Full wwPDB EM Validation Report (i)

Aug 26, 2026 – 05:57 pm BST

PDB ID	:	28JS / pdb_000028js
EMDB ID	:	EMD-56551
Title	:	Cryo-EM structure of the human holo-TFIIH-XPC complex bound to bulky lesion-mimic DNA (composite map)
Authors	:	de Martin Garrido, N.; Haste, C.A.F.; Feng, J.; Cronin, N.B.; Greber, B.J.
Deposited on	:	2026-02-03
Resolution	:	3.32 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

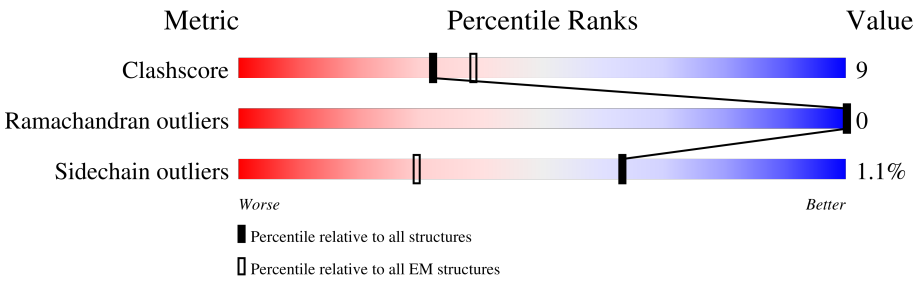
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

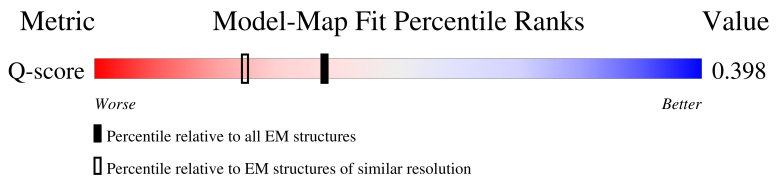
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.32 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	14518 (2.82 - 3.82)

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

Mol	Chain	Length	Quality of chain
1	A	797	• 63% 17% 20%
2	B	771	7% 77% 21% •
3	C	591	15% 52% 12% 37%
4	D	462	13% 80% 17% •

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Mol	Chain	Length	Quality of chain
5	E	395	7% 81% 11% 9%
6	F	308	• 71% 13% 15%
7	G	71	18% 69% 30% •
8	H	309	15% 11% 14% 75%
9	I	940	25% 43% 13% 43%
10	J	409	12% 11% • 85%
11	K	172	17% 26% 15% • 59%
12	L	71	6% 27% 21% 52%
13	M	92	• 21% 17% 62%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 30828 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 General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	636	5131	3276	890	935	30	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP P19447
A	-13	HIS	-	expression tag	UNP P19447
A	-12	HIS	-	expression tag	UNP P19447
A	-11	HIS	-	expression tag	UNP P19447
A	-10	HIS	-	expression tag	UNP P19447
A	-9	HIS	-	expression tag	UNP P19447
A	-8	GLU	-	expression tag	UNP P19447
A	-7	ASN	-	expression tag	UNP P19447
A	-6	LEU	-	expression tag	UNP P19447
A	-5	TYR	-	expression tag	UNP P19447
A	-4	PHE	-	expression tag	UNP P19447
A	-3	GLN	-	expression tag	UNP P19447
A	-2	SER	-	expression tag	UNP P19447
A	-1	ASN	-	expression tag	UNP P19447
A	0	ALA	-	expression tag	UNP P19447

- Molecule 2 is a protein called TFIIH basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	755	6080	3884	1059	1108	29	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	761	SER	-	expression tag	UNP P18074

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Chain	Residue	Modelled	Actual	Comment	Reference
B	762	SER	-	expression tag	UNP P18074
B	763	ASN	-	expression tag	UNP P18074
B	764	ASP	-	expression tag	UNP P18074
B	765	TYR	-	expression tag	UNP P18074
B	766	LYS	-	expression tag	UNP P18074
B	767	ASP	-	expression tag	UNP P18074
B	768	ASP	-	expression tag	UNP P18074
B	769	ASP	-	expression tag	UNP P18074
B	770	ASP	-	expression tag	UNP P18074
B	771	LYS	-	expression tag	UNP P18074

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	374	3014	1917	524	559	14	0	0

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	549	GLY	-	expression tag	UNP P32780
C	550	SER	-	expression tag	UNP P32780
C	551	GLY	-	expression tag	UNP P32780
C	552	GLY	-	expression tag	UNP P32780
C	553	GLU	-	expression tag	UNP P32780
C	554	ASN	-	expression tag	UNP P32780
C	555	LEU	-	expression tag	UNP P32780
C	556	TYR	-	expression tag	UNP P32780
C	557	PHE	-	expression tag	UNP P32780
C	558	GLN	-	expression tag	UNP P32780
C	559	SER	-	expression tag	UNP P32780
C	560	GLY	-	expression tag	UNP P32780
C	561	SER	-	expression tag	UNP P32780
C	562	TRP	-	expression tag	UNP P32780
C	563	SER	-	expression tag	UNP P32780
C	564	HIS	-	expression tag	UNP P32780
C	565	PRO	-	expression tag	UNP P32780
C	566	GLN	-	expression tag	UNP P32780
C	567	PHE	-	expression tag	UNP P32780
C	568	GLU	-	expression tag	UNP P32780
C	569	LYS	-	expression tag	UNP P32780
C	570	GLY	-	expression tag	UNP P32780

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Chain	Residue	Modelled	Actual	Comment	Reference
C	571	GLY	-	expression tag	UNP P32780
C	572	GLY	-	expression tag	UNP P32780
C	573	SER	-	expression tag	UNP P32780
C	574	GLY	-	expression tag	UNP P32780
C	575	GLY	-	expression tag	UNP P32780
C	576	GLY	-	expression tag	UNP P32780
C	577	SER	-	expression tag	UNP P32780
C	578	GLY	-	expression tag	UNP P32780
C	579	GLY	-	expression tag	UNP P32780
C	580	GLY	-	expression tag	UNP P32780
C	581	SER	-	expression tag	UNP P32780
C	582	TRP	-	expression tag	UNP P32780
C	583	SER	-	expression tag	UNP P32780
C	584	HIS	-	expression tag	UNP P32780
C	585	PRO	-	expression tag	UNP P32780
C	586	GLN	-	expression tag	UNP P32780
C	587	PHE	-	expression tag	UNP P32780
C	588	GLU	-	expression tag	UNP P32780
C	589	LYS	-	expression tag	UNP P32780
C	590	SER	-	expression tag	UNP P32780
C	591	GLY	-	expression tag	UNP P32780

- Molecule 4 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	449	3600	2317	630	639	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	360	2828	1780	489	532	27	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	261	2049	1313	339	378	19	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	70	556	357	89	107	3	0	0

- Molecule 8 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	77	659	417	109	132	1	0	0

- Molecule 9 is a protein called DNA repair protein complementing XP-C cells.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	534	4383	2801	773	789	20	0	0

- Molecule 10 is a protein called Lysine-specific demethylase RAD23B.

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

- Molecule 11 is a protein called Centrin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	71	578	357	94	125	2	0	0

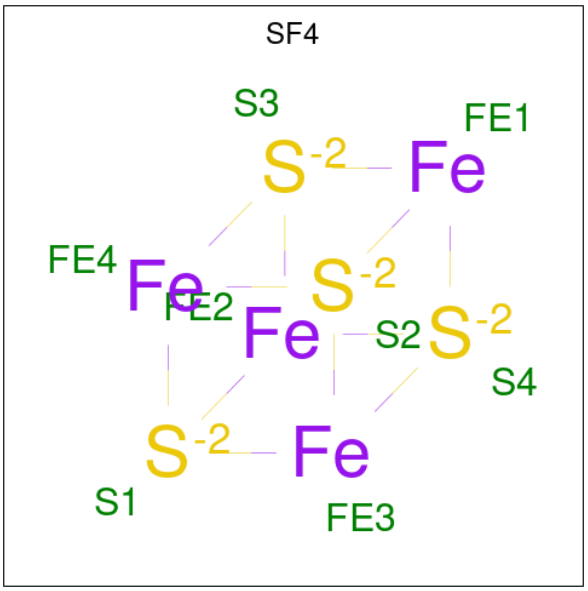
- Molecule 12 is a DNA chain called DNA (Cy5).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
12	L	34	690	345	108	203	34	0	0

- Molecule 13 is a DNA chain called DNA (biotinylated).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
13	M	35	741	349	149	208	35	0	0

- Molecule 14 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
15	E	3	3	3	0
15	F	2	Total 2	Zn 2	0

- Molecule 16 is CALCIUM ION (CCD ID: CA) (formula: Ca).

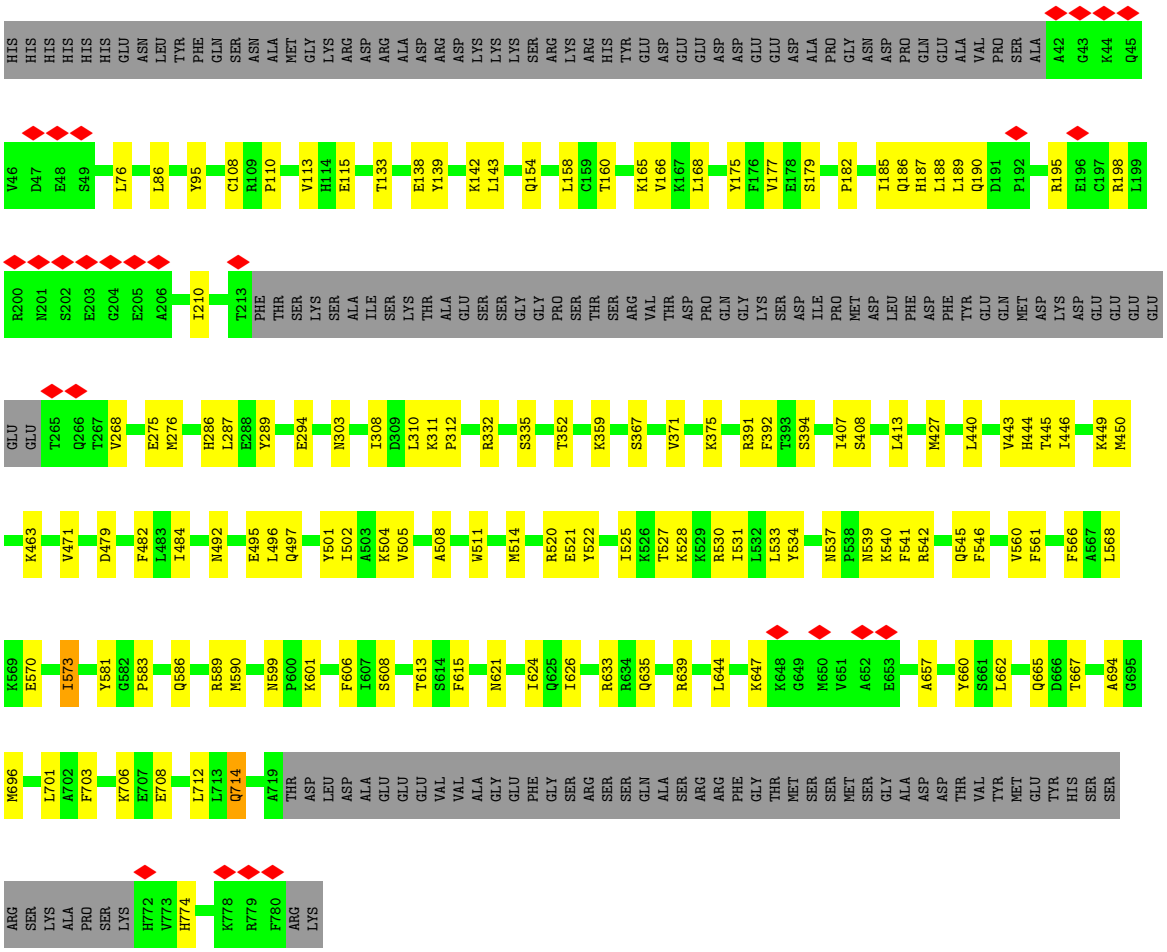
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
16	K	2	2	2	0

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: General transcription and DNA repair factor IIH helicase subunit XPB

