Full wwPDB EM Validation Report (i)

Sep 19, 2026 – 01:06 PM EDT

PDB ID	:	9Q2I / pdb_00009q2i
EMDB ID	:	EMD-72166
Title	:	Rad55-Rad57-SHU homologous recombination complex
Authors	:	Yatskevich, S.; Koo, C.W.; Ciferri, C.
Deposited on	:	2025-08-15
Resolution	:	3.00 Å(reported)

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

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

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

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

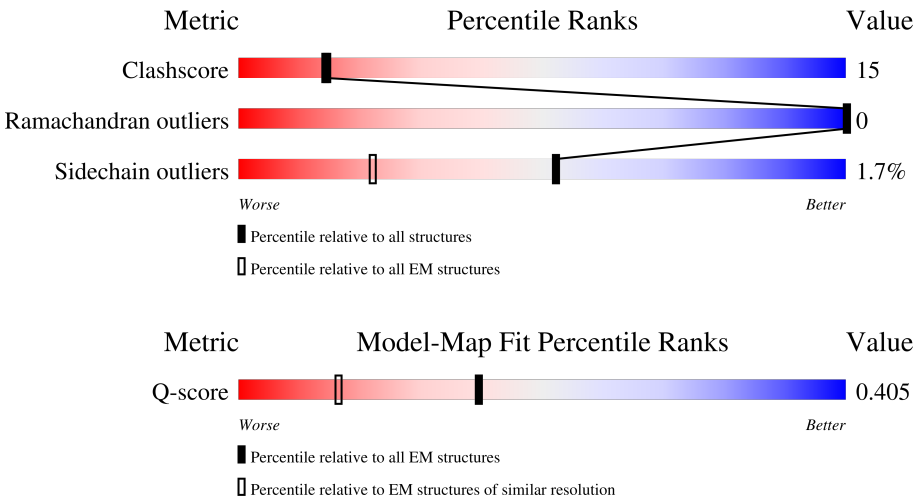
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.00 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	14081 (2.50 - 3.50)

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	631	34% 9% 57%
2	B	460	69% 19% 12%
3	C	213	62% 26% 12%
4	D	281	59% 21% • 18%

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Mol	Chain	Length	Quality of chain
5	E	150	39% 57%
6	F	262	16% 39% 39% 22%
7	G	418	5% 57% 18% 23%
7	I	418	59% 14% 27%
8	H	12	42% 58%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 16874 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 Methylated-DNA--protein-cysteine methyltransferase,DNA repair protein RAD55.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	272	2189	1410	373	395	11	0	0

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-224	MET	-	expression tag	UNP E5BBQ0
A	-223	SER	-	expression tag	UNP E5BBQ0
A	-222	ALA	-	expression tag	UNP E5BBQ0
A	-221	TRP	-	expression tag	UNP E5BBQ0
A	-220	SER	-	expression tag	UNP E5BBQ0
A	-219	HIS	-	expression tag	UNP E5BBQ0
A	-218	PRO	-	expression tag	UNP E5BBQ0
A	-217	GLN	-	expression tag	UNP E5BBQ0
A	-216	PHE	-	expression tag	UNP E5BBQ0
A	-215	GLU	-	expression tag	UNP E5BBQ0
A	-214	LYS	-	expression tag	UNP E5BBQ0
A	-213	GLY	-	expression tag	UNP E5BBQ0
A	-212	GLY	-	expression tag	UNP E5BBQ0
A	-211	GLY	-	expression tag	UNP E5BBQ0
A	-210	SER	-	expression tag	UNP E5BBQ0
A	-209	GLY	-	expression tag	UNP E5BBQ0
A	-208	GLY	-	expression tag	UNP E5BBQ0
A	-207	GLY	-	expression tag	UNP E5BBQ0
A	-206	SER	-	expression tag	UNP E5BBQ0
A	-205	GLY	-	expression tag	UNP E5BBQ0
A	-204	GLY	-	expression tag	UNP E5BBQ0
A	-203	SER	-	expression tag	UNP E5BBQ0
A	-202	ALA	-	expression tag	UNP E5BBQ0
A	-201	TRP	-	expression tag	UNP E5BBQ0
A	-200	SER	-	expression tag	UNP E5BBQ0
A	-199	HIS	-	expression tag	UNP E5BBQ0
A	-198	PRO	-	expression tag	UNP E5BBQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-197	GLN	-	expression tag	UNP E5BBQ0
A	-196	PHE	-	expression tag	UNP E5BBQ0
A	-195	GLU	-	expression tag	UNP E5BBQ0
A	-194	LYS	-	expression tag	UNP E5BBQ0
A	-193	GLY	-	expression tag	UNP E5BBQ0
A	-192	SER	-	expression tag	UNP E5BBQ0
A	-191	MET	-	expression tag	UNP E5BBQ0
A	-162	ARG	GLU	conflict	UNP E5BBQ0
A	-13	PRO	-	linker	UNP E5BBQ0
A	-12	GLY	-	linker	UNP E5BBQ0
A	-11	LEU	-	linker	UNP E5BBQ0
A	-10	GLY	-	linker	UNP E5BBQ0
A	-9	GLY	-	linker	UNP E5BBQ0
A	-8	SER	-	linker	UNP E5BBQ0
A	-7	GLU	-	linker	UNP E5BBQ0
A	-6	ASN	-	linker	UNP E5BBQ0
A	-5	LEU	-	linker	UNP E5BBQ0
A	-4	TYR	-	linker	UNP E5BBQ0
A	-3	PHE	-	linker	UNP E5BBQ0
A	-2	GLN	-	linker	UNP E5BBQ0
A	-1	GLY	-	linker	UNP E5BBQ0
A	0	SER	-	linker	UNP E5BBQ0

- Molecule 2 is a protein called DNA repair protein RAD57.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	406	3242	2054	551	624	13	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	161	GLN	GLU	engineered mutation	UNP P25301

- Molecule 3 is a protein called Chromosome segregation in meiosis protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	188	1552	1004	252	290	6	0	0

- Molecule 4 is a protein called Platinum sensitivity protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	231	1902	1230	316	347	9	0	0

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-38	MET	-	initiating methionine	UNP Q12318
D	-37	SER	-	expression tag	UNP Q12318
D	-36	ALA	-	expression tag	UNP Q12318
D	-35	TRP	-	expression tag	UNP Q12318
D	-34	SER	-	expression tag	UNP Q12318
D	-33	HIS	-	expression tag	UNP Q12318
D	-32	PRO	-	expression tag	UNP Q12318
D	-31	GLN	-	expression tag	UNP Q12318
D	-30	PHE	-	expression tag	UNP Q12318
D	-29	GLU	-	expression tag	UNP Q12318
D	-28	LYS	-	expression tag	UNP Q12318
D	-27	GLY	-	expression tag	UNP Q12318
D	-26	GLY	-	expression tag	UNP Q12318
D	-25	GLY	-	expression tag	UNP Q12318
D	-24	SER	-	expression tag	UNP Q12318
D	-23	GLY	-	expression tag	UNP Q12318
D	-22	GLY	-	expression tag	UNP Q12318
D	-21	GLY	-	expression tag	UNP Q12318
D	-20	SER	-	expression tag	UNP Q12318
D	-19	GLY	-	expression tag	UNP Q12318
D	-18	GLY	-	expression tag	UNP Q12318
D	-17	SER	-	expression tag	UNP Q12318
D	-16	ALA	-	expression tag	UNP Q12318
D	-15	TRP	-	expression tag	UNP Q12318
D	-14	SER	-	expression tag	UNP Q12318
D	-13	HIS	-	expression tag	UNP Q12318
D	-12	PRO	-	expression tag	UNP Q12318
D	-11	GLN	-	expression tag	UNP Q12318
D	-10	PHE	-	expression tag	UNP Q12318
D	-9	GLU	-	expression tag	UNP Q12318
D	-8	LYS	-	expression tag	UNP Q12318
D	-7	SER	-	expression tag	UNP Q12318
D	-6	GLY	-	expression tag	UNP Q12318
D	-5	GLU	-	expression tag	UNP Q12318
D	-4	ASN	-	expression tag	UNP Q12318
D	-3	LEU	-	expression tag	UNP Q12318
D	-2	TYR	-	expression tag	UNP Q12318

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	PHE	-	expression tag	UNP Q12318
D	0	GLN	-	expression tag	UNP Q12318

- Molecule 5 is a protein called Suppressor of HU sensitivity involved in recombination protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	147	1184	760	207	213	4	0	0

- Molecule 6 is a protein called Suppressor of hydroxyurea sensitivity protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	205	1703	1112	263	321	7	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-38	MET	-	initiating methionine	UNP C7GVQ9
F	-37	SER	-	expression tag	UNP C7GVQ9
F	-36	ALA	-	expression tag	UNP C7GVQ9
F	-35	TRP	-	expression tag	UNP C7GVQ9
F	-34	SER	-	expression tag	UNP C7GVQ9
F	-33	HIS	-	expression tag	UNP C7GVQ9
F	-32	PRO	-	expression tag	UNP C7GVQ9
F	-31	GLN	-	expression tag	UNP C7GVQ9
F	-30	PHE	-	expression tag	UNP C7GVQ9
F	-29	GLU	-	expression tag	UNP C7GVQ9
F	-28	LYS	-	expression tag	UNP C7GVQ9
F	-27	GLY	-	expression tag	UNP C7GVQ9
F	-26	GLY	-	expression tag	UNP C7GVQ9
F	-25	GLY	-	expression tag	UNP C7GVQ9
F	-24	SER	-	expression tag	UNP C7GVQ9
F	-23	GLY	-	expression tag	UNP C7GVQ9
F	-22	GLY	-	expression tag	UNP C7GVQ9
F	-21	GLY	-	expression tag	UNP C7GVQ9
F	-20	SER	-	expression tag	UNP C7GVQ9
F	-19	GLY	-	expression tag	UNP C7GVQ9
F	-18	GLY	-	expression tag	UNP C7GVQ9
F	-17	SER	-	expression tag	UNP C7GVQ9
F	-16	ALA	-	expression tag	UNP C7GVQ9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-15	TRP	-	expression tag	UNP C7GVQ9
F	-14	SER	-	expression tag	UNP C7GVQ9
F	-13	HIS	-	expression tag	UNP C7GVQ9
F	-12	PRO	-	expression tag	UNP C7GVQ9
F	-11	GLN	-	expression tag	UNP C7GVQ9
F	-10	PHE	-	expression tag	UNP C7GVQ9
F	-9	GLU	-	expression tag	UNP C7GVQ9
F	-8	LYS	-	expression tag	UNP C7GVQ9
F	-7	SER	-	expression tag	UNP C7GVQ9
F	-6	GLY	-	expression tag	UNP C7GVQ9
F	-5	GLU	-	expression tag	UNP C7GVQ9
F	-4	ASN	-	expression tag	UNP C7GVQ9
F	-3	LEU	-	expression tag	UNP C7GVQ9
F	-2	TYR	-	expression tag	UNP C7GVQ9
F	-1	PHE	-	expression tag	UNP C7GVQ9
F	0	GLN	-	expression tag	UNP C7GVQ9
F	1	GLY	-	expression tag	UNP C7GVQ9

- Molecule 7 is a protein called DNA repair protein RAD51.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	321	2442	1529	431	464	18	0	0
			Total	C	N	O	S		
7	I	307	2326	1461	412	436	17	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-17	MET	-	initiating methionine	UNP P25454
G	-16	HIS	-	expression tag	UNP P25454
G	-15	HIS	-	expression tag	UNP P25454
G	-14	HIS	-	expression tag	UNP P25454
G	-13	HIS	-	expression tag	UNP P25454
G	-12	HIS	-	expression tag	UNP P25454
G	-11	HIS	-	expression tag	UNP P25454
G	-10	HIS	-	expression tag	UNP P25454
G	-9	HIS	-	expression tag	UNP P25454
G	-8	GLY	-	expression tag	UNP P25454
G	-7	GLU	-	expression tag	UNP P25454
G	-6	ASN	-	expression tag	UNP P25454
G	-5	LEU	-	expression tag	UNP P25454

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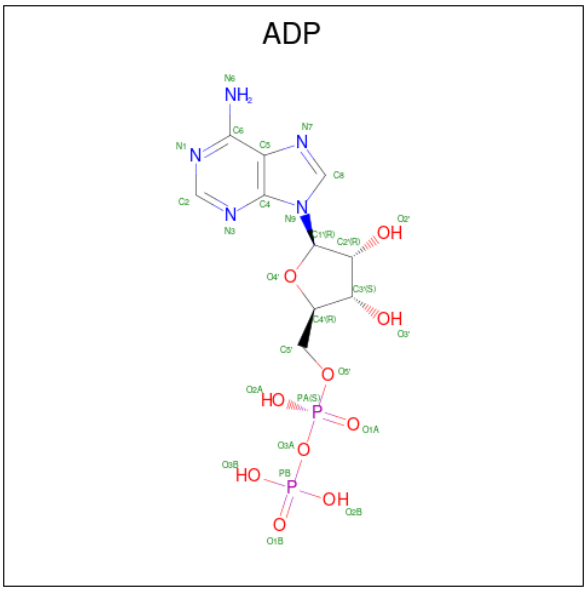
Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	TYR	-	expression tag	UNP P25454
G	-3	PHE	-	expression tag	UNP P25454
G	-2	GLN	-	expression tag	UNP P25454
G	-1	GLY	-	expression tag	UNP P25454
G	0	SER	-	expression tag	UNP P25454
I	-17	MET	-	initiating methionine	UNP P25454
I	-16	HIS	-	expression tag	UNP P25454
I	-15	HIS	-	expression tag	UNP P25454
I	-14	HIS	-	expression tag	UNP P25454
I	-13	HIS	-	expression tag	UNP P25454
I	-12	HIS	-	expression tag	UNP P25454
I	-11	HIS	-	expression tag	UNP P25454
I	-10	HIS	-	expression tag	UNP P25454
I	-9	HIS	-	expression tag	UNP P25454
I	-8	GLY	-	expression tag	UNP P25454
I	-7	GLU	-	expression tag	UNP P25454
I	-6	ASN	-	expression tag	UNP P25454
I	-5	LEU	-	expression tag	UNP P25454
I	-4	TYR	-	expression tag	UNP P25454
I	-3	PHE	-	expression tag	UNP P25454
I	-2	GLN	-	expression tag	UNP P25454
I	-1	GLY	-	expression tag	UNP P25454
I	0	SER	-	expression tag	UNP P25454

- Molecule 8 is a DNA chain called ssDNA (12-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	H	12	240	120	24	84	12	0	0

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

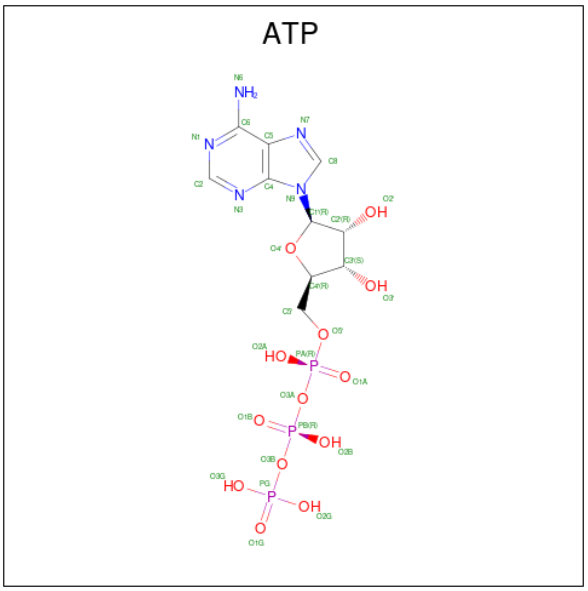


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
9	A	1	27	10	5	10	2	0

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
10	A	1	1	1	0
10	B	1	1	1	0
10	G	1	1	1	0
10	I	1	1	1	0

- Molecule 11 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
11	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
11	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

