10:L:200:VAL:HG21	1.82	0.44
5:D:59:LEU:HB2	10:L:619:GLU:HB3	1.99	0.44
10:L:548:LEU:HA	11:R:33:TRP:HA	2.00	0.44
3:B:54:PHE:HB3	3:B:75:MET:HG3	2.00	0.44
3:B:112:ILE:HD11	3:B:147:LEU:HD21	1.99	0.44
7:G:116:LEU:HD13	7:G:132:ILE:HD11	1.99	0.44
10:L:601:ILE:HG23	10:L:616:ILE:HG21	2.00	0.44
6:F:139:HIS:NE2	6:F:170:SER:HB3	2.33	0.44
8:H:204:VAL:O	8:H:208:GLU:N	2.51	0.44
10:L:102:LEU:HD23	10:L:102:LEU:H	1.83	0.44
10:L:467:THR:O	10:L:471:GLU:HG3	2.18	0.44
10:L:722:LEU:HD23	10:L:722:LEU:HA	1.77	0.44
2:A:122:VAL:HG13	2:A:127:ASN:HD22	1.83	0.44
2:A:365:ILE:HG23	2:A:377:CYS:SG	2.58	0.44
9:I:379:GLU:HG3	9:I:379:GLU:O	2.16	0.44
10:L:207:ALA:HB3	10:L:208:PRO:HD3	2.00	0.44
10:L:483:THR:HA	10:L:486:GLU:HG3	1.99	0.44
10:L:525:PRO:HD2	10:L:599:MET:HE3	2.00	0.44
2:A:108:PRO:C	2:A:110:LEU:H	2.25	0.44
3:B:294:PHE:HD2	3:B:315:VAL:HB	1.82	0.44
9:I:434:MET:HE2	9:I:455:ARG:NE	2.30	0.44
10:L:298:CYS:HA	10:L:301:LYS:HG2	1.99	0.44
10:L:451:GLU:HB3	10:L:474:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:397:ARG:HA	9:M:397:ARG:NE	2.33	0.44
9:M:503:ASP:HB3	9:M:506:LYS:HB2	1.98	0.44
3:B:252:GLU:HB3	11:R:95:PRO:HB3	1.99	0.44
4:C:245:THR:HB	4:C:246:SER:H	1.49	0.44
9:M:275:SER:N	9:M:575:LEU:O	2.51	0.44
11:R:42:CYS:HB2	11:R:48:HIS:O	2.17	0.44
1:E:60:LEU:CD2	6:F:53:ASP:CG	2.89	0.44
1:E:327:LEU:O	1:E:331:ILE:HB	2.18	0.44
3:B:359:LEU:HD21	3:B:389:LEU:HD23	2.00	0.44
6:F:138:VAL:O	6:F:142:VAL:HG23	2.18	0.44
6:F:217:VAL:HG22	6:F:221:LEU:HG	2.00	0.44
8:H:20:CYS:HB3	8:H:40:LEU:HG	1.98	0.44
9:I:107:THR:O	9:I:111:LEU:HG	2.18	0.44
10:L:605:PHE:CG	10:L:609:GLU:HG3	2.53	0.44
9:M:81:THR:OG1	9:M:107:THR:HG21	2.18	0.44
2:A:112:VAL:HG21	2:A:145:LEU:HD21	2.00	0.44
3:B:46:ASP:HA	3:B:47:PRO:HD3	1.89	0.44
3:B:262:PHE:CE2	3:B:297:GLN:HG2	2.53	0.44
6:F:210:GLY:HA3	6:F:214:ASN:N	2.26	0.44
11:R:27:TRP:CE2	11:R:29:ALA:HB2	2.53	0.44
3:B:76:ILE:HG23	3:B:88:MET:HG2	1.99	0.43
5:D:63:ARG:NH1	5:D:64:GLN:OE1	2.50	0.43
9:I:47:MET:HE2	9:M:24:PHE:CB	2.48	0.43
9:I:353:PHE:HB2	9:I:360:TRP:CH2	2.53	0.43
10:L:47:LYS:HA	10:L:47:LYS:HD2	1.34	0.43
1:E:311:THR:HG21	6:F:293:GLY:HA3	2.00	0.43
3:B:144:ASN:O	3:B:148:TRP:N	2.45	0.43
3:B:175:LEU:HB3	3:B:197:ILE:HD11	2.00	0.43
3:B:186:ASP:HB2	3:B:224:ILE:HG12	1.99	0.43
7:G:117:LEU:HA	7:G:122:MET:HB2	2.00	0.43
10:L:507:VAL:HG22	10:L:535:PHE:CZ	2.52	0.43
9:M:442:TYR:HB2	9:M:449:TRP:CZ3	2.53	0.43
3:B:181:THR:N	3:B:184:GLY:O	2.51	0.43
6:F:213:GLU:HB2	8:H:208:GLU:O	2.18	0.43
10:L:527:ALA:HB3	10:L:528:PRO:HD3	2.00	0.43
10:L:528:PRO:HB3	11:R:27:TRP:CZ2	2.53	0.43
3:B:367:THR:OG1	3:B:411:LEU:HB2	2.18	0.43
9:I:53:SER:HB3	9:I:56:PHE:CD2	2.53	0.43
9:I:195:ARG:O	9:I:199:MET:HG2	2.18	0.43
10:L:124:MET:HE3	10:L:124:MET:HB3	1.68	0.43
10:L:430:ARG:HG2	10:L:691:THR:OG1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:482:THR:HA	10:L:485:ASP:OD2	2.18	0.43
9:M:37:VAL:HG21	9:M:82:LEU:HD22	2.00	0.43
9:M:400:GLU:HG2	9:M:409:TRP:HE3	1.84	0.43
9:M:415:LEU:HD12	9:M:416:PRO:HD2	2.00	0.43
1:E:123:ASN:HB3	6:F:104:TYR:OH	2.19	0.43
2:A:491:LEU:HD23	4:C:167:MET:HA	2.01	0.43
3:B:73:LYS:HE2	3:B:77:LYS:HE3	2.00	0.43
5:D:271:ARG:HH21	5:D:274:ARG:HH11	1.65	0.43
9:I:275:SER:OG	9:I:574:ASP:O	2.21	0.43
9:M:108:ALA:HB1	9:M:117:LEU:HG	2.01	0.43
5:D:333:ALA:O	5:D:336:GLU:HG2	2.19	0.43
8:H:112:ALA:HA	8:H:115:ARG:HE	1.83	0.43
2:A:492:ARG:HG2	4:C:244:TYR:OH	2.18	0.43
5:D:208:TYR:HB3	5:D:229:ALA:HB2	2.00	0.43
5:D:297:SER:O	5:D:301:ASP:HB2	2.18	0.43
7:G:162:ILE:HG22	7:G:166:ASP:HB2	2.00	0.43
9:I:153:LYS:HE2	9:I:180:ILE:HA	2.00	0.43
9:I:244:VAL:O	9:I:247:GLN:HG3	2.19	0.43
10:L:61:ALA:O	10:L:64:MET:HB2	2.18	0.43
10:L:206:GLU:OE1	10:L:260:ILE:HG12	2.19	0.43
2:A:376:SER:O	2:A:379:LYS:HG3	2.18	0.43
6:F:74:GLY:HA2	6:F:119:LEU:HD22	2.01	0.43
10:L:593:GLN:HB2	10:L:671:ARG:HH22	1.84	0.43
10:L:657:HIS:CD2	10:L:659:PHE:CE1	3.06	0.43
2:A:341:GLU:HG3	2:A:344:ARG:NH2	2.34	0.43
3:B:269:GLY:HA2	3:B:273:ARG:NH2	2.34	0.43
3:B:344:ARG:O	3:B:347:ILE:HG22	2.19	0.43
6:F:42:ALA:HB3	6:F:82:GLU:HA	2.01	0.43
9:I:269:MET:HE3	9:I:530:ILE:HG22	1.99	0.43
9:M:513:ALA:HB3	9:M:561:TRP:HZ3	1.83	0.43
2:A:326:ALA:HB2	2:A:355:PHE:CD1	2.54	0.43
9:I:222:ILE:HG12	9:I:257:PHE:HB2	2.00	0.43
10:L:560:ASN:N	11:R:23:GLU:O	2.52	0.43
10:L:715:LYS:HB3	10:L:716:LYS:H	1.68	0.43
2:A:389:LEU:HD23	2:A:389:LEU:HA	1.75	0.42
3:B:326:PHE:HZ	3:B:350:LEU:HD21	1.84	0.42
5:D:157:GLU:H	5:D:157:GLU:HG2	1.51	0.42
9:M:346:THR:HG22	9:M:369:VAL:HB	2.01	0.42
9:M:379:GLU:O	9:M:379:GLU:HG3	2.18	0.42
3:B:262:PHE:CE1	3:B:277:LEU:HB2	2.54	0.42
5:D:262:GLY:O	5:D:266:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:243:LYS:HD3	6:F:243:LYS:HA	1.89	0.42
2:A:486:ALA:O	2:A:490:MET:HB2	2.18	0.42
2:A:502:VAL:HG22	4:C:178:ALA:HB3	2.01	0.42
3:B:301:PRO:HB3	10:L:544:SER:HB2	2.02	0.42
6:F:175:ILE:HD11	6:F:182:LEU:HD11	2.01	0.42
9:I:45:HIS:HB2	9:I:48:VAL:HG13	2.02	0.42
9:I:301:PRO:HB2	9:I:302:PRO:HD3	2.01	0.42
10:L:427:VAL:HG11	10:L:692:ARG:CZ	2.50	0.42
10:L:612:THR:HG23	10:L:614:GLU:H	1.85	0.42
1:E:228:TYR:CZ	6:F:206:MET:HE1	2.55	0.42
3:B:88:MET:HE3	3:B:88:MET:HB3	1.84	0.42
3:B:186:ASP:OD1	3:B:186:ASP:N	2.52	0.42
4:C:138:LEU:HB2	4:C:166:MET:HB2	2.01	0.42
4:C:380:MET:SD	8:H:203:TYR:CE1	3.13	0.42
6:F:262:ALA:HB2	7:G:159:GLY:HA3	2.01	0.42
10:L:86:ILE:HG23	10:L:90:ARG:HD2	2.01	0.42
9:M:181:LEU:HD22	9:M:219:GLN:HB2	2.01	0.42
9:M:372:LYS:NZ	9:M:580:ARG:HE	2.17	0.42
3:B:205:TYR:HD2	3:B:217:LEU:HD11	1.85	0.42
3:B:246:LEU:HD23	3:B:342:PHE:HE2	1.84	0.42
5:D:272:ILE:HG21	7:G:133:ILE:HD12	2.01	0.42
8:H:118:PHE:HZ	8:H:151:GLN:HG2	1.84	0.42
9:I:29:LEU:O	9:M:47:MET:HE3	2.20	0.42
9:I:539:ARG:HH22	9:I:577:ARG:HD3	1.84	0.42
9:M:68:LYS:HA	9:M:68:LYS:HD2	1.65	0.42
9:M:539:ARG:HH21	9:M:579:PHE:HE1	1.68	0.42
3:B:76:ILE:HG23	3:B:88:MET:CG	2.49	0.42
5:D:327:LEU:HB2	7:G:126:ARG:HH12	1.84	0.42
10:L:389:SER:O	10:L:392:ILE:HG22	2.19	0.42
2:A:172:LYS:HE3	2:A:172:LYS:HB3	1.83	0.42
5:D:312:ALA:O	5:D:316:TYR:N	2.53	0.42
8:H:23:GLN:HA	8:H:26:GLU:HG3	2.01	0.42
10:L:338:PRO:HB3	10:L:387:TYR:CG	2.54	0.42
10:L:425:LYS:HD2	10:L:462:CYS:SG	2.59	0.42
10:L:714:ARG:HE	10:L:714:ARG:HB3	1.72	0.42
9:M:269:MET:SD	9:M:528:VAL:HG21	2.60	0.42
9:I:18:LEU:HD22	9:M:14:ALA:CB	2.50	0.42
9:I:287:CYS:SG	9:I:288:TYR:N	2.92	0.42
10:L:419:PHE:HZ	10:L:425:LYS:HG3	1.85	0.42
3:B:58:LEU:HD21	3:B:72:LEU:HG	2.02	0.42