Chain A: 63% 17% 20%

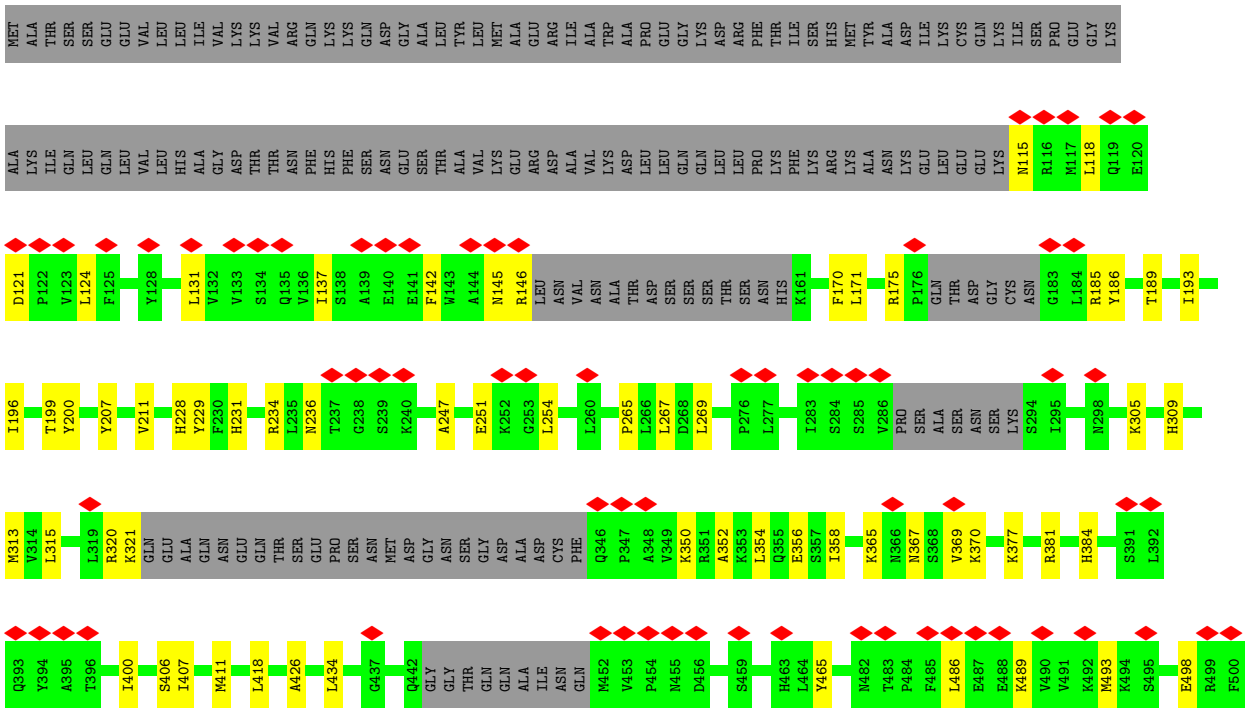


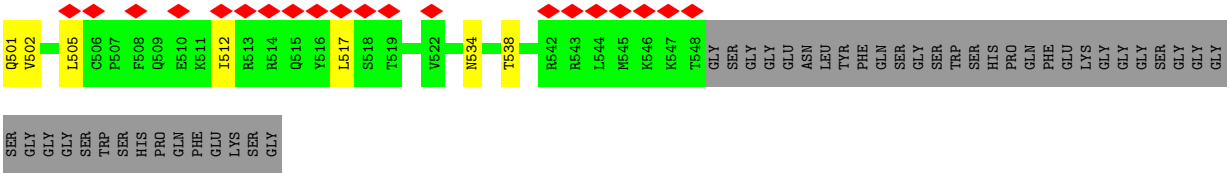
- Molecule 2: TFIIH basal transcription factor complex helicase XPD subunit

Chain B: 7% 77% 21%

• Molecule 3: General transcription factor IIH subunit 1

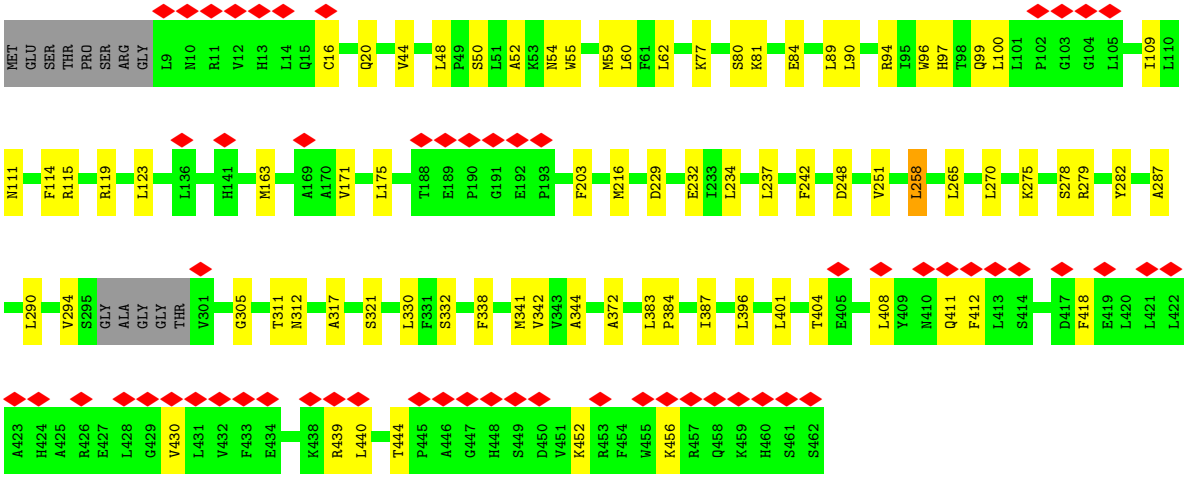
Chain C:





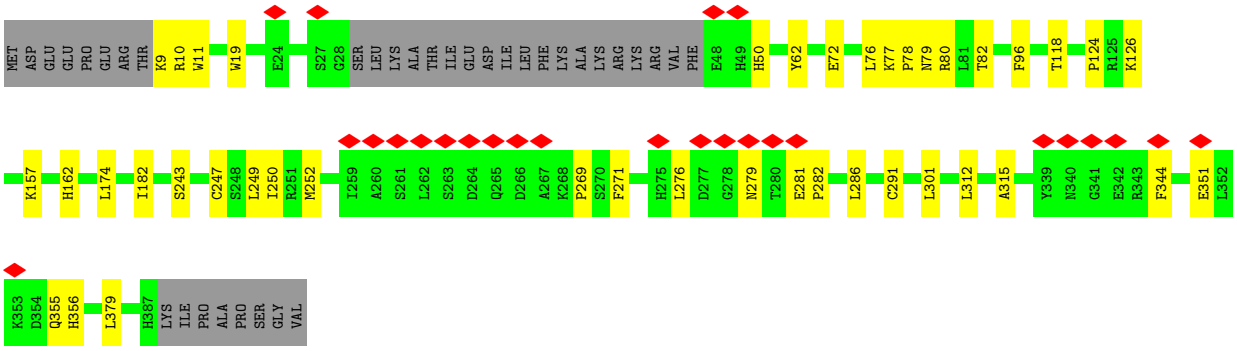
• Molecule 4: General transcription factor IIH subunit 4

Chain D:



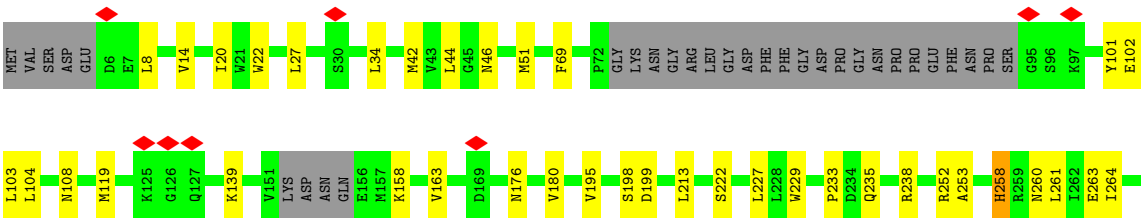
• Molecule 5: General transcription factor IIH subunit 2

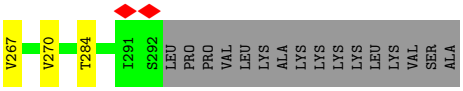
Chain E:



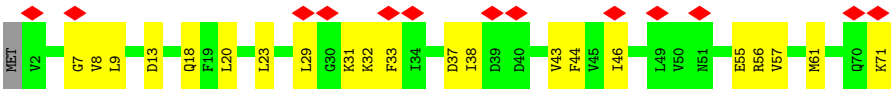
• Molecule 6: General transcription factor IIH subunit 3

Chain F:

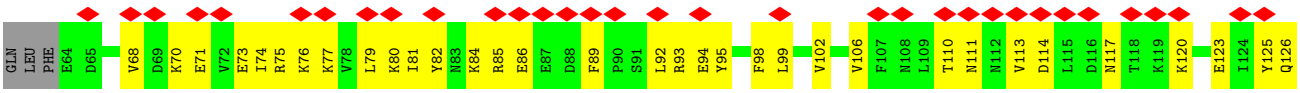


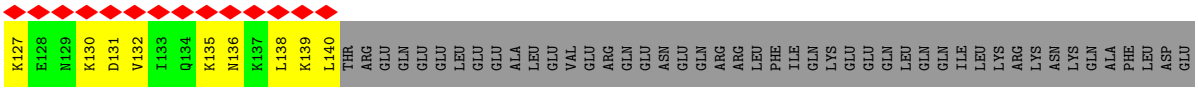


• Molecule 7: General transcription factor IIH subunit 5

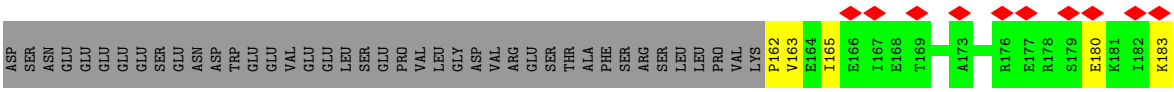


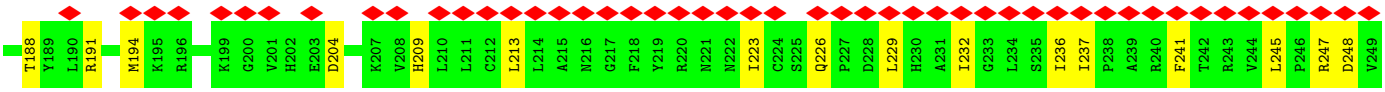
• Molecule 8: CDK-activating kinase assembly factor MAT1

