



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 10:30 PM UTC

PDB ID : 9UI8 / pdb_00009ui8
EMDB ID : EMD-64187
Title : structure of an 8 base pair Rad51 D-loop complex
Authors : Luo, S.C.; Ho, M.C.
Deposited on : 2025-04-15
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

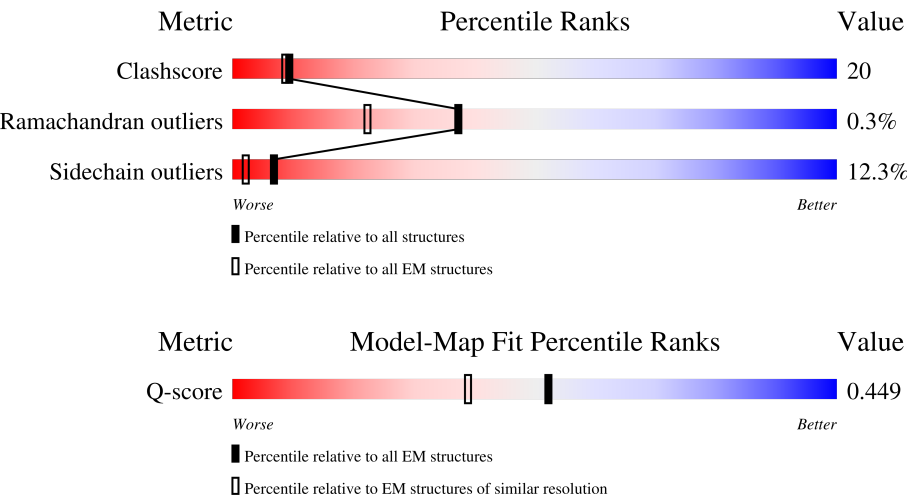
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 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.



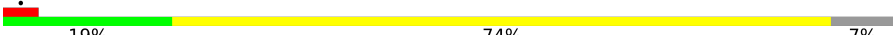
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	A	361	
1	B	361	
1	C	361	
1	D	361	

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Mol	Chain	Length	Quality of chain
1	E	361	
1	F	361	
1	G	361	
1	H	361	
1	I	361	
2	L	27	
3	T	48	
4	U	48	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23041 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 DNA repair protein RAD51 homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	315	Total	C	N	O	S	0	0
			2416	1513	424	465	14		
1	G	315	Total	C	N	O	S	0	0
			2416	1513	424	465	14		
1	C	308	Total	C	N	O	S	0	0
			2369	1483	417	456	13		
1	B	308	Total	C	N	O	S	0	0
			2369	1483	417	456	13		
1	A	308	Total	C	N	O	S	0	0
			2369	1483	417	456	13		
1	F	314	Total	C	N	O	S	0	0
			2408	1509	423	462	14		
1	I	308	Total	C	N	O	S	0	0
			2369	1483	417	456	13		
1	H	308	Total	C	N	O	S	0	0
			2369	1483	417	456	13		
1	D	308	Total	C	N	O	S	0	0
			2369	1483	417	456	13		

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
E	-10	GLY	-	expression tag	UNP Q08297

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
G	209	ASP	ALA	engineered mutation	UNP Q08297
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
C	-16	HIS	-	expression tag	UNP Q08297

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
F	-4	LYS	-	expression tag	UNP Q08297

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

- Molecule 2 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	25	Total	C	N	O	P	0	0
			500	243	69	163	25		

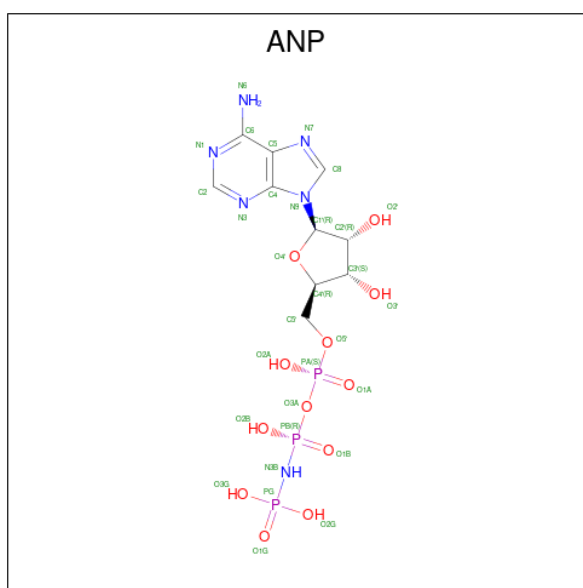
- Molecule 3 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	19	Total	C	N	O	P	0	0
			394	185	76	114	19		

- Molecule 4 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	20	Total	C	N	O	P	0	0
			405	196	62	127	20		

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

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Mol	Chain	Residues	Atoms					AltConf
5	I	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	H	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	D	1	Total	C	N	O	P	0
			31	10	6	12	3	

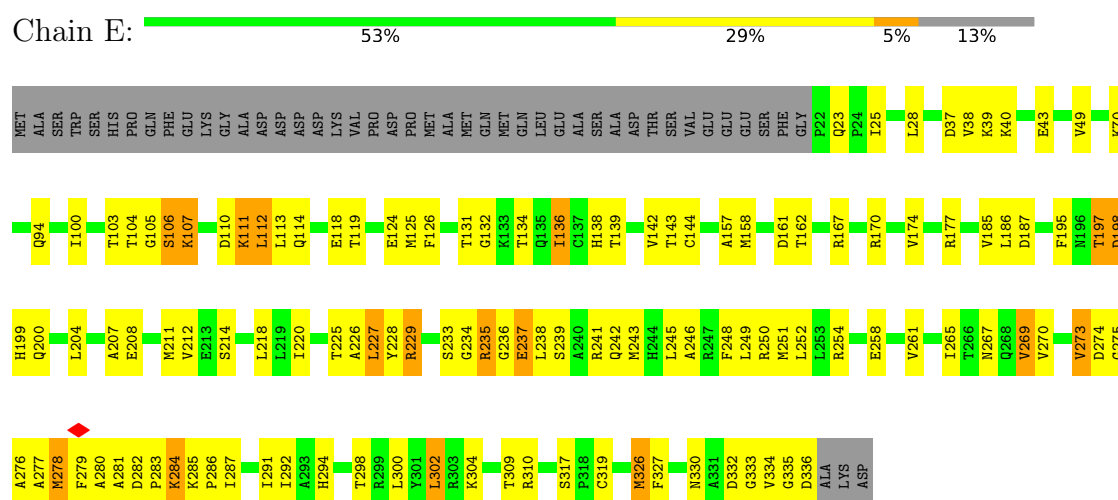
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	E	1	Total	Mg	0
			1	1	
6	G	1	Total	Mg	0
			1	1	
6	C	1	Total	Mg	0
			1	1	
6	B	1	Total	Mg	0
			1	1	
6	A	1	Total	Mg	0
			1	1	
6	F	1	Total	Mg	0
			1	1	
6	H	2	Total	Mg	0
			2	2	
6	D	1	Total	Mg	0
			1	1	

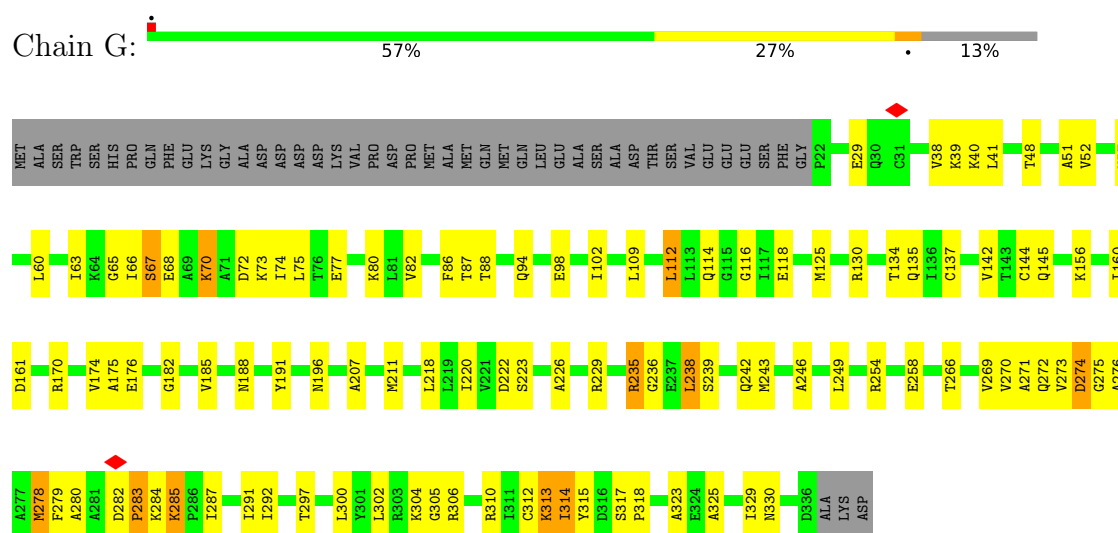
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA repair protein RAD51 homolog 1

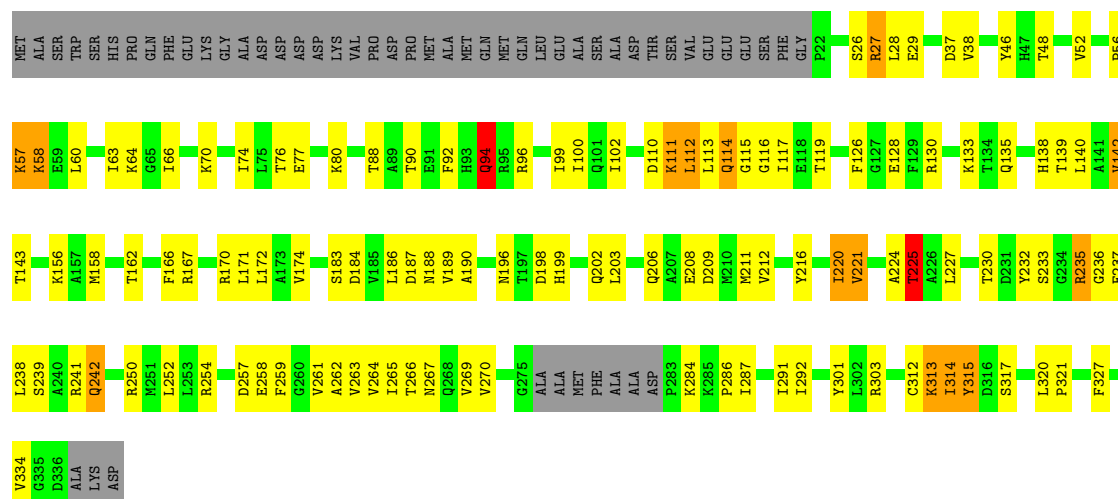


• Molecule 1: DNA repair protein RAD51 homolog 1

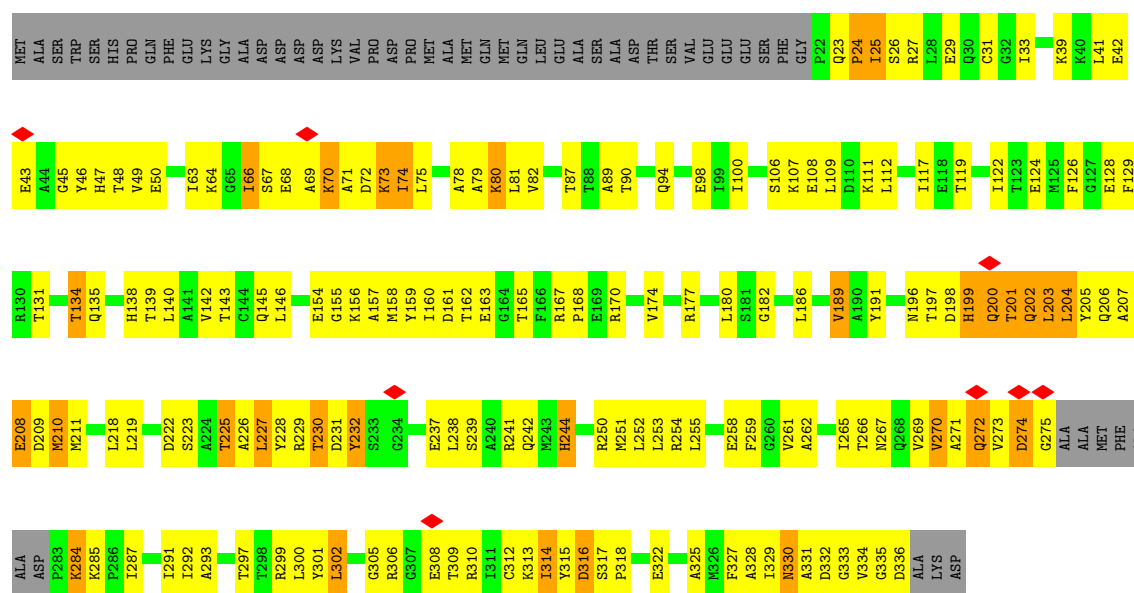
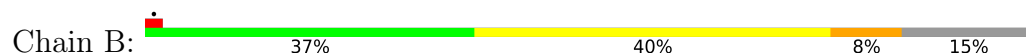


• Molecule 1: DNA repair protein RAD51 homolog 1

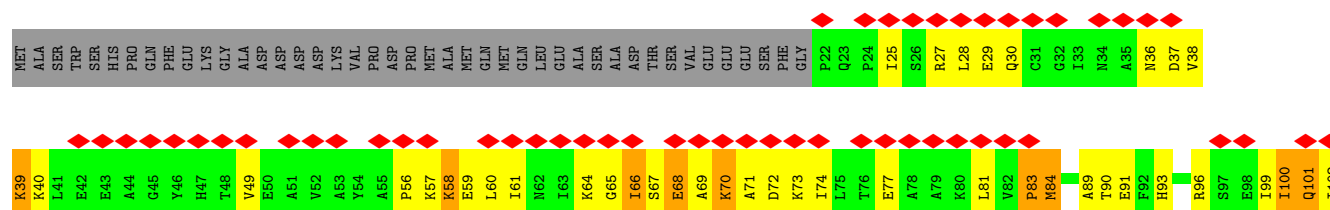


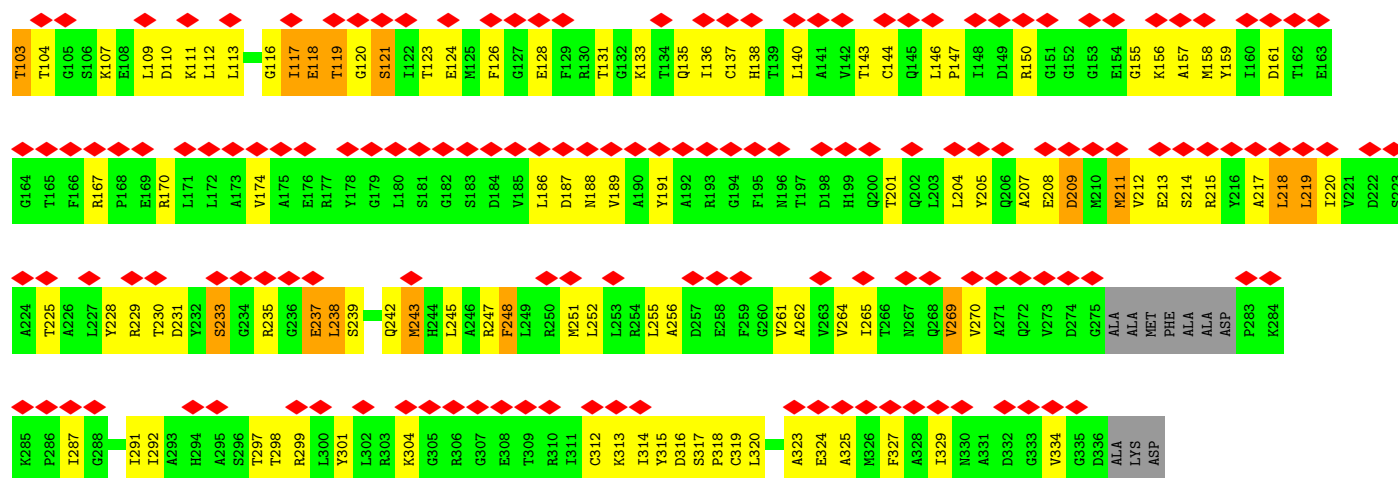


- Molecule 1: DNA repair protein RAD51 homolog 1



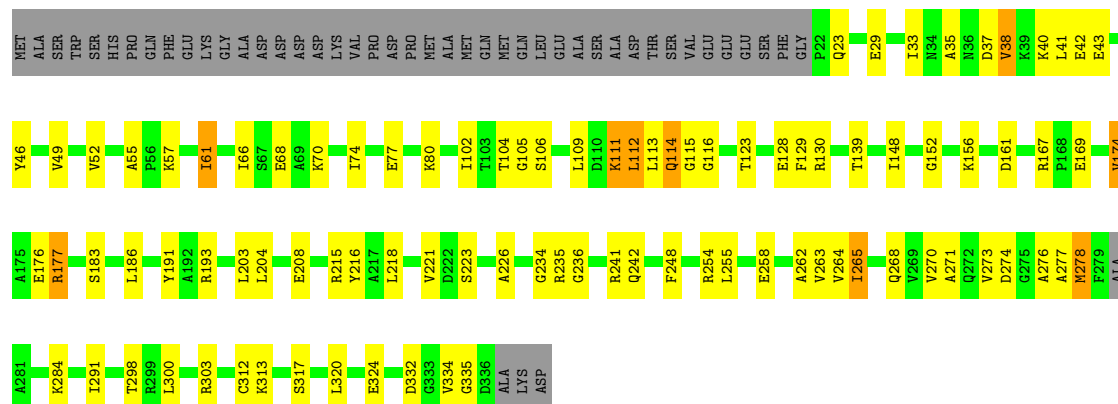
- Molecule 1: DNA repair protein RAD51 homolog 1





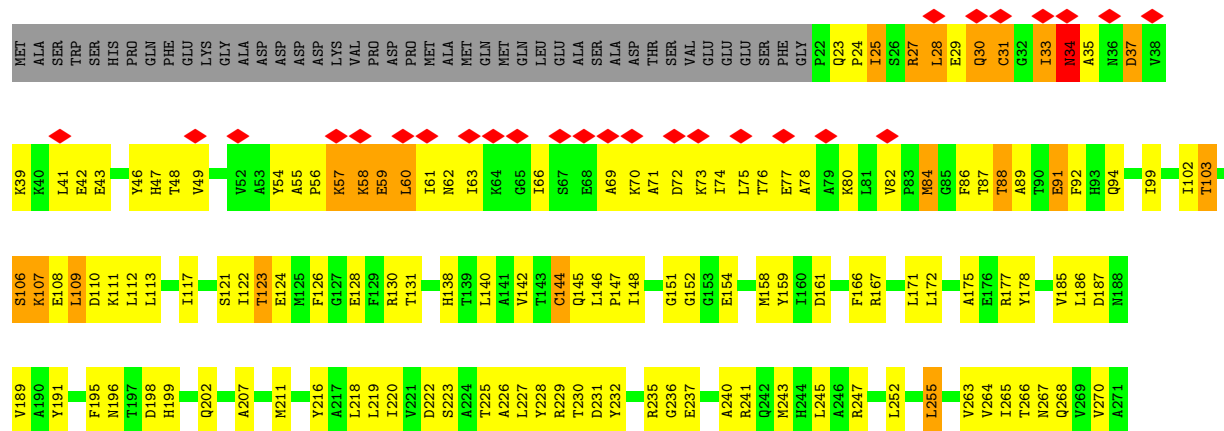
• Molecule 1: DNA repair protein RAD51 homolog 1

