



Full wwPDB EM Validation Report ⓘ

Apr 25, 2026 – 10:17 PM EDT

PDB ID : 9PCP / pdb_00009pcp
EMDB ID : EMD-71512
Title : NER dual incision complex - NoG
Authors : Kim, J.; Li, C.L.; Yang, W.
Deposited on : 2025-06-28
Resolution : 4.30 Å (reported)
Based on initial models : 8EBU, 8EBT, 8EBS

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

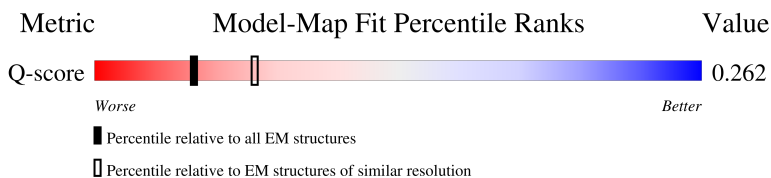
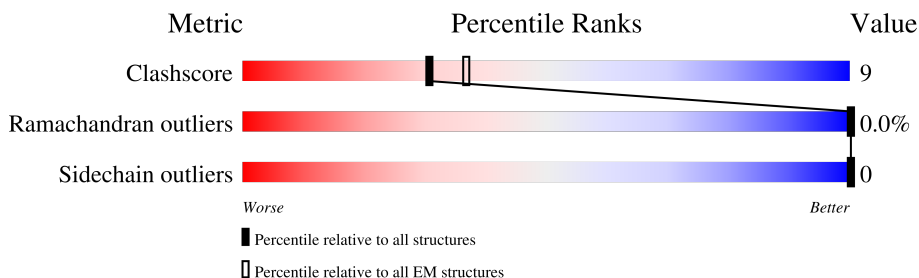
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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 4.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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

Mol	Chain	Length	Quality of chain
1	A	782	60% 18% 22%
2	B	768	69% 27% .
3	C	548	15% 19% 5% 76%
4	D	462	72% 21% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	395	
6	F	308	
7	G	71	
8	H	940	
9	I	409	
10	J	172	
11	K	273	
12	L	93	
13	M	94	
14	Q	916	
15	R	297	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 36356 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 TFIIF basal transcription factor complex helicase XPB subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	613	Total	C	N	O	S	0	0
			4947	3159	856	902	30		

- Molecule 2 is a protein called General transcription and DNA repair factor IIF helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	734	Total	C	N	O	S	0	0
			5913	3778	1033	1073	29		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	761	ASP	-	expression tag	UNP P18074
B	762	TYR	-	expression tag	UNP P18074
B	763	LYS	-	expression tag	UNP P18074
B	764	ASP	-	expression tag	UNP P18074
B	765	ASP	-	expression tag	UNP P18074
B	766	ASP	-	expression tag	UNP P18074
B	767	ASP	-	expression tag	UNP P18074
B	768	LYS	-	expression tag	UNP P18074

- Molecule 3 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	133	Total	C	N	O	S	0	0
			1076	684	185	200	7		

- Molecule 4 is a protein called General transcription factor IIF subunit 4, p52.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	427	Total	C	N	O	S	0	0
			3430	2212	593	612	13		

- Molecule 5 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	342	Total	C	N	O	S	0	0
			2668	1686	455	501	26		

- Molecule 6 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	255	Total	C	N	O	S	0	0
			2013	1289	333	372	19		

- Molecule 7 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	66	Total	C	N	O	S	0	0
			522	337	82	100	3		

- Molecule 8 is a protein called DNA repair protein complementing XP-C cells.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	503	Total	C	N	O	S	0	0
			4123	2632	729	742	20		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	499	VAL	ALA	variant	UNP Q01831
H	939	LYS	GLN	variant	UNP Q01831

- Molecule 9 is a protein called UV excision repair protein RAD23 homolog B.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	61	Total	C	N	O	S	0	0
			504	316	95	91	2		

- Molecule 10 is a protein called Centrin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	70	Total	C	N	O	S	1	0
			573	356	94	121	2		

- Molecule 11 is a protein called DNA repair protein complementing XP-A cells.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	206	Total	C	N	O	S	0	0
			1701	1062	309	314	16		

- Molecule 12 is a DNA chain called DNA (Cy5).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	54	Total	C	N	O	P	0	0
			1114	545	193	322	54		

- Molecule 13 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	44	Total	C	N	O	P	0	0
			905	432	162	267	44		

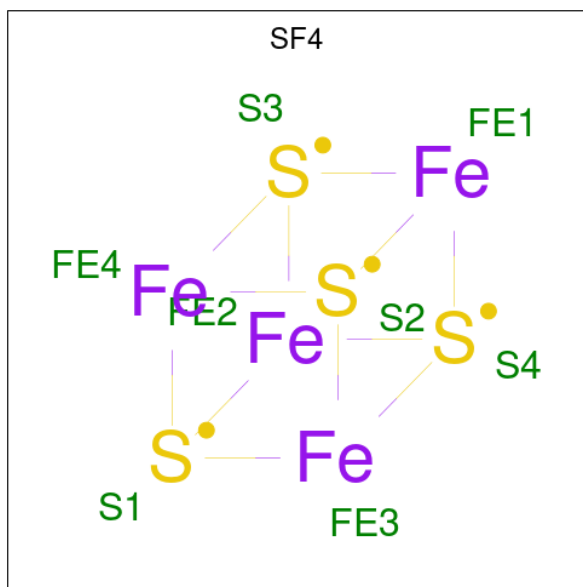
- Molecule 14 is a protein called DNA repair endonuclease XPF.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	713	Total	C	N	O	S	0	0
			5451	3497	949	984	21		

- Molecule 15 is a protein called DNA excision repair protein ERCC-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	196	Total	C	N	O	S	0	0
			1400	901	240	255	4		

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
16	B	1	Total	Fe	S	0
			8	4	4	

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	E	3	Total	Zn	0
			3	3	
17	F	2	Total	Zn	0
			2	2	
17	K	1	Total	Zn	0
			1	1	

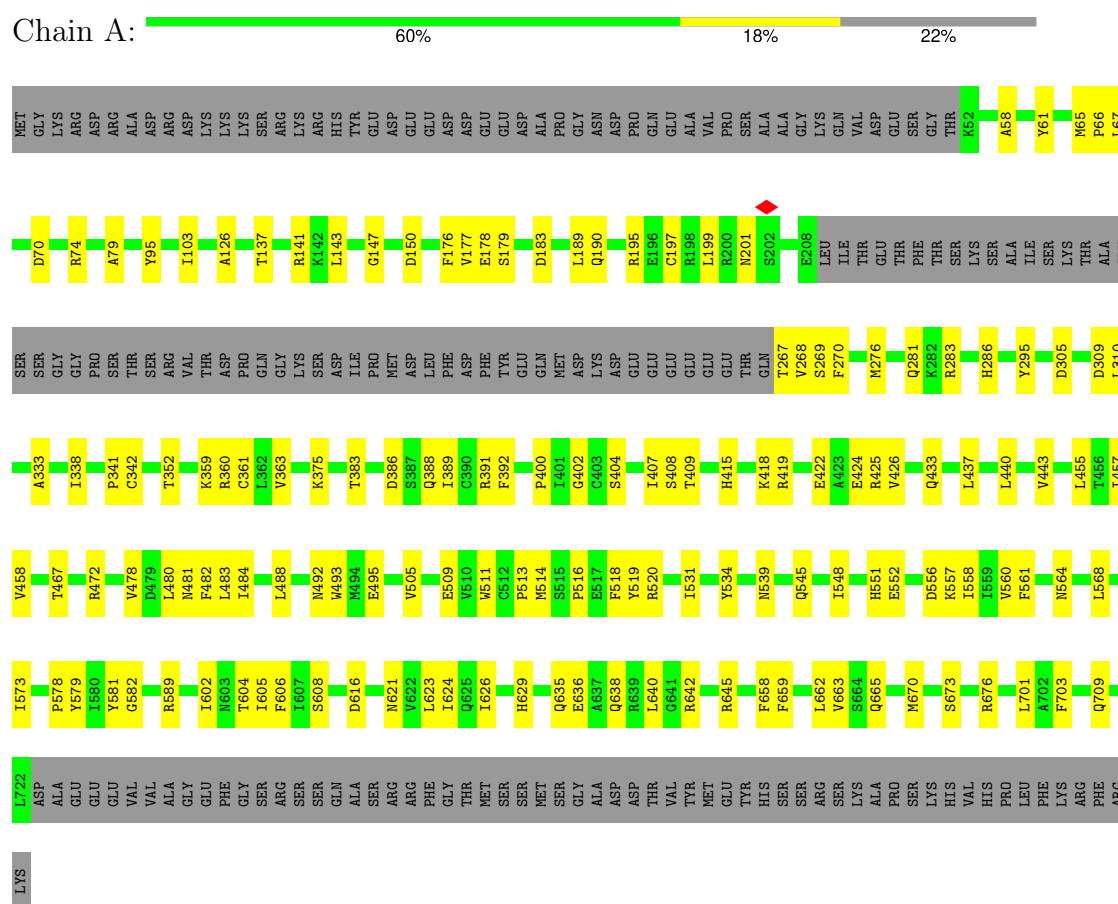
- Molecule 18 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
18	J	2	Total	Ca	0
			2	2	

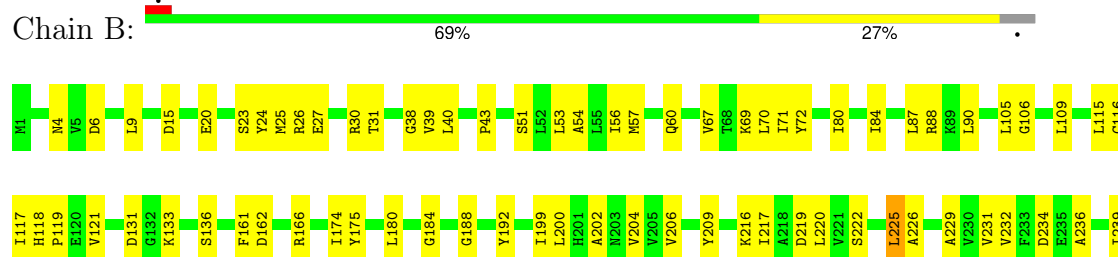
3 Residue-property plots

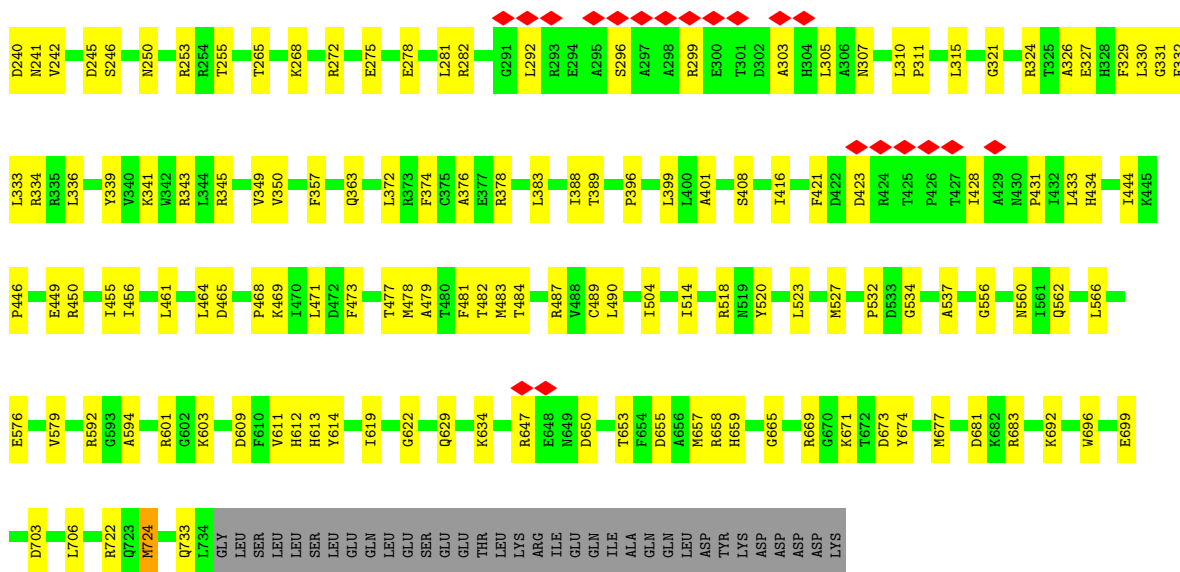
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

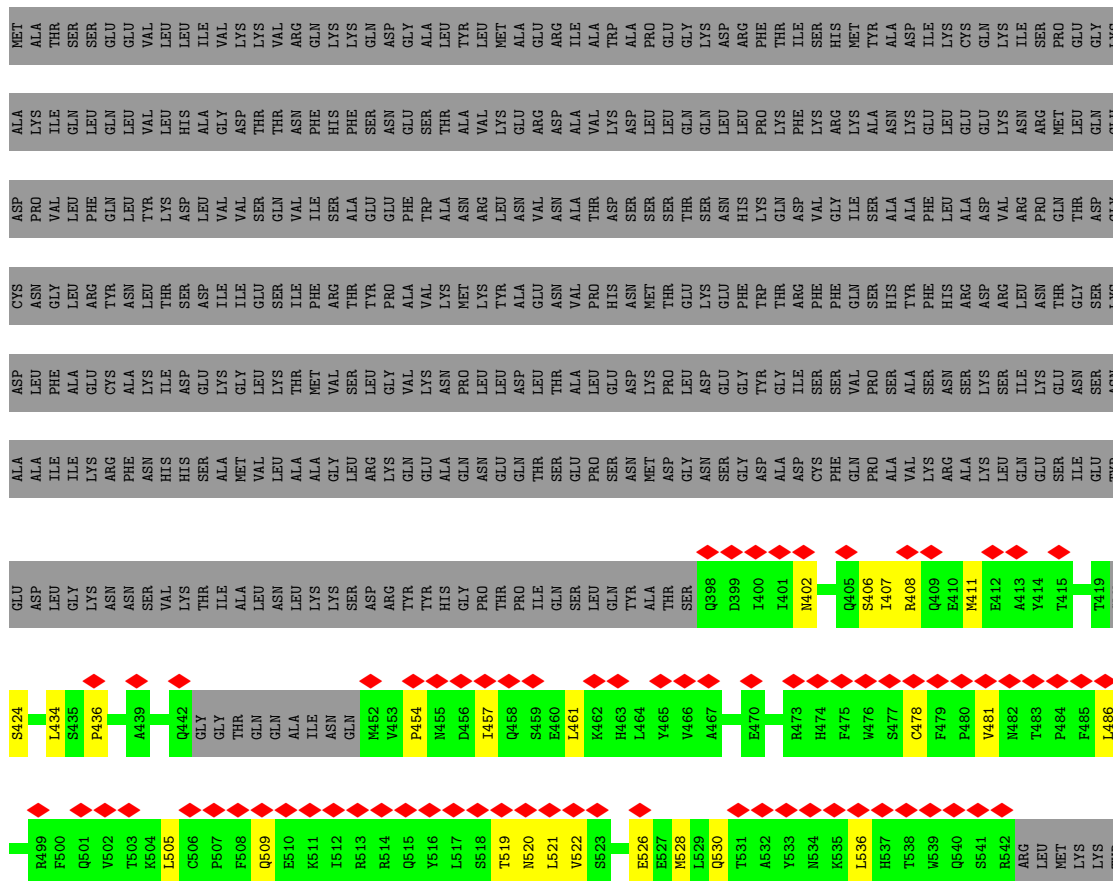


- Molecule 2: General transcription and DNA repair factor IIH helicase subunit XPD