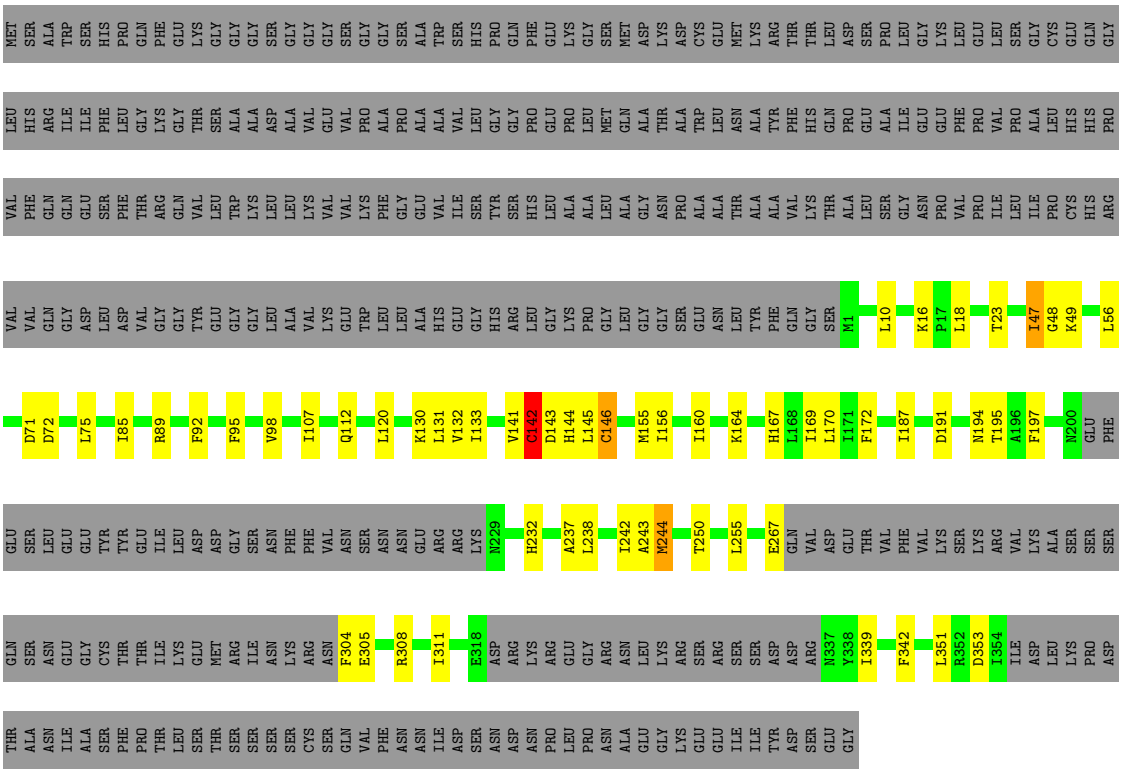
Mol	Chain	Residues	Atoms		AltConf
12	F	1	Total	Zn	0
			1	1	

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.

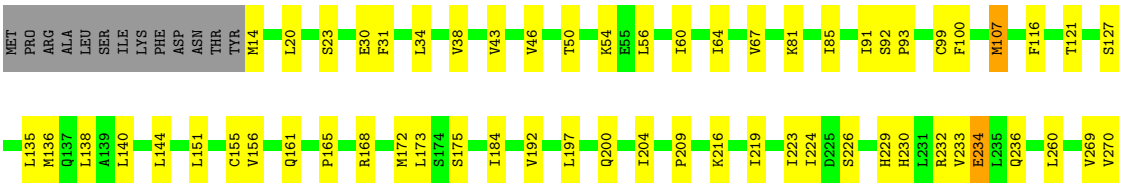
• Molecule 1: Methylated-DNA--protein-cysteine methyltransferase,DNA repair protein RAD55

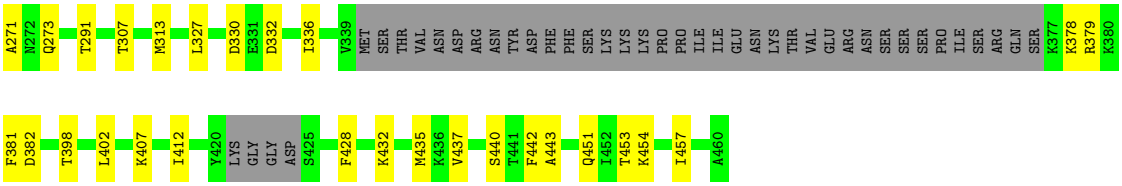
Chain A: 34% 9% 57%



• Molecule 2: DNA repair protein RAD57

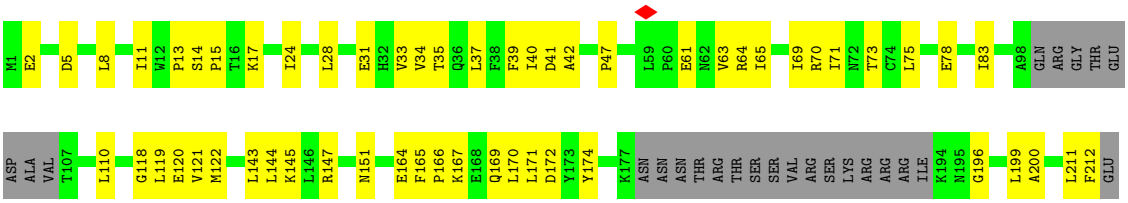
Chain B: 69% 19% 12%





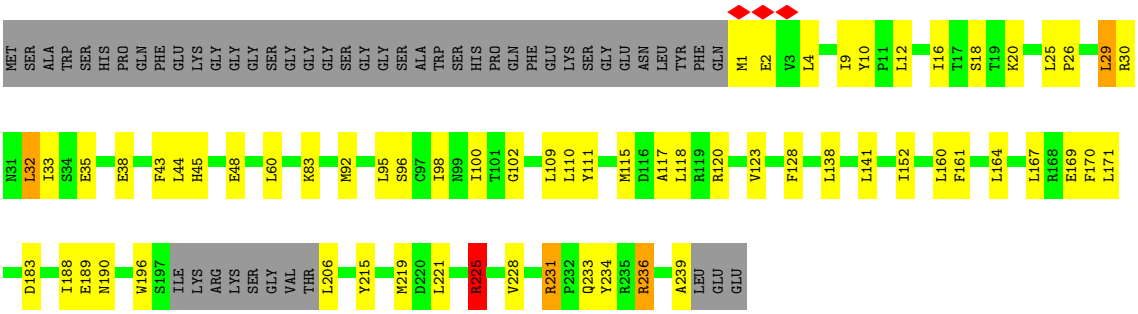
• Molecule 3: Chromosome segregation in meiosis protein 2

Chain C:



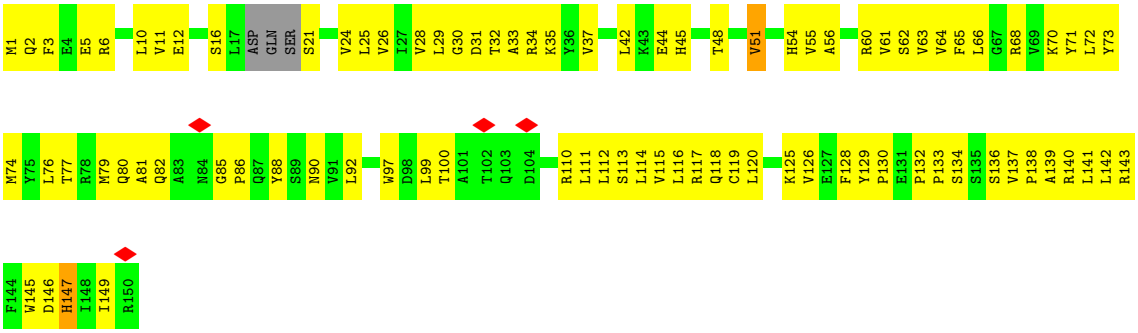
• Molecule 4: Platinum sensitivity protein 3

Chain D:



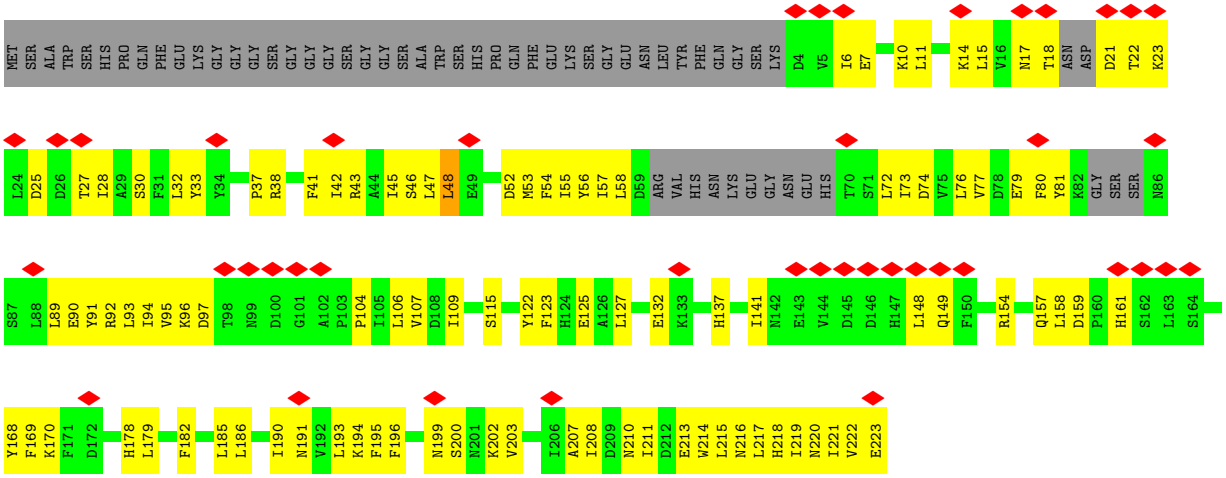
• Molecule 5: Suppressor of HU sensitivity involved in recombination protein 1

Chain E:



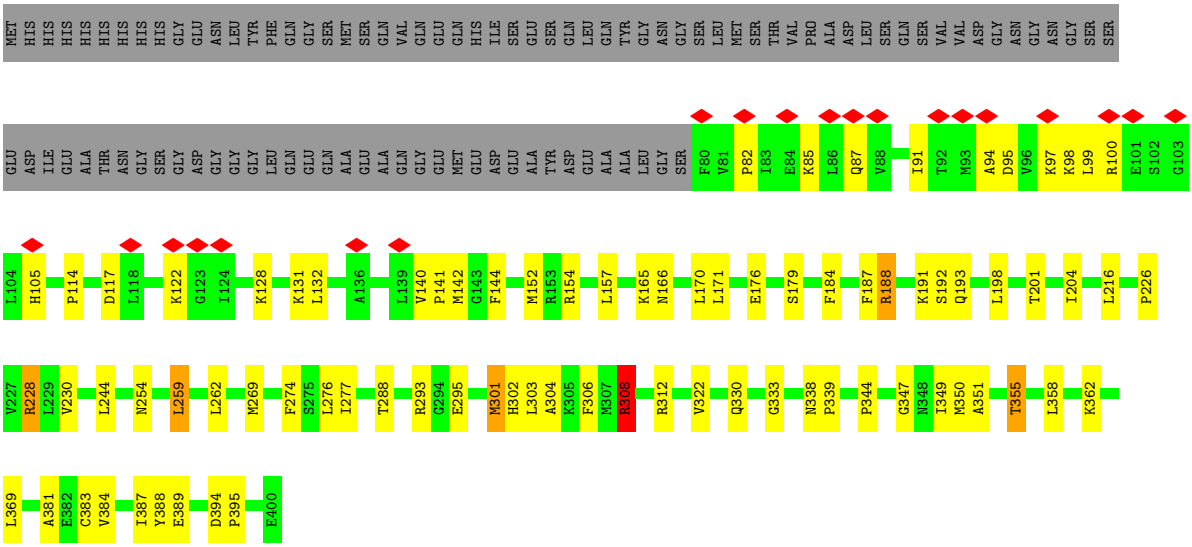
• Molecule 6: Suppressor of hydroxyurea sensitivity protein 2

Chain F:



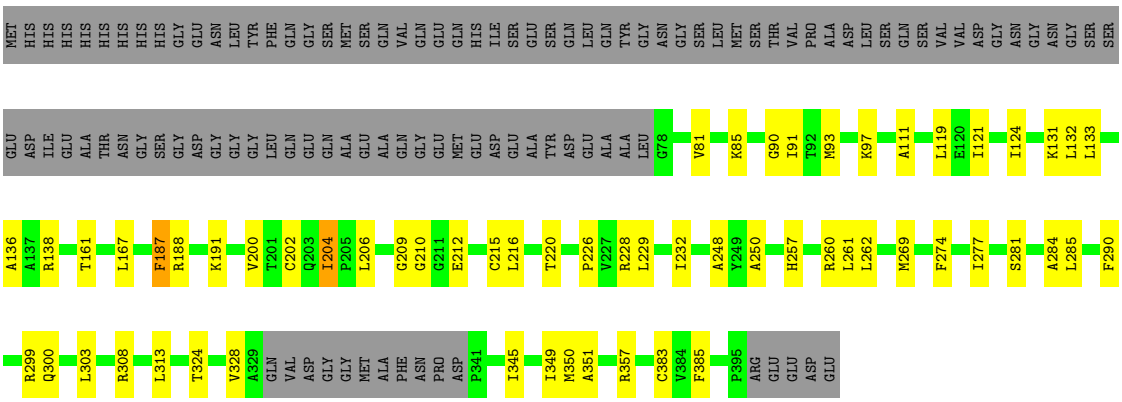
- Molecule 7: DNA repair protein RAD51

Chain G:



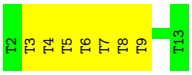
- Molecule 7: DNA repair protein RAD51

Chain I:



• Molecule 8: ssDNA (12-mer)

Chain H: 42% 58%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	155157	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 ($e^-/Å^2$)	56	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.414	Depositor
Minimum map value	-0.167	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	362.5, 362.5, 362.5	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.90625, 0.90625, 0.90625	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, MG, ADP, ATP

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	0.70	0/2227	0.75	5/2997 (0.2%)
2	B	0.67	0/3299	0.61	0/4459
3	C	0.57	0/1581	0.66	0/2136
4	D	0.56	0/1939	0.68	0/2618
5	E	0.43	0/1210	0.74	0/1645
6	F	0.29	0/1741	0.64	1/2357 (0.0%)
7	G	0.56	0/2479	0.62	1/3342 (0.0%)
7	I	0.41	0/2360	0.55	0/3180
8	H	0.66	0/263	0.75	0/404
All	All	0.56	0/17099	0.65	7/23138 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
4	D	0	1
7	G	0	2
7	I	0	1
All	All	0	6

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	146	CYS	CA-CB-SG	10.76	139.15	114.40
1	A	142	CYS	CA-CB-SG	7.57	131.82	114.40
1	A	142	CYS	N-CA-CB	6.85	120.27	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	146	CYS	CB-CA-C	6.75	123.55	110.46
6	F	48	LEU	CA-CB-CG	5.32	134.91	116.30
7	G	308	ARG	CB-CG-CD	-5.16	99.43	111.30
1	A	146	CYS	N-CA-CB	-5.16	101.99	110.14

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	CYS	Mainchain
1	A	308	ARG	Sidechain
4	D	225	ARG	Sidechain
7	G	228	ARG	Sidechain
7	G	308	ARG	Sidechain
7	I	357	ARG	Sidechain

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	2189	0	2229	49	0
2	B	3242	0	3241	74	0
3	C	1552	0	1586	45	0
4	D	1902	0	1938	64	0
5	E	1184	0	1202	110	0
6	F	1703	0	1658	98	0
7	G	2442	0	2458	69	0
7	I	2326	0	2364	41	0
8	H	240	0	145	9	0
9	A	27	0	12	1	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	G	1	0	0	0	0
10	I	1	0	0	0	0
11	B	31	0	12	0	0
11	G	31	0	12	4	0
12	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16874	0	16857	516	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 15.

