



Full wwPDB EM Validation Report ⓘ

Oct 27, 2025 – 02:22 PM JST

PDB ID : 9UI4 / pdb_00009ui4
EMDB ID : EMD-64183
Title : Rad51 presynaptic complex
Authors : Luo, S.C.; Ho, M.C.
Deposited on : 2025-04-15
Resolution : 2.91 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

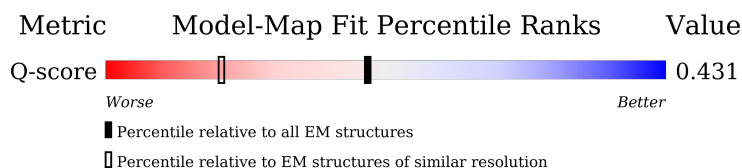
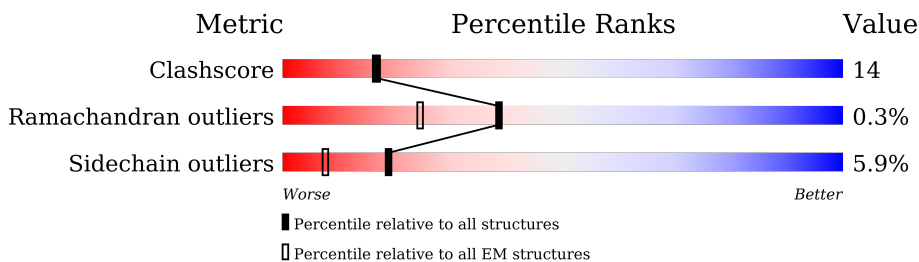
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.91 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.






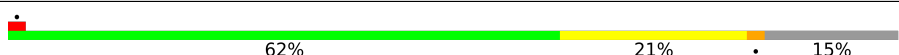
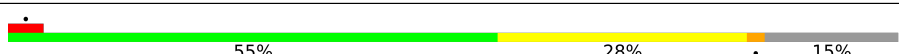
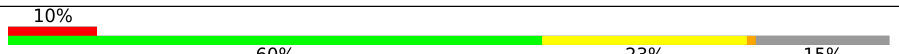
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	12972 (2.41 - 3.41)

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

Mol	Chain	Length	Quality of chain
1	L	27	<div> <div>70%</div> <div>30%</div> </div>
2	A	361	<div> <div>10%</div> <div>57%</div> <div>27%</div> <div>•</div> <div>15%</div> </div>
2	B	361	<div> <div>9%</div> <div>47%</div> <div>34%</div> <div>•</div> <div>16%</div> </div>
2	C	361	<div> <div>•</div> <div>58%</div> <div>26%</div> <div>•</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	361	
2	E	361	
2	F	361	
2	G	361	
2	H	361	
2	I	361	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22055 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 DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	27	Total	C	N	O	P	0	0
			540	263	73	177	27		

- Molecule 2 is a protein called DNA repair protein RAD51 homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	307	Total	C	N	O	S	0	0
			2365	1481	416	455	13		
2	B	302	Total	C	N	O	S	0	0
			2327	1458	408	448	13		
2	A	308	Total	C	N	O	S	0	0
			2369	1483	417	456	13		
2	F	306	Total	C	N	O	S	0	0
			2357	1477	415	452	13		
2	I	307	Total	C	N	O	S	0	0
			2365	1481	416	455	13		
2	E	306	Total	C	N	O	S	0	0
			2357	1477	415	452	13		
2	H	307	Total	C	N	O	S	0	0
			2365	1481	416	455	13		
2	D	306	Total	C	N	O	S	0	0
			2357	1477	415	452	13		
2	G	307	Total	C	N	O	S	0	0
			2365	1481	416	455	13		

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-21	MET	-	initiating methionine	UNP Q08297
C	-20	ALA	-	expression tag	UNP Q08297
C	-19	SER	-	expression tag	UNP Q08297
C	-18	TRP	-	expression tag	UNP Q08297
C	-17	SER	-	expression tag	UNP Q08297

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	HIS	-	expression tag	UNP Q08297
C	-15	PRO	-	expression tag	UNP Q08297
C	-14	GLN	-	expression tag	UNP Q08297
C	-13	PHE	-	expression tag	UNP Q08297
C	-12	GLU	-	expression tag	UNP Q08297
C	-11	LYS	-	expression tag	UNP Q08297
C	-10	GLY	-	expression tag	UNP Q08297
C	-9	ALA	-	expression tag	UNP Q08297
C	-8	ASP	-	expression tag	UNP Q08297
C	-7	ASP	-	expression tag	UNP Q08297
C	-6	ASP	-	expression tag	UNP Q08297
C	-5	ASP	-	expression tag	UNP Q08297
C	-4	LYS	-	expression tag	UNP Q08297
C	-3	VAL	-	expression tag	UNP Q08297
C	-2	PRO	-	expression tag	UNP Q08297
C	-1	ASP	-	expression tag	UNP Q08297
C	0	PRO	-	expression tag	UNP Q08297
C	208	GLU	SER	engineered mutation	UNP Q08297
C	209	ASP	ALA	engineered mutation	UNP Q08297
B	-21	MET	-	initiating methionine	UNP Q08297
B	-20	ALA	-	expression tag	UNP Q08297
B	-19	SER	-	expression tag	UNP Q08297
B	-18	TRP	-	expression tag	UNP Q08297
B	-17	SER	-	expression tag	UNP Q08297
B	-16	HIS	-	expression tag	UNP Q08297
B	-15	PRO	-	expression tag	UNP Q08297
B	-14	GLN	-	expression tag	UNP Q08297
B	-13	PHE	-	expression tag	UNP Q08297
B	-12	GLU	-	expression tag	UNP Q08297
B	-11	LYS	-	expression tag	UNP Q08297
B	-10	GLY	-	expression tag	UNP Q08297
B	-9	ALA	-	expression tag	UNP Q08297
B	-8	ASP	-	expression tag	UNP Q08297
B	-7	ASP	-	expression tag	UNP Q08297
B	-6	ASP	-	expression tag	UNP Q08297
B	-5	ASP	-	expression tag	UNP Q08297
B	-4	LYS	-	expression tag	UNP Q08297
B	-3	VAL	-	expression tag	UNP Q08297
B	-2	PRO	-	expression tag	UNP Q08297
B	-1	ASP	-	expression tag	UNP Q08297
B	0	PRO	-	expression tag	UNP Q08297
B	208	GLU	SER	engineered mutation	UNP Q08297

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Chain	Residue	Modelled	Actual	Comment	Reference
B	209	ASP	ALA	engineered mutation	UNP Q08297
A	-21	MET	-	initiating methionine	UNP Q08297
A	-20	ALA	-	expression tag	UNP Q08297
A	-19	SER	-	expression tag	UNP Q08297
A	-18	TRP	-	expression tag	UNP Q08297
A	-17	SER	-	expression tag	UNP Q08297
A	-16	HIS	-	expression tag	UNP Q08297
A	-15	PRO	-	expression tag	UNP Q08297
A	-14	GLN	-	expression tag	UNP Q08297
A	-13	PHE	-	expression tag	UNP Q08297
A	-12	GLU	-	expression tag	UNP Q08297
A	-11	LYS	-	expression tag	UNP Q08297
A	-10	GLY	-	expression tag	UNP Q08297
A	-9	ALA	-	expression tag	UNP Q08297
A	-8	ASP	-	expression tag	UNP Q08297
A	-7	ASP	-	expression tag	UNP Q08297
A	-6	ASP	-	expression tag	UNP Q08297
A	-5	ASP	-	expression tag	UNP Q08297
A	-4	LYS	-	expression tag	UNP Q08297
A	-3	VAL	-	expression tag	UNP Q08297
A	-2	PRO	-	expression tag	UNP Q08297
A	-1	ASP	-	expression tag	UNP Q08297
A	0	PRO	-	expression tag	UNP Q08297
A	208	GLU	SER	engineered mutation	UNP Q08297
A	209	ASP	ALA	engineered mutation	UNP Q08297
F	-21	MET	-	initiating methionine	UNP Q08297
F	-20	ALA	-	expression tag	UNP Q08297
F	-19	SER	-	expression tag	UNP Q08297
F	-18	TRP	-	expression tag	UNP Q08297
F	-17	SER	-	expression tag	UNP Q08297
F	-16	HIS	-	expression tag	UNP Q08297
F	-15	PRO	-	expression tag	UNP Q08297
F	-14	GLN	-	expression tag	UNP Q08297
F	-13	PHE	-	expression tag	UNP Q08297
F	-12	GLU	-	expression tag	UNP Q08297
F	-11	LYS	-	expression tag	UNP Q08297
F	-10	GLY	-	expression tag	UNP Q08297
F	-9	ALA	-	expression tag	UNP Q08297
F	-8	ASP	-	expression tag	UNP Q08297
F	-7	ASP	-	expression tag	UNP Q08297
F	-6	ASP	-	expression tag	UNP Q08297
F	-5	ASP	-	expression tag	UNP Q08297

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	LYS	-	expression tag	UNP Q08297
F	-3	VAL	-	expression tag	UNP Q08297
F	-2	PRO	-	expression tag	UNP Q08297
F	-1	ASP	-	expression tag	UNP Q08297
F	0	PRO	-	expression tag	UNP Q08297
F	208	GLU	SER	engineered mutation	UNP Q08297
F	209	ASP	ALA	engineered mutation	UNP Q08297
I	-21	MET	-	initiating methionine	UNP Q08297
I	-20	ALA	-	expression tag	UNP Q08297
I	-19	SER	-	expression tag	UNP Q08297
I	-18	TRP	-	expression tag	UNP Q08297
I	-17	SER	-	expression tag	UNP Q08297
I	-16	HIS	-	expression tag	UNP Q08297
I	-15	PRO	-	expression tag	UNP Q08297
I	-14	GLN	-	expression tag	UNP Q08297
I	-13	PHE	-	expression tag	UNP Q08297
I	-12	GLU	-	expression tag	UNP Q08297
I	-11	LYS	-	expression tag	UNP Q08297
I	-10	GLY	-	expression tag	UNP Q08297
I	-9	ALA	-	expression tag	UNP Q08297
I	-8	ASP	-	expression tag	UNP Q08297
I	-7	ASP	-	expression tag	UNP Q08297
I	-6	ASP	-	expression tag	UNP Q08297
I	-5	ASP	-	expression tag	UNP Q08297
I	-4	LYS	-	expression tag	UNP Q08297
I	-3	VAL	-	expression tag	UNP Q08297
I	-2	PRO	-	expression tag	UNP Q08297
I	-1	ASP	-	expression tag	UNP Q08297
I	0	PRO	-	expression tag	UNP Q08297
I	208	GLU	SER	engineered mutation	UNP Q08297
I	209	ASP	ALA	engineered mutation	UNP Q08297
E	-21	MET	-	initiating methionine	UNP Q08297
E	-20	ALA	-	expression tag	UNP Q08297
E	-19	SER	-	expression tag	UNP Q08297
E	-18	TRP	-	expression tag	UNP Q08297
E	-17	SER	-	expression tag	UNP Q08297
E	-16	HIS	-	expression tag	UNP Q08297
E	-15	PRO	-	expression tag	UNP Q08297
E	-14	GLN	-	expression tag	UNP Q08297
E	-13	PHE	-	expression tag	UNP Q08297
E	-12	GLU	-	expression tag	UNP Q08297
E	-11	LYS	-	expression tag	UNP Q08297

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	GLY	-	expression tag	UNP Q08297
E	-9	ALA	-	expression tag	UNP Q08297
E	-8	ASP	-	expression tag	UNP Q08297
E	-7	ASP	-	expression tag	UNP Q08297
E	-6	ASP	-	expression tag	UNP Q08297
E	-5	ASP	-	expression tag	UNP Q08297
E	-4	LYS	-	expression tag	UNP Q08297
E	-3	VAL	-	expression tag	UNP Q08297
E	-2	PRO	-	expression tag	UNP Q08297
E	-1	ASP	-	expression tag	UNP Q08297
E	0	PRO	-	expression tag	UNP Q08297
E	208	GLU	SER	engineered mutation	UNP Q08297
E	209	ASP	ALA	engineered mutation	UNP Q08297
H	-21	MET	-	initiating methionine	UNP Q08297
H	-20	ALA	-	expression tag	UNP Q08297
H	-19	SER	-	expression tag	UNP Q08297
H	-18	TRP	-	expression tag	UNP Q08297
H	-17	SER	-	expression tag	UNP Q08297
H	-16	HIS	-	expression tag	UNP Q08297
H	-15	PRO	-	expression tag	UNP Q08297
H	-14	GLN	-	expression tag	UNP Q08297
H	-13	PHE	-	expression tag	UNP Q08297
H	-12	GLU	-	expression tag	UNP Q08297
H	-11	LYS	-	expression tag	UNP Q08297
H	-10	GLY	-	expression tag	UNP Q08297
H	-9	ALA	-	expression tag	UNP Q08297
H	-8	ASP	-	expression tag	UNP Q08297
H	-7	ASP	-	expression tag	UNP Q08297
H	-6	ASP	-	expression tag	UNP Q08297
H	-5	ASP	-	expression tag	UNP Q08297
H	-4	LYS	-	expression tag	UNP Q08297
H	-3	VAL	-	expression tag	UNP Q08297
H	-2	PRO	-	expression tag	UNP Q08297
H	-1	ASP	-	expression tag	UNP Q08297
H	0	PRO	-	expression tag	UNP Q08297
H	208	GLU	SER	engineered mutation	UNP Q08297
H	209	ASP	ALA	engineered mutation	UNP Q08297
D	-21	MET	-	initiating methionine	UNP Q08297
D	-20	ALA	-	expression tag	UNP Q08297
D	-19	SER	-	expression tag	UNP Q08297
D	-18	TRP	-	expression tag	UNP Q08297
D	-17	SER	-	expression tag	UNP Q08297

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	HIS	-	expression tag	UNP Q08297
D	-15	PRO	-	expression tag	UNP Q08297
D	-14	GLN	-	expression tag	UNP Q08297
D	-13	PHE	-	expression tag	UNP Q08297
D	-12	GLU	-	expression tag	UNP Q08297
D	-11	LYS	-	expression tag	UNP Q08297
D	-10	GLY	-	expression tag	UNP Q08297
D	-9	ALA	-	expression tag	UNP Q08297
D	-8	ASP	-	expression tag	UNP Q08297
D	-7	ASP	-	expression tag	UNP Q08297
D	-6	ASP	-	expression tag	UNP Q08297
D	-5	ASP	-	expression tag	UNP Q08297
D	-4	LYS	-	expression tag	UNP Q08297
D	-3	VAL	-	expression tag	UNP Q08297
D	-2	PRO	-	expression tag	UNP Q08297
D	-1	ASP	-	expression tag	UNP Q08297
D	0	PRO	-	expression tag	UNP Q08297
D	208	GLU	SER	engineered mutation	UNP Q08297
D	209	ASP	ALA	engineered mutation	UNP Q08297
G	-21	MET	-	initiating methionine	UNP Q08297
G	-20	ALA	-	expression tag	UNP Q08297
G	-19	SER	-	expression tag	UNP Q08297
G	-18	TRP	-	expression tag	UNP Q08297
G	-17	SER	-	expression tag	UNP Q08297
G	-16	HIS	-	expression tag	UNP Q08297
G	-15	PRO	-	expression tag	UNP Q08297
G	-14	GLN	-	expression tag	UNP Q08297
G	-13	PHE	-	expression tag	UNP Q08297
G	-12	GLU	-	expression tag	UNP Q08297
G	-11	LYS	-	expression tag	UNP Q08297
G	-10	GLY	-	expression tag	UNP Q08297
G	-9	ALA	-	expression tag	UNP Q08297
G	-8	ASP	-	expression tag	UNP Q08297
G	-7	ASP	-	expression tag	UNP Q08297
G	-6	ASP	-	expression tag	UNP Q08297
G	-5	ASP	-	expression tag	UNP Q08297
G	-4	LYS	-	expression tag	UNP Q08297
G	-3	VAL	-	expression tag	UNP Q08297
G	-2	PRO	-	expression tag	UNP Q08297
G	-1	ASP	-	expression tag	UNP Q08297
G	0	PRO	-	expression tag	UNP Q08297
G	208	GLU	SER	engineered mutation	UNP Q08297

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Chain	Residue	Modelled	Actual	Comment	Reference
G	209	ASP	ALA	engineered mutation	UNP Q08297

- # ANP
-
- Chemical structure of ANP (Adenosine 3'-phosphate) showing the adenosine moiety and the triphosphate chain. The adenosine part consists of an adenine base (N1, N3, N7, N9, C2, C4, C6, C8) attached to a ribose sugar (C1', C2', C3', C4', C5'). The ribose is linked to a triphosphate chain (O1', O2', O3', O4', O5', O6', O7', O8', O9'). The triphosphate chain is shown as a series of phosphate groups (P1, P2, P3) connected by oxygen atoms (O1', O2', O3', O4', O5', O6', O7', O8', O9'). The terminal phosphate group (P3) is shown with a negative charge (O9').

Mol	Chain	Residues	Atoms					AltConf
3	C	1	Total 31	C 10	N 6	O 12	P 3	0
3	B	1	Total 31	C 10	N 6	O 12	P 3	0
3	A	1	Total 31	C 10	N 6	O 12	P 3	0
3	I	1	Total 31	C 10	N 6	O 12	P 3	0
3	E	1	Total 31	C 10	N 6	O 12	P 3	0
3	D	1	Total 31	C 10	N 6	O 12	P 3	0
3	D	1	Total 31	C 10	N 6	O 12	P 3	0
3	G	1	Total 31	C 10	N 6	O 12	P 3	0
3	G	1	Total 31	C 10	N 6	O 12	P 3	0

- 
- WORLD WIDE
PDB
PROTEIN DATA BANK

Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total 1	Mg 1	0
4	B	1	Total 1	Mg 1	0
4	A	1	Total 1	Mg 1	0
4	F	1	Total 1	Mg 1	0
4	I	1	Total 1	Mg 1	0
4	E	1	Total 1	Mg 1	0
4	H	1	Total 1	Mg 1	0
4	D	1	Total 1	Mg 1	0
4	G	1	Total 1	Mg 1	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.

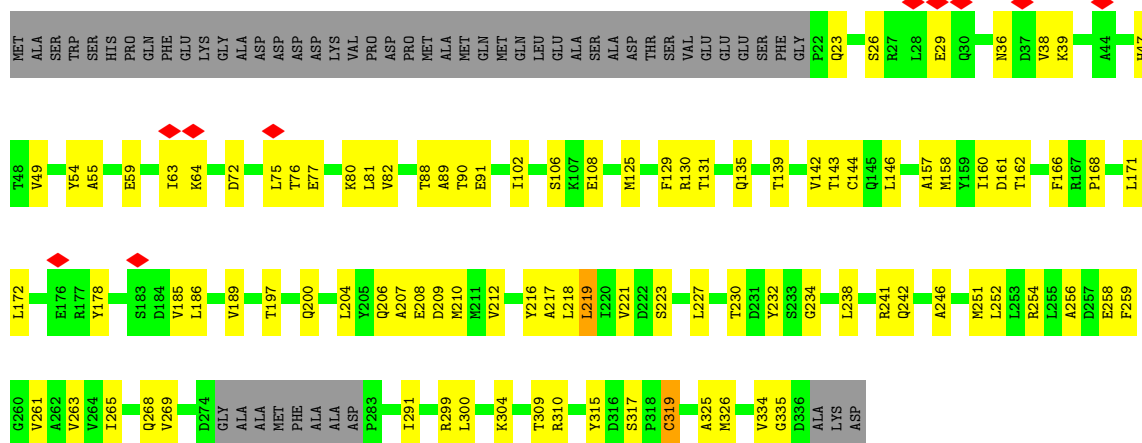
- Molecule 1: DNA (27-MER)

Chain L: 



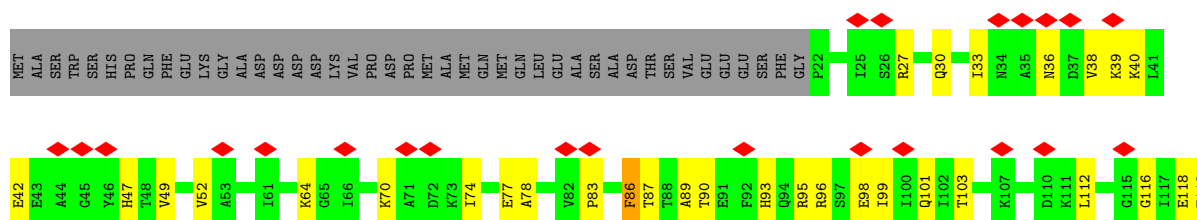
- Molecule 2: DNA repair protein RAD51 homolog 1

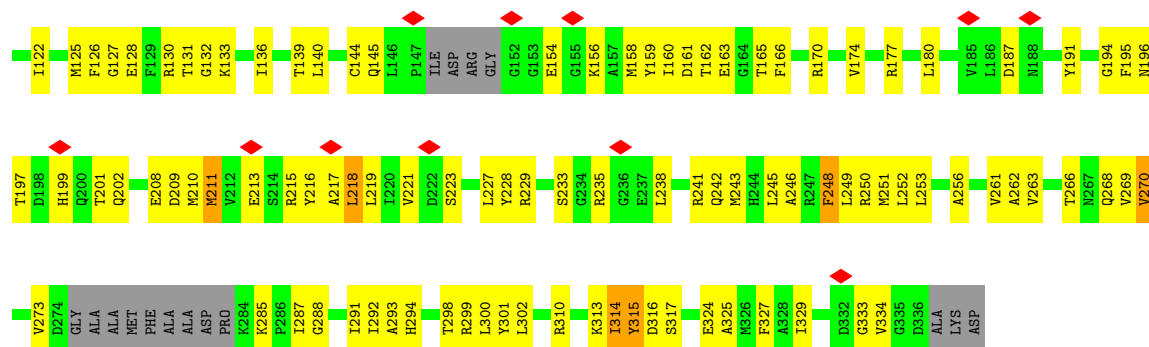
Chain C: 