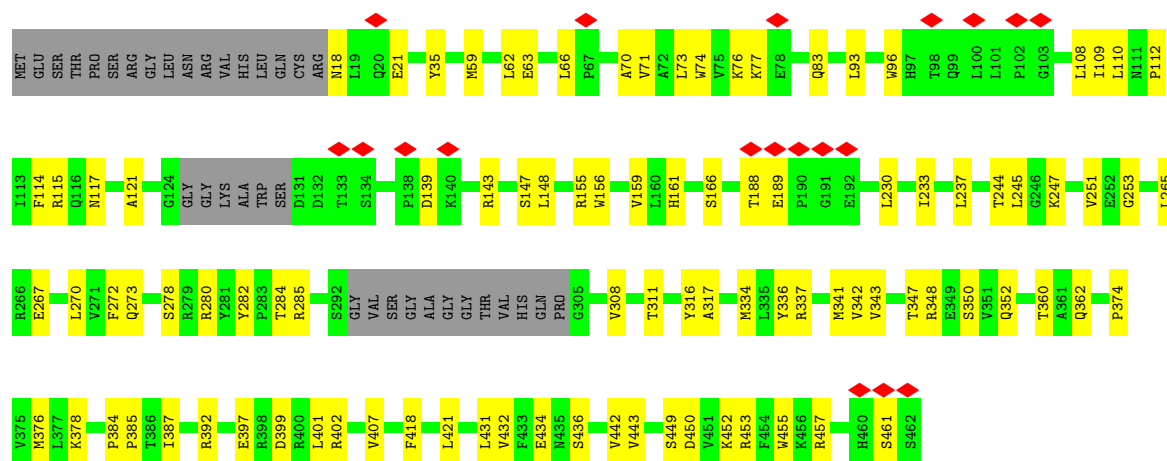


- Molecule 3: General transcription factor IIH subunit 1

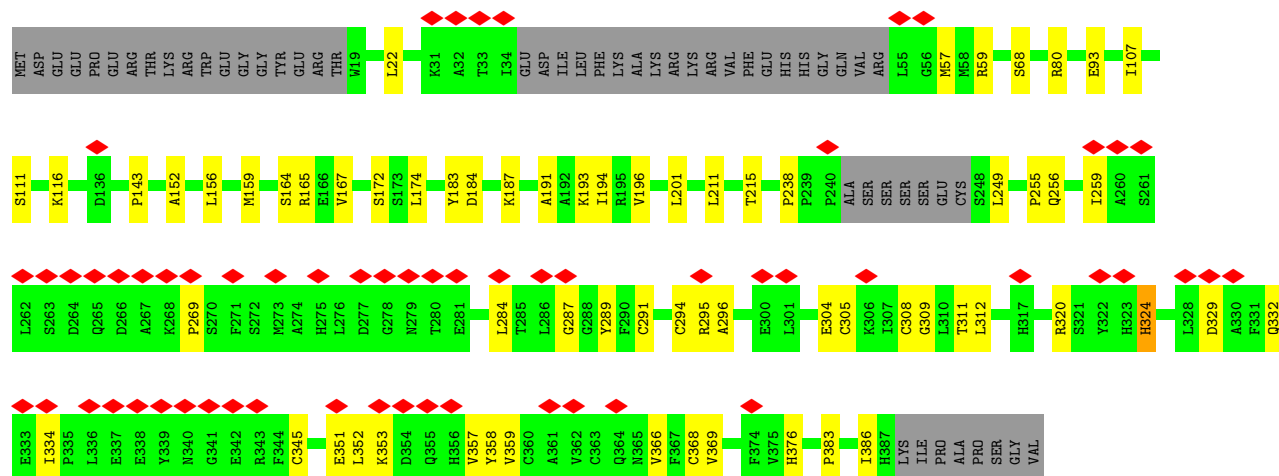


- Molecule 4: General transcription factor IIH subunit 4, p52

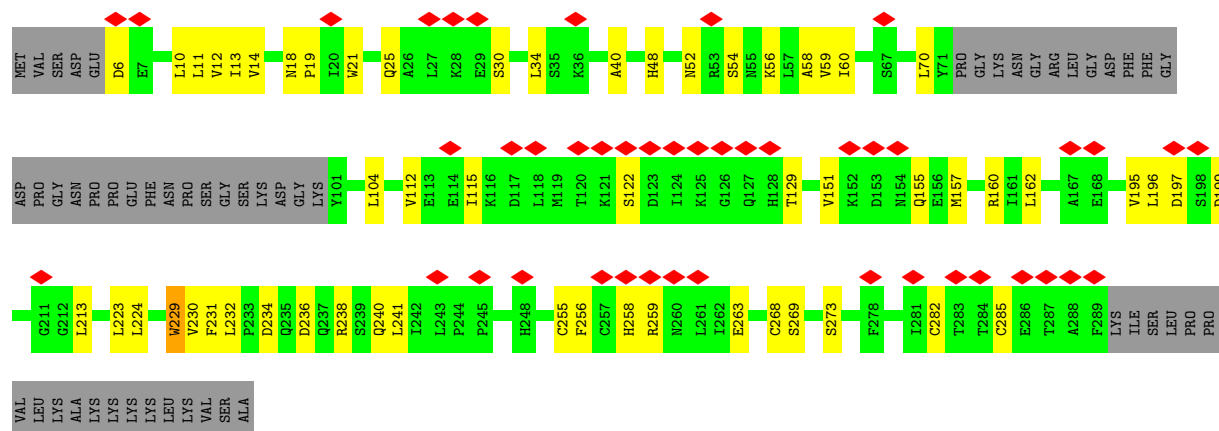


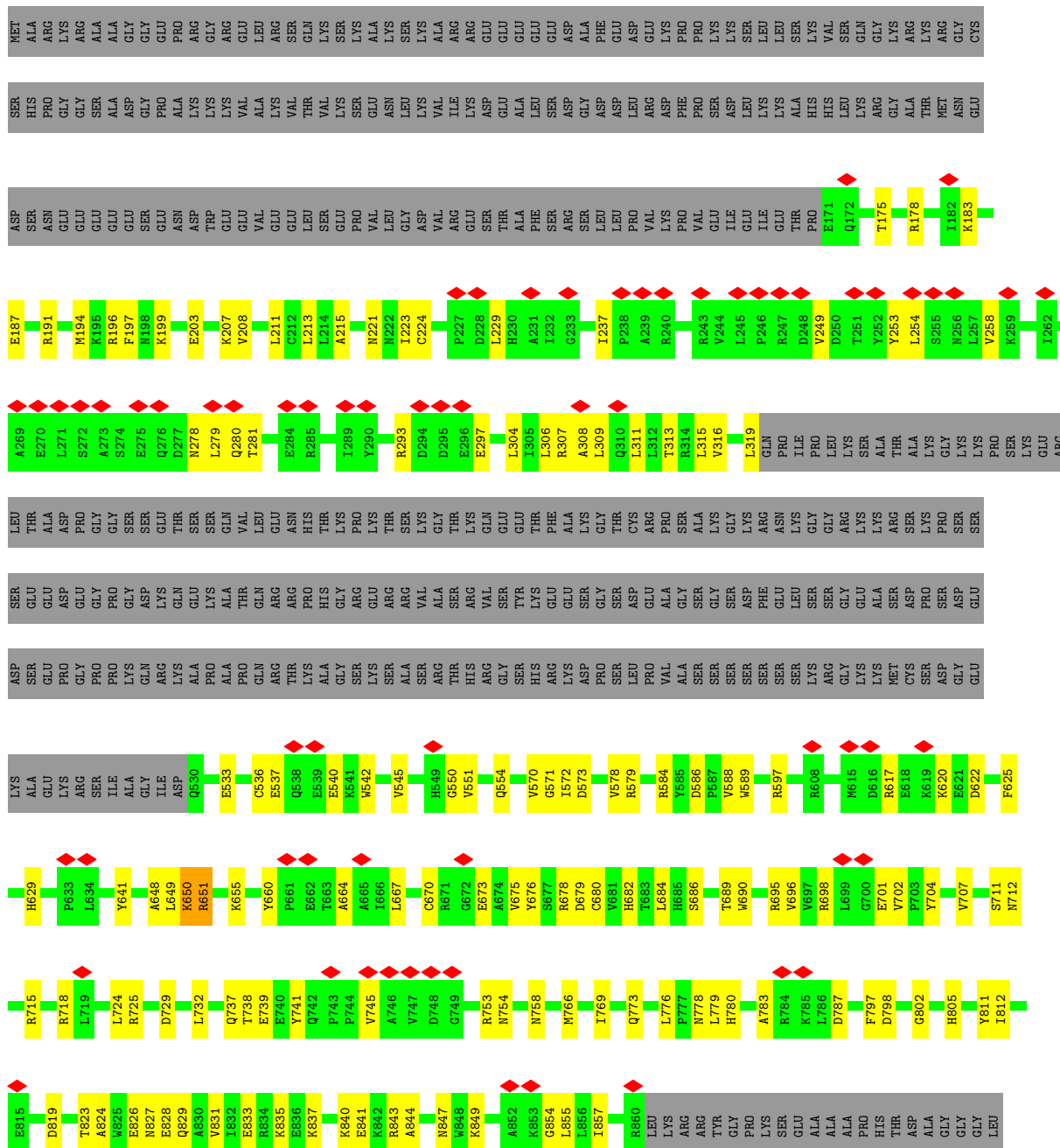


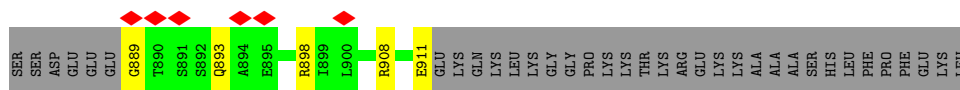
• Molecule 5: General transcription factor IIH subunit 2



• Molecule 6: General transcription factor IIH subunit 3

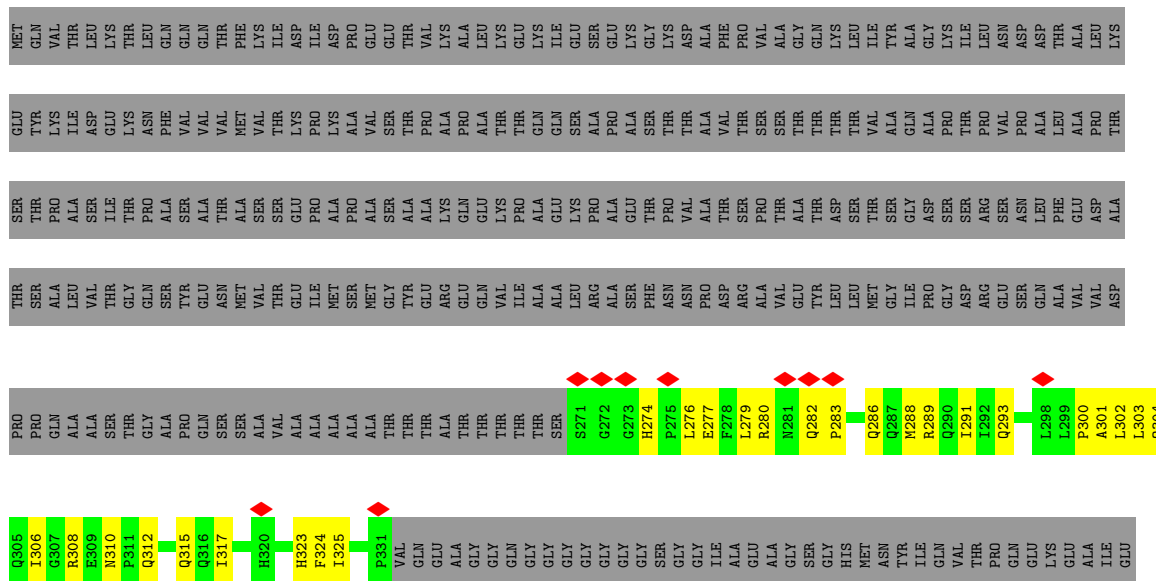






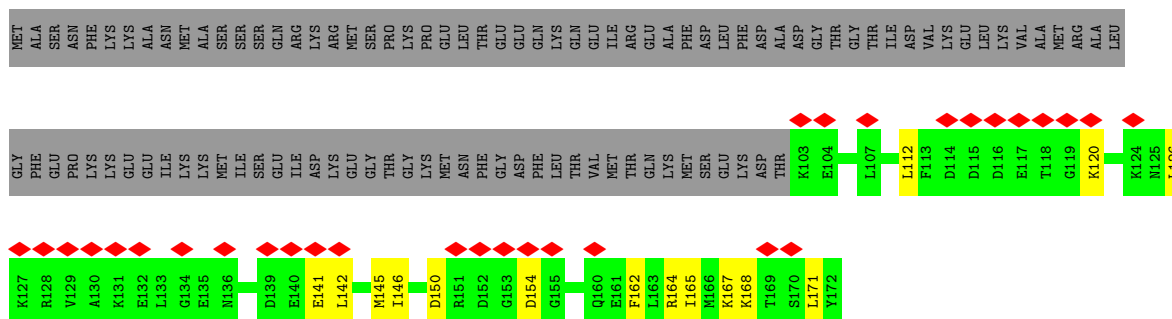
• Molecule 9: UV excision repair protein RAD23 homolog B

Chain I: 9% 6% 85%



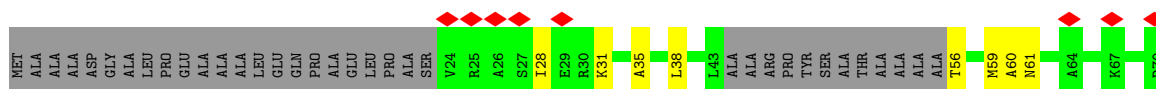
• Molecule 10: Centrin-2

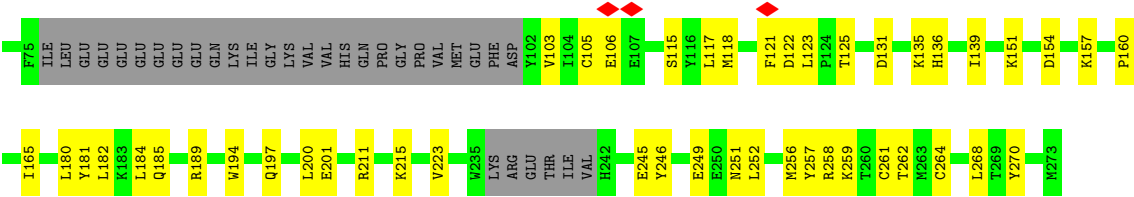
Chain J: 18% 32% 9% 59%



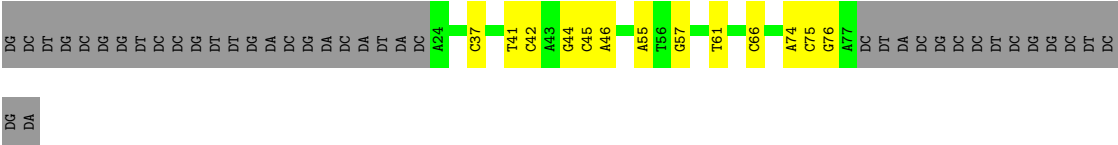
• Molecule 11: DNA repair protein complementing XP-A cells

Chain K: 56% 20% 25%

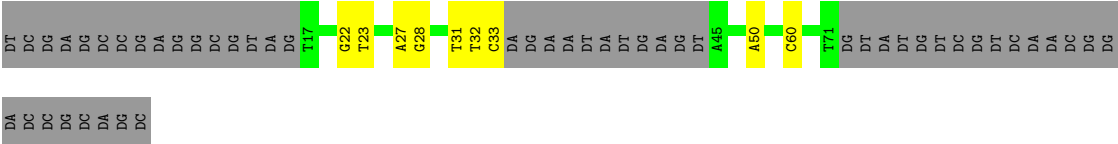
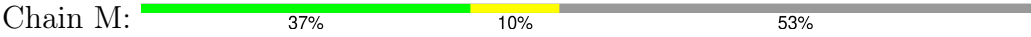




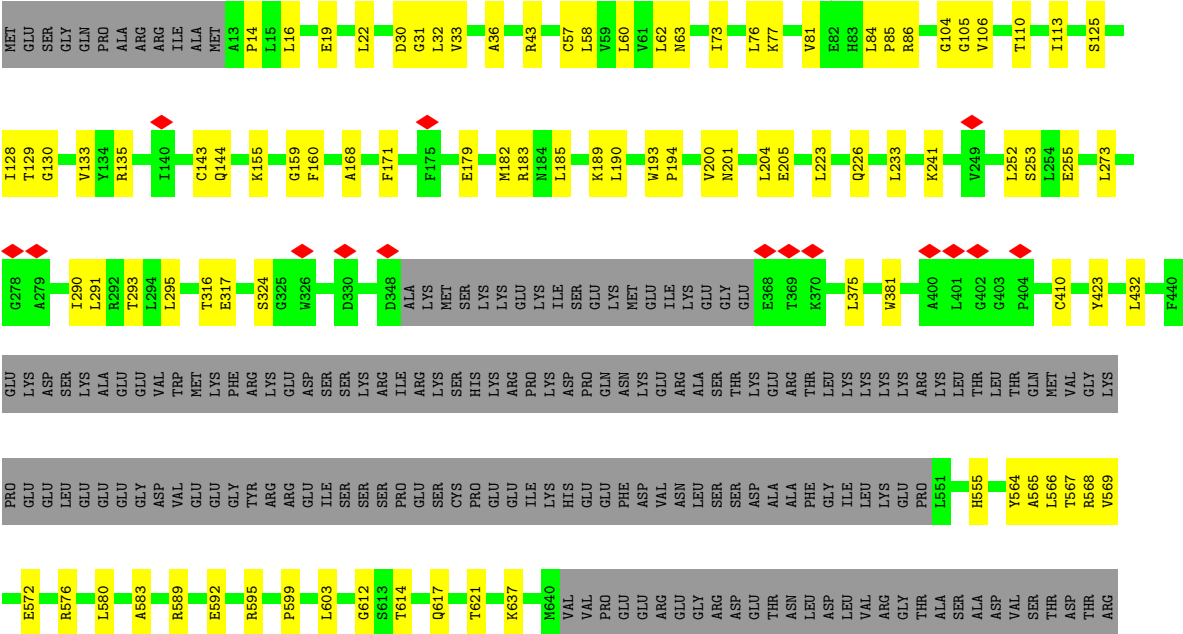
• Molecule 12: DNA (Cy5)