9:I:45:HIS:CD2	9:M:47:MET:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:93:ASN:ND2	9:M:10:ASN:HB2	2.35	0.42
9:I:221:ARG:HE	9:I:260:ARG:HG2	1.85	0.42
1:E:162:GLN:HE21	1:E:162:GLN:HB2	1.55	0.42
3:B:61:GLU:H	3:B:61:GLU:HG3	1.39	0.42
4:C:167:MET:SD	4:C:167:MET:N	2.92	0.42
5:D:208:TYR:CB	5:D:229:ALA:HB2	2.50	0.42
10:L:202:GLU:O	10:L:206:GLU:HB2	2.20	0.42
3:B:169:GLN:NE2	9:I:451:GLU:HG3	2.35	0.41
3:B:416:ARG:HH12	3:B:419:ALA:HB2	1.85	0.41
7:G:164:LYS:HG3	7:G:165:LYS:HG2	2.01	0.41
9:I:53:SER:CB	9:I:111:LEU:HB3	2.50	0.41
9:I:289:SER:HG	9:I:294:LYS:H	1.65	0.41
10:L:507:VAL:HG22	10:L:535:PHE:HZ	1.84	0.41
5:D:342:MET:HG2	5:D:347:ARG:NH2	2.35	0.41
10:L:342:ILE:HD13	10:L:342:ILE:HA	1.95	0.41
9:M:66:GLU:HA	9:M:69:GLN:HB2	2.03	0.41
1:E:219:LYS:HA	1:E:219:LYS:HD3	1.41	0.41
3:B:33:GLU:HG2	3:B:67:TRP:CE2	2.56	0.41
4:C:368:ASN:HD21	6:F:277:THR:HG23	1.85	0.41
5:D:124:ALA:HB1	5:D:155:TYR:CE2	2.55	0.41
5:D:273:ILE:HB	5:D:304:VAL:HG13	2.03	0.41
6:F:217:VAL:HB	8:H:204:VAL:HG21	2.02	0.41
7:G:95:LYS:HE3	7:G:95:LYS:HB2	1.87	0.41
9:I:189:GLU:HB3	9:I:265:LYS:HE2	2.03	0.41
10:L:126:MET:C	10:L:128:ARG:H	2.28	0.41
3:B:47:PRO:HB2	3:B:82:LEU:HD23	2.01	0.41
3:B:212:LYS:O	3:B:215:LYS:HG2	2.20	0.41
3:B:288:LYS:HB3	3:B:289:SER:H	1.61	0.41
4:C:77:LEU:HD12	4:C:77:LEU:HA	1.81	0.41
4:C:400:ASN:ND2	6:F:312:LEU:HG	2.34	0.41
5:D:230:LEU:HD11	5:D:264:LEU:HB3	2.03	0.41
6:F:85:ASN:OD1	6:F:86:SER:N	2.53	0.41
6:F:231:LEU:O	6:F:235:VAL:HG23	2.20	0.41
10:L:68:LYS:HB3	10:L:69:HIS:H	1.68	0.41
10:L:153:ARG:HH21	10:L:200:VAL:HG13	1.85	0.41
10:L:606:ASN:ND2	11:R:22:PHE:O	2.54	0.41
9:M:133:CYS:HB2	9:M:156:VAL:HG22	2.02	0.41
9:M:152:ALA:O	9:M:153:LYS:C	2.63	0.41
3:B:314:LEU:HD11	3:B:337:ILE:HD12	2.02	0.41
4:C:224:TYR:CG	4:C:253:ILE:HG21	2.55	0.41
7:G:111:ILE:HB	7:G:152:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:153:TRP:CD2	8:H:164:PRO:HA	2.56	0.41
9:I:145:CYS:SG	9:I:148:LEU:HB3	2.60	0.41
9:I:205:ASN:ND2	9:I:206:THR:H	2.18	0.41
10:L:374:PHE:HA	10:L:377:PHE:CE2	2.55	0.41
1:E:162:GLN:O	1:E:163:GLU:C	2.63	0.41
3:B:416:ARG:HD2	3:B:417:GLY:N	2.36	0.41
4:C:52:GLN:O	4:C:55:SER:OG	2.34	0.41
5:D:155:TYR:CE2	5:D:167:TYR:HE2	2.39	0.41
9:I:81:THR:OG1	9:I:107:THR:HG21	2.21	0.41
9:I:435:THR:HG22	9:I:438:LEU:O	2.20	0.41
10:L:647:GLU:HB2	10:L:648:PRO:HD3	2.02	0.41
10:L:687:GLU:O	10:L:690:GLU:HG3	2.20	0.41
11:R:48:HIS:HD2	11:R:50:MET:H	1.66	0.41
11:R:48:HIS:HB3	11:R:50:MET:O	2.20	0.41
2:A:420:ALA:O	2:A:460:LEU:N	2.45	0.41
2:A:468:ARG:HH12	6:F:281:ASP:CB	2.34	0.41
4:C:20:GLN:HB3	4:C:23:GLN:HB2	2.01	0.41
4:C:404:VAL:HG11	7:G:216:ILE:HG21	2.03	0.41
5:D:48:PHE:CZ	5:D:65:LEU:HB3	2.53	0.41
5:D:49:VAL:O	5:D:53:VAL:HG23	2.21	0.41
5:D:185:ILE:HD13	5:D:185:ILE:HA	1.95	0.41
5:D:352:ILE:HG12	5:D:359:VAL:HG13	2.01	0.41
6:F:126:THR:HG23	6:F:153:LYS:HG3	2.03	0.41
2:A:349:SER:C	2:A:351:SER:H	2.28	0.41
2:A:498:ASN:O	4:C:171:LYS:HG2	2.21	0.41
4:C:65:LYS:HE3	4:C:71:VAL:HA	2.02	0.41
10:L:685:ASP:HB3	10:L:686:PRO:HD3	2.03	0.41
11:R:44:ILE:HD13	11:R:87:TRP:HB2	2.02	0.41
1:E:304:THR:HG23	6:F:296:THR:HG22	2.02	0.41
2:A:135:HIS:NE2	2:A:162:LEU:HB3	2.35	0.41
3:B:258:PHE:HB3	3:B:280:LEU:HB2	2.03	0.41
3:B:298:GLU:O	3:B:303:LYS:HB2	2.21	0.41
3:B:408:LEU:HD12	3:B:409:LEU:H	1.85	0.41
4:C:49:LEU:HD23	4:C:49:LEU:HA	1.94	0.41
4:C:209:ILE:HD11	4:C:224:TYR:HA	2.03	0.41
4:C:247:GLN:C	4:C:249:VAL:H	2.29	0.41
6:F:230:MET:O	6:F:234:ARG:HG2	2.21	0.41
7:G:194:ARG:HE	7:G:198:TYR:HE2	1.69	0.41
8:H:147:GLY:O	8:H:150:GLU:HG3	2.21	0.41
9:I:221:ARG:NE	9:I:260:ARG:HG2	2.36	0.41
9:I:539:ARG:HD3	9:I:549:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:45:GLN:OE1	10:L:84:HIS:HB2	2.21	0.41
10:L:168:MET:HE2	10:L:168:MET:HB3	1.91	0.41
10:L:459:LYS:HE3	10:L:471:GLU:OE2	2.21	0.41
10:L:681:GLN:NE2	10:L:683:GLU:OE2	2.54	0.41
9:M:234:PHE:CD1	9:M:245:VAL:HG12	2.56	0.41
9:M:539:ARG:HD3	9:M:549:TYR:CZ	2.56	0.41
2:A:166:TRP:HE3	9:I:345:ARG:HH22	1.68	0.41
3:B:214:LEU:HD22	3:B:240:CYS:SG	2.61	0.41
3:B:298:GLU:HA	3:B:302:TYR:HB2	2.03	0.41
9:I:597:LYS:HA	9:I:598:PRO:HD2	1.95	0.41
9:M:125:ILE:O	9:M:128:ILE:HG22	2.21	0.41
2:A:291:LEU:HD22	2:A:320:LEU:HB2	2.03	0.40
3:B:136:LEU:O	3:B:140:LYS:HG3	2.21	0.40
5:D:73:LEU:N	5:D:74:PRO:HD2	2.37	0.40
9:I:455:ARG:NH1	9:I:457:THR:O	2.55	0.40
9:M:127:LYS:HA	9:M:127:LYS:HD2	1.88	0.40
9:M:133:CYS:SG	9:M:134:VAL:N	2.94	0.40
1:E:106:ARG:H	1:E:106:ARG:HG2	1.73	0.40
2:A:127:ASN:OD1	2:A:128:VAL:N	2.53	0.40
3:B:93:LYS:HA	3:B:96:LEU:HD12	2.04	0.40
4:C:347:ILE:HD12	4:C:347:ILE:HA	1.93	0.40
5:D:81:ALA:HA	5:D:84:ILE:HG22	2.02	0.40
5:D:81:ALA:O	5:D:84:ILE:HG22	2.21	0.40
5:D:130:ILE:HG23	5:D:132:LEU:HG	2.03	0.40
5:D:319:ILE:HG13	7:G:147:GLN:OE1	2.22	0.40
9:I:57:ARG:HA	9:M:30:PHE:CE1	2.56	0.40
10:L:717:MET:HB3	10:L:721:VAL:HB	2.04	0.40
9:M:327:LEU:HG	9:M:343:ALA:HB1	2.02	0.40
2:A:193:ILE:HG22	2:A:196:SER:H	1.86	0.40
3:B:230:HIS:HB3	3:B:233:ILE:HD12	2.03	0.40
3:B:375:SER:OG	3:B:380:ILE:O	2.39	0.40
4:C:246:SER:OG	4:C:247:GLN:N	2.54	0.40
6:F:49:LEU:HD12	6:F:49:LEU:HA	1.86	0.40
9:I:56:PHE:O	9:M:30:PHE:HZ	2.03	0.40
9:M:137:LEU:HG	9:M:176:LEU:HD21	2.03	0.40
3:B:228:ILE:HD12	3:B:229:PRO:HD2	2.03	0.40
3:B:292:ASN:HB3	11:R:43:ALA:HA	2.03	0.40
6:F:71:ALA:HB2	6:F:89:LEU:HD11	2.03	0.40
8:H:70:GLU:O	8:H:74:ILE:HG13	2.21	0.40
10:L:756:ARG:HG3	10:L:764:TYR:CE1	2.57	0.40
9:M:88:TYR:CD1	9:M:94:LEU:HB2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:237:LEU:HD13	6:F:203:VAL:HG11	2.04	0.40
3:B:220:GLN:O	3:B:224:ILE:HG22	2.22	0.40
10:L:518:ALA:O	10:L:519:THR:OG1	2.31	0.40
10:L:526:PRO:HD3	10:L:603:MET:HG3	2.03	0.40
10:L:633:SER:HA	10:L:676:THR:HG21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	307/334 (92%)	271 (88%)	30 (10%)	6 (2%)	6 31
2	A	406/527 (77%)	382 (94%)	23 (6%)	1 (0%)	43 78
3	B	418/443 (94%)	381 (91%)	32 (8%)	5 (1%)	10 44
4	C	405/423 (96%)	385 (95%)	17 (4%)	3 (1%)	18 56
5	D	404/406 (100%)	373 (92%)	27 (7%)	4 (1%)	12 48
6	F	286/327 (88%)	272 (95%)	14 (5%)	0	100 100
7	G	212/264 (80%)	207 (98%)	5 (2%)	0	100 100
8	H	173/209 (83%)	171 (99%)	2 (1%)	0	100 100
9	I	550/623 (88%)	508 (92%)	41 (8%)	1 (0%)	43 78
9	M	558/623 (90%)	524 (94%)	34 (6%)	0	100 100
10	L	714/768 (93%)	639 (90%)	64 (9%)	11 (2%)	8 40
11	R	87/108 (81%)	70 (80%)	16 (18%)	1 (1%)	11 46
All	All	4520/5055 (89%)	4183 (92%)	305 (7%)	32 (1%)	20 56