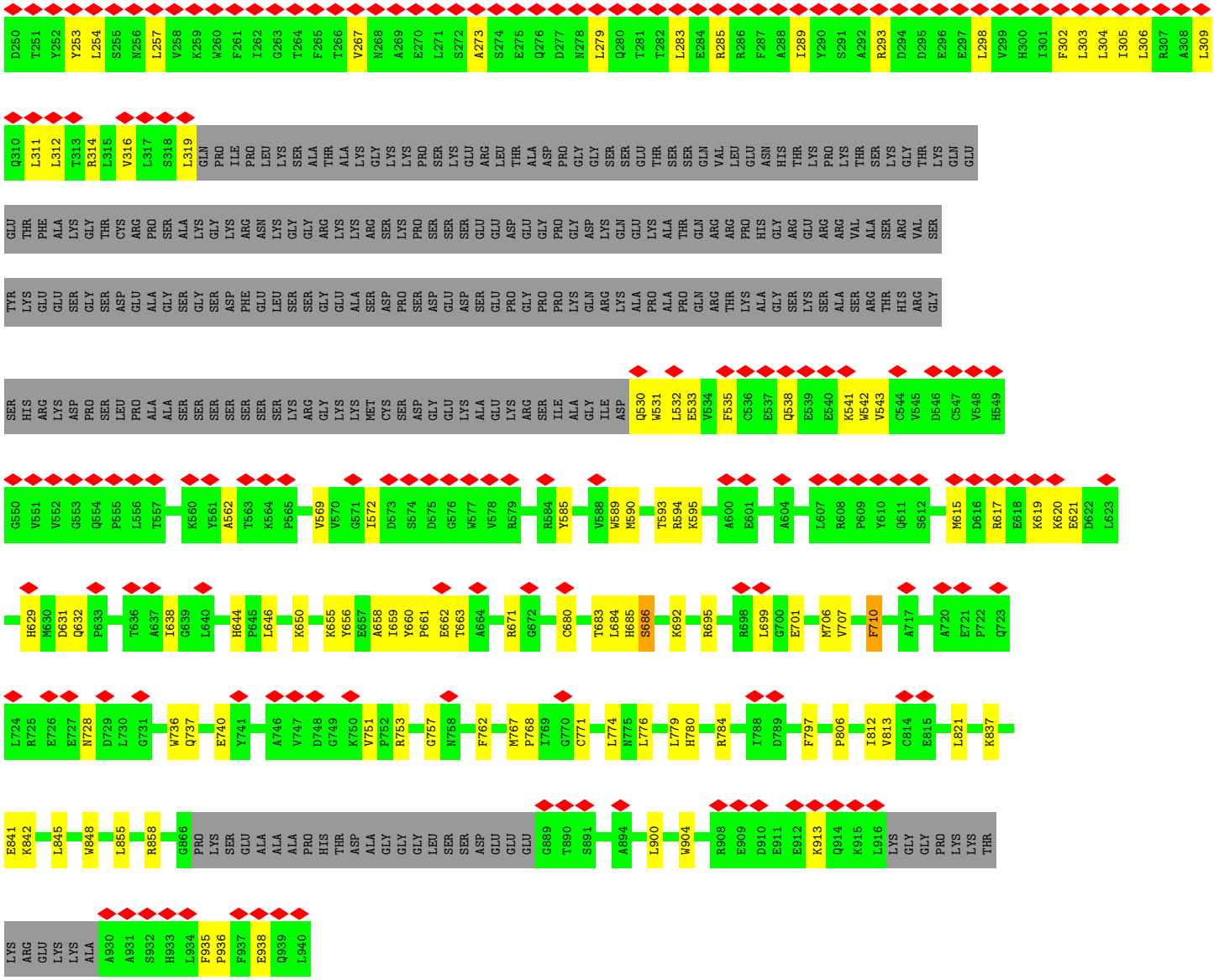




• Molecule 9: DNA repair protein complementing XP-C cells

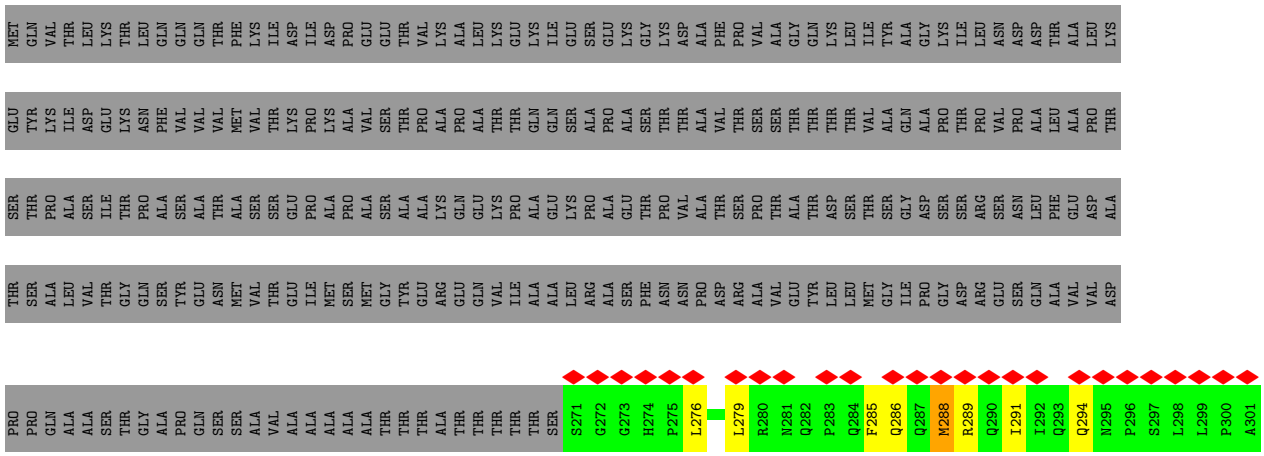


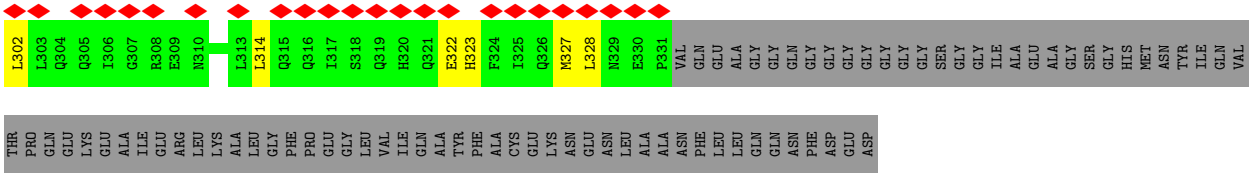




• Molecule 10: Lysine-specific demethylase RAD23B

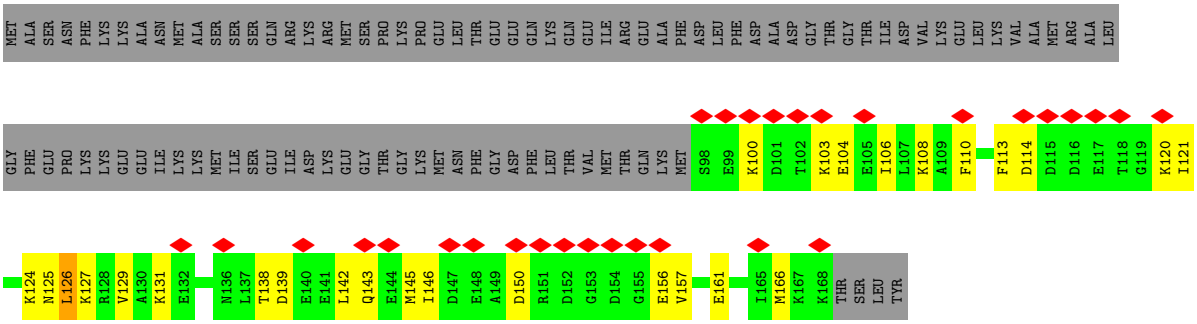
Chain J: 12% 11% 85%





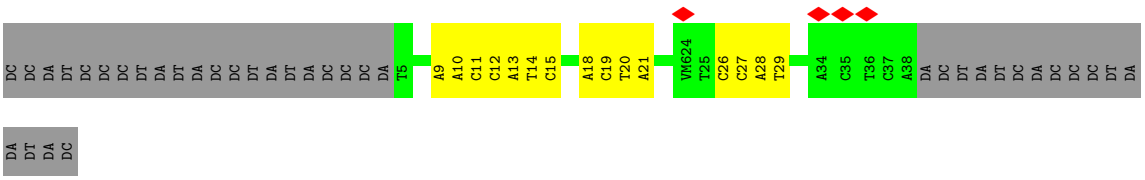
- Molecule 11: Centrin-2

Chain K:



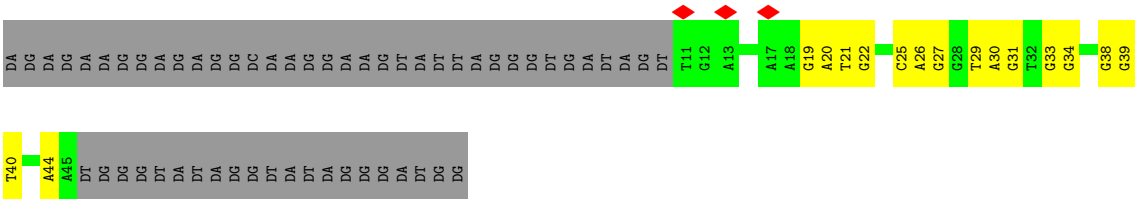
- Molecule 12: DNA (Cy5)

Chain L:



- Molecule 13: DNA (biotinylated)

Chain M:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	166008	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.195	Depositor
Minimum map value	0.084	Depositor
Average map value	0.095	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.106	Depositor
Map size (Å)	375.2, 375.2, 375.2	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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: ZN, CA, SF4, VM6

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	0.09	0/5239	0.29	0/7074
2	B	0.12	0/6205	0.33	0/8397
3	C	0.10	0/3071	0.27	0/4138
4	D	0.12	0/3684	0.32	0/4991
5	E	0.10	0/2893	0.26	0/3917
6	F	0.10	0/2085	0.27	0/2821
7	G	0.18	0/562	0.45	0/757
8	H	0.25	0/666	0.78	0/891
9	I	0.10	0/4486	0.28	0/6068
10	J	0.19	0/515	0.47	1/696 (0.1%)
11	K	0.15	0/581	0.49	0/770
12	L	0.19	0/724	0.38	0/1106
13	M	0.22	0/836	0.40	0/1294
All	All	0.12	0/31547	0.33	1/42920 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	288	MET	CB-CG-SD	5.44	129.01	112.70