• Molecule 13: DNA



• Molecule 14: DNA repair endonuclease XPF



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	81380	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.123	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.026	Depositor
Map size (Å)	365.19998, 365.19998, 365.19998	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.66, 1.66, 1.66	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SF4, VM6, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.38	0/5051	0.68	1/6822 (0.0%)
2	B	0.32	0/6040	0.73	2/8179 (0.0%)
3	C	3.40	1/1097 (0.1%)	0.75	0/1480
4	D	0.32	0/3508	0.70	2/4751 (0.0%)
5	E	0.29	0/2725	0.69	4/3690 (0.1%)
6	F	0.87	6/2049 (0.3%)	0.66	0/2776
7	G	0.43	0/528	0.80	0/713
8	H	0.32	0/4220	0.76	1/5713 (0.0%)
9	I	0.36	0/515	0.88	0/696
10	J	0.34	0/577	0.71	0/762
11	K	0.30	0/1728	0.68	0/2301
12	L	0.39	0/1203	0.57	0/1849
13	M	0.42	0/1013	0.57	0/1560
14	Q	0.26	0/5560	0.64	3/7568 (0.0%)
15	R	0.28	0/1431	0.67	0/1968
All	All	0.69	7/37245 (0.0%)	0.69	13/50828 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	434	LEU	CG-CD2	112.25	5.22	1.52
6	F	229	TRP	CE3-CZ3	20.07	1.98	1.38
6	F	229	TRP	CE2-CZ2	17.39	1.76	1.39
6	F	229	TRP	CZ3-CH2	15.24	1.78	1.40
6	F	229	TRP	CD2-CE2	13.21	1.63	1.41
6	F	229	TRP	CZ2-CH2	12.60	1.61	1.37
6	F	229	TRP	CD2-CE3	11.83	1.59	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	324	HIS	N-CA-C	-7.84	100.08	111.30
1	A	484	ILE	N-CA-C	-7.20	106.07	112.12
2	B	724	MET	CB-CG-SD	-6.39	93.54	112.70
4	D	77	LYS	CA-C-N	6.10	133.19	121.54
4	D	77	LYS	C-N-CA	6.10	133.19	121.54
5	E	183	TYR	CA-C-N	5.86	132.72	121.54
5	E	183	TYR	C-N-CA	5.86	132.72	121.54
14	Q	273	LEU	CA-CB-CG	5.36	135.07	116.30
5	E	93	GLU	N-CA-CB	5.30	118.50	110.28
2	B	225	LEU	N-CA-C	5.18	117.34	111.02
8	H	588	VAL	N-CA-C	-5.13	107.34	111.91
14	Q	768	SER	CA-C-N	5.01	131.12	121.54
14	Q	768	SER	C-N-CA	5.01	131.12	121.54

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	A	4947	0	4993	92	0
2	B	5913	0	5947	134	0
3	C	1076	0	1078	19	0
4	D	3430	0	3473	63	0
5	E	2668	0	2637	46	0
6	F	2013	0	2030	41	0
7	G	522	0	531	20	0
8	H	4123	0	4106	105	0
9	I	504	0	497	23	0
10	J	573	0	554	12	0
11	K	1701	0	1703	38	0
12	L	1114	0	598	14	0
13	M	905	0	500	8	0
14	Q	5451	0	5321	71	0
15	R	1400	0	1292	12	0
16	B	8	0	0	1	0
17	E	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	F	2	0	0	0	0
17	K	1	0	0	0	0
18	J	2	0	0	0	0
All	All	36356	0	35260	636	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 9.