All (516) 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:56:TYR:HB2	6:F:92:ARG:HB2	1.53	0.89
7:G:87:GLN:HA	7:G:91:ILE:HB	1.54	0.89
6:F:57:ILE:HD11	6:F:89:LEU:HB2	1.54	0.88
6:F:79:GLU:HG2	6:F:89:LEU:HD11	1.54	0.88
4:D:45:HIS:HB2	4:D:219:MET:HE2	1.57	0.87
3:C:120:GLU:HA	3:C:199:LEU:HD23	1.61	0.83
5:E:133:PRO:HG2	5:E:136:SER:HB3	1.63	0.80
5:E:60:ARG:HH11	5:E:60:ARG:HA	1.47	0.80
3:C:119:LEU:HA	3:C:122:MET:HE3	1.65	0.78
7:G:154:ARG:HA	7:G:157:LEU:HD23	1.66	0.78
6:F:107:VAL:HG13	6:F:179:LEU:HD23	1.66	0.77
2:B:233:VAL:HG22	7:G:308:ARG:NH1	2.00	0.76
7:I:93:MET:HE3	7:I:93:MET:H	1.52	0.74
6:F:42:ILE:HD12	6:F:45:ILE:HD11	1.67	0.74
7:I:216:LEU:HD12	7:I:277:ILE:HG12	1.66	0.74
7:G:152:MET:HA	7:G:152:MET:HE2	1.69	0.74
2:B:56:LEU:HD12	2:B:67:VAL:HG13	1.67	0.74
7:G:192:SER:OG	11:G:501:ATP:O2B	2.05	0.74
6:F:92:ARG:HH11	6:F:218:HIS:HE1	1.35	0.73
6:F:214:TRP:HD1	6:F:215:LEU:HD23	1.55	0.72
6:F:54:PHE:HB3	6:F:56:TYR:HE1	1.55	0.71
6:F:73:ILE:HD12	6:F:76:LEU:HD11	1.72	0.70
7:G:142:MET:HE2	7:G:142:MET:HA	1.73	0.70
5:E:82:GLN:HE22	5:E:85:GLY:HA3	1.56	0.70
6:F:22:THR:HA	6:F:195:PHE:HE1	1.55	0.70
5:E:29:LEU:HD23	5:E:66:LEU:HB2	1.72	0.70
2:B:56:LEU:HD12	2:B:67:VAL:CG1	2.21	0.69
5:E:60:ARG:HA	5:E:60:ARG:NH1	2.08	0.69
2:B:38:VAL:HG22	2:B:60:ILE:HD13	1.74	0.68
2:B:307:THR:HG23	2:B:381:PHE:HB2	1.75	0.68
2:B:230:HIS:HA	7:G:308:ARG:CZ	2.24	0.68
6:F:54:PHE:HB3	6:F:56:TYR:CE1	2.29	0.68
7:G:154:ARG:HH22	7:G:176:GLU:HB3	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:ILE:HD13	2:B:428:PHE:HB3	1.75	0.67
6:F:57:ILE:HD12	6:F:90:GLU:O	1.94	0.67
5:E:74:MET:HA	5:E:74:MET:HE2	1.76	0.67
6:F:11:LEU:HG	6:F:32:LEU:HD21	1.77	0.66
6:F:53:MET:HE1	6:F:95:VAL:HG23	1.78	0.66
5:E:16:SER:HG	5:E:21:SER:N	1.94	0.65
2:B:56:LEU:CD1	2:B:60:ILE:HD12	2.26	0.65
5:E:119:CYS:HG	5:E:128:PHE:HZ	1.42	0.65
7:I:250:ALA:HB1	7:I:261:LEU:HD13	1.78	0.65
4:D:231:ARG:HB3	4:D:233:GLN:HG3	1.79	0.65
1:A:169:ILE:HD11	1:A:250:THR:HG22	1.77	0.65
6:F:221:ILE:HD12	6:F:222:VAL:N	2.11	0.65
2:B:330:ASP:HB3	2:B:379:ARG:HG3	1.78	0.64
2:B:140:LEU:HD22	2:B:173:LEU:HD13	1.78	0.64
5:E:25:LEU:HB2	5:E:88:TYR:CD2	2.32	0.64
7:G:193:GLN:OE1	7:G:387:ILE:HG21	1.98	0.64
2:B:336:ILE:HG12	2:B:412:ILE:HD13	1.79	0.64
2:B:136:MET:HE1	2:B:165:PRO:HB2	1.80	0.63
1:A:170:LEU:HD13	2:B:50:THR:HG21	1.80	0.63
4:D:138:LEU:HA	4:D:141:LEU:HD23	1.78	0.63
6:F:193:LEU:HD12	6:F:194:LYS:N	2.14	0.63
6:F:218:HIS:O	6:F:221:ILE:HG13	1.98	0.63
4:D:206:LEU:HD12	4:D:239:ALA:HB1	1.81	0.63
5:E:82:GLN:NE2	5:E:85:GLY:HA3	2.14	0.62
2:B:56:LEU:HD13	2:B:60:ILE:HD12	1.82	0.62
2:B:233:VAL:HG13	7:G:308:ARG:NH2	2.16	0.61
1:A:144:HIS:HE1	1:A:167:HIS:ND1	1.99	0.61
6:F:216:ASN:O	6:F:219:ILE:HG22	2.00	0.61
6:F:195:PHE:HD2	6:F:196:PHE:CD1	2.19	0.61
7:G:166:ASN:HB3	7:G:383:CYS:SG	2.41	0.61
1:A:18:LEU:HD11	1:A:131:LEU:HD11	1.83	0.60
5:E:29:LEU:HA	5:E:66:LEU:O	2.01	0.60
6:F:79:GLU:CG	6:F:89:LEU:HD11	2.30	0.60
6:F:190:ILE:O	6:F:193:LEU:HG	2.01	0.60
7:G:269:MET:SD	7:G:277:ILE:HD11	2.41	0.60
3:C:13:PRO:HA	3:C:165:PHE:O	2.01	0.60
3:C:118:GLY:O	3:C:121:VAL:HG12	2.01	0.60
5:E:100:THR:HG21	5:E:112:LEU:HD21	1.84	0.60
6:F:45:ILE:HD12	6:F:46:SER:N	2.17	0.60
7:G:262:LEU:HD22	7:G:306:PHE:CE1	2.37	0.60
5:E:113:SER:HA	5:E:141:LEU:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:93:LEU:HD22	6:F:93:LEU:H	1.66	0.60
6:F:154:ARG:HA	6:F:157:GLN:CD	2.27	0.59
7:G:226:PRO:HB3	7:G:244:LEU:HD11	1.84	0.59
8:H:5:DT:H3'	8:H:6:DT:H3'	1.83	0.59
6:F:45:ILE:O	6:F:48:LEU:HD12	2.02	0.59
2:B:14:MET:HE2	2:B:38:VAL:HG11	1.84	0.59
4:D:225:ARG:HG2	4:D:225:ARG:HH11	1.67	0.59
8:H:8:DT:H5"	8:H:8:DT:H6	1.66	0.59
7:I:269:MET:HG2	7:I:274:PHE:HB2	1.84	0.59
5:E:73:TYR:O	5:E:77:THR:HG22	2.02	0.59
6:F:94:ILE:HD13	6:F:106:LEU:HA	1.83	0.59
7:G:193:GLN:HB2	7:G:228:ARG:HH21	1.68	0.59
5:E:24:VAL:HG12	5:E:61:VAL:HG22	1.83	0.59
8:H:3:DT:H2"	8:H:4:DT:OP1	2.02	0.59
4:D:4:LEU:HB3	5:E:71:TYR:CD2	2.37	0.58
5:E:3:PHE:HB2	5:E:129:TYR:HB3	1.84	0.58
3:C:11:ILE:HB	3:C:211:LEU:HD12	1.85	0.58
8:H:6:DT:H4'	8:H:7:DT:O5'	2.02	0.58
3:C:119:LEU:HA	3:C:122:MET:CE	2.33	0.58
7:G:171:LEU:HD21	7:G:358:LEU:HD11	1.85	0.58
6:F:122:TYR:O	6:F:125:GLU:HG2	2.03	0.58
7:I:229:LEU:HA	7:I:232:ILE:HD12	1.84	0.58
5:E:1:MET:SD	5:E:5:GLU:HB2	2.44	0.57
6:F:30:SER:HA	6:F:33:TYR:CD2	2.39	0.57
6:F:137:HIS:CG	6:F:141:ILE:HG13	2.39	0.57
4:D:170:PHE:HD1	4:D:171:LEU:HG	1.70	0.57
2:B:38:VAL:HG13	2:B:43:VAL:HB	1.86	0.57
6:F:6:ILE:HD13	6:F:11:LEU:HD21	1.86	0.57
4:D:92:MET:HE3	4:D:92:MET:O	2.04	0.57
6:F:77:VAL:HG12	6:F:193:LEU:CD1	2.35	0.57
5:E:25:LEU:HD11	5:E:64:VAL:HG23	1.87	0.56
6:F:18:THR:HA	6:F:21:ASP:HA	1.85	0.56
7:I:200:VAL:HG21	7:I:232:ILE:HB	1.87	0.56
2:B:233:VAL:H	7:G:308:ARG:HH22	1.52	0.56
4:D:35:GLU:O	4:D:38:GLU:HG3	2.05	0.56
5:E:51:VAL:HA	5:E:54:HIS:HD2	1.69	0.56
6:F:89:LEU:O	6:F:89:LEU:HD12	2.05	0.56
7:I:111:ALA:HB2	7:I:136:ALA:HB1	1.87	0.56
3:C:17:LYS:HG3	3:C:47:PRO:HB3	1.87	0.56
5:E:119:CYS:SG	5:E:128:PHE:HZ	2.27	0.56
6:F:72:LEU:HD11	6:F:207:ALA:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:41:PHE:O	6:F:45:ILE:HG13	2.06	0.56
4:D:115:MET:HE3	5:E:55:VAL:HG11	1.87	0.56
5:E:24:VAL:HG13	5:E:61:VAL:HG13	1.88	0.56
3:C:143:LEU:O	3:C:147:ARG:HG3	2.06	0.55
4:D:1:MET:CG	4:D:2:GLU:H	2.19	0.55
6:F:58:LEU:HD11	6:F:211:ILE:HD13	1.88	0.55
2:B:402:LEU:HD21	2:B:435:MET:HE2	1.87	0.55
4:D:118:LEU:O	4:D:123:VAL:HB	2.06	0.55
7:G:193:GLN:HB2	7:G:228:ARG:NH2	2.21	0.55
5:E:28:VAL:HG12	5:E:28:VAL:O	2.05	0.55
5:E:134:SER:HA	5:E:143:ARG:HH22	1.70	0.55
6:F:28:ILE:O	6:F:32:LEU:HG	2.06	0.55
7:I:216:LEU:HD23	7:I:248:ALA:HB3	1.89	0.55
5:E:76:LEU:HD11	5:E:119:CYS:HA	1.88	0.55
6:F:11:LEU:O	6:F:15:LEU:HG	2.07	0.55
6:F:73:ILE:O	6:F:77:VAL:HG13	2.06	0.55
6:F:95:VAL:HG11	6:F:178:HIS:HB3	1.88	0.55
7:I:257:HIS:HE1	7:I:261:LEU:HD21	1.70	0.55
5:E:79:MET:O	5:E:82:GLN:HG3	2.07	0.54
7:G:389:GLU:HA	11:G:501:ATP:HN62	1.71	0.54
2:B:54:LYS:HA	2:B:64:ILE:CD1	2.38	0.54
5:E:26:VAL:HB	5:E:63:VAL:HG22	1.89	0.54
6:F:154:ARG:HA	6:F:157:GLN:NE2	2.23	0.54
7:I:303:LEU:HD21	7:I:350:MET:HG2	1.89	0.54
1:A:351:LEU:HD12	1:A:351:LEU:H	1.73	0.54
4:D:44:LEU:HD12	4:D:45:HIS:N	2.23	0.54
6:F:22:THR:HA	6:F:195:PHE:CE1	2.38	0.54
3:C:42:ALA:HB1	3:C:75:LEU:HD23	1.90	0.54
1:A:167:HIS:CD2	2:B:46:VAL:HG11	2.43	0.54
2:B:107:MET:HE1	2:B:457:ILE:HG21	1.90	0.54
2:B:135:LEU:HD11	2:B:271:ALA:HB2	1.90	0.54
3:C:14:SER:HB3	3:C:166:PRO:HA	1.90	0.54
5:E:29:LEU:HD11	5:E:72:LEU:HG	1.90	0.54
3:C:40:ILE:HD11	3:C:83:ILE:HG21	1.89	0.53
1:A:267:GLU:OE2	1:A:304:PHE:HB3	2.09	0.53
1:A:95:PHE:HE1	1:A:98:VAL:HG11	1.73	0.53
7:G:128:LYS:HA	7:G:131:LYS:HE2	1.89	0.53
3:C:15:PRO:HD2	3:C:164:GLU:CD	2.33	0.53
3:C:171:LEU:HD12	3:C:172:ASP:N	2.23	0.53
4:D:225:ARG:HG2	4:D:234:TYR:CE1	2.44	0.53
6:F:185:LEU:HD13	6:F:203:VAL:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:225:ARG:O	4:D:225:ARG:HD3	2.09	0.53
2:B:230:HIS:HA	7:G:308:ARG:NH1	2.24	0.53
3:C:65:ILE:O	3:C:69:ILE:HG13	2.08	0.53
1:A:339:ILE:HD12	1:A:339:ILE:O	2.09	0.52
5:E:70:LYS:HZ1	6:F:223:GLU:HA	1.74	0.52
6:F:157:GLN:HG2	6:F:168:TYR:HE1	1.72	0.52
2:B:407:LYS:HE3	2:B:432:LYS:HD3	1.91	0.52
7:G:95:ASP:O	7:G:99:LEU:HG	2.09	0.52
5:E:81:ALA:HB2	6:F:214:TRP:CD1	2.45	0.52
1:A:142:CYS:C	1:A:144:HIS:N	2.66	0.52
3:C:39:PHE:HB3	3:C:71:ILE:HD13	1.90	0.52
4:D:4:LEU:HD22	5:E:71:TYR:HA	1.91	0.52
4:D:26:PRO:HD3	4:D:60:LEU:HD13	1.92	0.52
5:E:68:ARG:HB2	5:E:71:TYR:CD1	2.45	0.52
5:E:140:ARG:HA	5:E:143:ARG:NE	2.25	0.52
6:F:14:LYS:HG3	6:F:28:ILE:HG13	1.92	0.52
6:F:195:PHE:HD2	6:F:196:PHE:HD1	1.56	0.52
5:E:68:ARG:HB2	5:E:71:TYR:HD1	1.73	0.52
1:A:197:PHE:HB3	1:A:244:MET:CE	2.40	0.51
5:E:29:LEU:CD2	5:E:72:LEU:HB2	2.41	0.51
5:E:73:TYR:CD2	5:E:114:LEU:HD11	2.45	0.51
2:B:156:VAL:HG23	2:B:219:ILE:HG21	1.91	0.51
2:B:161:GLN:HG2	2:B:229:HIS:CE1	2.45	0.51
3:C:41:ASP:O	3:C:73:THR:HA	2.10	0.51
5:E:140:ARG:NH2	6:F:132:GLU:HG2	2.25	0.51
4:D:33:ILE:HG23	4:D:38:GLU:HG2	1.92	0.51
5:E:66:LEU:HD22	5:E:71:TYR:HB3	1.91	0.51
7:G:389:GLU:HA	11:G:501:ATP:N6	2.25	0.51
5:E:44:GLU:HG2	5:E:45:HIS:CE1	2.45	0.51
2:B:229:HIS:O	7:G:308:ARG:NH2	2.43	0.51
3:C:14:SER:OG	3:C:167:LYS:HG3	2.10	0.51
4:D:128:PHE:O	5:E:51:VAL:HG12	2.10	0.51
4:D:152:ILE:HG12	4:D:196:TRP:CE3	2.45	0.51
5:E:31:ASP:HB2	5:E:34:ARG:HH22	1.75	0.51
5:E:73:TYR:CZ	6:F:221:ILE:HD11	2.45	0.51
5:E:28:VAL:HB	5:E:65:PHE:HA	1.92	0.51
5:E:111:LEU:O	5:E:115:VAL:HG12	2.11	0.51
7:G:82:PRO:HG2	7:G:85:LYS:HE3	1.93	0.51
7:G:154:ARG:NH1	7:G:157:LEU:HG	2.25	0.51
1:A:342:PHE:HE1	1:A:351:LEU:HD23	1.76	0.51
5:E:70:LYS:NZ	6:F:223:GLU:HA	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:208:ILE:HG23	6:F:213:GLU:HB2	1.93	0.51
7:G:140:VAL:HB	7:G:141:PRO:HD2	1.92	0.51
4:D:25:LEU:HD12	4:D:33:ILE:HG21	1.92	0.51
5:E:31:ASP:OD1	5:E:32:THR:N	2.43	0.50
6:F:52:ASP:HB3	6:F:96:LYS:O	2.11	0.50
1:A:146:CYS:HA	1:A:242:ILE:HD13	1.92	0.50
3:C:63:VAL:H	3:C:64:ARG:NH2	2.10	0.50
4:D:1:MET:HG2	4:D:2:GLU:H	1.76	0.50
6:F:137:HIS:CE1	6:F:141:ILE:HG13	2.46	0.50
7:I:257:HIS:CE1	7:I:261:LEU:HD21	2.46	0.50
1:A:191:ASP:O	1:A:237:ALA:HB2	2.12	0.50
3:C:34:VAL:HG12	3:C:34:VAL:O	2.11	0.50
6:F:37:PRO:HA	6:F:38:ARG:NH2	2.26	0.50
6:F:45:ILE:HD12	6:F:46:SER:H	1.76	0.50
6:F:77:VAL:HG12	6:F:193:LEU:HD13	1.94	0.50
6:F:92:ARG:O	6:F:94:ILE:HG12	2.11	0.50
1:A:342:PHE:CE1	1:A:351:LEU:HD23	2.47	0.49
3:C:13:PRO:HG2	3:C:212:PHE:HE1	1.77	0.49
4:D:109:LEU:HD13	4:D:117:ALA:HB2	1.94	0.49
4:D:111:TYR:HE1	4:D:170:PHE:HB2	1.77	0.49
4:D:120:ARG:HB2	4:D:120:ARG:CZ	2.42	0.49
7:G:170:LEU:HD22	7:G:383:CYS:HB2	1.94	0.49
4:D:9:ILE:HG23	5:E:62:SER:OG	2.12	0.49
1:A:232:HIS:CG	8:H:5:DT:H1'	2.48	0.49
4:D:33:ILE:HG23	4:D:38:GLU:OE2	2.13	0.49
7:I:167:LEU:HD13	7:I:385:PHE:HB3	1.95	0.49
2:B:135:LEU:HD22	2:B:223:ILE:HD12	1.95	0.49
3:C:11:ILE:HB	3:C:211:LEU:CD1	2.43	0.49
4:D:12:LEU:O	4:D:16:ILE:HG12	2.13	0.49
7:I:281:SER:OG	7:I:284:ALA:HB2	2.13	0.49
1:A:47:ILE:HD11	1:A:49:LYS:HE3	1.95	0.49
2:B:224:ILE:HB	2:B:270:VAL:HG12	1.94	0.49
4:D:32:LEU:HD21	4:D:236:ARG:HB3	1.95	0.49
5:E:37:VAL:HA	5:E:42:LEU:HD23	1.93	0.49
7:G:216:LEU:HB2	7:G:274:PHE:CD2	2.48	0.49
7:I:290:PHE:CD1	7:I:299:ARG:HG3	2.48	0.49
3:C:61:GLU:C	3:C:64:ARG:HH21	2.20	0.49
5:E:145:TRP:HA	5:E:145:TRP:CE3	2.48	0.49
7:I:161:THR:HG22	7:I:209:GLY:O	2.13	0.49
6:F:220:ASN:OD1	6:F:220:ASN:O	2.31	0.48
7:I:81:VAL:HG13	7:I:85:LYS:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:ARG:HB2	7:G:308:ARG:HH21	1.78	0.48
6:F:43:ARG:O	6:F:47:LEU:HG	2.12	0.48
2:B:161:GLN:NE2	2:B:273:GLN:HE22	2.11	0.48
5:E:30:GLY:HA2	5:E:99:LEU:HD21	1.95	0.48
5:E:79:MET:HE1	5:E:80:GLN:HG2	1.93	0.48
5:E:117:ARG:HG3	5:E:117:ARG:HH11	1.79	0.48
6:F:96:LYS:HE3	6:F:97:ASP:H	1.77	0.48
6:F:158:LEU:HD23	6:F:169:PHE:HB2	1.96	0.48
7:I:206:LEU:HG	7:I:212:GLU:CD	2.38	0.48
7:I:328:VAL:HG23	7:I:345:ILE:HD11	1.95	0.48
5:E:76:LEU:O	5:E:79:MET:HE3	2.14	0.48
5:E:116:LEU:HA	5:E:119:CYS:SG	2.53	0.48
1:A:112:GLN:NE2	2:B:81:LYS:HE2	2.28	0.48
7:G:187:PHE:CG	7:I:351:ALA:HB1	2.49	0.48
4:D:18:SER:HB2	5:E:54:HIS:CE1	2.49	0.48
4:D:100:ILE:HA	4:D:141:LEU:HD12	1.96	0.48
6:F:210:ASN:OD1	6:F:213:GLU:HG3	2.12	0.48
5:E:33:ALA:O	5:E:37:VAL:HG12	2.14	0.48
1:A:75:LEU:HD23	1:A:132:VAL:HG13	1.95	0.48
1:A:197:PHE:HB3	1:A:244:MET:HE1	1.96	0.48
2:B:56:LEU:HD11	2:B:60:ILE:HD12	1.96	0.48
5:E:76:LEU:HD22	5:E:118:GLN:HB3	1.94	0.48
3:C:34:VAL:HB	3:C:110:LEU:HA	1.94	0.48
4:D:83:LYS:O	4:D:83:LYS:HD3	2.14	0.48
6:F:195:PHE:HA	6:F:199:ASN:HB2	1.96	0.48
5:E:114:LEU:C	5:E:114:LEU:HD13	2.38	0.47
7:G:100:ARG:HG3	7:G:105:HIS:CD2	2.48	0.47
1:A:107:ILE:HD13	2:B:85:ILE:HD13	1.96	0.47
5:E:137:VAL:HG23	5:E:138:PRO:HD3	1.96	0.47
6:F:53:MET:HB2	6:F:203:VAL:HG22	1.96	0.47