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	5131	0	5175	88	0
2	B	6080	0	6125	101	0
3	C	3014	0	3039	53	0
4	D	3600	0	3644	53	0
5	E	2828	0	2767	33	0
6	F	2049	0	2075	29	0
7	G	556	0	567	18	0
8	H	659	0	669	40	0
9	I	4383	0	4373	91	0
10	J	504	0	497	11	0
11	K	578	0	565	21	0
12	L	690	0	373	15	0
13	M	741	0	394	18	0
14	B	8	0	0	1	0
15	E	3	0	0	0	0
15	F	2	0	0	0	0
16	K	2	0	0	0	0
All	All	30828	0	30263	524	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 (524) 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)
5:E:279:ASN:HB3	5:E:282:PRO:HG3	1.65	0.78
3:C:254:LEU:HD13	3:C:305:LYS:HE2	1.67	0.77
13:M:33:DG:H2'	13:M:34:DG:C8	2.21	0.76
12:L:18:DA:H2"	12:L:19:DC:H5"	1.66	0.76
1:A:511:TRP:HB3	1:A:665:GLN:HE21	1.51	0.75
4:D:408:LEU:HD11	4:D:440:LEU:HD12	1.70	0.74
1:A:694:ALA:HB3	9:I:938:GLU:HG3	1.69	0.73
3:C:465:TYR:HB3	5:E:276:LEU:HD21	1.72	0.72
5:E:252:MET:HE2	6:F:267:VAL:HG21	1.72	0.71
6:F:195:VAL:HG11	6:F:199:ASP:H	1.55	0.70
8:H:77:LYS:O	8:H:81:ILE:HD12	1.92	0.70
2:B:232:VAL:HG12	2:B:455:ILE:HB	1.73	0.70
8:H:136:ASN:HA	8:H:139:LYS:HG2	1.74	0.69
2:B:70:LEU:HD22	2:B:204:VAL:HG22	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:30:DA:H2'	13:M:31:DG:C8	2.28	0.69
11:K:142:LEU:O	11:K:146:ILE:HG13	1.93	0.69
5:E:72:GLU:HA	5:E:79:ASN:HD21	1.57	0.69
2:B:54:ALA:HB2	2:B:90:LEU:HD11	1.74	0.68
9:I:316:VAL:O	9:I:530:GLN:HA	1.93	0.68
2:B:72:TYR:HB3	2:B:206:VAL:HG12	1.76	0.67
3:C:501:GLN:HA	3:C:505:LEU:HD13	1.76	0.67
1:A:303:ASN:HD21	1:A:359:LYS:HD2	1.58	0.67
11:K:121:ILE:HB	11:K:157:VAL:HB	1.76	0.67
1:A:537:ASN:HD22	1:A:540:LYS:H	1.43	0.66
1:A:195:ARG:HG2	1:A:198:ARG:HH22	1.61	0.66
2:B:249:VAL:HG22	2:B:435:PHE:HB3	1.76	0.65
8:H:117:ASN:HA	8:H:120:LYS:NZ	2.12	0.65
2:B:338:GLU:HG3	8:H:68:VAL:HG11	1.78	0.65
9:I:303:LEU:HD13	9:I:532:LEU:HD11	1.79	0.65
9:I:223:ILE:HG21	9:I:279:LEU:HB3	1.77	0.65
9:I:590:MET:HB2	9:I:644:HIS:HE1	1.60	0.65
1:A:542:ARG:HB3	1:A:701:LEU:HD23	1.78	0.64
3:C:186:TYR:HB2	9:I:165:ILE:HB	1.78	0.64
9:I:305:ILE:HG23	9:I:306:LEU:HD22	1.79	0.64
9:I:213:LEU:HD22	9:I:319:LEU:HD22	1.79	0.64
3:C:131:LEU:HB3	3:C:137:ILE:HG12	1.80	0.64
1:A:561:PHE:HB3	1:A:639:ARG:HH21	1.63	0.64
2:B:21:GLN:O	2:B:25:MET:HG3	1.98	0.63
2:B:84:ILE:HG21	2:B:176:ASN:HB3	1.80	0.63
4:D:411:GLN:HG2	4:D:439:ARG:HB2	1.80	0.63
9:I:254:LEU:HD23	9:I:257:LEU:HD21	1.78	0.63
9:I:312:LEU:HB3	9:I:535:PHE:HB3	1.80	0.63
2:B:353:SER:HB3	2:B:355:PRO:HD2	1.81	0.63
4:D:401:LEU:HD11	7:G:57:VAL:HG21	1.81	0.63
12:L:20:DT:H2"	12:L:21:DA:C8	2.34	0.63
4:D:77:LYS:HA	4:D:77:LYS:HE3	1.81	0.62
12:L:13:DA:H2'	12:L:14:DT:C6	2.35	0.62
2:B:530:VAL:HG21	2:B:714:VAL:HG13	1.82	0.62
3:C:309:HIS:O	3:C:313:MET:HG2	1.99	0.62
1:A:392:PHE:HB3	1:A:408:SER:HB2	1.81	0.62
9:I:541:LYS:HE3	9:I:543:VAL:HG22	1.82	0.62
6:F:263:GLU:HG2	6:F:264:ILE:HG13	1.82	0.61
7:G:7:GLY:HA3	7:G:46:ILE:HG12	1.83	0.61
9:I:848:TRP:CD1	11:K:166:MET:HE1	2.36	0.61
2:B:134:CYS:HB2	14:B:1000:SF4:S4	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:TYR:HB2	2:B:21:GLN:HG3	1.82	0.60
2:B:747:GLU:HA	2:B:750:LEU:HD12	1.83	0.60
1:A:294:GLU:HG3	1:A:332:ARG:HD3	1.84	0.60
10:J:288:MET:HB3	10:J:302:LEU:HD11	1.82	0.60
2:B:170:LEU:HD11	2:B:194:LEU:HD11	1.85	0.59
8:H:74:ILE:HA	8:H:77:LYS:HE2	1.85	0.59
1:A:520:ARG:HD3	7:G:18:GLN:HG3	1.83	0.59
12:L:12:DC:H2'	12:L:13:DA:C8	2.38	0.59
10:J:276:LEU:HB3	10:J:279:LEU:HD12	1.85	0.59
12:L:9:DA:H2"	12:L:10:DA:C8	2.38	0.59
1:A:371:VAL:HG13	1:A:407:ILE:HG22	1.84	0.58
1:A:375:LYS:HD2	1:A:391:ARG:HD3	1.85	0.58
1:A:139:TYR:HA	1:A:142:LYS:HG2	1.85	0.58
4:D:311:THR:HA	4:D:387:ILE:HD11	1.84	0.58
5:E:76:LEU:HD12	5:E:80:ARG:HA	1.86	0.58
2:B:323:ILE:HD12	2:B:329:PHE:HD1	1.69	0.57
4:D:270:LEU:HB3	4:D:287:ALA:HB2	1.86	0.57
8:H:86:GLU:HG2	8:H:95:TYR:HE1	1.69	0.57
11:K:104:GLU:O	11:K:108:LYS:HG2	2.05	0.57
11:K:127:LYS:O	11:K:131:LYS:HG2	2.05	0.57
2:B:517:ILE:HG23	2:B:548:THR:HG23	1.86	0.57
13:M:39:DG:H2"	13:M:40:DT:H5'	1.87	0.57
1:A:541:PHE:HE1	1:A:545:GLN:HE21	1.52	0.57
12:L:12:DC:H2'	12:L:13:DA:H8	1.69	0.57
1:A:440:LEU:HD12	1:A:484:ILE:HD11	1.87	0.56
9:I:204:ASP:HB2	10:J:314:LEU:HD12	1.86	0.56
1:A:76:LEU:HB3	1:A:86:LEU:HD12	1.87	0.56
3:C:189:THR:HA	9:I:162:PRO:HG2	1.88	0.56
10:J:285:PHE:HA	10:J:288:MET:HE2	1.86	0.56
2:B:230:VAL:HG22	2:B:453:SER:HB2	1.88	0.56
3:C:171:LEU:HD11	3:C:196:ILE:HD13	1.88	0.56
9:I:283:LEU:HD13	9:I:304:LEU:HD11	1.87	0.56
12:L:28:DA:H5"	12:L:28:DA:H8	1.71	0.56
1:A:497:GLN:HE21	1:A:504:LYS:HG3	1.70	0.55
2:B:109:LEU:HD23	2:B:220:LEU:HD21	1.87	0.55
9:I:533:GLU:HB3	9:I:542:TRP:CE3	2.42	0.55
2:B:668:ILE:HG23	2:B:673:ASP:HB3	1.87	0.55
9:I:569:VAL:HG11	9:I:585:TYR:HE2	1.72	0.55
13:M:20:DA:C8	13:M:20:DA:H5'	2.42	0.55
2:B:532:PRO:HA	5:E:174:LEU:HD13	1.89	0.55
3:C:418:LEU:O	4:D:123:LEU:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:404:THR:HG22	7:G:9:LEU:HB3	1.89	0.55
8:H:114:ASP:HB3	8:H:117:ASN:HB3	1.89	0.55
9:I:229:LEU:HB3	9:I:304:LEU:HD13	1.88	0.54
9:I:655:LYS:HG2	9:I:656:TYR:CZ	2.42	0.54
3:C:406:SER:HB2	6:F:27:LEU:HD21	1.89	0.54
4:D:16:CYS:HB2	4:D:294:VAL:HG21	1.90	0.54
2:B:28:LEU:HD23	2:B:55:LEU:HD23	1.90	0.54
9:I:594:ARG:HB2	9:I:595:LYS:NZ	2.22	0.54
2:B:25:MET:HE3	2:B:55:LEU:HB2	1.89	0.54
3:C:498:GLU:HA	3:C:501:GLN:HG2	1.88	0.54
9:I:768:PRO:HG2	9:I:771:CYS:HB2	1.90	0.54
1:A:505:VAL:HG22	1:A:657:ALA:HB3	1.90	0.53
6:F:46:ASN:HB3	6:F:104:LEU:HD21	1.90	0.53
2:B:165:GLY:HA3	2:B:189:TRP:CZ2	2.43	0.53
2:B:748:GLU:HA	2:B:751:LYS:HE2	1.89	0.53
4:D:317:ALA:O	4:D:341:MET:HA	2.07	0.53
1:A:168:LEU:HD11	1:A:175:TYR:HB3	1.89	0.53
8:H:135:LYS:O	8:H:138:LEU:HG	2.08	0.53
1:A:521:GLU:O	1:A:525:ILE:HG12	2.09	0.53
3:C:400:ILE:HG23	6:F:20:ILE:HD11	1.90	0.53
4:D:55:TRP:O	4:D:59:MET:HG2	2.08	0.53
8:H:106:VAL:O	8:H:110:THR:HG23	2.08	0.53
9:I:302:PHE:HD2	9:I:532:LEU:HD23	1.74	0.53
2:B:484:THR:HG23	2:B:756:ILE:HD11	1.90	0.53
3:C:426:ALA:HB1	6:F:222:SER:HB2	1.90	0.53
7:G:31:LYS:HD3	7:G:31:LYS:N	2.24	0.53
1:A:367:SER:O	1:A:371:VAL:HG23	2.08	0.52
9:I:848:TRP:HH2	11:K:126:LEU:HD11	1.74	0.52
12:L:13:DA:H2'	12:L:14:DT:H6	1.74	0.52
6:F:119:MET:HE2	6:F:119:MET:HA	1.91	0.52
10:J:279:LEU:HA	10:J:285:PHE:CD2	2.45	0.52
11:K:106:ILE:HD11	11:K:166:MET:HG3	1.91	0.52
8:H:85:ARG:HH12	8:H:140:LEU:HD21	1.74	0.52
9:I:774:LEU:HD12	9:I:813:VAL:HB	1.92	0.52
1:A:394:SER:HB2	12:L:15:DC:H5"	1.91	0.52
1:A:471:VAL:HG11	1:A:633:ARG:HB2	1.90	0.52
1:A:444:HIS:CD2	1:A:445:THR:HG23	2.45	0.52
5:E:379:LEU:HD11	6:F:180:VAL:HG12	1.91	0.52
4:D:94:ARG:HB3	4:D:97:HIS:HE1	1.74	0.52
12:L:14:DT:H2'	12:L:15:DC:C6	2.44	0.52
2:B:349:VAL:HG12	2:B:419:GLU:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:19:DG:H2"	13:M:20:DA:C8	2.44	0.52
5:E:162:HIS:CD2	5:E:250:ILE:HD11	2.45	0.52
8:H:73:GLU:O	8:H:76:LYS:HG2	2.09	0.52
9:I:180:GLU:HA	9:I:183:LYS:HE3	1.91	0.52
12:L:28:DA:H2'	12:L:29:DT:H71	1.91	0.52
2:B:135:HIS:HD2	2:B:391:LEU:HD22	1.74	0.52
1:A:185:ILE:HG21	1:A:268:VAL:HG11	1.91	0.51
11:K:138:THR:O	11:K:142:LEU:HD12	2.10	0.51
3:C:465:TYR:CE2	5:E:271:PHE:HB2	2.45	0.51
8:H:77:LYS:O	8:H:80:LYS:HB3	2.10	0.51
9:I:273:ALA:HB2	9:I:293:ARG:HD2	1.91	0.51
1:A:108:CYS:SG	1:A:115:GLU:HB3	2.50	0.51
1:A:568:LEU:HD22	1:A:608:SER:HB3	1.92	0.51
9:I:257:LEU:HD13	9:I:306:LEU:HD11	1.92	0.51
2:B:603:LYS:HG2	3:C:269:LEU:HD22	1.92	0.51
8:H:74:ILE:HG22	8:H:77:LYS:NZ	2.26	0.51
3:C:137:ILE:HD11	3:C:142:PHE:HD1	1.75	0.51
8:H:75:ARG:HG2	8:H:106:VAL:HG11	1.92	0.51
9:I:658:ALA:HB3	9:I:684:LEU:HD13	1.92	0.51
2:B:2:LYS:HE3	2:B:11:TYR:HE1	1.74	0.51
6:F:69:PHE:HE1	6:F:139:LYS:HE3	1.75	0.51
9:I:589:TRP:HD1	9:I:593:THR:HB	1.74	0.51
9:I:685:HIS:CG	9:I:686:SER:H	2.29	0.51
9:I:848:TRP:CG	11:K:145:MET:HE2	2.46	0.51
13:M:30:DA:H2'	13:M:31:DG:H8	1.75	0.51
2:B:346:VAL:HG12	2:B:348:HIS:H	1.75	0.50
3:C:534:ASN:O	3:C:538:THR:HG23	2.12	0.50
1:A:168:LEU:HD13	1:A:177:VAL:HG22	1.94	0.50
3:C:465:TYR:HE2	5:E:271:PHE:H	1.60	0.50
4:D:312:ASN:OD1	4:D:312:ASN:O	2.29	0.50
8:H:117:ASN:HA	8:H:120:LYS:HZ2	1.75	0.50
3:C:228:HIS:CG	3:C:236:ASN:HD21	2.29	0.50
12:L:11:DC:H2'	12:L:12:DC:C6	2.46	0.50
2:B:404:ALA:HA	2:B:407:VAL:HG12	1.93	0.50
3:C:489:LYS:HG2	3:C:493:MET:HE2	1.93	0.50
1:A:310:LEU:HD11	1:A:352:THR:HG23	1.93	0.49
1:A:539:ASN:HD21	9:I:900:LEU:HD13	1.77	0.49
7:G:32:LYS:HE2	7:G:32:LYS:HA	1.93	0.49
9:I:695:ARG:HH22	9:I:740:GLU:HG2	1.76	0.49
9:I:706:MET:HE1	9:I:728:ASN:HB2	1.94	0.49
12:L:28:DA:H5"	12:L:28:DA:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:GLN:O	1:A:158:LEU:HG	2.12	0.49
1:A:413:LEU:HA	1:A:427:MET:HE1	1.94	0.49
1:A:531:ILE:HA	1:A:534:TYR:CE2	2.47	0.49
3:C:381:ARG:HA	3:C:384:HIS:CE1	2.48	0.49
7:G:37:ASP:HB2	7:G:43:VAL:HG22	1.94	0.49
1:A:182:PRO:O	1:A:186:GLN:HG2	2.12	0.49
2:B:272:ARG:NH2	2:B:273:ILE:HA	2.27	0.49
2:B:583:LYS:HD2	3:C:315:LEU:HD23	1.94	0.49
3:C:247:ALA:O	3:C:251:GLU:HG2	2.12	0.49
2:B:210:HIS:CE1	2:B:242:VAL:HG13	2.48	0.49
2:B:358:LEU:HD11	2:B:369:ARG:HG3	1.95	0.49
2:B:745:GLU:O	2:B:745:GLU:HG2	2.13	0.49
9:I:248:ASP:HA	9:I:538:GLN:HE21	1.76	0.49
2:B:161:PHE:HB2	2:B:189:TRP:HD1	1.77	0.49
8:H:86:GLU:HG2	8:H:95:TYR:CE1	2.46	0.49
1:A:525:ILE:HG22	1:A:527:THR:H	1.77	0.48
2:B:24:TYR:HE2	2:B:52:LEU:HD21	1.78	0.48
5:E:269:PRO:HB3	5:E:286:LEU:HD22	1.95	0.48
8:H:85:ARG:HH21	8:H:139:LYS:HE3	1.77	0.48
2:B:285:TYR:O	2:B:289:VAL:HG13	2.12	0.48
4:D:163:MET:HE1	4:D:203:PHE:CE2	2.48	0.48
5:E:355:GLN:HG2	5:E:356:HIS:ND1	2.28	0.48
8:H:74:ILE:HG22	8:H:77:LYS:HZ3	1.78	0.48
9:I:188:THR:HG22	9:I:191:ARG:HH22	1.78	0.48
2:B:264:GLU:O	2:B:268:LYS:HD3	2.13	0.48
5:E:182:ILE:HD12	5:E:182:ILE:H	1.79	0.48
9:I:245:LEU:HD13	9:I:247:ARG:HE	1.79	0.48
4:D:275:LYS:H	4:D:278:SER:HB2	1.78	0.48
8:H:99:LEU:O	8:H:102:VAL:HG22	2.14	0.48
8:H:127:LYS:HA	8:H:130:LYS:HZ3	1.79	0.48
1:A:95:TYR:HD2	5:E:19:TRP:HA	1.79	0.48
2:B:497:ARG:HH21	2:B:709:THR:HG23	1.78	0.48
11:K:166:MET:HE3	11:K:166:MET:HA	1.95	0.48
1:A:626:ILE:HG22	1:A:662:LEU:HD12	1.96	0.48
2:B:321:GLY:HA3	8:H:99:LEU:HB2	1.95	0.48
1:A:479:ASP:HA	1:A:482:PHE:CE2	2.49	0.47
1:A:586:GLN:HA	1:A:589:ARG:HG3	1.96	0.47
2:B:28:LEU:HD22	2:B:52:LEU:HD22	1.96	0.47
3:C:121:ASP:HB3	3:C:124:LEU:HB3	1.95	0.47
3:C:193:ILE:HA	3:C:196:ILE:HG22	1.96	0.47
4:D:229:ASP:HB3	4:D:232:GLU:HG2	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:370:LYS:HE3	2:B:370:LYS:HB3	1.77	0.47
4:D:412:PHE:H	4:D:418:PHE:HZ	1.62	0.47
8:H:74:ILE:HA	8:H:77:LYS:CE	2.45	0.47
11:K:146:ILE:O	11:K:150:ASP:HB2	2.13	0.47
2:B:28:LEU:HD11	2:B:455:ILE:HD13	1.97	0.47
2:B:29:LYS:HD3	2:B:29:LYS:C	2.39	0.47
9:I:237:ILE:HD13	9:I:309:LEU:HD21	1.95	0.47
1:A:138:GLU:HG3	1:A:139:TYR:HD1	1.79	0.47
4:D:265:LEU:CD1	4:D:270:LEU:HB2	2.44	0.47
6:F:213:LEU:HD12	6:F:238:ARG:HD3	1.96	0.47
12:L:26:DC:H1'	12:L:27:DC:C5	2.49	0.47
2:B:616:ARG:HA	2:B:616:ARG:HD3	1.72	0.47
1:A:492:ASN:HB3	1:A:495:GLU:HB3	1.97	0.47
3:C:489:LYS:O	3:C:493:MET:HG2	2.14	0.47
8:H:89:PHE:CD2	8:H:94:GLU:HG3	2.49	0.47
9:I:285:ARG:O	9:I:289:ILE:HG13	2.15	0.47
9:I:659:ILE:HG22	9:I:663:THR:HG22	1.97	0.47
1:A:714:GLN:HG3	9:I:858:ARG:HD2	1.97	0.47
2:B:60:GLN:HG3	2:B:67:VAL:O	2.14	0.47
2:B:514:ILE:HG23	2:B:518:ARG:HH12	1.80	0.47
9:I:629:HIS:CE1	9:I:646:LEU:HD21	2.48	0.47
9:I:701:GLU:HG3	9:I:737:GLN:HB3	1.96	0.47
2:B:746:SER:O	2:B:750:LEU:HG	2.15	0.47
3:C:170:PHE:HZ	3:C:199:THR:HG21	1.79	0.47
9:I:797:PHE:HA	9:I:806:PRO:HA	1.97	0.47
1:A:520:ARG:CD	7:G:18:GLN:HG3	2.44	0.47
9:I:707:VAL:C	9:I:728:ASN:HB3	2.40	0.47
3:C:200:TYR:CG	3:C:229:TYR:HE2	2.33	0.47
9:I:241:PHE:HD1	9:I:253:TYR:HE1	1.63	0.47
2:B:657:MET:HE2	2:B:689:LYS:O	2.15	0.46
2:B:679:PHE:HB3	2:B:684:PHE:CD2	2.50	0.46
9:I:661:PRO:HA	9:I:663:THR:N	2.29	0.46
1:A:525:ILE:HG13	1:A:533:LEU:HD12	1.97	0.46
2:B:243:CYS:HB3	2:B:443:ALA:HB3	1.96	0.46
2:B:420:PRO:HA	2:B:431:PRO:HB3	1.97	0.46
9:I:617:ARG:HA	9:I:620:LYS:HE3	1.96	0.46
11:K:114:ASP:HB3	11:K:125:ASN:CG	2.40	0.46
13:M:21:DT:H2"	13:M:22:DG:C8	2.50	0.46
4:D:171:VAL:HB	4:D:175:LEU:HD12	1.98	0.46
1:A:335:SER:HB3	1:A:463:LYS:H	1.80	0.46
3:C:498:GLU:O	3:C:502:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:44:PHE:CZ	7:G:46:ILE:HD11	2.50	0.46
8:H:117:ASN:HA	8:H:120:LYS:HZ3	1.77	0.46
1:A:774:HIS:HD2	4:D:330:LEU:HD23	1.81	0.46
9:I:935:PHE:CD2	9:I:936:PRO:HD2	2.50	0.46
2:B:165:GLY:HA2	2:B:168:VAL:HG22	1.97	0.46
2:B:634:LYS:HE3	2:B:634:LYS:HB2	1.77	0.46
9:I:797:PHE:HD2	13:M:25:DC:H2'	1.81	0.46
2:B:24:TYR:CE2	2:B:52:LEU:HD21	2.51	0.46