All (636) 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)
6:F:229:TRP:CZ3	6:F:229:TRP:CH2	1.78	1.72
6:F:229:TRP:CE2	6:F:229:TRP:CZ2	1.76	1.65
6:F:229:TRP:CZ3	6:F:229:TRP:CE3	1.98	1.47
2:B:479:ALA:HA	11:K:60:ALA:O	1.68	0.91
8:H:826:GLU:O	8:H:829:GLN:HB2	1.72	0.90
2:B:416:ILE:HA	2:B:434:HIS:O	1.73	0.87
2:B:324:ARG:O	2:B:327:GLU:HB2	1.74	0.86
8:H:316:VAL:HA	8:H:570:VAL:O	1.80	0.81
8:H:625:PHE:O	8:H:629:HIS:HB2	1.81	0.81
9:I:300:PRO:O	9:I:303:LEU:HB2	1.83	0.79
2:B:54:ALA:HA	2:B:57:MET:HE2	1.68	0.76
5:E:294:CYS:SG	5:E:308:CYS:HB3	2.25	0.76
8:H:707:VAL:O	8:H:729:ASP:HA	1.87	0.75
14:Q:576:ARG:O	14:Q:603:LEU:HA	1.87	0.74
2:B:6:ASP:H	2:B:26:ARG:HH22	1.40	0.70
8:H:701:GLU:HB3	8:H:737:GLN:HE21	1.56	0.69
8:H:824:ALA:O	8:H:827:ASN:HB3	1.92	0.69
14:Q:129:THR:O	14:Q:159:GLY:HA2	1.92	0.69
4:D:244:THR:HB	4:D:247:LYS:HD2	1.76	0.67
4:D:308:VAL:HB	4:D:316:TYR:HB2	1.75	0.66
7:G:32:LYS:NZ	11:K:264:CYS:SG	2.69	0.66
10:J:141:GLU:O	10:J:145:MET:HB2	1.96	0.66
1:A:665:GLN:HA	1:A:670:MET:HE2	1.76	0.66
2:B:232:VAL:HG12	2:B:455:ILE:HB	1.79	0.64
2:B:292:LEU:HB3	2:B:305:LEU:HD13	1.80	0.64
14:Q:130:GLY:HA3	14:Q:160:PHE:O	1.98	0.64
8:H:183:LYS:O	8:H:187:GLU:HB2	1.98	0.64
2:B:116:CYS:SG	2:B:117:ILE:N	2.70	0.63
9:I:289:ARG:O	9:I:293:GLN:HB2	1.98	0.63
14:Q:724:VAL:HA	14:Q:756:VAL:O	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:304:LEU:O	8:H:308:ALA:HB2	1.99	0.63
2:B:38:GLY:O	2:B:455:ILE:HA	1.98	0.63
3:C:494:LYS:HD2	3:C:536:LEU:HD23	1.81	0.63
11:K:246:TYR:HA	11:K:261:CYS:HA	1.80	0.62
14:Q:685:VAL:HB	14:Q:717:ILE:HB	1.81	0.62
3:C:528:MET:HE1	5:E:296:ALA:HA	1.79	0.62
8:H:586:ASP:HB3	8:H:589:TRP:HB2	1.80	0.62
4:D:251:VAL:HG12	4:D:253:GLY:H	1.65	0.62
6:F:151:VAL:HG21	6:F:157:MET:HB2	1.82	0.62
8:H:208:VAL:HG22	9:I:317:ILE:HD13	1.82	0.62
9:I:301:ALA:O	9:I:304:GLN:HB3	2.00	0.62
6:F:268:CYS:SG	6:F:269:SER:N	2.73	0.61
2:B:703:ASP:HA	2:B:706:LEU:HD23	1.82	0.61
2:B:490:LEU:HB2	2:B:677:MET:HE1	1.81	0.61
1:A:361:CYS:HA	1:A:437:LEU:O	2.01	0.61
8:H:641:TYR:HB2	8:H:649:LEU:HD22	1.82	0.60
9:I:306:ILE:HG13	9:I:310:ASN:HB2	1.83	0.60
8:H:841:GLU:O	8:H:844:ALA:HB3	2.02	0.60
1:A:629:HIS:O	1:A:676:ARG:NH1	2.35	0.60
2:B:468:PRO:HA	2:B:473:PHE:HB3	1.82	0.60
8:H:824:ALA:O	8:H:828:GLU:N	2.34	0.60
8:H:844:ALA:HA	10:J:145:MET:HE1	1.82	0.60
1:A:392:PHE:HB3	1:A:408:SER:HB2	1.83	0.60
2:B:109:LEU:HD21	2:B:199:ILE:HD11	1.83	0.60
8:H:684:LEU:HB2	8:H:732:LEU:HD13	1.84	0.60
2:B:39:VAL:HG12	2:B:456:ILE:HB	1.84	0.60
5:E:156:LEU:HA	5:E:159:MET:HE3	1.84	0.60
5:E:308:CYS:SG	5:E:309:GLY:N	2.75	0.59
11:K:160:PRO:O	11:K:189:ARG:NH2	2.35	0.59
4:D:432:VAL:HB	4:D:442:VAL:HG13	1.84	0.59
2:B:653:THR:HG22	2:B:692:LYS:HD2	1.85	0.59
3:C:436:PRO:HG2	4:D:70:ALA:HB3	1.85	0.59
10:J:162:PHE:HA	10:J:165:ILE:HG12	1.85	0.59
11:K:115:SER:H	11:K:118:MET:HB2	1.66	0.59
1:A:177:VAL:O	1:A:269:SER:HA	2.02	0.59
3:C:526:GLU:OE1	3:C:530:GLN:NE2	2.36	0.58
9:I:283:PRO:HA	9:I:286:GLN:HB2	1.85	0.58
1:A:66:PRO:HD2	1:A:67:LEU:HD12	1.85	0.58
5:E:291:CYS:O	5:E:295:ARG:N	2.35	0.58
2:B:136:SER:HA	2:B:389:THR:HB	1.86	0.58
8:H:175:THR:HA	8:H:178:ARG:HD2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:540:GLU:HB3	8:H:620:LYS:HD3	1.86	0.58
1:A:199:LEU:HG	1:A:201:ASN:H	1.69	0.58
8:H:718:ARG:HD2	8:H:725:ARG:HA	1.85	0.58
11:K:117:LEU:HD12	11:K:125:THR:HB	1.86	0.58
8:H:533:GLU:OE2	8:H:584:ARG:NH1	2.36	0.58
8:H:686:SER:O	8:H:690:TRP:N	2.36	0.58
1:A:520:ARG:HH22	7:G:25:GLU:HG2	1.69	0.57
1:A:281:GLN:NE2	1:A:482:PHE:O	2.37	0.57
1:A:568:LEU:HD22	1:A:608:SER:HB3	1.86	0.57
2:B:272:ARG:NH2	2:B:275:GLU:OE1	2.37	0.57
14:Q:871:LYS:HD3	14:Q:872:ASN:HB2	1.86	0.57
2:B:199:ILE:HG22	2:B:225:LEU:HD11	1.86	0.57
2:B:278:GLU:HG2	2:B:315:LEU:HD11	1.86	0.57
2:B:523:LEU:HG	2:B:527:MET:HE1	1.84	0.57
15:R:129:ASP:HB2	15:R:139:LEU:HD23	1.86	0.57
2:B:303:ALA:O	9:I:308:ARG:NH2	2.38	0.57
12:L:45:DC:H42	13:M:50:DA:H61	1.52	0.57
14:Q:143:CYS:SG	14:Q:144:GLN:N	2.77	0.57
9:I:300:PRO:HA	9:I:303:LEU:HD13	1.85	0.57
2:B:70:LEU:HB3	2:B:204:VAL:HG12	1.86	0.57
8:H:194:MET:HA	8:H:197:PHE:HB3	1.86	0.57
2:B:534:GLY:HA2	2:B:594:ALA:O	2.05	0.57
4:D:399:ASP:O	8:H:908:ARG:NH1	2.38	0.57
5:E:80:ARG:NH1	5:E:172:SER:OG	2.37	0.57
9:I:280:ARG:HH21	9:I:289:ARG:HH11	1.53	0.57
11:K:249:GLU:HB2	11:K:257:TYR:HB3	1.87	0.57
14:Q:758:LEU:HA	14:Q:801:LEU:HB2	1.86	0.57
5:E:291:CYS:O	5:E:295:ARG:HA	2.05	0.56
2:B:321:GLY:HA2	2:B:324:ARG:HB3	1.87	0.56
2:B:383:LEU:HA	2:B:388:ILE:HD12	1.88	0.56
8:H:650:LYS:HE3	8:H:673:GLU:HG2	1.87	0.56
14:Q:565:ALA:HA	14:Q:568:ARG:HE	1.69	0.56
1:A:513:PRO:O	1:A:539:ASN:ND2	2.36	0.56
2:B:250:ASN:HA	2:B:433:LEU:O	2.06	0.56
8:H:651:ARG:NH1	13:M:23:DT:OP2	2.39	0.56
8:H:840:LYS:HA	8:H:843:ARG:HH11	1.71	0.56
1:A:415:HIS:O	1:A:419:ARG:NH2	2.35	0.56
1:A:568:LEU:HD11	1:A:606:PHE:HB3	1.86	0.56
14:Q:255:GLU:HB3	14:Q:621:THR:HG21	1.87	0.56
8:H:589:TRP:HH2	8:H:597:ARG:HH11	1.53	0.56
9:I:276:LEU:O	9:I:280:ARG:N	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:O	1:A:195:ARG:NH1	2.39	0.56
1:A:400:PRO:HG3	1:A:426:VAL:HG22	1.88	0.56
3:C:526:GLU:O	3:C:530:GLN:NE2	2.38	0.56
14:Q:580:LEU:HB3	14:Q:583:ALA:HB2	1.88	0.56
14:Q:595:ARG:HH12	14:Q:599:PRO:HA	1.71	0.56
1:A:65:MET:HE1	1:A:79:ALA:HA	1.87	0.56
14:Q:125:SER:O	14:Q:155:LYS:NZ	2.38	0.56
8:H:667:LEU:N	8:H:675:VAL:O	2.39	0.55
1:A:342:CYS:SG	1:A:642:ARG:NH2	2.80	0.55
4:D:402:ARG:NH2	8:H:911:GLU:OE1	2.39	0.55
9:I:304:GLN:OE1	9:I:308:ARG:NH1	2.40	0.55
15:R:143:LEU:HD23	15:R:173:VAL:HA	1.89	0.55
2:B:226:ALA:HB3	2:B:229:ALA:HB2	1.89	0.55
2:B:655:ASP:OD1	2:B:658:ARG:NH2	2.39	0.55
4:D:272:PHE:HB3	4:D:282:TYR:HB2	1.87	0.55
8:H:798:ASP:N	8:H:805:HIS:O	2.39	0.55
8:H:215:ALA:HB2	9:I:325:ILE:HG12	1.89	0.55
5:E:329:ASP:O	5:E:376:HIS:NE2	2.40	0.55
6:F:160:ARG:NH1	6:F:231:PHE:O	2.39	0.55
2:B:461:LEU:HB3	2:B:464:LEU:HD21	1.89	0.54
9:I:304:GLN:O	9:I:308:ARG:NH1	2.40	0.54
14:Q:14:PRO:O	14:Q:43:ARG:NH2	2.39	0.54
2:B:612:HIS:O	2:B:613:HIS:ND1	2.39	0.54
4:D:59:MET:HE3	4:D:109:ILE:HA	1.89	0.54
8:H:854:GLY:HA2	8:H:857:ILE:HD12	1.89	0.54
1:A:418:LYS:HZ3	12:L:42:DC:H5'	1.72	0.54
14:Q:31:GLY:HA3	14:Q:189:LYS:HB2	1.90	0.54
14:Q:740:ARG:HH22	14:Q:744:GLN:HE21	1.56	0.54
14:Q:190:LEU:O	14:Q:637:LYS:NZ	2.41	0.54
2:B:219:ASP:N	2:B:219:ASP:OD1	2.40	0.54
2:B:241:ASN:O	2:B:245:ASP:N	2.41	0.54
2:B:281:LEU:HD12	2:B:315:LEU:HD12	1.89	0.54
4:D:308:VAL:HG13	4:D:376:MET:HE1	1.90	0.54
14:Q:84:LEU:O	14:Q:86:ARG:NH1	2.41	0.54
2:B:217:ILE:HA	2:B:220:LEU:HB3	1.89	0.54
2:B:444:ILE:HG21	2:B:471:LEU:HD23	1.90	0.54
11:K:154:ASP:O	11:K:189:ARG:NH1	2.36	0.54
1:A:95:TYR:HB3	5:E:22:LEU:HA	1.88	0.54
1:A:703:PHE:O	1:A:709:GLN:NE2	2.38	0.54
2:B:363:GLN:OE1	8:H:778:ASN:ND2	2.41	0.54
6:F:52:ASN:ND2	6:F:54:SER:OG	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:651:ARG:HH22	13:M:22:DG:H3'	1.73	0.54
1:A:424:GLU:OE1	1:A:425:ARG:NH1	2.41	0.53
5:E:291:CYS:O	5:E:295:ARG:CA	2.56	0.53
6:F:196:LEU:HD21	6:F:223:LEU:HD12	1.89	0.53
10:J:120:LYS:NZ	10:J:154:ASP:OD2	2.41	0.53
8:H:773:GLN:HB3	8:H:812:ILE:HG12	1.90	0.53
2:B:483:MET:O	11:K:56:THR:N	2.41	0.53
4:D:63:GLU:OE1	4:D:115:ARG:NH2	2.41	0.53
2:B:6:ASP:OD1	2:B:6:ASP:N	2.40	0.53
2:B:222:SER:HA	2:B:225:LEU:HD23	1.89	0.53
2:B:671:LYS:HB3	2:B:733:GLN:HE22	1.74	0.53
3:C:481:VAL:HA	3:C:486:LEU:HD23	1.89	0.53
8:H:536:CYS:O	8:H:540:GLU:N	2.42	0.53
2:B:72:TYR:HB3	2:B:206:VAL:HG22	1.91	0.53
2:B:184:GLY:O	2:B:188:GLY:N	2.41	0.53
5:E:256:GLN:NE2	6:F:263:GLU:OE1	2.42	0.53
1:A:74:ARG:HB3	1:A:143:LEU:HA	1.91	0.53
5:E:383:PRO:HA	5:E:386:ILE:HD12	1.91	0.53
14:Q:223:LEU:HA	14:Q:226:GLN:HB3	1.89	0.53
2:B:478:MET:O	11:K:61:ASN:HA	2.09	0.53
1:A:635:GLN:OE1	1:A:676:ARG:NH2	2.42	0.53
2:B:446:PRO:O	2:B:450:ARG:HB2	2.08	0.53
4:D:337:ARG:HA	4:D:342:VAL:HG12	1.90	0.52
4:D:450:ASP:OD1	4:D:453:ARG:NH2	2.42	0.52
7:G:40:ASP:OD2	8:H:898:ARG:NH1	2.43	0.52
1:A:582:GLY:O	1:A:589:ARG:NH2	2.41	0.52
8:H:221:ASN:OD1	8:H:307:ARG:NH1	2.38	0.52
8:H:715:ARG:NH1	8:H:802:GLY:O	2.41	0.52
9:I:277:GLU:O	9:I:280:ARG:HB3	2.10	0.52
1:A:360:ARG:NH2	1:A:433:GLN:OE1	2.43	0.52
2:B:88:ARG:NH2	2:B:174:ILE:O	2.42	0.52
4:D:317:ALA:O	4:D:341:MET:HA	2.10	0.52
1:A:511:TRP:HB3	1:A:663:VAL:HG23	1.91	0.52
3:C:478:CYS:SG	3:C:489:LYS:NZ	2.71	0.52
4:D:352:GLN:NE2	4:D:397:GLU:OE2	2.43	0.52
14:Q:201:ASN:O	14:Q:205:GLU:HB2	2.09	0.52
1:A:388:GLN:NE2	1:A:402:GLY:O	2.43	0.52
1:A:514:MET:HE2	1:A:519:TYR:HD1	1.73	0.52
1:A:626:ILE:HG22	1:A:662:LEU:HD12	1.90	0.52
4:D:35:TYR:OH	4:D:93:LEU:O	2.27	0.52
14:Q:728:SER:OG	14:Q:729:ILE:N	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:223:ILE:HD13	8:H:279:LEU:HB3	1.92	0.52
8:H:783:ALA:O	8:H:787:ASP:N	2.43	0.52
8:H:854:GLY:O	8:H:857:ILE:HB	2.10	0.52
1:A:557:LYS:NZ	1:A:602:ILE:O	2.39	0.51
4:D:273:GLN:NE2	4:D:278:SER:O	2.41	0.51
1:A:418:LYS:NZ	12:L:41:DT:O3'	2.44	0.51
1:A:556:ASP:OD1	1:A:621:ASN:ND2	2.42	0.51
2:B:69:LYS:NZ	2:B:200:LEU:O	2.43	0.51
2:B:161:PHE:O	2:B:166:ARG:N	2.42	0.51
15:R:170:LEU:HD21	15:R:205:ALA:HB1	1.92	0.51
3:C:461:LEU:HD11	3:C:521:LEU:HD13	1.93	0.51
8:H:819:ASP:N	8:H:819:ASP:OD1	2.44	0.51
8:H:833:GLU:O	8:H:837:LYS:N	2.40	0.51
5:E:332:GLN:HB3	5:E:334:ILE:HG13	1.92	0.51
3:C:520:ASN:H	5:E:269:PRO:HD2	1.76	0.51
4:D:143:ARG:HH21	4:D:147:SER:HB2	1.76	0.51
8:H:696:VAL:HG23	8:H:741:TYR:HB2	1.93	0.51
8:H:819:ASP:O	8:H:823:THR:N	2.43	0.51
1:A:440:LEU:HD21	1:A:455:LEU:HD21	1.93	0.51
2:B:341:LYS:O	2:B:345:ARG:NH1	2.44	0.51
11:K:246:TYR:HB3	11:K:259:LYS:HB3	1.93	0.51
14:Q:73:ILE:HG22	14:Q:77:LYS:HE2	1.92	0.51
1:A:176:PHE:HA	1:A:270:PHE:O	2.11	0.51
1:A:623:LEU:HB3	1:A:659:PHE:HB2	1.93	0.51
6:F:11:LEU:HD11	6:F:162:LEU:HD23	1.92	0.51
14:Q:614:THR:HA	14:Q:617:GLN:HB2	1.92	0.51
10:J:164:ARG:HG2	10:J:167:LYS:HE3	1.92	0.51
2:B:200:LEU:HD13	2:B:225:LEU:HD13	1.92	0.50
5:E:191:ALA:O	5:E:193:LYS:NZ	2.44	0.50
5:E:57:MET:HE1	5:E:164:SER:HB2	1.92	0.50
11:K:105:CYS:SG	11:K:106:GLU:N	2.85	0.50
5:E:184:ASP:HA	5:E:187:LYS:HD3	1.94	0.50
8:H:798:ASP:HB3	8:H:805:HIS:HB2	1.94	0.50
10:J:165:ILE:HG22	10:J:168:LYS:HZ3	1.77	0.50
2:B:57:MET:HE1	2:B:90:LEU:HD11	1.94	0.50
2:B:209:TYR:OH	2:B:234:ASP:O	2.29	0.50
3:C:454:PRO:HD2	3:C:457:ILE:HD12	1.93	0.50
3:C:489:LYS:HA	3:C:492:LYS:HG2	1.94	0.50
4:D:155:ARG:NH2	4:D:267:GLU:O	2.44	0.50
4:D:360:THR:HG22	4:D:362:GLN:H	1.77	0.50
8:H:221:ASN:ND2	8:H:573:ASP:O	2.43	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:683:SER:O	14:Q:817:LYS:NZ	2.39	0.50
2:B:4:ASN:HA	2:B:9:LEU:HA	1.94	0.50
2:B:296:SER:HB3	2:B:299:ARG:HB2	1.93	0.50
8:H:551:VAL:HG13	8:H:554:GLN:HB2	1.94	0.50
2:B:423:ASP:HB2	12:L:55:DA:H61	1.77	0.50
8:H:315:LEU:O	8:H:571:GLY:HA2	2.12	0.50
4:D:362:GLN:OE1	4:D:392:ARG:NH1	2.44	0.50
1:A:472:ARG:NH2	13:M:60:DC:OP2	2.45	0.49
2:B:80:ILE:HG12	2:B:206:VAL:HG12	1.93	0.49
2:B:253:ARG:HD2	2:B:431:PRO:HD2	1.93	0.49
3:C:408:ARG:NH2	6:F:122:SER:O	2.40	0.49
4:D:139:ASP:OD1	4:D:280:ARG:NH1	2.45	0.49
8:H:754:ASN:OD1	8:H:758:ASN:N	2.44	0.49
11:K:215:LYS:NZ	12:L:45:DC:OP1	2.39	0.49
14:Q:204:LEU:HD22	14:Q:592:GLU:HG2	1.94	0.49
1:A:516:PRO:O	7:G:18:GLN:NE2	2.43	0.49
2:B:216:LYS:HD3	12:L:61:DT:H3	1.77	0.49
8:H:855:LEU:HB2	10:J:112:LEU:HD13	1.93	0.49
15:R:141:LEU:HD22	15:R:171:VAL:HG13	1.92	0.49
5:E:359:VAL:HG22	5:E:366:VAL:HG23	1.95	0.49
8:H:753:ARG:HH22	8:H:812:ILE:HB	1.77	0.49
14:Q:110:THR:HB	14:Q:113:ILE:HD12	1.94	0.49
2:B:69:LYS:NZ	2:B:202:ALA:O	2.46	0.49
6:F:268:CYS:HB3	6:F:273:SER:H	1.78	0.49
14:Q:30:ASP:N	14:Q:30:ASP:OD1	2.44	0.49
14:Q:740:ARG:NH1	14:Q:743:SER:OG	2.45	0.49
2:B:31:THR:HG21	2:B:477:THR:HG22	1.94	0.49
2:B:241:ASN:OD1	2:B:658:ARG:NH2	2.45	0.49
2:B:514:ILE:HG23	2:B:518:ARG:HH12	1.77	0.49
2:B:611:VAL:HB	2:B:614:TYR:HD2	1.76	0.49
5:E:291:CYS:HB2	5:E:312:LEU:HD11	1.95	0.49
15:R:103:VAL:HG21	15:R:113:LEU:HD11	1.95	0.49
3:C:407:ILE:HD11	6:F:19:PRO:HB3	1.95	0.49
1:A:67:LEU:HD13	1:A:147:GLY:HA3	1.95	0.49
2:B:482:THR:OG1	2:B:699:GLU:OE2	2.30	0.49
5:E:68:SER:HB3	5:E:143:PRO:HD3	1.95	0.49
5:E:259:ILE:HA	5:E:287:GLY:HA3	1.95	0.49
8:H:221:ASN:HA	8:H:224:CYS:HB2	1.94	0.49
8:H:660:TYR:HB3	8:H:680:CYS:HB3	1.95	0.49
2:B:329:PHE:HA	2:B:332:PHE:HB3	1.95	0.49
4:D:188:THR:OG1	4:D:189:GLU:OE1	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:698:ARG:HD2	8:H:739:GLU:HG3	1.94	0.49
1:A:638:GLN:O	1:A:642:ARG:NH1	2.46	0.49
9:I:312:GLN:HA	9:I:315:GLN:HG2	1.94	0.49
14:Q:726:ARG:NH2	14:Q:760:GLU:OE1	2.46	0.49
1:A:408:SER:OG	1:A:409:THR:N	2.46	0.48
7:G:29:LEU:HD23	7:G:49:LEU:HD13	1.95	0.48
14:Q:233:LEU:HD12	14:Q:291:LEU:HB3	1.94	0.48
14:Q:241:LYS:HE2	14:Q:252:LEU:HA	1.95	0.48
2:B:115:LEU:HD23	2:B:192:TYR:HA	1.96	0.48
4:D:431:LEU:HA	4:D:443:VAL:HG12	1.95	0.48
2:B:118:HIS:ND1	16:B:1000:SF4:S3	2.73	0.48
6:F:21:TRP:NE1	6:F:197:ASP:OD2	2.46	0.48
8:H:203:GLU:HG3	8:H:207:LYS:HE3	1.96	0.48
8:H:313:THR:HA	8:H:533:GLU:O	2.12	0.48
13:M:27:DA:H2'	13:M:28:DG:C8	2.48	0.48
1:A:480:LEU:HA	1:A:483:LEU:HB2	1.95	0.48
8:H:655:LYS:NZ	12:L:66:DC:OP1	2.36	0.48
9:I:276:LEU:HG	9:I:279:LEU:HD12	1.96	0.48
2:B:622:GLY:HA2	2:B:681:ASP:HB2	1.96	0.48
6:F:59:VAL:HG23	6:F:70:LEU:HB2	1.95	0.48
1:A:564:ASN:ND2	12:L:37:DC:OP1	2.46	0.48
2:B:15:ASP:OD1	2:B:15:ASP:N	2.44	0.48
2:B:240:ASP:OD1	2:B:240:ASP:N	2.47	0.48
2:B:339:TYR:OH	2:B:343:ARG:NH2	2.47	0.48
2:B:562:GLN:O	2:B:592:ARG:NH2	2.46	0.48
2:B:647:ARG:HB3	2:B:650:ASP:HB2	1.95	0.48
6:F:282:CYS:HB3	6:F:285:CYS:HB2	1.96	0.48
11:K:28:ILE:O	11:K:31:LYS:HB2	2.14	0.48
5:E:320:ARG:HH21	5:E:324:HIS:HB2	1.78	0.48
6:F:13:ILE:HB	6:F:59:VAL:HG12	1.94	0.48
6:F:48:HIS:NE2	6:F:56:LYS:O	2.43	0.48
8:H:306:LEU:HD22	8:H:311:LEU:HD12	1.96	0.48
11:K:165:ILE:HB	11:K:180:LEU:HB2	1.95	0.48
11:K:197:GLN:NE2	11:K:201:GLU:OE2	2.47	0.48
14:Q:57:CYS:SG	14:Q:129:THR:OG1	2.64	0.48
2:B:20:GLU:O	2:B:24:TYR:HB2	2.14	0.48
2:B:105:LEU:HD23	2:B:202:ALA:HA	1.95	0.48
4:D:148:LEU:HD12	4:D:284:THR:HG22	1.95	0.48
5:E:167:VAL:O	5:E:196:VAL:HA	2.14	0.48
5:E:211:LEU:O	5:E:215:THR:CB	2.62	0.48
14:Q:719:THR:HG23	14:Q:721:GLU:H	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:ILE:O	1:A:552:GLU:HB2	2.14	0.47
2:B:53:LEU:HD13	2:B:87:LEU:HD13	1.96	0.47
5:E:152:ALA:O	5:E:156:LEU:HB2	2.14	0.47
5:E:255:PRO:HG3	5:E:312:LEU:HB3	1.95	0.47
1:A:513:PRO:HA	1:A:665:GLN:HB2	1.94	0.47
6:F:112:VAL:HA	6:F:115:ILE:HG22	1.96	0.47
6:F:236:ASP:N	6:F:236:ASP:OD1	2.47	0.47
8:H:537:GLU:HG2	8:H:540:GLU:HG2	1.96	0.47
8:H:695:ARG:NH2	8:H:738:THR:O	2.47	0.47
10:J:146:ILE:O	10:J:150:ASP:N	2.47	0.47
1:A:183:ASP:OD1	1:A:183:ASP:N	2.45	0.47
2:B:131:ASP:OD1	2:B:131:ASP:N	2.48	0.47
8:H:533:GLU:HB3	8:H:542:TRP:HB3	1.96	0.47
11:K:35:ALA:O	11:K:38:LEU:HB2	2.14	0.47
11:K:223:VAL:HG21	14:Q:612:GLY:HA2	1.97	0.47
3:C:505:LEU:O	3:C:509:GLN:N	2.46	0.47
7:G:11:GLU:OE1	8:H:908:ARG:NH2	2.47	0.47
14:Q:375:LEU:HD23	14:Q:432:LEU:HD12	1.95	0.47
2:B:504:ILE:O	2:B:520:TYR:OH	2.27	0.47
6:F:25:GLN:OE1	6:F:30:SER:OG	2.32	0.47
14:Q:317:GLU:HB3	14:Q:324:SER:HB2	1.97	0.47
1:A:703:PHE:HB3	1:A:709:GLN:HG2	1.96	0.47
4:D:407:VAL:HG22	7:G:6:LYS:HD3	1.97	0.47
4:D:431:LEU:HD21	4:D:434:GLU:HB3	1.97	0.47
5:E:59:ARG:HB3	5:E:164:SER:HB3	1.97	0.47
7:G:50:VAL:O	7:G:53:LEU:HB2	2.14	0.47