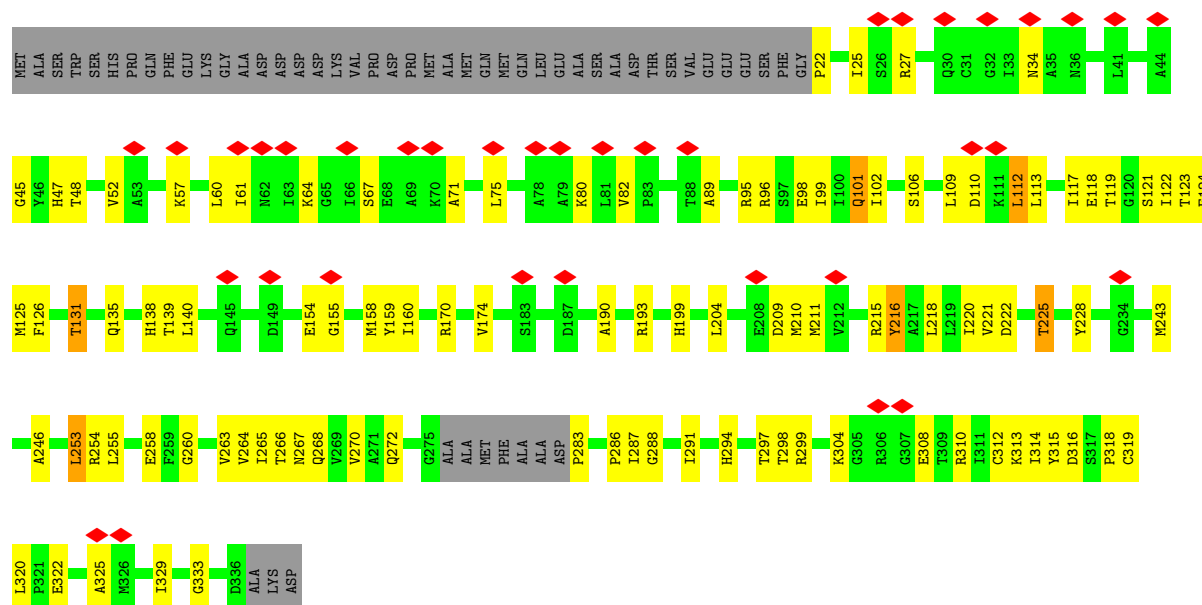
- Molecule 2: DNA repair protein RAD51 homolog 1

Chain B: 

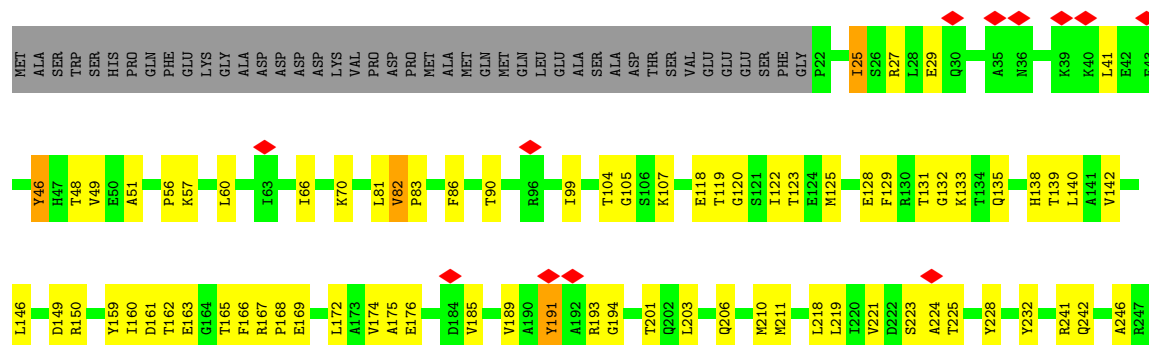




• Molecule 2: DNA repair protein RAD51 homolog 1

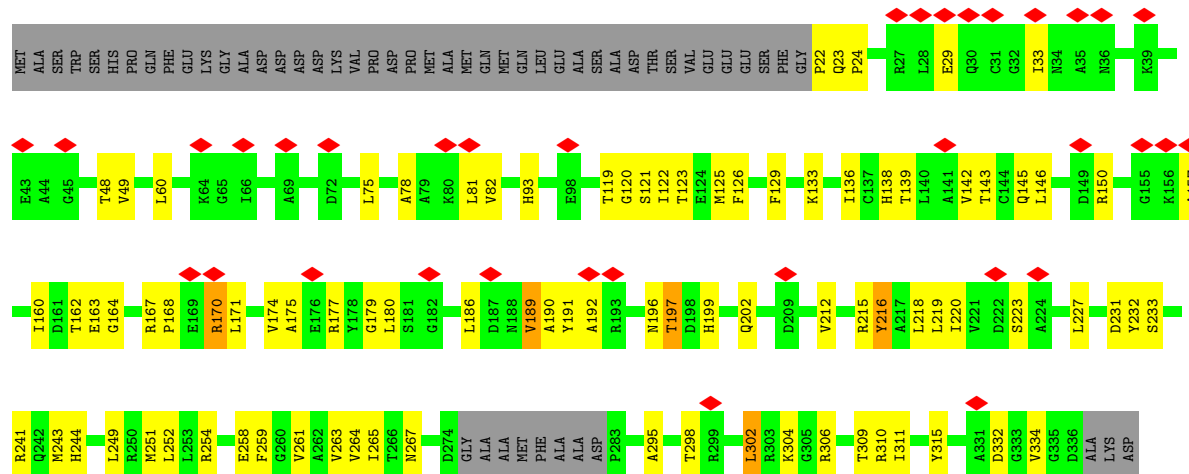


• Molecule 2: DNA repair protein RAD51 homolog 1

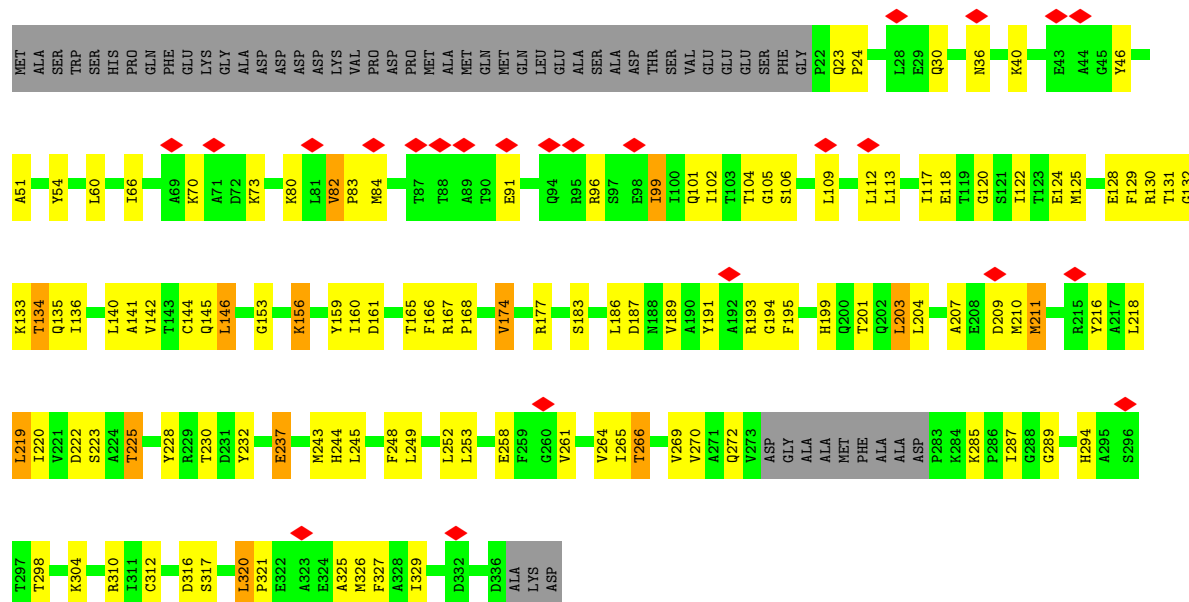




• Molecule 2: DNA repair protein RAD51 homolog 1



• Molecule 2: DNA repair protein RAD51 homolog 1



• Molecule 2: DNA repair protein RAD51 homolog 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67329	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.804	Depositor
Minimum map value	-2.066	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.071	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	318.72, 318.72, 318.72	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: ANP, MG

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	L	0.23	0/597	0.43	0/918
2	A	0.14	0/2403	0.39	0/3239
2	B	0.14	0/2359	0.40	0/3179
2	C	0.12	0/2399	0.32	0/3234
2	D	0.12	0/2391	0.27	0/3223
2	E	0.17	0/2391	0.38	0/3223
2	F	0.14	0/2391	0.39	0/3223
2	G	0.12	0/2399	0.29	0/3234
2	H	0.13	0/2399	0.33	0/3234
2	I	0.12	0/2399	0.33	0/3234
All	All	0.14	0/22128	0.35	0/29941

There are no bond length outliers.

There are no bond angle outliers.

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	L	540	0	314	8	0
2	A	2369	0	2384	77	0
2	B	2327	0	2341	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2365	0	2382	68	0
2	D	2357	0	2378	57	0
2	E	2357	0	2378	81	0
2	F	2357	0	2378	68	0
2	G	2365	0	2382	58	0
2	H	2365	0	2382	81	0
2	I	2365	0	2381	59	0
3	A	31	0	13	3	0
3	B	31	0	13	4	0
3	C	31	0	13	1	0
3	D	62	0	26	2	0
3	E	31	0	13	2	0
3	G	62	0	26	4	0
3	I	31	0	13	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
All	All	22055	0	21817	606	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 14.