2:B:461:LEU:HD23	2:B:464:LEU:HD22	1.98	0.46
4:D:251:VAL:HG11	4:D:279:ARG:HA	1.97	0.46
4:D:341:MET:HG2	4:D:342:VAL:N	2.30	0.46
11:K:124:LYS:HA	11:K:127:LYS:HE3	1.98	0.46
1:A:443:VAL:O	1:A:446:ILE:HG22	2.16	0.46
9:I:309:LEU:HB2	9:I:311:LEU:HG	1.98	0.46
1:A:514:MET:HE2	1:A:667:THR:HG22	1.98	0.46
2:B:537:ALA:HB3	2:B:597:LEU:HD22	1.98	0.46
6:F:102:GLU:O	6:F:103:LEU:HB3	2.16	0.46
10:J:289:ARG:HB2	10:J:328:LEU:HA	1.96	0.45
2:B:511:ARG:HH22	2:B:627:TYR:HE1	1.64	0.45
3:C:175:ARG:HH12	3:C:185:ARG:HG3	1.81	0.45
5:E:344:PHE:CE2	5:E:351:GLU:HG3	2.52	0.45
7:G:23:LEU:HD13	7:G:29:LEU:HD12	1.97	0.45
9:I:302:PHE:HA	9:I:305:ILE:HG22	1.98	0.45
10:J:291:ILE:HA	10:J:294:GLN:HG2	1.98	0.45
3:C:199:THR:HG23	3:C:200:TYR:CD2	2.52	0.45
4:D:54:ASN:OD1	6:F:233:PRO:HG3	2.16	0.45
1:A:311:LYS:HG2	1:A:312:PRO:HD2	1.98	0.45
2:B:215:PRO:HA	2:B:218:ALA:HB3	1.97	0.45
5:E:301:LEU:HD23	5:E:301:LEU:HA	1.69	0.45
9:I:661:PRO:HA	9:I:662:GLU:C	2.41	0.45
13:M:29:DT:H2"	13:M:30:DA:C8	2.51	0.45
1:A:502:ILE:HG23	1:A:644:LEU:HD22	1.99	0.45
2:B:223:LYS:HD2	2:B:223:LYS:HA	1.77	0.45
8:H:127:LYS:HA	8:H:130:LYS:NZ	2.31	0.45
1:A:522:TYR:CE2	1:A:530:ARG:HB2	2.52	0.45
3:C:365:LYS:HA	3:C:365:LYS:HD3	1.69	0.45
6:F:22:TRP:CE2	6:F:34:LEU:HD13	2.51	0.45
2:B:492:PRO:HB2	2:B:701:LEU:HD12	1.98	0.45
11:K:103:LYS:HA	11:K:106:ILE:HG22	1.99	0.45
1:A:187:HIS:HD2	1:A:289:TYR:HE2	1.64	0.45
4:D:305:GLY:HA3	4:D:372:ALA:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:322:GLU:HG2	10:J:323:HIS:CD2	2.52	0.45
6:F:252:ARG:HD2	6:F:261:LEU:HD12	1.99	0.44
9:I:736:TRP:CD1	9:I:737:GLN:HG3	2.52	0.44
11:K:120:LYS:HB3	11:K:156:GLU:HB3	1.99	0.44
13:M:38:DG:H2'	13:M:39:DG:C8	2.53	0.44
1:A:133:THR:HB	1:A:160:THR:HG21	1.99	0.44
1:A:624:ILE:HD13	1:A:660:TYR:HB2	1.99	0.44
2:B:42:MET:HB3	2:B:48:LYS:HE2	1.98	0.44
4:D:81:LYS:O	4:D:84:GLU:HG2	2.17	0.44
8:H:70:LYS:O	8:H:73:GLU:HG3	2.17	0.44
9:I:314:ARG:HG3	9:I:572:ILE:C	2.42	0.44
13:M:29:DT:H2"	13:M:30:DA:H8	1.82	0.44
2:B:448:PHE:HE1	2:B:454:VAL:HG11	1.83	0.44
8:H:71:GLU:O	8:H:75:ARG:HG3	2.16	0.44
9:I:660:TYR:CD2	9:I:661:PRO:HD2	2.53	0.44
2:B:657:MET:HE3	2:B:657:MET:HB3	1.82	0.44
3:C:370:LYS:HZ3	5:E:243:SER:H	1.65	0.44
2:B:323:ILE:HG21	2:B:378:ARG:HG2	1.98	0.44
9:I:797:PHE:HD1	9:I:806:PRO:HB3	1.82	0.44
3:C:512:ILE:HG23	3:C:517:LEU:HB2	1.99	0.44
4:D:20:GLN:HE21	4:D:44:VAL:HA	1.83	0.44
4:D:332:SER:OG	4:D:344:ALA:HB1	2.17	0.44
5:E:10:ARG:HH21	5:E:11:TRP:HZ3	1.63	0.44
5:E:96:PHE:CD2	5:E:124:PRO:HB3	2.53	0.44
7:G:61:MET:HE2	7:G:61:MET:HA	1.99	0.44
9:I:267:VAL:HG22	9:I:298:LEU:HD11	1.99	0.44
11:K:125:ASN:O	11:K:129:VAL:HG23	2.18	0.44
2:B:339:TYR:CD2	2:B:361:LEU:HD23	2.52	0.44
2:B:349:VAL:HA	2:B:418:ILE:O	2.18	0.44
7:G:20:LEU:HD23	7:G:23:LEU:HD21	2.00	0.44
7:G:38:ILE:N	7:G:38:ILE:HD12	2.32	0.44
9:I:631:ASP:HB3	9:I:632:GLN:H	1.52	0.44
1:A:566:PHE:O	1:A:570:GLU:HG2	2.18	0.44
4:D:216:MET:SD	4:D:290:LEU:HD21	2.58	0.44
6:F:102:GLU:C	6:F:104:LEU:H	2.24	0.44
1:A:703:PHE:CD1	1:A:712:LEU:HB2	2.53	0.43
2:B:72:TYR:CE1	2:B:234:ASP:HB2	2.53	0.43
2:B:263:LEU:HD23	2:B:263:LEU:HA	1.86	0.43
5:E:249:LEU:HD23	5:E:249:LEU:HA	1.85	0.43
8:H:79:LEU:HA	8:H:82:TYR:O	2.18	0.43
8:H:92:LEU:HD12	8:H:93:ARG:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:162:PRO:HB2	9:I:163:VAL:H	1.64	0.43
9:I:302:PHE:CD2	9:I:532:LEU:HD23	2.52	0.43
9:I:659:ILE:HG23	9:I:680:CYS:HB3	1.99	0.43
13:M:33:DG:H2'	13:M:34:DG:H8	1.76	0.43
1:A:533:LEU:HD23	1:A:533:LEU:HA	1.83	0.43
3:C:370:LYS:NZ	5:E:243:SER:H	2.16	0.43
6:F:14:VAL:HB	6:F:163:VAL:HG22	1.99	0.43
1:A:275:GLU:C	1:A:276:MET:HE2	2.43	0.43
3:C:207:TYR:CZ	3:C:211:VAL:HG21	2.53	0.43
3:C:434:LEU:HD11	6:F:229:TRP:CE2	2.53	0.43
4:D:248:ASP:HB2	4:D:282:TYR:CZ	2.53	0.43
5:E:315:ALA:HB2	6:F:253:ALA:HB2	1.99	0.43
10:J:288:MET:HA	10:J:291:ILE:HG12	1.99	0.43
1:A:560:VAL:HG22	1:A:624:ILE:HB	1.99	0.43
3:C:381:ARG:HH11	6:F:284:THR:HB	1.83	0.43
4:D:99:GLN:HG3	4:D:100:LEU:N	2.32	0.43
5:E:271:PHE:CE2	5:E:282:PRO:HB2	2.54	0.43
5:E:271:PHE:HE2	5:E:282:PRO:HB2	1.83	0.43
8:H:123:GLU:O	8:H:126:GLN:HG3	2.19	0.43
8:H:131:ASP:CG	8:H:132:VAL:HG23	2.42	0.43
2:B:681:ASP:HB3	2:B:684:PHE:HD2	1.83	0.43
4:D:77:LYS:HA	4:D:80:SER:HB3	2.01	0.43
4:D:396:LEU:HD23	4:D:396:LEU:HA	1.83	0.43
9:I:855:LEU:HD23	11:K:113:PHE:CE2	2.54	0.43
9:I:684:LEU:HD11	9:I:736:TRP:CH2	2.54	0.43
9:I:797:PHE:CD2	13:M:25:DC:H2'	2.53	0.43
1:A:166:VAL:HA	1:A:179:SER:HB2	2.00	0.43
2:B:391:LEU:HD23	2:B:391:LEU:H	1.84	0.43
2:B:537:ALA:HB1	2:B:621:PHE:HE2	1.83	0.43
6:F:176:ASN:O	6:F:180:VAL:HG13	2.19	0.43
8:H:84:LYS:HB3	8:H:84:LYS:HE3	1.75	0.43
9:I:226:GLN:HB2	9:I:229:LEU:HD12	2.00	0.43
9:I:569:VAL:HG11	9:I:585:TYR:CE2	2.54	0.43
9:I:837:LYS:O	9:I:841:GLU:HG2	2.17	0.43
3:C:170:PHE:CE2	3:C:171:LEU:HG	2.54	0.43
3:C:231:HIS:HB2	3:C:234:ARG:HB2	2.01	0.43
1:A:185:ILE:O	1:A:189:LEU:HG	2.18	0.43
1:A:581:TYR:CE2	1:A:583:PRO:HD2	2.54	0.43
2:B:105:LEU:HD12	2:B:173:GLY:H	1.83	0.43
4:D:338:PHE:HB2	4:D:341:MET:O	2.18	0.43
2:B:332:PHE:HE2	2:B:367:ILE:HG23	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:603:LYS:HB2	2:B:603:LYS:HE3	1.83	0.43
3:C:115:ASN:HA	3:C:118:LEU:HD12	2.00	0.43
9:I:620:LYS:HD2	9:I:620:LYS:C	2.44	0.43
9:I:779:LEU:HD21	9:I:821:LEU:HD21	2.01	0.43
11:K:100:LYS:O	11:K:103:LYS:HG2	2.19	0.43
2:B:82:LYS:O	2:B:86:GLU:HG3	2.19	0.42
4:D:383:LEU:HD13	4:D:383:LEU:HA	1.92	0.42
7:G:32:LYS:HD3	7:G:33:PHE:N	2.34	0.42
9:I:620:LYS:HD2	9:I:621:GLU:N	2.34	0.42
7:G:55:GLU:HB3	7:G:56:ARG:HH22	1.84	0.42
8:H:70:LYS:O	8:H:74:ILE:HG23	2.20	0.42
9:I:806:PRO:HG3	13:M:26:DA:N1	2.33	0.42
9:I:842:LYS:HD2	9:I:845:LEU:HD11	2.00	0.42
1:A:568:LEU:HD11	1:A:606:PHE:HB3	2.00	0.42
3:C:265:PRO:HG2	3:C:350:LYS:HG3	2.01	0.42
4:D:50:SER:C	4:D:52:ALA:H	2.26	0.42
6:F:42:MET:HE3	6:F:108:ASN:CG	2.45	0.42
9:I:531:TRP:HZ3	9:I:562:ALA:HB2	1.84	0.42
9:I:615:MET:O	9:I:619:LYS:HG2	2.19	0.42
1:A:613:THR:HB	1:A:615:PHE:CD1	2.54	0.42
2:B:606:GLU:HG2	2:B:662:GLN:NE2	2.35	0.42
3:C:352:ALA:O	3:C:356:GLU:HG2	2.19	0.42
5:E:281:GLU:O	5:E:281:GLU:HG2	2.19	0.42
6:F:258:HIS:HB2	6:F:260:ASN:ND2	2.35	0.42
5:E:276:LEU:HD12	5:E:276:LEU:HA	1.86	0.42
9:I:751:VAL:HG21	9:I:812:ILE:HG21	2.01	0.42
2:B:20:GLU:OE1	2:B:42:MET:HE3	2.19	0.42
2:B:526:GLU:HB3	2:B:714:VAL:HG21	2.01	0.42
3:C:465:TYR:CD2	5:E:271:PHE:HB2	2.55	0.42
4:D:111:ASN:HB3	4:D:114:PHE:HB3	2.01	0.42
10:J:286:GLN:HA	10:J:289:ARG:NE	2.35	0.42
1:A:496:LEU:HD22	1:A:501:TYR:HD2	1.85	0.42
1:A:621:ASN:HD22	1:A:647:LYS:NZ	2.18	0.42
2:B:94:TYR:CE2	2:B:102:LEU:HD12	2.55	0.42
4:D:418:PHE:CZ	4:D:439:ARG:HB3	2.55	0.42
9:I:183:LYS:HE3	9:I:183:LYS:HB3	1.90	0.42
1:A:546:PHE:CG	1:A:696:MET:HE1	2.55	0.42
1:A:647:LYS:HE2	1:A:647:LYS:HB3	1.81	0.42
2:B:381:SER:O	2:B:385:THR:HG23	2.19	0.42
13:M:26:DA:H2"	13:M:27:DG:H5"	2.02	0.42
1:A:166:VAL:HG21	1:A:188:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:ALA:HB2	9:I:935:PHE:CZ	2.55	0.42
2:B:118:HIS:ND1	2:B:119:PRO:HD2	2.35	0.42
2:B:738:LEU:HD12	2:B:738:LEU:HA	1.88	0.42
4:D:387:ILE:H	4:D:387:ILE:HG12	1.68	0.42
6:F:8:LEU:HD12	6:F:8:LEU:H	1.85	0.42
9:I:638:ILE:HD11	9:I:671:ARG:HB3	2.01	0.42
9:I:650:LYS:HA	9:I:650:LYS:HD3	1.88	0.42
1:A:599:ASN:HB3	1:A:601:LYS:HG2	2.02	0.41
1:A:706:LYS:HA	1:A:706:LYS:HD2	1.71	0.41
2:B:622:GLY:HA2	2:B:681:ASP:HB2	2.01	0.41
2:B:660:ALA:O	2:B:664:VAL:HG23	2.20	0.41
3:C:377:LYS:HB3	3:C:377:LYS:HE3	1.79	0.41
4:D:234:LEU:HD23	4:D:237:LEU:HD12	2.02	0.41
4:D:258:LEU:HD12	4:D:258:LEU:HA	1.87	0.41
7:G:71:LYS:HE2	7:G:71:LYS:HB2	1.75	0.41
8:H:95:TYR:HD2	8:H:98:PHE:HD1	1.67	0.41
8:H:126:GLN:NE2	8:H:127:LYS:HG2	2.35	0.41
9:I:683:THR:C	9:I:684:LEU:HD12	2.45	0.41
10:J:279:LEU:HB2	10:J:327:MET:HE1	2.02	0.41
2:B:52:LEU:O	2:B:56:ILE:HG13	2.20	0.41
3:C:354:LEU:O	3:C:358:ILE:HG13	2.20	0.41
6:F:44:LEU:HD22	6:F:227:LEU:HD13	2.02	0.41
1:A:287:LEU:HD12	1:A:287:LEU:HA	1.88	0.41
4:D:430:VAL:HB	4:D:444:THR:OG1	2.21	0.41
5:E:77:LYS:HB2	5:E:78:PRO:HD3	2.02	0.41
1:A:546:PHE:CD2	1:A:696:MET:HE1	2.55	0.41
1:A:573:ILE:HD13	1:A:573:ILE:HA	1.87	0.41
2:B:161:PHE:HA	2:B:189:TRP:HE1	1.86	0.41
3:C:411:MET:HG3	6:F:119:MET:HG3	2.03	0.41
4:D:242:PHE:HB3	6:F:101:TYR:CE1	2.56	0.41
8:H:70:LYS:HD3	8:H:70:LYS:HA	1.91	0.41
8:H:131:ASP:O	8:H:135:LYS:HE2	2.21	0.41
9:I:753:ARG:HB3	9:I:757:GLY:HA2	2.02	0.41
1:A:210:ILE:HD13	1:A:210:ILE:HA	1.89	0.41
1:A:703:PHE:CD2	1:A:712:LEU:HD22	2.55	0.41
2:B:377:GLU:OE2	2:B:377:GLU:N	2.47	0.41
2:B:730:ARG:HG3	2:B:738:LEU:HD23	2.03	0.41
4:D:48:LEU:HD23	4:D:48:LEU:HA	1.91	0.41
4:D:60:LEU:HD21	4:D:119:ARG:HG2	2.01	0.41
4:D:265:LEU:HD11	4:D:270:LEU:HB2	2.01	0.41
1:A:110:PRO:HD2	1:A:113:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:LYS:HG3	1:A:450:MET:SD	2.61	0.41
5:E:79:ASN:HB3	5:E:82:THR:HG23	2.03	0.41
5:E:118:THR:HG23	5:E:126:LYS:HD3	2.01	0.41
9:I:710:PHE:CE1	13:M:25:DC:H5'	2.55	0.41
2:B:118:HIS:O	2:B:122:THR:HG23	2.21	0.41
2:B:280:ARG:HA	2:B:283:ASP:OD2	2.20	0.41
2:B:587:ALA:HB3	2:B:594:ALA:HB2	2.03	0.41
5:E:9:LYS:HE2	5:E:9:LYS:HB2	1.91	0.41
6:F:158:LYS:HD2	6:F:235:GLN:HE21	1.85	0.41
8:H:111:ASN:HB3	8:H:113:VAL:HG22	2.03	0.41
1:A:165:LYS:HD3	1:A:165:LYS:HA	1.91	0.41
1:A:528:LYS:HE2	13:M:44:DA:H5'	2.03	0.41
1:A:635:GLN:HG2	1:A:639:ARG:HH11	1.85	0.41
1:A:665:GLN:O	1:A:667:THR:HG23	2.20	0.41
2:B:553:TYR:HB2	2:B:558:LEU:HD12	2.03	0.41
2:B:693:LEU:HD22	2:B:697:ILE:HD11	2.02	0.41
8:H:82:TYR:CZ	8:H:125:TYR:HD2	2.39	0.41
13:M:34:DG:H8	13:M:34:DG:OP2	2.03	0.41
3:C:313:MET:HE3	3:C:313:MET:HB3	1.88	0.41
4:D:62:LEU:HD23	4:D:62:LEU:HA	1.90	0.41
4:D:163:MET:HE1	4:D:203:PHE:HE2	1.86	0.41
4:D:175:LEU:HD23	4:D:175:LEU:HA	1.84	0.41
7:G:13:ASP:OD2	9:I:904:TRP:HB2	2.21	0.41
8:H:131:ASP:C	8:H:135:LYS:HE2	2.45	0.41
9:I:913:LYS:HA	9:I:913:LYS:HD2	1.76	0.41
11:K:157:VAL:HA	11:K:161:GLU:OE1	2.21	0.41
12:L:14:DT:H2'	12:L:15:DC:H6	1.83	0.41
1:A:537:ASN:HD21	1:A:539:ASN:HB2	1.85	0.41
1:A:703:PHE:HA	1:A:708:GLU:HB3	2.03	0.41
3:C:145:ASN:HB2	3:C:146:ARG:NH1	2.35	0.41
4:D:90:LEU:HD23	4:D:96:TRP:CH2	2.56	0.41
4:D:115:ARG:O	4:D:119:ARG:HG3	2.21	0.41
4:D:452:LYS:HG2	4:D:456:LYS:HE3	2.03	0.41
7:G:55:GLU:HB3	7:G:56:ARG:NH2	2.36	0.41
9:I:232:ILE:O	9:I:236:ILE:HG22	2.20	0.41
11:K:139:ASP:O	11:K:143:GLN:HG2	2.21	0.41
3:C:486:LEU:HD23	3:C:486:LEU:HA	1.90	0.40
1:A:586:GLN:O	1:A:590:MET:SD	2.79	0.40
2:B:56:ILE:HG21	2:B:70:LEU:HD12	2.03	0.40
9:I:780:HIS:CD2	9:I:784:ARG:HG3	2.56	0.40
2:B:337:LEU:HD12	2:B:337:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:383:LEU:O	4:D:384:PRO:C	2.64	0.40
6:F:195:VAL:HG13	6:F:198:SER:HB3	2.04	0.40
1:A:76:LEU:HD21	1:A:143:LEU:HB3	2.04	0.40
2:B:117:ILE:HG21	2:B:185:ARG:HG3	2.02	0.40
3:C:269:LEU:HD23	3:C:269:LEU:HA	1.86	0.40
3:C:320:ARG:HD3	3:C:321:LYS:H	1.86	0.40
3:C:407:ILE:HD13	3:C:407:ILE:HA	1.88	0.40
5:E:157:LYS:HB3	5:E:157:LYS:HE2	1.76	0.40
9:I:692:LYS:HG2	9:I:762:PHE:CZ	2.57	0.40
9:I:699:LEU:O	9:I:701:GLU:HG2	2.21	0.40
9:I:776:LEU:HD23	9:I:776:LEU:HA	1.87	0.40
1:A:537:ASN:ND2	1:A:540:LYS:H	2.16	0.40
2:B:5:VAL:HG13	2:B:26:ARG:HG2	2.03	0.40
2:B:62:ALA:C	2:B:63:TYR:HD1	2.30	0.40
4:D:341:MET:HB3	4:D:341:MET:HE2	1.79	0.40
5:E:291:CYS:HB2	5:E:312:LEU:HD11	2.03	0.40
9:I:194:MET:HE3	9:I:194:MET:HB3	1.93	0.40
11:K:110:PHE:HE2	11:K:121:ILE:HG13	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	630/797 (79%)	606 (96%)	24 (4%)	0	100	100
2	B	751/771 (97%)	716 (95%)	35 (5%)	0	100	100
3	C	362/591 (61%)	345 (95%)	17 (5%)	0	100	100
4	D	445/462 (96%)	430 (97%)	15 (3%)	0	100	100
5	E	356/395 (90%)	346 (97%)	10 (3%)	0	100	100
6	F	255/308 (83%)	249 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
8	H	75/309 (24%)	72 (96%)	3 (4%)	0	100	100
9	I	526/940 (56%)	508 (97%)	18 (3%)	0	100	100
10	J	59/409 (14%)	54 (92%)	5 (8%)	0	100	100
11	K	69/172 (40%)	69 (100%)	0	0	100	100
All	All	3596/5225 (69%)	3461 (96%)	135 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	562/702 (80%)	557 (99%)	5 (1%)	70	77
2	B	659/675 (98%)	646 (98%)	13 (2%)	48	67
3	C	335/513 (65%)	332 (99%)	3 (1%)	70	77
4	D	391/399 (98%)	387 (99%)	4 (1%)	68	75
5	E	321/352 (91%)	318 (99%)	3 (1%)	70	77
6	F	232/272 (85%)	229 (99%)	3 (1%)	61	73
7	G	63/64 (98%)	62 (98%)	1 (2%)	55	71
8	H	77/283 (27%)	77 (100%)	0	100	100
9	I	470/804 (58%)	466 (99%)	4 (1%)	70	77
10	J	57/328 (17%)	57 (100%)	0	100	100
11	K	64/152 (42%)	63 (98%)	1 (2%)	55	71
All	All	3231/4544 (71%)	3194 (99%)	37 (1%)	63	74