14:Q:316:THR:HG21	15:R:252:THR:HG22	1.97	0.47
4:D:112:PRO:HG2	4:D:115:ARG:HG3	1.97	0.47
11:K:258:ARG:HA	11:K:268:LEU:O	2.14	0.47
14:Q:179:GLU:HB3	14:Q:183:ARG:HH12	1.79	0.47
1:A:150:ASP:OD1	1:A:150:ASP:N	2.47	0.47
1:A:363:VAL:HB	1:A:407:ILE:HG12	1.97	0.47
2:B:242:VAL:HA	2:B:245:ASP:HB2	1.96	0.47
2:B:556:GLY:O	2:B:560:ASN:ND2	2.48	0.47
5:E:59:ARG:HH11	5:E:238:PRO:HA	1.80	0.47
5:E:107:ILE:HG12	5:E:116:LYS:HD2	1.96	0.47
8:H:670:CYS:HB3	8:H:673:GLU:HB2	1.96	0.47
2:B:465:ASP:O	2:B:469:LYS:NZ	2.42	0.46
6:F:240:GLN:HG3	6:F:241:LEU:HD12	1.97	0.46
6:F:256:PHE:HD1	6:F:259:ARG:HH22	1.62	0.46
8:H:849:LYS:HE2	10:J:171:LEU:H	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:GLU:HA	2:B:30:ARG:HE	1.80	0.46
6:F:213:LEU:HB2	6:F:231:PHE:HE1	1.81	0.46
8:H:711:SER:OG	8:H:715:ARG:N	2.48	0.46
14:Q:32:LEU:HD11	14:Q:190:LEU:HG	1.97	0.46
1:A:309:ASP:OD1	1:A:309:ASP:N	2.48	0.46
2:B:307:ASN:ND2	9:I:308:ARG:O	2.36	0.46
3:C:402:ASN:O	3:C:406:SER:HB3	2.15	0.46
5:E:304:GLU:HA	5:E:311:THR:HA	1.95	0.46
6:F:255:CYS:SG	6:F:258:HIS:HD2	2.38	0.46
14:Q:253:SER:OG	14:Q:255:GLU:OE2	2.30	0.46
8:H:229:LEU:HD21	8:H:280:GLN:HG3	1.97	0.46
14:Q:744:GLN:O	14:Q:748:MET:HB2	2.16	0.46
2:B:629:GLN:HA	2:B:634:LYS:HE2	1.96	0.46
4:D:59:MET:HA	4:D:66:LEU:HD22	1.98	0.46
4:D:457:ARG:O	4:D:461:SER:CB	2.63	0.46
8:H:776:LEU:HD12	8:H:779:LEU:HD13	1.98	0.46
4:D:421:LEU:HD21	4:D:455:TRP:HB2	1.98	0.46
8:H:753:ARG:HD2	8:H:758:ASN:HA	1.97	0.46
2:B:236:ALA:O	2:B:239:ILE:HB	2.15	0.46
8:H:237:ILE:HG21	8:H:309:LEU:HD21	1.97	0.46
8:H:249:VAL:HG13	8:H:253:TYR:HD2	1.79	0.46
8:H:889:GLY:O	8:H:893:GLN:NE2	2.48	0.46
14:Q:182:MET:HA	14:Q:185:LEU:HB3	1.98	0.46
14:Q:381:TRP:HB3	14:Q:423:TYR:CZ	2.50	0.46
5:E:111:SER:O	5:E:111:SER:OG	2.33	0.46
5:E:165:ARG:HB3	5:E:194:ILE:HG23	1.98	0.46
9:I:274:HIS:CD2	9:I:323:HIS:HB3	2.50	0.46
2:B:23:SER:HB2	11:K:59:MET:HE2	1.98	0.46
2:B:487:ARG:NH1	2:B:724:MET:O	2.48	0.46
11:K:245:GLU:O	11:K:262:THR:N	2.44	0.46
14:Q:410:CYS:HA	14:Q:555:HIS:O	2.16	0.46
14:Q:564:TYR:O	14:Q:567:THR:OG1	2.29	0.46
1:A:305:ASP:HA	1:A:359:LYS:HD3	1.98	0.46
4:D:114:PHE:HD1	4:D:117:ASN:HB2	1.81	0.46
14:Q:290:ILE:HA	14:Q:293:THR:HG22	1.98	0.46
1:A:505:VAL:HG23	1:A:658:PHE:HA	1.98	0.45
1:A:558:ILE:O	1:A:604:THR:HA	2.16	0.45
4:D:76:LYS:HG2	6:F:240:GLN:HA	1.98	0.45
8:H:660:TYR:N	8:H:680:CYS:O	2.47	0.45
14:Q:728:SER:O	14:Q:732:LEU:N	2.46	0.45
1:A:190:GLN:HA	1:A:195:ARG:HH12	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601:ARG:HG3	2:B:659:HIS:CE1	2.51	0.45
4:D:70:ALA:O	4:D:74:TRP:N	2.49	0.45
4:D:384:PRO:HA	4:D:385:PRO:HD3	1.85	0.45
8:H:698:ARG:HH21	8:H:737:GLN:HA	1.81	0.45
1:A:179:SER:O	1:A:267:THR:HA	2.16	0.45
4:D:70:ALA:HB1	4:D:73:LEU:HB2	1.97	0.45
7:G:9:LEU:HD11	7:G:42:HIS:HB3	1.97	0.45
7:G:27:ASN:HD21	7:G:32:LYS:HD3	1.80	0.45
14:Q:36:ALA:HB2	14:Q:194:PRO:HA	1.97	0.45
1:A:478:VAL:O	1:A:481:ASN:HB2	2.16	0.45
2:B:421:PHE:HA	2:B:428:ILE:HG22	1.99	0.45
3:C:519:THR:HG21	5:E:284:LEU:HD13	1.98	0.45
1:A:295:TYR:HB3	1:A:333:ALA:HB3	1.98	0.45
4:D:449:SER:HA	4:D:452:LYS:HE2	1.98	0.45
14:Q:36:ALA:O	14:Q:589:ARG:NH1	2.49	0.45
2:B:106:GLY:O	2:B:175:TYR:N	2.48	0.45
2:B:331:GLY:O	2:B:334:ARG:HB2	2.16	0.45
2:B:374:PHE:HD2	2:B:378:ARG:HH21	1.65	0.45
8:H:211:LEU:HB3	9:I:324:PHE:HE2	1.81	0.45
8:H:780:HIS:HB2	8:H:811:TYR:CZ	2.52	0.45
14:Q:687:ASP:HB2	14:Q:711:LEU:HB2	1.99	0.45
12:L:74:DA:H2''	12:L:75:DC:H5''	1.99	0.45
1:A:578:PRO:HG2	1:A:605:ILE:HG22	1.99	0.45
5:E:255:PRO:HB2	5:E:289:TYR:HB3	1.99	0.45
7:G:22:TYR:O	7:G:26:SER:OG	2.31	0.45
8:H:254:LEU:HD13	8:H:545:VAL:HG21	1.99	0.45
8:H:293:ARG:NH2	8:H:297:GLU:OE1	2.50	0.45
1:A:386:ASP:HA	1:A:389:ILE:HD12	1.98	0.45
2:B:60:GLN:HG2	2:B:67:VAL:HG23	1.99	0.45
2:B:175:TYR:HB3	2:B:180:LEU:HG	1.98	0.45
6:F:18:ASN:ND2	6:F:129:THR:O	2.50	0.45
11:K:249:GLU:OE1	11:K:270:TYR:OH	2.33	0.44
2:B:657:MET:HG2	2:B:692:LYS:HG3	1.99	0.44
14:Q:715:ASP:OD2	14:Q:726:ARG:N	2.47	0.44
1:A:551:HIS:HB3	1:A:556:ASP:HB2	2.00	0.44
2:B:265:THR:HA	2:B:268:LYS:HG2	1.99	0.44
2:B:537:ALA:HA	2:B:619:ILE:O	2.18	0.44
3:C:509:GLN:HG2	3:C:522:VAL:HG11	1.99	0.44
5:E:167:VAL:HB	5:E:196:VAL:HG22	1.99	0.44
7:G:62:ASP:OD1	7:G:62:ASP:N	2.51	0.44
1:A:514:MET:HE3	1:A:518:PHE:HB3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:311:THR:HA	4:D:387:ILE:HD11	2.00	0.44
4:D:336:TYR:HB2	4:D:343:VAL:HG12	2.00	0.44
6:F:12:VAL:HG22	6:F:58:ALA:HB3	1.99	0.44
12:L:75:DC:H2''	12:L:76:DG:H2'	1.99	0.44
1:A:509:GLU:OE1	1:A:673:SER:OG	2.35	0.44
4:D:265:LEU:HD22	4:D:270:LEU:HD21	1.98	0.44
15:R:131:VAL:HA	15:R:136:THR:O	2.17	0.44
2:B:40:LEU:HD22	2:B:481:PHE:HE1	1.82	0.44
2:B:71:ILE:HB	2:B:231:VAL:HG12	1.99	0.44
4:D:272:PHE:N	4:D:282:TYR:O	2.42	0.44
8:H:579:ARG:NH2	8:H:622:ASP:OD1	2.47	0.44
8:H:690:TRP:O	8:H:695:ARG:N	2.50	0.44
8:H:797:PHE:HB2	13:M:32:DT:H6	1.81	0.44
14:Q:62:LEU:HD12	14:Q:133:VAL:HG12	2.00	0.44
2:B:330:LEU:HD23	2:B:330:LEU:HA	1.88	0.44
5:E:211:LEU:O	5:E:215:THR:HB	2.18	0.44
8:H:745:VAL:HG22	8:H:769:ILE:HD12	2.00	0.44
1:A:197:CYS:HB3	1:A:276:MET:HB2	1.99	0.44
3:C:424:SER:HB2	4:D:62:LEU:HA	1.99	0.44
8:H:847:ASN:HB3	10:J:145:MET:HE2	1.98	0.44
1:A:61:TYR:HB3	1:A:65:MET:HE3	2.00	0.44
6:F:195:VAL:HG11	6:F:199:ASP:HA	2.00	0.44
1:A:309:ASP:OD1	1:A:383:THR:OG1	2.27	0.43
6:F:234:ASP:O	6:F:238:ARG:N	2.48	0.43
8:H:690:TRP:HB3	8:H:695:ARG:HB2	1.99	0.43
1:A:531:ILE:HA	1:A:534:TYR:CZ	2.54	0.43
9:I:288:MET:HA	9:I:291:ILE:HD12	2.00	0.43
14:Q:76:LEU:HD23	14:Q:81:VAL:HG11	1.99	0.43
15:R:128:PRO:HG3	15:R:164:PHE:HE2	1.82	0.43
2:B:532:PRO:HB3	5:E:174:LEU:HD22	1.99	0.43
4:D:59:MET:HE1	4:D:96:TRP:HB3	1.99	0.43
4:D:96:TRP:HA	4:D:110:LEU:HB3	2.00	0.43
5:E:345:CYS:HB3	5:E:352:LEU:HD11	2.01	0.43
9:I:282:GLN:O	9:I:286:GLN:N	2.39	0.43
1:A:341:PRO:HB3	1:A:493:TRP:CE2	2.53	0.43
4:D:156:TRP:HA	4:D:159:VAL:HG12	2.00	0.43
4:D:401:LEU:HG	7:G:12:CYS:HB3	2.00	0.43
6:F:40:ALA:HA	6:F:224:LEU:HD13	2.01	0.43
8:H:773:GLN:HA	8:H:812:ILE:HA	2.00	0.43
14:Q:568:ARG:O	14:Q:572:GLU:CB	2.66	0.43
14:Q:726:ARG:HG3	14:Q:758:LEU:HD22	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ASP:OD1	1:A:386:ASP:N	2.41	0.43
1:A:422:GLU:HG2	11:K:157:LYS:HG2	1.99	0.43
1:A:492:ASN:HB3	1:A:495:GLU:HG2	1.99	0.43
2:B:39:VAL:N	2:B:477:THR:OG1	2.51	0.43
2:B:56:ILE:HG21	2:B:70:LEU:HD22	2.01	0.43
2:B:566:LEU:HG	2:B:592:ARG:HG2	2.01	0.43
5:E:345:CYS:SG	5:E:368:CYS:N	2.92	0.43
11:K:117:LEU:HA	11:K:121:PHE:HD2	1.83	0.43
11:K:211:ARG:NE	12:L:44:DG:OP1	2.51	0.43
14:Q:63:ASN:O	14:Q:135:ARG:NH2	2.52	0.43
14:Q:566:LEU:HA	14:Q:569:VAL:HG12	2.00	0.43
14:Q:691:PHE:HZ	14:Q:708:PRO:HB3	1.83	0.43
1:A:305:ASP:OD1	1:A:305:ASP:N	2.43	0.43
1:A:560:VAL:HG22	1:A:624:ILE:HB	1.99	0.43
2:B:376:ALA:HA	2:B:401:ALA:HB1	2.01	0.43
6:F:6:ASP:HA	6:F:155:GLN:HG2	2.01	0.43
7:G:46:ILE:HG22	7:G:48:GLU:HG3	2.01	0.43
11:K:117:LEU:HB3	11:K:123:LEU:HB3	2.01	0.43
7:G:8:VAL:HG11	7:G:50:VAL:HG11	2.01	0.43
7:G:40:ASP:OD1	7:G:40:ASP:N	2.51	0.43
8:H:617:ARG:HA	8:H:620:LYS:HD2	1.99	0.43
8:H:908:ARG:HA	8:H:908:ARG:HD3	1.85	0.43
2:B:25:MET:HE3	2:B:51:SER:HB2	2.00	0.43
2:B:255:THR:HB	2:B:396:PRO:HB3	2.00	0.43
2:B:326:ALA:O	2:B:330:LEU:N	2.49	0.43
4:D:407:VAL:O	4:D:442:VAL:HA	2.19	0.43
8:H:664:ALA:HB1	8:H:676:TYR:HB3	2.01	0.43
11:K:117:LEU:HD13	11:K:123:LEU:HD23	2.01	0.43
14:Q:16:LEU:H	14:Q:19:GLU:HB2	1.83	0.43
15:R:194:CYS:SG	15:R:195:THR:N	2.92	0.43
1:A:70:ASP:OD2	1:A:74:ARG:NE	2.50	0.43
2:B:343:ARG:HG2	2:B:357:PHE:HE1	1.84	0.43
5:E:305:CYS:HB3	5:E:308:CYS:SG	2.58	0.43
11:K:135:LYS:HG2	11:K:184:LEU:HD11	2.00	0.43
8:H:648:ALA:HB3	8:H:678:ARG:HA	2.01	0.42
11:K:251:ASN:HA	11:K:256:MET:O	2.19	0.42
14:Q:193:TRP:HZ3	14:Q:200:VAL:HB	1.84	0.42
8:H:191:ARG:HA	8:H:191:ARG:HD3	1.79	0.42
11:K:139:ILE:O	11:K:181:TYR:N	2.52	0.42
1:A:388:GLN:OE1	1:A:404:SER:OG	2.31	0.42
1:A:573:ILE:HD13	1:A:573:ILE:HA	1.91	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:722:ARG:NH2	5:E:201:LEU:O	2.49	0.42
4:D:121:ALA:HB2	6:F:104:LEU:HB2	2.00	0.42
8:H:712:ASN:HD22	13:M:33:DC:H4'	1.83	0.42
11:K:103:VAL:HG21	11:K:118:MET:HG3	2.02	0.42
14:Q:750:ARG:NH2	14:Q:832:THR:OG1	2.51	0.42
1:A:310:LEU:HD11	1:A:352:THR:HG23	2.01	0.42
1:A:375:LYS:HE3	1:A:391:ARG:HD3	2.01	0.42
2:B:69:LYS:HE3	2:B:225:LEU:HD12	2.00	0.42
4:D:418:PHE:HE2	4:D:436:SER:HA	1.85	0.42
8:H:831:VAL:HG13	8:H:835:LYS:HE2	2.01	0.42
10:J:126:LEU:HG	10:J:142:LEU:HD22	2.01	0.42
14:Q:799:ARG:HA	15:R:195:THR:HG22	2.01	0.42
15:R:106:ARG:NH2	15:R:152:TYR:OH	2.53	0.42
2:B:372:LEU:HG	2:B:408:SER:HB3	2.02	0.42
14:Q:22:LEU:HD21	14:Q:33:VAL:HG11	2.02	0.42
14:Q:58:LEU:HB3	14:Q:104:GLY:HA2	2.01	0.42
1:A:616:ASP:OD2	1:A:645:ARG:NH1	2.53	0.42
4:D:457:ARG:O	4:D:461:SER:HB2	2.19	0.42
6:F:12:VAL:HA	6:F:58:ALA:O	2.19	0.42
1:A:103:ILE:HA	1:A:126:ALA:HB2	2.02	0.42
1:A:443:VAL:HG12	1:A:467:THR:HB	2.01	0.42
2:B:603:LYS:HB3	12:L:57:DG:H5'	2.01	0.42
8:H:572:ILE:HG23	8:H:578:VAL:HG22	2.02	0.42
9:I:302:LEU:O	9:I:306:ILE:N	2.51	0.42
14:Q:32:LEU:HG	14:Q:190:LEU:HA	2.02	0.42
2:B:118:HIS:HA	2:B:119:PRO:HD3	1.77	0.42
4:D:374:PRO:O	4:D:378:LYS:NZ	2.41	0.42
8:H:213:LEU:HD13	8:H:319:LEU:HD22	2.01	0.42
11:K:194:TRP:CD1	11:K:200:LEU:HD12	2.55	0.42
1:A:375:LYS:HG3	1:A:389:ILE:HG21	2.01	0.42
1:A:545:GLN:HB3	1:A:701:LEU:HD23	2.01	0.42
2:B:236:ALA:HB1	2:B:239:ILE:HB	2.02	0.41
5:E:249:LEU:HD22	6:F:268:CYS:HA	2.01	0.41
8:H:660:TYR:HD1	8:H:704:TYR:HE2	1.67	0.41
8:H:689:THR:HG21	13:M:31:DT:H3	1.85	0.41
14:Q:295:LEU:HD21	14:Q:614:THR:HG21	2.01	0.41
2:B:242:VAL:O	2:B:246:SER:N	2.53	0.41
2:B:333:LEU:HA	2:B:336:LEU:HD12	2.02	0.41
5:E:334:ILE:O	5:E:357:VAL:N	2.43	0.41
8:H:258:VAL:HG11	8:H:550:GLY:HA2	2.01	0.41
14:Q:57:CYS:O	14:Q:105:GLY:N	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:160:ARG:NH2	6:F:232:LEU:O	2.54	0.41
2:B:121:VAL:HG23	2:B:133:LYS:HE2	2.02	0.41
2:B:612:HIS:HB3	2:B:673:ASP:HA	2.02	0.41
4:D:71:VAL:O	4:D:83:GLN:NE2	2.53	0.41
4:D:245:LEU:HD21	4:D:285:ARG:HH21	1.85	0.41
5:E:358:TYR:HE1	5:E:369:VAL:HG22	1.86	0.41
6:F:10:LEU:HA	6:F:56:LYS:O	2.21	0.41
8:H:679:ASP:O	8:H:682:HIS:NE2	2.54	0.41
11:K:131:ASP:H	11:K:136:HIS:HD2	1.68	0.41
11:K:252:LEU:HB2	11:K:256:MET:HE3	2.01	0.41
6:F:255:CYS:HB3	6:F:258:HIS:HB2	2.02	0.41
14:Q:769:LEU:HA	14:Q:784:ILE:HD12	2.03	0.41
1:A:283:ARG:HA	1:A:286:HIS:HB3	2.02	0.41
2:B:609:ASP:HB3	2:B:669:ARG:HG3	2.02	0.41
4:D:233:ILE:O	4:D:237:LEU:HB2	2.21	0.41
8:H:741:TYR:CD2	8:H:766:MET:HG3	2.55	0.41
14:Q:85:PRO:HB3	14:Q:106:VAL:HB	2.03	0.41
1:A:58:ALA:HB2	4:D:334:MET:HB3	2.02	0.41
4:D:18:ASN:HB3	4:D:21:GLU:HG2	2.02	0.41
4:D:348:ARG:NH2	7:G:61:MET:O	2.53	0.41
4:D:402:ARG:NH1	7:G:11:GLU:OE1	2.54	0.41
8:H:278:ASN:O	8:H:281:THR:OG1	2.36	0.41
14:Q:60:LEU:HD23	14:Q:128:ILE:HD12	2.01	0.41
1:A:295:TYR:N	1:A:333:ALA:O	2.53	0.41
1:A:338:ILE:HD13	1:A:488:LEU:HB2	2.03	0.41
2:B:40:LEU:HD23	2:B:40:LEU:HA	1.81	0.41
15:R:160:LEU:HD23	15:R:160:LEU:HA	1.89	0.41
2:B:43:PRO:HG3	2:B:696:TRP:CE2	2.55	0.41
2:B:537:ALA:HA	2:B:619:ILE:HG23	2.02	0.41
3:C:411:MET:HE3	6:F:34:LEU:HB3	2.02	0.41
4:D:449:SER:HA	4:D:452:LYS:HB3	2.03	0.41
5:E:351:GLU:HG2	5:E:353:LYS:HG2	2.03	0.41
6:F:14:VAL:HA	6:F:60:ILE:HG23	2.02	0.41
11:K:151:LYS:HE3	12:L:42:DC:H3'	2.03	0.41
12:L:45:DC:H2''	12:L:46:DA:C8	2.55	0.41
4:D:230:LEU:HD12	4:D:230:LEU:HA	1.94	0.41
4:D:347:THR:HG1	4:D:350:SER:H	1.67	0.41
8:H:695:ARG:HB3	8:H:738:THR:HB	2.03	0.41
11:K:121:PHE:HD1	11:K:182:LEU:HB2	1.86	0.41
14:Q:168:ALA:HA	14:Q:171:PHE:HD2	1.86	0.41
1:A:640:LEU:HD12	1:A:640:LEU:HA	1.91	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:ILE:HD13	2:B:84:ILE:HA	1.96	0.40
2:B:489:CYS:HB3	2:B:674:TYR:HA	2.02	0.40
2:B:576:GLU:HA	2:B:579:VAL:HG12	2.02	0.40
4:D:96:TRP:CD2	4:D:108:LEU:HD21	2.56	0.40
8:H:702:VAL:O	8:H:737:GLN:NE2	2.49	0.40
11:K:182:LEU:HD23	11:K:185:GLN:HB2	2.03	0.40
1:A:457:ILE:HG13	1:A:458:VAL:HG23	2.02	0.40
1:A:561:PHE:HD2	1:A:623:LEU:HD11	1.85	0.40
2:B:20:GLU:OE2	2:B:484:THR:N	2.55	0.40
2:B:278:GLU:HB3	2:B:282:ARG:HE	1.86	0.40
2:B:349:VAL:HG12	2:B:350:VAL:HG13	2.04	0.40
2:B:446:PRO:HA	2:B:449:GLU:HG3	2.03	0.40
4:D:161:HIS:CD2	4:D:166:SER:HB2	2.56	0.40
5:E:211:LEU:O	5:E:215:THR:OG1	2.38	0.40
6:F:229:TRP:HE3	6:F:230:VAL:HG22	1.87	0.40
7:G:38:ILE:HD11	7:G:44:PHE:HB2	2.02	0.40
8:H:196:ARG:HA	8:H:199:LYS:HE2	2.03	0.40
9:I:289:ARG:O	9:I:293:GLN:CB	2.66	0.40
10:J:120:LYS:HA	10:J:120:LYS:HD3	1.98	0.40
11:K:118:MET:HA	11:K:122:ASP:HA	2.02	0.40
1:A:137:THR:HG23	1:A:141:ARG:HH21	1.86	0.40
1:A:178:GLU:HA	1:A:268:VAL:O	2.22	0.40
2:B:310:LEU:HA	2:B:311:PRO:HD3	1.94	0.40
7:G:51:ASN:OD1	7:G:52:VAL:N	2.54	0.40
1:A:579:TYR:CE2	1:A:581:TYR:HB2	2.57	0.40
2:B:665:GLY:O	2:B:669:ARG:NH2	2.54	0.40
8:H:718:ARG:HG2	8:H:724:LEU:HB2	2.04	0.40
1:A:636:GLU:HG3	1:A:676:ARG:HE	1.86	0.40
2:B:162:ASP:HA	2:B:166:ARG:HG3	2.03	0.40
2:B:396:PRO:HA	2:B:399:LEU:HB2	2.04	0.40
2:B:681:ASP:OD2	2:B:683:ARG:NE	2.51	0.40
8:H:304:LEU:O	8:H:308:ALA:CB	2.67	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	A	609/782 (78%)	569 (93%)	40 (7%)	0	100	100
2	B	732/768 (95%)	666 (91%)	66 (9%)	0	100	100
3	C	127/548 (23%)	124 (98%)	3 (2%)	0	100	100
4	D	421/462 (91%)	395 (94%)	26 (6%)	0	100	100
5	E	336/395 (85%)	304 (90%)	32 (10%)	0	100	100
6	F	251/308 (82%)	242 (96%)	9 (4%)	0	100	100
7	G	64/71 (90%)	62 (97%)	2 (3%)	0	100	100
8	H	497/940 (53%)	460 (93%)	35 (7%)	2 (0%)	30	66
9	I	59/409 (14%)	52 (88%)	7 (12%)	0	100	100
10	J	69/172 (40%)	66 (96%)	3 (4%)	0	100	100
11	K	198/273 (72%)	182 (92%)	16 (8%)	0	100	100
14	Q	701/916 (76%)	654 (93%)	47 (7%)	0	100	100
15	R	194/297 (65%)	170 (88%)	24 (12%)	0	100	100
All	All	4258/6341 (67%)	3946 (93%)	310 (7%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	651	ARG
8	H	650	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	542/688 (79%)	542 (100%)	0	100	100
2	B	640/672 (95%)	640 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	123/484 (25%)	123 (100%)	0	100	100
4	D	373/399 (94%)	373 (100%)	0	100	100
5	E	305/352 (87%)	305 (100%)	0	100	100
6	F	228/272 (84%)	228 (100%)	0	100	100
7	G	59/64 (92%)	59 (100%)	0	100	100
8	H	442/805 (55%)	442 (100%)	0	100	100
9	I	57/328 (17%)	57 (100%)	0	100	100
10	J	61/152 (40%)	61 (100%)	0	100	100
11	K	185/233 (79%)	185 (100%)	0	100	100
14	Q	562/815 (69%)	562 (100%)	0	100	100
15	R	132/254 (52%)	132 (100%)	0	100	100
All	All	3709/5518 (67%)	3709 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	154	GLN
1	A	201	ASN
1	A	497	GLN
1	A	555	ASN
1	A	711	GLN
2	B	135	HIS
2	B	238	ASN
2	B	347	GLN
2	B	368	GLN
2	B	402	ASN
2	B	645	GLN
2	B	649	ASN
2	B	698	GLN
2	B	723	GLN
2	B	733	GLN
3	C	442	GLN
3	C	524	HIS
3	C	530	GLN
4	D	173	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	224	GLN
4	D	390	GLN
4	D	415	GLN
4	D	424	HIS
5	E	98	GLN
5	E	147	ASN
5	E	365	ASN
6	F	52	ASN
6	F	145	HIS
6	F	240	GLN
7	G	27	ASN
7	G	63	GLN
8	H	206	HIS
8	H	712	ASN
8	H	728	ASN
8	H	780	HIS
9	I	319	GLN
9	I	320	HIS
9	I	323	HIS
9	I	326	GLN
11	K	136	HIS
14	Q	395	ASN
14	Q	859	ASN
15	R	118	ASN
15	R	154	HIS
15	R	172	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	SF4	B	1000	2	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	SF4	B	1000	2	-	-	0/6/5/5