All (606) 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)
3:I:600:ANP:H8	2:H:321:PRO:HG3	1.58	0.85
2:B:301:TYR:HB3	2:B:313:LYS:HG3	1.63	0.80
2:A:126:PHE:HB3	2:A:267:ASN:HB3	1.62	0.80
2:C:252:LEU:HD11	2:C:263:VAL:HG11	1.62	0.80
2:G:143:THR:HA	2:G:146:LEU:HD13	1.64	0.79
2:G:204:LEU:HD12	2:G:255:LEU:HD13	1.65	0.79
2:E:141:ALA:HA	2:E:218:LEU:HG	1.64	0.79
2:A:113:LEU:HB2	2:A:320:LEU:HD11	1.65	0.78
2:E:145:GLN:HG2	2:E:146:LEU:HG	1.65	0.77
2:B:130:ARG:HH21	2:B:165:THR:HG23	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:25:ILE:HG12	2:F:27:ARG:H	1.50	0.75
2:G:223:SER:H	2:G:266:THR:HB	1.52	0.74
3:I:600:ANP:H3'	2:H:321:PRO:HB3	1.70	0.74
2:A:135:GLN:HA	2:A:138:HIS:HB2	1.69	0.74
2:E:120:GLY:HA2	2:E:261:VAL:H	1.52	0.74
2:G:157:ALA:HB3	2:G:189:VAL:HG12	1.68	0.74
2:F:104:THR:HB	2:F:140:LEU:HD13	1.68	0.74
2:H:142:VAL:HG12	2:H:185:VAL:HG21	1.68	0.73
2:B:119:THR:HA	2:B:262:ALA:HB2	1.71	0.73
2:A:254:ARG:O	2:A:258:GLU:HG3	1.89	0.73
2:D:299:ARG:HB2	2:D:315:TYR:HB3	1.69	0.73
2:B:158:MET:HE1	2:B:216:TYR:CG	2.23	0.73
2:B:162:THR:HG22	2:B:163:GLU:HG3	1.72	0.72
2:F:219:LEU:HB3	2:F:263:VAL:HG12	1.71	0.72
2:E:211:MET:HE3	2:E:219:LEU:HD23	1.71	0.72
2:G:146:LEU:HB3	2:G:150:ARG:HE	1.54	0.72
2:D:158:MET:HG3	2:D:211:MET:HE3	1.72	0.72
2:E:113:LEU:HA	2:E:320:LEU:HD21	1.73	0.71
2:H:142:VAL:HG21	2:H:174:VAL:HG13	1.72	0.71
2:D:223:SER:H	2:D:266:THR:HB	1.55	0.71
2:I:160:ILE:HA	2:I:192:ALA:HA	1.72	0.70
2:H:119:THR:HA	2:H:262:ALA:HB2	1.73	0.70
2:B:131:THR:HG21	3:B:600:ANP:H5'2	1.73	0.69
2:D:64:LYS:HE3	2:D:65:GLY:H	1.57	0.69
2:C:185:VAL:HG23	2:C:186:LEU:HD22	1.73	0.69
2:B:270:VAL:HG22	2:B:287:ILE:HD13	1.74	0.69
2:F:314:ILE:HG22	2:F:316:ASP:H	1.58	0.69
2:G:125:MET:HG2	2:G:300:LEU:HD23	1.75	0.68
2:A:123:THR:HA	2:A:298:THR:HB	1.75	0.68
2:G:242:GLN:HE21	2:G:291:ILE:HD13	1.58	0.68
2:D:314:ILE:HD12	2:D:320:LEU:HD23	1.76	0.68
2:B:145:GLN:HG2	2:B:180:LEU:HD22	1.76	0.68
2:A:158:MET:HG3	2:A:190:ALA:HB3	1.75	0.67
2:D:28:LEU:HD23	2:D:49:VAL:HG22	1.77	0.67
2:E:70:LYS:HD3	2:E:73:LYS:HE3	1.76	0.67
2:C:204:LEU:HD13	2:C:251:MET:HE1	1.77	0.66
2:I:122:ILE:HG22	2:I:263:VAL:HB	1.76	0.66
2:F:125:MET:HB2	2:F:266:THR:HG23	1.76	0.66
2:B:249:LEU:HD21	2:B:292:ILE:HG22	1.78	0.66
2:E:141:ALA:HB2	2:E:220:ILE:HD11	1.77	0.66
2:G:70:LYS:O	2:G:74:ILE:HG13	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:103:THR:HG23	2:H:143:THR:HB	1.78	0.65
2:B:241:ARG:O	2:B:245:LEU:HD12	1.96	0.65
2:G:299:ARG:HB2	2:G:315:TYR:HB3	1.77	0.65
2:B:208:GLU:HA	2:B:211:MET:HB2	1.79	0.65
2:C:139:THR:O	2:C:143:THR:HG23	1.96	0.64
2:B:27:ARG:HA	2:B:30:GLN:HG2	1.78	0.64
2:A:304:LYS:HB2	2:A:308:GLU:HA	1.78	0.64
2:D:147:PRO:HA	2:D:154:GLU:HG2	1.78	0.64
2:I:311:ILE:HD12	2:I:311:ILE:H	1.63	0.64
2:C:319:CYS:HA	2:D:170:ARG:HD3	1.80	0.64
2:G:135:GLN:HE21	3:G:402:ANP:H5'1	1.62	0.64
2:D:73:LYS:O	2:D:77:GLU:HG2	1.98	0.64
2:B:313:LYS:HB3	2:B:324:GLU:HG2	1.79	0.63
2:I:249:LEU:HD13	2:I:295:ALA:HB3	1.80	0.63
2:B:103:THR:HA	2:B:116:GLY:HA3	1.81	0.63
2:I:138:HIS:CE1	2:I:170:ARG:HE	2.16	0.63
2:F:246:ALA:HB2	2:F:291:ILE:HD13	1.81	0.63
2:A:160:ILE:HD11	2:A:221:VAL:HG13	1.81	0.62
2:I:162:THR:HG22	2:I:196:ASN:HB2	1.81	0.62
2:H:252:LEU:HA	2:H:255:LEU:HD12	1.82	0.62
2:A:139:THR:HG21	2:A:333:GLY:HA3	1.82	0.62
2:I:170:ARG:O	2:I:174:VAL:HG23	2.00	0.61
2:I:157:ALA:HA	2:I:218:LEU:HB2	1.82	0.61
2:H:71:ALA:O	2:H:75:LEU:HD22	2.00	0.61
2:C:157:ALA:HB3	2:C:189:VAL:HG12	1.82	0.61
2:H:46:TYR:H	2:H:254:ARG:HH22	1.49	0.61
2:D:128:GLU:HG3	2:D:129:PHE:H	1.65	0.61
2:I:304:LYS:HA	2:I:310:ARG:HG3	1.83	0.61
2:B:133:LYS:HA	2:B:136:ILE:HG12	1.83	0.60
2:E:122:ILE:HG21	2:E:252:LEU:HD13	1.83	0.60
2:A:210:MET:HB3	2:A:216:TYR:HD2	1.66	0.60
2:E:232:TYR:HD2	2:E:237:GLU:HG2	1.65	0.60
2:B:170:ARG:HD3	2:A:319:CYS:HB2	1.84	0.60
2:A:61:ILE:HD13	2:A:67:SER:HB3	1.84	0.60
2:C:206:GLN:HB3	2:B:86:PHE:HE2	1.67	0.59
2:I:126:PHE:HB3	2:I:267:ASN:HB3	1.84	0.59
2:H:249:LEU:HA	2:H:252:LEU:HD12	1.83	0.59
2:C:49:VAL:HG11	2:C:81:LEU:HD12	1.84	0.59
2:B:300:LEU:HB2	2:B:314:ILE:HA	1.84	0.59
2:C:256:ALA:HA	2:C:261:VAL:HG12	1.84	0.59
2:A:57:LYS:HA	2:A:60:LEU:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:99:ILE:HG23	2:D:101:GLN:HG3	1.84	0.59
2:B:228:TYR:HB2	2:B:241:ARG:HE	1.68	0.58
2:H:70:LYS:O	2:H:74:ILE:HG13	2.03	0.58
2:E:99:ILE:HG22	2:E:101:GLN:HG3	1.84	0.58
2:H:158:MET:HA	2:H:190:ALA:HB3	1.85	0.58
2:D:133:LYS:HG2	2:D:302:LEU:HD12	1.85	0.58
2:C:144:CYS:HB3	2:C:218:LEU:HD23	1.85	0.58
2:E:117:ILE:HG12	2:E:298:THR:HG21	1.84	0.58
2:F:225:THR:HA	2:F:228:TYR:HD2	1.69	0.58
2:I:125:MET:SD	2:I:302:LEU:HB3	2.44	0.58
2:E:96:ARG:HB2	2:E:99:ILE:HD13	1.85	0.58
2:A:102:ILE:HD13	2:A:140:LEU:HD11	1.86	0.57
2:H:293:ALA:HA	2:H:299:ARG:NH2	2.19	0.57
2:E:207:ALA:O	2:E:210:MET:HG2	2.03	0.57
2:H:25:ILE:HG22	2:H:50:GLU:HG3	1.87	0.57
2:H:248:PHE:O	2:H:251:MET:HB3	2.05	0.57
2:F:48:THR:HG22	2:F:51:ALA:H	1.68	0.57
2:E:199:HIS:O	2:E:203:LEU:HD12	2.04	0.57
2:A:60:LEU:HD11	2:A:75:LEU:HD13	1.85	0.57
2:A:170:ARG:HE	3:A:600:ANP:H2	1.68	0.57
2:E:204:LEU:HD11	2:E:248:PHE:CE1	2.40	0.57
2:G:126:PHE:HB3	2:G:267:ASN:HB3	1.86	0.57
2:G:218:LEU:HD12	2:G:262:ALA:HB3	1.85	0.57
2:C:234:GLY:HA2	2:B:243:MET:HE3	1.86	0.56
2:F:160:ILE:HB	2:F:221:VAL:HG22	1.87	0.56
2:C:135:GLN:HE21	3:C:600:ANP:H5'1	1.70	0.56
2:B:287:ILE:O	2:B:292:ILE:HD11	2.06	0.56
2:H:128:GLU:HG3	2:H:129:PHE:N	2.21	0.56
2:E:105:GLY:HA3	2:E:109:LEU:HD22	1.87	0.56
2:E:230:THR:HA	2:D:243:MET:HE1	1.88	0.56
2:C:162:THR:HB	2:C:223:SER:HB2	1.88	0.56
2:C:246:ALA:HB2	2:C:291:ILE:HD12	1.88	0.56
2:F:168:PRO:HG2	2:E:96:ARG:HG3	1.86	0.56
2:I:29:GLU:HB3	2:I:33:ILE:HB	1.88	0.56
2:E:161:ASP:HA	2:E:222:ASP:HB2	1.88	0.56
2:A:119:THR:HB	2:A:260:GLY:HA2	1.88	0.56
2:I:191:TYR:HB3	2:H:92:PHE:HD2	1.71	0.56
2:A:266:THR:HG22	2:A:267:ASN:H	1.70	0.55
2:B:219:LEU:HB3	2:B:263:VAL:HG12	1.88	0.55
2:F:105:GLY:HA3	2:F:334:VAL:HB	1.88	0.55
2:F:128:GLU:HG3	2:F:129:PHE:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:70:LYS:O	2:D:74:ILE:HG22	2.06	0.55
2:C:26:SER:O	2:C:29:GLU:HG3	2.06	0.55
2:B:90:THR:HA	2:B:93:HIS:HB3	1.88	0.55
2:F:268:GLN:HG2	2:E:294:HIS:CG	2.41	0.55
2:I:120:GLY:HA2	2:I:261:VAL:H	1.72	0.55
2:E:159:TYR:HD2	2:E:160:ILE:N	2.04	0.55
2:A:64:LYS:HD3	2:A:67:SER:HA	1.88	0.55
2:I:232:TYR:CG	2:I:241:ARG:HB2	2.42	0.55
2:D:38:VAL:HA	2:D:41:LEU:HD12	1.89	0.55
2:C:144:CYS:HB2	2:C:217:ALA:HB3	1.87	0.55
2:F:118:GLU:HG2	2:F:120:GLY:H	1.72	0.54
2:I:219:LEU:HD23	2:I:263:VAL:HG22	1.89	0.54
2:E:80:LYS:O	2:E:80:LYS:HG2	2.05	0.54
2:C:108:GLU:HG3	2:C:325:ALA:HB1	1.88	0.54
2:I:122:ILE:HG21	2:I:252:LEU:HD13	1.88	0.54
2:D:298:THR:HG23	2:D:317:SER:HB2	1.90	0.54
2:C:207:ALA:HA	2:C:210:MET:HB3	1.89	0.54
2:A:135:GLN:HG3	2:A:329:ILE:HD11	1.90	0.54
2:D:112:LEU:HD22	2:D:325:ALA:HB2	1.89	0.54
2:B:174:VAL:HG22	2:B:177:ARG:HH21	1.73	0.54
2:C:29:GLU:HB3	2:C:38:VAL:HG21	1.89	0.54
2:F:107:LYS:HD2	2:F:107:LYS:O	2.08	0.54
2:B:144:CYS:HA	2:B:154:GLU:HB2	1.90	0.53
2:E:144:CYS:HA	2:E:153:GLY:HA2	1.90	0.53
2:B:125:MET:HB2	2:B:266:THR:HG22	1.90	0.53
2:A:225:THR:HA	2:A:228:TYR:HD2	1.73	0.53
2:F:162:THR:HB	2:F:223:SER:O	2.09	0.53
2:D:143:THR:HG23	2:D:146:LEU:HD12	1.89	0.53
2:F:125:MET:HE3	2:F:300:LEU:HD13	1.91	0.53
2:F:232:TYR:CG	2:F:241:ARG:HB2	2.43	0.53
2:G:211:MET:HG3	2:G:216:TYR:HB2	1.90	0.53
2:A:25:ILE:HD11	2:A:48:THR:HA	1.89	0.53
2:E:136:ILE:O	2:E:140:LEU:HD12	2.08	0.53
2:G:168:PRO:HA	2:G:171:LEU:HD12	1.91	0.53
2:G:298:THR:HG23	2:G:317:SER:HB2	1.91	0.53
2:C:125:MET:HG2	2:C:300:LEU:HB2	1.91	0.53
2:E:130:ARG:NH2	2:D:316:ASP:H	2.07	0.53
2:H:207:ALA:O	2:H:211:MET:HG2	2.09	0.53
2:B:38:VAL:O	2:B:42:GLU:HG2	2.09	0.52
2:F:161:ASP:HB3	2:F:162:THR:HG23	1.91	0.52
2:H:66:ILE:HG23	2:H:70:LYS:HD2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:THR:O	2:B:201:THR:HG23	2.09	0.52
2:I:123:THR:HB	2:I:265:ILE:H	1.74	0.52
2:I:150:ARG:HH22	2:I:179:GLY:H	1.56	0.52
2:F:25:ILE:HG13	2:F:49:VAL:HG23	1.92	0.52
2:F:57:LYS:HA	2:F:60:LEU:HB3	1.91	0.52
2:F:165:THR:HG23	2:F:193:ARG:HH21	1.74	0.52
2:B:133:LYS:HD2	2:B:266:THR:HB	1.91	0.52
2:A:154:GLU:HG2	2:A:215:ARG:HD2	1.91	0.52
2:B:83:PRO:HB2	2:B:87:THR:HB	1.92	0.52
2:E:165:THR:HG22	2:E:165:THR:O	2.09	0.52
2:G:42:GLU:HG3	2:G:47:HIS:HD2	1.75	0.52
2:E:135:GLN:HG3	2:E:329:ILE:HD13	1.92	0.52
2:B:329:ILE:HG22	2:B:334:VAL:HG22	1.92	0.52
2:F:135:GLN:HE22	2:F:329:ILE:HA	1.74	0.52
2:A:287:ILE:HG13	2:A:288:GLY:N	2.24	0.52
2:E:199:HIS:NE2	2:D:84:MET:HB3	2.25	0.52
2:G:45:GLY:HA2	2:G:47:HIS:CE1	2.45	0.52
2:G:158:MET:HB2	2:G:216:TYR:HD2	1.74	0.52
2:I:167:ARG:HB3	2:I:170:ARG:HG3	1.91	0.51
2:D:157:ALA:HB3	2:D:189:VAL:HG22	1.93	0.51
2:C:227:LEU:HD23	2:B:250:ARG:HH22	1.76	0.51
2:H:56:PRO:HG2	2:H:59:GLU:HG3	1.93	0.51
2:I:220:ILE:HA	2:I:264:VAL:HB	1.91	0.51
2:E:36:ASN:HA	2:E:40:LYS:HG3	1.92	0.51
2:E:80:LYS:NZ	2:E:82:VAL:HG23	2.25	0.51
1:L:3:DT:H4'	2:H:242:GLN:HG3	1.92	0.51
2:G:23:GLN:HE21	2:G:82:VAL:HG12	1.74	0.51
2:E:193:ARG:HG3	2:E:194:GLY:N	2.25	0.51
2:F:56:PRO:HB3	2:G:196:ASN:HB2	1.93	0.51
2:D:223:SER:HB2	2:D:226:ALA:HB2	1.93	0.51
2:F:122:ILE:O	2:F:298:THR:HB	2.11	0.51
2:E:159:TYR:HE2	2:E:222:ASP:HB2	1.75	0.51
2:B:293:ALA:HA	2:B:299:ARG:NH2	2.25	0.51
2:F:142:VAL:HG21	2:F:175:ALA:HB2	1.93	0.51
2:H:148:ILE:HG12	2:H:154:GLU:HB3	1.93	0.51
2:F:41:LEU:O	2:F:46:TYR:HB3	2.10	0.51
2:C:258:GLU:HG3	2:C:259:PHE:HD1	1.76	0.50
2:B:36:ASN:O	2:B:40:LYS:HG2	2.10	0.50
2:F:210:MET:HE2	2:F:210:MET:N	2.26	0.50
2:C:168:PRO:HD2	2:B:96:ARG:HD2	1.93	0.50
2:F:161:ASP:OD1	2:F:194:GLY:HA3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:310:ARG:HH12	2:A:312:CYS:HB2	1.76	0.50
2:E:298:THR:HA	2:E:316:ASP:O	2.12	0.50
2:A:220:ILE:HG22	2:A:222:ASP:H	1.77	0.50
2:E:113:LEU:HB3	2:E:320:LEU:HD11	1.93	0.50
2:D:218:LEU:HD12	2:D:262:ALA:HB3	1.93	0.50
2:F:317:SER:OG	2:F:320:LEU:HG	2.12	0.50
2:I:233:SER:HB2	2:H:243:MET:HE3	1.94	0.50
1:L:4:DC:H5'	2:H:289:GLY:HA3	1.93	0.50
2:C:102:ILE:HG21	2:C:218:LEU:HD21	1.93	0.50
2:A:193:ARG:HG3	2:A:199:HIS:HE1	1.77	0.50
2:I:142:VAL:HG21	2:I:174:VAL:HB	1.94	0.50
2:G:158:MET:HB3	2:G:219:LEU:HA	1.93	0.50
2:C:232:TYR:CG	2:C:241:ARG:HB2	2.47	0.49
2:B:160:ILE:HG22	2:B:161:ASP:H	1.77	0.49
2:H:125:MET:HB2	2:H:300:LEU:HB2	1.93	0.49
2:A:135:GLN:HE22	3:A:600:ANP:H5'2	1.77	0.49
1:L:13:DC:H5'	2:E:289:GLY:HA3	1.95	0.49
2:B:228:TYR:HD2	2:B:241:ARG:HG3	1.77	0.49
2:A:95:ARG:HA	2:A:98:GLU:HG3	1.94	0.49
2:A:99:ILE:O	2:A:101:GLN:NE2	2.45	0.49
2:B:96:ARG:HA	2:B:99:ILE:HB	1.95	0.49
2:C:238:LEU:HD23	2:D:273:VAL:HG21	1.94	0.49
2:I:160:ILE:HD12	2:I:160:ILE:O	2.12	0.49
2:H:285:LYS:HG3	2:H:286:PRO:HD2	1.95	0.49
2:H:88:THR:H	2:H:91:GLU:HB3	1.78	0.49
2:C:160:ILE:HD12	2:C:221:VAL:HG22	1.94	0.49
2:B:256:ALA:HA	2:B:261:VAL:HG22	1.95	0.49
2:A:314:ILE:HG21	2:A:320:LEU:HD23	1.95	0.49
2:E:70:LYS:O	2:E:73:LYS:HG3	2.13	0.49
2:G:52:VAL:HG23	2:G:60:LEU:HD11	1.94	0.49
2:C:77:GLU:HA	2:C:80:LYS:HZ3	1.77	0.49
2:G:221:VAL:HG11	2:G:248:PHE:HZ	1.77	0.49
2:B:95:ARG:O	2:B:98:GLU:HG2	2.13	0.49
2:B:228:TYR:CD2	2:B:241:ARG:HG3	2.48	0.49
2:B:301:TYR:HD1	2:B:302:LEU:N	2.10	0.48
2:I:143:THR:HA	2:I:146:LEU:HD23	1.94	0.48
2:G:310:ARG:HE	2:G:329:ILE:HD13	1.78	0.48
2:A:204:LEU:HD11	2:A:255:LEU:HD12	1.93	0.48
2:H:24:PRO:HD2	2:H:83:PRO:HG2	1.95	0.48
1:L:19:DT:OP1	2:C:242:GLN:HG3	2.13	0.48
2:I:49:VAL:HG21	2:I:81:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:126:PHE:HB3	2:D:267:ASN:HB3	1.94	0.48
2:C:221:VAL:HB	2:C:265:ILE:HG22	1.95	0.48
2:B:52:VAL:HG11	2:B:74:ILE:HG22	1.96	0.48
2:A:139:THR:HA	2:A:174:VAL:HG11	1.95	0.48
2:H:89:ALA:HB1	2:H:93:HIS:HE2	1.78	0.48
2:G:124:GLU:O	2:G:299:ARG:HA	2.13	0.48
2:G:145:GLN:HE22	2:G:189:VAL:HG13	1.77	0.48
2:A:131:THR:HG22	2:A:304:LYS:HD2	1.95	0.48
2:B:299:ARG:HG2	2:B:300:LEU:N	2.28	0.48
2:A:101:GLN:HB3	2:A:118:GLU:HG2	1.95	0.48
2:F:99:ILE:HG21	2:F:118:GLU:HG3	1.95	0.48
2:I:215:ARG:NH1	2:I:216:TYR:H	2.11	0.48
2:E:104:THR:HG22	2:E:113:LEU:HD11	1.96	0.48
2:E:156:LYS:HE3	2:E:216:TYR:HA	1.95	0.48
2:G:172:LEU:HA	2:G:185:VAL:HG11	1.95	0.48
2:C:36:ASN:O	2:C:39:LYS:HG2	2.14	0.48
2:B:270:VAL:HG23	2:B:285:LYS:O	2.13	0.48
2:F:224:ALA:HB3	2:F:265:ILE:HD11	1.95	0.48
2:E:264:VAL:HG23	2:E:264:VAL:O	2.14	0.48
2:H:186:LEU:HB3	2:G:90:THR:HG22	1.95	0.48
2:E:272:GLN:HB3	2:E:285:LYS:HZ2	1.79	0.48
2:H:167:ARG:HA	2:H:167:ARG:HD3	1.68	0.48
2:D:259:PHE:HB3	2:D:261:VAL:HG13	1.96	0.48
2:B:33:ILE:HG21	2:B:74:ILE:HG12	1.96	0.48
2:E:122:ILE:HG12	2:E:252:LEU:HD22	1.96	0.48
2:B:194:GLY:HA2	2:B:199:HIS:CD2	2.49	0.47
2:B:218:LEU:HD12	2:B:219:LEU:N	2.29	0.47
2:I:177:ARG:HD3	2:I:332:ASP:OD2	2.14	0.47
2:E:201:THR:HA	2:E:204:LEU:HD12	1.96	0.47
2:H:103:THR:HG22	2:H:152:GLY:HA3	1.94	0.47
2:H:218:LEU:HA	2:H:261:VAL:HG13	1.96	0.47
2:H:221:VAL:O	2:H:265:ILE:HA	2.14	0.47
2:F:250:ARG:NH1	2:F:254:ARG:HG3	2.29	0.47
2:E:66:ILE:HG13	2:E:70:LYS:HG2	1.96	0.47
2:F:86:PHE:CZ	2:G:158:MET:HE1	2.49	0.47
2:H:104:THR:HG22	2:H:140:LEU:HD21	1.95	0.47
2:D:100:ILE:HB	2:D:119:THR:HG21	1.97	0.47
2:G:53:ALA:HB2	2:G:78:ALA:HB1	1.96	0.47
2:C:47:HIS:CD2	2:C:209:ASP:HB3	2.50	0.47
2:F:119:THR:HA	2:F:262:ALA:HB2	1.96	0.47
2:E:54:TYR:CE2	2:E:258:GLU:HG2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:28:LEU:HA	2:H:49:VAL:HG22	1.96	0.47
2:C:326:MET:HE3	2:C:326:MET:N	2.30	0.47
2:E:199:HIS:HE2	2:D:84:MET:HB3	1.79	0.47
2:H:57:LYS:HE2	2:H:75:LEU:HD23	1.96	0.47
2:C:251:MET:HE3	2:C:252:LEU:N	2.30	0.47
2:B:299:ARG:HB3	2:B:316:ASP:OD1	2.14	0.47
2:A:27:ARG:HD3	2:A:80:LYS:HD3	1.96	0.47
2:F:66:ILE:HG12	2:F:70:LYS:HD2	1.97	0.47
3:I:600:ANP:H5'1	2:H:321:PRO:HA	1.95	0.47
2:H:126:PHE:HD2	2:H:269:VAL:HG12	1.80	0.47
2:D:47:HIS:CE1	2:D:209:ASP:HB2	2.50	0.47
2:I:75:LEU:O	2:I:78:ALA:HB3	2.15	0.47
2:E:46:TYR:HA	2:E:51:ALA:HB1	1.96	0.47
2:F:132:GLY:O	2:F:135:GLN:HG2	2.15	0.47
2:F:138:HIS:NE2	2:F:166:PHE:HB2	2.30	0.47
2:F:250:ARG:HG3	2:G:230:THR:HG21	1.96	0.47
2:H:167:ARG:HG3	2:G:319:CYS:HB3	1.97	0.47
2:H:205:TYR:CE1	2:H:251:MET:HE1	2.50	0.47
2:H:233:SER:HB2	2:G:243:MET:HE3	1.95	0.47
2:D:299:ARG:HG3	2:D:316:ASP:HB3	1.97	0.47
2:A:314:ILE:HD12	2:A:320:LEU:HG	1.97	0.47
2:H:293:ALA:HA	2:H:299:ARG:HH22	1.80	0.47
2:D:232:TYR:CG	2:D:241:ARG:HB2	2.50	0.46
2:C:129:PHE:O	2:C:130:ARG:HG3	2.15	0.46
2:F:203:LEU:HD22	2:F:206:GLN:HE21	1.80	0.46
2:I:197:THR:HB	2:I:231:ASP:OD2	2.15	0.46
2:B:101:GLN:HG3	2:B:118:GLU:HA	1.96	0.46
2:B:245:LEU:HB2	2:B:291:ILE:HG21	1.98	0.46
2:B:298:THR:HG23	2:B:317:SER:HB3	1.97	0.46
2:A:138:HIS:HA	2:A:159:TYR:HE2	1.81	0.46
2:H:133:LYS:HA	2:H:136:ILE:HD12	1.96	0.46
2:E:304:LYS:HE2	2:E:310:ARG:NH2	2.30	0.46
2:H:177:ARG:HH22	2:H:335:GLY:HA3	1.81	0.46
2:D:252:LEU:HD22	2:D:263:VAL:HG11	1.97	0.46
2:B:36:ASN:O	2:B:39:LYS:HG2	2.15	0.46
2:B:125:MET:HE1	2:B:300:LEU:HD21	1.98	0.46
2:G:170:ARG:NH2	2:G:331:ALA:HA	2.30	0.46
2:G:211:MET:HA	2:G:214:SER:O	2.15	0.46
2:A:27:ARG:HB2	2:A:80:LYS:HE2	1.98	0.46
2:B:49:VAL:HG23	2:B:78:ALA:HB1	1.98	0.46
2:F:27:ARG:HG3	2:F:29:GLU:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:221:VAL:H	2:F:264:VAL:HG22	1.79	0.46
2:E:134:THR:HG21	2:E:165:THR:HG22	1.97	0.46
2:E:326:MET:HE3	2:E:326:MET:H	1.81	0.46
2:C:47:HIS:HB2	2:C:208:GLU:HG3	1.97	0.46
2:B:131:THR:HG22	3:B:600:ANP:O3G	2.16	0.46
2:I:197:THR:HG21	2:H:250:ARG:HE	1.81	0.46
2:H:89:ALA:HB1	2:H:93:HIS:NE2	2.31	0.46
2:C:304:LYS:HA	2:C:310:ARG:HD3	1.98	0.46
3:B:600:ANP:H5'1	2:A:316:ASP:H	1.80	0.46
2:E:133:LYS:HE3	3:D:401:ANP:O2G	2.15	0.46
2:H:136:ILE:HA	2:H:334:VAL:HG21	1.96	0.46
2:F:82:VAL:HG12	2:F:83:PRO:HD2	1.98	0.46
2:D:156:LYS:HB2	2:D:216:TYR:CD2	2.50	0.46
2:B:128:GLU:HG3	2:B:132:GLY:HA3	1.97	0.45
2:F:159:TYR:HB3	2:F:191:TYR:HA	1.98	0.45
2:F:211:MET:HB2	2:F:259:PHE:CD2	2.51	0.45
2:E:145:GLN:H	2:E:153:GLY:HA2	1.82	0.45
2:D:102:ILE:HG12	2:D:152:GLY:HA2	1.97	0.45
2:G:170:ARG:HH21	2:G:331:ALA:HA	1.81	0.45
2:B:122:ILE:HA	2:B:263:VAL:HG23	1.97	0.45
2:E:30:GLN:OE1	2:E:30:GLN:HA	2.16	0.45
2:E:189:VAL:HG23	2:D:89:ALA:HB3	1.98	0.45
2:H:256:ALA:HA	2:H:261:VAL:HB	1.98	0.45
2:D:317:SER:OG	2:D:320:LEU:HB2	2.16	0.45
2:C:230:THR:HG22	2:B:246:ALA:HB1	1.98	0.45
2:B:70:LYS:HA	2:B:70:LYS:HD3	1.82	0.45
2:I:157:ALA:HB1	2:I:189:VAL:HG13	1.98	0.45
2:C:227:LEU:HD23	2:B:250:ARG:NH2	2.31	0.45
2:I:190:ALA:HB1	2:H:86:PHE:HD2	1.82	0.45
2:B:238:LEU:O	2:B:242:GLN:HG2	2.17	0.45
2:F:301:TYR:HD2	2:F:315:TYR:HB2	1.81	0.45
2:H:205:TYR:HE1	2:H:251:MET:HE1	1.82	0.45
2:C:269:VAL:HG22	2:B:294:HIS:NE2	2.32	0.45
2:B:127:GLY:HA2	2:B:269:VAL:HG13	1.99	0.45
2:A:160:ILE:HD12	2:A:160:ILE:C	2.41	0.45
2:F:161:ASP:CG	2:F:194:GLY:HA3	2.42	0.45
2:I:175:ALA:HA	2:I:180:LEU:HD21	1.99	0.45
2:E:220:ILE:HG23	2:E:264:VAL:O	2.16	0.45
2:H:25:ILE:HB	2:H:49:VAL:HB	1.98	0.45
2:D:177:ARG:HD2	2:D:332:ASP:HB2	1.97	0.45
2:C:161:ASP:CG	2:C:166:PHE:HB2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:212:VAL:HA	2:C:259:PHE:CZ	2.51	0.45
2:B:249:LEU:CD2	2:B:292:ILE:HG22	2.46	0.45
2:C:315:TYR:O	2:D:130:ARG:HD3	2.17	0.45
2:B:159:TYR:CE1	2:B:166:PHE:HB2	2.52	0.45
2:F:86:PHE:HZ	2:G:158:MET:HE1	1.82	0.45
2:E:210:MET:HE2	2:E:210:MET:HB3	1.80	0.45
2:G:56:PRO:HD2	2:G:59:GLU:HG3	1.99	0.45
2:G:221:VAL:HG11	2:G:248:PHE:CZ	2.52	0.45
1:L:18:DT:H4'	2:C:242:GLN:HG3	1.98	0.45
2:B:112:LEU:HD23	2:B:325:ALA:HB2	1.99	0.45
2:B:170:ARG:HH22	2:B:333:GLY:HA2	1.82	0.45
2:H:159:TYR:HE1	2:H:161:ASP:HB2	1.82	0.45
2:H:252:LEU:HD13	2:H:265:ILE:HD11	1.98	0.45
2:D:119:THR:HG22	2:D:262:ALA:HB2	1.99	0.45
2:D:133:LYS:HD2	2:D:266:THR:HG23	1.98	0.45
2:C:64:LYS:HA	2:C:64:LYS:HD3	1.79	0.45
2:A:112:LEU:HA	2:A:314:ILE:HD11	1.98	0.45
2:A:272:GLN:HE21	2:A:283:PRO:HA	1.81	0.45
2:I:23:GLN:N	2:I:24:PRO:HD3	2.31	0.45
2:C:204:LEU:HD21	2:C:219:LEU:HD11	1.99	0.44
2:B:139:THR:HG23	2:B:140:LEU:HG	1.98	0.44
2:B:156:LYS:HE3	2:B:156:LYS:HB2	1.65	0.44
2:B:229:ARG:O	2:B:233:SER:HB3	2.17	0.44
2:A:210:MET:HB3	2:A:216:TYR:CD2	2.50	0.44
2:D:208:GLU:HB2	2:D:255:LEU:HD11	1.98	0.44
2:C:106:SER:HB2	2:C:335:GLY:O	2.16	0.44
2:B:313:LYS:H	2:B:313:LYS:HG2	1.59	0.44
2:A:106:SER:O	2:A:110:ASP:HB2	2.18	0.44
2:A:155:GLY:HA3	2:A:215:ARG:O	2.17	0.44
2:F:146:LEU:HD11	2:F:150:ARG:NH1	2.32	0.44
2:C:23:GLN:HE22	2:C:49:VAL:HB	1.82	0.44
2:G:170:ARG:HH22	3:G:402:ANP:HN61	1.64	0.44
2:C:72:ASP:O	2:C:76:THR:HG22	2.17	0.44
2:C:325:ALA:C	2:C:326:MET:HE3	2.43	0.44
2:B:233:SER:HB2	2:A:243:MET:HE3	1.99	0.44
2:A:122:ILE:HA	2:A:263:VAL:HG13	1.99	0.44
2:H:243:MET:HB3	2:H:247:ARG:HH21	1.81	0.44
2:D:198:ASP:O	2:D:202:GLN:HG3	2.18	0.44
2:C:131:THR:HA	2:C:310:ARG:HD2	1.99	0.44
2:B:268:GLN:CD	2:A:294:HIS:HE1	2.25	0.44
2:F:167:ARG:NE	2:E:118:GLU:HG3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:129:PHE:HE1	2:H:316:ASP:HB2	1.83	0.44
2:D:113:LEU:HA	2:D:320:LEU:HD21	1.99	0.44
2:D:124:GLU:O	2:D:299:ARG:HA	2.18	0.44
2:A:122:ILE:HG22	2:A:124:GLU:HG3	1.98	0.44
2:A:299:ARG:HH21	2:A:315:TYR:HB3	1.82	0.44
2:C:268:GLN:NE2	2:B:294:HIS:HB3	2.32	0.44
2:B:156:LYS:HE3	2:B:217:ALA:HB2	1.99	0.44
2:A:22:PRO:HB3	2:A:211:MET:HE1	1.98	0.44
2:I:232:TYR:CD1	2:I:241:ARG:HB2	2.52	0.44
2:C:88:THR:HG23	2:C:91:GLU:H	1.83	0.44
2:B:139:THR:HA	2:B:174:VAL:HG11	1.99	0.44
2:A:246:ALA:HB2	2:A:291:ILE:HG12	1.99	0.44
2:H:156:LYS:HB2	2:H:216:TYR:CD2	2.53	0.44
2:H:158:MET:HE2	2:H:216:TYR:CD2	2.52	0.44
2:H:250:ARG:O	2:H:253:LEU:HB2	2.18	0.44
2:B:126:PHE:O	2:B:302:LEU:HB2	2.18	0.44
2:B:156:LYS:HD2	2:B:215:ARG:O	2.18	0.44
2:A:96:ARG:HA	2:A:96:ARG:HD2	1.77	0.44
2:I:139:THR:HG21	2:I:334:VAL:HG22	2.00	0.44
2:H:146:LEU:HD13	2:H:150:ARG:HB3	1.99	0.44
2:H:249:LEU:HD21	2:H:292:ILE:HD12	1.99	0.44
2:G:259:PHE:HB3	2:G:261:VAL:HG13	1.99	0.44
2:B:219:LEU:O	2:B:263:VAL:HA	2.18	0.43
2:F:133:LYS:HB2	2:F:133:LYS:HE2	1.63	0.43
2:I:22:PRO:HB2	2:I:24:PRO:HD3	2.00	0.43
2:I:258:GLU:HG3	2:I:259:PHE:HD1	1.83	0.43
2:E:102:ILE:HD12	2:E:102:ILE:HA	1.90	0.43
2:A:320:LEU:HD12	2:A:320:LEU:HA	1.68	0.43
2:F:317:SER:O	3:G:402:ANP:H2'	2.18	0.43
2:I:129:PHE:HZ	2:H:315:TYR:HB3	1.82	0.43
2:D:252:LEU:HD23	2:D:252:LEU:HA	1.89	0.43
2:B:199:HIS:O	2:B:202:GLN:HG3	2.18	0.43
2:I:120:GLY:CA	2:I:261:VAL:H	2.32	0.43
2:H:208:GLU:HA	2:H:211:MET:HG2	2.00	0.43
2:G:303:ARG:O	2:G:310:ARG:HG3	2.17	0.43
2:C:125:MET:HB2	2:C:125:MET:HE3	1.74	0.43
2:B:160:ILE:HB	2:B:221:VAL:HG13	2.01	0.43
2:I:168:PRO:HG2	2:H:95:ARG:HH22	1.84	0.43
2:E:167:ARG:HG2	2:D:319:CYS:HB2	2.01	0.43
2:B:158:MET:HE1	2:B:216:TYR:CD2	2.53	0.43
2:B:160:ILE:HB	2:B:221:VAL:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:41:LEU:HB3	2:F:46:TYR:CD2	2.53	0.43
2:I:186:LEU:O	2:H:89:ALA:HB2	2.18	0.43
2:E:132:GLY:O	2:E:136:ILE:HD12	2.19	0.43
2:G:96:ARG:HA	2:G:99:ILE:HD13	1.99	0.43
2:C:158:MET:HB2	2:C:216:TYR:CE2	2.53	0.43
2:C:317:SER:O	3:D:402:ANP:H8	2.19	0.43
2:B:47:HIS:NE2	2:B:208:GLU:HB2	2.33	0.43
3:B:600:ANP:N7	2:A:318:PRO:HA	2.33	0.43
2:A:126:PHE:HZ	2:A:315:TYR:CD2	2.36	0.43
2:F:139:THR:HA	2:F:174:VAL:HG11	2.01	0.43
2:F:185:VAL:O	2:F:189:VAL:HG23	2.18	0.43
2:I:60:LEU:HD12	2:I:60:LEU:HA	1.81	0.43
2:E:104:THR:HG23	2:E:109:LEU:HB3	2.00	0.43
2:G:135:GLN:HG3	3:G:402:ANP:H8	1.99	0.43
2:A:312:CYS:H	2:A:325:ALA:HB3	1.83	0.43
2:G:47:HIS:ND1	2:G:208:GLU:HB3	2.33	0.43
2:C:142:VAL:HG11	2:C:178:TYR:CD1	2.54	0.43
2:A:109:LEU:HA	2:A:112:LEU:HD23	2.00	0.43
2:A:25:ILE:HD12	2:A:25:ILE:N	2.34	0.43
2:A:125:MET:HE1	2:A:264:VAL:HG13	2.01	0.43
2:H:172:LEU:HD11	2:H:186:LEU:HD22	2.01	0.43
2:C:89:ALA:HB3	2:D:186:LEU:O	2.18	0.43
2:F:86:PHE:CE1	2:G:210:MET:HE2	2.54	0.43
2:I:170:ARG:HH12	2:H:318:PRO:HB2	1.84	0.43
2:G:220:ILE:HG22	2:G:222:ASP:H	1.84	0.43
2:I:306:ARG:HD3	2:I:306:ARG:HA	1.83	0.42
2:D:124:GLU:HG3	2:D:267:ASN:HB2	2.00	0.42
2:B:40:LYS:HD2	2:B:64:LYS:HD2	2.01	0.42
2:A:170:ARG:O	2:A:174:VAL:HG23	2.18	0.42
2:E:270:VAL:HB	2:E:287:ILE:HG22	2.00	0.42
2:H:99:ILE:HG21	2:H:118:GLU:HB3	2.01	0.42
2:E:80:LYS:HB3	2:E:80:LYS:HE3	1.77	0.42
2:E:191:TYR:HB3	2:D:89:ALA:HB2	2.01	0.42
2:B:156:LYS:HD2	2:B:216:TYR:HA	2.02	0.42
2:B:162:THR:HB	2:B:223:SER:O	2.19	0.42
2:B:288:GLY:HA3	2:B:292:ILE:HG12	2.02	0.42
2:A:122:ILE:HG12	2:A:253:LEU:HD23	2.00	0.42
2:A:313:LYS:HG3	2:A:322:GLU:HB3	2.01	0.42
2:D:204:LEU:HD12	2:D:204:LEU:HA	1.82	0.42
2:B:201:THR:HA	2:B:248:PHE:HZ	1.85	0.42
2:B:210:MET:HE3	2:B:210:MET:HB2	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:45:GLY:H	2:A:47:HIS:HE1	1.68	0.42
2:E:106:SER:H	2:E:109:LEU:HB2	1.84	0.42
2:G:41:LEU:O	2:G:46:TYR:HB2	2.20	0.42
2:A:287:ILE:HG13	2:A:288:GLY:H	1.84	0.42
2:E:220:ILE:HG22	2:E:222:ASP:H	1.84	0.42
2:G:112:LEU:HD11	2:G:314:ILE:HG12	2.01	0.42
2:B:235:ARG:HD2	2:B:235:ARG:HA	1.85	0.42
2:E:174:VAL:O	2:E:177:ARG:HB3	2.20	0.42
2:H:106:SER:OG	2:H:109:LEU:HB2	2.19	0.42
2:A:126:PHE:CE2	2:A:286:PRO:HG3	2.54	0.42
2:F:122:ILE:HG13	2:F:296:SER:HA	2.01	0.42
2:I:298:THR:HA	2:I:315:TYR:CE2	2.55	0.42
2:E:128:GLU:HG3	2:E:129:PHE:H	1.85	0.42
2:E:312:CYS:HB2	2:E:327:PHE:CE1	2.55	0.42
2:E:223:SER:HA	2:E:266:THR:HB	2.02	0.42
2:G:119:THR:HA	2:G:262:ALA:HB2	2.01	0.42
2:A:170:ARG:NE	3:A:600:ANP:H2	2.34	0.42
2:E:23:GLN:HB2	2:E:24:PRO:HD3	2.02	0.42
2:D:224:ALA:HB2	2:D:265:ILE:HB	2.01	0.42
2:C:54:TYR:HD2	2:C:254:ARG:HG3	1.85	0.41
2:H:186:LEU:HD12	2:H:186:LEU:HA	1.89	0.41
2:B:158:MET:HE1	2:B:216:TYR:CD1	2.55	0.41
2:H:134:THR:HG22	2:H:138:HIS:CE1	2.55	0.41
2:D:125:MET:HE3	2:D:125:MET:HB2	1.86	0.41
2:E:228:TYR:HE1	2:E:244:HIS:HB3	1.85	0.41
2:C:166:PHE:CE1	2:C:171:LEU:HD11	2.55	0.41
2:E:112:LEU:HD22	2:E:325:ALA:HB3	2.02	0.41
2:E:317:SER:O	3:E:600:ANP:H3'	2.19	0.41
2:H:147:PRO:HD2	2:H:150:ARG:HD3	2.03	0.41
2:G:58:LYS:HB2	2:G:58:LYS:HE3	1.83	0.41
2:B:315:TYR:HD1	2:B:315:TYR:HA	1.75	0.41
2:F:140:LEU:HD12	2:F:140:LEU:HA	1.83	0.41
2:E:193:ARG:HG2	2:E:195:PHE:CE1	2.56	0.41
2:H:267:ASN:HD22	2:H:286:PRO:HB2	1.85	0.41
2:D:165:THR:HG22	2:D:165:THR:O	2.20	0.41
2:C:189:VAL:HG23	2:B:89:ALA:HB3	2.01	0.41
2:B:47:HIS:CE1	2:B:209:ASP:HA	2.56	0.41
2:B:158:MET:HB2	2:B:219:LEU:HA	2.02	0.41
2:B:187:ASP:HA	2:A:89:ALA:HB3	2.02	0.41
2:A:117:ILE:HG23	2:A:123:THR:HG21	2.02	0.41
2:A:124:GLU:O	2:A:299:ARG:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:133:LYS:HE2	2:H:294:HIS:ND1	2.35	0.41
2:I:168:PRO:HA	2:I:171:LEU:HD12	2.03	0.41
2:I:199:HIS:O	2:I:202:GLN:HG3	2.21	0.41
2:H:102:ILE:HA	2:H:152:GLY:HA2	2.02	0.41
2:G:74:ILE:HG13	2:G:74:ILE:H	1.70	0.41
2:C:75:LEU:HD23	2:C:75:LEU:HA	1.82	0.41
2:C:197:THR:O	2:C:200:GLN:HG2	2.21	0.41
2:C:299:ARG:HB2	2:C:315:TYR:HB3	2.02	0.41
2:I:163:GLU:HG2	2:I:164:GLY:H	1.86	0.41
2:I:167:ARG:HB2	2:I:170:ARG:CZ	2.50	0.41
2:E:320:LEU:HD23	2:E:321:PRO:HD2	2.03	0.41
2:H:141:ALA:HB1	2:H:189:VAL:HG11	2.03	0.41
2:I:142:VAL:HG13	2:I:180:LEU:HD11	2.02	0.41
2:E:183:SER:HB2	2:E:187:ASP:HB2	2.02	0.41
2:D:232:TYR:HB2	2:D:241:ARG:HD3	2.02	0.41
2:G:142:VAL:HG21	2:G:174:VAL:HG13	2.02	0.41
2:G:205:TYR:O	2:G:208:GLU:HB2	2.21	0.41
2:A:67:SER:HA	2:A:71:ALA:HB3	2.03	0.41
2:A:124:GLU:HA	2:A:265:ILE:O	2.21	0.41
2:A:139:THR:HG22	2:A:174:VAL:HG21	2.03	0.41
2:A:215:ARG:O	2:A:215:ARG:HD3	2.19	0.41
2:A:265:ILE:HD12	2:A:265:ILE:N	2.35	0.41
2:F:211:MET:HG2	2:F:261:VAL:HG11	2.03	0.41
2:I:24:PRO:HG3	2:I:48:THR:HG23	2.02	0.41
2:I:251:MET:O	2:I:254:ARG:HG3	2.20	0.41
2:E:166:PHE:CE1	2:E:168:PRO:HG3	2.55	0.41
2:H:46:TYR:HA	2:H:51:ALA:HB1	2.03	0.41
2:G:107:LYS:HD2	2:G:107:LYS:HA	1.91	0.41
2:G:146:LEU:HD23	2:G:150:ARG:HD2	2.02	0.41
1:L:9:DC:O3'	2:F:242:GLN:HG3	2.20	0.41
2:H:159:TYR:CE1	2:H:161:ASP:HB2	2.56	0.41
2:H:207:ALA:O	2:H:210:MET:HG2	2.21	0.41
2:H:242:GLN:HB3	2:H:291:ILE:HD12	2.02	0.41
2:G:185:VAL:HG13	2:G:186:LEU:HD23	2.03	0.41
1:L:14:DG:H5'	1:L:14:DG:C8	2.56	0.40
2:C:55:ALA:HB1	2:C:59:GLU:HB2	2.02	0.40
2:A:265:ILE:HD12	2:A:265:ILE:H	1.85	0.40
2:F:131:THR:HA	2:F:310:ARG:NH1	2.36	0.40
2:I:196:ASN:CG	2:I:199:HIS:HB2	2.46	0.40
2:E:245:LEU:O	2:E:249:LEU:HG	2.21	0.40
1:L:25:DT:C4	2:B:273:VAL:HG12	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:HIS:H	2:B:47:HIS:CD2	2.40	0.40
2:F:163:GLU:HA	2:F:193:ARG:HH12	1.86	0.40
2:F:165:THR:HG23	2:F:193:ARG:NH2	2.36	0.40
2:F:201:THR:HA	2:F:248:PHE:HZ	1.86	0.40
2:F:329:ILE:HD11	3:E:600:ANP:O4'	2.20	0.40
2:I:186:LEU:HD12	2:I:186:LEU:HA	1.95	0.40
2:E:159:TYR:HB3	2:E:166:PHE:CE2	2.56	0.40
2:E:225:THR:O	2:E:287:ILE:HD11	2.22	0.40
2:H:28:LEU:HD12	2:H:49:VAL:HG22	2.02	0.40
2:G:145:GLN:NE2	2:G:189:VAL:HG13	2.36	0.40
2:C:36:ASN:HA	2:C:39:LYS:HD3	2.04	0.40
2:C:63:ILE:H	2:C:63:ILE:HG13	1.75	0.40
2:F:228:TYR:O	2:F:241:ARG:HD2	2.21	0.40
2:D:309:THR:HB	2:D:326:MET:HE3	2.02	0.40
2:I:197:THR:HA	2:I:227:LEU:HD13	2.02	0.40
2:E:91:GLU:H	2:E:91:GLU:HG2	1.65	0.40
2:D:158:MET:HB2	2:D:219:LEU:HA	2.03	0.40
2:C:172:LEU:HD23	2:C:172:LEU:HA	1.88	0.40
2:B:310:ARG:HE	2:B:310:ARG:HB2	1.65	0.40
2:F:218:LEU:HD12	2:F:218:LEU:HA	1.92	0.40
2:F:314:ILE:H	2:F:322:GLU:HG3	1.85	0.40
2:D:146:LEU:HD22	2:D:150:ARG:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	304/361 (84%)	274 (90%)	30 (10%)	0	100	100
2	B	296/361 (82%)	267 (90%)	28 (10%)	1 (0%)	37	65
2	C	303/361 (84%)	287 (95%)	16 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	302/361 (84%)	291 (96%)	11 (4%)	0	100	100
2	E	302/361 (84%)	267 (88%)	32 (11%)	3 (1%)	13	38
2	F	302/361 (84%)	272 (90%)	30 (10%)	0	100	100
2	G	303/361 (84%)	289 (95%)	14 (5%)	0	100	100
2	H	303/361 (84%)	273 (90%)	28 (9%)	2 (1%)	19	47
2	I	303/361 (84%)	284 (94%)	18 (6%)	1 (0%)	37	65
All	All	2718/3249 (84%)	2504 (92%)	207 (8%)	7 (0%)	38	65