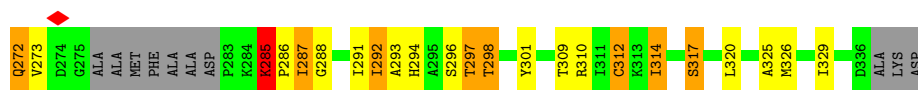
Chain F: 61% 24% 13%



• Molecule 1: DNA repair protein RAD51 homolog 1

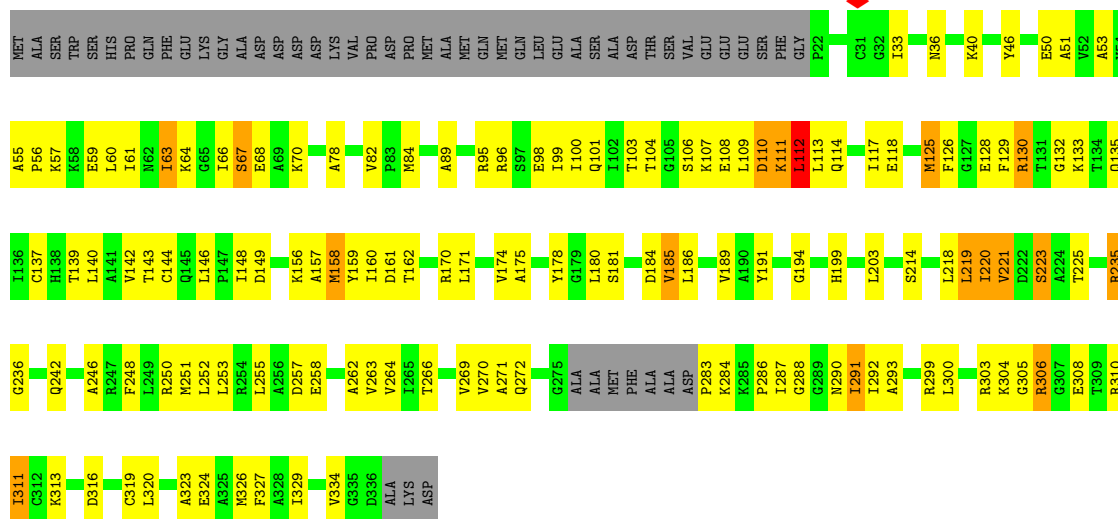
Chain I: 8% 42% 35% 8% 15%





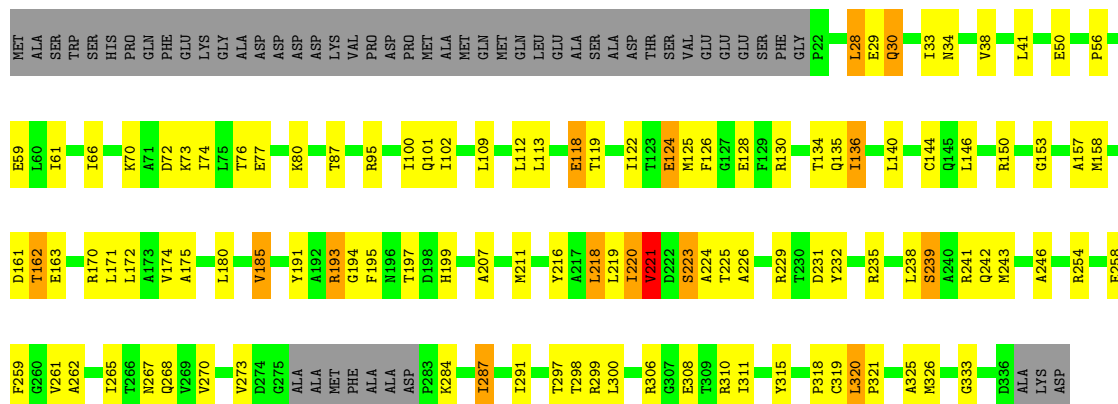
- Molecule 1: DNA repair protein RAD51 homolog 1

Chain H: 48% 33% 15%



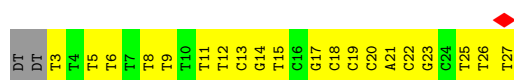
- Molecule 1: DNA repair protein RAD51 homolog 1

Chain D: 55% 27% 15%



- Molecule 2: DNA (27-MER)

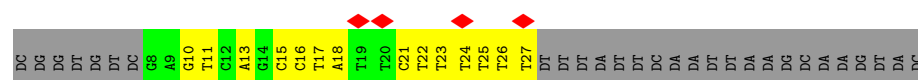
Chain L: 19% 74% 7%



- Molecule 3: DNA (48-MER)

DG	DT	DA	DC	DT	DT	DG	DC	DT	DT	DA	DA	DT	DT	DG	DA	DA	DA	DA	DA	G23	G24	G25		A28	A29	G30	T31	A32	G33	G34	C35	T36	G37	A38		G41	DG	DA	DC	DA	DA	DC	DC	DC
----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	-----	-----	-----	--	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	--	-----	----	----	----	----	----	----	----	----

Chain U:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53493	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	2.413	Depositor
Minimum map value	-1.190	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.18	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 ⓘ

5.1 Standard geometry ⓘ

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	A	0.22	0/2403	0.64	2/3239 (0.1%)
1	B	0.26	0/2403	0.58	0/3239
1	C	0.27	0/2403	0.64	3/3239 (0.1%)
1	D	0.29	0/2403	0.65	4/3239 (0.1%)
1	E	0.34	0/2452	0.67	4/3308 (0.1%)
1	F	0.29	0/2443	0.65	3/3294 (0.1%)
1	G	0.29	0/2452	0.64	3/3308 (0.1%)
1	H	0.33	0/2403	0.68	2/3239 (0.1%)
1	I	0.27	0/2403	0.67	3/3239 (0.1%)
2	L	0.26	0/553	0.46	0/850
3	T	0.28	0/442	0.52	0/681
4	U	0.25	0/450	0.53	0/692
All	All	0.29	0/23210	0.64	24/31567 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	236	GLY	N-CA-C	-9.54	103.34	114.69
1	H	112	LEU	N-CA-C	-9.18	98.42	110.53
1	A	65	GLY	N-CA-C	-8.97	103.80	114.48
1	E	197	THR	N-CA-C	-8.27	102.21	111.14
1	C	236	GLY	N-CA-C	-8.10	105.06	114.69
1	G	236	GLY	N-CA-C	-7.73	105.49	114.69
1	E	229	ARG	N-CA-C	-7.05	101.74	110.41
1	D	95	ARG	N-CA-C	-6.49	106.57	114.75
1	A	243	MET	N-CA-C	-6.25	105.97	113.97
1	F	115	GLY	N-CA-C	-6.21	103.86	112.18
1	F	176	GLU	N-CA-C	-6.15	107.00	114.75
1	G	68	GLU	CB-CA-C	-6.09	109.54	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	115	GLY	N-CA-C	-6.03	105.19	112.48
1	I	285	LYS	CA-C-N	-5.71	114.86	120.52
1	I	285	LYS	C-N-CA	-5.71	114.86	120.52
1	D	174	VAL	N-CA-C	-5.58	106.36	113.22
1	D	136	ILE	N-CA-C	-5.41	107.10	113.42
1	C	94	GLN	N-CA-C	-5.29	106.15	113.18
1	F	66	ILE	N-CA-C	5.25	115.16	108.12
1	E	136	ILE	N-CA-C	-5.25	106.77	112.80
1	D	226	ALA	N-CA-C	-5.16	106.07	112.93
1	E	226	ALA	N-CA-C	-5.12	106.97	113.43
1	G	67	SER	CB-CA-C	-5.07	109.76	115.79
1	I	297	THR	CB-CA-C	-5.03	109.82	117.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2369	0	2384	132	0
1	B	2369	0	2384	163	0
1	C	2369	0	2385	83	0
1	D	2369	0	2385	72	0
1	E	2416	0	2427	107	0
1	F	2408	0	2418	64	0
1	G	2416	0	2427	78	0
1	H	2369	0	2384	98	0
1	I	2369	0	2385	144	0
2	L	500	0	290	39	0
3	T	394	0	213	13	0
4	U	405	0	231	25	0
5	A	31	0	13	0	0
5	B	31	0	13	0	0
5	C	31	0	13	0	0
5	D	31	0	13	1	0
5	E	31	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	31	0	13	2	0
5	G	31	0	13	2	0
5	H	31	0	13	2	0
5	I	31	0	13	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	2	0	0	0	0
All	All	23041	0	22430	918	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 20.