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1000	SF4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

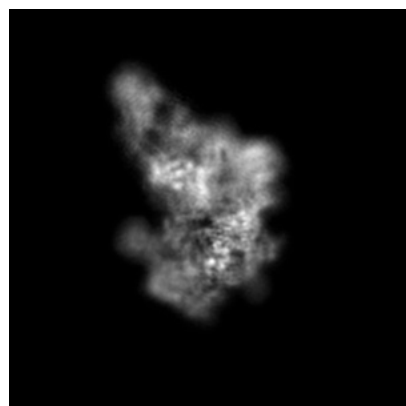
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71512. These allow visual inspection of the internal detail of the map and identification of artifacts.

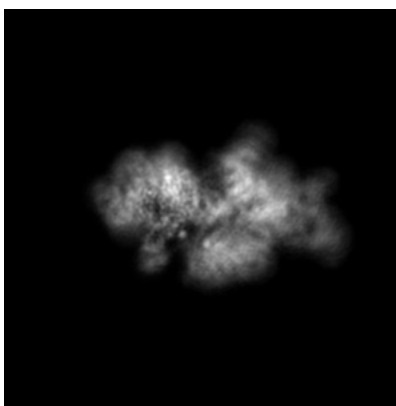
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

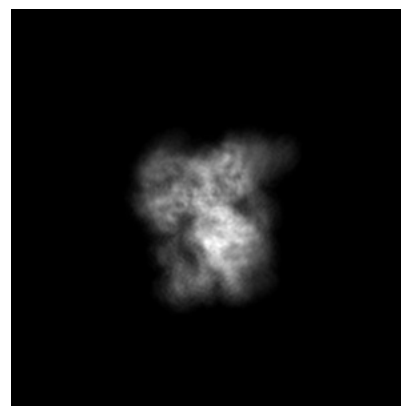
6.1.1 Primary map



X

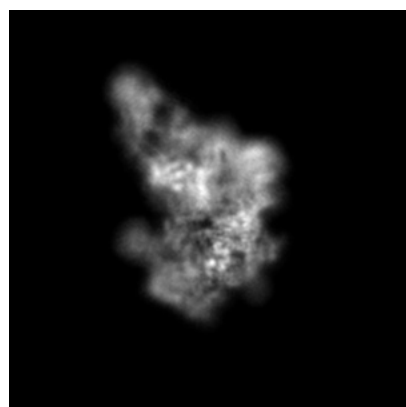


Y

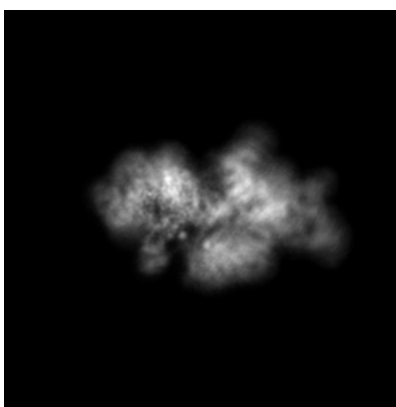


Z

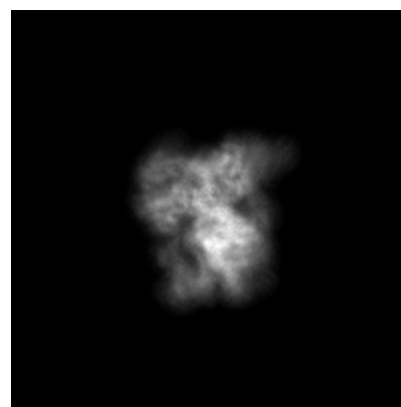
6.1.2 Raw map



X



Y

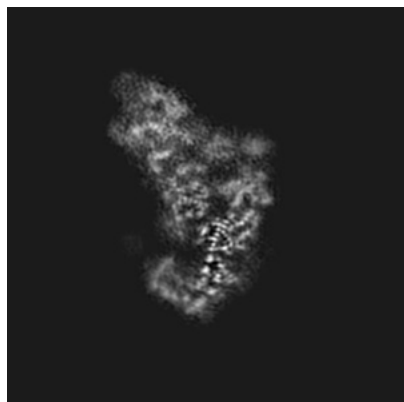


Z

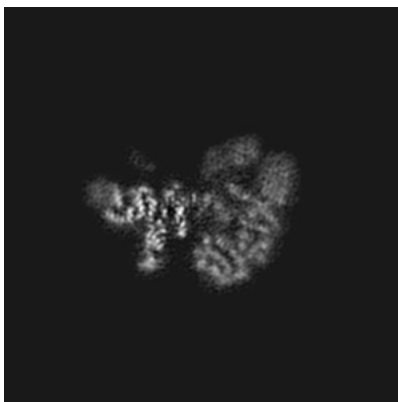
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