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	253	SER
5	D	93	GLN
5	D	287	PRO
5	D	288	HIS
10	L	117	VAL
10	L	280	GLU
10	L	516	GLN
1	E	164	PRO
1	E	181	VAL
10	L	116	MET
10	L	257	GLU
10	L	496	VAL
1	E	163	GLU
3	B	66	GLU
3	B	182	ASP
4	C	72	PRO
4	C	248	ILE
10	L	120	ARG
10	L	755	ALA
1	E	71	SER
3	B	65	GLY
5	D	298	SER
10	L	757	THR
1	E	141	PRO
2	A	76	VAL
3	B	28	PRO
4	C	52	GLN
10	L	756	ARG
3	B	25	ASN
10	L	495	GLY
9	I	113	VAL
11	R	37	ILE

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	E	265/283 (94%)	221 (83%)	44 (17%)	2 10
2	A	360/458 (79%)	356 (99%)	4 (1%)	65 76
3	B	382/405 (94%)	378 (99%)	4 (1%)	68 78
4	C	363/377 (96%)	360 (99%)	3 (1%)	73 80
5	D	347/347 (100%)	341 (98%)	6 (2%)	53 69
6	F	255/276 (92%)	253 (99%)	2 (1%)	73 80
7	G	187/229 (82%)	187 (100%)	0	100 100
8	H	147/173 (85%)	147 (100%)	0	100 100
9	I	500/560 (89%)	492 (98%)	8 (2%)	55 70
9	M	507/560 (90%)	503 (99%)	4 (1%)	73 80
10	L	651/693 (94%)	610 (94%)	41 (6%)	16 37
11	R	78/90 (87%)	78 (100%)	0	100 100
All	All	4042/4451 (91%)	3926 (97%)	116 (3%)	38 58