All (918) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:ASP:HB2	1:B:202:GLN:HA	1.37	1.07
1:B:329:ILE:HA	1:B:333:GLY:HA2	1.45	0.95
1:E:235:ARG:HG2	3:T:29:DC:H5''	1.51	0.93
1:I:41:LEU:HD23	1:I:63:ILE:HD12	1.51	0.89
1:B:24:PRO:HA	1:B:48:THR:HA	1.55	0.89
1:E:136:ILE:HG12	1:E:334:VAL:HG21	1.55	0.89
1:I:88:THR:HG23	1:I:91:GLU:HB3	1.55	0.88
1:B:329:ILE:HA	1:B:333:GLY:CA	2.03	0.88
1:I:158:MET:HE1	1:I:207:ALA:HB1	1.56	0.88
1:I:23:GLN:HG3	1:I:27:ARG:HG3	1.56	0.86
1:B:182:GLY:O	1:B:186:LEU:HB2	1.77	0.85
1:H:113:LEU:HD21	1:H:300:LEU:HD11	1.56	0.84
4:U:16:DC:H2'	4:U:18:DA:H62	1.44	0.83
1:A:143:THR:HA	1:A:146:LEU:HD13	1.59	0.83
1:D:161:ASP:HB3	1:D:191:TYR:HE1	1.45	0.81
1:D:163:GLU:HG3	1:D:223:SER:HB3	1.62	0.81
1:A:158:MET:HG2	1:A:219:LEU:HD13	1.61	0.80
1:B:143:THR:HA	1:B:146:LEU:HD13	1.62	0.80
1:E:278:MET:HE3	1:E:279:PHE:H	1.47	0.79
2:L:27:DT:C4	1:B:273:VAL:HA	2.18	0.79
1:D:113:LEU:HA	1:D:320:LEU:HD11	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ALA:O	1:A:93:HIS:HB2	1.83	0.79
1:E:103:THR:HG22	1:E:105:GLY:H	1.48	0.78
1:A:135:GLN:HB2	1:A:329:ILE:HD11	1.66	0.78
1:B:170:ARG:HD3	1:A:319:CYS:HA	1.65	0.78
1:B:242:GLN:HB3	1:B:291:ILE:HG13	1.67	0.77
1:E:113:LEU:HD21	1:E:300:LEU:HD21	1.66	0.77
1:G:145:GLN:HE21	1:G:188:ASN:HB2	1.49	0.77
4:U:22:DT:H1'	1:F:278:MET:HB2	1.67	0.76
1:G:315:TYR:O	1:H:130:ARG:HD3	1.87	0.75
1:F:139:THR:HG21	1:F:334:VAL:HG22	1.68	0.75
1:B:329:ILE:CA	1:B:333:GLY:HA2	2.17	0.75
1:A:229:ARG:HD2	1:A:230:THR:HG23	1.69	0.74
1:I:189:VAL:HG22	1:H:89:ALA:HB2	1.68	0.74
1:B:330:ASN:N	1:B:333:GLY:HA2	2.02	0.74
1:B:167:ARG:HD3	1:A:319:CYS:HB2	1.70	0.74
1:B:140:LEU:HB3	1:B:218:LEU:HD21	1.70	0.74
1:D:268:GLN:HB2	1:D:287:ILE:HD11	1.69	0.73
1:B:330:ASN:H	1:B:333:GLY:HA2	1.53	0.73
1:A:126:PHE:HB2	1:A:301:TYR:HA	1.68	0.73
1:I:42:GLU:HB2	1:I:47:HIS:HA	1.70	0.73
1:C:139:THR:HG21	1:C:334:VAL:HG12	1.71	0.72
1:D:77:GLU:HA	1:D:80:LYS:HD3	1.70	0.72
1:E:278:MET:HE2	4:U:27:DT:H5'	1.71	0.72
1:G:223:SER:HB3	1:G:226:ALA:HB2	1.71	0.72
1:C:172:LEU:HD21	1:C:186:LEU:HD22	1.72	0.72
1:A:28:LEU:HG	1:A:49:VAL:HG22	1.70	0.71
1:A:71:ALA:HA	1:A:74:ILE:HD12	1.72	0.71
1:A:25:ILE:HG13	1:A:28:LEU:HD12	1.71	0.71
1:E:278:MET:HG3	1:E:283:PRO:HG2	1.73	0.71
1:B:162:THR:HG21	1:B:227:LEU:HD21	1.72	0.71
1:I:142:VAL:HG13	1:I:171:LEU:HD22	1.73	0.70
1:B:158:MET:HG3	1:B:160:ILE:HG23	1.73	0.70
1:B:201:THR:HG22	1:B:204:LEU:H	1.56	0.70
1:C:130:ARG:HD2	1:B:315:TYR:O	1.90	0.70
1:B:201:THR:HB	1:B:204:LEU:HB2	1.74	0.70
3:T:29:DC:H41	1:F:274:ASP:CG	2.00	0.70
1:I:33:ILE:HD13	1:I:74:ILE:HG12	1.74	0.69
1:I:34:ASN:HD21	1:I:70:LYS:HB3	1.56	0.69
1:D:161:ASP:HB3	1:D:191:TYR:CE1	2.27	0.69
1:C:102:ILE:O	1:C:116:GLY:HA3	1.92	0.69
1:G:66:ILE:HG12	1:G:70:LYS:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ALA:HB3	1:B:189:VAL:HG12	1.74	0.69
1:I:272:GLN:HB3	1:I:285:LYS:HE2	1.75	0.69
1:H:175:ALA:HB2	1:H:185:VAL:HG11	1.75	0.69
1:H:82:VAL:HG13	1:H:84:MET:HE2	1.74	0.69
1:B:68:GLU:HA	1:B:71:ALA:HB3	1.74	0.68
1:A:57:LYS:O	1:A:61:ILE:HB	1.93	0.68
1:H:242:GLN:HB3	1:H:291:ILE:HD12	1.76	0.68
1:E:235:ARG:HH21	1:F:274:ASP:HA	1.57	0.68
1:C:270:VAL:HB	1:C:287:ILE:HG22	1.76	0.68
1:F:223:SER:HB2	1:F:226:ALA:HB2	1.75	0.68
1:I:126:PHE:CE2	1:I:286:PRO:HB3	2.28	0.68
1:B:200:GLN:NE2	1:B:201:THR:H	1.92	0.67
1:I:46:TYR:HE2	1:I:55:ALA:HB2	1.59	0.67
1:A:61:ILE:HD11	1:A:68:GLU:H	1.59	0.67
1:G:238:LEU:HD12	2:L:8:DT:H2"	1.77	0.67
1:A:329:ILE:HA	1:A:334:VAL:HA	1.76	0.67
1:A:158:MET:HB3	1:A:219:LEU:HB2	1.77	0.67
1:A:204:LEU:HD23	1:A:251:MET:HG3	1.76	0.67
1:G:272:GLN:HB2	1:G:283:PRO:HB2	1.77	0.67
1:I:189:VAL:HG23	1:I:191:TYR:H	1.59	0.67
1:H:219:LEU:HD22	1:H:221:VAL:HG22	1.77	0.67
3:T:32:DA:H2"	3:T:33:DG:C8	2.31	0.66
4:U:10:DG:H2'	4:U:11:DT:C6	2.30	0.66
1:B:66:ILE:HG23	1:B:70:LYS:HB3	1.77	0.66
1:A:113:LEU:HD21	1:A:117:ILE:HG22	1.77	0.66
1:H:310:ARG:HE	1:H:329:ILE:HD12	1.60	0.66
1:I:161:ASP:HA	1:I:222:ASP:HB2	1.78	0.66
1:I:268:GLN:HB2	1:I:287:ILE:HD11	1.76	0.66
1:A:61:ILE:HD11	1:A:68:GLU:HA	1.78	0.66
1:I:131:THR:HA	1:I:310:ARG:HE	1.61	0.66
1:A:66:ILE:HD12	1:A:71:ALA:HB2	1.77	0.65
1:A:156:LYS:HA	1:A:188:ASN:HD22	1.62	0.65
1:I:91:GLU:HA	1:I:94:GLN:HG2	1.78	0.65
1:E:124:GLU:HA	1:E:265:ILE:HG23	1.78	0.65
1:C:135:GLN:HE22	1:C:170:ARG:HE	1.45	0.65
1:H:303:ARG:HH21	1:H:311:ILE:HG13	1.62	0.65
1:D:162:THR:HG23	1:D:194:GLY:HA3	1.78	0.65
1:I:144:CYS:HB3	1:I:218:LEU:HD22	1.79	0.64
1:D:61:ILE:H	1:D:61:ILE:HD12	1.62	0.64
1:E:235:ARG:CG	3:T:29:DC:H5"	2.26	0.64
1:A:292:ILE:HG12	1:A:299:ARG:HH22	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:272:GLN:H	1:I:272:GLN:CD	2.05	0.64
1:C:117:ILE:HD12	1:C:117:ILE:H	1.63	0.64
1:E:103:THR:HB	1:E:143:THR:HG21	1.79	0.64
1:C:225:THR:HB	1:C:287:ILE:HD11	1.80	0.63
1:B:33:ILE:HG23	1:B:70:LYS:HE3	1.79	0.63
1:A:157:ALA:HB3	1:A:189:VAL:HB	1.80	0.63
1:C:258:GLU:HG3	1:C:259:PHE:H	1.64	0.63
1:I:123:THR:HB	1:I:298:THR:HG23	1.79	0.63
1:E:319:CYS:HB2	1:F:167:ARG:HG3	1.80	0.63
1:D:30:GLN:H	1:D:33:ILE:HB	1.64	0.63
1:H:104:THR:HG23	1:H:106:SER:H	1.63	0.63
1:A:313:LYS:HG2	1:A:324:GLU:HB3	1.81	0.62
1:A:56:PRO:HG2	1:A:59:GLU:HB2	1.79	0.62
1:D:219:LEU:HG	1:D:221:VAL:HG22	1.80	0.62
1:G:40:LYS:HG2	1:G:65:GLY:HA3	1.81	0.62
1:B:197:THR:HG22	1:B:227:LEU:HB2	1.80	0.62
1:B:24:PRO:O	1:B:49:VAL:HG23	2.00	0.62
1:A:112:LEU:HD11	1:A:325:ALA:HB3	1.81	0.62
1:D:70:LYS:HA	1:D:73:LYS:HD2	1.81	0.62
1:D:126:PHE:HE1	1:D:299:ARG:HG2	1.65	0.62
1:E:195:PHE:H	1:E:199:HIS:HD2	1.47	0.61
1:I:89:ALA:HA	1:I:92:PHE:CD2	2.35	0.61
1:B:269:VAL:HG21	1:B:284:LYS:HG3	1.83	0.61
1:B:196:ASN:H	1:B:202:GLN:HE22	1.47	0.61
1:B:63:ILE:HG23	1:B:64:LYS:HE3	1.82	0.61
2:L:21:DA:C5	1:D:273:VAL:HG12	2.35	0.61
2:L:20:DC:H2"	1:C:238:LEU:HG	1.83	0.61
1:B:41:LEU:HB2	1:B:46:TYR:HD2	1.65	0.61
1:A:314:ILE:HD12	1:A:323:ALA:HB3	1.81	0.61
1:I:232:TYR:HB2	1:I:241:ARG:HD3	1.82	0.61
1:F:148:ILE:HD12	1:F:148:ILE:H	1.65	0.61
1:G:242:GLN:HB3	1:G:291:ILE:HG13	1.83	0.60
1:E:37:ASP:HA	1:E:40:LYS:HD2	1.83	0.60
1:B:309:THR:HA	1:B:328:ALA:HA	1.84	0.60
1:E:225:THR:O	1:E:287:ILE:HD11	2.01	0.60
1:I:35:ALA:O	1:I:39:LYS:HG2	2.02	0.60
1:B:69:ALA:O	1:B:73:LYS:HB2	2.01	0.60
1:A:242:GLN:HG3	1:A:291:ILE:HD12	1.83	0.60
1:H:225:THR:HG21	1:H:292:ILE:HD13	1.84	0.60
1:H:246:ALA:HB2	1:H:291:ILE:HD13	1.83	0.60
1:A:103:THR:HA	1:A:110:ASP:OD1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:229:ARG:HH21	1:G:270:VAL:HG12	1.66	0.60
1:F:102:ILE:O	1:F:116:GLY:HA3	2.01	0.60
1:I:31:CYS:HB3	1:I:33:ILE:HG13	1.82	0.60
1:A:131:THR:HG23	1:A:304:LYS:HB2	1.84	0.60
1:C:100:ILE:HD12	1:C:119:THR:HG21	1.83	0.59
1:I:230:THR:HG21	1:H:250:ARG:HG3	1.83	0.59
1:H:129:PHE:O	5:H:602:ANP:N3B	2.35	0.59
1:B:259:PHE:HB3	1:B:261:VAL:HG13	1.84	0.59
1:I:71:ALA:HA	1:I:74:ILE:HD12	1.84	0.59
1:A:140:LEU:HB3	1:A:218:LEU:HD21	1.84	0.59
1:F:313:LYS:HB2	1:F:324:GLU:HG3	1.82	0.59
1:E:242:GLN:HB3	1:E:291:ILE:HD12	1.85	0.59
1:C:156:LYS:HG3	1:C:216:TYR:CD1	2.36	0.59
1:B:145:GLN:HA	1:B:154:GLU:HA	1.84	0.59
1:B:222:ASP:HA	1:B:266:THR:HB	1.85	0.59
1:A:61:ILE:HD11	1:A:68:GLU:N	2.18	0.59
1:A:243:MET:HE3	1:A:243:MET:O	2.02	0.59
1:I:112:LEU:HD12	1:I:325:ALA:HB3	1.84	0.59
1:C:133:LYS:HB3	1:C:266:THR:HG23	1.84	0.59
1:I:111:LYS:O	1:I:111:LYS:HD3	2.03	0.59
1:I:175:ALA:HB2	1:I:185:VAL:HG11	1.83	0.59
1:C:317:SER:HB2	1:C:320:LEU:HD12	1.85	0.59
1:I:24:PRO:O	1:I:27:ARG:HG2	2.02	0.59
1:I:24:PRO:HD2	1:I:27:ARG:CZ	2.33	0.59
1:B:223:SER:HB3	1:B:226:ALA:HB3	1.85	0.58
1:I:288:GLY:O	1:I:292:ILE:HB	2.02	0.58
2:L:25:DT:H2"	2:L:26:DT:H5"	1.84	0.58
1:B:186:LEU:HB3	1:A:90:THR:HG22	1.84	0.58
1:E:283:PRO:HB3	4:U:27:DT:OP1	2.04	0.58
1:F:221:VAL:HB	1:F:265:ILE:HG12	1.86	0.58
1:H:126:PHE:HE1	1:H:299:ARG:HD2	1.68	0.58
1:B:273:VAL:HB	1:A:238:LEU:HD13	1.86	0.58
1:A:58:LYS:O	1:A:61:ILE:HG22	2.03	0.58
1:B:131:THR:HA	1:B:310:ARG:HE	1.68	0.58
1:B:207:ALA:HA	1:B:210:MET:HG2	1.86	0.58
1:F:177:ARG:HG2	1:F:332:ASP:HB3	1.86	0.58
1:D:66:ILE:HG23	1:D:70:LYS:HB3	1.85	0.58
2:L:27:DT:H72	1:B:272:GLN:C	2.29	0.57
1:C:88:THR:HG22	1:C:90:THR:H	1.68	0.57
1:B:45:GLY:HA3	1:B:254:ARG:HH22	1.68	0.57
1:E:273:VAL:HA	2:L:18:DC:C4	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:252:LEU:HD13	1:H:263:VAL:HG11	1.84	0.57
1:D:119:THR:HG22	1:D:262:ALA:HB2	1.87	0.57
1:D:219:LEU:HG	1:D:221:VAL:CG2	2.33	0.57
1:E:238:LEU:HD23	1:F:273:VAL:HG21	1.86	0.57
1:A:225:THR:HG22	1:A:248:PHE:HZ	1.69	0.57
1:A:248:PHE:O	1:A:252:LEU:HG	2.04	0.57
1:B:50:GLU:HG3	1:B:82:VAL:HG22	1.86	0.57
1:H:110:ASP:O	1:H:112:LEU:O	2.23	0.57
1:E:139:THR:HG21	1:E:334:VAL:HB	1.87	0.57
1:B:161:ASP:HB2	1:B:222:ASP:HB3	1.87	0.57
1:A:220:ILE:HG13	1:A:264:VAL:HG23	1.86	0.57
1:H:113:LEU:HA	1:H:320:LEU:HD22	1.86	0.57
1:G:310:ARG:HH21	1:G:329:ILE:HD12	1.70	0.57
1:A:131:THR:HA	1:A:304:LYS:HD3	1.87	0.57
1:F:242:GLN:HB3	1:F:291:ILE:HG13	1.87	0.57
3:T:35:DC:H2"	3:T:36:DT:C4	2.40	0.57
1:A:312:CYS:HB2	1:A:327:PHE:CE1	2.40	0.57
1:E:235:ARG:NH2	1:F:274:ASP:HA	2.20	0.56
1:E:239:SER:O	1:E:243:MET:HG3	2.05	0.56
1:I:199:HIS:NE2	1:H:84:MET:HB3	2.20	0.56
1:G:77:GLU:HA	1:G:80:LYS:HD3	1.88	0.56
1:H:109:LEU:HG	1:H:327:PHE:HB3	1.87	0.56
1:C:269:VAL:HG21	1:C:284:LYS:HG3	1.86	0.56
1:A:124:GLU:HG2	1:A:265:ILE:HB	1.87	0.56
1:C:162:THR:HB	1:C:227:LEU:HG	1.88	0.56
1:F:128:GLU:HG3	1:F:129:PHE:H	1.69	0.56
1:E:126:PHE:CD2	1:E:286:PRO:HG3	2.41	0.56
1:D:220:ILE:O	1:D:221:VAL:C	2.49	0.56
1:A:36:ASN:O	1:A:39:LYS:HG3	2.05	0.56
1:I:33:ILE:O	1:I:34:ASN:C	2.49	0.56
1:I:219:LEU:HD22	1:I:255:LEU:HD11	1.88	0.56
1:E:310:ARG:HB2	1:E:327:PHE:CE1	2.41	0.56
1:G:161:ASP:HB3	1:G:191:TYR:HE1	1.71	0.56
1:B:78:ALA:O	1:B:81:LEU:HB2	2.06	0.56
1:H:56:PRO:HD2	1:H:59:GLU:HG2	1.88	0.56
1:H:161:ASP:HB3	1:H:191:TYR:HE1	1.71	0.56
1:A:133:LYS:O	1:A:136:ILE:HG22	2.06	0.55
1:B:139:THR:HG21	1:B:334:VAL:HG21	1.88	0.55
1:A:29:GLU:HB3	1:A:38:VAL:HG21	1.89	0.55
1:A:107:LYS:O	1:A:111:LYS:HB2	2.05	0.55
1:I:55:ALA:HB1	1:I:60:LEU:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:22:DT:H2'	4:U:23:DT:H2'	1.89	0.55
1:I:225:THR:HA	1:I:228:TYR:HD2	1.72	0.55
1:E:228:TYR:HD1	1:E:241:ARG:HG3	1.70	0.55
1:C:130:ARG:HG3	1:B:316:ASP:HB2	1.88	0.55
1:C:235:ARG:HH11	1:C:238:LEU:HB2	1.70	0.55
1:B:200:GLN:OE1	1:B:251:MET:HG2	2.06	0.55
1:F:109:LEU:HD11	1:F:312:CYS:HB3	1.89	0.55
1:H:100:ILE:HG12	1:H:148:ILE:HD11	1.89	0.55
1:H:171:LEU:HD21	1:H:186:LEU:HD21	1.88	0.55
1:C:156:LYS:HB3	1:C:188:ASN:HB3	1.87	0.55
1:A:204:LEU:HD21	1:A:252:LEU:HD23	1.89	0.55
1:A:205:TYR:HA	1:A:208:GLU:CD	2.32	0.55
1:D:56:PRO:HG2	1:D:59:GLU:HB2	1.86	0.55
1:E:309:THR:HB	1:E:326:MET:SD	2.46	0.55
2:L:6:DT:C4	1:I:273:VAL:HA	2.42	0.55
2:L:22:DC:H2''	2:L:23:DG:C8	2.42	0.55
1:B:117:ILE:HD12	1:B:117:ILE:H	1.72	0.55
1:A:204:LEU:HB3	1:A:251:MET:HE2	1.88	0.55
1:D:194:GLY:O	1:D:199:HIS:HB3	2.07	0.55
1:E:281:ALA:O	1:E:282:ASP:C	2.49	0.55
1:B:33:ILE:HA	1:B:73:LYS:HE3	1.87	0.55
1:B:270:VAL:HG22	1:B:285:LYS:HB3	1.88	0.55
1:E:162:THR:HB	1:E:227:LEU:HD22	1.88	0.55
1:E:278:MET:HE1	4:U:27:DT:C6	2.42	0.55
1:A:61:ILE:HD11	1:A:68:GLU:CA	2.37	0.55
1:E:234:GLY:O	1:E:236:GLY:N	2.40	0.55
1:A:138:HIS:HE1	1:A:167:ARG:HB3	1.72	0.55
1:H:299:ARG:HB2	1:H:316:ASP:HB3	1.88	0.55
1:G:239:SER:O	1:G:243:MET:HG3	2.08	0.54
1:B:196:ASN:H	1:B:202:GLN:NE2	2.05	0.54
1:H:112:LEU:O	1:H:113:LEU:HB2	2.07	0.54
1:E:278:MET:HE3	1:E:280:ALA:H	1.72	0.54
1:B:200:GLN:HG2	1:B:251:MET:HG2	1.90	0.54
1:D:158:MET:HG2	1:D:219:LEU:CD1	2.37	0.54
1:B:163:GLU:HB3	1:B:165:THR:HG23	1.90	0.54
1:F:113:LEU:HD21	1:F:300:LEU:HD21	1.90	0.54
1:F:161:ASP:HB3	1:F:191:TYR:HE1	1.71	0.54
1:I:196:ASN:OD1	1:I:199:HIS:HB2	2.07	0.54
1:D:102:ILE:HD13	1:D:218:LEU:HD12	1.90	0.54
1:I:106:SER:O	1:I:110:ASP:HB2	2.08	0.54
1:D:170:ARG:HH22	1:D:333:GLY:H	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:GLU:HB2	1:C:38:VAL:HG11	1.90	0.54
1:C:76:THR:O	1:C:80:LYS:HG3	2.06	0.54
1:D:239:SER:O	1:D:243:MET:HG3	2.08	0.54
1:I:148:ILE:HG13	1:I:154:GLU:CD	2.33	0.53
1:I:314:ILE:HG23	1:I:317:SER:OG	2.08	0.53
1:I:126:PHE:CZ	1:I:286:PRO:HB3	2.43	0.53
1:I:195:PHE:HE2	1:H:84:MET:HG2	1.74	0.53
1:I:309:THR:HG23	1:I:326:MET:HG2	1.90	0.53
1:E:238:LEU:HG	2:L:14:DG:H2''	1.89	0.53
2:L:6:DT:H3	1:H:235:ARG:CZ	2.21	0.53
1:C:315:TYR:O	1:D:130:ARG:HD3	2.09	0.53
4:U:21:DC:N3	1:F:277:ALA:HB1	2.23	0.53
1:C:242:GLN:HB3	1:C:291:ILE:HD12	1.89	0.53
1:G:170:ARG:O	1:G:174:VAL:HG23	2.09	0.53
1:A:170:ARG:O	1:A:174:VAL:HG23	2.09	0.53
1:G:41:LEU:HD11	1:G:74:ILE:HD12	1.89	0.53
1:B:48:THR:HG22	1:B:50:GLU:H	1.73	0.53
1:E:238:LEU:HD21	2:L:15:DT:O4'	2.09	0.53
4:U:24:DT:O3'	1:F:303:ARG:HD2	2.08	0.53
1:C:140:LEU:HA	1:C:143:THR:HG22	1.89	0.53
1:D:311:ILE:HD11	1:D:326:MET:HE2	1.91	0.53
1:G:273:VAL:CG2	2:L:11:DT:H2'	2.39	0.53
1:G:314:ILE:HG13	1:G:323:ALA:H	1.74	0.53
1:B:252:LEU:HD22	1:B:265:ILE:HD11	1.91	0.53
1:I:198:ASP:O	1:I:202:GLN:HG3	2.09	0.53
1:A:101:GLN:HB3	1:A:116:GLY:HA3	1.89	0.52
1:G:279:PHE:HB3	4:U:18:DA:H1'	1.92	0.52
1:A:218:LEU:HB2	1:A:262:ALA:HB3	1.90	0.52
1:I:145:GLN:OE1	1:I:185:VAL:HA	2.10	0.52
1:H:143:THR:HG22	1:H:178:TYR:HE2	1.75	0.52
1:I:107:LYS:HZ1	1:I:111:LYS:HB2	1.74	0.52
1:I:314:ILE:HD12	1:I:317:SER:OG	2.09	0.52
1:H:144:CYS:SG	1:H:157:ALA:HB2	2.49	0.52
1:C:221:VAL:CG1	1:C:265:ILE:HG12	2.39	0.52
1:H:109:LEU:O	1:H:112:LEU:O	2.28	0.52
1:E:204:LEU:HD11	1:E:248:PHE:CE1	2.45	0.52
1:A:252:LEU:O	1:A:255:LEU:HG	2.09	0.52
1:I:267:ASN:HD21	1:I:292:ILE:HG12	1.74	0.52
1:E:177:ARG:HB2	1:E:332:ASP:HB3	1.92	0.52
1:G:302:LEU:HD23	1:G:312:CYS:HB2	1.90	0.52