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	GLN

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Mol	Chain	Res	Type
1	A	286	HIS
1	A	308	ILE
1	A	573	ILE
1	A	714	GLN
2	B	12	PHE
2	B	27	GLU
2	B	46	THR
2	B	121	VAL
2	B	148	HIS
2	B	217	ILE
2	B	225	LEU
2	B	325	THR
2	B	447	VAL
2	B	493	MET
2	B	541	SER
2	B	673	ASP
2	B	688	ASP
3	C	267	LEU
3	C	367	ASN
3	C	369	VAL
4	D	89	LEU
4	D	109	ILE
4	D	258	LEU
4	D	321	SER
5	E	50	HIS
5	E	62	TYR
5	E	247	CYS
6	F	51	MET
6	F	258	HIS
6	F	270	VAL
7	G	8	VAL
9	I	209	HIS
9	I	686	SER
9	I	710	PHE
9	I	767	MET
11	K	126	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	A	187	HIS

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Mol	Chain	Res	Type
1	A	266	GLN
1	A	299	ASN
1	A	388	GLN
1	A	433	GLN
1	A	444	HIS
1	A	497	GLN
1	A	537	ASN
1	A	539	ASN
1	A	545	GLN
1	A	591	GLN
1	A	625	GLN
1	A	665	GLN
1	A	774	HIS
2	B	135	HIS
2	B	210	HIS
2	B	260	GLN
2	B	351	GLN
2	B	434	HIS
2	B	560	ASN
2	B	562	GLN
2	B	662	GLN
2	B	733	GLN
3	C	236	ASN
3	C	264	ASN
3	C	393	GLN
3	C	501	GLN
3	C	534	ASN
4	D	20	GLN
4	D	97	HIS
4	D	117	ASN
4	D	177	GLN
4	D	260	ASN
4	D	312	ASN
4	D	390	GLN
5	E	60	HIS
5	E	79	ASN
5	E	220	HIS
5	E	317	HIS
5	E	324	HIS
6	F	48	HIS
6	F	52	ASN
6	F	63	HIS

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Mol	Chain	Res	Type
6	F	205	GLN
9	I	202	HIS
9	I	206	HIS
9	I	222	ASN
9	I	538	GLN
9	I	685	HIS
9	I	728	ASN
9	I	758	ASN
9	I	778	ASN
9	I	780	HIS
9	I	800	HIS
9	I	829	GLN
9	I	907	ASN
10	J	312	GLN
10	J	315	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 7 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	$\#\|Z\| > 2$
14	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
14	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
14	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.