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	40	LEU
1	E	63	LEU
1	E	74	ASN
1	E	75	LEU
1	E	76	GLU
1	E	100	VAL
1	E	103	THR
1	E	104	GLU
1	E	105	THR
1	E	106	ARG
1	E	107	VAL
1	E	108	ASN
1	E	125	LYS
1	E	129	ARG
1	E	130	LEU
1	E	150	ILE
1	E	156	MET
1	E	159	GLN
1	E	160	GLN
1	E	162	GLN
1	E	166	VAL
1	E	170	ILE

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Mol	Chain	Res	Type
1	E	173	THR
1	E	174	ARG
1	E	176	ILE
1	E	180	LYS
1	E	181	VAL
1	E	197	ASP
1	E	206	ILE
1	E	212	GLU
1	E	219	LYS
1	E	227	SER
1	E	230	LYS
1	E	232	SER
1	E	234	ASP
1	E	235	ARG
1	E	236	LYS
1	E	238	LEU
1	E	242	TRP
1	E	244	LYS
1	E	246	TRP
1	E	248	ASN
1	E	249	THR
1	E	295	LYS
2	A	389	LEU
2	A	390	LEU
2	A	391	ASP
2	A	392	MET
3	B	56	LYS
3	B	61	GLU
3	B	64	LYS
3	B	66	GLU
4	C	71	VAL
4	C	73	ASP
4	C	77	LEU
5	D	157	GLU
5	D	158	ASP
5	D	162	VAL
5	D	289	GLN
5	D	290	LYS
5	D	292	THR
6	F	265	HIS
6	F	270	LEU
9	I	51	THR

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Mol	Chain	Res	Type
9	I	52	CYS
9	I	55	TYR
9	I	62	SER
9	I	112	GLN
9	I	113	VAL
9	I	115	ASP
9	I	116	VAL
10	L	47	LYS
10	L	49	ASN
10	L	50	SER
10	L	52	LEU
10	L	56	GLU
10	L	59	ARG
10	L	63	THR
10	L	65	VAL
10	L	68	LYS
10	L	69	HIS
10	L	71	GLU
10	L	72	LYS
10	L	102	LEU
10	L	114	THR
10	L	116	MET
10	L	120	ARG
10	L	123	LEU
10	L	124	MET
10	L	127	ASP
10	L	128	ARG
10	L	491	LEU
10	L	492	GLN
10	L	712	LYS
10	L	713	SER
10	L	714	ARG
10	L	716	LYS
10	L	717	MET
10	L	718	GLN
10	L	722	LEU
10	L	723	VAL
10	L	750	GLU
10	L	751	ARG
10	L	752	GLU
10	L	753	TYR
10	L	754	LEU

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Mol	Chain	Res	Type
10	L	756	ARG
10	L	761	ARG
10	L	762	LYS
10	L	763	VAL
10	L	765	THR
10	L	766	TYR
9	M	61	MET
9	M	62	SER
9	M	64	LEU
9	M	68	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	123	ASN
1	E	126	GLN
1	E	243	ASN
2	A	101	GLN
2	A	387	ASN
2	A	397	HIS
2	A	423	HIS
2	A	456	HIS
3	B	35	GLN
3	B	79	ASN
3	B	124	GLN
3	B	169	GLN
3	B	203	GLN
3	B	223	HIS
3	B	297	GLN
3	B	319	GLN
4	C	29	ASN
4	C	258	ASN
4	C	261	HIS
4	C	297	GLN
4	C	363	ASN
4	C	368	ASN
5	D	86	HIS
5	D	136	GLN
5	D	360	HIS
5	D	406	GLN
6	F	50	ASN
6	F	141	GLN

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Mol	Chain	Res	Type
6	F	214	ASN
7	G	53	GLN
7	G	208	GLN
8	H	23	GLN
8	H	103	GLN
9	I	69	GLN
9	I	93	ASN
9	I	112	GLN
9	I	150	GLN
9	I	166	GLN
9	I	205	ASN
9	I	356	GLN
9	I	357	GLN
10	L	31	ASN
10	L	45	GLN
10	L	87	ASN
10	L	103	GLN
10	L	163	GLN
10	L	228	ASN
10	L	423	GLN
10	L	434	GLN
10	L	552	HIS
10	L	606	ASN
10	L	618	GLN
10	L	657	HIS
10	L	664	GLN
10	L	719	HIS
10	L	720	ASN
9	M	8	GLN
9	M	27	GLN
9	M	28	GLN
9	M	129	ASN
9	M	150	GLN
9	M	171	GLN
9	M	187	ASN
9	M	219	GLN
9	M	230	GLN
9	M	235	GLN
11	R	28	ASN
11	R	41	ASN
11	R	47	ASN
11	R	48	HIS

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Mol	Chain	Res	Type
11	R	108	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 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.

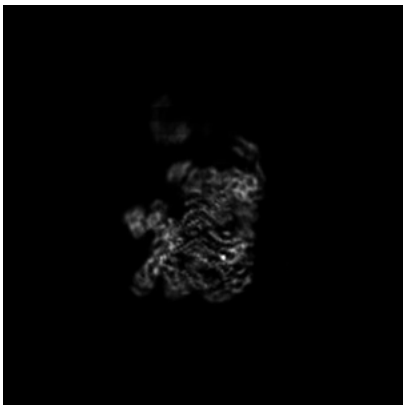
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34462. These allow visual inspection of the internal detail of the map and identification of artifacts.

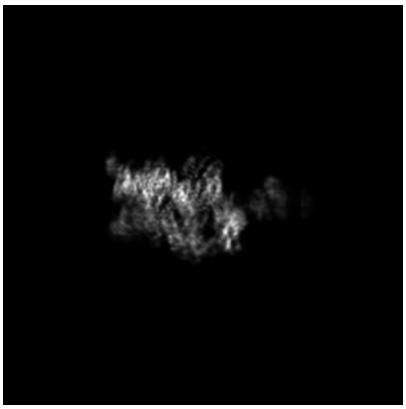
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