1:D:320:LEU:HD23	1:D:321:PRO:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:LEU:HD23	1:E:49:VAL:HG23	1.90	0.52
1:G:175:ALA:HB2	1:G:185:VAL:HG11	1.92	0.52
1:C:158:MET:HG2	1:C:190:ALA:HB3	1.91	0.52
1:I:34:ASN:OD1	1:I:70:LYS:HD2	2.09	0.52
1:H:220:ILE:O	1:H:221:VAL:C	2.53	0.52
1:E:249:LEU:HD11	1:E:292:ILE:HG13	1.91	0.52
1:B:72:ASP:HA	1:B:75:LEU:HB2	1.92	0.52
1:B:174:VAL:HG12	1:B:332:ASP:HB3	1.92	0.52
1:I:63:ILE:HB	1:I:66:ILE:HG12	1.92	0.52
1:B:200:GLN:OE1	1:B:204:LEU:HB3	2.11	0.51
1:B:200:GLN:HE21	1:B:201:THR:H	1.57	0.51
1:G:273:VAL:HG13	2:L:12:DT:N3	2.25	0.51
2:L:27:DT:C5	1:B:273:VAL:HA	2.45	0.51
1:C:211:MET:HA	1:C:216:TYR:HD2	1.74	0.51
1:H:162:THR:OG1	1:H:223:SER:HB2	2.09	0.51
1:I:103:THR:HG23	1:I:151:GLY:HA3	1.91	0.51
2:L:12:DT:H1'	2:L:13:DC:H5'	1.93	0.51
1:A:118:GLU:HB2	1:A:121:SER:HB3	1.93	0.51
1:E:170:ARG:O	1:E:174:VAL:HG23	2.11	0.51
1:B:300:LEU:HD12	1:B:312:CYS:SG	2.51	0.51
1:F:112:LEU:HD23	1:F:113:LEU:HG	1.93	0.51
1:F:270:VAL:HG22	1:F:271:ALA:H	1.76	0.51
1:H:135:GLN:O	1:H:139:THR:HG23	2.11	0.51
1:E:142:VAL:HG13	1:E:185:VAL:HG21	1.92	0.51
1:G:94:GLN:O	1:G:98:GLU:HG2	2.10	0.51
1:I:186:LEU:O	1:H:89:ALA:HB3	2.11	0.51
1:E:291:ILE:HD11	2:L:14:DG:H5'	1.92	0.51
4:U:24:DT:H2'	4:U:25:DT:N3	2.26	0.51
1:C:317:SER:OG	1:C:320:LEU:HB2	2.10	0.51
1:B:50:GLU:HB3	1:B:258:GLU:HG2	1.93	0.51
1:A:37:ASP:HA	1:A:40:LYS:HG2	1.93	0.51
1:I:138:HIS:O	1:I:142:VAL:HG22	2.11	0.51
1:F:123:THR:HG23	1:F:298:THR:HB	1.91	0.51
1:I:229:ARG:NH2	1:I:270:VAL:HG12	2.26	0.51
1:E:267:ASN:HD22	1:E:286:PRO:HB3	1.75	0.51
1:B:106:SER:HB3	1:B:335:GLY:HA3	1.92	0.51
1:F:41:LEU:HD11	1:F:74:ILE:HD13	1.93	0.51
1:C:77:GLU:HA	1:C:80:LYS:HD2	1.91	0.50
1:I:78:ALA:O	1:I:82:VAL:HG13	2.11	0.50
1:I:159:TYR:O	1:I:191:TYR:HA	2.11	0.50
1:B:112:LEU:HG	1:B:314:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LEU:HD23	1:A:150:ARG:HB3	1.91	0.50
1:G:161:ASP:HA	1:G:222:ASP:HB3	1.92	0.50
1:G:112:LEU:HD13	1:G:325:ALA:HB2	1.92	0.50
1:B:112:LEU:HD22	1:B:325:ALA:HB2	1.92	0.50
1:F:298:THR:HG23	1:F:317:SER:HB3	1.93	0.50
1:E:195:PHE:H	1:E:199:HIS:CD2	2.28	0.50
1:G:207:ALA:O	1:G:211:MET:HG3	2.11	0.50
1:B:177:ARG:CZ	1:B:332:ASP:HB2	2.42	0.50
1:G:235:ARG:NH1	2:L:9:DT:H3	2.10	0.50
1:I:57:LYS:C	1:I:59:GLU:H	2.20	0.50
1:E:273:VAL:HG23	1:D:235:ARG:HD2	1.94	0.50
4:U:23:DT:H4'	4:U:24:DT:O5'	2.11	0.50
1:F:254:ARG:O	1:F:258:GLU:HB2	2.12	0.50
1:I:107:LYS:NZ	1:I:110:ASP:HB3	2.26	0.50
1:E:208:GLU:O	1:E:212:VAL:HG23	2.12	0.50
1:G:280:ALA:H	4:U:18:DA:H2	1.60	0.50
1:A:99:ILE:HG23	1:A:119:THR:HG23	1.93	0.50
1:E:243:MET:HE1	1:F:234:GLY:HA2	1.94	0.49
1:E:126:PHE:HB3	1:E:267:ASN:HB3	1.94	0.49
1:E:278:MET:CG	1:E:283:PRO:HG2	2.42	0.49
1:G:246:ALA:HB2	1:G:291:ILE:HD12	1.94	0.49
1:A:69:ALA:C	1:A:71:ALA:H	2.20	0.49
1:A:119:THR:HA	1:A:262:ALA:HA	1.94	0.49
1:I:28:LEU:HB2	1:I:49:VAL:CG2	2.42	0.49
1:H:313:LYS:HB2	1:H:324:GLU:HG3	1.94	0.49
1:B:71:ALA:O	1:B:74:ILE:HG12	2.12	0.49
1:A:109:LEU:HA	1:A:112:LEU:HD12	1.93	0.49
1:E:158:MET:HE1	1:E:207:ALA:HA	1.94	0.49
1:G:102:ILE:O	1:G:116:GLY:HA3	2.12	0.49
1:B:94:GLN:O	1:B:98:GLU:HG3	2.12	0.49
1:A:83:PRO:C	1:A:84:MET:HG3	2.36	0.49
1:A:91:GLU:CD	1:A:91:GLU:H	2.19	0.49
1:C:117:ILE:HD13	1:C:140:LEU:HD21	1.94	0.49
1:B:126:PHE:O	1:B:301:TYR:HA	2.12	0.49
1:I:131:THR:O	1:I:329:ILE:HD11	2.11	0.49
1:D:113:LEU:HD21	1:D:300:LEU:HD21	1.94	0.49
1:G:135:GLN:HG3	5:G:600:ANP:H5'2	1.93	0.49
1:C:209:ASP:O	1:C:212:VAL:HG12	2.13	0.49
1:A:27:ARG:HB2	1:A:49:VAL:HG21	1.94	0.49
1:A:301:TYR:HD2	1:A:313:LYS:HB2	1.77	0.49
1:I:25:ILE:H	1:I:25:ILE:HD13	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:THR:HG21	1:D:232:TYR:CE1	2.48	0.49
1:G:270:VAL:HG22	1:G:285:LYS:O	2.12	0.49
1:B:47:HIS:CD2	1:B:208:GLU:HG2	2.48	0.49
1:B:206:GLN:HE21	1:B:210:MET:HB3	1.78	0.49
1:I:140:LEU:HB3	1:I:218:LEU:HD21	1.95	0.49
1:H:146:LEU:HD23	1:H:180:LEU:HD21	1.94	0.49
1:D:146:LEU:HD22	1:D:150:ARG:HD3	1.93	0.49
1:B:139:THR:OG1	1:B:334:VAL:HG11	2.12	0.49
1:B:208:GLU:HB2	1:B:255:LEU:HD11	1.94	0.49
1:A:124:GLU:CD	1:A:299:ARG:HH21	2.21	0.49
1:H:287:ILE:HG12	1:H:288:GLY:H	1.76	0.49
1:E:278:MET:HG3	1:E:283:PRO:CG	2.41	0.49
3:T:31:DT:H1'	3:T:32:DA:N7	2.27	0.49
1:C:237:GLU:O	1:C:238:LEU:C	2.56	0.49
1:B:168:PRO:HB2	1:A:93:HIS:CE1	2.48	0.49
1:A:136:ILE:HD13	1:A:334:VAL:HG21	1.95	0.49
1:D:128:GLU:HG3	1:D:284:LYS:HZ1	1.78	0.49
1:G:254:ARG:O	1:G:258:GLU:HB2	2.12	0.49
1:C:220:ILE:HG23	1:C:264:VAL:HB	1.94	0.49
1:I:196:ASN:HD22	1:H:55:ALA:C	2.20	0.49
1:D:259:PHE:HB2	1:D:261:VAL:HG13	1.95	0.49
1:E:70:LYS:HA	1:E:70:LYS:HD3	1.63	0.48
1:G:273:VAL:HG23	2:L:11:DT:H2'	1.94	0.48
1:A:117:ILE:HD13	1:A:264:VAL:HG13	1.96	0.48
1:C:70:LYS:O	1:C:74:ILE:HG13	2.13	0.48
1:B:308:GLU:HB2	1:B:329:ILE:H	1.77	0.48
1:A:147:PRO:HD2	1:A:150:ARG:HD2	1.95	0.48
1:E:132:GLY:O	1:E:136:ILE:HG13	2.13	0.48
1:B:128:GLU:HA	1:B:269:VAL:HG11	1.95	0.48
1:A:251:MET:HE3	1:A:255:LEU:HD23	1.95	0.48
1:H:67:SER:O	1:H:68:GLU:C	2.56	0.48
1:D:180:LEU:HD22	1:D:185:VAL:HG23	1.96	0.48
1:A:100:ILE:O	1:A:101:GLN:HB2	2.13	0.48
1:I:159:TYR:CE1	1:I:161:ASP:HB2	2.48	0.48
1:C:250:ARG:HG3	1:C:250:ARG:O	2.13	0.48
1:A:301:TYR:HB2	1:A:315:TYR:HB2	1.96	0.48
1:E:275:GLY:C	1:E:277:ALA:N	2.70	0.48
1:I:24:PRO:HD2	1:I:27:ARG:NH2	2.29	0.48
1:G:160:ILE:HG22	1:G:160:ILE:O	2.13	0.48
2:L:25:DT:H5'	1:B:241:ARG:HH22	1.79	0.48
1:C:66:ILE:HD13	1:C:70:LYS:HE3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:ARG:O	1:C:258:GLU:HG2	2.13	0.48
1:B:119:THR:HA	1:B:262:ALA:HA	1.95	0.48
1:I:106:SER:O	1:I:110:ASP:N	2.47	0.48
1:H:221:VAL:HG11	1:H:248:PHE:HZ	1.79	0.48
1:E:111:LYS:HB2	1:E:111:LYS:HE3	1.46	0.48
1:E:138:HIS:HD2	1:E:170:ARG:HB2	1.78	0.48
1:B:31:CYS:HB3	1:B:33:ILE:HD13	1.96	0.48
1:B:186:LEU:O	1:A:89:ALA:HB3	2.13	0.48
1:A:137:CYS:SG	1:A:220:ILE:HG21	2.53	0.48
1:H:175:ALA:CB	1:H:185:VAL:HG11	2.44	0.48
1:D:158:MET:HE3	1:D:211:MET:HE3	1.96	0.48
1:H:158:MET:HE2	1:H:219:LEU:HG	1.96	0.48
1:H:170:ARG:O	1:H:174:VAL:HG23	2.14	0.48
1:A:299:ARG:HB2	1:A:316:ASP:H	1.79	0.47
1:I:211:MET:SD	1:I:216:TYR:HB2	2.54	0.47
1:G:112:LEU:HG	1:G:314:ILE:HD11	1.96	0.47
1:H:125:MET:HE1	1:H:137:CYS:SG	2.54	0.47
1:G:70:LYS:O	1:G:74:ILE:HG12	2.14	0.47
1:B:329:ILE:C	1:B:333:GLY:HA2	2.39	0.47
1:A:102:ILE:HB	1:A:117:ILE:HG23	1.95	0.47
1:I:117:ILE:HD12	1:I:140:LEU:HD21	1.95	0.47
1:I:147:PRO:HA	1:I:154:GLU:HG3	1.96	0.47
1:H:112:LEU:HD21	1:H:323:ALA:HB3	1.96	0.47
1:E:106:SER:HB2	1:E:335:GLY:O	2.14	0.47
1:E:144:CYS:SG	1:E:157:ALA:HB2	2.55	0.47
1:C:221:VAL:HG21	1:C:224:ALA:HB2	1.95	0.47
1:B:25:ILE:HD13	1:B:25:ILE:H	1.78	0.47
1:B:189:VAL:HG22	1:A:89:ALA:HB2	1.96	0.47
1:B:210:MET:HG3	1:B:211:MET:HG3	1.96	0.47
1:B:225:THR:O	1:B:229:ARG:N	2.47	0.47
1:E:198:ASP:O	1:E:199:HIS:HB3	2.14	0.47
1:E:304:LYS:HZ3	1:E:310:ARG:NH1	2.13	0.47
4:U:24:DT:H5'	1:F:303:ARG:CZ	2.44	0.47
1:B:108:GLU:HA	1:B:111:LYS:HD2	1.97	0.47
1:B:329:ILE:HG23	1:B:333:GLY:HA3	1.97	0.47
1:I:107:LYS:HZ3	1:I:110:ASP:HB3	1.79	0.47
1:I:225:THR:HG21	1:I:292:ILE:HD11	1.96	0.47
1:E:134:THR:HG23	5:E:600:ANP:O2B	2.15	0.47
1:G:279:PHE:HD2	4:U:18:DA:C1'	2.27	0.47
4:U:25:DT:H1'	4:U:26:DT:C2	2.50	0.47
1:C:135:GLN:HE22	1:C:170:ARG:NE	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:LEU:HD22	1:C:263:VAL:HG11	1.96	0.47
1:I:291:ILE:H	1:I:294:HIS:CD2	2.33	0.47
1:E:211:MET:HE2	1:E:261:VAL:HG11	1.97	0.47
1:G:272:GLN:HB2	1:G:283:PRO:CB	2.44	0.47
2:L:27:DT:OP2	1:B:271:ALA:HB3	2.15	0.47
1:B:155:GLY:O	1:B:156:LYS:C	2.56	0.47
1:F:284:LYS:HA	1:F:284:LYS:HD3	1.61	0.47
1:I:34:ASN:HB2	1:I:37:ASP:HB3	1.97	0.47
1:H:113:LEU:CD2	1:H:300:LEU:HD11	2.39	0.47
1:B:207:ALA:O	1:B:211:MET:HG3	2.15	0.47
1:F:102:ILE:HA	1:F:152:GLY:HA2	1.97	0.47
1:H:112:LEU:HD23	1:H:112:LEU:HA	1.69	0.47
1:C:232:TYR:CD2	1:C:241:ARG:HG3	2.50	0.47
1:C:327:PHE:CD2	1:C:334:VAL:HG23	2.50	0.47
1:I:272:GLN:HB3	1:I:285:LYS:CE	2.45	0.47
1:H:108:GLU:HA	1:H:111:LYS:HE2	1.96	0.47
1:D:100:ILE:HG21	1:D:153:GLY:HA2	1.97	0.47
1:G:73:LYS:HD2	1:G:73:LYS:C	2.40	0.47
1:C:126:PHE:CD2	1:C:286:PRO:HG3	2.50	0.47
1:C:183:SER:O	1:C:187:ASP:HB2	2.14	0.47
1:B:308:GLU:HG3	1:B:328:ALA:HB1	1.97	0.47
1:A:287:ILE:HD12	1:A:287:ILE:H	1.80	0.47
2:L:27:DT:C6	1:B:273:VAL:HG12	2.50	0.46
1:E:233:SER:H	1:E:237:GLU:HG3	1.80	0.46
1:E:112:LEU:HD23	1:E:113:LEU:HG	1.98	0.46
1:C:37:ASP:HB3	1:C:66:ILE:HD11	1.96	0.46
1:B:80:LYS:H	1:B:80:LYS:HZ2	1.63	0.46
1:B:238:LEU:HD12	1:B:241:ARG:NH2	2.30	0.46
1:F:57:LYS:O	1:F:61:ILE:HB	2.15	0.46
1:I:33:ILE:O	1:I:35:ALA:N	2.49	0.46
1:D:161:ASP:CB	1:D:191:TYR:HE1	2.23	0.46
1:E:103:THR:HG23	1:E:110:ASP:OD2	2.16	0.46
1:B:90:THR:O	1:B:94:GLN:HG3	2.15	0.46
1:B:297:THR:O	1:B:318:PRO:HD3	2.16	0.46
1:I:236:GLY:O	1:I:237:GLU:HB2	2.14	0.46
1:D:175:ALA:HB2	1:D:185:VAL:HG11	1.97	0.46
1:E:218:LEU:HD13	1:E:220:ILE:HD11	1.97	0.46
1:B:198:ASP:O	1:B:199:HIS:C	2.58	0.46
1:I:56:PRO:HB2	1:I:59:GLU:HB3	1.95	0.46
2:L:21:DA:H1'	2:L:22:DC:H5'	1.97	0.46
1:B:273:VAL:HG11	1:A:238:LEU:HD22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:VAL:O	1:F:177:ARG:HG3	2.16	0.46
1:I:33:ILE:HD11	1:I:77:GLU:HB2	1.97	0.46
1:G:229:ARG:NH2	1:G:270:VAL:HG12	2.30	0.46
2:L:26:DT:O5'	1:B:270:VAL:HB	2.15	0.46
1:I:70:LYS:HD3	1:I:73:LYS:HE3	1.98	0.46
1:G:276:ALA:O	1:G:279:PHE:HE1	1.99	0.46
1:I:287:ILE:O	1:I:292:ILE:HD13	2.16	0.46
1:G:29:GLU:HB3	1:G:38:VAL:HG11	1.98	0.46
1:G:144:CYS:SG	1:G:218:LEU:HB2	2.55	0.46
2:L:14:DG:H5''	1:F:270:VAL:HG23	1.97	0.46
1:A:101:GLN:HA	1:A:117:ILE:O	2.15	0.46
1:A:104:THR:HA	1:A:143:THR:HG21	1.97	0.46
1:A:140:LEU:HB3	1:A:218:LEU:CD2	2.45	0.46
1:F:38:VAL:O	1:F:42:GLU:HG2	2.16	0.46
1:I:172:LEU:HD11	1:I:186:LEU:HD22	1.97	0.46
1:H:46:TYR:HA	1:H:51:ALA:HB3	1.98	0.46
1:E:25:ILE:HG22	1:E:38:VAL:HG13	1.98	0.46
1:C:313:LYS:HE2	1:C:313:LYS:HB2	1.47	0.46
1:B:301:TYR:HD2	1:B:313:LYS:HD2	1.81	0.46
1:A:117:ILE:HD11	1:A:262:ALA:HB1	1.98	0.46
1:H:113:LEU:HA	1:H:320:LEU:CD2	2.46	0.46
1:G:109:LEU:HD23	1:G:109:LEU:HA	1.83	0.45
1:G:156:LYS:HB2	1:G:188:ASN:HB3	1.97	0.45
1:G:278:MET:HE3	1:G:278:MET:HB3	1.71	0.45
1:A:228:TYR:HA	1:A:231:ASP:HB2	1.98	0.45
1:I:41:LEU:HA	1:I:63:ILE:HD13	1.98	0.45
1:I:227:LEU:O	1:I:231:ASP:HB2	2.16	0.45
1:H:290:ASN:HA	1:H:293:ALA:HB3	1.98	0.45
1:D:308:GLU:HA	1:D:310:ARG:HH21	1.80	0.45
2:L:27:DT:O4	1:B:273:VAL:HA	2.14	0.45
1:C:46:TYR:N	1:C:46:TYR:CD1	2.84	0.45
1:C:57:LYS:HA	1:C:57:LYS:HD3	1.64	0.45
1:B:33:ILE:HG23	1:B:70:LYS:CE	2.47	0.45
1:A:156:LYS:O	1:A:217:ALA:N	2.46	0.45
1:E:235:ARG:NH1	3:T:28:DA:H2'	2.31	0.45
1:G:249:LEU:HD11	1:G:292:ILE:HG13	1.97	0.45
1:C:167:ARG:HA	1:C:167:ARG:HD3	1.58	0.45
1:B:228:TYR:HE2	1:B:244:HIS:HB3	1.82	0.45
1:I:24:PRO:HA	1:I:48:THR:HA	1.97	0.45
1:I:34:ASN:O	1:I:35:ALA:C	2.60	0.45
1:I:177:ARG:HH21	1:I:178:TYR:HE2	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:225:THR:CG2	1:I:292:ILE:HD11	2.46	0.45
1:D:144:CYS:SG	1:D:157:ALA:HB2	2.57	0.45
1:E:317:SER:O	5:F:600:ANP:H3'	2.17	0.45
1:A:61:ILE:CD1	1:A:68:GLU:H	2.29	0.45
1:A:120:GLY:H	1:A:261:VAL:C	2.23	0.45
1:I:58:LYS:HA	1:I:61:ILE:HG13	1.98	0.45
1:I:223:SER:HB2	1:I:226:ALA:HB2	1.98	0.45
1:E:186:LEU:HA	1:E:186:LEU:HD23	1.80	0.45
1:E:273:VAL:HG13	2:L:17:DG:C5	2.52	0.45
1:G:86:PHE:CE1	1:H:203:LEU:HD22	2.51	0.45
1:C:221:VAL:HG11	1:C:265:ILE:HG12	1.99	0.45
1:H:57:LYS:O	1:H:61:ILE:HG23	2.16	0.45
1:E:170:ARG:HD3	1:D:319:CYS:HA	1.99	0.45
1:E:304:LYS:HG3	1:E:310:ARG:HH11	1.82	0.45
2:L:26:DT:H4'	2:L:26:DT:OP1	2.15	0.45
1:B:254:ARG:O	1:B:258:GLU:HB2	2.16	0.45
1:A:239:SER:O	1:A:243:MET:CB	2.64	0.45
1:D:134:THR:HG23	5:D:600:ANP:O2B	2.17	0.45
1:C:235:ARG:HA	1:C:235:ARG:HD3	1.60	0.45
1:B:119:THR:HG22	1:B:262:ALA:N	2.31	0.45
5:F:600:ANP:H5'1	5:F:600:ANP:H8	1.98	0.45
1:H:50:GLU:OE2	1:H:82:VAL:HG21	2.17	0.45
1:H:143:THR:HG22	1:H:178:TYR:CE2	2.52	0.45
1:H:270:VAL:HG22	1:H:271:ALA:H	1.81	0.45
1:G:176:GLU:OE1	1:G:176:GLU:HA	2.16	0.45
1:H:272:GLN:HB2	1:H:283:PRO:HB3	1.99	0.45
1:H:287:ILE:HG12	1:H:288:GLY:N	2.31	0.45
1:C:138:HIS:HD2	1:C:171:LEU:HD13	1.81	0.45
1:B:310:ARG:HB2	1:B:327:PHE:CZ	2.52	0.45
1:F:161:ASP:O	1:F:193:ARG:HD2	2.17	0.45
1:I:57:LYS:HD3	1:I:57:LYS:HA	1.41	0.45
1:D:310:ARG:O	1:D:311:ILE:HD13	2.16	0.45
1:G:52:VAL:HG13	1:G:60:LEU:HD21	1.99	0.45
1:G:161:ASP:OD1	1:G:161:ASP:C	2.60	0.45
1:G:273:VAL:HG12	1:F:235:ARG:HD3	1.98	0.45
2:L:5:DT:H4'	1:H:242:GLN:HG3	1.99	0.45
1:C:92:PHE:C	1:C:94:GLN:H	2.25	0.45
1:C:196:ASN:HB3	1:C:198:ASP:H	1.82	0.45
1:C:230:THR:HG21	1:B:250:ARG:HB2	1.98	0.45
1:A:66:ILE:HD13	1:A:66:ILE:HA	1.78	0.45
1:I:27:ARG:HA	1:I:30:GLN:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:72:ASP:HA	1:I:75:LEU:HG	1.99	0.45
1:H:139:THR:HG21	1:H:334:VAL:H	1.81	0.45
1:D:207:ALA:O	1:D:211:MET:HG3	2.17	0.45
1:G:125:MET:HG2	1:G:300:LEU:HD12	1.99	0.44
1:G:182:GLY:HA2	1:G:185:VAL:HG12	1.99	0.44
1:B:305:GLY:H	1:B:310:ARG:HA	1.81	0.44
1:I:87:THR:HB	1:I:91:GLU:OE2	2.18	0.44
1:I:243:MET:O	1:I:247:ARG:HG2	2.17	0.44
1:D:140:LEU:O	1:D:218:LEU:HD13	2.17	0.44
1:E:273:VAL:HG11	1:D:238:LEU:HD23	1.99	0.44
1:G:51:ALA:HB1	1:G:254:ARG:HH21	1.82	0.44
1:C:167:ARG:NH1	1:B:318:PRO:HG2	2.32	0.44
1:A:161:ASP:H	1:A:191:TYR:HE1	1.66	0.44
1:H:218:LEU:HD12	1:H:262:ALA:HB3	2.00	0.44
1:D:229:ARG:NH2	1:D:270:VAL:HG12	2.32	0.44
1:D:306:ARG:HA	1:D:306:ARG:NE	2.33	0.44
1:E:278:MET:SD	4:U:26:DT:H1'	2.57	0.44
1:B:200:GLN:NE2	1:B:205:TYR:HB2	2.32	0.44
1:A:128:GLU:HA	1:A:269:VAL:HG12	2.00	0.44
1:A:155:GLY:CA	1:A:215:ARG:HH21	2.30	0.44
1:F:156:LYS:HB2	1:F:216:TYR:CD2	2.51	0.44
1:H:101:GLN:HA	1:H:117:ILE:O	2.17	0.44