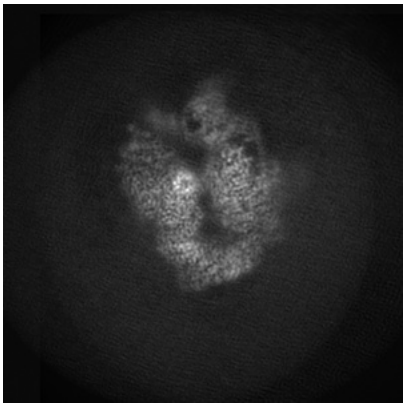
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-56551. These allow visual inspection of the internal detail of the map and identification of artifacts.

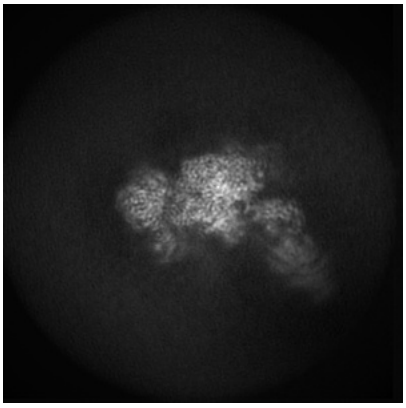
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

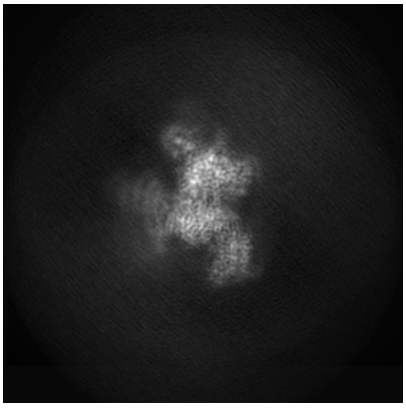
6.1.1 Primary map



X



Y

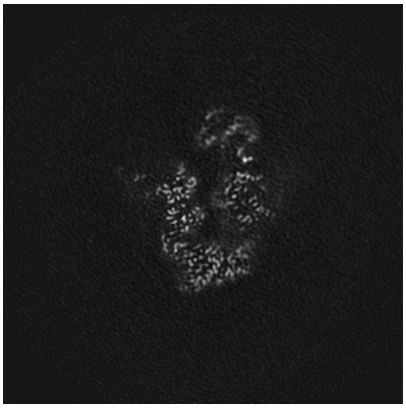


Z

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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 140

Y Index: 140

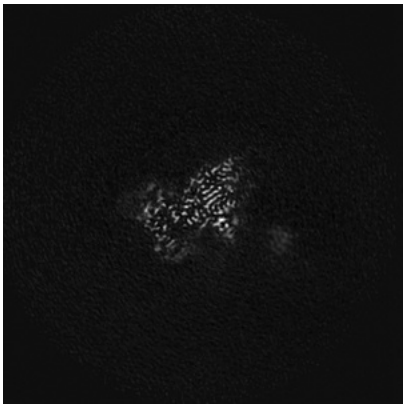
Z Index: 140

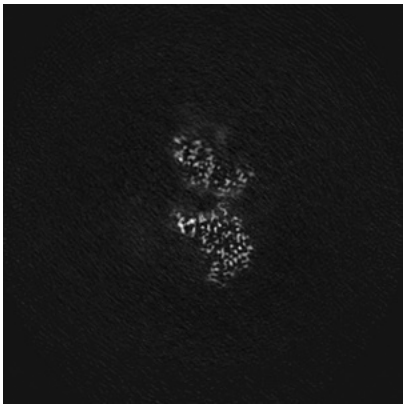
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 134

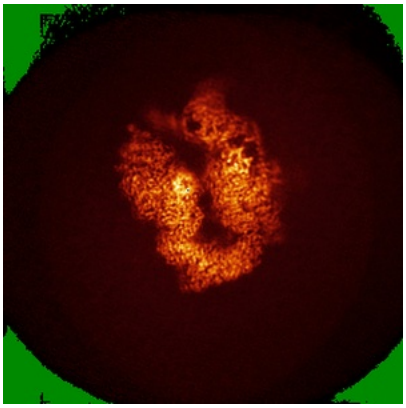

Y Index: 122

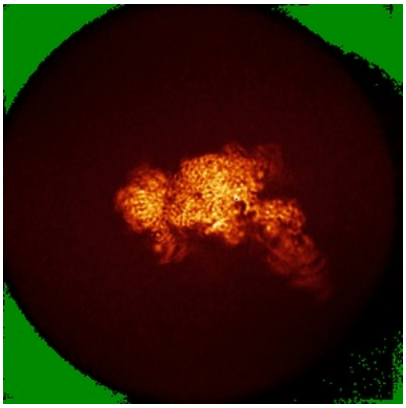

Z Index: 148

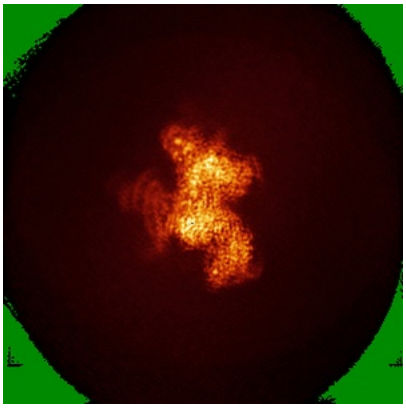
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X


Y


Z

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 0.106. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

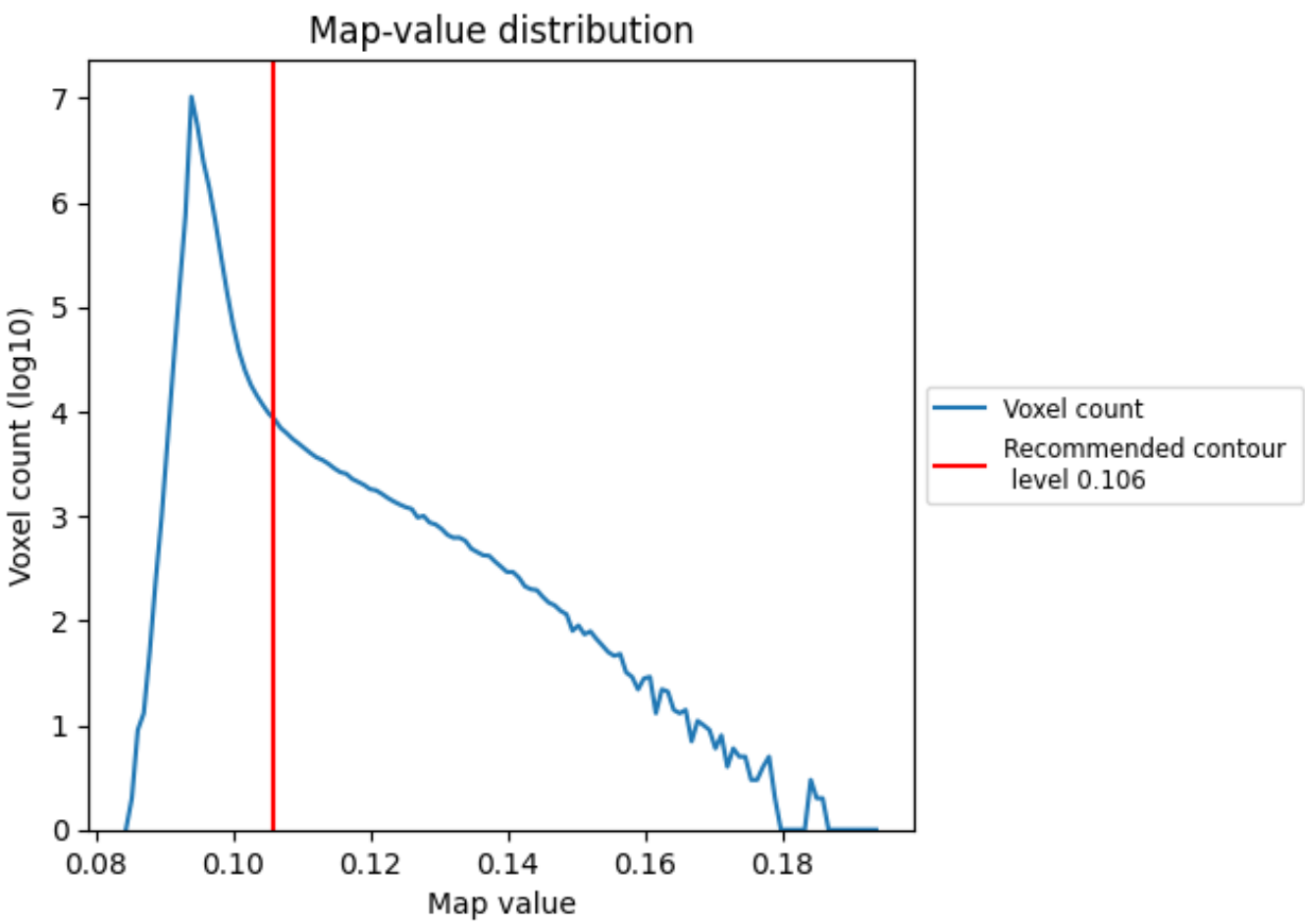
6.6 Mask visualisation (i)

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

7 Map analysis (i)

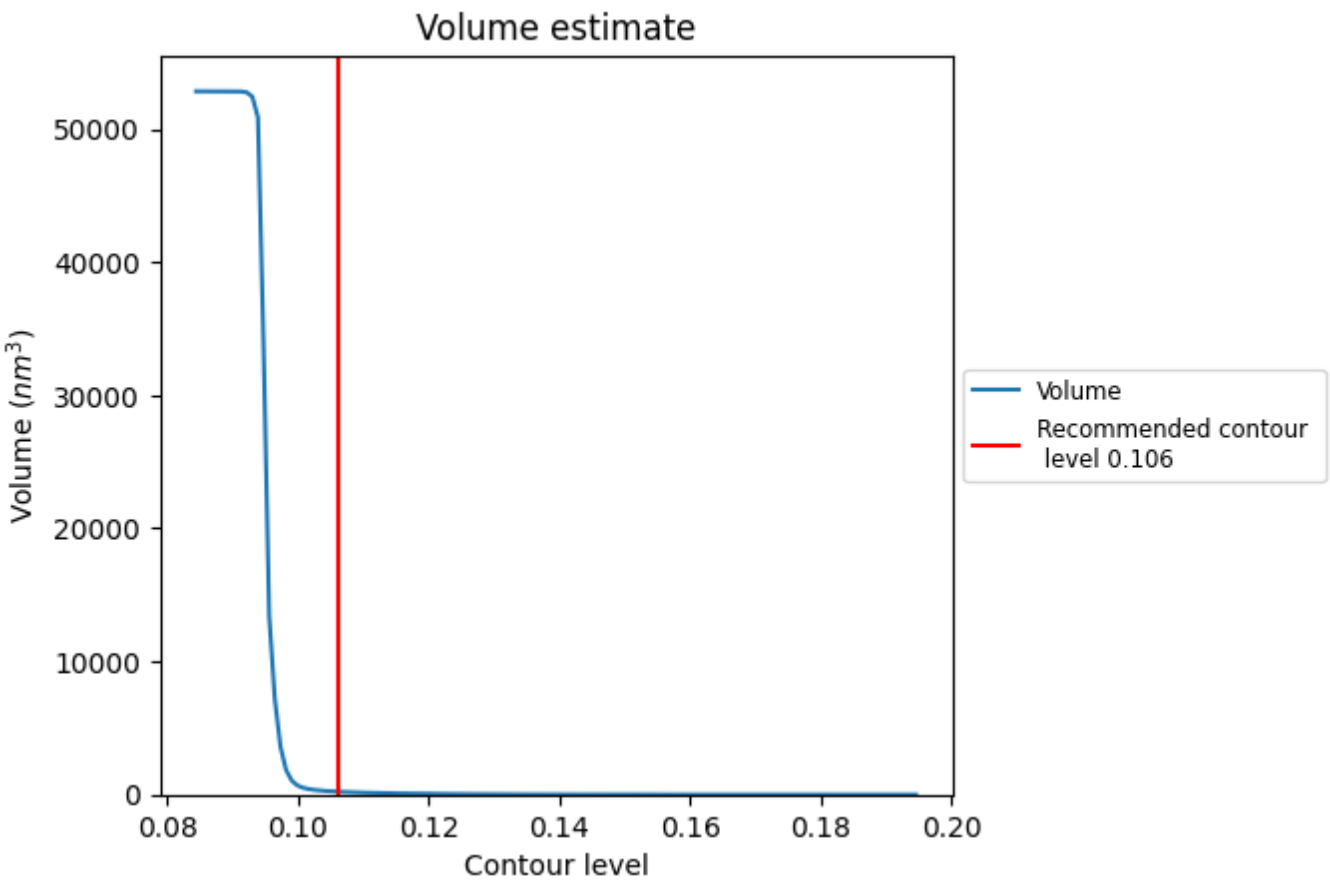
This section contains the results of statistical analysis of the map.