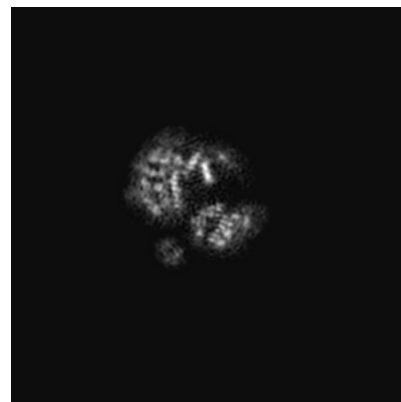
6.2.1 Primary map



X Index: 110

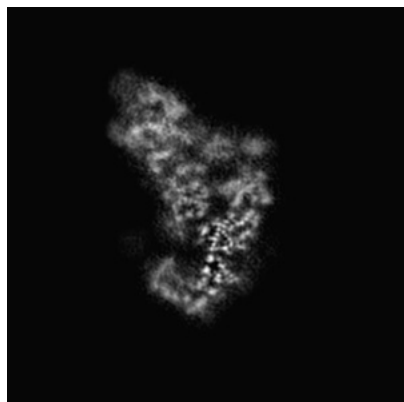


Y Index: 110

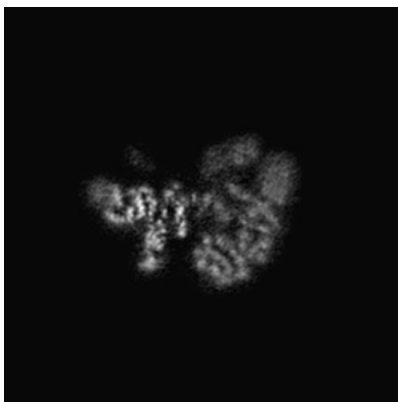


Z Index: 110

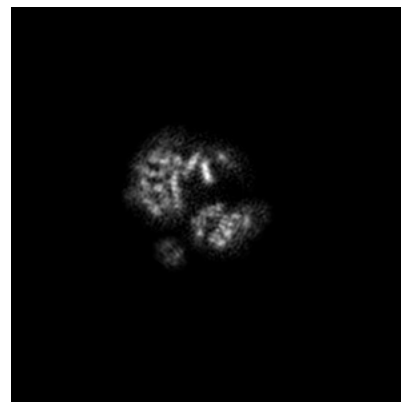
6.2.2 Raw map



X Index: 110



Y Index: 110

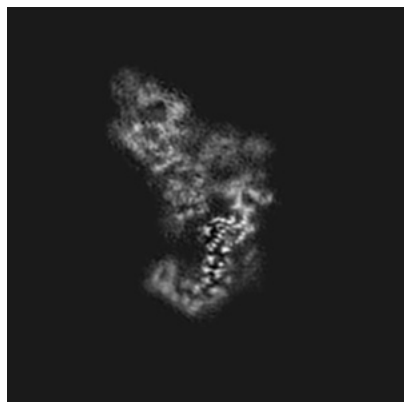


Z Index: 110

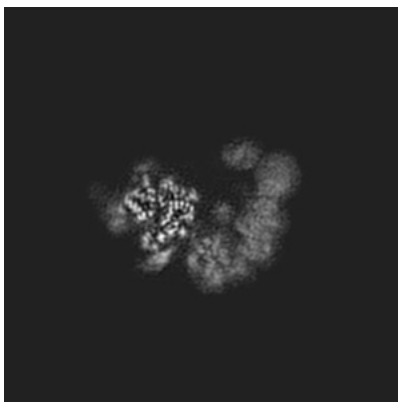
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

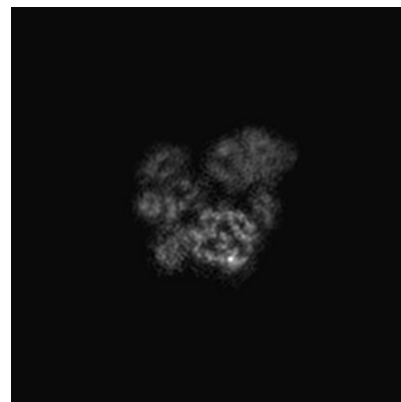
6.3.1 Primary map



X Index: 108

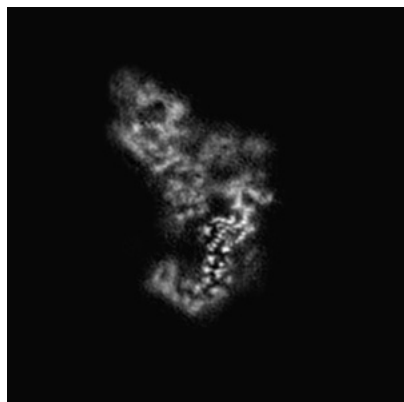


Y Index: 115

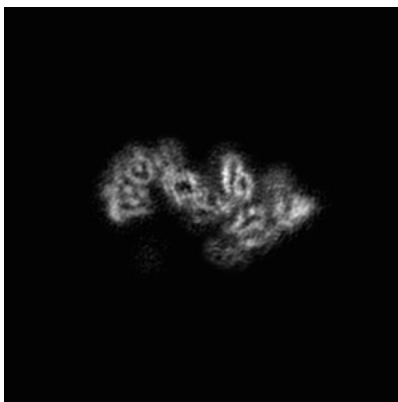


Z Index: 130

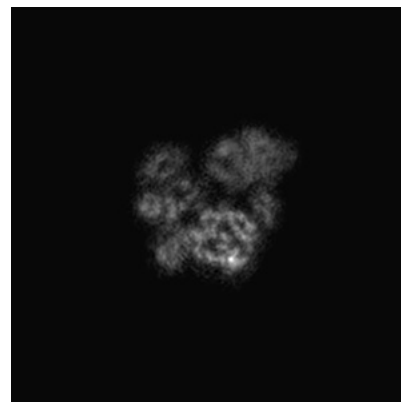
6.3.2 Raw map



X Index: 108



Y Index: 92

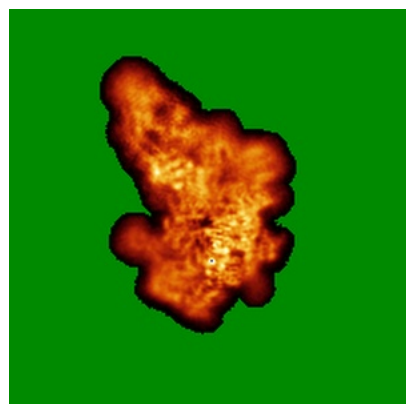


Z Index: 130

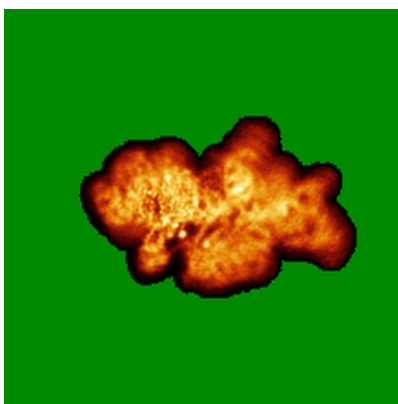
The images above show the largest variance slices of the map in three orthogonal directions.

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

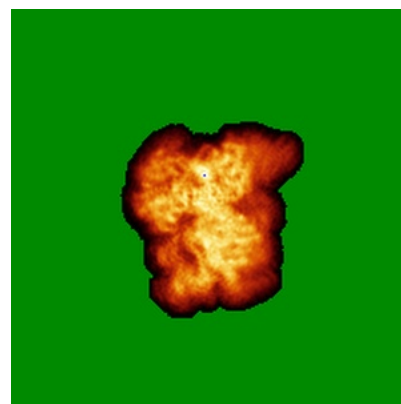
6.4.1 Primary map



X

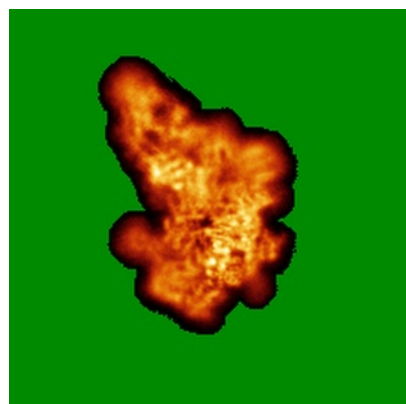


Y

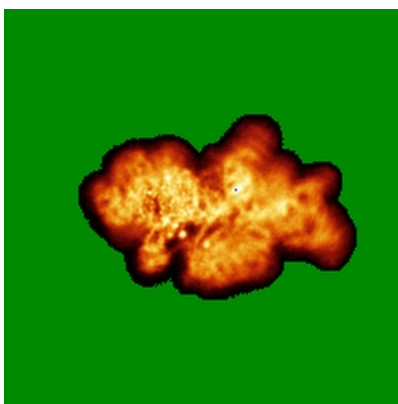


Z

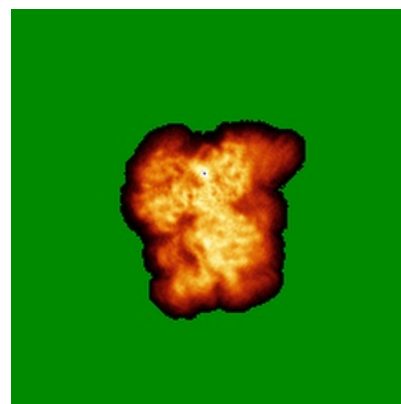
6.4.2 Raw map



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 0.026. 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.

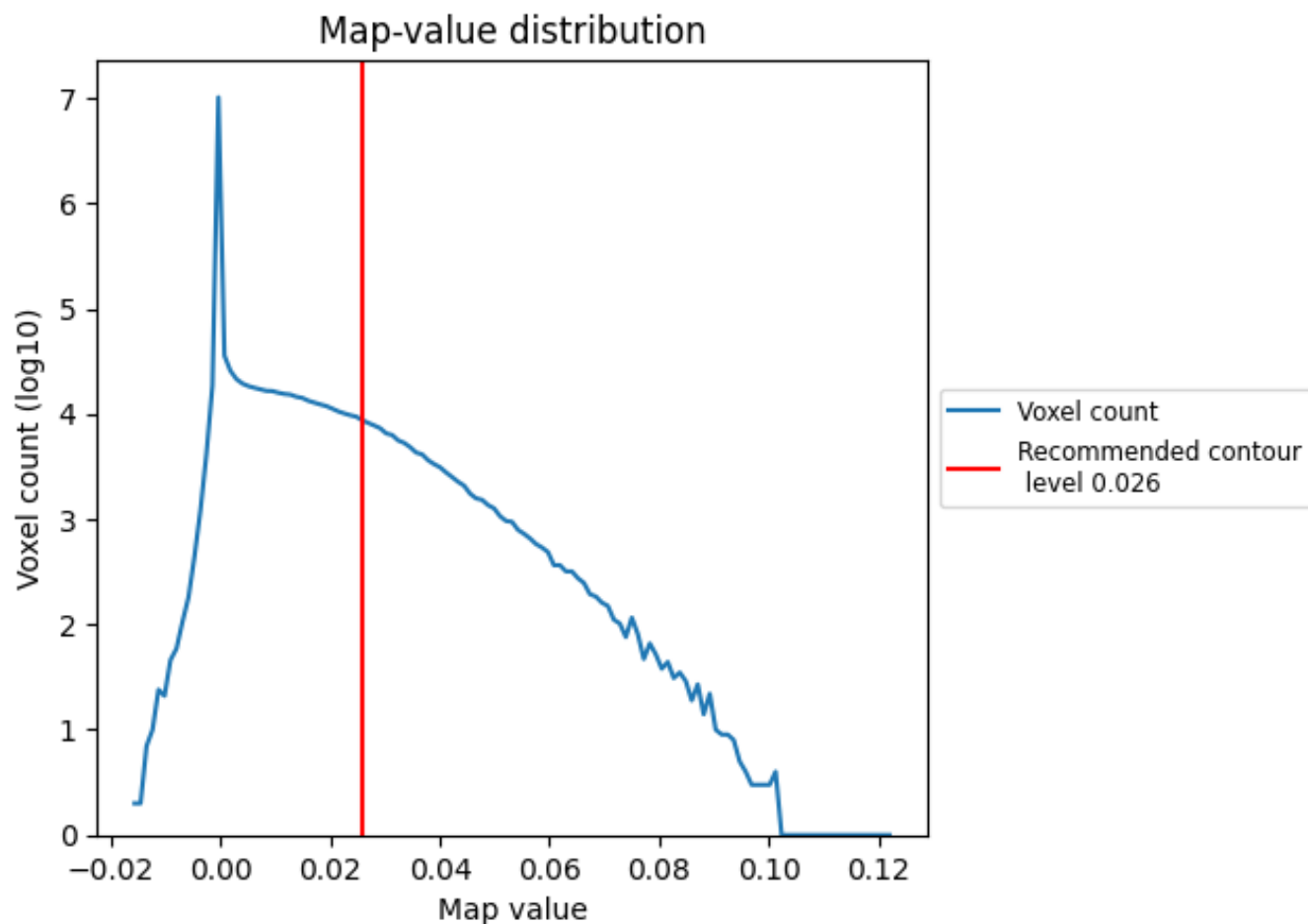
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

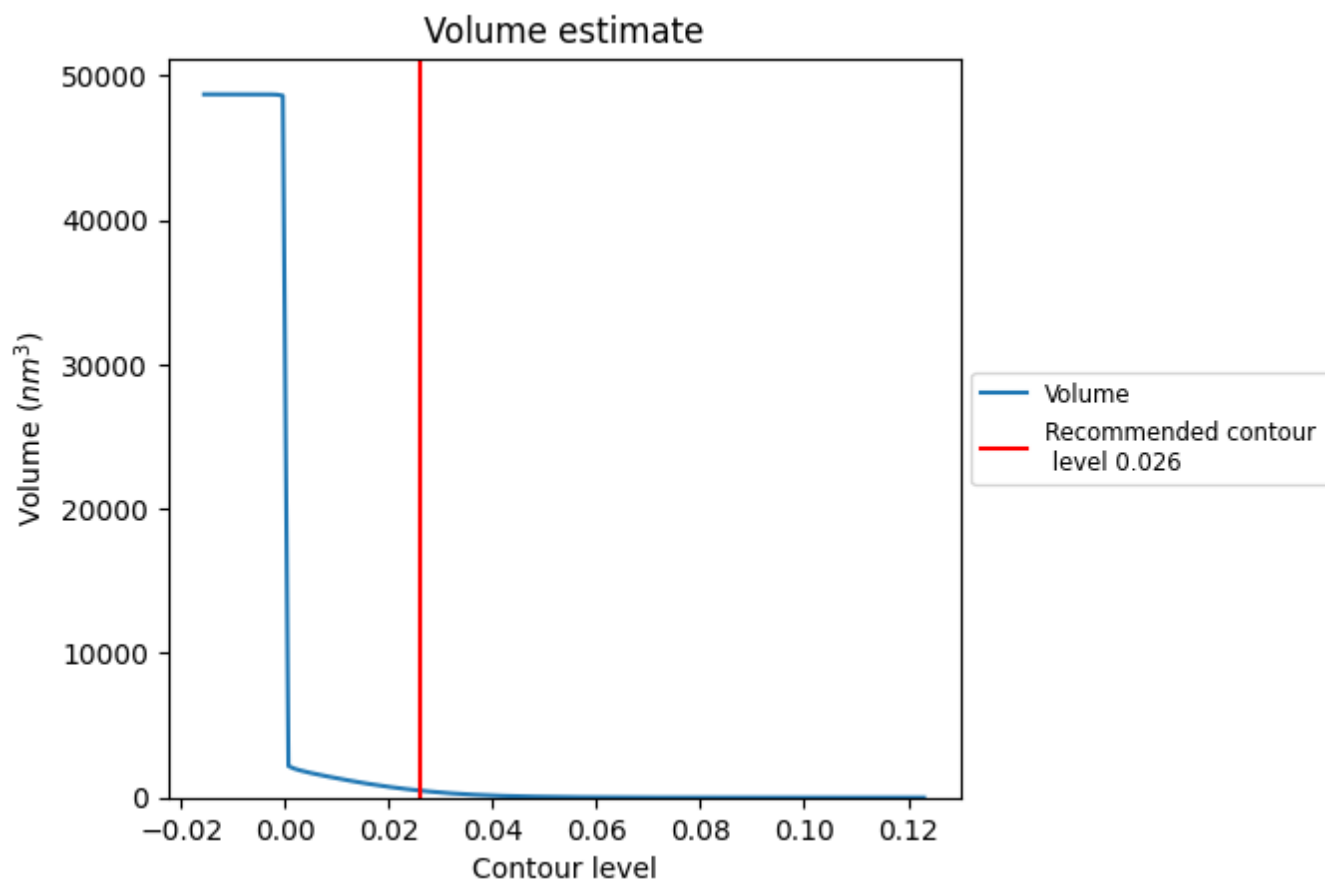
This section contains the results of statistical analysis of the map.

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.