1:D:125:MET:HE1	1:D:136:ILE:HB	1.99	0.44
1:E:279:PHE:HE1	4:U:26:DT:H72	1.82	0.44
3:T:24:DG:H2''	3:T:25:DG:O5'	2.18	0.44
1:C:257:ASP:OD1	1:C:258:GLU:N	2.50	0.44
1:A:70:LYS:HE3	1:A:74:ILE:HD11	1.99	0.44
1:A:119:THR:HB	1:A:262:ALA:HB2	1.99	0.44
1:F:111:LYS:HE3	1:F:111:LYS:HB2	1.61	0.44
1:F:203:LEU:HD12	1:F:203:LEU:HA	1.88	0.44
1:H:305:GLY:C	1:H:306:ARG:HE	2.26	0.44
1:D:254:ARG:O	1:D:258:GLU:HG3	2.17	0.44
1:G:279:PHE:HD2	4:U:18:DA:N9	2.16	0.44
3:T:23:DG:N3	3:T:23:DG:H2'	2.33	0.44
1:B:23:GLN:O	1:B:48:THR:HG23	2.17	0.44
1:B:197:THR:CG2	1:B:227:LEU:HB2	2.45	0.44
1:H:159:TYR:HE1	1:H:161:ASP:HB2	1.83	0.44
1:D:219:LEU:O	1:D:221:VAL:HG23	2.17	0.44
1:G:297:THR:O	1:G:318:PRO:HD3	2.17	0.44
1:C:142:VAL:HG21	1:C:174:VAL:HG13	1.99	0.44
1:C:156:LYS:HG3	1:C:216:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ILE:HG12	1:A:299:ARG:NH2	2.29	0.44
1:F:37:ASP:HA	1:F:40:LYS:NZ	2.33	0.44
1:D:101:GLN:HA	1:D:118:GLU:HA	1.99	0.44
1:G:130:ARG:HE	1:G:130:ARG:HB3	1.42	0.44
1:G:313:LYS:HE3	1:G:315:TYR:HA	1.99	0.44
3:T:37:DG:H1'	3:T:38:DA:H5'	2.00	0.44
1:E:229:ARG:HD2	1:E:287:ILE:HD13	1.99	0.44
1:B:200:GLN:HE22	1:B:205:TYR:H	1.66	0.44
1:A:126:PHE:CE2	1:A:299:ARG:HD2	2.53	0.44
1:F:29:GLU:CD	1:F:29:GLU:O	2.61	0.44
1:H:36:ASN:O	1:H:40:LYS:HG2	2.17	0.44
1:D:158:MET:HE2	1:D:216:TYR:CD2	2.53	0.44
1:A:207:ALA:C	1:A:209:ASP:N	2.74	0.44
1:A:233:SER:HB2	1:A:237:GLU:OE1	2.18	0.44
1:G:317:SER:O	5:H:602:ANP:H3'	2.18	0.43
1:A:136:ILE:HD12	1:A:136:ILE:HA	1.84	0.43
1:F:70:LYS:HD3	1:F:70:LYS:HA	1.87	0.43
1:I:130:ARG:HE	1:I:130:ARG:HB3	1.69	0.43
1:I:268:GLN:HB2	1:I:287:ILE:CD1	2.44	0.43
1:H:284:LYS:HA	1:H:284:LYS:HD3	1.74	0.43
1:E:269:VAL:HG11	1:E:284:LYS:HE3	2.00	0.43
1:B:329:ILE:HA	1:B:333:GLY:HA3	1.94	0.43
1:I:33:ILE:HD11	1:I:77:GLU:CB	2.48	0.43
1:I:199:HIS:HE2	1:H:84:MET:HB3	1.83	0.43
1:I:297:THR:O	1:I:298:THR:C	2.58	0.43
1:H:142:VAL:HG23	1:H:171:LEU:HB2	2.00	0.43
1:C:189:VAL:HB	1:B:89:ALA:HB2	2.00	0.43
1:C:203:LEU:HD23	1:C:203:LEU:HA	1.85	0.43
1:B:180:LEU:HD23	1:B:180:LEU:HA	1.86	0.43
1:D:161:ASP:O	1:D:193:ARG:HA	2.18	0.43
1:E:227:LEU:HD12	1:E:227:LEU:HA	1.80	0.43
2:L:13:DC:H5''	1:F:241:ARG:HH22	1.83	0.43
1:A:239:SER:O	1:A:243:MET:HB2	2.18	0.43
1:I:107:LYS:HD2	1:I:107:LYS:HA	1.27	0.43
1:D:297:THR:O	1:D:318:PRO:HD3	2.17	0.43
1:B:309:THR:O	1:B:310:ARG:HD3	2.19	0.43
1:A:144:CYS:HB3	1:A:217:ALA:HB3	2.00	0.43
1:I:77:GLU:O	1:I:80:LYS:HB2	2.19	0.43
1:D:224:ALA:O	1:D:225:THR:C	2.61	0.43
1:D:241:ARG:NH2	1:D:242:GLN:HE22	2.16	0.43
2:L:21:DA:O4'	1:C:238:LEU:HD21	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:SER:CB	1:C:320:LEU:HD12	2.48	0.43
1:B:122:ILE:HD11	1:B:253:LEU:HB2	2.01	0.43
1:F:183:SER:HA	1:F:186:LEU:HB2	2.01	0.43
1:I:63:ILE:HB	1:I:66:ILE:CG1	2.47	0.43
1:I:124:GLU:HG3	1:I:296:SER:HB2	2.00	0.43
1:H:53:ALA:HB2	1:H:78:ALA:HB1	2.00	0.43
1:H:66:ILE:HG23	1:H:70:LYS:HB2	2.00	0.43
1:H:158:MET:HE3	1:H:158:MET:HB3	1.69	0.43
1:D:28:LEU:HD22	1:D:28:LEU:HA	1.80	0.43
1:D:194:GLY:O	1:D:195:PHE:HB2	2.18	0.43
1:G:304:LYS:HD2	1:G:305:GLY:H	1.83	0.43
1:A:298:THR:HA	1:A:316:ASP:O	2.18	0.43
1:F:114:GLN:NE2	1:F:320:LEU:HD23	2.34	0.43
1:E:94:GLN:OE1	1:E:94:GLN:HA	2.17	0.43
1:E:284:LYS:HE3	1:E:284:LYS:HB3	1.46	0.43
1:G:134:THR:HG23	5:G:600:ANP:O2B	2.18	0.43
1:G:279:PHE:CE2	4:U:17:DT:C5	3.06	0.43
1:C:267:ASN:HD21	1:C:292:ILE:HG12	1.82	0.43
1:B:138:HIS:O	1:B:142:VAL:HG12	2.19	0.43
1:B:142:VAL:HG11	1:B:174:VAL:HG21	2.01	0.43
1:B:198:ASP:C	1:B:199:HIS:CG	2.96	0.43
1:B:238:LEU:HD12	1:B:241:ARG:HH22	1.83	0.43
1:H:269:VAL:HG11	1:H:284:LYS:HD2	2.01	0.43
1:E:228:TYR:HB3	1:E:241:ARG:HD2	2.00	0.43
1:B:25:ILE:HD12	1:B:46:TYR:O	2.19	0.43
1:B:135:GLN:HE22	1:A:318:PRO:HB3	1.83	0.43
1:B:199:HIS:HB2	1:B:200:GLN:H	1.55	0.43
1:B:203:LEU:O	1:B:204:LEU:C	2.61	0.43
1:A:159:TYR:CD1	1:A:220:ILE:HB	2.53	0.43
1:I:121:SER:HB2	1:I:297:THR:OG1	2.18	0.43
1:H:194:GLY:HA2	1:H:199:HIS:ND1	2.34	0.43
1:D:124:GLU:HG2	1:D:267:ASN:ND2	2.34	0.43
1:E:124:GLU:HG2	1:E:125:MET:N	2.34	0.43
4:U:15:DC:H2''	4:U:16:DC:C5	2.54	0.43
1:A:113:LEU:O	1:A:113:LEU:HG	2.19	0.43
1:A:317:SER:C	1:A:319:CYS:H	2.26	0.43
1:C:58:LYS:NZ	1:D:231:ASP:HB3	2.33	0.42
1:B:135:GLN:H	1:B:135:GLN:HG2	1.67	0.42
1:B:293:ALA:HA	1:B:299:ARG:NH2	2.34	0.42
1:D:50:GLU:H	1:D:50:GLU:HG2	1.65	0.42
1:E:218:LEU:HD23	1:E:218:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:29:DC:H41	1:F:274:ASP:CB	2.32	0.42
4:U:24:DT:H2'	4:U:25:DT:C2	2.54	0.42
1:C:138:HIS:NE2	1:C:166:PHE:HA	2.34	0.42
1:A:140:LEU:HD13	1:A:218:LEU:HD11	2.00	0.42
1:F:208:GLU:HB2	1:F:255:LEU:HD21	2.01	0.42
1:I:28:LEU:HD11	1:I:33:ILE:HD12	2.01	0.42
1:H:251:MET:HE3	1:H:251:MET:HB2	1.96	0.42
1:E:40:LYS:HA	1:E:43:GLU:HG2	2.02	0.42
1:E:246:ALA:HB2	1:E:291:ILE:HG21	1.99	0.42
1:E:270:VAL:HG12	1:E:287:ILE:HG22	2.01	0.42
1:G:57:LYS:HD3	1:G:75:LEU:HD12	2.01	0.42
1:G:238:LEU:O	1:G:242:GLN:HG2	2.19	0.42
1:C:110:ASP:OD1	1:C:111:LYS:HG2	2.19	0.42
1:A:77:GLU:O	1:A:81:LEU:HG	2.19	0.42
1:A:245:LEU:HA	1:A:248:PHE:HD1	1.85	0.42
1:A:312:CYS:HB2	1:A:327:PHE:CD1	2.55	0.42
1:I:25:ILE:HA	1:I:49:VAL:HG23	2.01	0.42
1:I:84:MET:HE3	1:I:84:MET:HB3	1.78	0.42
1:I:292:ILE:HG22	1:I:293:ALA:N	2.34	0.42
1:G:305:GLY:C	1:G:306:ARG:HD3	2.44	0.42
2:L:3:DT:H3	1:I:235:ARG:CZ	2.33	0.42
1:C:56:PRO:C	1:C:58:LYS:N	2.74	0.42
1:C:262:ALA:O	1:C:264:VAL:HG23	2.19	0.42
1:B:48:THR:HG22	1:B:50:GLU:N	2.35	0.42
1:I:25:ILE:HG21	1:I:42:GLU:HB3	2.02	0.42
1:I:219:LEU:HD12	1:I:220:ILE:N	2.34	0.42
1:H:95:ARG:O	1:H:98:GLU:HG2	2.20	0.42
1:H:133:LYS:HB2	1:H:133:LYS:HE2	1.85	0.42
1:E:254:ARG:O	1:E:258:GLU:HB3	2.20	0.42
1:E:278:MET:CE	1:E:279:PHE:H	2.27	0.42
1:B:168:PRO:HD2	1:A:96:ARG:HG2	2.01	0.42
1:B:210:MET:HE2	1:B:210:MET:HB2	1.71	0.42
1:A:61:ILE:HD12	1:A:66:ILE:CG2	2.49	0.42
1:A:256:ALA:HA	1:A:261:VAL:HB	2.00	0.42
1:I:69:ALA:O	1:I:73:LYS:HG3	2.19	0.42
1:E:278:MET:CB	1:E:283:PRO:HG2	2.49	0.42
1:B:198:ASP:H	1:B:202:GLN:CD	2.27	0.42
1:B:314:ILE:HB	1:B:322:GLU:HA	2.01	0.42
1:F:218:LEU:HD12	1:F:262:ALA:HB3	2.02	0.42
1:I:285:LYS:HB2	1:I:285:LYS:HE3	1.29	0.42
1:H:159:TYR:CE1	1:H:161:ASP:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:LYS:O	1:D:74:ILE:HG12	2.19	0.42
1:E:282:ASP:O	1:E:283:PRO:C	2.61	0.42
1:G:142:VAL:HG22	1:G:185:VAL:HG21	2.00	0.42
1:B:230:THR:HG21	1:A:247:ARG:HA	2.01	0.42
1:A:301:TYR:CD2	1:A:313:LYS:HD2	2.54	0.42
1:I:252:LEU:HD12	1:I:263:VAL:HG11	2.01	0.42
1:H:156:LYS:NZ	1:H:214:SER:HB2	2.34	0.42
1:D:246:ALA:HB2	1:D:291:ILE:HD12	2.01	0.42
1:G:60:LEU:HA	1:G:63:ILE:HG12	2.02	0.42
2:L:5:DT:H5''	1:H:242:GLN:HB2	2.02	0.42
1:I:167:ARG:HG2	1:H:319:CYS:HB3	2.01	0.42
1:H:60:LEU:O	1:H:63:ILE:HG12	2.18	0.42
1:E:167:ARG:HG3	1:D:319:CYS:HB2	2.02	0.42
1:C:70:LYS:HB2	1:C:70:LYS:HE2	1.88	0.42
1:B:201:THR:O	1:B:202:GLN:C	2.62	0.42
1:A:58:LYS:HE3	1:A:58:LYS:HB2	1.89	0.42
1:I:113:LEU:HD23	1:I:113:LEU:H	1.85	0.42
1:I:166:PHE:CZ	1:I:189:VAL:HG21	2.55	0.42
1:D:30:GLN:O	1:D:33:ILE:HG12	2.20	0.42
1:C:26:SER:HA	1:C:29:GLU:HB3	2.02	0.42
1:C:301:TYR:CE2	1:C:303:ARG:HB3	2.55	0.42
1:B:39:LYS:NZ	1:B:42:GLU:HG2	2.35	0.42
1:B:139:THR:HG21	1:B:334:VAL:CG2	2.50	0.42
1:I:89:ALA:HA	1:I:92:PHE:CE2	2.54	0.42
1:I:218:LEU:HD12	1:I:218:LEU:HA	1.83	0.42
1:E:131:THR:HB	1:E:302:LEU:HB3	2.02	0.41
1:E:238:LEU:HD11	2:L:15:DT:H4'	2.02	0.41
1:E:278:MET:HB3	1:E:283:PRO:HG2	2.02	0.41
1:B:207:ALA:O	1:B:208:GLU:C	2.63	0.41
1:A:107:LYS:H	1:A:107:LYS:HG2	1.62	0.41
1:A:218:LEU:HD21	1:A:220:ILE:HD11	2.02	0.41
1:F:46:TYR:CD2	1:F:52:VAL:HG12	2.55	0.41
1:F:104:THR:HG22	1:F:105:GLY:H	1.84	0.41
1:I:199:HIS:CE1	1:H:84:MET:HB3	2.54	0.41
1:I:230:THR:OG1	1:H:250:ARG:HD3	2.20	0.41
1:G:279:PHE:CD2	4:U:18:DA:C1'	3.03	0.41
4:U:25:DT:H2''	4:U:26:DT:O5'	2.18	0.41
1:B:78:ALA:O	1:B:79:ALA:C	2.63	0.41
1:B:107:LYS:H	1:B:107:LYS:HG3	1.73	0.41
1:B:267:ASN:ND2	1:B:287:ILE:O	2.53	0.41
1:B:274:ASP:O	1:B:275:GLY:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ARG:O	1:A:99:ILE:HG13	2.20	0.41
1:A:123:THR:HA	1:A:298:THR:O	2.19	0.41
1:I:195:PHE:CE2	1:H:84:MET:HG2	2.54	0.41
1:I:225:THR:HG22	1:I:245:LEU:HD11	2.01	0.41
1:I:272:GLN:HB3	1:I:285:LYS:HD3	2.02	0.41
1:H:126:PHE:CG	1:H:286:PRO:HB3	2.55	0.41
1:H:223:SER:H	1:H:266:THR:HB	1.85	0.41
1:E:274:ASP:C	1:E:276:ALA:H	2.27	0.41
1:B:134:THR:HG23	1:B:222:ASP:CG	2.46	0.41
1:B:299:ARG:HE	1:B:299:ARG:HB2	1.62	0.41
1:I:109:LEU:HD23	1:I:312:CYS:SG	2.60	0.41
1:I:231:ASP:OD2	1:H:56:PRO:HG3	2.20	0.41
1:G:137:CYS:HB3	1:G:220:ILE:HG21	2.02	0.41
3:T:33:DG:C4	3:T:34:DG:C6	3.08	0.41
1:C:170:ARG:HA	1:C:170:ARG:HD2	1.79	0.41
1:A:69:ALA:C	1:A:71:ALA:N	2.79	0.41
1:A:137:CYS:HB3	1:A:159:TYR:CE1	2.56	0.41
1:A:207:ALA:C	1:A:209:ASP:H	2.28	0.41
1:F:23:GLN:O	1:F:49:VAL:HG23	2.21	0.41
1:I:219:LEU:CD2	1:I:255:LEU:HD11	2.49	0.41
1:E:302:LEU:HD12	1:E:327:PHE:CE1	2.55	0.41
1:G:39:LYS:HE2	1:G:39:LYS:HB2	1.94	0.41
1:G:271:ALA:HA	1:G:283:PRO:O	2.21	0.41
1:G:310:ARG:HE	1:G:329:ILE:HD12	1.86	0.41
1:B:68:GLU:HA	1:B:71:ALA:CB	2.46	0.41
1:B:238:LEU:O	1:B:239:SER:C	2.62	0.41
1:F:218:LEU:HD12	1:F:218:LEU:HA	1.93	0.41
1:F:273:VAL:HG23	1:F:273:VAL:O	2.20	0.41
1:I:146:LEU:O	1:I:152:GLY:HA3	2.20	0.41
1:H:132:GLY:HA3	1:H:329:ILE:HD11	2.02	0.41
1:G:75:LEU:HD23	1:G:75:LEU:HA	1.89	0.41
1:C:128:GLU:HA	1:C:269:VAL:HG11	2.02	0.41
1:B:251:MET:O	1:B:255:LEU:HD22	2.20	0.41
1:I:28:LEU:HG	1:I:49:VAL:HG22	2.02	0.41
1:I:122:ILE:HA	1:I:263:VAL:HB	2.01	0.41
1:I:220:ILE:HG12	1:I:264:VAL:HB	2.03	0.41
1:H:139:THR:HG22	1:H:174:VAL:HG21	2.03	0.41
1:D:326:MET:HE3	1:D:326:MET:HB2	1.95	0.41
1:E:294:HIS:N	1:E:294:HIS:CD2	2.88	0.41
1:G:235:ARG:CZ	2:L:9:DT:H3	2.33	0.41
3:T:36:DT:H3	4:U:13:DA:H2	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:MET:HG3	1:B:160:ILE:CG2	2.47	0.41
1:F:35:ALA:O	1:F:38:VAL:HG22	2.21	0.41
1:F:130:ARG:HE	1:F:130:ARG:HB3	1.41	0.41
1:C:156:LYS:O	1:C:216:TYR:HD1	2.04	0.41
1:A:71:ALA:O	1:A:74:ILE:HB	2.20	0.41
1:I:41:LEU:O	1:I:46:TYR:HB2	2.21	0.41
1:H:326:MET:HE2	1:H:326:MET:HB2	1.94	0.41
1:E:275:GLY:O	1:E:276:ALA:C	2.64	0.41
1:E:285:LYS:HE2	1:E:285:LYS:HB2	1.78	0.41
1:E:294:HIS:CE1	1:F:268:GLN:HB3	2.55	0.41
2:L:21:DA:N6	1:D:273:VAL:HA	2.35	0.41
1:C:114:GLN:HE22	1:C:321:PRO:HD2	1.86	0.41
1:C:196:ASN:HB2	1:C:199:HIS:CB	2.51	0.41
1:B:196:ASN:ND2	1:A:56:PRO:HB3	2.36	0.41
1:B:231:ASP:O	1:B:232:TYR:C	2.64	0.41
1:B:333:GLY:O	1:B:334:VAL:C	2.63	0.41
1:A:39:LYS:HE3	1:A:40:LYS:HB3	2.03	0.41
1:H:125:MET:HE2	1:H:125:MET:HB2	1.82	0.41
1:H:126:PHE:CE1	1:H:299:ARG:HD2	2.53	0.41
1:C:96:ARG:O	1:C:99:ILE:HG12	2.21	0.41
1:B:158:MET:HB2	1:B:219:LEU:HA	2.02	0.41
1:B:302:LEU:HA	1:B:312:CYS:HA	2.03	0.41
1:F:33:ILE:HG23	1:F:70:LYS:NZ	2.36	0.41
1:F:106:SER:HB2	1:F:335:GLY:O	2.21	0.41
1:I:196:ASN:HD22	1:H:56:PRO:N	2.19	0.41
1:H:160:ILE:HB	1:H:221:VAL:HA	2.03	0.41
1:D:221:VAL:HB	1:D:265:ILE:HD13	2.03	0.41
1:E:39:LYS:HD2	1:E:39:LYS:O	2.21	0.40
1:E:238:LEU:O	1:E:242:GLN:HG2	2.21	0.40
1:E:252:LEU:HD23	1:E:252:LEU:HA	1.88	0.40
1:E:284:LYS:H	1:E:284:LYS:HG2	1.69	0.40
1:C:112:LEU:HG	1:C:314:ILE:HD11	2.02	0.40
1:B:41:LEU:O	1:B:46:TYR:HB2	2.20	0.40
1:B:159:TYR:O	1:B:191:TYR:HA	2.21	0.40
1:B:167:ARG:NH2	1:A:297:THR:HB	2.36	0.40
1:B:204:LEU:HD23	1:B:204:LEU:HA	1.75	0.40
1:E:198:ASP:O	1:E:200:GLN:N	2.47	0.40
1:G:274:ASP:O	1:G:275:GLY:C	2.65	0.40
1:C:27:ARG:HD3	1:C:27:ARG:HA	1.76	0.40
1:B:134:THR:HG21	1:B:165:THR:OG1	2.22	0.40
1:B:309:THR:HA	1:B:327:PHE:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:204:LEU:HD11	1:F:248:PHE:CE1	2.56	0.40
1:I:41:LEU:HA	1:I:63:ILE:CD1	2.51	0.40
1:H:33:ILE:HG12	1:H:70:LYS:NZ	2.36	0.40
1:H:157:ALA:O	1:H:189:VAL:HA	2.21	0.40
1:E:107:LYS:HG3	1:E:336:ASP:OD2	2.22	0.40
1:E:333:GLY:O	1:E:334:VAL:C	2.65	0.40
1:G:196:ASN:HD22	1:F:55:ALA:C	2.29	0.40
1:G:218:LEU:HD23	1:G:220:ILE:HD11	2.04	0.40
2:L:19:DC:H2''	2:L:20:DC:C6	2.56	0.40
1:B:109:LEU:HD11	1:B:327:PHE:HD2	1.86	0.40
1:A:104:THR:HB	1:A:140:LEU:HD23	2.03	0.40
1:A:207:ALA:O	1:A:211:MET:HB3	2.22	0.40
1:F:70:LYS:O	1:F:74:ILE:HG13	2.22	0.40
1:I:25:ILE:O	1:I:28:LEU:N	2.48	0.40
1:I:39:LYS:O	1:I:42:GLU:HG3	2.21	0.40
1:I:56:PRO:HD2	1:I:59:GLU:CD	2.46	0.40
1:D:29:GLU:HB2	1:D:38:VAL:HG21	2.04	0.40
1:E:273:VAL:O	2:L:18:DC:N4	2.55	0.40
1:C:208:GLU:HG3	1:C:259:PHE:CE2	2.56	0.40
1:C:312:CYS:O	1:C:313:LYS:C	2.64	0.40
1:B:330:ASN:O	1:B:331:ALA:C	2.63	0.40
1:F:77:GLU:HA	1:F:80:LYS:HG2	2.04	0.40
1:F:234:GLY:C	1:F:236:GLY:H	2.29	0.40
1:F:276:ALA:C	1:F:278:MET:N	2.79	0.40
1:I:41:LEU:HD11	1:I:74:ILE:HD13	2.03	0.40
1:I:240:ALA:HA	1:I:243:MET:HG3	2.03	0.40
1:H:140:LEU:HD23	1:H:140:LEU:HA	1.95	0.40
2:L:18:DC:O4'	1:D:238:LEU:HD21	2.21	0.40
1:B:128:GLU:HA	1:B:269:VAL:CG1	2.52	0.40
1:A:157:ALA:H	1:A:188:ASN:HB3	1.85	0.40
1:A:212:VAL:O	1:A:213:GLU:C	2.64	0.40
1:I:28:LEU:O	1:I:31:CYS:HB2	2.21	0.40
1:I:33:ILE:HG21	1:I:74:ILE:HG12	2.04	0.40
1:I:126:PHE:HB2	1:I:301:TYR:HA	2.04	0.40
1:D:72:ASP:O	1:D:76:THR:HG23	2.21	0.40
1:D:112:LEU:HB2	1:D:325:ALA:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	304/361 (84%)	279 (92%)	24 (8%)	1 (0%)	36	68
1	B	304/361 (84%)	265 (87%)	38 (12%)	1 (0%)	36	68
1	C	304/361 (84%)	268 (88%)	35 (12%)	1 (0%)	36	68
1	D	304/361 (84%)	275 (90%)	28 (9%)	1 (0%)	36	68
1	E	313/361 (87%)	287 (92%)	24 (8%)	2 (1%)	21	56
1	F	310/361 (86%)	273 (88%)	37 (12%)	0	100	100
1	G	313/361 (87%)	274 (88%)	38 (12%)	1 (0%)	36	68
1	H	304/361 (84%)	280 (92%)	24 (8%)	0	100	100
1	I	304/361 (84%)	266 (88%)	37 (12%)	1 (0%)	36	68
All	All	2760/3249 (85%)	2467 (89%)	285 (10%)	8 (0%)	37	68