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.

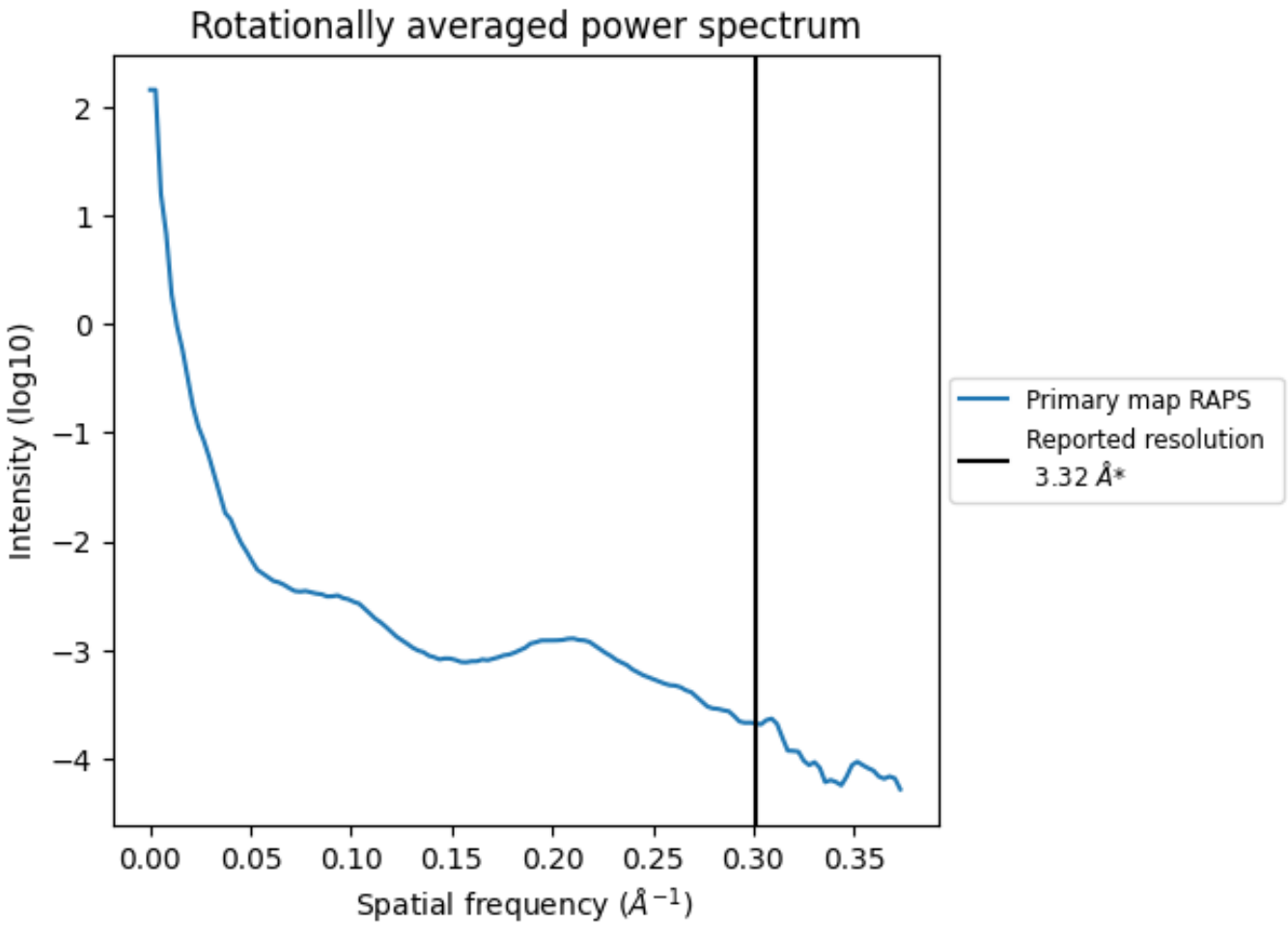
7.2 Volume estimate (i)



The volume at the recommended contour level is 217 nm^3; this corresponds to an approximate mass of 196 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 0.301 Å^{-1}

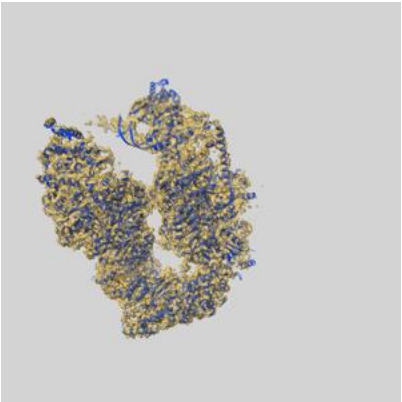
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

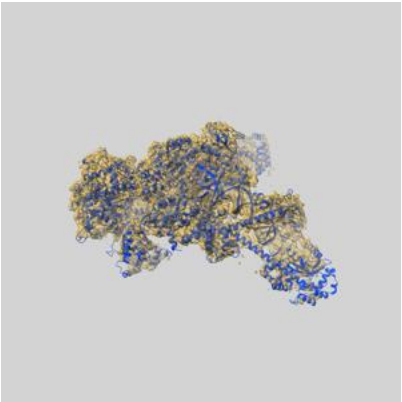
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-56551 and PDB model 28JS. Per-residue inclusion information can be found in section 3 on page 9.

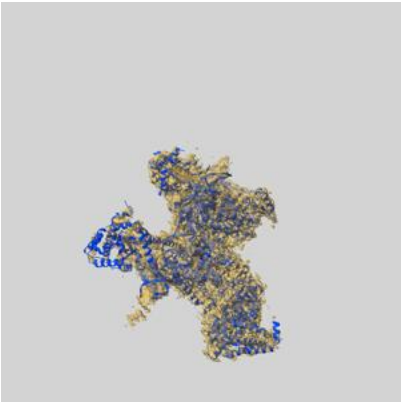
9.1 Map-model overlay (i)



X



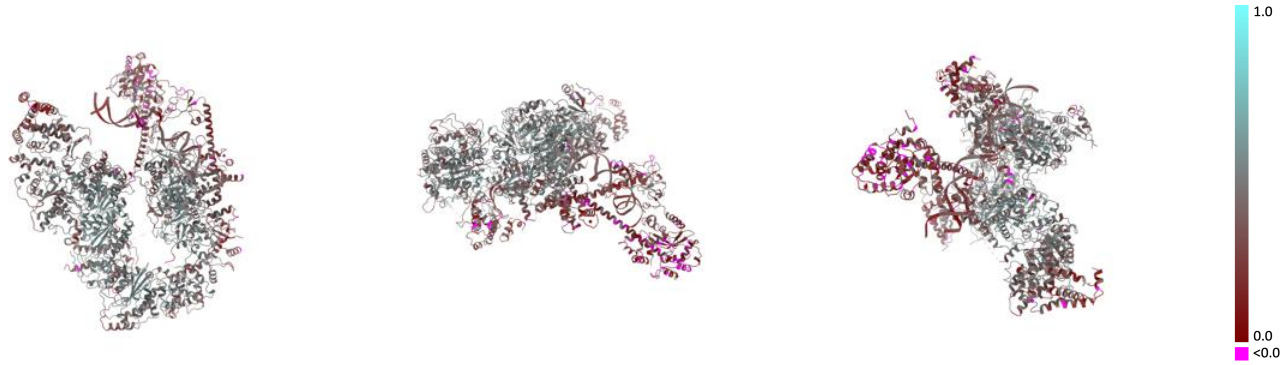
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.106 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.

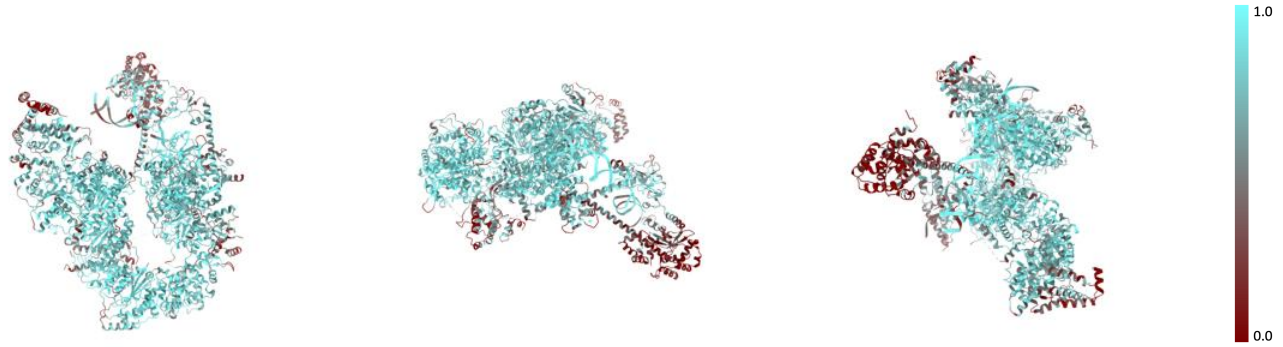
9.2 Q-score mapped to coordinate model (i)



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.

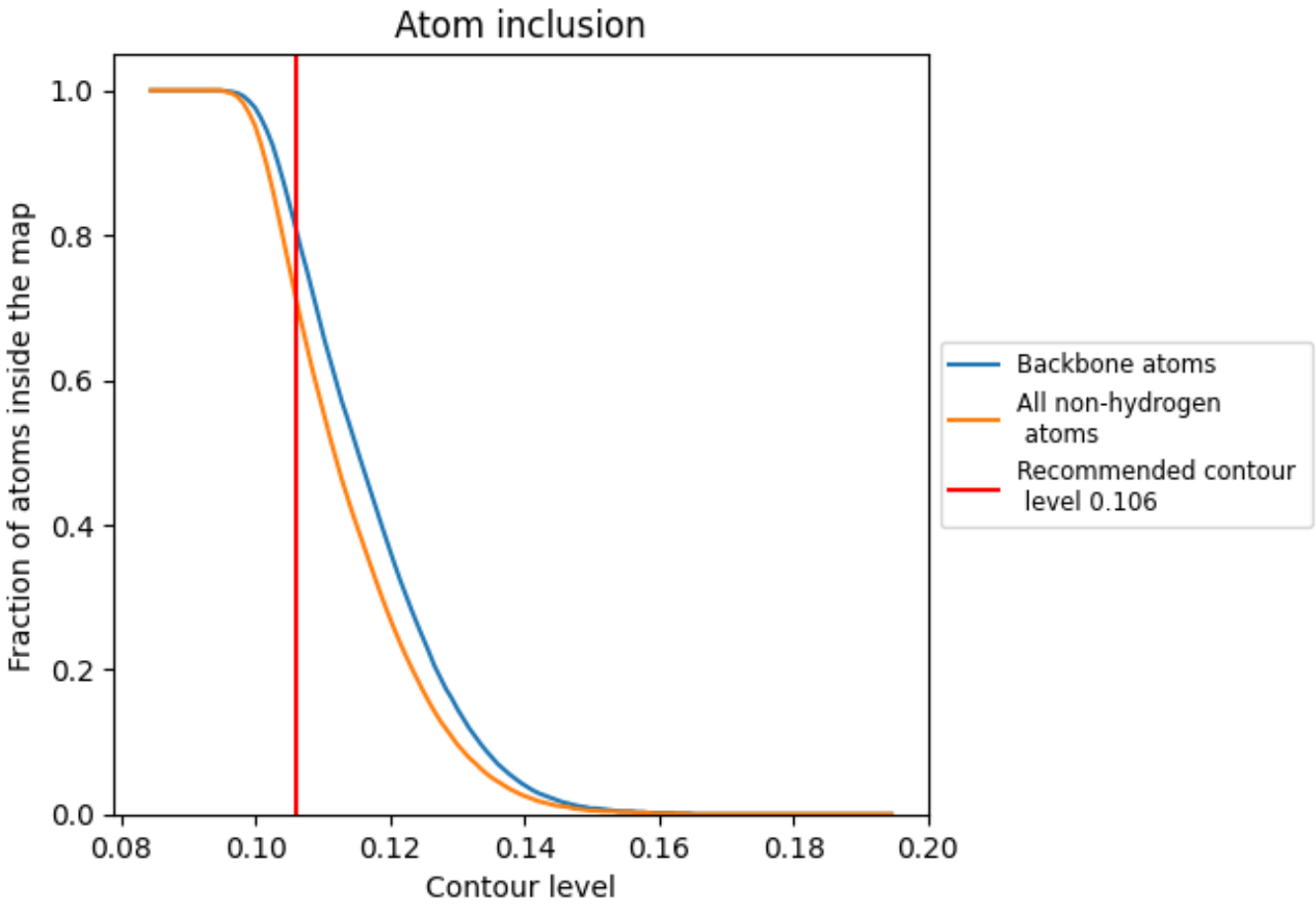
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.106).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.106) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7110	0.3980
A	0.8160	0.4580
B	0.7860	0.4450
C	0.6340	0.3670
D	0.7440	0.4260
E	0.8410	0.4970
F	0.8790	0.5000
G	0.6440	0.3490
H	0.3090	0.2410
I	0.4720	0.2600
J	0.1970	0.1710
K	0.4840	0.2030
L	0.8000	0.3150
M	0.8260	0.3100