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	83	PRO
2	B	86	PHE
2	I	212	VAL
2	E	146	LEU
2	H	95	ARG
2	E	99	ILE
2	H	321	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	249/290 (86%)	234 (94%)	15 (6%)	16	42
2	B	245/290 (84%)	229 (94%)	16 (6%)	14	39
2	C	249/290 (86%)	242 (97%)	7 (3%)	38	71
2	D	248/290 (86%)	236 (95%)	12 (5%)	21	52
2	E	248/290 (86%)	225 (91%)	23 (9%)	7	22
2	F	248/290 (86%)	233 (94%)	15 (6%)	16	42
2	G	249/290 (86%)	235 (94%)	14 (6%)	17	46
2	H	249/290 (86%)	235 (94%)	14 (6%)	17	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	249/290 (86%)	234 (94%)	15 (6%)	16	42
All	All	2234/2610 (86%)	2103 (94%)	131 (6%)	19	43

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	82	VAL
2	C	90	THR
2	C	146	LEU
2	C	219	LEU
2	C	309	THR
2	C	319	CYS
2	C	334	VAL
2	B	77	GLU
2	B	191	TYR
2	B	195	PHE
2	B	196	ASN
2	B	211	MET
2	B	213	GLU
2	B	218	LEU
2	B	227	LEU
2	B	248	PHE
2	B	251	MET
2	B	252	LEU
2	B	253	LEU
2	B	270	VAL
2	B	314	ILE
2	B	315	TYR
2	B	327	PHE
2	A	34	ASN
2	A	52	VAL
2	A	82	VAL
2	A	101	GLN
2	A	112	LEU
2	A	121	SER
2	A	131	THR
2	A	209	ASP
2	A	216	TYR
2	A	218	LEU
2	A	225	THR
2	A	253	LEU
2	A	268	GLN

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Mol	Chain	Res	Type
2	A	270	VAL
2	A	297	THR
2	F	25	ILE
2	F	46	TYR
2	F	81	LEU
2	F	82	VAL
2	F	90	THR
2	F	123	THR
2	F	149	ASP
2	F	169	GLU
2	F	172	LEU
2	F	176	GLU
2	F	191	TYR
2	F	265	ILE
2	F	297	THR
2	F	311	ILE
2	F	329	ILE
2	I	82	VAL
2	I	93	HIS
2	I	119	THR
2	I	121	SER
2	I	136	ILE
2	I	145	GLN
2	I	170	ARG
2	I	189	VAL
2	I	197	THR
2	I	216	TYR
2	I	223	SER
2	I	243	MET
2	I	244	HIS
2	I	302	LEU
2	I	309	THR
2	E	60	LEU
2	E	82	VAL
2	E	84	MET
2	E	124	GLU
2	E	125	MET
2	E	131	THR
2	E	134	THR
2	E	142	VAL
2	E	156	LYS
2	E	174	VAL

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Mol	Chain	Res	Type
2	E	186	LEU
2	E	203	LEU
2	E	209	ASP
2	E	211	MET
2	E	219	LEU
2	E	225	THR
2	E	237	GLU
2	E	243	MET
2	E	253	LEU
2	E	265	ILE
2	E	266	THR
2	E	269	VAL
2	E	320	LEU
2	H	49	VAL
2	H	61	ILE
2	H	82	VAL
2	H	103	THR
2	H	106	SER
2	H	111	LYS
2	H	139	THR
2	H	172	LEU
2	H	200	GLN
2	H	210	MET
2	H	212	VAL
2	H	222	ASP
2	H	249	LEU
2	H	315	TYR
2	D	48	THR
2	D	62	ASN
2	D	128	GLU
2	D	135	GLN
2	D	158	MET
2	D	162	THR
2	D	163	GLU
2	D	203	LEU
2	D	214	SER
2	D	221	VAL
2	D	269	VAL
2	D	315	TYR
2	G	47	HIS
2	G	48	THR
2	G	82	VAL

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Mol	Chain	Res	Type
2	G	99	ILE
2	G	102	ILE
2	G	113	LEU
2	G	124	GLU
2	G	163	GLU
2	G	172	LEU
2	G	300	LEU
2	G	306	ARG
2	G	310	ARG
2	G	315	TYR
2	G	330	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	23	GLN
2	C	62	ASN
2	C	196	ASN
2	C	290	ASN
2	B	30	GLN
2	B	34	ASN
2	B	93	HIS
2	B	101	GLN
2	B	290	ASN
2	A	114	GLN
2	A	188	ASN
2	A	202	GLN
2	F	23	GLN
2	F	62	ASN
2	F	188	ASN
2	F	242	GLN
2	I	199	HIS
2	I	268	GLN
2	H	47	HIS
2	H	62	ASN
2	H	200	GLN
2	G	135	GLN
2	G	145	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 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	$\# Z > 2$
3	ANP	D	402	4	29,33,33	2.40	6 (20%)	31,52,52	1.50	4 (12%)
3	ANP	A	600	-	29,33,33	2.49	6 (20%)	31,52,52	1.48	5 (16%)
3	ANP	I	600	-	29,33,33	2.44	6 (20%)	31,52,52	1.53	5 (16%)
3	ANP	B	600	-	29,33,33	2.44	6 (20%)	31,52,52	1.64	5 (16%)
3	ANP	G	401	4	29,33,33	2.45	6 (20%)	31,52,52	1.46	5 (16%)
3	ANP	E	600	4	29,33,33	2.45	6 (20%)	31,52,52	1.49	5 (16%)
3	ANP	G	402	4	29,33,33	2.49	6 (20%)	31,52,52	1.46	4 (12%)
3	ANP	C	600	4	29,33,33	2.52	6 (20%)	31,52,52	1.46	4 (12%)
3	ANP	D	401	4	29,33,33	2.44	6 (20%)	31,52,52	1.55	5 (16%)