8:H:7:DT:H2"	8:H:8:DT:H5"	1.95	0.47
2:B:127:SER:HB3	7:G:351:ALA:HB1	1.97	0.47
1:A:311:ILE:HG12	1:A:339:ILE:HG22	1.96	0.47
7:G:304:ALA:HB2	7:G:349:ILE:HG21	1.95	0.47
3:C:24:ILE:O	3:C:28:LEU:HB2	2.15	0.47
3:C:63:VAL:H	3:C:64:ARG:HH21	1.62	0.47
8:H:8:DT:H6	8:H:8:DT:C5'	2.27	0.47
1:A:72:ASP:HB2	1:A:130:LYS:NZ	2.30	0.47
1:A:194:ASN:ND2	1:A:232:HIS:HD2	2.12	0.47
1:A:71:ASP:OD1	1:A:71:ASP:N	2.48	0.47
2:B:30:GLU:OE1	2:B:31:PHE:CE1	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:303:LEU:HD21	7:G:350:MET:HG2	1.97	0.47
2:B:34:LEU:O	2:B:38:VAL:HG23	2.15	0.46
2:B:161:GLN:HE21	2:B:273:GLN:HE22	1.63	0.46
5:E:68:ARG:HD3	5:E:71:TYR:HE1	1.80	0.46
5:E:141:LEU:C	5:E:141:LEU:HD13	2.41	0.46
7:I:257:HIS:HA	7:I:260:ARG:HE	1.79	0.46
6:F:214:TRP:O	6:F:218:HIS:HD2	1.98	0.46
7:G:114:PRO:HG2	7:G:117:ASP:CG	2.41	0.46
7:G:276:LEU:HD11	7:G:322:VAL:HG23	1.98	0.46
2:B:20:LEU:HB3	2:B:23:SER:HB2	1.98	0.46
2:B:209:PRO:HB3	2:B:260:LEU:HD21	1.96	0.46
2:B:233:VAL:H	7:G:308:ARG:NH2	2.12	0.46
4:D:228:VAL:HG21	4:D:233:GLN:OE1	2.16	0.46
6:F:73:ILE:O	6:F:76:LEU:HD12	2.15	0.46
1:A:85:ILE:HG12	2:B:91:ILE:HD11	1.97	0.46
2:B:121:THR:HG23	2:B:398:THR:HB	1.97	0.46
4:D:152:ILE:HD12	4:D:152:ILE:O	2.16	0.46
5:E:2:GLN:HB3	5:E:5:GLU:OE1	2.15	0.46
5:E:139:ALA:HB1	5:E:143:ARG:HH21	1.80	0.46
5:E:147:HIS:HD1	5:E:147:HIS:C	2.24	0.46
2:B:92:SER:HB2	2:B:93:PRO:HD2	1.97	0.46
5:E:11:VAL:HG23	5:E:12:GLU:HG2	1.98	0.46
5:E:24:VAL:HA	5:E:90:ASN:O	2.16	0.46
7:G:191:LYS:HE3	7:G:191:LYS:HB2	1.75	0.46
1:A:142:CYS:O	1:A:146:CYS:HB3	2.16	0.46
7:G:188:ARG:CZ	7:G:362:LYS:HG3	2.45	0.46
1:A:194:ASN:HD22	1:A:232:HIS:HD2	1.64	0.46
5:E:66:LEU:HD13	5:E:72:LEU:HA	1.97	0.46
1:A:89:ARG:HH11	1:A:95:PHE:HE2	1.64	0.46
2:B:175:SER:HB2	2:B:454:LYS:HE3	1.97	0.46
5:E:28:VAL:HG11	5:E:65:PHE:CD1	2.51	0.45
1:A:172:PHE:CZ	1:A:255:LEU:HD21	2.51	0.45
3:C:78:GLU:OE1	3:C:78:GLU:N	2.49	0.45
4:D:10:TYR:HD2	5:E:65:PHE:CE2	2.34	0.45
7:I:269:MET:HG2	7:I:274:PHE:CG	2.52	0.45
2:B:192:VAL:HG23	7:G:144:PHE:HA	1.98	0.45
3:C:196:GLY:HA2	4:D:190:ASN:OD1	2.17	0.45
1:A:142:CYS:HB3	1:A:146:CYS:HB3	1.60	0.45
4:D:92:MET:HE3	4:D:92:MET:C	2.41	0.45
7:G:184:PHE:CG	7:G:344:PRO:HB3	2.51	0.45
1:A:155:MET:HG3	1:A:156:ILE:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:20:LYS:HE3	4:D:169:GLU:HA	1.99	0.45
6:F:122:TYR:HA	6:F:125:GLU:HG2	1.99	0.45
1:A:145:LEU:HD21	1:A:164:LYS:HG3	1.98	0.45
3:C:199:LEU:HD12	3:C:199:LEU:O	2.16	0.45
6:F:47:LEU:HB3	6:F:53:MET:CE	2.46	0.45
6:F:190:ILE:HD12	6:F:191:ASN:N	2.31	0.45
2:B:155:CYS:SG	2:B:156:VAL:N	2.90	0.45
4:D:183:ASP:C	4:D:183:ASP:OD1	2.60	0.45
7:I:220:THR:HB	7:I:285:LEU:CD2	2.47	0.45
4:D:110:LEU:HG	4:D:167:LEU:HD11	1.99	0.44
7:G:99:LEU:HD11	7:G:132:LEU:HD11	1.99	0.44
7:G:82:PRO:HD2	7:G:85:LYS:HE3	1.99	0.44
7:I:262:LEU:HD21	7:I:313:LEU:HD11	1.99	0.44
3:C:33:VAL:HG23	3:C:35:THR:HG23	1.99	0.44
4:D:4:LEU:HB3	5:E:71:TYR:HD2	1.79	0.44
6:F:159:ASP:C	6:F:161:HIS:H	2.25	0.44
6:F:195:PHE:CD2	6:F:196:PHE:HD1	2.36	0.44
2:B:327:LEU:HD21	2:B:381:PHE:HB3	2.00	0.44
3:C:167:LYS:HG2	3:C:174:TYR:OH	2.18	0.44
4:D:10:TYR:HD2	5:E:65:PHE:HE2	1.64	0.44
7:G:388:TYR:OH	7:G:395:PRO:HA	2.18	0.44
7:I:204:ILE:O	7:I:210:GLY:HA3	2.18	0.44
2:B:451:GLN:HG3	2:B:453:THR:HG23	1.99	0.44
4:D:30:ARG:HH11	4:D:30:ARG:HG2	1.82	0.44
5:E:10:LEU:HD13	5:E:24:VAL:HG11	1.99	0.44
5:E:120:LEU:CD2	5:E:146:ASP:HA	2.47	0.44
6:F:45:ILE:HA	6:F:48:LEU:HG	1.98	0.44
2:B:327:LEU:HA	2:B:327:LEU:HD23	1.76	0.44
5:E:137:VAL:HA	5:E:140:ARG:HD2	1.99	0.44
6:F:137:HIS:ND1	6:F:141:ILE:HG13	2.33	0.44
6:F:141:ILE:N	6:F:170:LYS:HG2	2.32	0.44
6:F:148:LEU:HD13	6:F:149:GLN:HG3	1.99	0.44
7:G:142:MET:HG3	7:G:144:PHE:H	1.82	0.44
1:A:131:LEU:HD13	1:A:133:ILE:HD11	2.00	0.44
7:I:285:LEU:HD13	7:I:285:LEU:HA	1.70	0.44
6:F:53:MET:HB3	6:F:203:VAL:HG13	2.00	0.44
2:B:200:GLN:O	2:B:204:ILE:HG12	2.18	0.44
1:A:195:THR:OG1	1:A:244:MET:HE1	2.18	0.43
4:D:236:ARG:HD3	4:D:236:ARG:C	2.43	0.43
5:E:29:LEU:HD21	5:E:72:LEU:HB2	2.00	0.43
6:F:17:ASN:HB2	6:F:23:LYS:NZ	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:369:LEU:HD12	7:G:384:VAL:HG22	2.00	0.43
4:D:111:TYR:HB2	4:D:167:LEU:HD22	1.99	0.43
6:F:74:ASP:O	6:F:77:VAL:HG22	2.18	0.43
7:G:165:LYS:HB2	7:G:394:ASP:OD2	2.17	0.43
3:C:31:GLU:OE1	3:C:31:GLU:N	2.49	0.43
3:C:70:ARG:H	3:C:70:ARG:HG2	1.50	0.43
3:C:120:GLU:HG3	3:C:169:GLN:HE22	1.83	0.43
4:D:48:GLU:CB	4:D:225:ARG:HD2	2.47	0.43
7:G:128:LYS:HA	7:G:131:LYS:HG2	2.00	0.43
7:I:121:ILE:HB	7:I:124:ILE:HG13	2.00	0.43
2:B:378:LYS:N	2:B:378:LYS:HD2	2.33	0.43
3:C:69:ILE:O	3:C:69:ILE:HG22	2.17	0.43
3:C:144:LEU:HD12	4:D:98:ILE:HG23	2.00	0.43
5:E:117:ARG:HB2	5:E:117:ARG:CZ	2.49	0.43
5:E:118:GLN:OE1	5:E:118:GLN:HA	2.18	0.43
6:F:48:LEU:HA	6:F:53:MET:HG2	2.01	0.43
6:F:104:PRO:HD2	6:F:220:ASN:OD1	2.19	0.43
7:G:91:ILE:HG12	7:G:131:LYS:HE3	2.00	0.43
1:A:142:CYS:O	1:A:143:ASP:C	2.60	0.43
2:B:99:CYS:HB3	2:B:116:PHE:CD1	2.53	0.43
5:E:10:LEU:HD13	5:E:24:VAL:HG21	1.99	0.43
5:E:16:SER:H	5:E:21:SER:N	2.16	0.43
7:I:187:PHE:CZ	7:I:188:ARG:HB2	2.54	0.43
4:D:96:SER:O	4:D:102:GLY:HA3	2.18	0.43
5:E:1:MET:O	5:E:129:TYR:HE2	2.02	0.43
5:E:70:LYS:HE3	5:E:70:LYS:HA	2.01	0.43
7:I:226:PRO:HA	7:I:229:LEU:HD13	2.00	0.43
6:F:95:VAL:HG11	6:F:178:HIS:CD2	2.54	0.43
6:F:104:PRO:HG2	6:F:221:ILE:HA	2.00	0.43
7:G:187:PHE:HB3	7:I:351:ALA:HB1	2.00	0.43
7:G:198:LEU:HD23	7:G:198:LEU:HA	1.86	0.43
5:E:70:LYS:O	5:E:70:LYS:HD3	2.18	0.43
5:E:120:LEU:HD23	5:E:149:ILE:HB	2.01	0.43
5:E:136:SER:HB2	5:E:138:PRO:HD2	2.01	0.43
7:G:288:THR:HB	7:I:308:ARG:HD2	2.01	0.43
6:F:208:ILE:CG2	6:F:213:GLU:HB2	2.48	0.43
7:G:94:ALA:O	7:G:97:LYS:HG3	2.19	0.43
1:A:72:ASP:HB3	1:A:130:LYS:HB2	2.00	0.43
7:G:98:LYS:HE2	7:G:122:LYS:O	2.18	0.43
1:A:95:PHE:CD1	1:A:98:VAL:HB	2.54	0.42
5:E:10:LEU:CD1	5:E:24:VAL:HG21	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:97:TRP:HE1	5:E:132:PRO:HD3	1.84	0.42
5:E:110:ARG:NH2	6:F:115:SER:HB2	2.33	0.42
7:G:201:THR:HA	7:G:204:ILE:HG23	2.00	0.42
7:I:90:GLY:HA3	7:I:131:LYS:NZ	2.34	0.42
1:A:120:LEU:HD23	1:A:120:LEU:HA	1.90	0.42
4:D:45:HIS:CD2	4:D:45:HIS:C	2.97	0.42
5:E:5:GLU:OE1	5:E:5:GLU:N	2.45	0.42
5:E:24:VAL:HG21	5:E:92:LEU:HD13	2.00	0.42
5:E:32:THR:O	5:E:35:LYS:HE3	2.19	0.42
6:F:92:ARG:HH11	6:F:218:HIS:CE1	2.26	0.42
1:A:16:LYS:HE3	1:A:16:LYS:HA	2.01	0.42
5:E:79:MET:SD	5:E:79:MET:C	3.03	0.42
7:G:198:LEU:HA	7:G:201:THR:OG1	2.20	0.42
2:B:223:ILE:CD1	2:B:269:VAL:HB	2.49	0.42
2:B:332:ASP:OD2	2:B:407:LYS:HD2	2.19	0.42
1:A:145:LEU:CD2	1:A:164:LYS:HG3	2.48	0.42
1:A:146:CYS:HA	1:A:242:ILE:CD1	2.50	0.42
6:F:104:PRO:HG2	6:F:221:ILE:HG22	2.02	0.42
7:I:202:CYS:SG	7:I:215:CYS:HB2	2.59	0.42
1:A:23:THR:HG22	1:A:353:ASP:HB3	2.01	0.42
2:B:175:SER:HB2	2:B:454:LYS:HG2	2.01	0.42
2:B:197:LEU:HD12	2:B:234:GLU:HG2	2.02	0.42
4:D:45:HIS:CB	4:D:219:MET:HE2	2.39	0.42
5:E:1:MET:HE1	5:E:6:ARG:N	2.34	0.42
9:A:501:ADP:H3'	2:B:440:SER:O	2.20	0.42
2:B:138:LEU:HA	2:B:138:LEU:HD23	1.81	0.42
5:E:86:PRO:HB2	5:E:88:TYR:CE1	2.55	0.42
6:F:7:GLU:HG2	6:F:10:LYS:H	1.84	0.42
7:G:192:SER:CB	11:G:501:ATP:O2B	2.68	0.42
7:G:216:LEU:HD22	7:G:277:ILE:HD12	2.01	0.42
1:A:47:ILE:HD12	1:A:48:GLY:H	1.84	0.42
2:B:440:SER:HB3	2:B:443:ALA:HB3	2.02	0.42
4:D:32:LEU:C	4:D:32:LEU:HD23	2.45	0.42
4:D:43:PHE:HB3	4:D:219:MET:SD	2.60	0.42
5:E:29:LEU:HD22	5:E:72:LEU:HB2	2.02	0.42
6:F:80:PHE:CD2	6:F:186:LEU:HD21	2.55	0.42
6:F:137:HIS:CD2	6:F:141:ILE:HG13	2.53	0.42
3:C:8:LEU:HD21	3:C:151:ASN:HB2	2.00	0.42
5:E:25:LEU:HD12	5:E:26:VAL:H	1.85	0.42
7:G:170:LEU:HD11	7:G:381:ALA:HB3	2.01	0.42
2:B:437:VAL:O	2:B:437:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:18:SER:HB2	5:E:54:HIS:HE1	1.84	0.41
5:E:56:ALA:HA	5:E:60:ARG:HB3	2.02	0.41
5:E:72:LEU:C	5:E:72:LEU:HD13	2.45	0.41
6:F:214:TRP:O	6:F:217:LEU:HG	2.20	0.41
7:G:179:SER:HB2	7:G:355:THR:CB	2.50	0.41
6:F:195:PHE:CD2	6:F:196:PHE:CD1	3.05	0.41
6:F:221:ILE:HD12	6:F:222:VAL:HB	2.02	0.41
7:I:191:LYS:HB2	7:I:191:LYS:HE2	1.82	0.41
3:C:170:LEU:CD2	3:C:200:ALA:HB1	2.51	0.41
5:E:10:LEU:HD23	5:E:10:LEU:HA	1.83	0.41
5:E:129:TYR:HA	5:E:130:PRO:C	2.44	0.41
7:G:347:GLY:HA3	8:H:9:DT:H5'	2.01	0.41
1:A:141:VAL:HG21	1:A:238:LEU:CD2	2.50	0.41
3:C:28:LEU:HA	3:C:35:THR:OG1	2.20	0.41
3:C:145:LYS:HG2	4:D:95:LEU:HD22	2.02	0.41
5:E:117:ARG:HH11	5:E:117:ARG:CG	2.32	0.41
7:I:133:LEU:HD23	7:I:133:LEU:HA	1.94	0.41
4:D:110:LEU:HD12	4:D:110:LEU:O	2.20	0.41
5:E:34:ARG:HB3	5:E:34:ARG:CZ	2.51	0.41
5:E:142:LEU:C	5:E:142:LEU:HD23	2.45	0.41
6:F:123:PHE:O	6:F:127:LEU:HD23	2.20	0.41
7:G:188:ARG:NE	7:G:362:LYS:HG3	2.36	0.41
7:I:132:LEU:HD23	7:I:132:LEU:HA	1.93	0.41
3:C:37:LEU:HD23	3:C:37:LEU:C	2.46	0.41
3:C:199:LEU:HD13	4:D:188:ILE:HD11	2.03	0.41
5:E:116:LEU:HD12	5:E:141:LEU:CD1	2.50	0.41
6:F:55:ILE:C	6:F:56:TYR:HD1	2.29	0.41
7:G:330:GLN:HG3	7:G:333:GLY:HA3	2.02	0.41
7:I:91:ILE:HD13	7:I:132:LEU:HD23	2.03	0.41
1:A:10:LEU:HD12	1:A:10:LEU:HA	1.84	0.41
8:H:8:DT:H5"	8:H:8:DT:C6	2.53	0.41
7:I:97:LYS:HE2	7:I:97:LYS:HB2	1.82	0.41
2:B:197:LEU:HA	2:B:197:LEU:HD23	1.92	0.41
2:B:216:LYS:H	2:B:216:LYS:HD3	1.86	0.41
7:G:259:LEU:HD12	7:G:302:HIS:CE1	2.55	0.41
1:A:160:ILE:HG13	1:A:243:ALA:HB2	2.03	0.41
2:B:307:THR:HG21	2:B:382:ASP:O	2.20	0.41
4:D:161:PHE:HB2	4:D:215:TYR:CD1	2.56	0.41
5:E:73:TYR:CD1	5:E:73:TYR:C	2.99	0.41
6:F:25:ASP:OD1	6:F:27:THR:HG22	2.20	0.41
7:G:301:MET:HB2	7:G:301:MET:HE2	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:338:ASN:OD1	7:G:339:PRO:HD2	2.20	0.41
7:I:93:MET:O	7:I:97:LYS:HD3	2.20	0.41
2:B:100:PHE:HB3	2:B:151:LEU:HG	2.03	0.41
2:B:168:ARG:NH1	2:B:172:MET:HG3	2.35	0.41
2:B:226:SER:HA	2:B:271:ALA:O	2.21	0.41
7:G:170:LEU:HD22	7:G:383:CYS:CB	2.51	0.41
7:G:293:ARG:C	7:G:295:GLU:H	2.29	0.41
4:D:12:LEU:HD22	5:E:61:VAL:HG11	2.03	0.40
4:D:33:ILE:HD13	4:D:221:LEU:HD13	2.03	0.40
4:D:48:GLU:HB2	4:D:225:ARG:HD2	2.03	0.40
7:I:228:ARG:O	7:I:232:ILE:HG13	2.21	0.40
1:A:56:LEU:HD13	1:A:187:ILE:HD13	2.02	0.40
2:B:116:PHE:CD2	2:B:442:PHE:CD2	3.10	0.40
3:C:199:LEU:HD13	4:D:188:ILE:CD1	2.51	0.40
4:D:26:PRO:HD2	4:D:29:LEU:HD23	2.02	0.40
1:A:47:ILE:HD12	1:A:48:GLY:N	2.36	0.40
2:B:38:VAL:HG22	2:B:60:ILE:CD1	2.47	0.40
2:B:144:LEU:HG	2:B:184:ILE:HD11	2.03	0.40
3:C:2:GLU:HB2	3:C:5:ASP:OD1	2.21	0.40
7:I:138:ARG:NE	7:I:138:ARG:HA	2.35	0.40
2:B:216:LYS:HD3	2:B:216:LYS:N	2.36	0.40
3:C:196:GLY:HA3	4:D:189:GLU:HA	2.03	0.40
4:D:160:LEU:O	4:D:164:LEU:HD23	2.22	0.40
6:F:200:SER:HB2	6:F:202:LYS:HG2	2.02	0.40
2:B:34:LEU:C	2:B:34:LEU:HD13	2.46	0.40
2:B:402:LEU:CD2	2:B:435:MET:HE2	2.49	0.40
3:C:11:ILE:HD13	3:C:11:ILE:HG21	1.81	0.40
5:E:37:VAL:HA	5:E:42:LEU:CD2	2.52	0.40
5:E:125:LYS:HD2	5:E:126:VAL:N	2.37	0.40
5:E:140:ARG:O	5:E:143:ARG:HG2	2.21	0.40
6:F:93:LEU:HB3	6:F:182:PHE:CE1	2.57	0.40
7:I:300:GLN:HB3	7:I:349:ILE:CD1	2.52	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	264/631 (42%)	245 (93%)	19 (7%)	0	100	100
2	B	400/460 (87%)	380 (95%)	20 (5%)	0	100	100
3	C	182/213 (85%)	170 (93%)	12 (7%)	0	100	100
4	D	227/281 (81%)	210 (92%)	17 (8%)	0	100	100
5	E	143/150 (95%)	137 (96%)	6 (4%)	0	100	100
6	F	197/262 (75%)	180 (91%)	17 (9%)	0	100	100
7	G	319/418 (76%)	303 (95%)	16 (5%)	0	100	100
7	I	303/418 (72%)	296 (98%)	7 (2%)	0	100	100
All	All	2035/2833 (72%)	1921 (94%)	114 (6%)	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	246/543 (45%)	242 (98%)	4 (2%)	55	79
2	B	364/415 (88%)	359 (99%)	5 (1%)	59	80
3	C	179/202 (89%)	179 (100%)	0	100	100
4	D	217/255 (85%)	212 (98%)	5 (2%)	44	74
5	E	132/135 (98%)	129 (98%)	3 (2%)	44	74
6	F	195/238 (82%)	192 (98%)	3 (2%)	57	80
7	G	260/336 (77%)	253 (97%)	7 (3%)	39	71
7	I	248/336 (74%)	243 (98%)	5 (2%)	48	76
All	All	1841/2460 (75%)	1809 (98%)	32 (2%)	52	78