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	34	ASN
1	G	283	PRO
1	C	225	THR
1	E	235	ARG
1	E	330	ASN
1	B	24	PRO
1	A	83	PRO
1	D	221	VAL

5.3.2 Protein sidechains

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	249/290 (86%)	214 (86%)	35 (14%)	3	17
1	B	249/290 (86%)	205 (82%)	44 (18%)	2	10
1	C	249/290 (86%)	220 (88%)	29 (12%)	5	24
1	D	249/290 (86%)	225 (90%)	24 (10%)	8	32
1	E	252/290 (87%)	225 (89%)	27 (11%)	6	27
1	F	251/290 (87%)	236 (94%)	15 (6%)	17	50
1	G	252/290 (87%)	229 (91%)	23 (9%)	9	34
1	H	249/290 (86%)	214 (86%)	35 (14%)	3	17
1	I	249/290 (86%)	205 (82%)	44 (18%)	2	10
All	All	2249/2610 (86%)	1973 (88%)	276 (12%)	7	22

All (276) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	23	GLN
1	E	100	ILE
1	E	104	THR
1	E	106	SER
1	E	107	LYS
1	E	111	LYS
1	E	112	LEU
1	E	114	GLN
1	E	118	GLU
1	E	119	THR
1	E	161	ASP
1	E	187	ASP
1	E	197	THR
1	E	198	ASP
1	E	214	SER
1	E	227	LEU
1	E	237	GLU
1	E	245	LEU
1	E	250	ARG
1	E	251	MET
1	E	269	VAL
1	E	273	VAL
1	E	278	MET
1	E	284	LYS

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Mol	Chain	Res	Type
1	E	298	THR
1	E	302	LEU
1	E	326	MET
1	G	48	THR
1	G	67	SER
1	G	70	LYS
1	G	72	ASP
1	G	82	VAL
1	G	87	THR
1	G	88	THR
1	G	112	LEU
1	G	114	GLN
1	G	118	GLU
1	G	235	ARG
1	G	238	LEU
1	G	266	THR
1	G	269	VAL
1	G	274	ASP
1	G	278	MET
1	G	282	ASP
1	G	284	LYS
1	G	285	LYS
1	G	287	ILE
1	G	313	LYS
1	G	314	ILE
1	G	330	ASN
1	C	27	ARG
1	C	28	LEU
1	C	48	THR
1	C	52	VAL
1	C	57	LYS
1	C	58	LYS
1	C	60	LEU
1	C	63	ILE
1	C	64	LYS
1	C	94	GLN
1	C	111	LYS
1	C	112	LEU
1	C	113	LEU
1	C	114	GLN
1	C	142	VAL
1	C	184	ASP

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Mol	Chain	Res	Type
1	C	202	GLN
1	C	206	GLN
1	C	220	ILE
1	C	221	VAL
1	C	225	THR
1	C	233	SER
1	C	235	ARG
1	C	239	SER
1	C	242	GLN
1	C	261	VAL
1	C	313	LYS
1	C	314	ILE
1	C	315	TYR
1	B	25	ILE
1	B	26	SER
1	B	27	ARG
1	B	29	GLU
1	B	43	GLU
1	B	66	ILE
1	B	67	SER
1	B	70	LYS
1	B	73	LYS
1	B	74	ILE
1	B	80	LYS
1	B	87	THR
1	B	100	ILE
1	B	124	GLU
1	B	129	PHE
1	B	134	THR
1	B	189	VAL
1	B	199	HIS
1	B	200	GLN
1	B	201	THR
1	B	202	GLN
1	B	203	LEU
1	B	204	LEU
1	B	208	GLU
1	B	209	ASP
1	B	210	MET
1	B	225	THR
1	B	227	LEU
1	B	230	THR

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Mol	Chain	Res	Type
1	B	232	TYR
1	B	237	GLU
1	B	244	HIS
1	B	270	VAL
1	B	272	GLN
1	B	274	ASP
1	B	284	LYS
1	B	292	ILE
1	B	302	LEU
1	B	306	ARG
1	B	314	ILE
1	B	316	ASP
1	B	317	SER
1	B	330	ASN
1	B	336	ASP
1	A	30	GLN
1	A	39	LYS
1	A	58	LYS
1	A	60	LEU
1	A	64	LYS
1	A	66	ILE
1	A	67	SER
1	A	68	GLU
1	A	70	LYS
1	A	72	ASP
1	A	73	LYS
1	A	84	MET
1	A	100	ILE
1	A	101	GLN
1	A	103	THR
1	A	117	ILE
1	A	118	GLU
1	A	119	THR
1	A	121	SER
1	A	186	LEU
1	A	187	ASP
1	A	201	THR
1	A	209	ASP
1	A	211	MET
1	A	214	SER
1	A	218	LEU
1	A	219	LEU

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Mol	Chain	Res	Type
1	A	233	SER
1	A	235	ARG
1	A	237	GLU
1	A	238	LEU
1	A	248	PHE
1	A	269	VAL
1	A	270	VAL
1	A	320	LEU
1	F	38	VAL
1	F	43	GLU
1	F	61	ILE
1	F	68	GLU
1	F	111	LYS
1	F	112	LEU
1	F	114	GLN
1	F	169	GLU
1	F	174	VAL
1	F	177	ARG
1	F	215	ARG
1	F	263	VAL
1	F	264	VAL
1	F	265	ILE
1	F	278	MET
1	I	25	ILE
1	I	27	ARG
1	I	28	LEU
1	I	29	GLU
1	I	30	GLN
1	I	31	CYS
1	I	33	ILE
1	I	34	ASN
1	I	37	ASP
1	I	43	GLU
1	I	54	TYR
1	I	57	LYS
1	I	58	LYS
1	I	59	GLU
1	I	60	LEU
1	I	62	ASN
1	I	76	THR
1	I	84	MET
1	I	86	PHE

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Mol	Chain	Res	Type
1	I	88	THR
1	I	91	GLU
1	I	99	ILE
1	I	102	ILE
1	I	103	THR
1	I	106	SER
1	I	107	LYS
1	I	108	GLU
1	I	109	LEU
1	I	123	THR
1	I	128	GLU
1	I	144	CYS
1	I	187	ASP
1	I	255	LEU
1	I	265	ILE
1	I	266	THR
1	I	272	GLN
1	I	285	LYS
1	I	287	ILE
1	I	292	ILE
1	I	298	THR
1	I	312	CYS
1	I	314	ILE
1	I	317	SER
1	I	320	LEU
1	H	63	ILE
1	H	64	LYS
1	H	67	SER
1	H	96	ARG
1	H	99	ILE
1	H	103	THR
1	H	107	LYS
1	H	110	ASP
1	H	111	LYS
1	H	112	LEU
1	H	114	GLN
1	H	118	GLU
1	H	125	MET
1	H	128	GLU
1	H	130	ARG
1	H	149	ASP
1	H	158	MET

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Mol	Chain	Res	Type
1	H	181	SER
1	H	184	ASP
1	H	185	VAL
1	H	219	LEU
1	H	220	ILE
1	H	221	VAL
1	H	223	SER
1	H	235	ARG
1	H	253	LEU
1	H	255	LEU
1	H	257	ASP
1	H	258	GLU
1	H	264	VAL
1	H	291	ILE
1	H	304	LYS
1	H	306	ARG
1	H	308	GLU
1	H	311	ILE
1	D	28	LEU
1	D	30	GLN
1	D	34	ASN
1	D	41	LEU
1	D	87	THR
1	D	109	LEU
1	D	118	GLU
1	D	122	ILE
1	D	124	GLU
1	D	135	GLN
1	D	162	THR
1	D	171	LEU
1	D	172	LEU
1	D	185	VAL
1	D	193	ARG
1	D	218	LEU
1	D	220	ILE
1	D	221	VAL
1	D	223	SER
1	D	239	SER
1	D	287	ILE
1	D	298	THR
1	D	315	TYR
1	D	320	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	199	HIS
1	E	202	GLN
1	E	330	ASN
1	G	101	GLN
1	G	199	HIS
1	G	242	GLN
1	G	272	GLN
1	G	330	ASN
1	C	135	GLN
1	B	34	ASN
1	B	135	GLN
1	B	196	ASN
1	B	206	GLN
1	A	101	GLN
1	A	188	ASN
1	A	200	GLN
1	F	23	GLN
1	F	47	HIS
1	F	94	GLN
1	F	101	GLN
1	F	114	GLN
1	F	200	GLN
1	I	34	ASN
1	I	114	GLN
1	I	202	GLN
1	I	206	GLN
1	I	267	ASN
1	I	294	HIS
1	H	242	GLN
1	D	23	GLN
1	D	267	ASN
1	D	272	GLN
1	D	290	ASN