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
3	ANP	D	402	4	-	7/14/38/38	0/3/3/3
3	ANP	A	600	-	-	5/14/38/38	0/3/3/3
3	ANP	I	600	-	-	8/14/38/38	0/3/3/3
3	ANP	B	600	-	-	6/14/38/38	0/3/3/3
3	ANP	G	401	4	-	6/14/38/38	0/3/3/3
3	ANP	E	600	4	-	5/14/38/38	0/3/3/3
3	ANP	G	402	4	-	7/14/38/38	0/3/3/3
3	ANP	C	600	4	-	7/14/38/38	0/3/3/3
3	ANP	D	401	4	-	5/14/38/38	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	600	ANP	PB-O3A	9.15	1.70	1.59
3	A	600	ANP	PB-O3A	9.10	1.70	1.59
3	G	402	ANP	PB-O3A	8.91	1.70	1.59
3	E	600	ANP	PB-O3A	8.84	1.70	1.59
3	D	401	ANP	PB-O3A	8.74	1.70	1.59
3	B	600	ANP	PB-O3A	8.72	1.70	1.59
3	G	401	ANP	PB-O3A	8.70	1.70	1.59
3	I	600	ANP	PB-O3A	8.67	1.70	1.59
3	D	402	ANP	PB-O3A	8.65	1.70	1.59
3	C	600	ANP	PG-N3B	6.48	1.80	1.63
3	G	402	ANP	PG-N3B	6.38	1.80	1.63
3	G	401	ANP	PG-N3B	6.33	1.79	1.63
3	I	600	ANP	PG-N3B	6.30	1.79	1.63
3	A	600	ANP	PG-N3B	6.26	1.79	1.63
3	D	402	ANP	PG-N3B	6.20	1.79	1.63
3	B	600	ANP	PG-N3B	6.19	1.79	1.63
3	E	600	ANP	PG-N3B	6.16	1.79	1.63
3	D	401	ANP	PG-N3B	6.12	1.79	1.63
3	C	600	ANP	PG-O1G	4.56	1.53	1.46
3	G	402	ANP	PG-O1G	4.56	1.53	1.46
3	I	600	ANP	PG-O1G	4.55	1.53	1.46
3	A	600	ANP	PG-O1G	4.54	1.53	1.46
3	B	600	ANP	PG-O1G	4.51	1.53	1.46
3	D	401	ANP	PG-O1G	4.51	1.53	1.46
3	E	600	ANP	PG-O1G	4.48	1.53	1.46
3	G	401	ANP	PG-O1G	4.47	1.53	1.46
3	D	402	ANP	PG-O1G	4.20	1.52	1.46
3	B	600	ANP	PB-O1B	2.80	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	ANP	PB-O1B	2.70	1.50	1.46
3	E	600	ANP	PB-O1B	2.66	1.50	1.46
3	D	401	ANP	PB-O1B	2.66	1.50	1.46
3	G	401	ANP	PB-O1B	2.59	1.50	1.46
3	G	402	ANP	PB-O1B	2.58	1.50	1.46
3	C	600	ANP	PB-O1B	2.54	1.50	1.46
3	I	600	ANP	PB-O1B	2.46	1.50	1.46
3	D	402	ANP	PB-O1B	2.45	1.50	1.46
3	D	401	ANP	C8-N7	-2.39	1.30	1.34
3	A	600	ANP	C8-N7	-2.35	1.30	1.34
3	E	600	ANP	C8-N7	-2.34	1.30	1.34
3	C	600	ANP	C8-N7	-2.31	1.30	1.34
3	G	402	ANP	C8-N7	-2.30	1.30	1.34
3	G	401	ANP	PB-O2B	-2.30	1.50	1.56
3	D	402	ANP	C8-N7	-2.29	1.30	1.34
3	G	401	ANP	C8-N7	-2.29	1.30	1.34
3	B	600	ANP	C8-N7	-2.25	1.30	1.34
3	I	600	ANP	C8-N7	-2.22	1.30	1.34
3	E	600	ANP	PB-O2B	-2.19	1.50	1.56
3	D	402	ANP	PB-O2B	-2.15	1.51	1.56
3	A	600	ANP	PB-O2B	-2.14	1.51	1.56
3	G	402	ANP	PB-O2B	-2.14	1.51	1.56
3	I	600	ANP	PB-O2B	-2.12	1.51	1.56
3	D	401	ANP	PB-O2B	-2.10	1.51	1.56
3	C	600	ANP	PB-O2B	-2.09	1.51	1.56
3	B	600	ANP	PB-O2B	-2.08	1.51	1.56

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	600	ANP	O2B-PB-O1B	5.05	120.52	109.92
3	B	600	ANP	O2B-PB-O1B	5.04	120.50	109.92
3	G	402	ANP	O2B-PB-O1B	4.81	120.01	109.92
3	D	402	ANP	O2B-PB-O1B	4.77	119.93	109.92
3	A	600	ANP	O2B-PB-O1B	4.68	119.74	109.92
3	D	401	ANP	O2B-PB-O1B	4.58	119.53	109.92
3	C	600	ANP	O2B-PB-O1B	4.57	119.50	109.92
3	E	600	ANP	O2B-PB-O1B	4.52	119.41	109.92
3	G	401	ANP	O2B-PB-O1B	4.45	119.25	109.92
3	B	600	ANP	O1G-PG-N3B	-4.02	105.86	111.77
3	D	401	ANP	O1G-PG-N3B	-3.82	106.15	111.77
3	D	402	ANP	O1G-PG-N3B	-3.81	106.16	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	ANP	O1G-PG-N3B	-3.68	106.35	111.77
3	E	600	ANP	O1G-PG-N3B	-3.65	106.40	111.77
3	G	402	ANP	O1G-PG-N3B	-3.57	106.51	111.77
3	G	401	ANP	O1G-PG-N3B	-3.54	106.56	111.77
3	C	600	ANP	O1G-PG-N3B	-3.45	106.68	111.77
3	I	600	ANP	O1G-PG-N3B	-3.43	106.72	111.77
3	D	401	ANP	O3A-PB-N3B	-2.99	98.29	106.59
3	B	600	ANP	O2G-PG-O3G	2.77	115.01	107.64
3	D	402	ANP	O2G-PG-O3G	2.74	114.92	107.64
3	G	401	ANP	O2G-PG-O3G	2.68	114.79	107.64
3	E	600	ANP	O2G-PG-O3G	2.64	114.68	107.64
3	E	600	ANP	O3A-PB-N3B	-2.59	99.40	106.59
3	I	600	ANP	O2G-PG-O3G	2.58	114.52	107.64
3	B	600	ANP	PB-O3A-PA	-2.52	123.74	132.62
3	D	401	ANP	O2G-PG-O3G	2.49	114.27	107.64
3	A	600	ANP	O2G-PG-O3G	2.48	114.23	107.64
3	G	401	ANP	PB-O3A-PA	-2.43	124.04	132.62
3	G	402	ANP	O2G-PG-O3G	2.42	114.07	107.64
3	C	600	ANP	O2G-PG-O3G	2.36	113.93	107.64
3	D	402	ANP	PB-O3A-PA	-2.34	124.39	132.62
3	I	600	ANP	PB-O3A-PA	-2.24	124.74	132.62
3	B	600	ANP	O3A-PB-N3B	-2.21	100.47	106.59
3	C	600	ANP	PB-O3A-PA	-2.18	124.94	132.62
3	D	401	ANP	PB-O3A-PA	-2.14	125.09	132.62
3	G	402	ANP	PB-O3A-PA	-2.10	125.22	132.62
3	A	600	ANP	PB-O3A-PA	-2.09	125.27	132.62
3	G	401	ANP	O3A-PB-N3B	-2.08	100.83	106.59
3	I	600	ANP	O3A-PB-N3B	-2.02	100.98	106.59
3	E	600	ANP	PB-O3A-PA	-2.02	125.50	132.62
3	A	600	ANP	O3A-PB-N3B	-2.00	101.04	106.59

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	600	ANP	PG-N3B-PB-O1B
3	C	600	ANP	PA-O3A-PB-O1B
3	C	600	ANP	PA-O3A-PB-O2B
3	C	600	ANP	C5'-O5'-PA-O3A
3	B	600	ANP	C5'-O5'-PA-O1A
3	B	600	ANP	C5'-O5'-PA-O2A
3	B	600	ANP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	A	600	ANP	PB-N3B-PG-O1G
3	A	600	ANP	PG-N3B-PB-O1B
3	I	600	ANP	PA-O3A-PB-O1B
3	I	600	ANP	C5'-O5'-PA-O2A
3	I	600	ANP	O4'-C4'-C5'-O5'
3	E	600	ANP	PB-N3B-PG-O1G
3	E	600	ANP	C5'-O5'-PA-O1A
3	E	600	ANP	C5'-O5'-PA-O2A
3	E	600	ANP	C5'-O5'-PA-O3A
3	D	401	ANP	PB-N3B-PG-O1G
3	D	401	ANP	PG-N3B-PB-O1B
3	D	402	ANP	PB-N3B-PG-O1G
3	D	402	ANP	PG-N3B-PB-O1B
3	D	402	ANP	PA-O3A-PB-O1B
3	D	402	ANP	PA-O3A-PB-O2B
3	G	401	ANP	PB-N3B-PG-O1G
3	G	401	ANP	PG-N3B-PB-O1B
3	G	401	ANP	C5'-O5'-PA-O3A
3	G	402	ANP	PB-N3B-PG-O1G
3	G	402	ANP	C5'-O5'-PA-O1A
3	B	600	ANP	C3'-C4'-C5'-O5'
3	G	401	ANP	O4'-C4'-C5'-O5'
3	G	401	ANP	C3'-C4'-C5'-O5'
3	I	600	ANP	C3'-C4'-C5'-O5'
3	A	600	ANP	O4'-C4'-C5'-O5'
3	G	402	ANP	C4'-C5'-O5'-PA
3	A	600	ANP	C4'-C5'-O5'-PA
3	D	401	ANP	O4'-C4'-C5'-O5'
3	I	600	ANP	C5'-O5'-PA-O3A
3	G	402	ANP	C5'-O5'-PA-O3A
3	A	600	ANP	C3'-C4'-C5'-O5'
3	D	401	ANP	C4'-C5'-O5'-PA
3	C	600	ANP	C5'-O5'-PA-O2A
3	I	600	ANP	C5'-O5'-PA-O1A
3	G	401	ANP	C5'-O5'-PA-O2A
3	G	402	ANP	C5'-O5'-PA-O2A
3	B	600	ANP	C4'-C5'-O5'-PA
3	I	600	ANP	C4'-C5'-O5'-PA
3	G	402	ANP	PG-N3B-PB-O1B
3	D	401	ANP	C3'-C4'-C5'-O5'
3	I	600	ANP	PA-O3A-PB-O2B
3	B	600	ANP	C5'-O5'-PA-O3A

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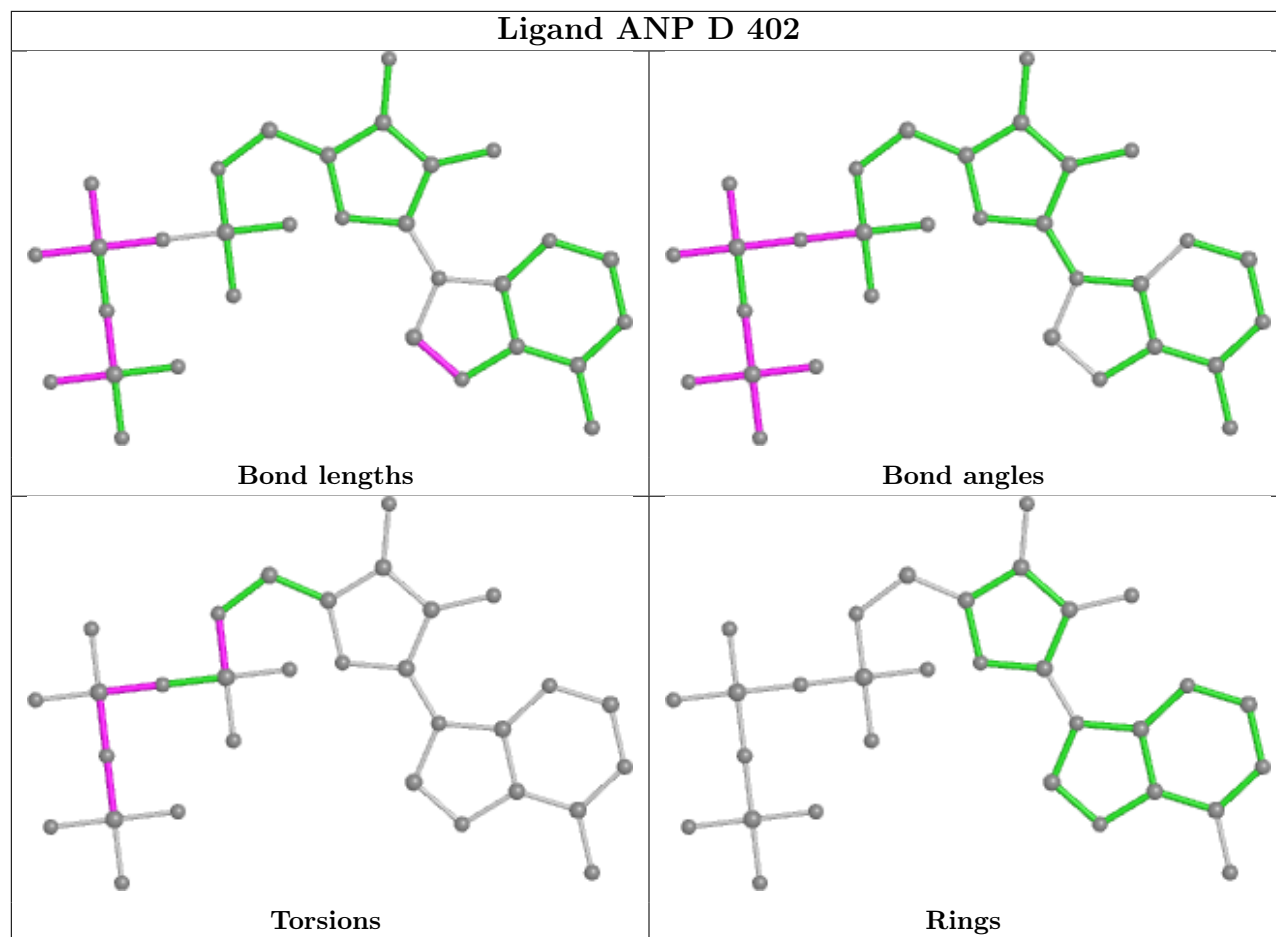
Mol	Chain	Res	Type	Atoms
3	D	402	ANP	C5'-O5'-PA-O3A
3	C	600	ANP	O4'-C4'-C5'-O5'
3	G	402	ANP	O4'-C4'-C5'-O5'
3	D	402	ANP	C5'-O5'-PA-O1A
3	D	402	ANP	C5'-O5'-PA-O2A
3	E	600	ANP	O4'-C4'-C5'-O5'
3	C	600	ANP	PB-N3B-PG-O1G

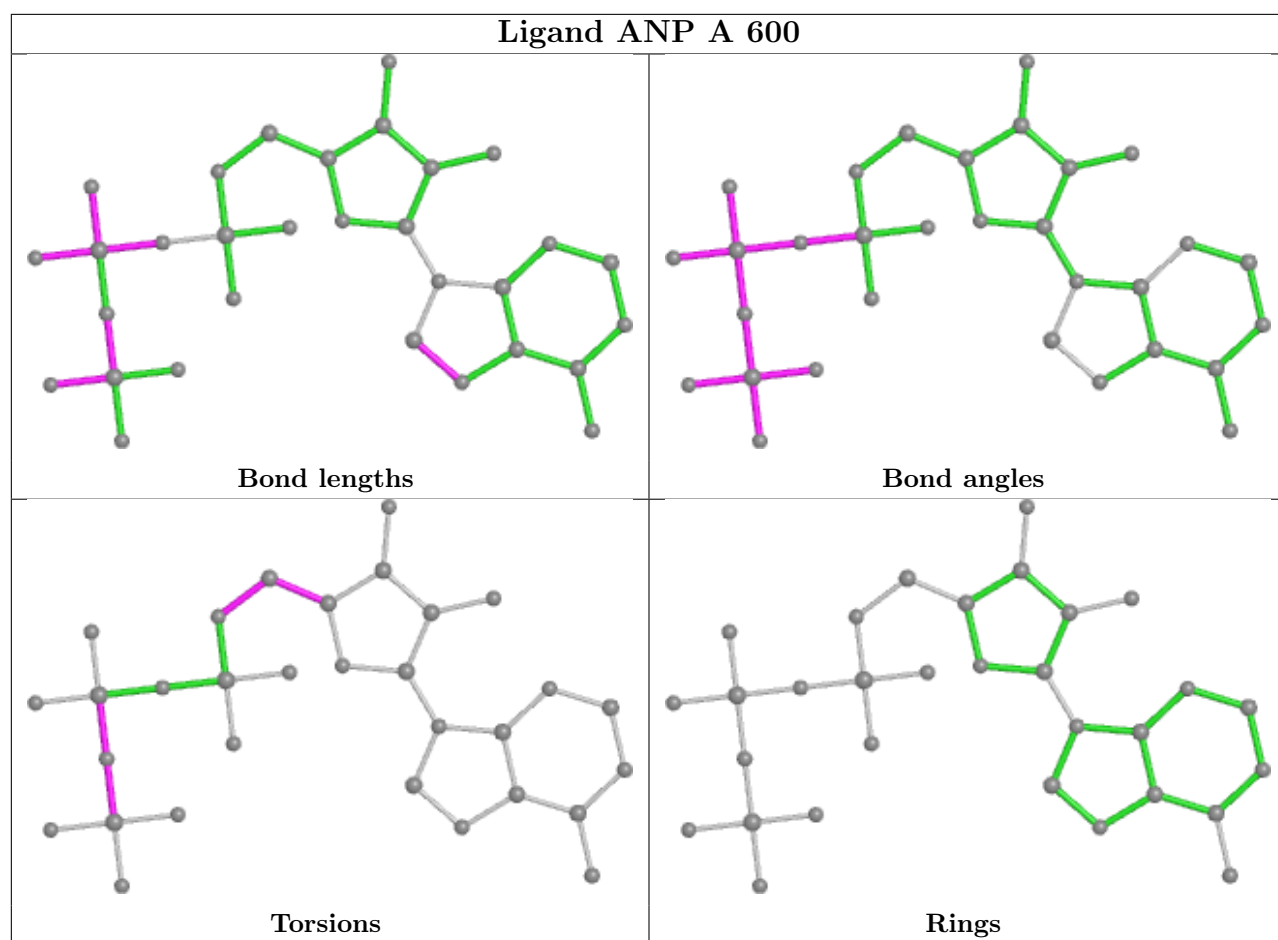
There are no ring outliers.