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ILE
1	A	92	PHE
1	A	244	MET
1	A	305	GLU
2	B	107	MET
2	B	234	GLU
2	B	236	GLN
2	B	291	THR
2	B	313	MET
4	D	29	LEU
4	D	32	LEU
4	D	225	ARG
4	D	231	ARG
4	D	236	ARG
5	E	48	THR
5	E	51	VAL
5	E	147	HIS
6	F	81	TYR
6	F	91	TYR
6	F	109	ILE
7	G	188	ARG
7	G	230	VAL
7	G	254	ASN
7	G	259	LEU
7	G	301	MET
7	G	312	ARG
7	G	355	THR
7	I	119	LEU
7	I	187	PHE
7	I	204	ILE
7	I	324	THR
7	I	383	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	101	ASN
1	A	144	HIS
1	A	232	HIS
2	B	41	ASN
2	B	79	ASN
2	B	161	GLN

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Mol	Chain	Res	Type
2	B	195	ASN
2	B	230	HIS
3	C	27	ASN
3	C	97	ASN
3	C	151	ASN
4	D	62	ASN
4	D	84	GLN
5	E	54	HIS
6	F	17	ASN
7	G	203	GLN
7	G	257	HIS
7	G	302	HIS
7	G	316	GLN
7	G	348	ASN
7	I	203	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, 5 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
9	ADP	A	501	10	28,29,29	1.46	5 (17%)	43,45,45	1.79	8 (18%)
11	ATP	G	501	10	32,33,33	1.50	2 (6%)	48,52,52	0.69	1 (2%)
11	ATP	B	502	10	32,33,33	1.77	2 (6%)	48,52,52	0.62	1 (2%)

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
9	ADP	A	501	10	-	2/16/32/32	0/3/3/3
11	ATP	G	501	10	-	3/22/38/38	0/3/3/3
11	ATP	B	502	10	-	8/22/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	502	ATP	PA-O3A	-7.03	1.51	1.59
11	G	501	ATP	PB-O3B	-6.93	1.52	1.59
11	B	502	ATP	PB-O3B	-6.33	1.52	1.59
11	G	501	ATP	PA-O3A	-4.00	1.55	1.59
9	A	501	ADP	C5-C4	3.42	1.45	1.39
9	A	501	ADP	C5-N7	-3.12	1.33	1.39
9	A	501	ADP	C4-N9	-2.77	1.31	1.37
9	A	501	ADP	C8-N9	-2.11	1.34	1.37
9	A	501	ADP	C2'-C3'	-2.09	1.47	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	501	ADP	C5-C4-N3	-6.22	118.16	126.72
9	A	501	ADP	N3-C4-N9	4.51	134.84	127.17
9	A	501	ADP	C2-N3-C4	3.66	120.76	111.83
9	A	501	ADP	C4-C5-N7	-2.83	107.35	110.58
9	A	501	ADP	N3-C2-N1	-2.61	124.63	128.58
9	A	501	ADP	O3'-C3'-C2'	-2.30	104.43	111.82
11	G	501	ATP	O3G-PG-O1G	2.28	119.70	110.83
9	A	501	ADP	O5'-C5'-C4'	2.27	116.71	108.99
9	A	501	ADP	O3B-PB-O2B	2.19	116.01	107.80
11	B	502	ATP	O3'-C3'-C2'	-2.03	105.30	111.82

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	501	ADP	C5'-O5'-PA-O1A
11	B	502	ATP	O4'-C4'-C5'-O5'
11	B	502	ATP	C3'-C4'-C5'-O5'
11	B	502	ATP	C4'-C5'-O5'-PA
9	A	501	ADP	C4'-C5'-O5'-PA
11	G	501	ATP	PG-O3B-PB-O1B
11	G	501	ATP	PG-O3B-PB-O2B
11	B	502	ATP	PB-O3B-PG-O1G
11	B	502	ATP	PB-O3B-PG-O2G
11	B	502	ATP	PB-O3B-PG-O3G
11	B	502	ATP	PB-O3A-PA-O1A
11	B	502	ATP	PB-O3A-PA-O2A
11	G	501	ATP	PB-O3A-PA-O2A