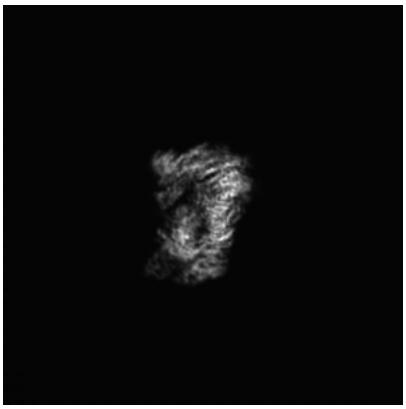
6.1.1 Primary map



X

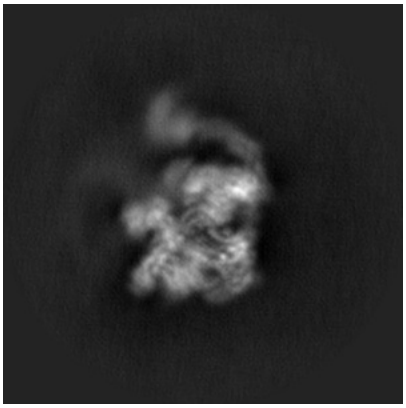


Y

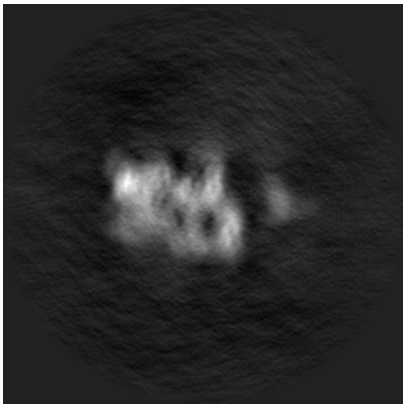


Z

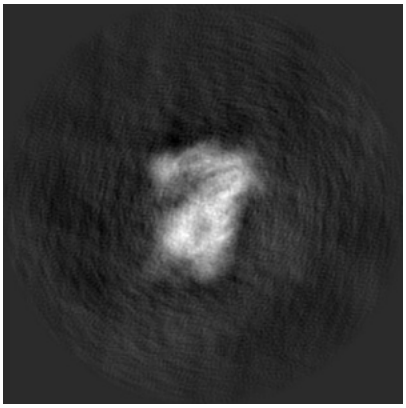
6.1.2 Raw map



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: 108

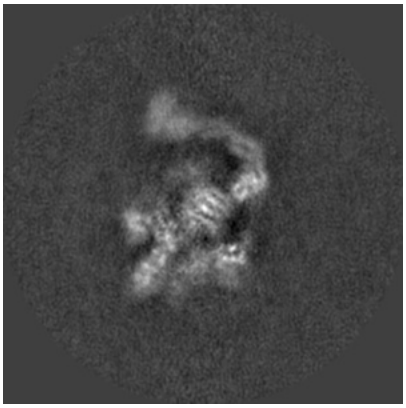


Y Index: 108

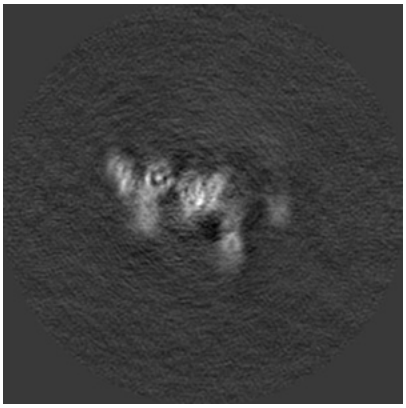


Z Index: 108

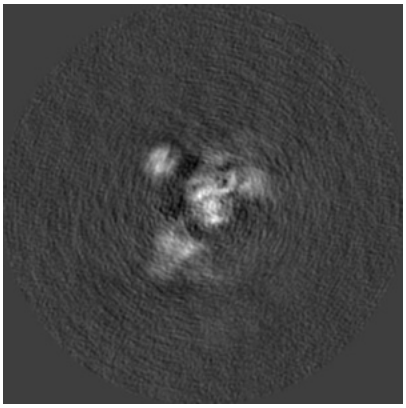
6.2.2 Raw map



X Index: 108



Y Index: 108

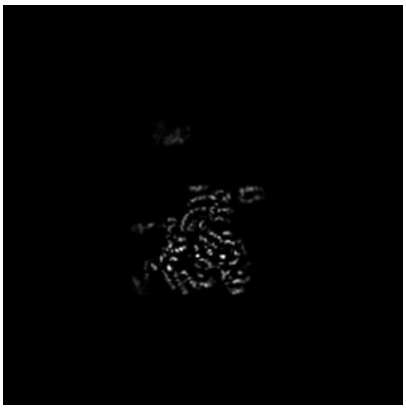


Z Index: 108

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: 118

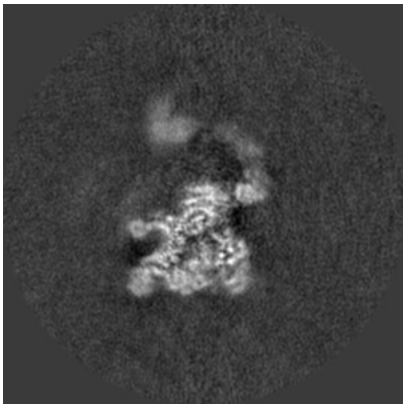


Y Index: 119

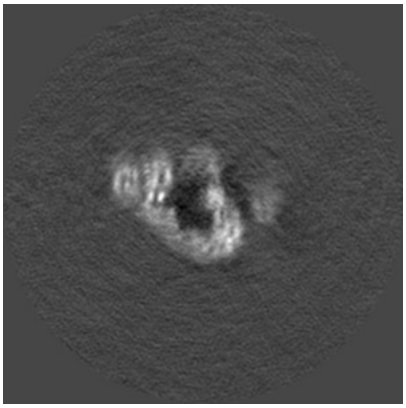


Z Index: 83

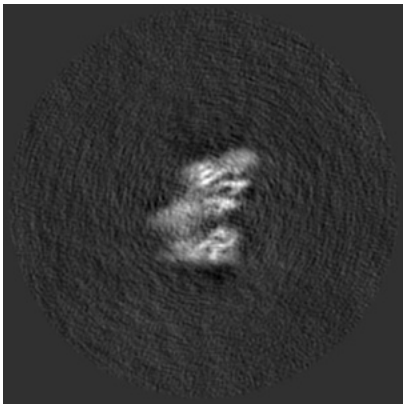
6.3.2 Raw map



X Index: 115



Y Index: 126

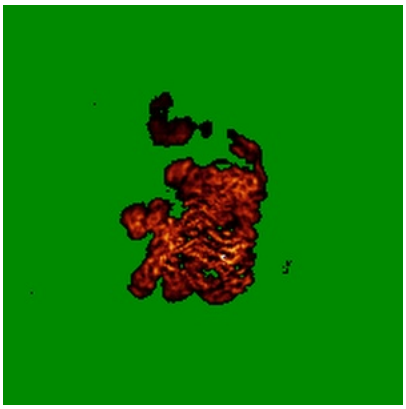


Z Index: 78

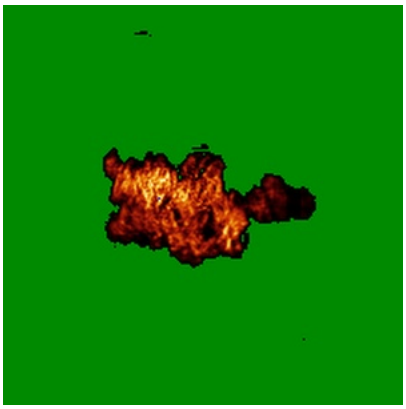
The images above show the largest variance slices of the map in three orthogonal directions.

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

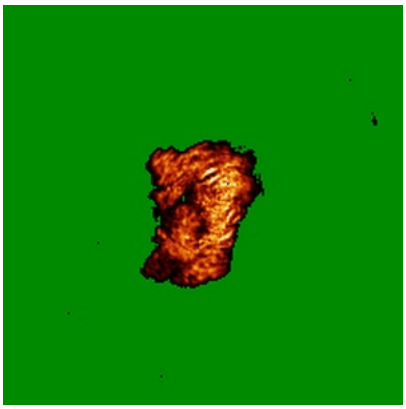
6.4.1 Primary map



X

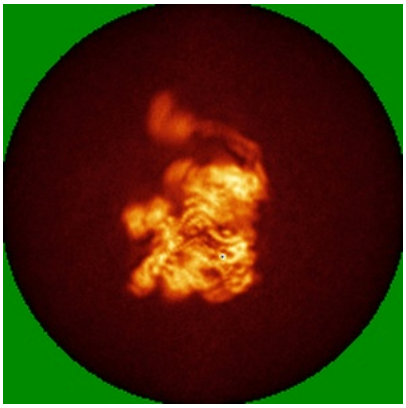


Y

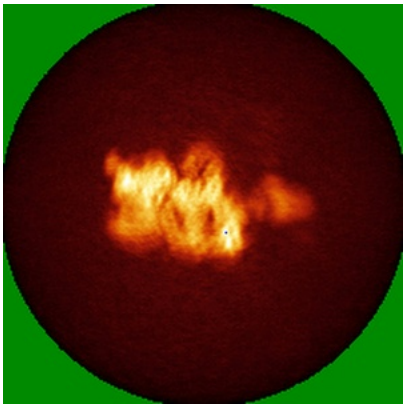


Z

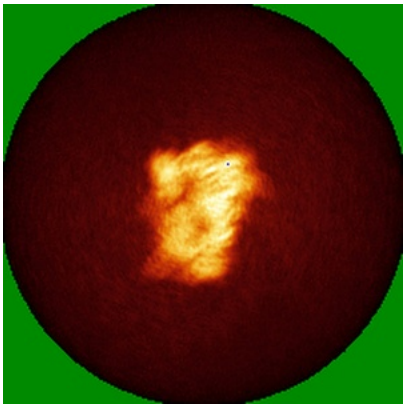
6.4.2 Raw map



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 0.001. 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



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.