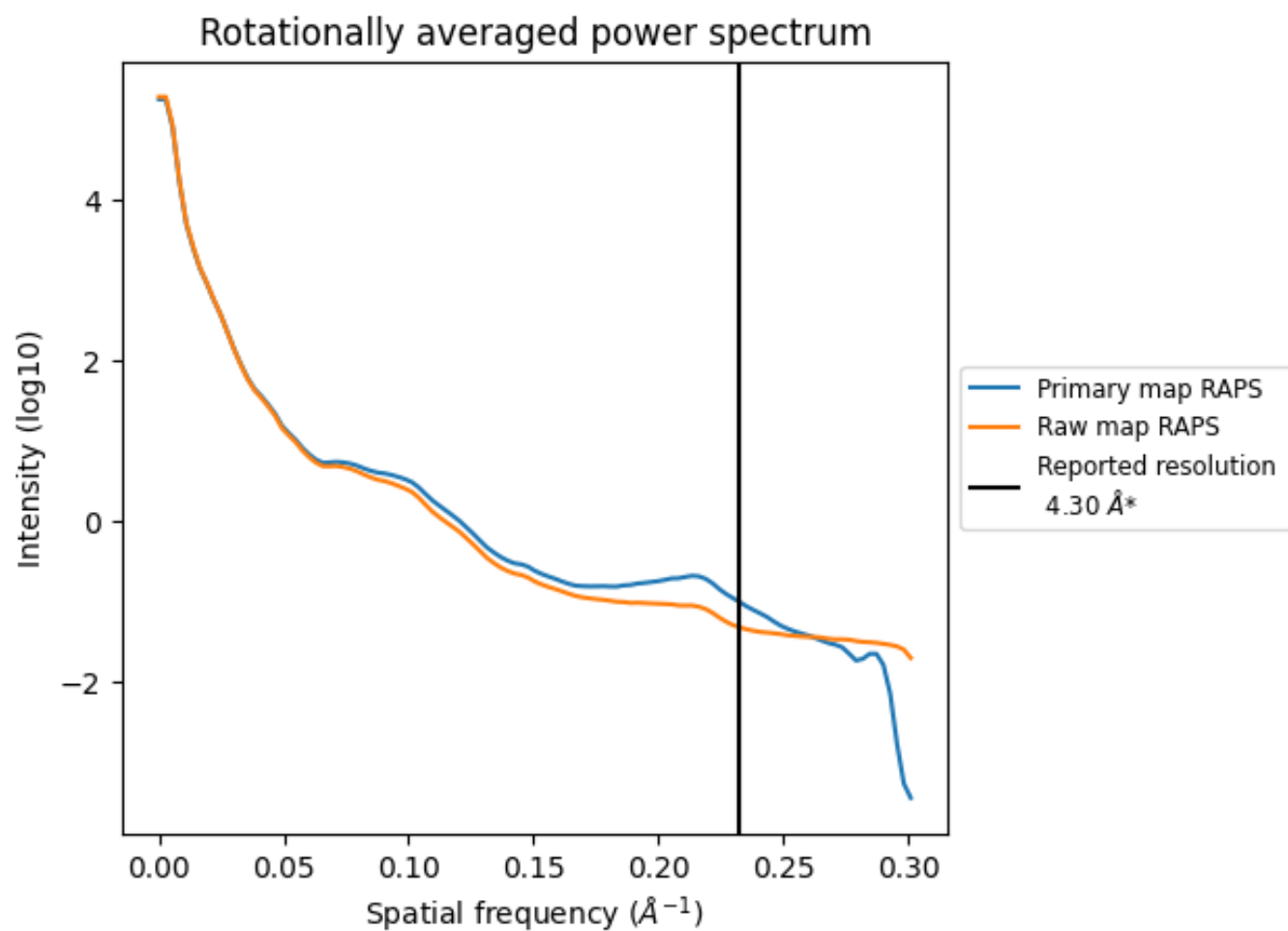
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 483 nm³; this corresponds to an approximate mass of 437 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 ⓘ

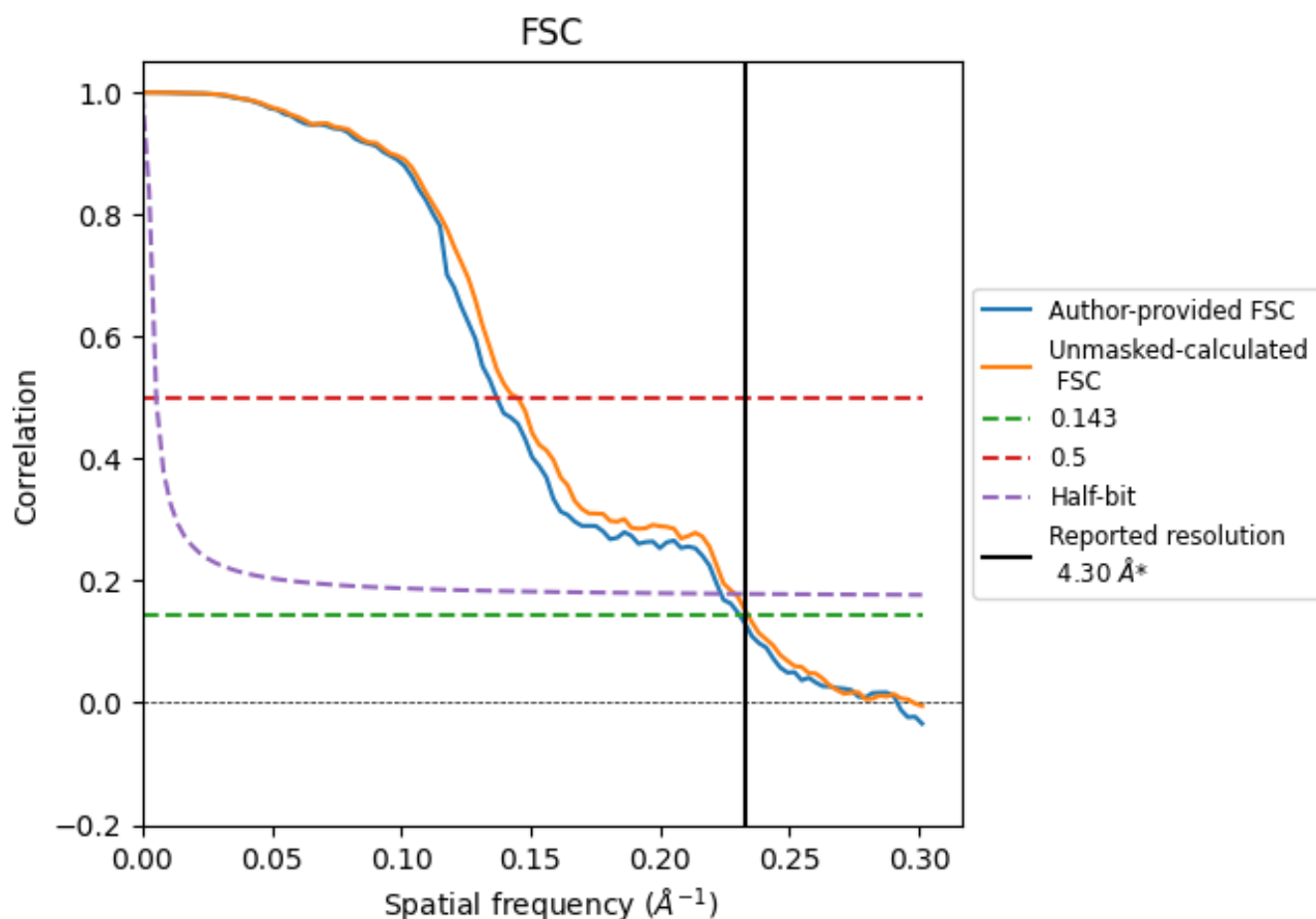


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 0.233 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

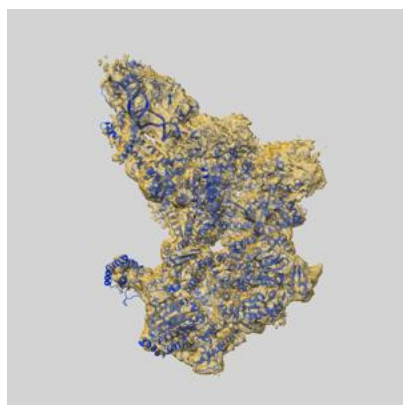
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.33	7.30	4.47
Unmasked-calculated*	4.27	6.90	4.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

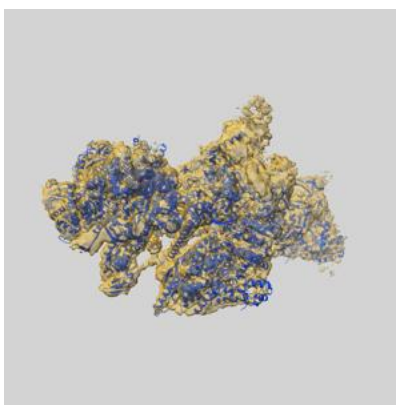
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71512 and PDB model 9PCP. Per-residue inclusion information can be found in section 3 on page 8.

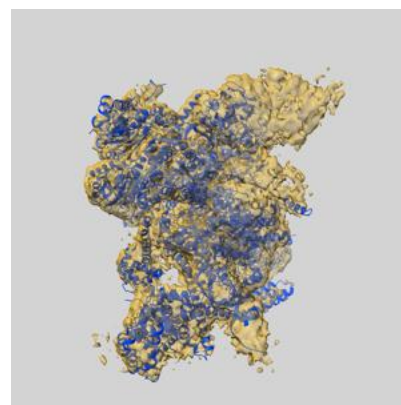
9.1 Map-model overlay [i](#)



X



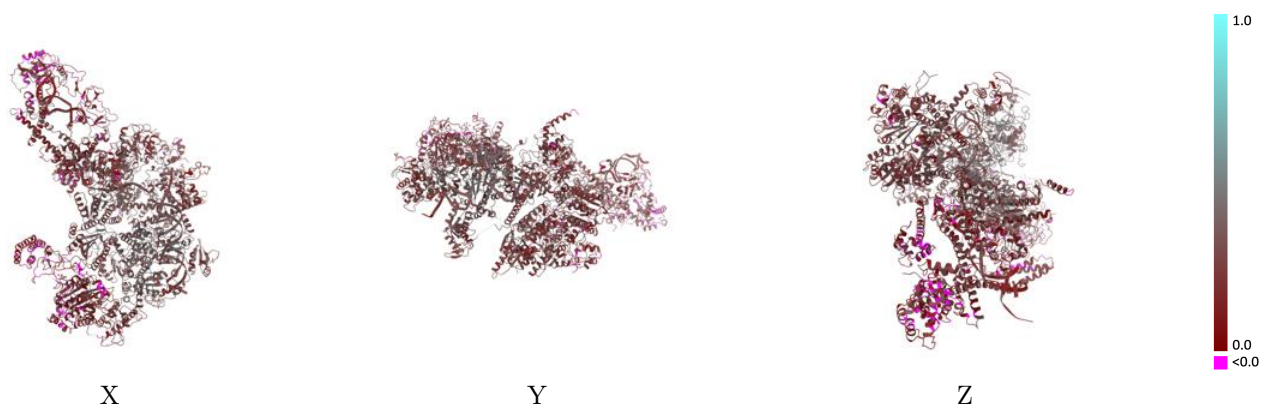
Y



Z

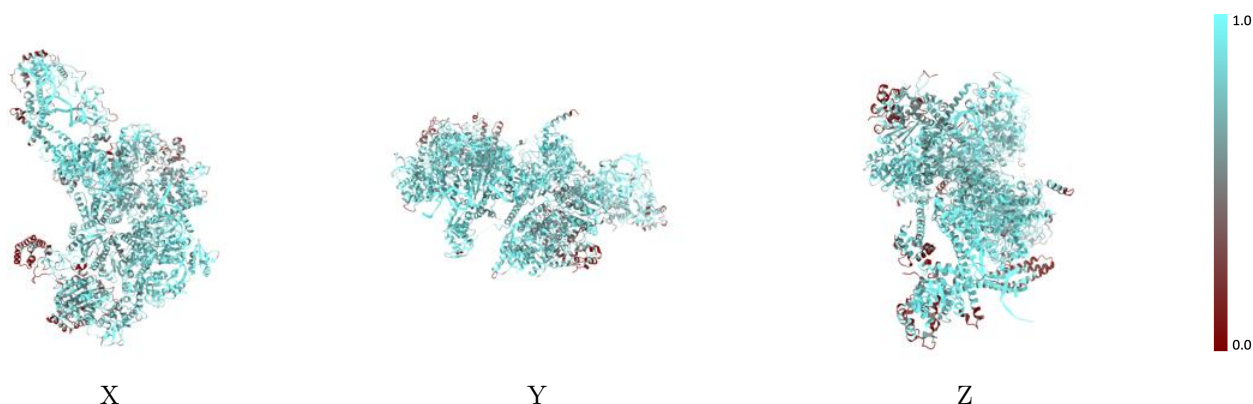
The images above show the 3D surface view of the map at the recommended contour level 0.026 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



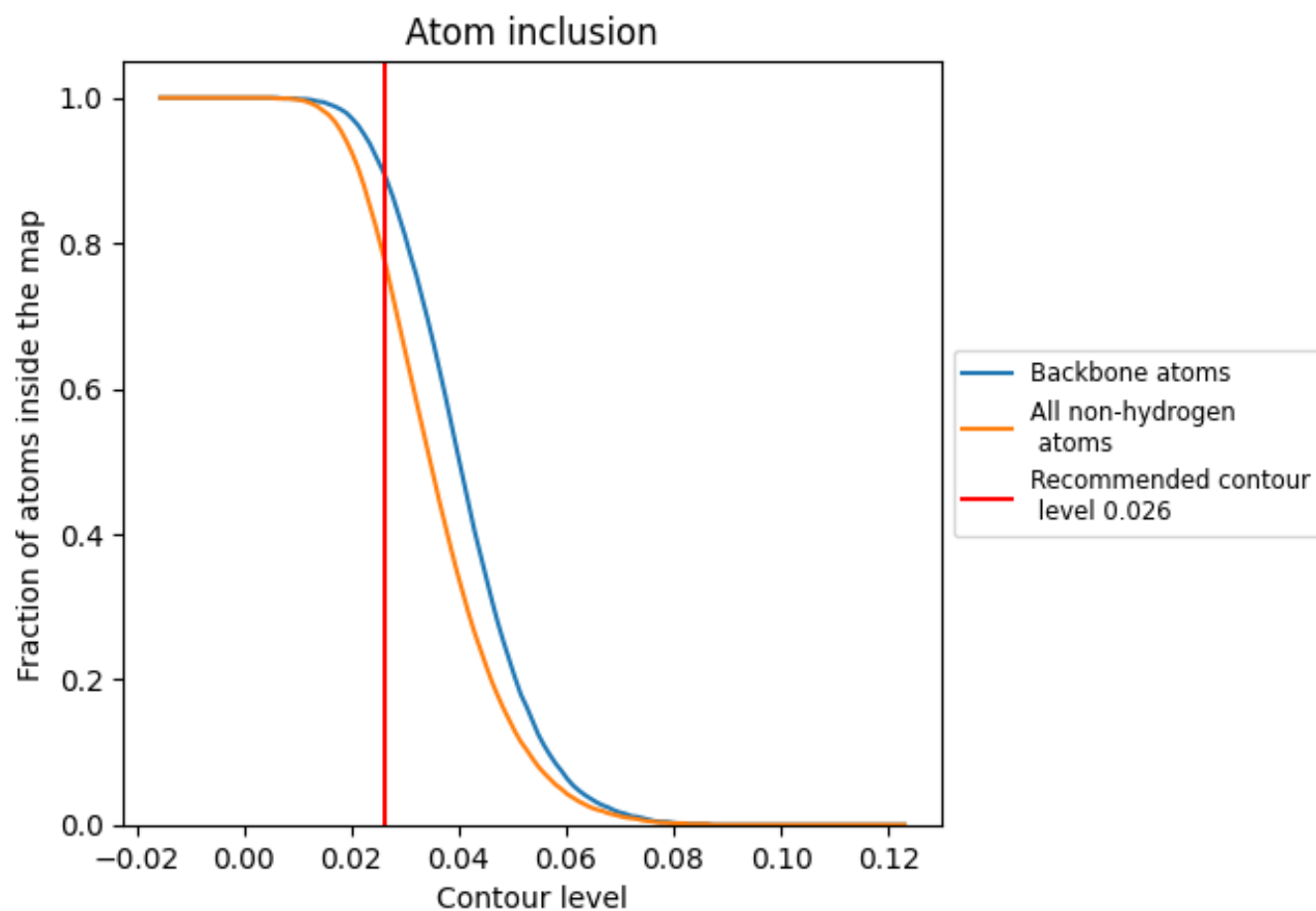
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.026).

9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 78% 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 (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7810	0.2620
A	0.8720	0.3650
B	0.8620	0.2740
C	0.3400	0.1450
D	0.8240	0.2790
E	0.6950	0.2480
F	0.6570	0.1760
G	0.8820	0.3470
H	0.7590	0.1880
I	0.7110	0.1850
J	0.5330	0.1300
K	0.7890	0.2530
L	0.9480	0.2880
M	0.9470	0.2780
Q	0.7650	0.2710
R	0.6480	0.2620

1.0

0.0

<0.0