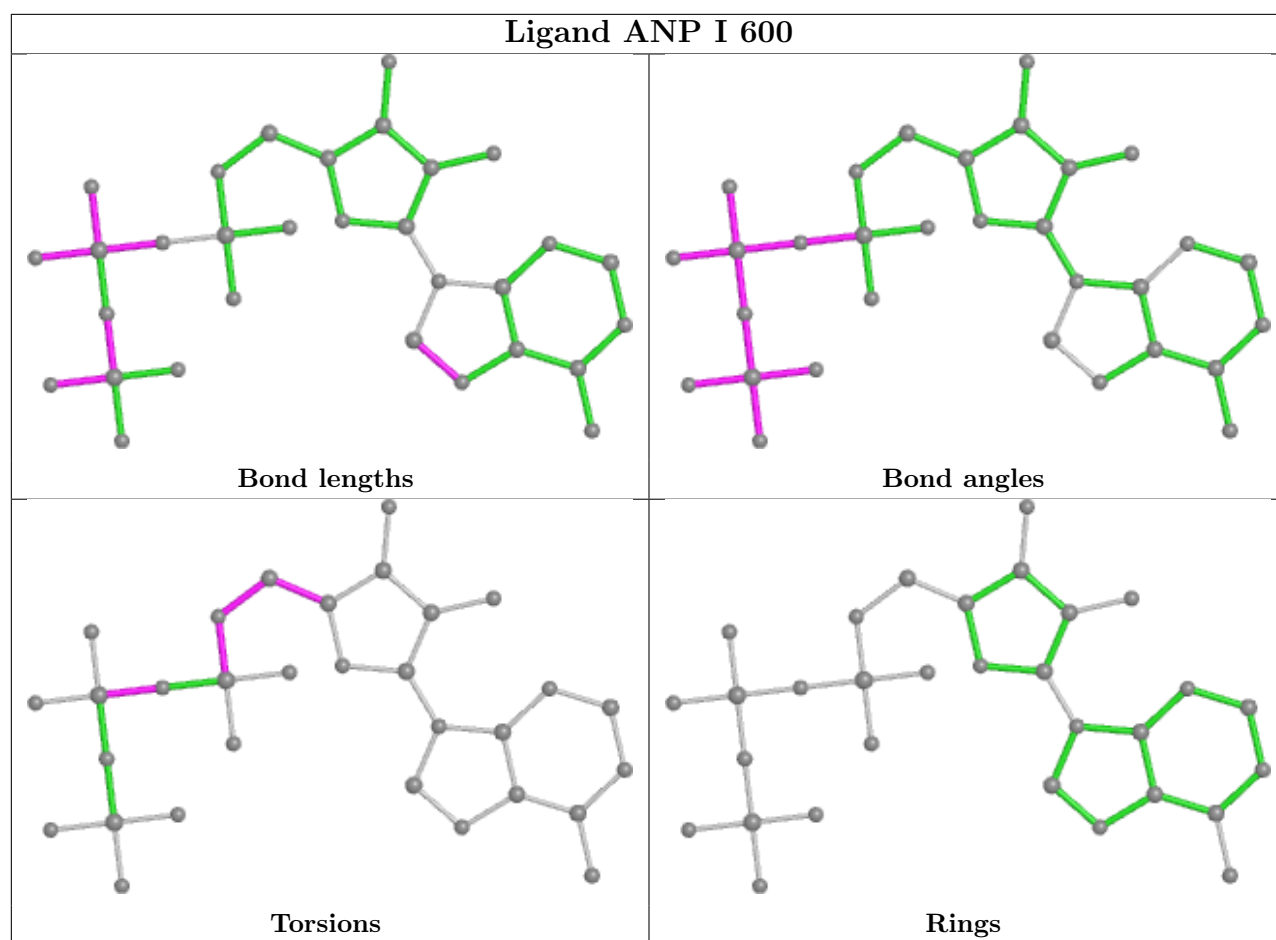
8 monomers are involved in 19 short contacts:

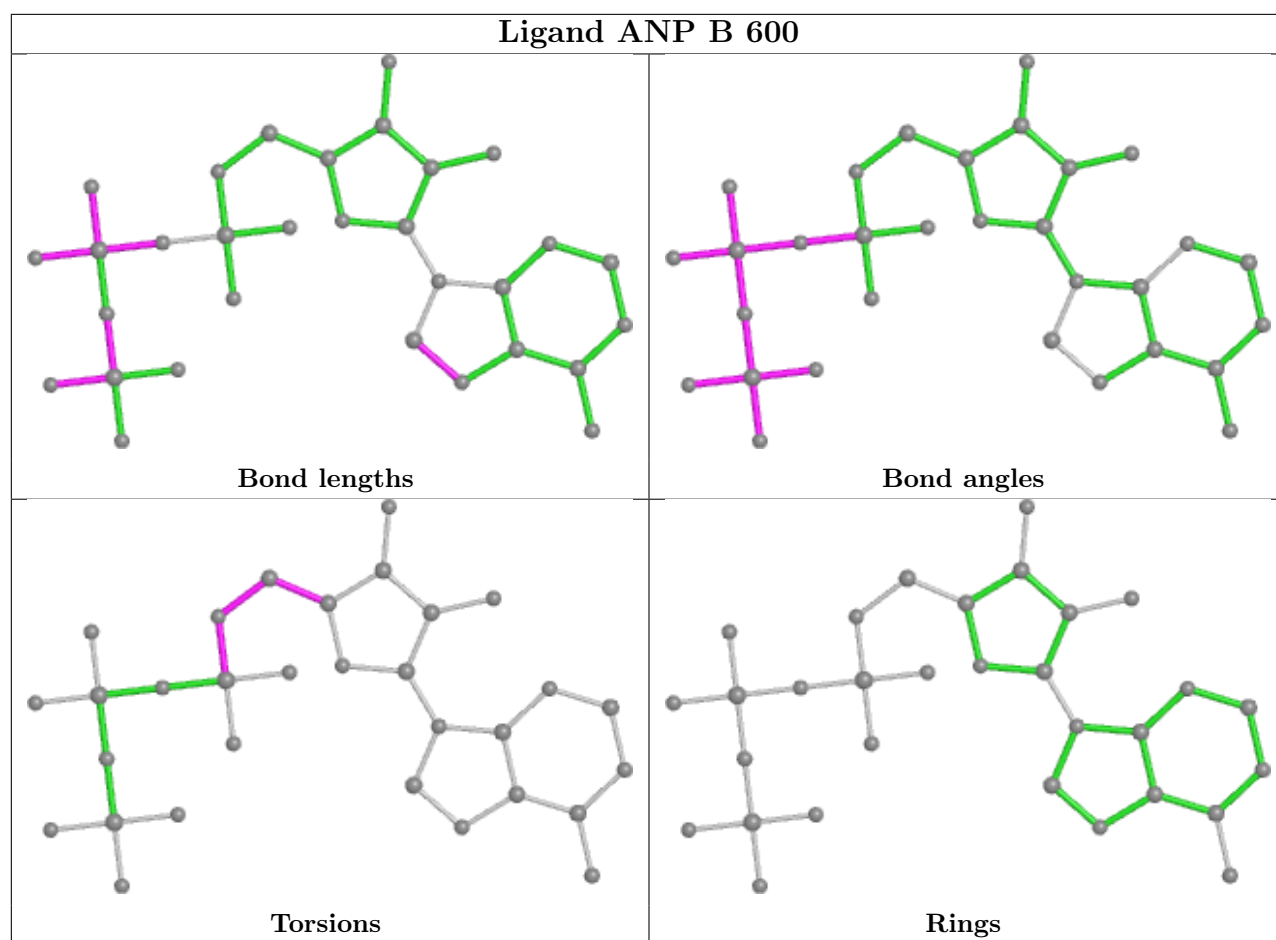
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	ANP	1	0
3	A	600	ANP	3	0
3	I	600	ANP	3	0
3	B	600	ANP	4	0
3	E	600	ANP	2	0
3	G	402	ANP	4	0
3	C	600	ANP	1	0
3	D	401	ANP	1	0

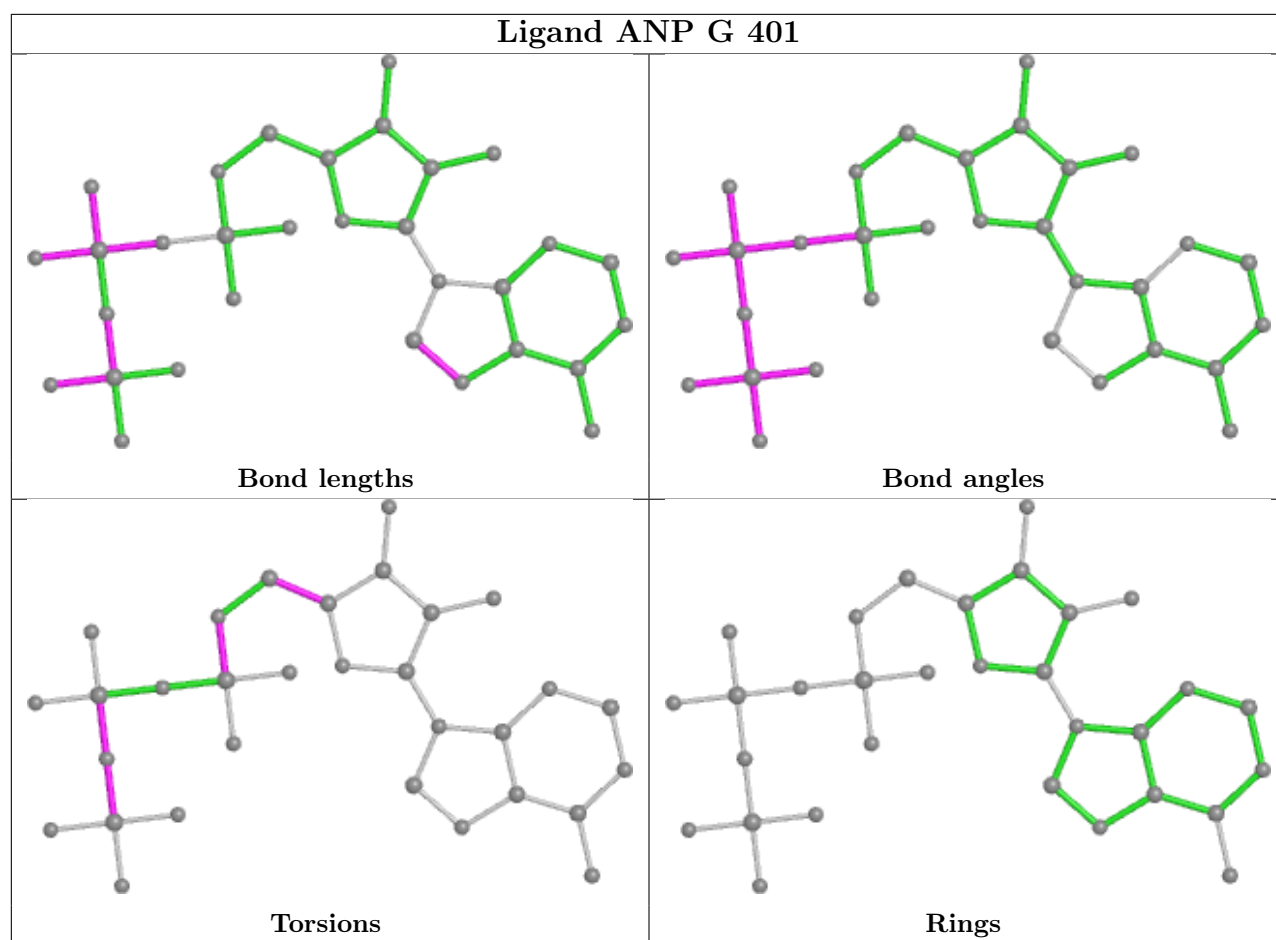
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

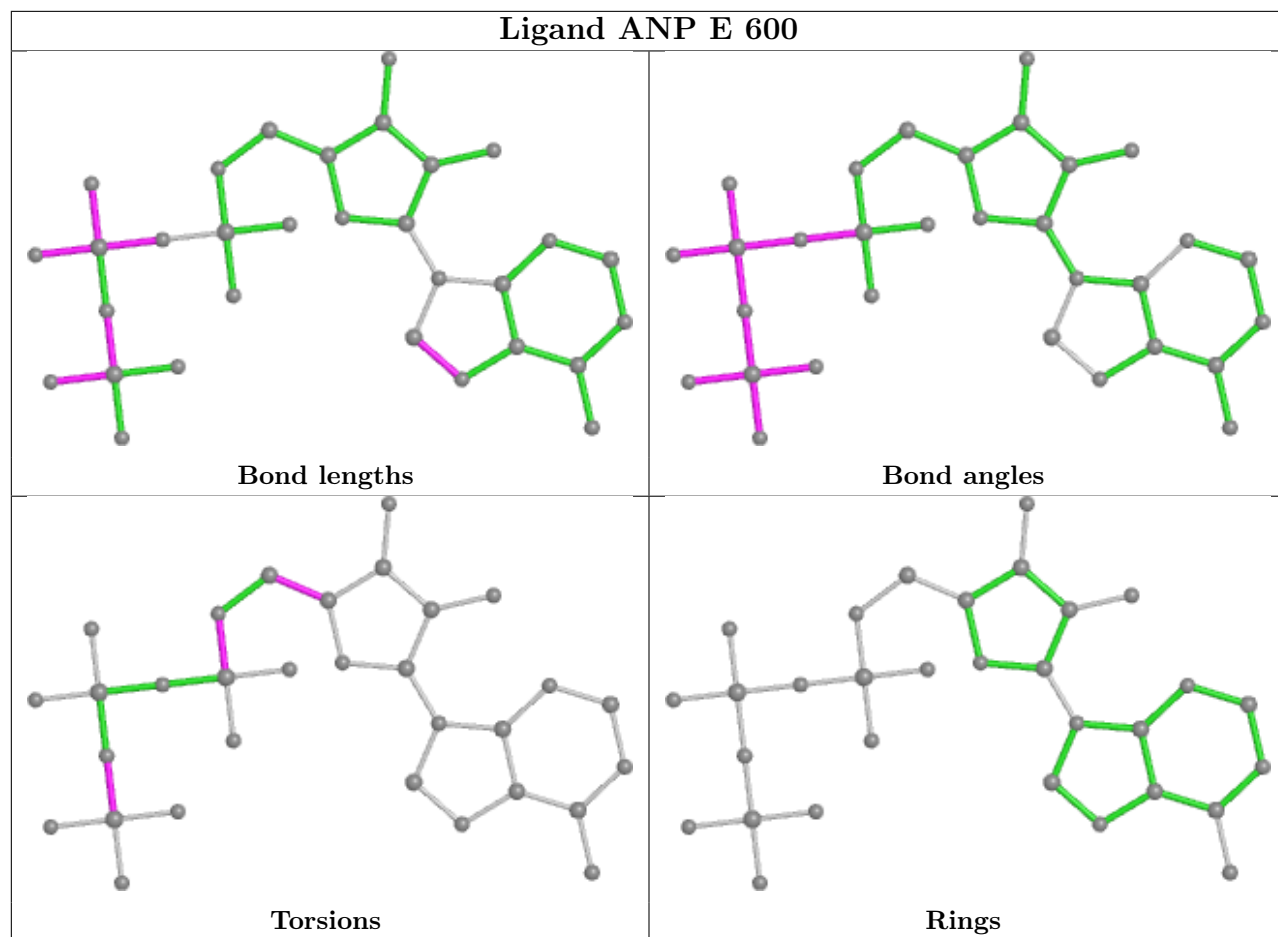


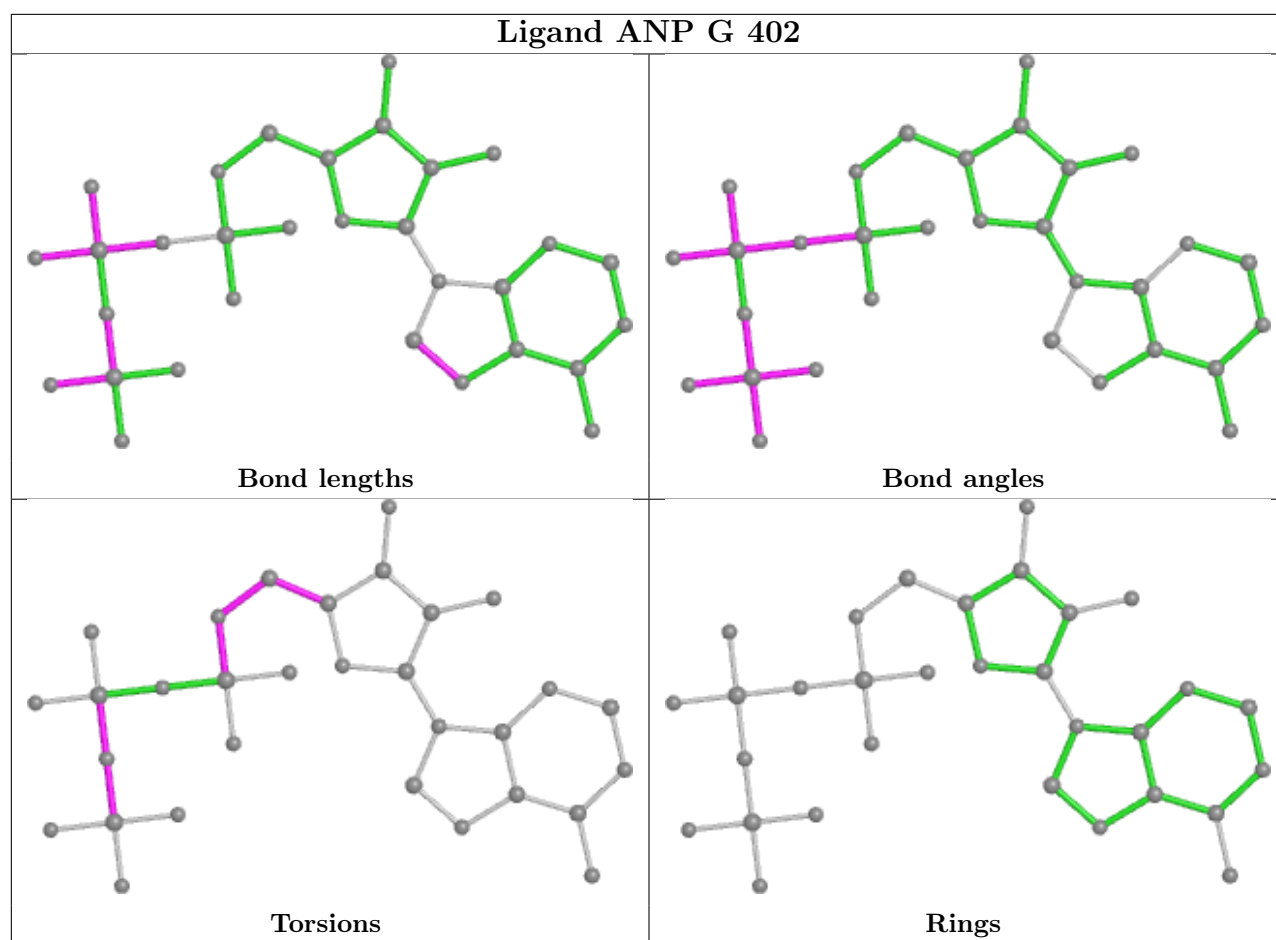


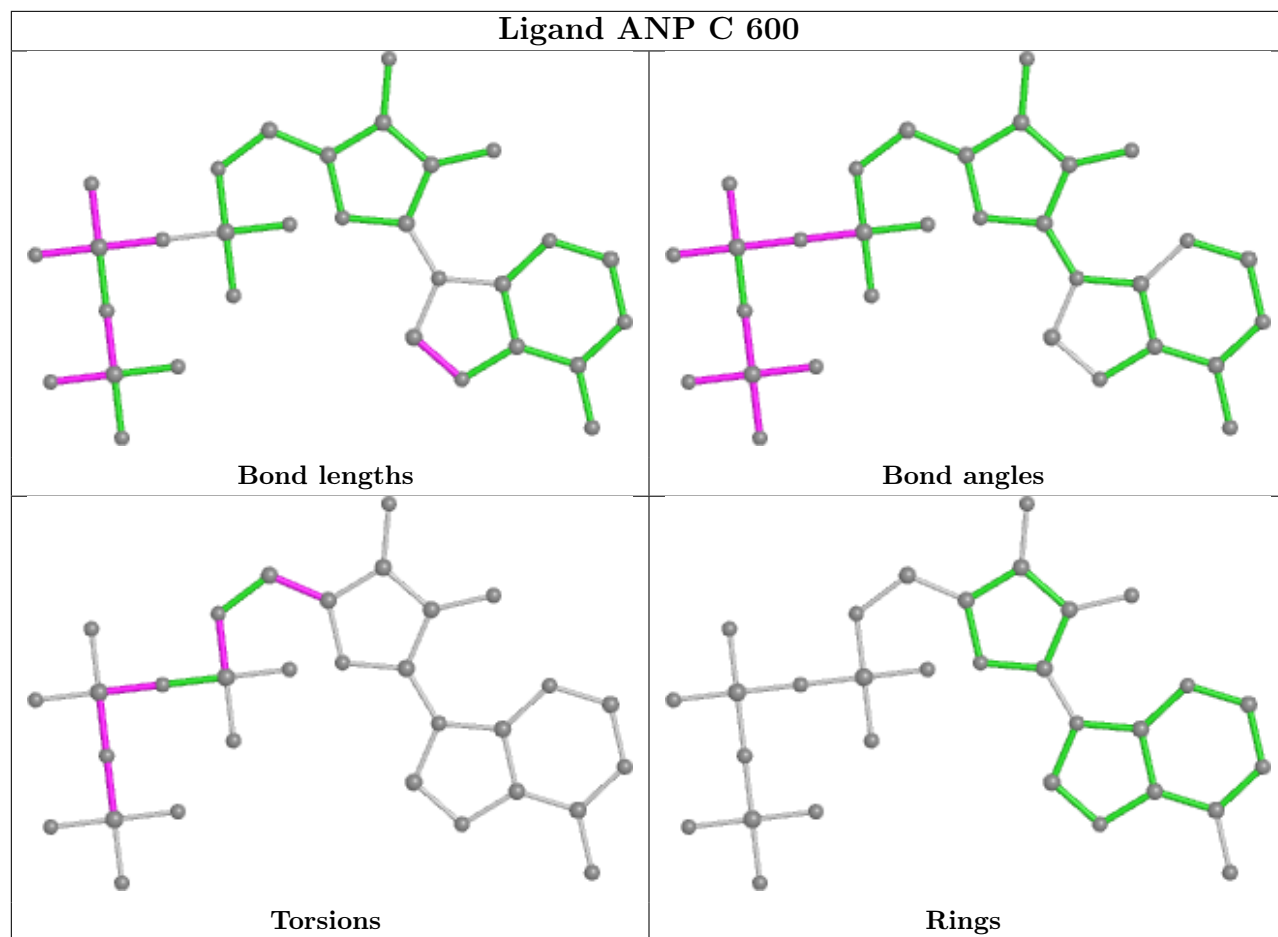


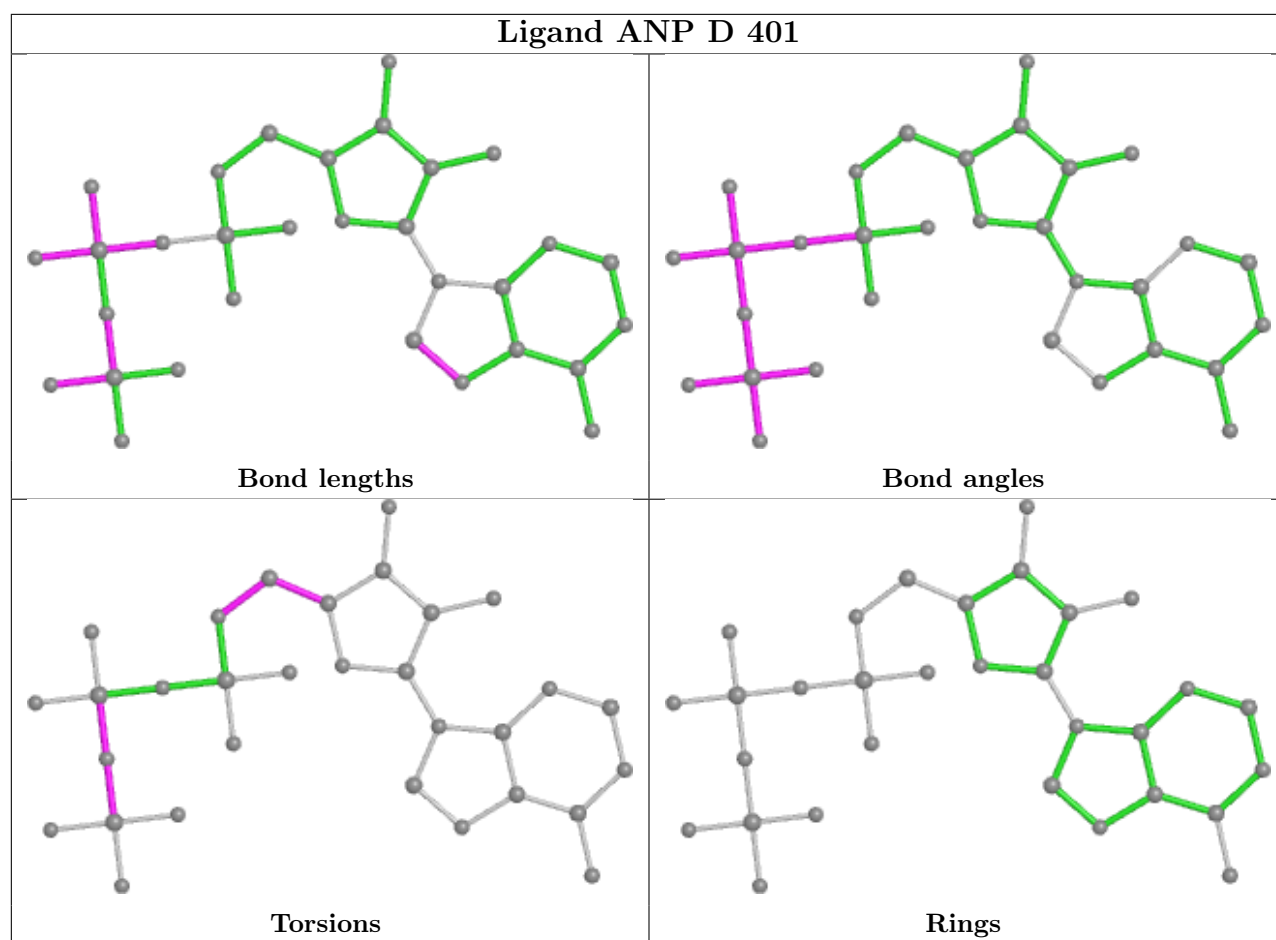












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

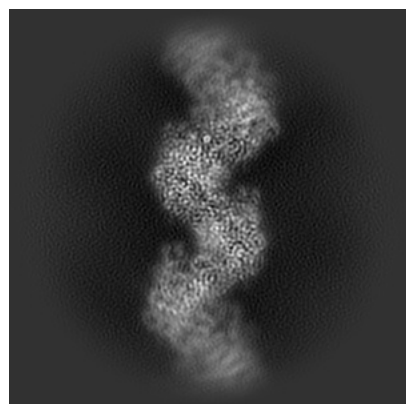
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64183. These allow visual inspection of the internal detail of the map and identification of artifacts.