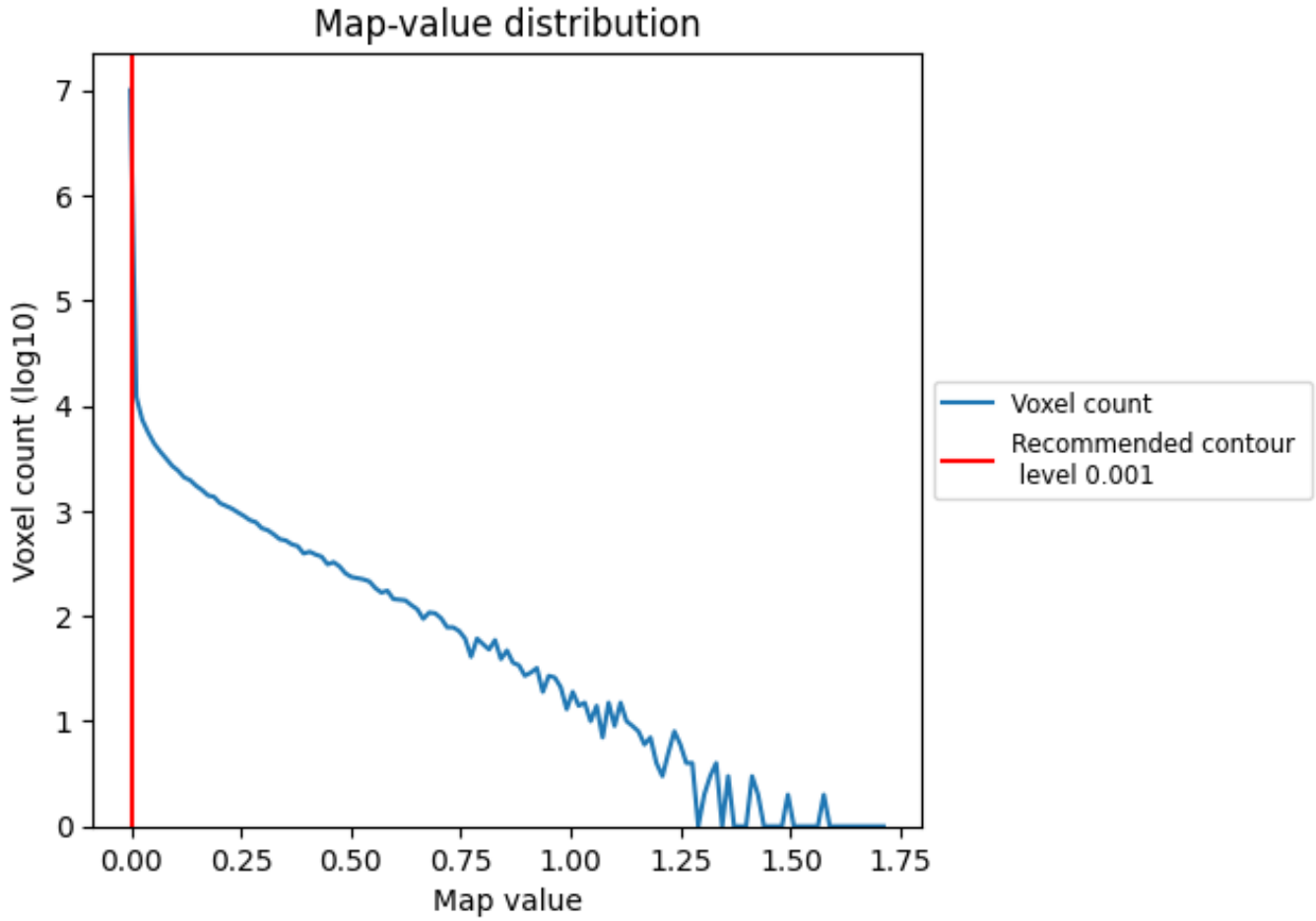
6.6 Mask visualisation (i)

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

7 Map analysis

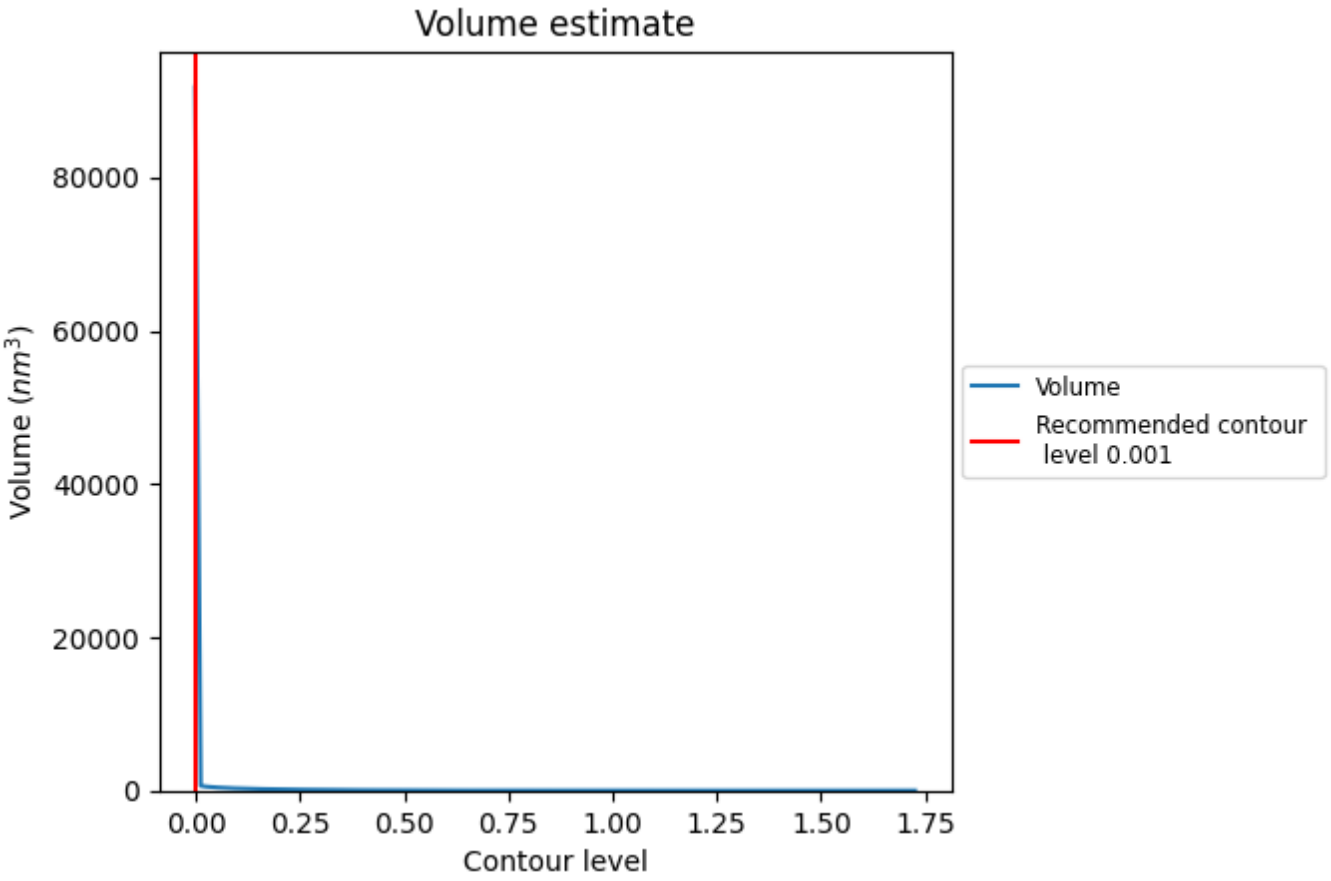
This section contains the results of statistical analysis of the map.