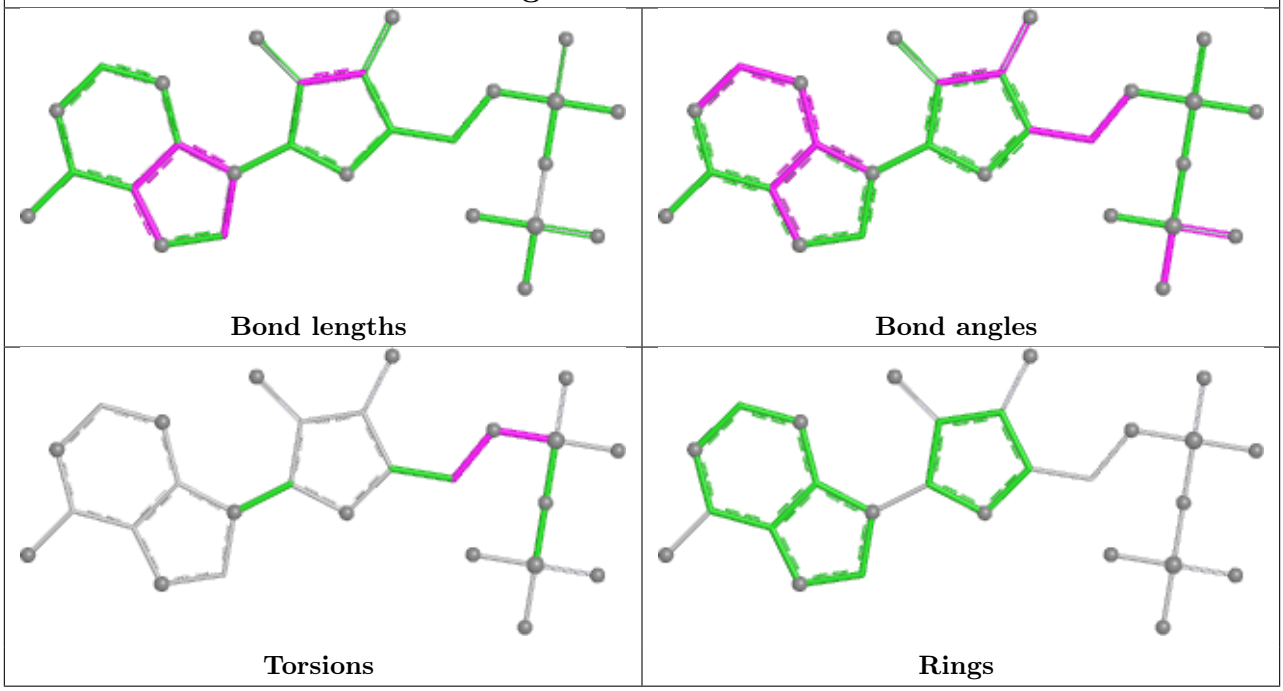
There are no ring outliers.

2 monomers are involved in 5 short contacts:

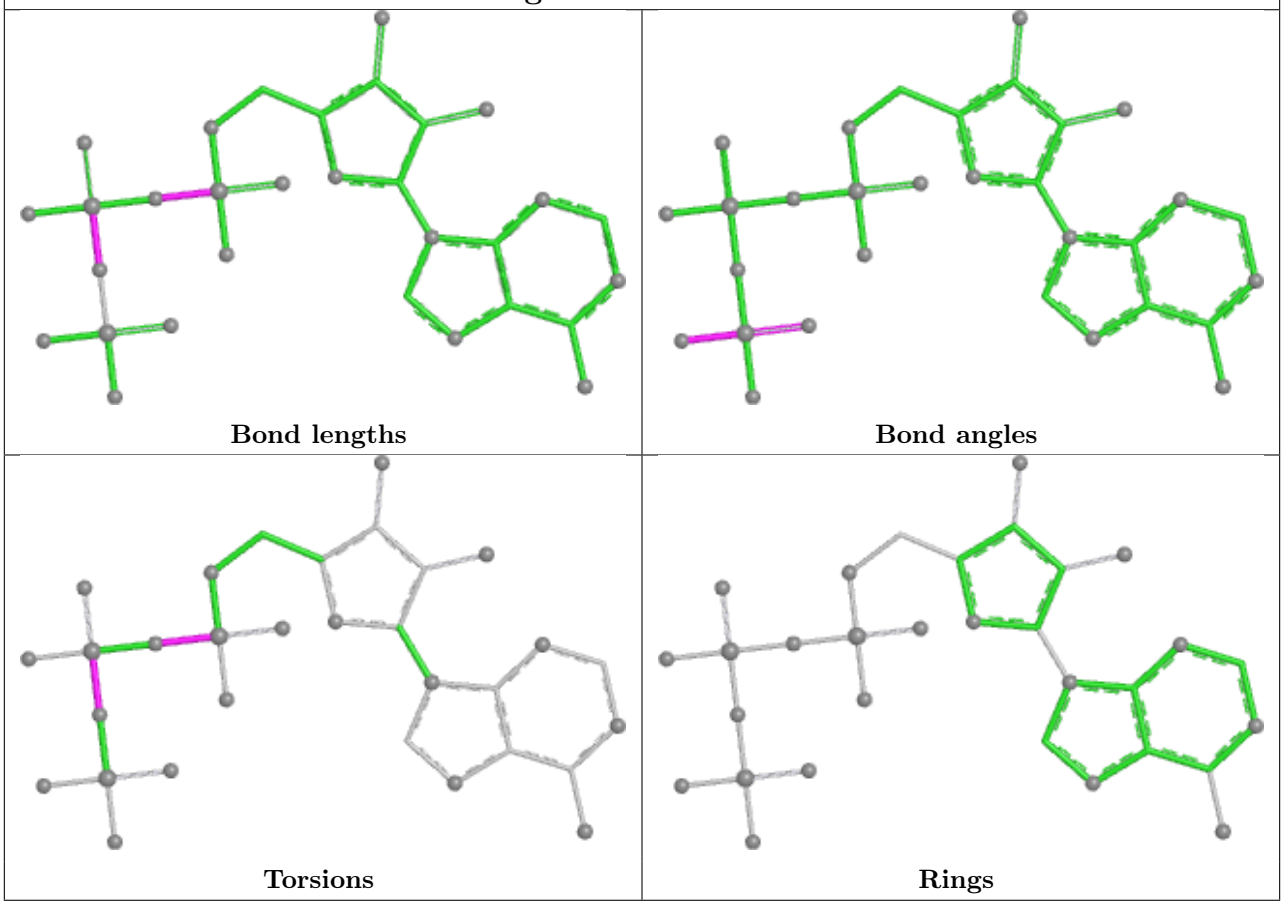
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	501	ADP	1	0
11	G	501	ATP	4	0

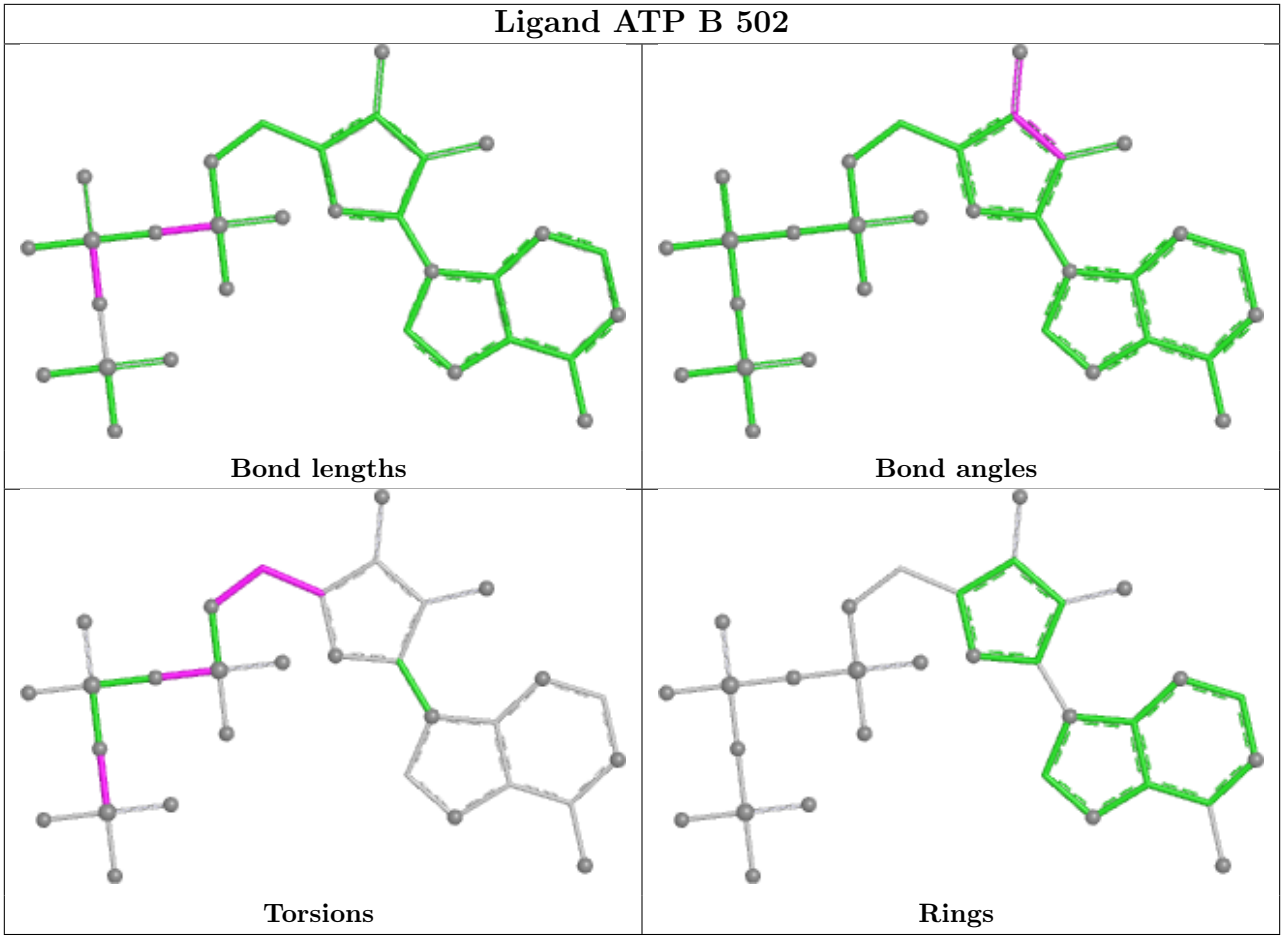
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP A 501



Ligand ATP G 501





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.

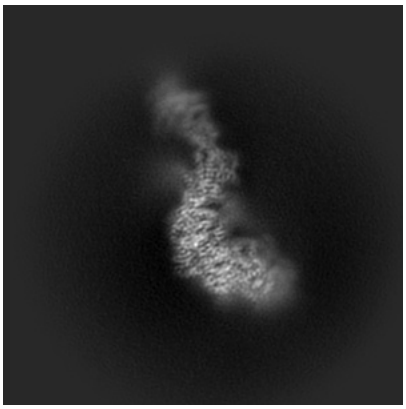
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-72166. These allow visual inspection of the internal detail of the map and identification of artifacts.

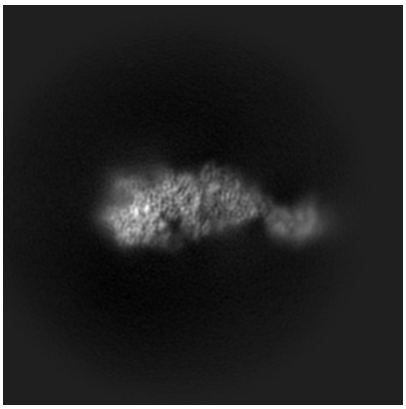
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

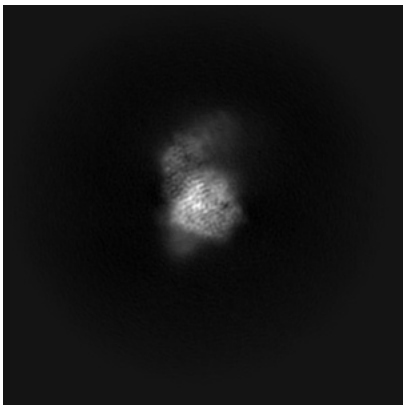
6.1.1 Primary map



X

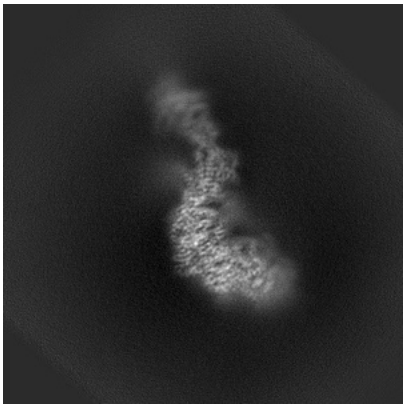


Y

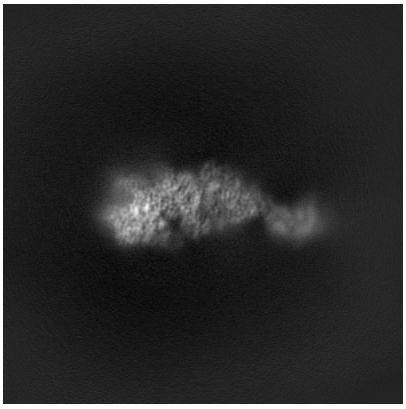


Z

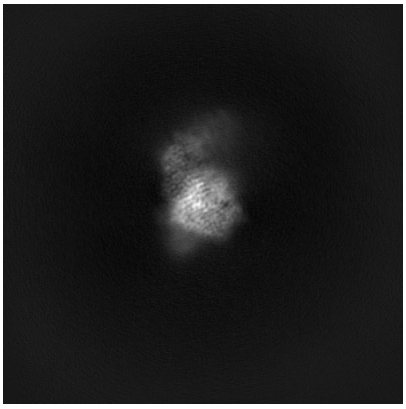
6.1.2 Raw map



X



Y

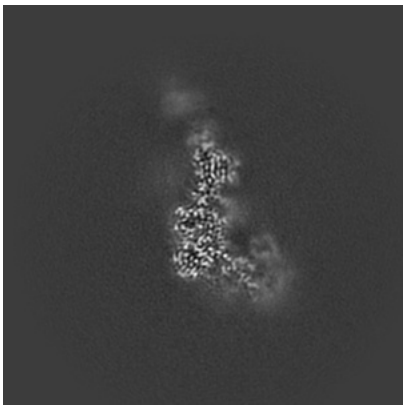


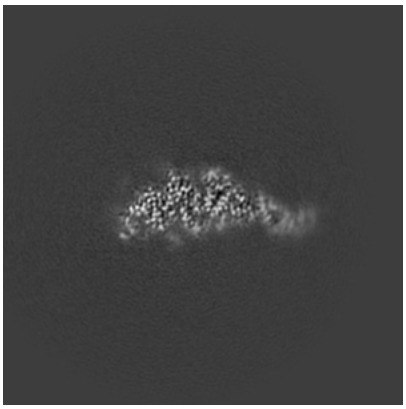
Z

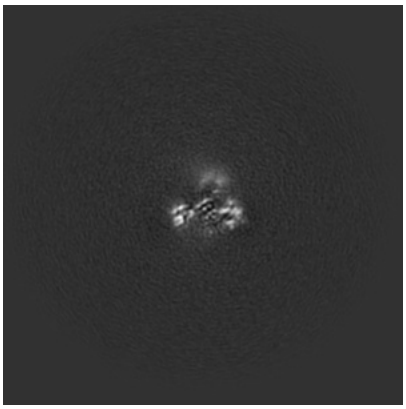
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