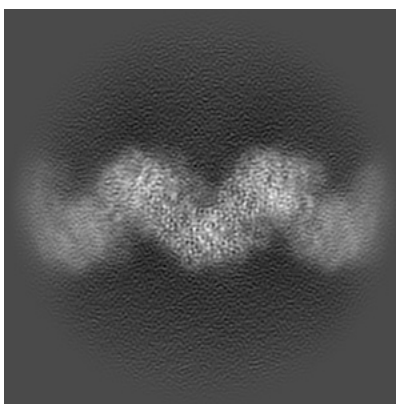
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

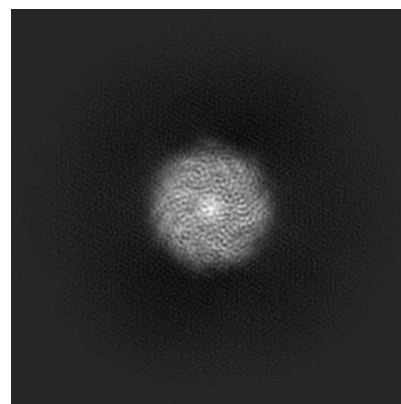
6.1.1 Primary map



X

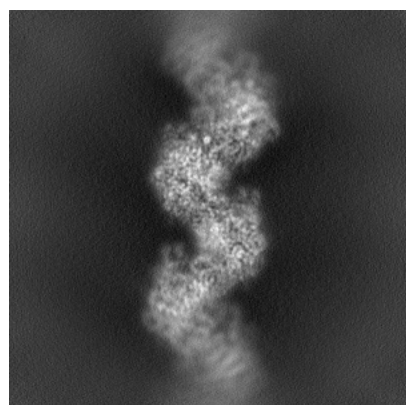


Y

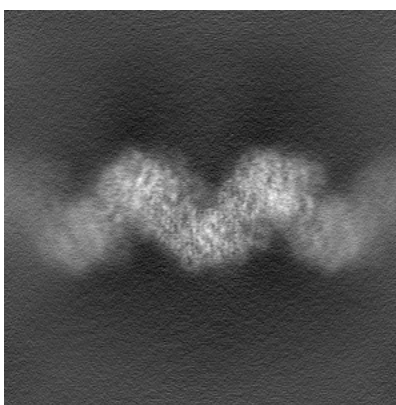


Z

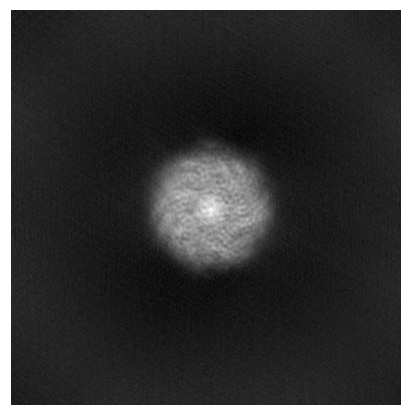
6.1.2 Raw map



X



Y

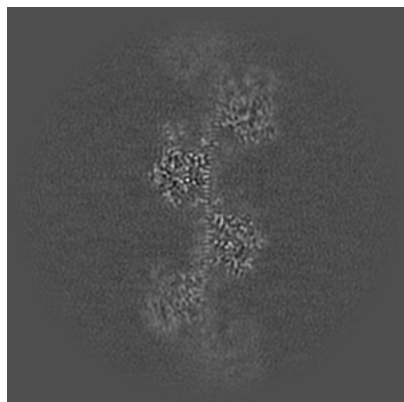


Z

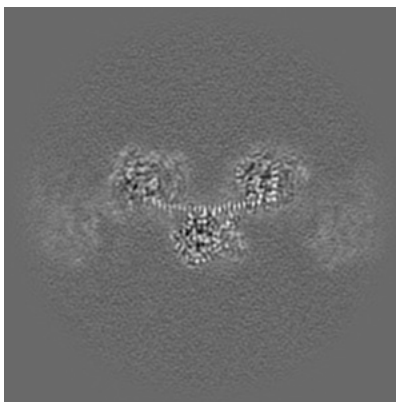
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

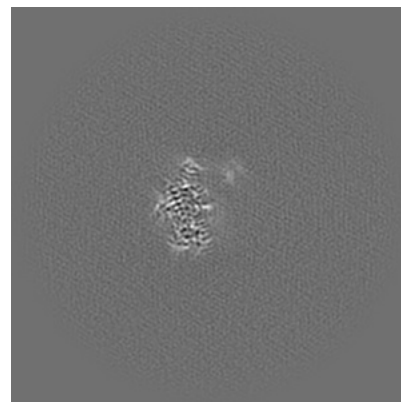
6.2.1 Primary map



X Index: 192

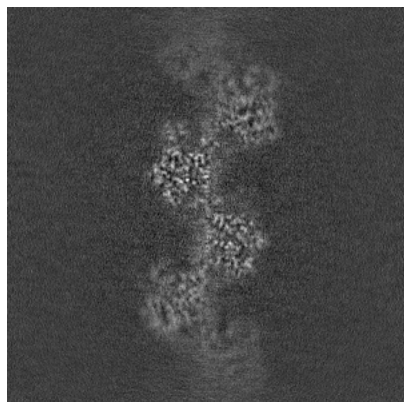


Y Index: 192

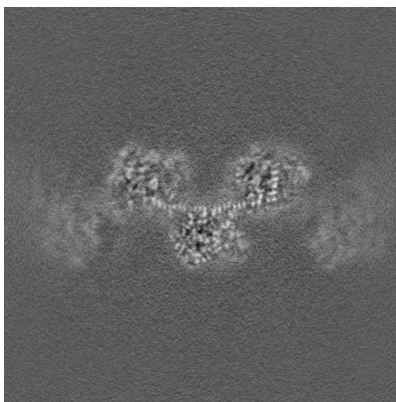


Z Index: 192

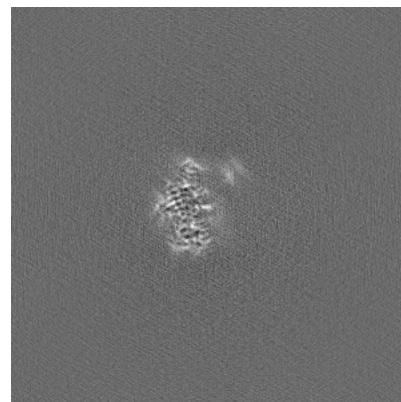
6.2.2 Raw map



X Index: 192



Y Index: 192

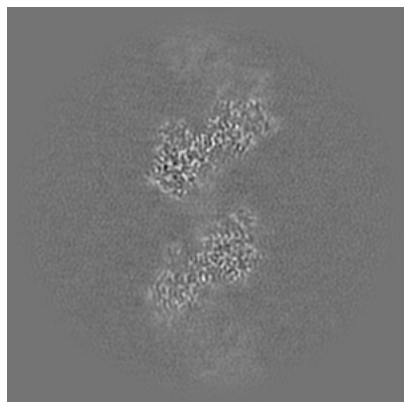


Z Index: 192

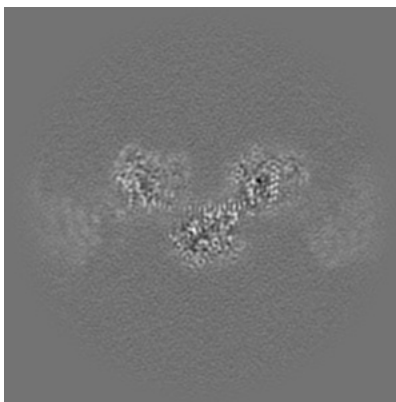
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

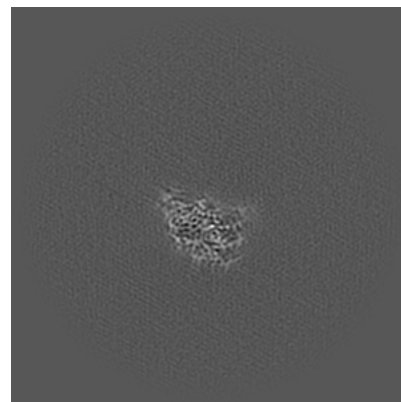
6.3.1 Primary map



X Index: 202

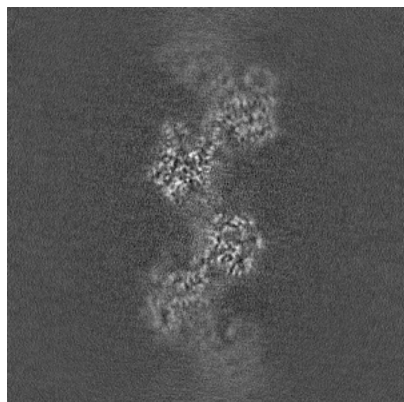


Y Index: 190

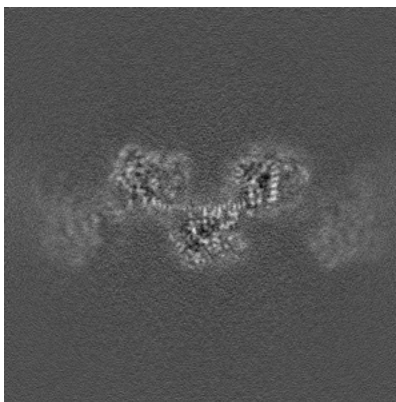


Z Index: 218

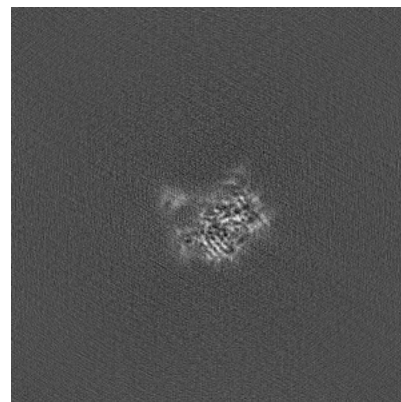
6.3.2 Raw map



X Index: 194



Y Index: 191

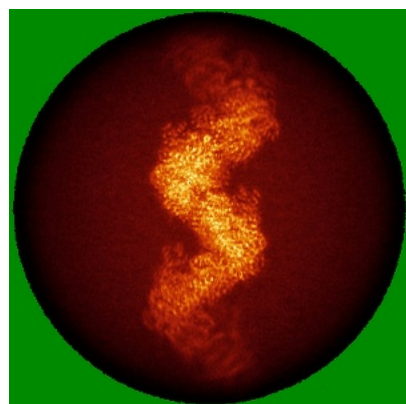


Z Index: 232

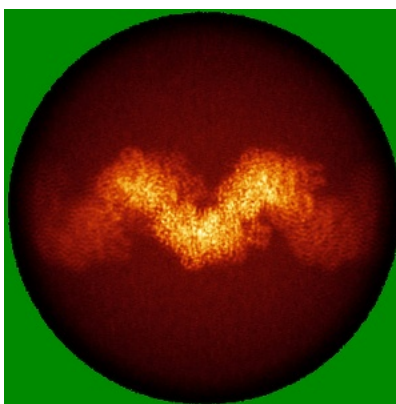
The images above show the largest variance slices of the map in three orthogonal directions.

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

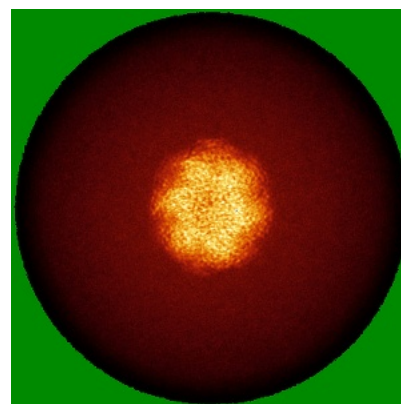
6.4.1 Primary map



X

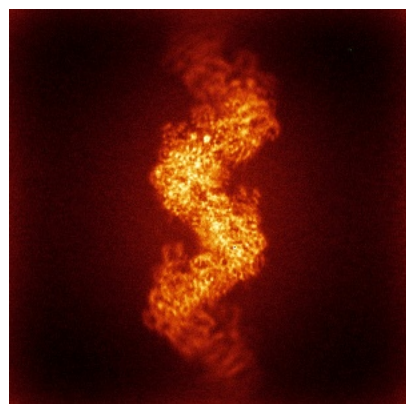


Y

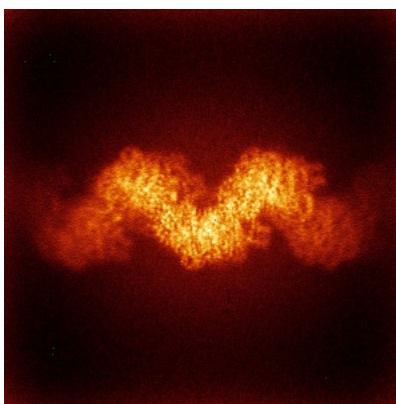


Z

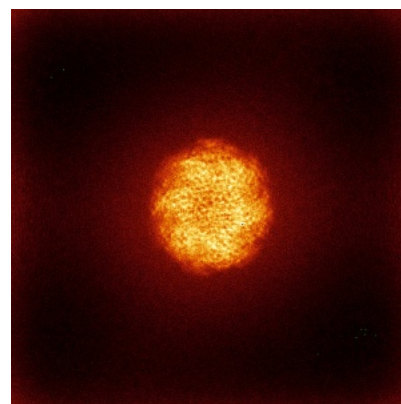
6.4.2 Raw map



X



Y

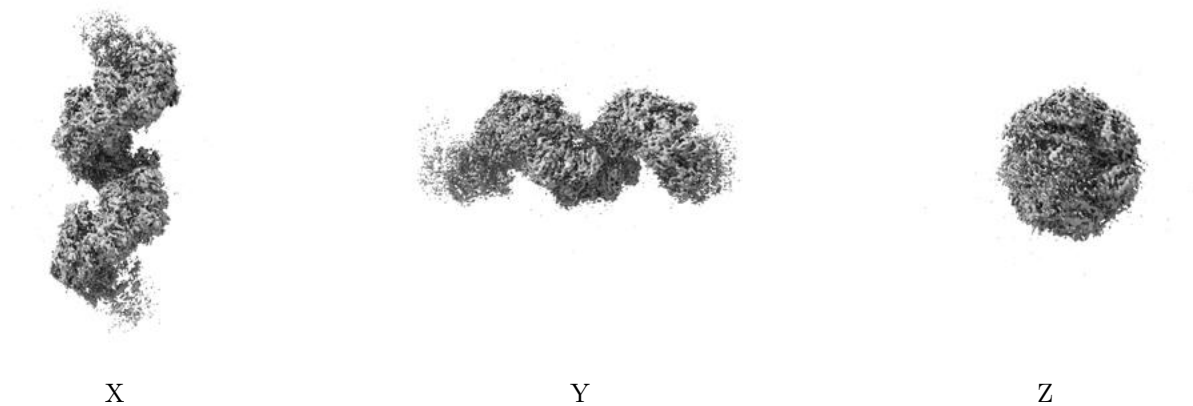


Z

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

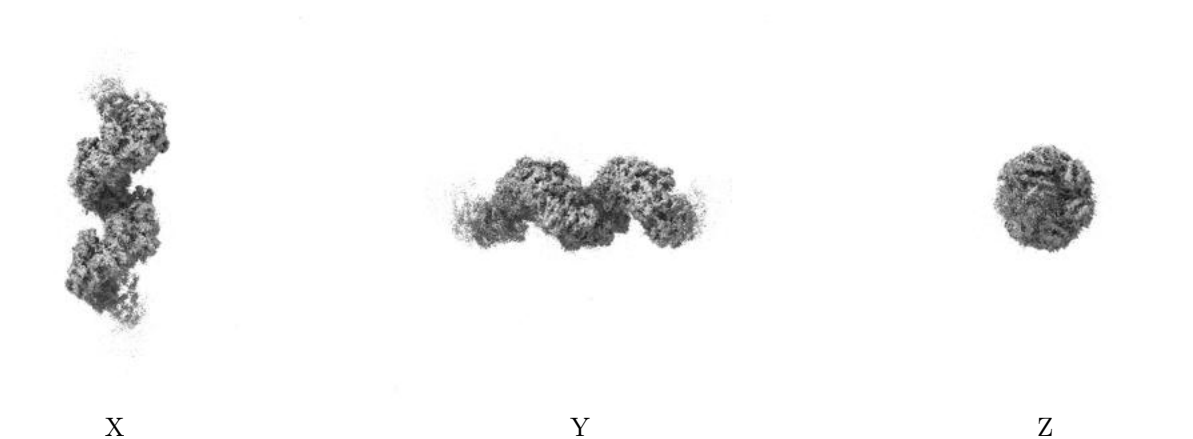
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

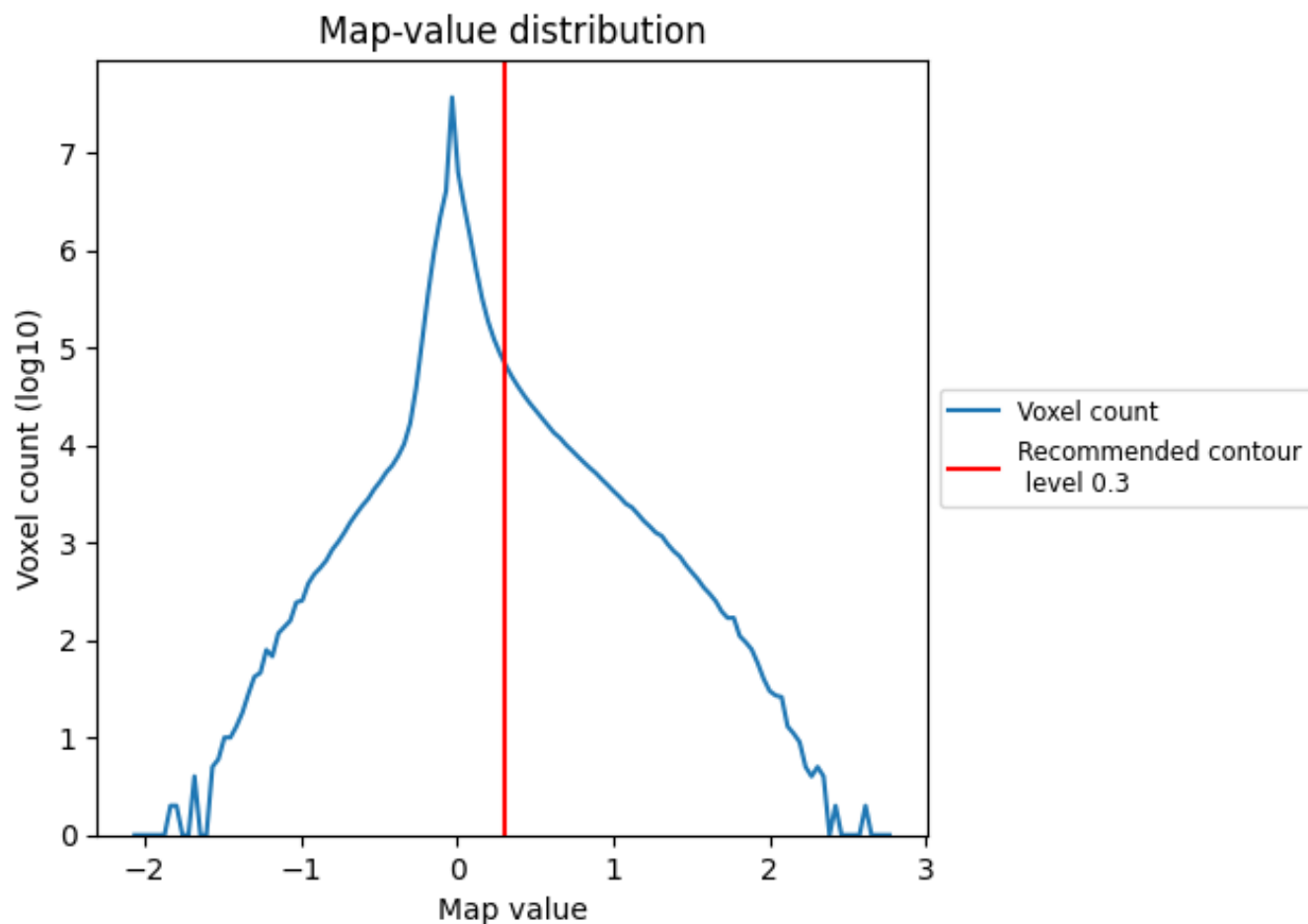
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