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.

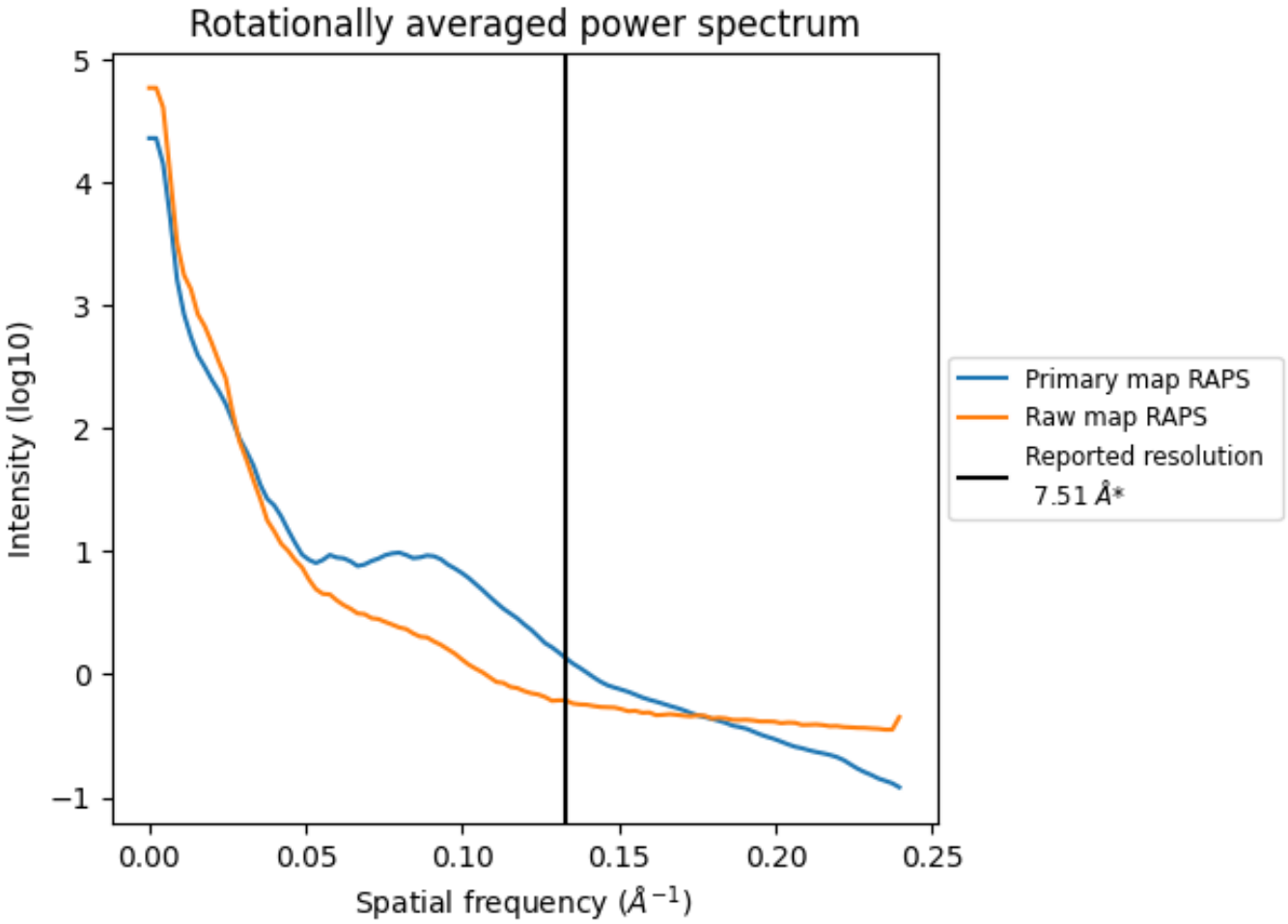
7.2 Volume estimate



The volume at the recommended contour level is 71810 nm^3; this corresponds to an approximate mass of 64868 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)

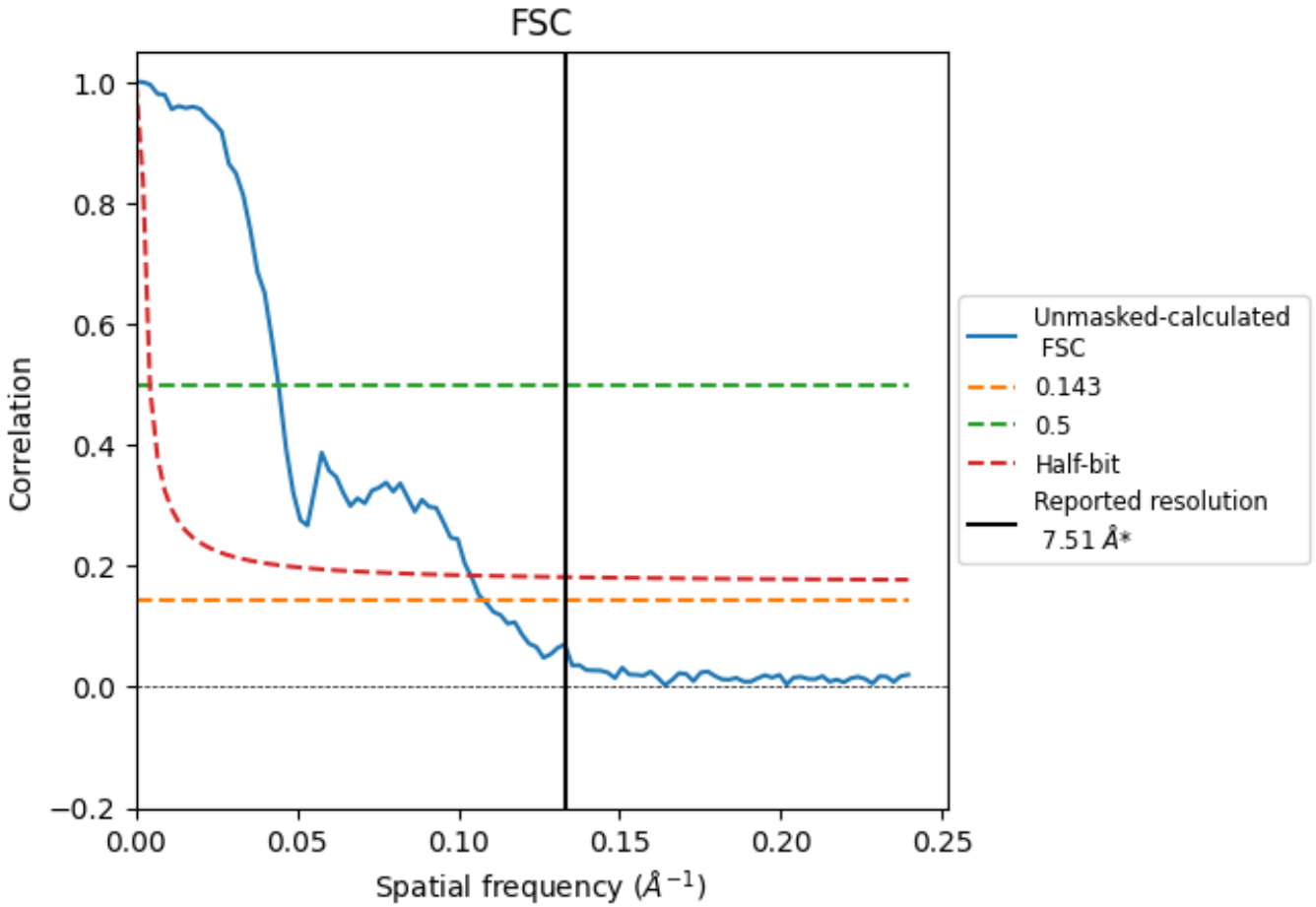


*Reported resolution corresponds to spatial frequency of 0.133 Å^{-1}

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 0.133 Å^{-1}

8.2 Resolution estimates (i)

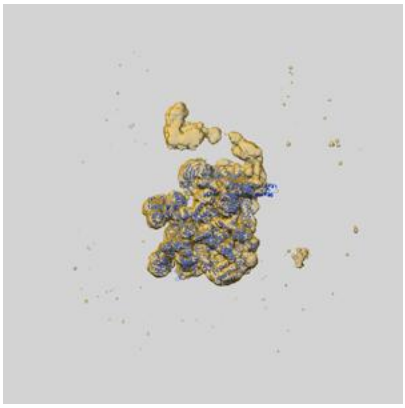
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.51	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.26	22.62	9.63