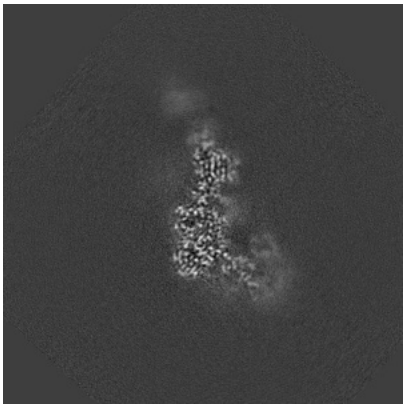
6.2.1 Primary map

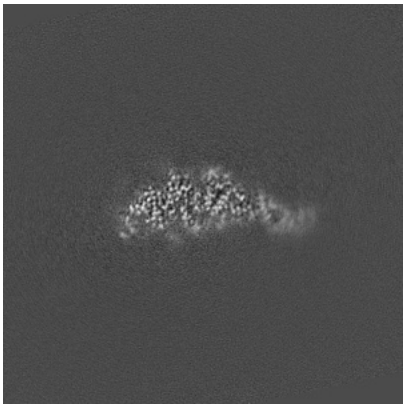

X Index: 200

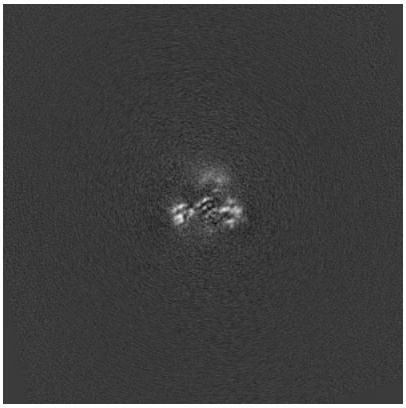

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

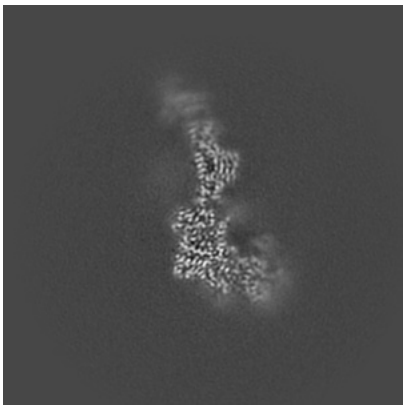

Y Index: 200

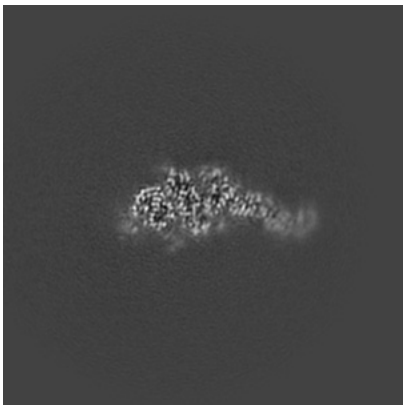

Z Index: 200

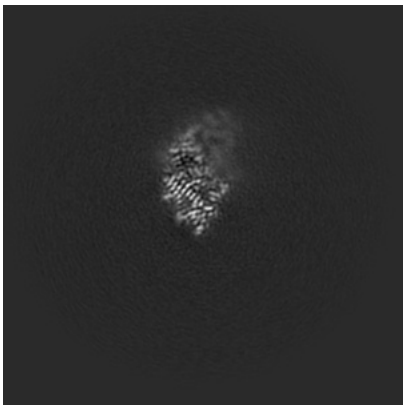
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

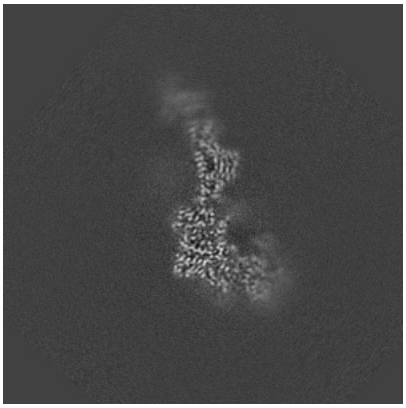
6.3.1 Primary map

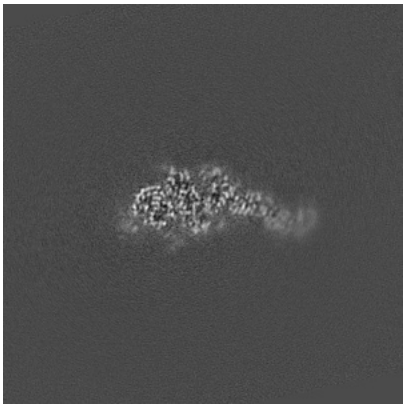

X Index: 195

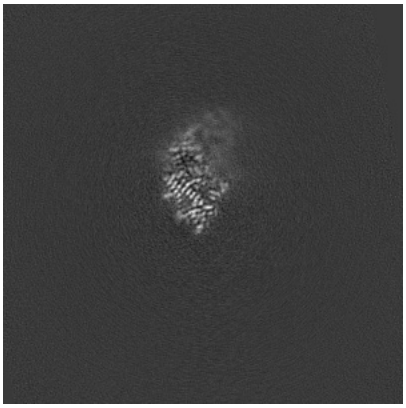

Y Index: 197


Z Index: 134

6.3.2 Raw map


X Index: 195

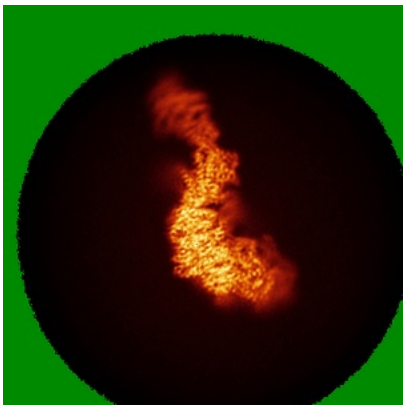

Y Index: 197

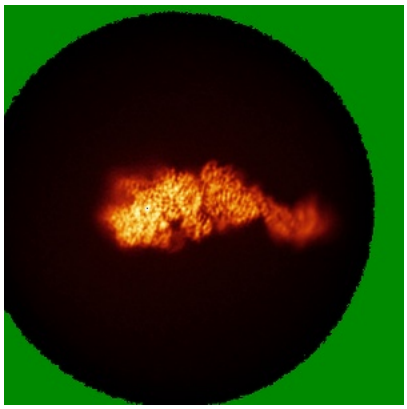

Z Index: 134

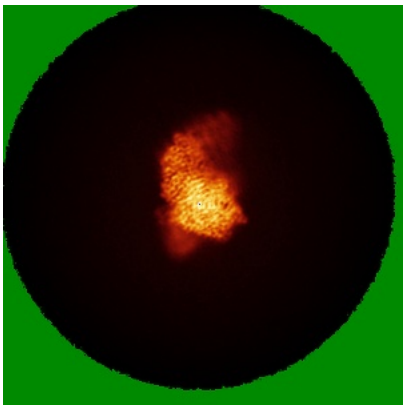
The images above show the largest variance slices of the map in three orthogonal directions.

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

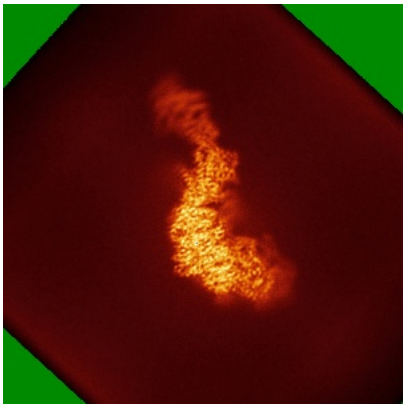
6.4.1 Primary map

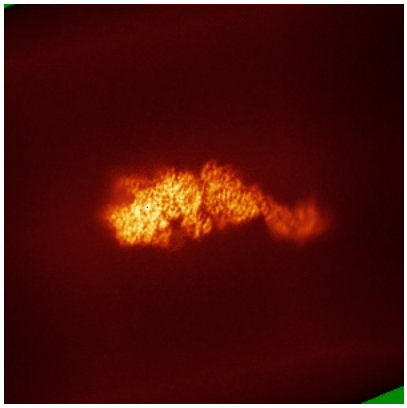

X

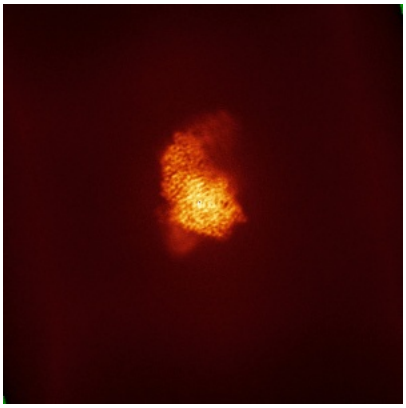

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

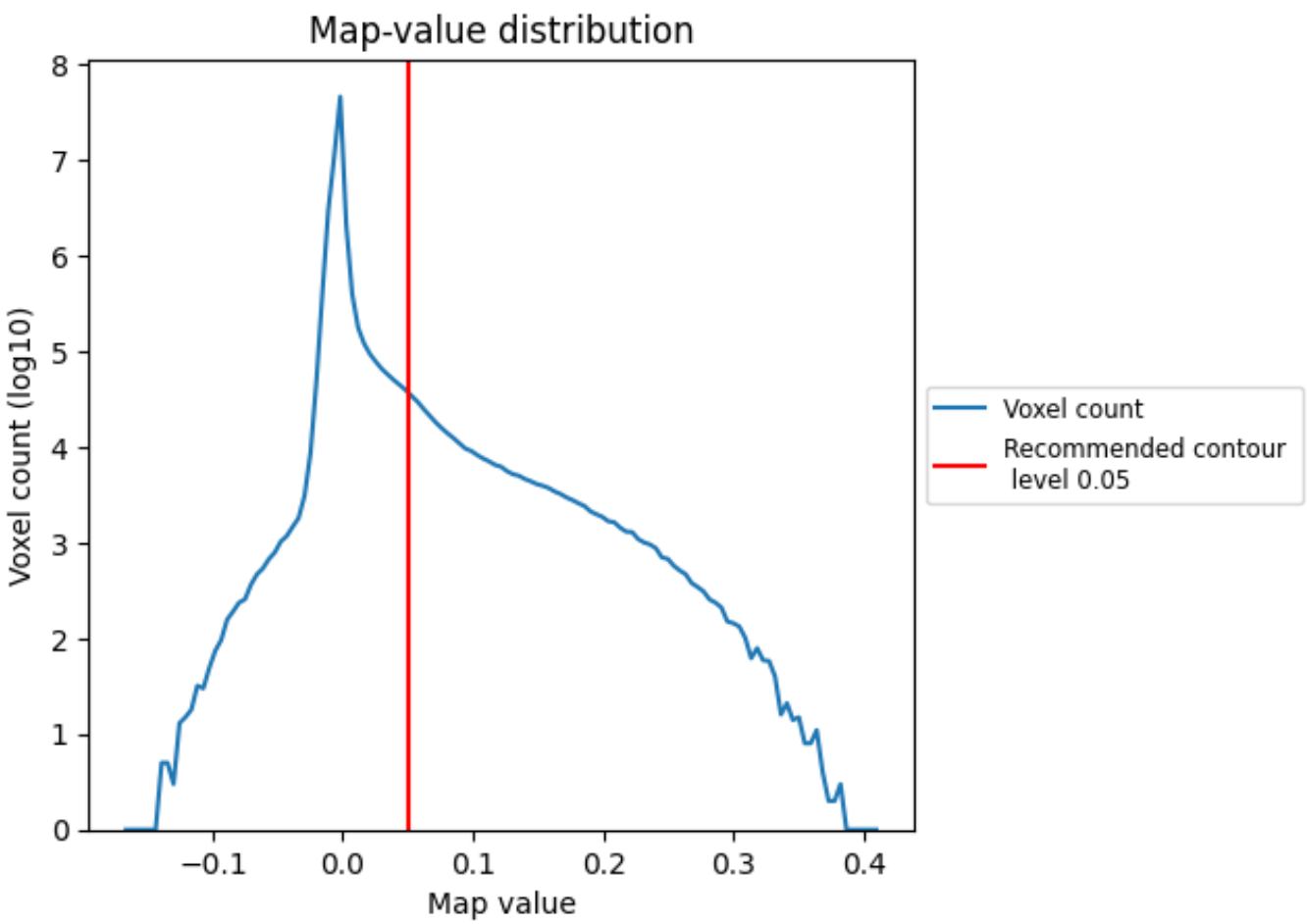
6.6 Mask visualisation (i)

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

7 Map analysis (i)

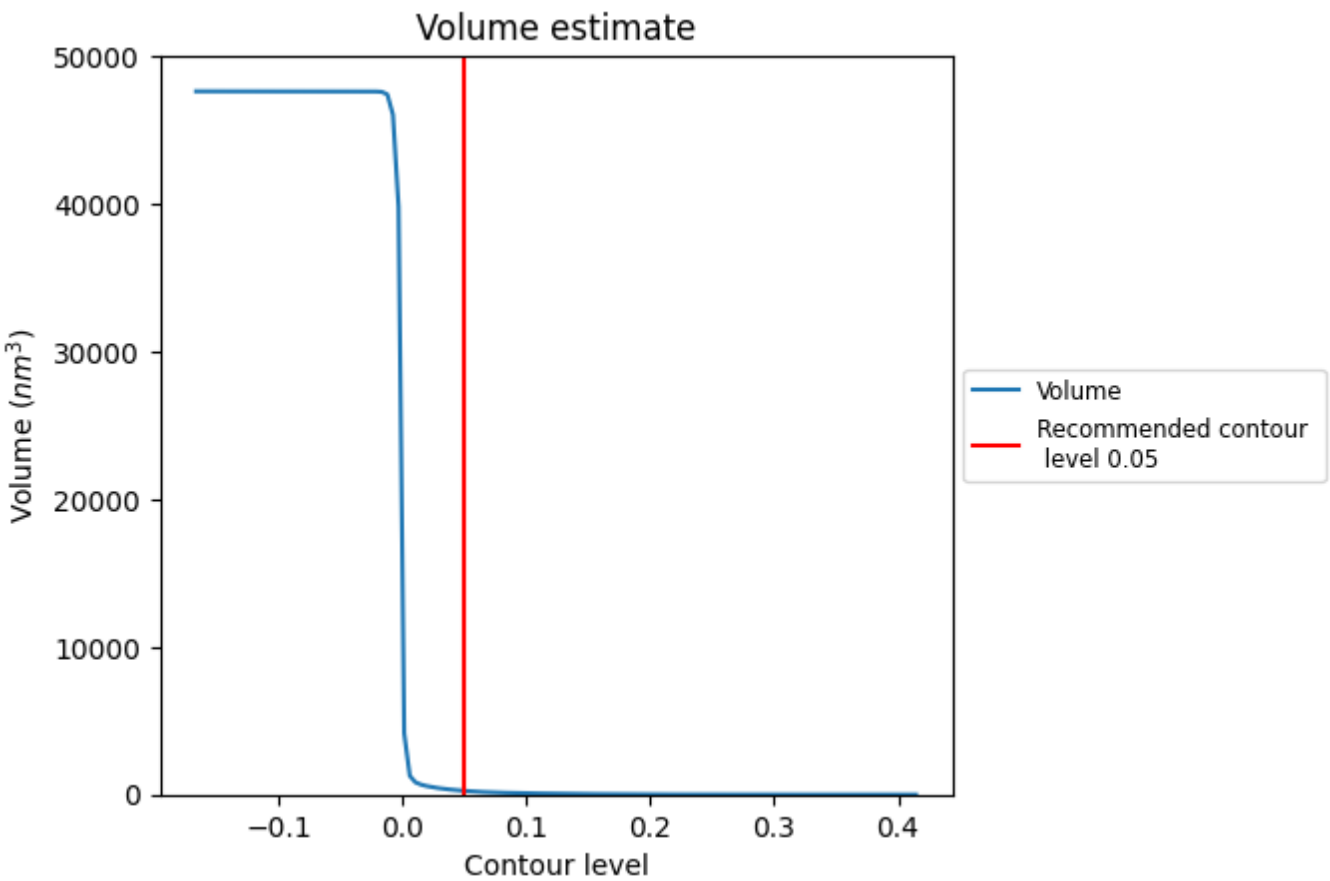
This section contains the results of statistical analysis of the map.

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.