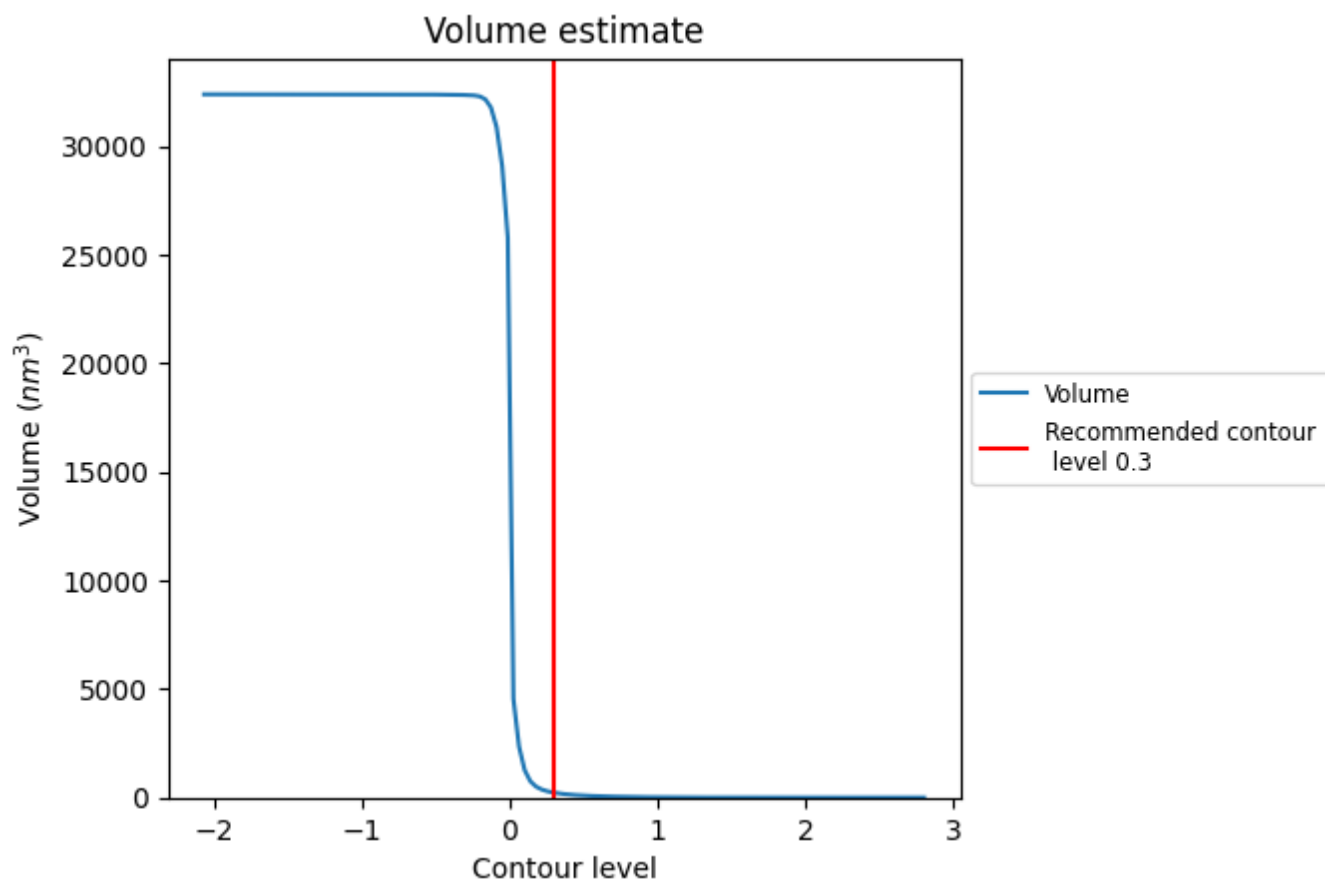
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

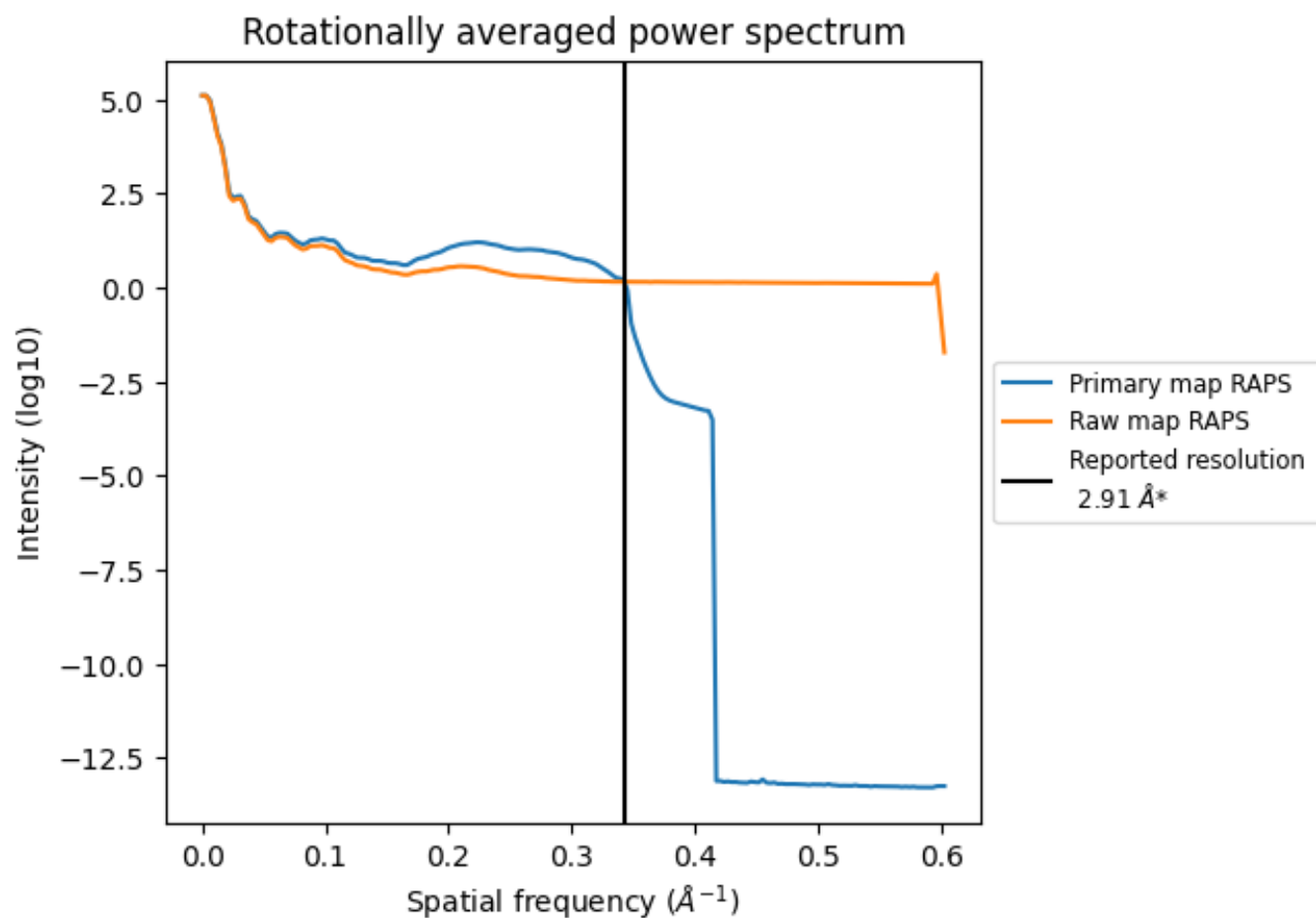
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 227 nm³; this corresponds to an approximate mass of 205 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

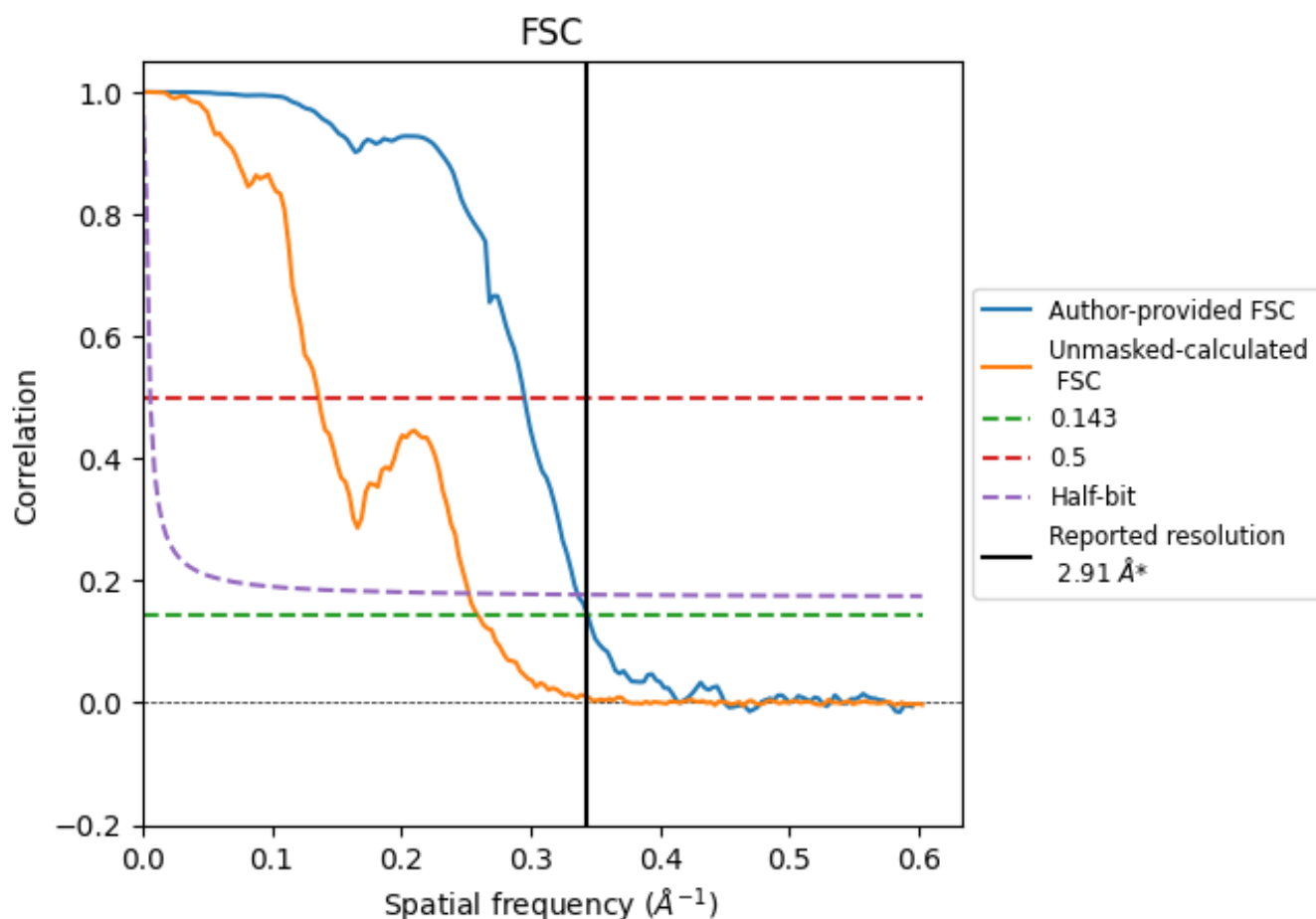


*Reported resolution corresponds to spatial frequency of 0.344 \AA^{-1}

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 0.344 \AA^{-1}

8.2 Resolution estimates [i](#)

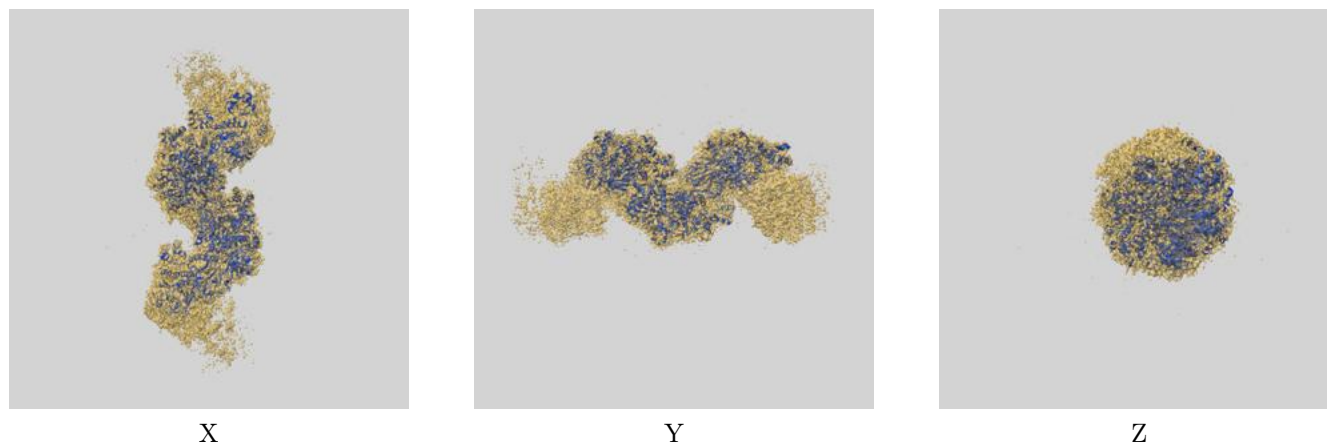
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	2.91	3.39	2.97
Unmasked-calculated*	3.86	7.34	3.97

*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 3.86 differs from the reported value 2.91 by more than 10 %

9 Map-model fit [i](#)

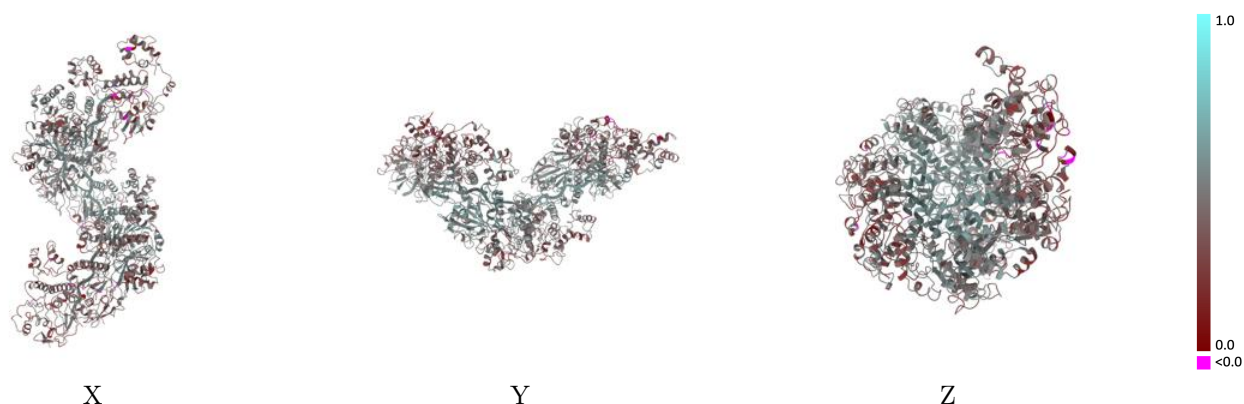
This section contains information regarding the fit between EMDB map EMD-64183 and PDB model 9UI4. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



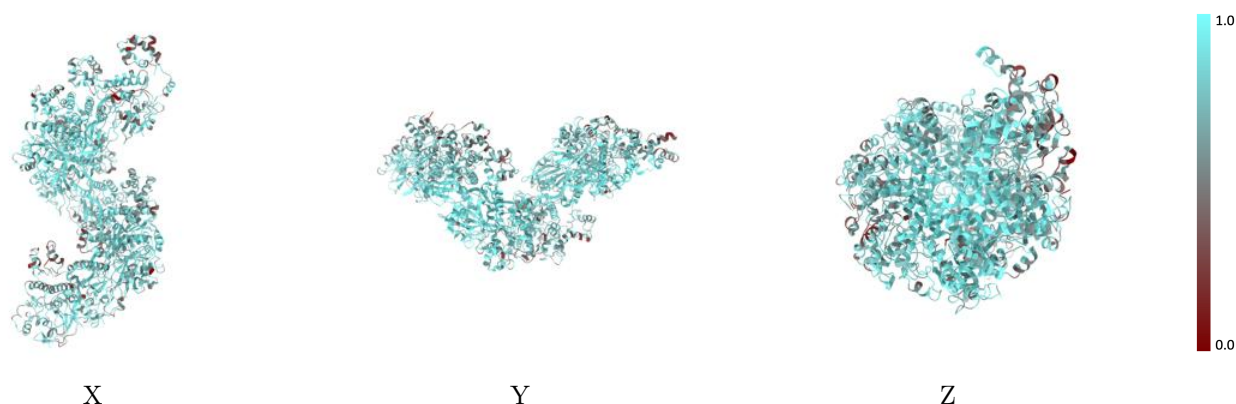
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



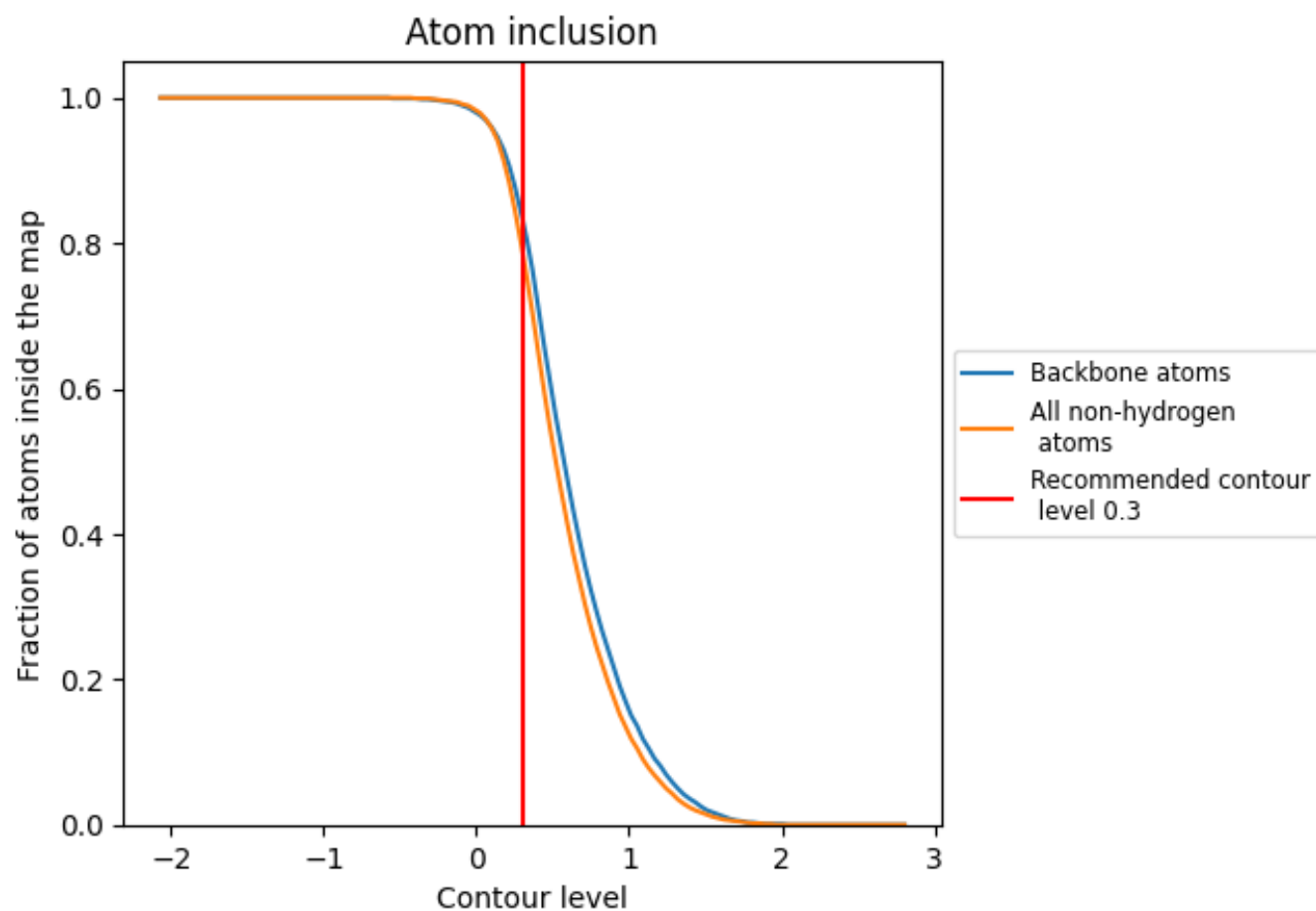
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7920	<div></div> 0.4310
A	<div></div> 0.6920	<div></div> 0.3670
B	<div></div> 0.7270	<div></div> 0.3670
C	<div></div> 0.8160	<div></div> 0.4520
D	<div></div> 0.8720	<div></div> 0.5190
E	<div></div> 0.7870	<div></div> 0.4210
F	<div></div> 0.8040	<div></div> 0.4170
G	<div></div> 0.8600	<div></div> 0.4780
H	<div></div> 0.8080	<div></div> 0.4420
I	<div></div> 0.7270	<div></div> 0.3860
L	<div></div> 0.9410	<div></div> 0.5580

1.0

0.0

<0.0