*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 9.26 differs from the reported value 7.51 by more than 10 %

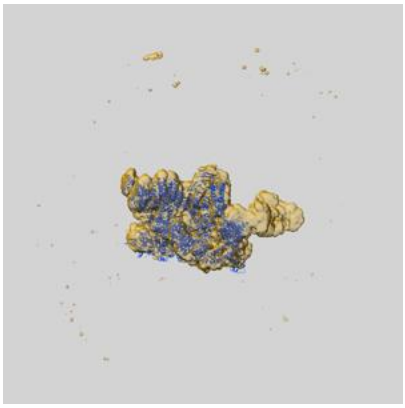
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34462 and PDB model 8H3A. Per-residue inclusion information can be found in section 3 on page 8.

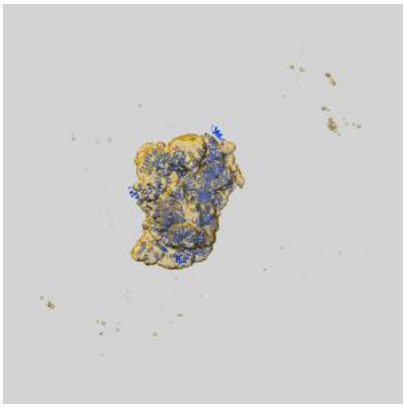
9.1 Map-model overlay



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.001 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.

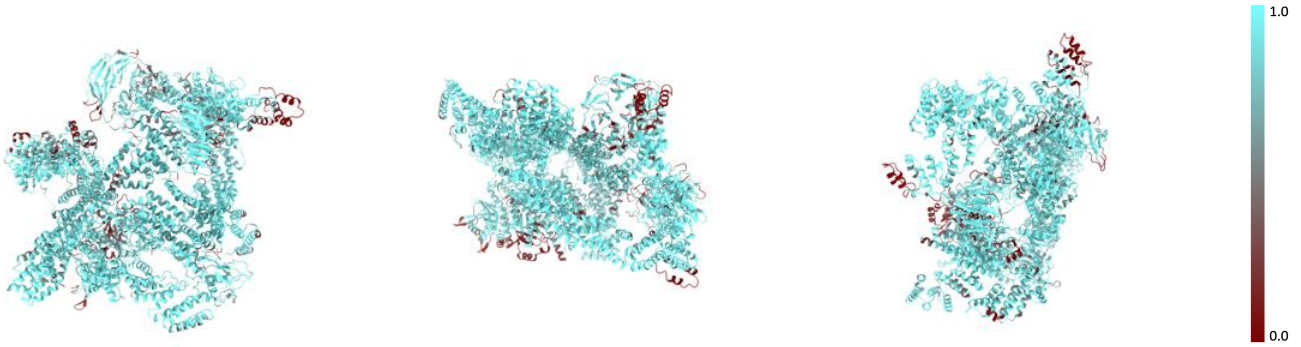
9.2 Q-score mapped to coordinate model (i)



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.

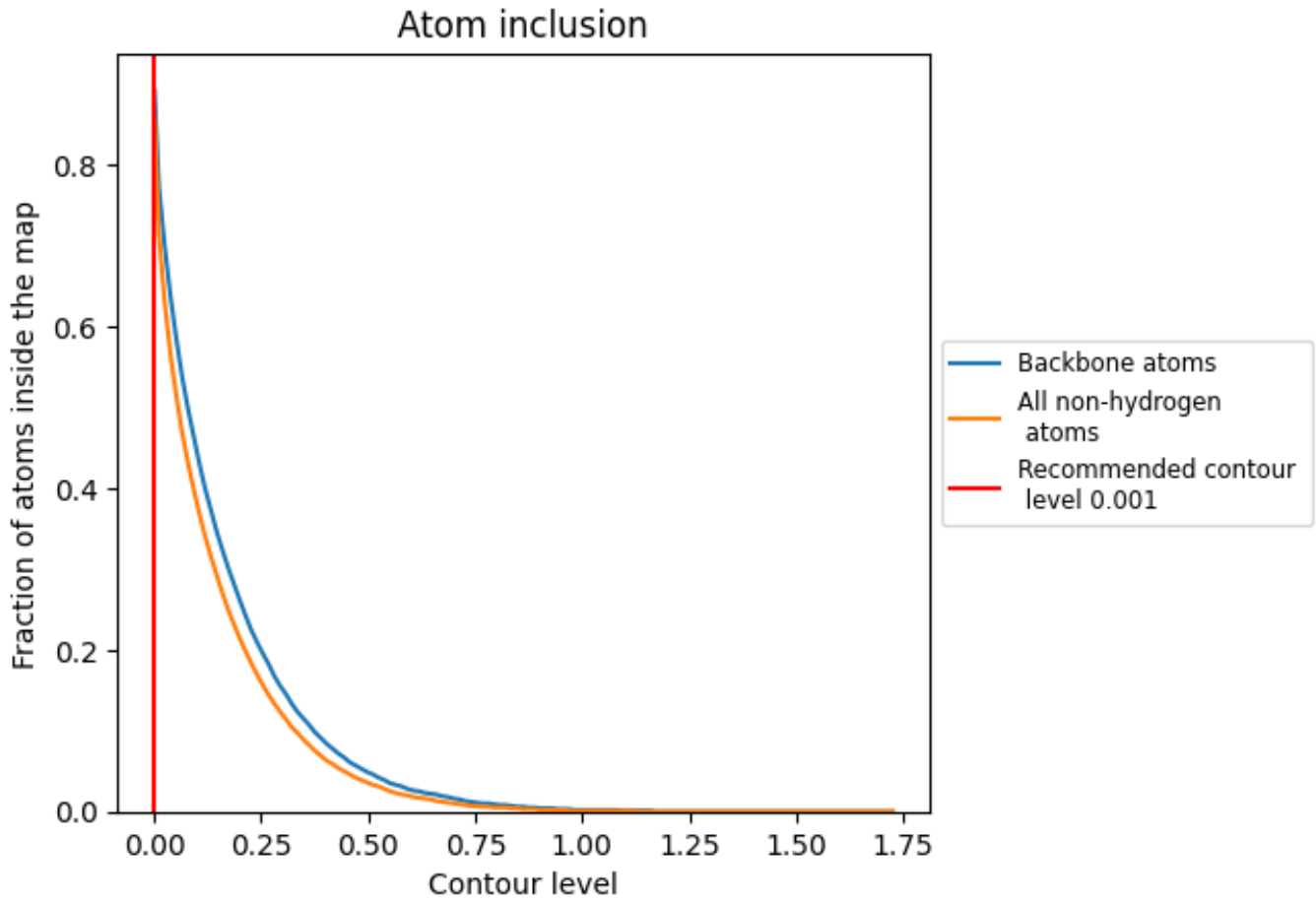
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.001).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 86% 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	0.8600	-0.0240
A	0.9230	-0.0370
B	0.9190	-0.0410
C	0.8870	-0.0320
D	0.9500	0.0090
E	0.6120	-0.0570
F	0.8080	-0.0290
G	0.9020	0.0020
H	0.8840	-0.0390
I	0.7650	-0.0410
L	0.9350	0.0070
M	0.8110	-0.0260
R	0.9420	-0.0410