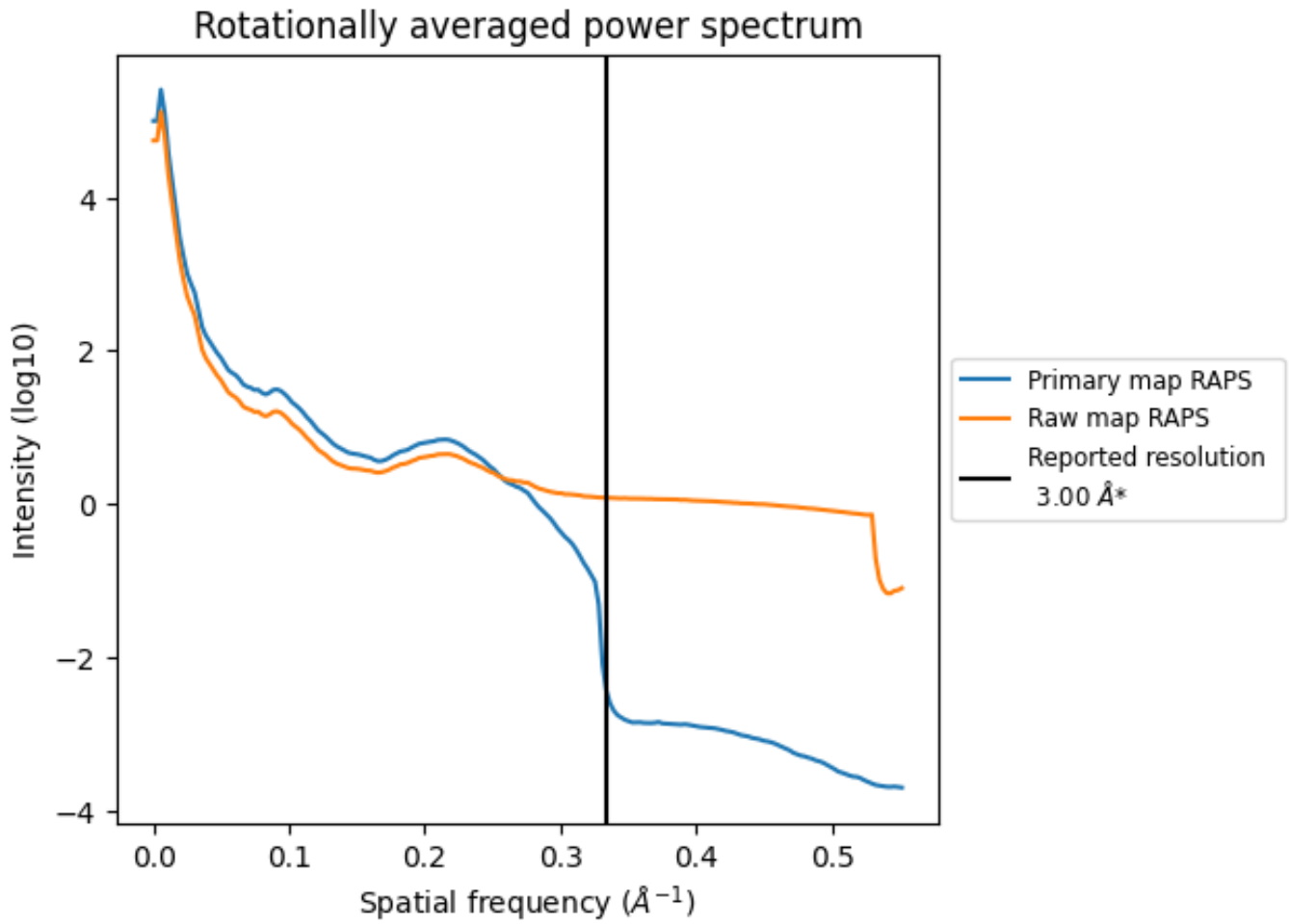
7.2 Volume estimate (i)



The volume at the recommended contour level is 251 nm^3; this corresponds to an approximate mass of 227 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)

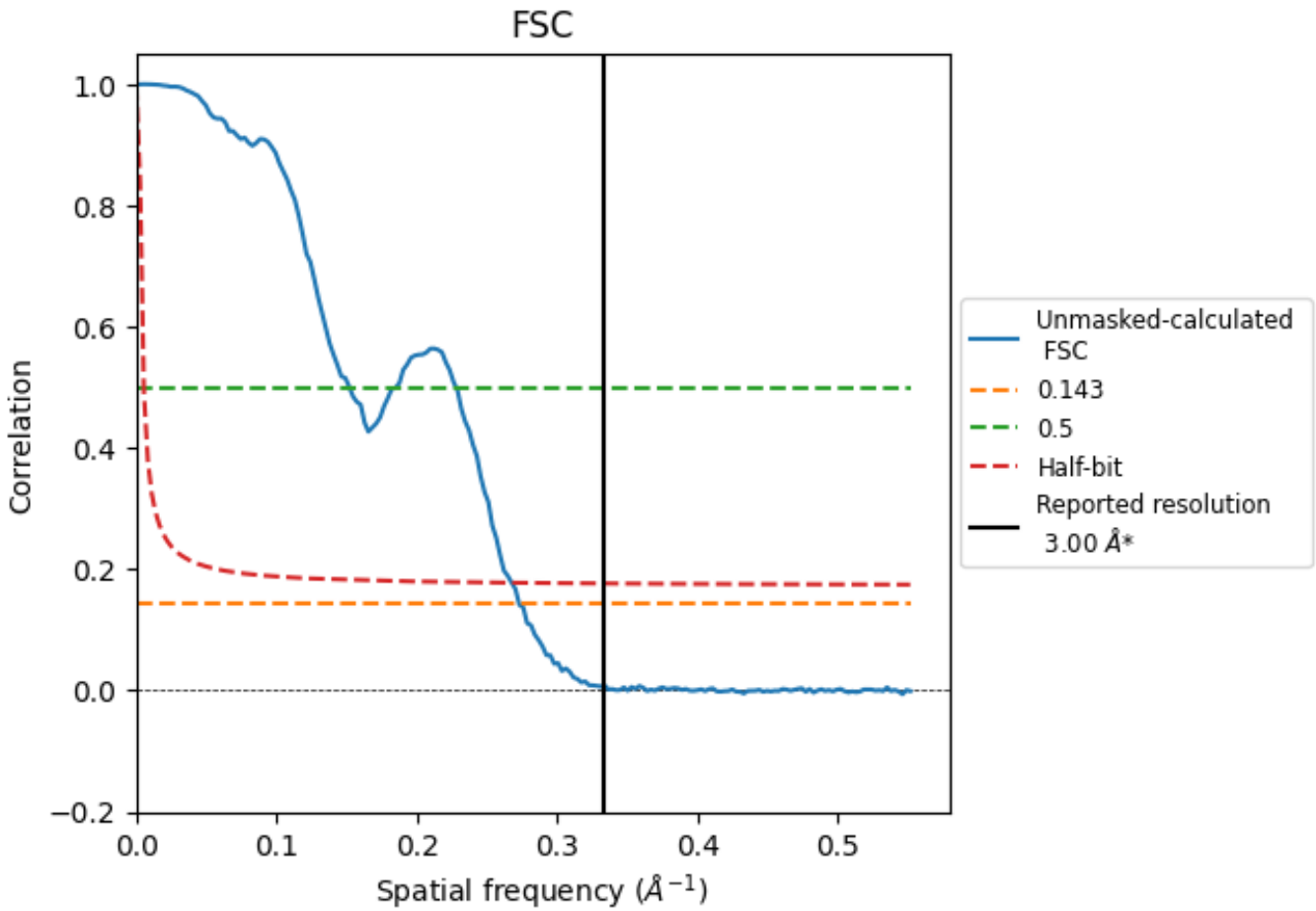


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

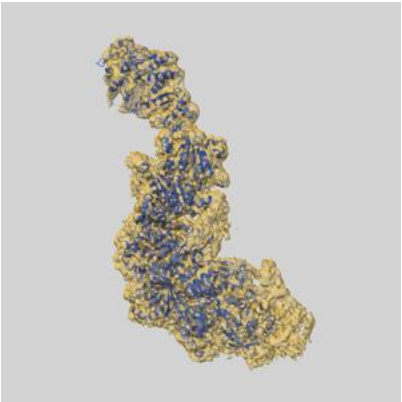
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.66	6.58	3.74

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.66 differs from the reported value 3.0 by more than 10 %

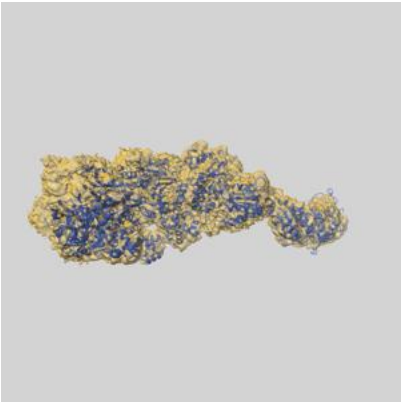
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-72166 and PDB model 9Q2I. Per-residue inclusion information can be found in section 3 on page 12.

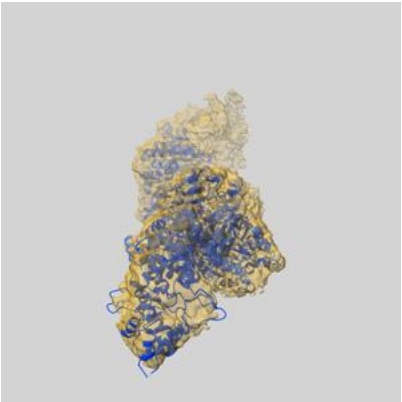
9.1 Map-model overlay (i)



X



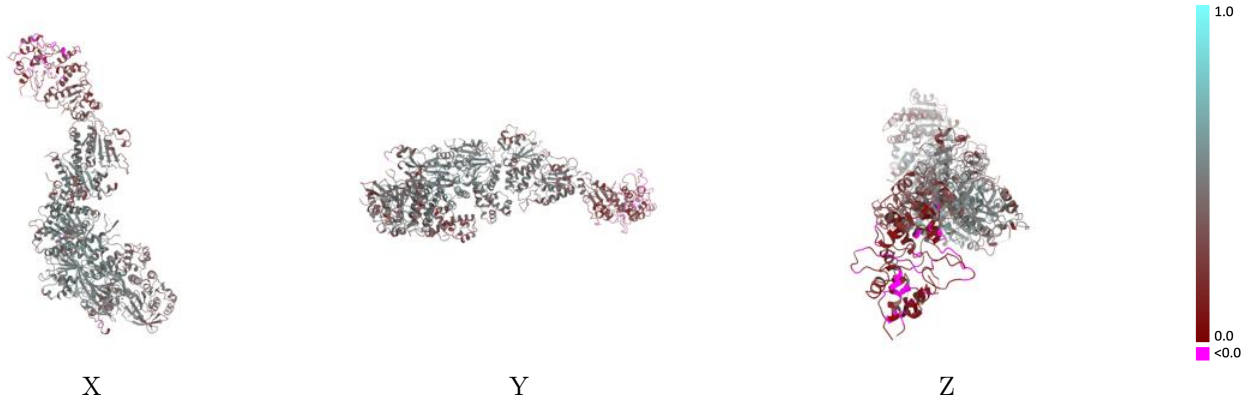
Y



Z

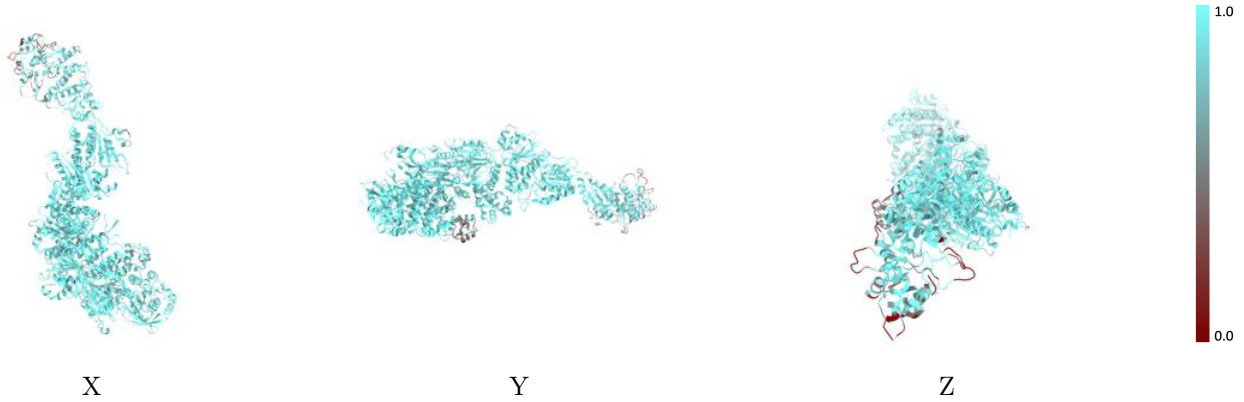
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



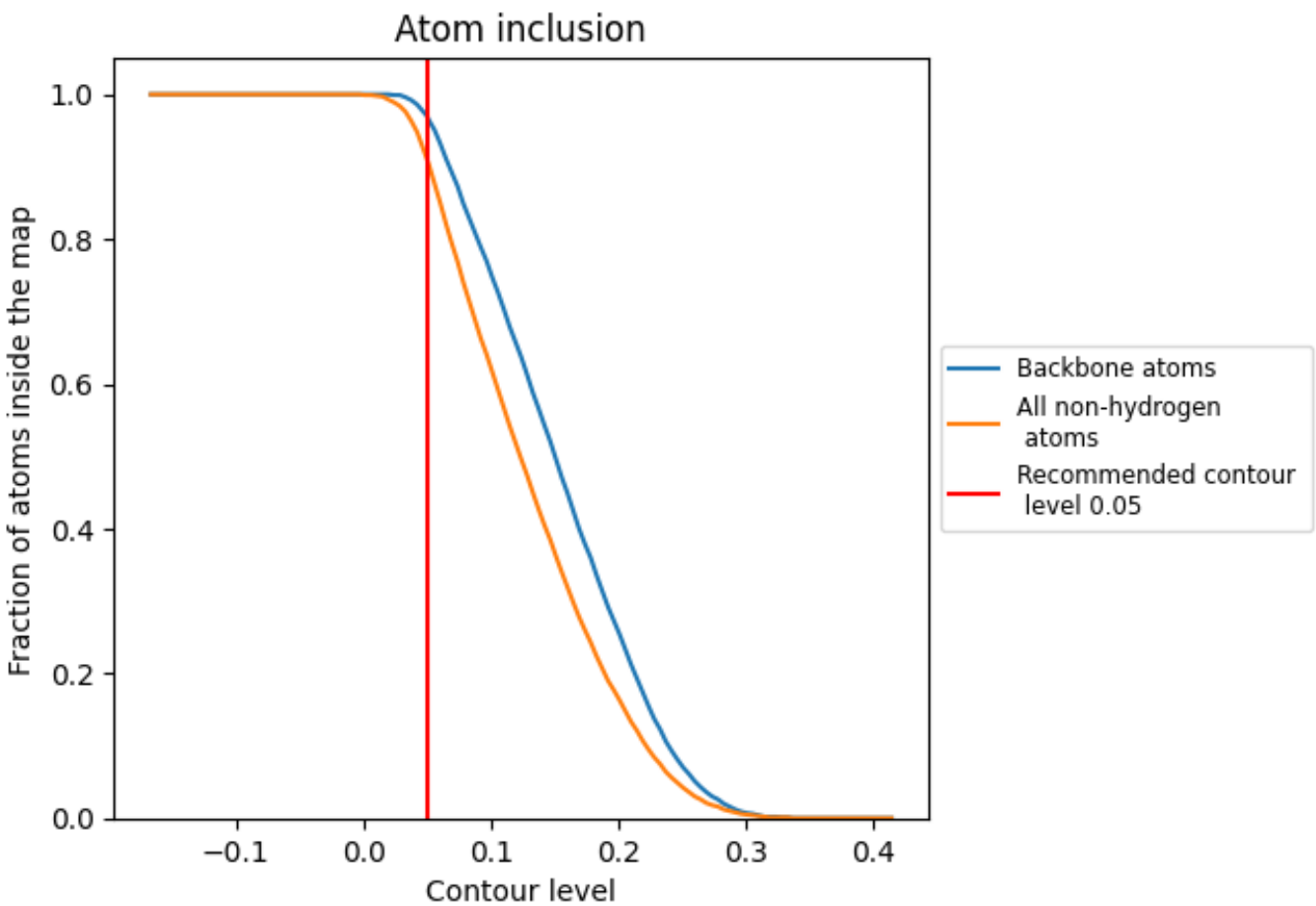
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 91% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9110	0.4050
A	0.9700	0.4920
B	0.9690	0.4840
C	0.9570	0.4560
D	0.9150	0.4090
E	0.8860	0.2570
F	0.6860	0.1200
G	0.8800	0.4330
H	0.9880	0.5100
I	0.9460	0.4140