5.3.3 RNA ⓘ

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 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
5	ANP	I	600	6	33,33,33	2.34	5 (15%)	45,52,52	1.18	3 (6%)
5	ANP	H	602	-	33,33,33	2.20	5 (15%)	45,52,52	1.27	3 (6%)
5	ANP	B	600	6	33,33,33	2.31	5 (15%)	45,52,52	1.24	3 (6%)
5	ANP	E	600	6	33,33,33	2.25	5 (15%)	45,52,52	1.20	3 (6%)
5	ANP	F	600	-	33,33,33	2.29	5 (15%)	45,52,52	1.23	3 (6%)
5	ANP	G	600	-	33,33,33	2.27	5 (15%)	45,52,52	1.24	3 (6%)
5	ANP	C	600	6	33,33,33	2.29	5 (15%)	45,52,52	1.21	4 (8%)
5	ANP	A	600	6	33,33,33	2.36	6 (18%)	45,52,52	1.19	3 (6%)
5	ANP	D	600	6	33,33,33	2.27	5 (15%)	45,52,52	1.23	3 (6%)

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
5	ANP	I	600	6	-	7/18/38/38	0/3/3/3
5	ANP	H	602	-	-	8/18/38/38	0/3/3/3
5	ANP	B	600	6	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ANP	E	600	6	-	4/18/38/38	0/3/3/3
5	ANP	F	600	-	-	5/18/38/38	0/3/3/3
5	ANP	G	600	-	-	7/18/38/38	0/3/3/3
5	ANP	C	600	6	-	8/18/38/38	0/3/3/3
5	ANP	A	600	6	-	10/18/38/38	0/3/3/3
5	ANP	D	600	6	-	3/18/38/38	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	600	ANP	PB-O3A	9.29	1.70	1.59
5	I	600	ANP	PB-O3A	9.13	1.70	1.59
5	B	600	ANP	PB-O3A	8.95	1.70	1.59
5	C	600	ANP	PB-O3A	8.85	1.70	1.59
5	F	600	ANP	PB-O3A	8.77	1.70	1.59
5	G	600	ANP	PB-O3A	8.72	1.69	1.59
5	D	600	ANP	PB-O3A	8.62	1.69	1.59
5	E	600	ANP	PB-O3A	8.42	1.69	1.59
5	H	602	ANP	PB-O3A	8.36	1.69	1.59
5	I	600	ANP	PG-N3B	6.35	1.79	1.63
5	B	600	ANP	PG-N3B	6.33	1.79	1.63
5	A	600	ANP	PG-N3B	6.30	1.79	1.63
5	C	600	ANP	PG-N3B	6.17	1.79	1.63
5	D	600	ANP	PG-N3B	6.10	1.79	1.63
5	F	600	ANP	PG-N3B	6.09	1.79	1.63
5	E	600	ANP	PG-N3B	6.00	1.79	1.63
5	G	600	ANP	PG-N3B	5.97	1.79	1.63
5	H	602	ANP	PG-N3B	5.96	1.78	1.63
5	G	600	ANP	PG-O1G	4.89	1.53	1.46
5	F	600	ANP	PG-O1G	4.88	1.53	1.46
5	D	600	ANP	PG-O1G	4.88	1.53	1.46
5	E	600	ANP	PG-O1G	4.85	1.53	1.46
5	A	600	ANP	PG-O1G	4.78	1.53	1.46
5	B	600	ANP	PG-O1G	4.73	1.53	1.46
5	I	600	ANP	PG-O1G	4.73	1.53	1.46
5	C	600	ANP	PG-O1G	4.71	1.53	1.46
5	H	602	ANP	PG-O1G	4.49	1.53	1.46
5	A	600	ANP	PB-O1B	2.87	1.50	1.46
5	B	600	ANP	PB-O1B	2.80	1.50	1.46
5	I	600	ANP	PB-O1B	2.67	1.50	1.46
5	C	600	ANP	PB-O1B	2.65	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	600	ANP	PB-O2B	-2.53	1.50	1.56
5	G	600	ANP	PB-O2B	-2.50	1.50	1.56
5	H	602	ANP	PB-O1B	2.50	1.50	1.46
5	F	600	ANP	PB-O1B	2.47	1.49	1.46
5	D	600	ANP	PB-O2B	-2.47	1.50	1.56
5	E	600	ANP	PB-O1B	2.46	1.49	1.46
5	F	600	ANP	PB-O2B	-2.46	1.50	1.56
5	D	600	ANP	PB-O1B	2.43	1.49	1.46
5	H	602	ANP	PB-O2B	-2.42	1.50	1.56
5	G	600	ANP	PB-O1B	2.36	1.49	1.46
5	I	600	ANP	PB-O2B	-2.21	1.50	1.56
5	C	600	ANP	PB-O2B	-2.14	1.51	1.56
5	B	600	ANP	PB-O2B	-2.12	1.51	1.56
5	A	600	ANP	PB-O2B	-2.10	1.51	1.56
5	A	600	ANP	PA-O3A	2.10	1.61	1.59

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	600	ANP	O2B-PB-O1B	4.95	120.49	109.87
5	H	602	ANP	O2B-PB-O1B	4.92	120.43	109.87
5	I	600	ANP	O2B-PB-O1B	4.86	120.28	109.87
5	E	600	ANP	O2B-PB-O1B	4.77	120.09	109.87
5	H	602	ANP	O1G-PG-N3B	-4.76	104.76	111.77
5	F	600	ANP	O2B-PB-O1B	4.75	120.05	109.87
5	G	600	ANP	O2B-PB-O1B	4.73	120.02	109.87
5	A	600	ANP	O2B-PB-O1B	4.62	119.78	109.87
5	C	600	ANP	O2B-PB-O1B	4.57	119.67	109.87
5	D	600	ANP	O2B-PB-O1B	4.50	119.53	109.87
5	B	600	ANP	O1G-PG-N3B	-4.50	105.15	111.77
5	C	600	ANP	O1G-PG-N3B	-3.99	105.89	111.77
5	G	600	ANP	O1G-PG-N3B	-3.85	106.11	111.77
5	D	600	ANP	O1G-PG-N3B	-3.75	106.25	111.77
5	A	600	ANP	O1G-PG-N3B	-3.75	106.25	111.77
5	E	600	ANP	O1G-PG-N3B	-3.73	106.28	111.77
5	F	600	ANP	O1G-PG-N3B	-3.43	106.72	111.77
5	I	600	ANP	O1G-PG-N3B	-3.27	106.95	111.77
5	H	602	ANP	O2G-PG-O3G	2.75	114.97	107.59
5	C	600	ANP	O2G-PG-O3G	2.61	114.60	107.59
5	A	600	ANP	O2G-PG-O3G	2.55	114.45	107.59
5	F	600	ANP	O2G-PG-O3G	2.50	114.31	107.59
5	I	600	ANP	O2G-PG-O3G	2.50	114.30	107.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	600	ANP	O2G-PG-O3G	2.49	114.28	107.59
5	G	600	ANP	O2G-PG-O3G	2.47	114.23	107.59
5	E	600	ANP	O2G-PG-O3G	2.46	114.19	107.59
5	C	600	ANP	O3A-PB-N3B	-2.40	99.93	106.59
5	B	600	ANP	O2G-PG-O3G	2.28	113.70	107.59

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	600	ANP	PG-N3B-PB-O1B
5	E	600	ANP	PA-O3A-PB-O2B
5	G	600	ANP	PB-N3B-PG-O1G
5	G	600	ANP	PG-N3B-PB-O1B
5	C	600	ANP	PB-N3B-PG-O1G
5	C	600	ANP	PG-N3B-PB-O1B
5	C	600	ANP	C5'-O5'-PA-O1A
5	C	600	ANP	C5'-O5'-PA-O2A
5	C	600	ANP	C5'-O5'-PA-O3A
5	B	600	ANP	PG-N3B-PB-O1B
5	B	600	ANP	PG-N3B-PB-O3A
5	B	600	ANP	C5'-O5'-PA-O1A
5	B	600	ANP	O4'-C4'-C5'-O5'
5	B	600	ANP	C3'-C4'-C5'-O5'
5	A	600	ANP	PG-N3B-PB-O1B
5	A	600	ANP	PA-O3A-PB-O2B
5	A	600	ANP	C5'-O5'-PA-O2A
5	A	600	ANP	C5'-O5'-PA-O3A
5	F	600	ANP	PG-N3B-PB-O1B
5	F	600	ANP	C5'-O5'-PA-O1A
5	I	600	ANP	PB-N3B-PG-O1G
5	I	600	ANP	PG-N3B-PB-O1B
5	I	600	ANP	C5'-O5'-PA-O2A
5	I	600	ANP	C5'-O5'-PA-O3A
5	H	602	ANP	PB-N3B-PG-O1G
5	H	602	ANP	PG-N3B-PB-O1B
5	H	602	ANP	PG-N3B-PB-O3A
5	H	602	ANP	C5'-O5'-PA-O1A
5	H	602	ANP	C5'-O5'-PA-O2A
5	H	602	ANP	C5'-O5'-PA-O3A
5	D	600	ANP	PG-N3B-PB-O1B
5	D	600	ANP	PG-N3B-PB-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	I	600	ANP	C3'-C4'-C5'-O5'
5	B	600	ANP	C4'-C5'-O5'-PA
5	G	600	ANP	C3'-C4'-C5'-O5'
5	G	600	ANP	O4'-C4'-C5'-O5'
5	A	600	ANP	O4'-C4'-C5'-O5'
5	I	600	ANP	O4'-C4'-C5'-O5'
5	G	600	ANP	C4'-C5'-O5'-PA
5	A	600	ANP	C3'-C4'-C5'-O5'
5	A	600	ANP	O4'-C1'-N9-C4
5	C	600	ANP	C4'-C5'-O5'-PA
5	A	600	ANP	O4'-C1'-N9-C8
5	C	600	ANP	O4'-C4'-C5'-O5'
5	A	600	ANP	C2'-C1'-N9-C8
5	F	600	ANP	C4'-C5'-O5'-PA
5	G	600	ANP	C5'-O5'-PA-O1A
5	I	600	ANP	C5'-O5'-PA-O1A
5	C	600	ANP	C3'-C4'-C5'-O5'
5	F	600	ANP	O4'-C4'-C5'-O5'
5	H	602	ANP	PA-O3A-PB-O2B
5	E	600	ANP	C3'-C4'-C5'-O5'
5	D	600	ANP	C3'-C4'-C5'-O5'
5	E	600	ANP	PA-O3A-PB-O1B
5	G	600	ANP	PA-O3A-PB-O1B
5	A	600	ANP	PA-O3A-PB-O1B
5	H	602	ANP	PA-O3A-PB-O1B
5	F	600	ANP	PB-N3B-PG-O1G

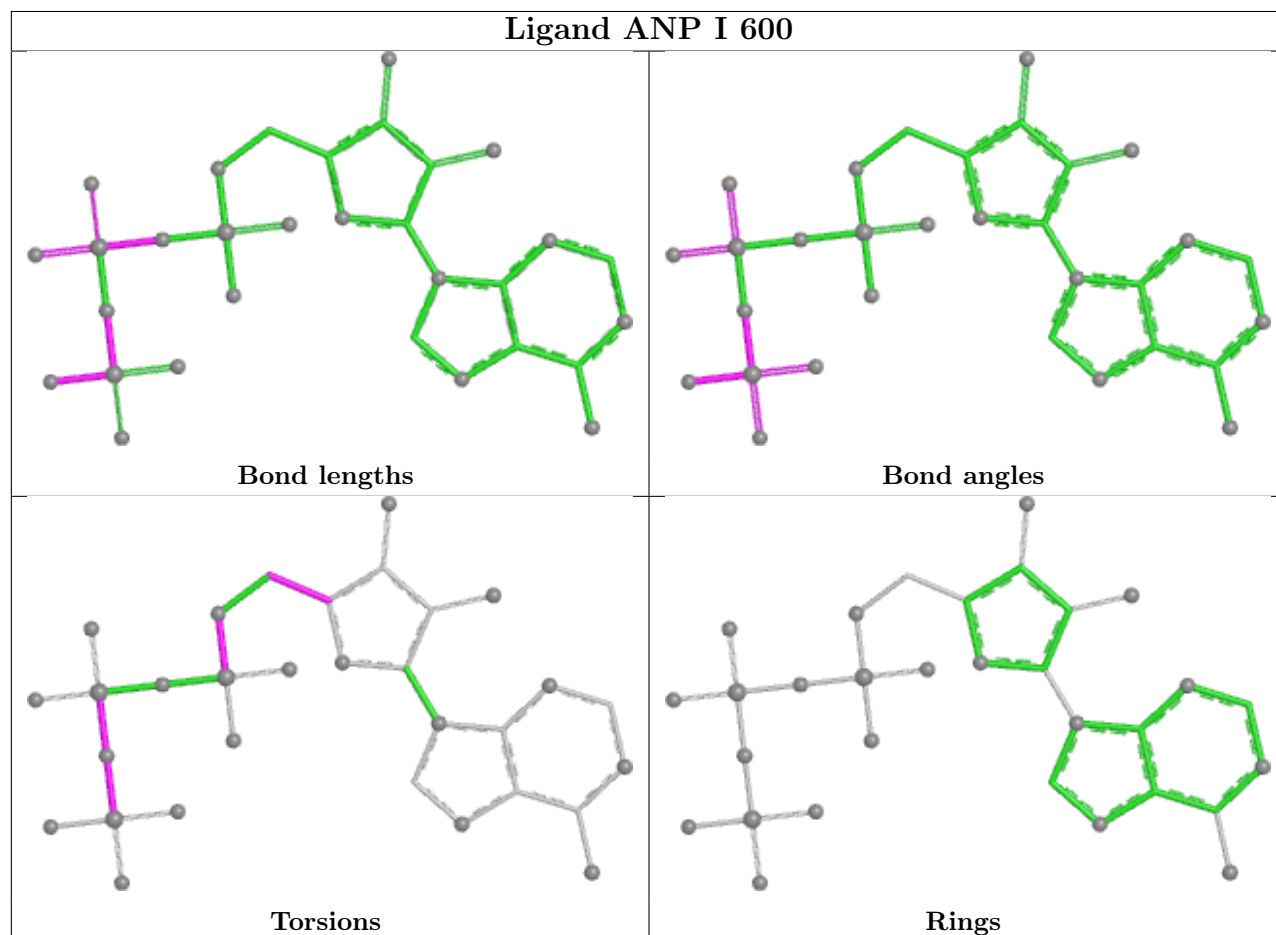
There are no ring outliers.

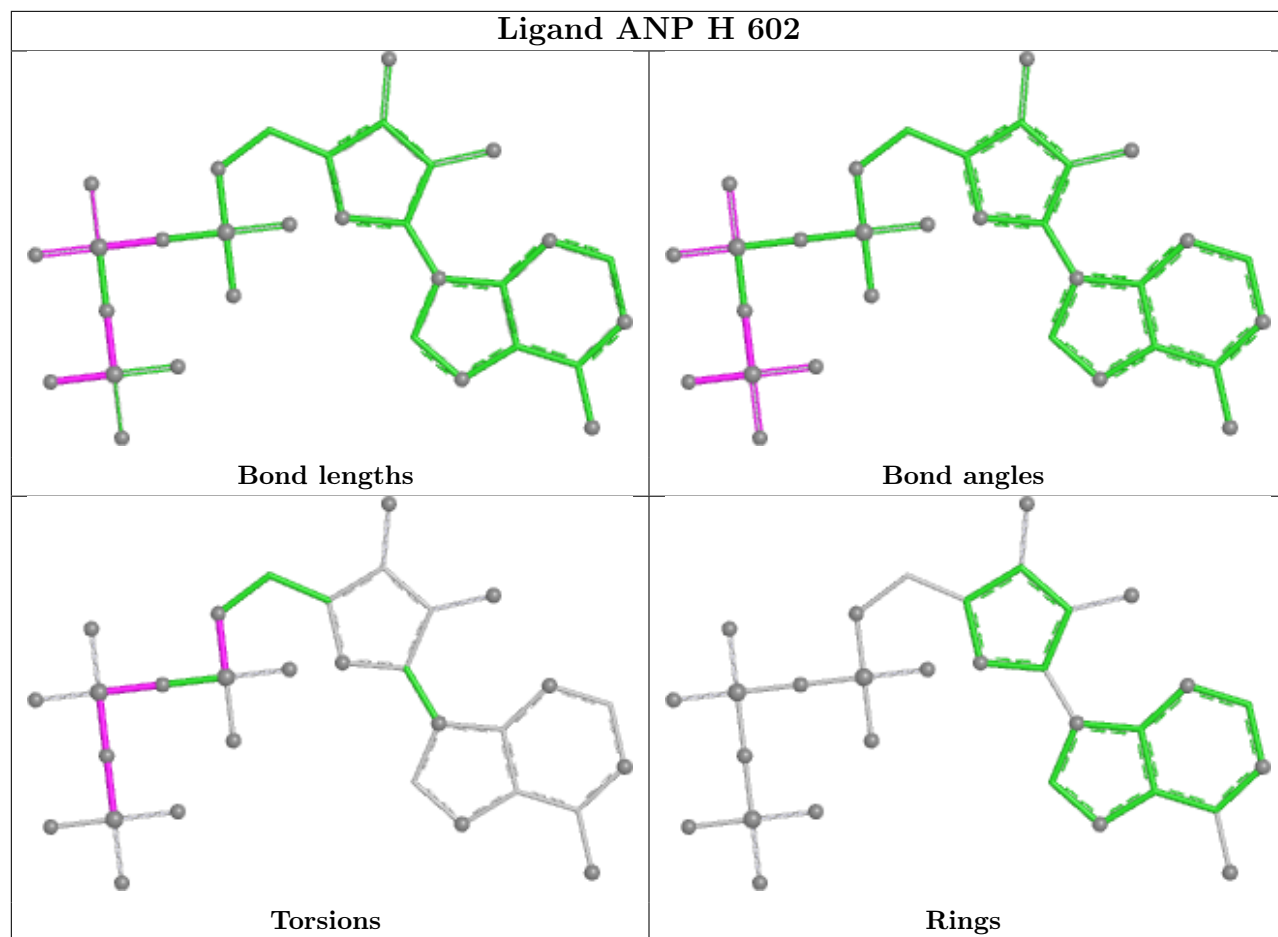
5 monomers are involved in 8 short contacts:

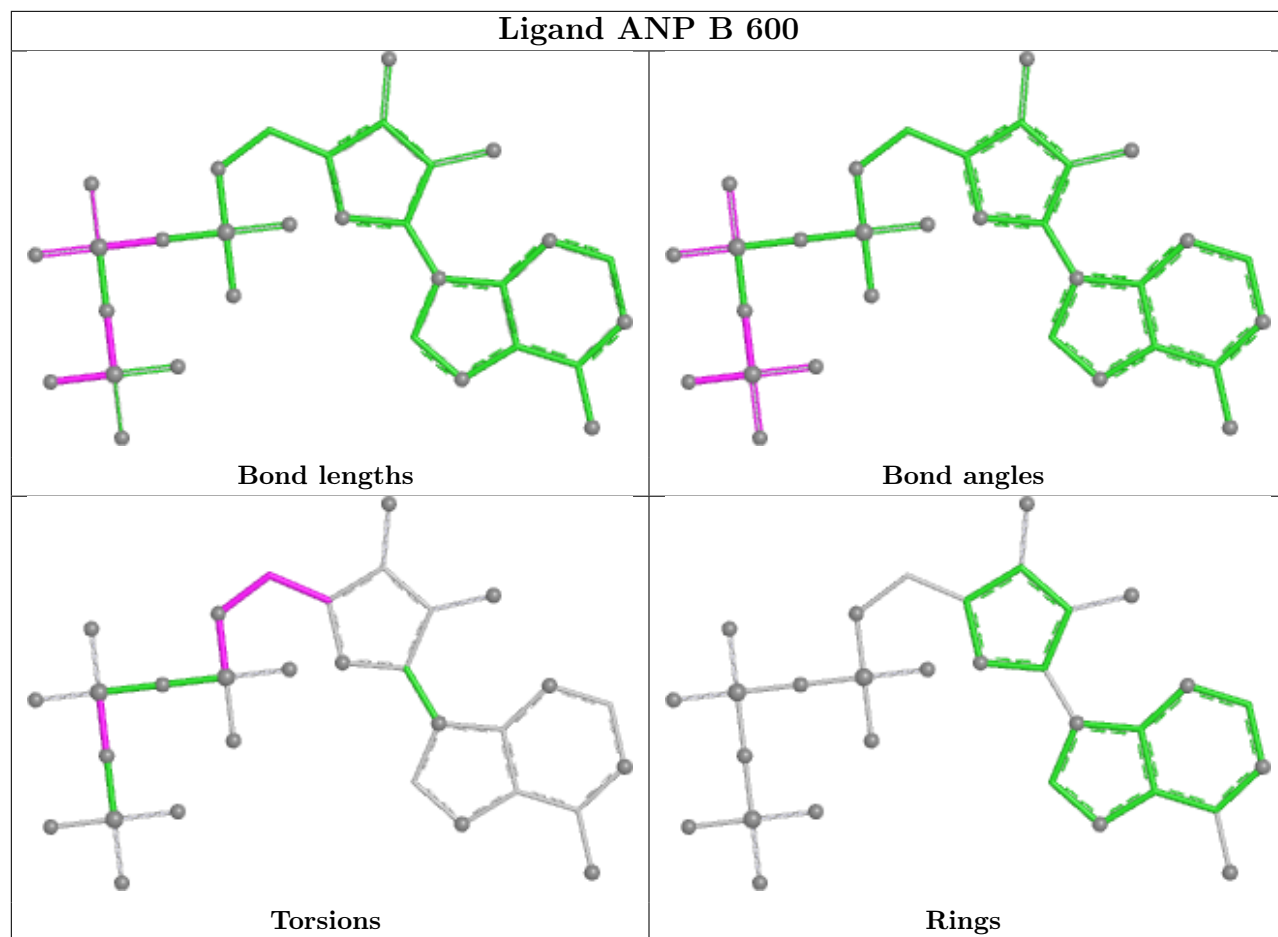
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	602	ANP	2	0
5	E	600	ANP	1	0
5	F	600	ANP	2	0
5	G	600	ANP	2	0
5	D	600	ANP	1	0

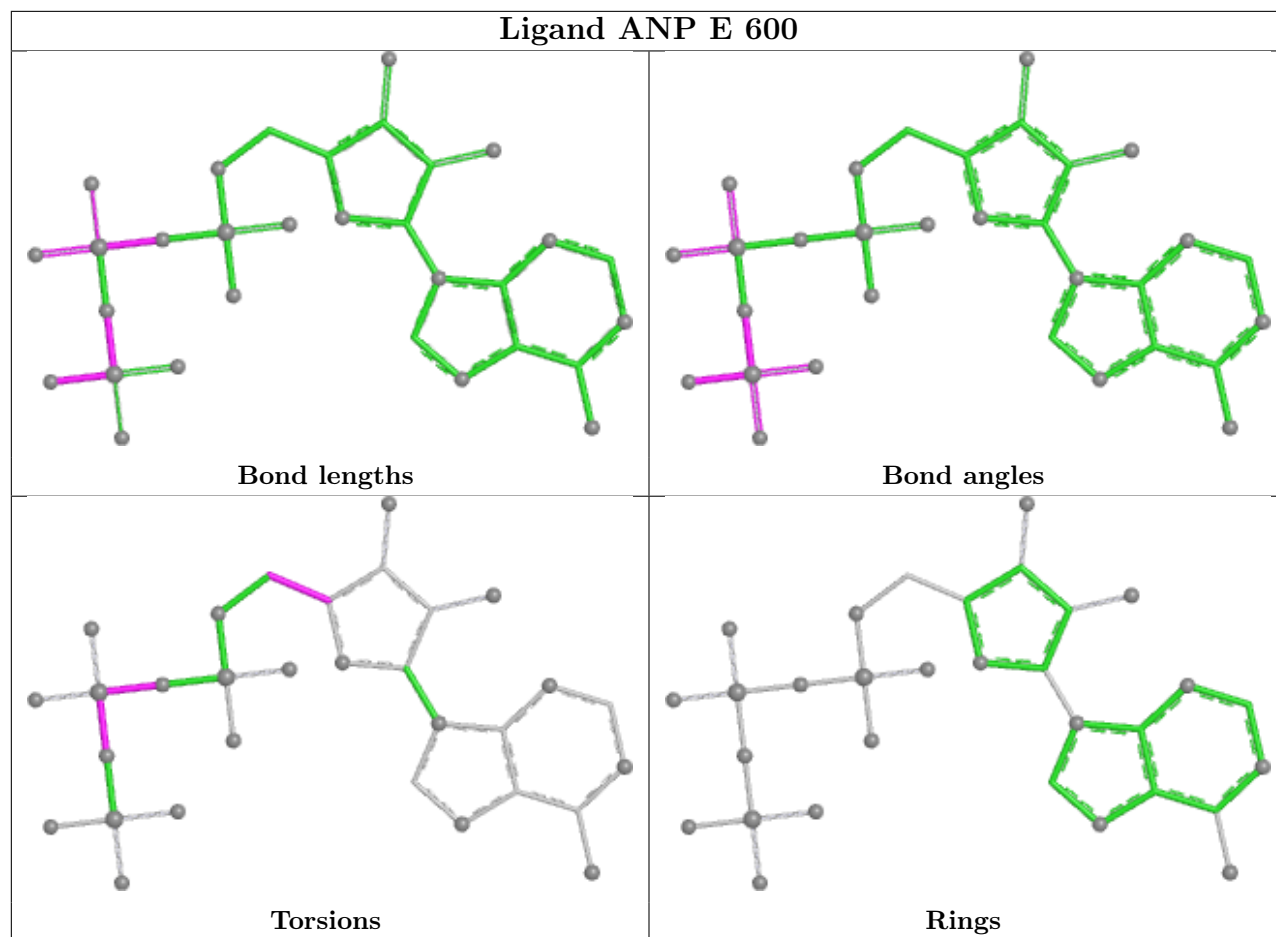
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

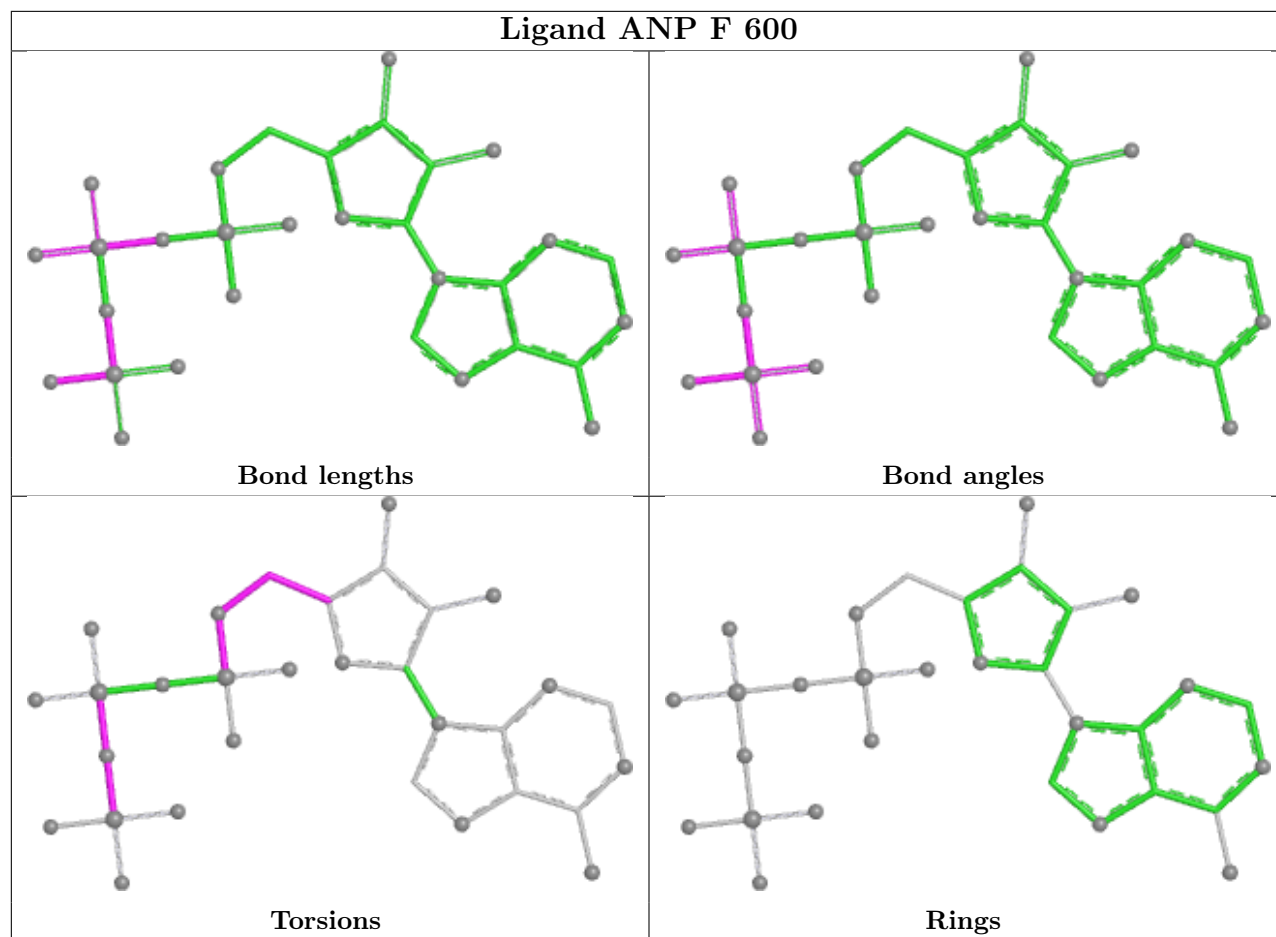
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

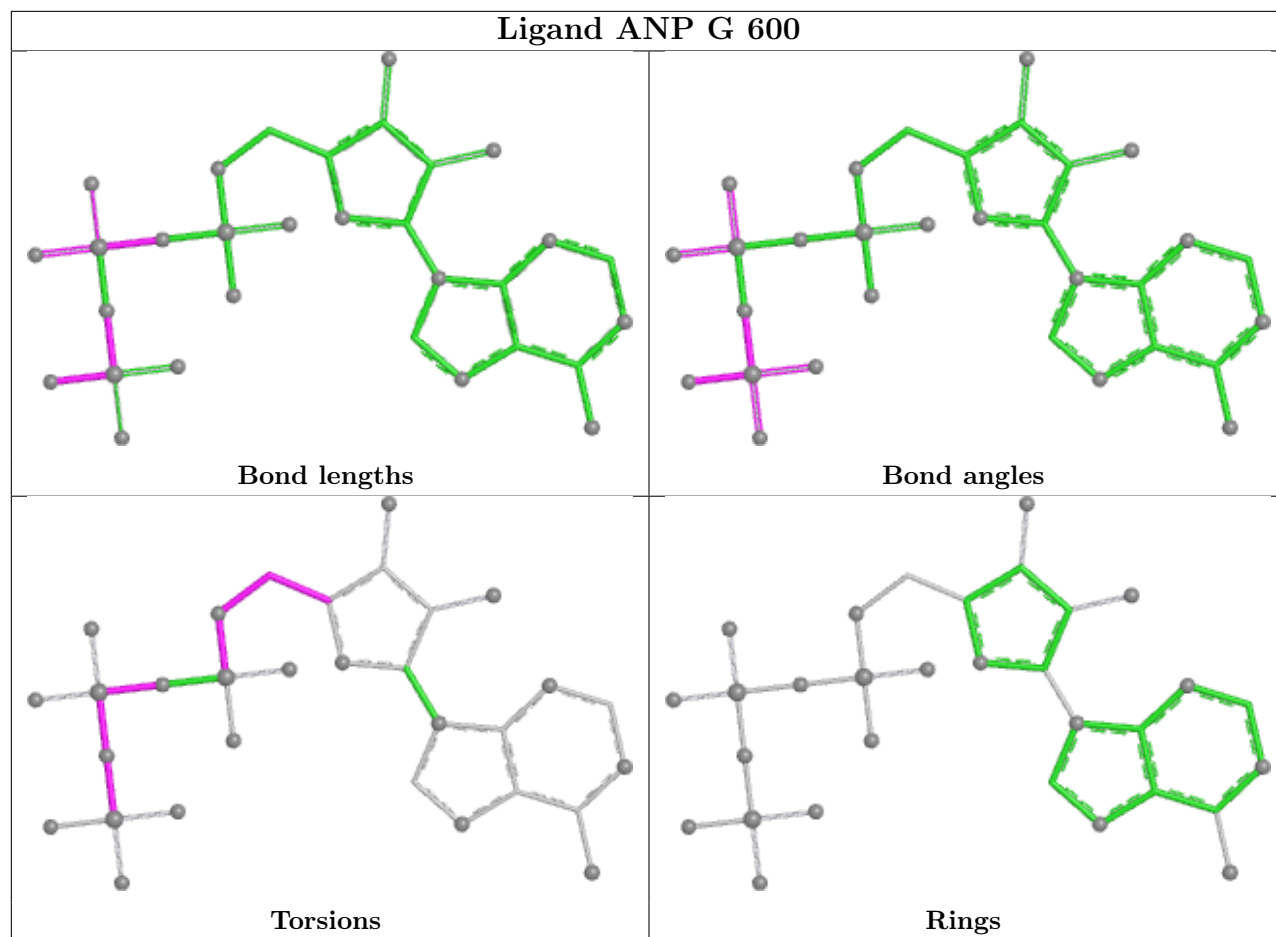


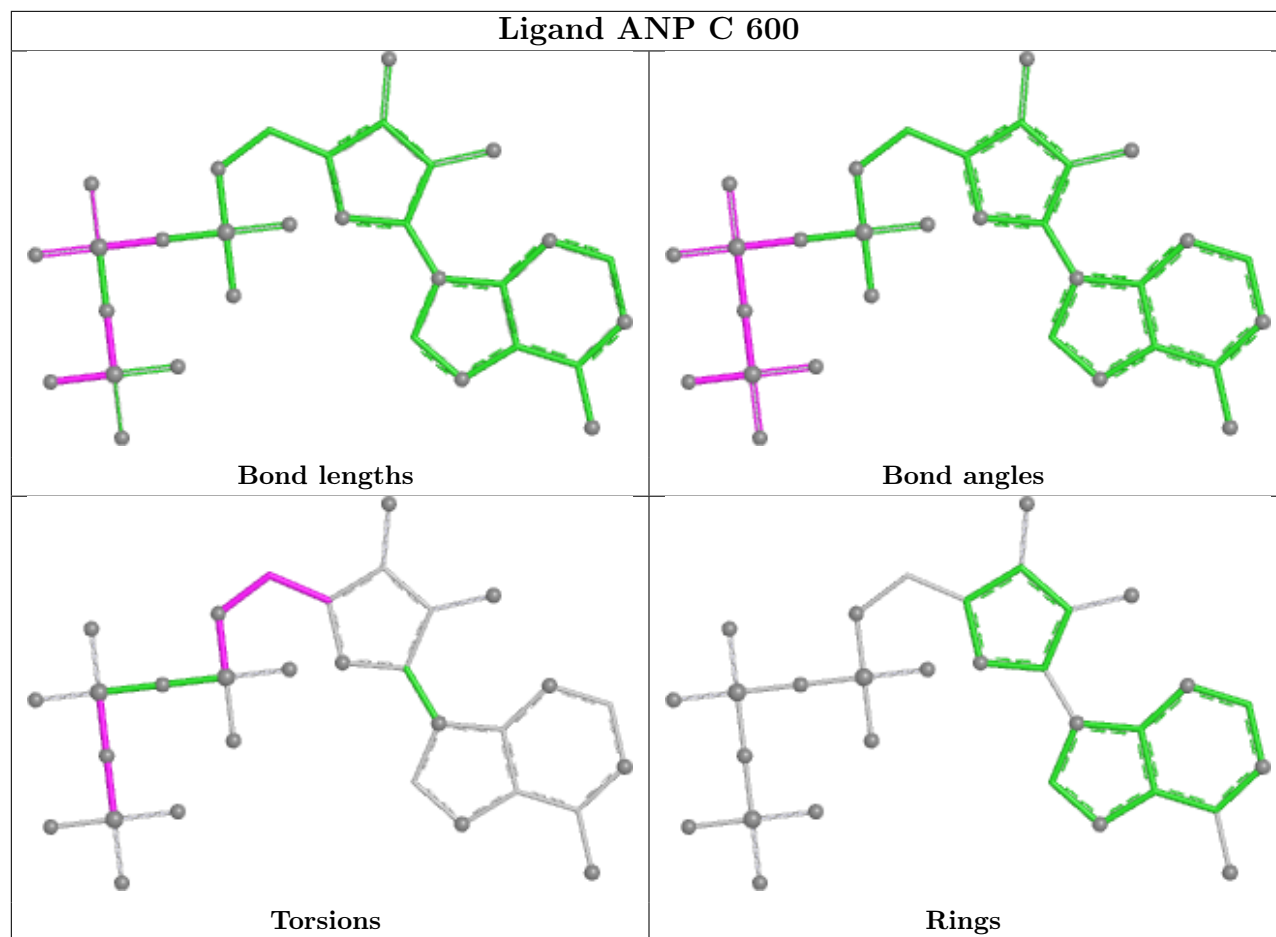


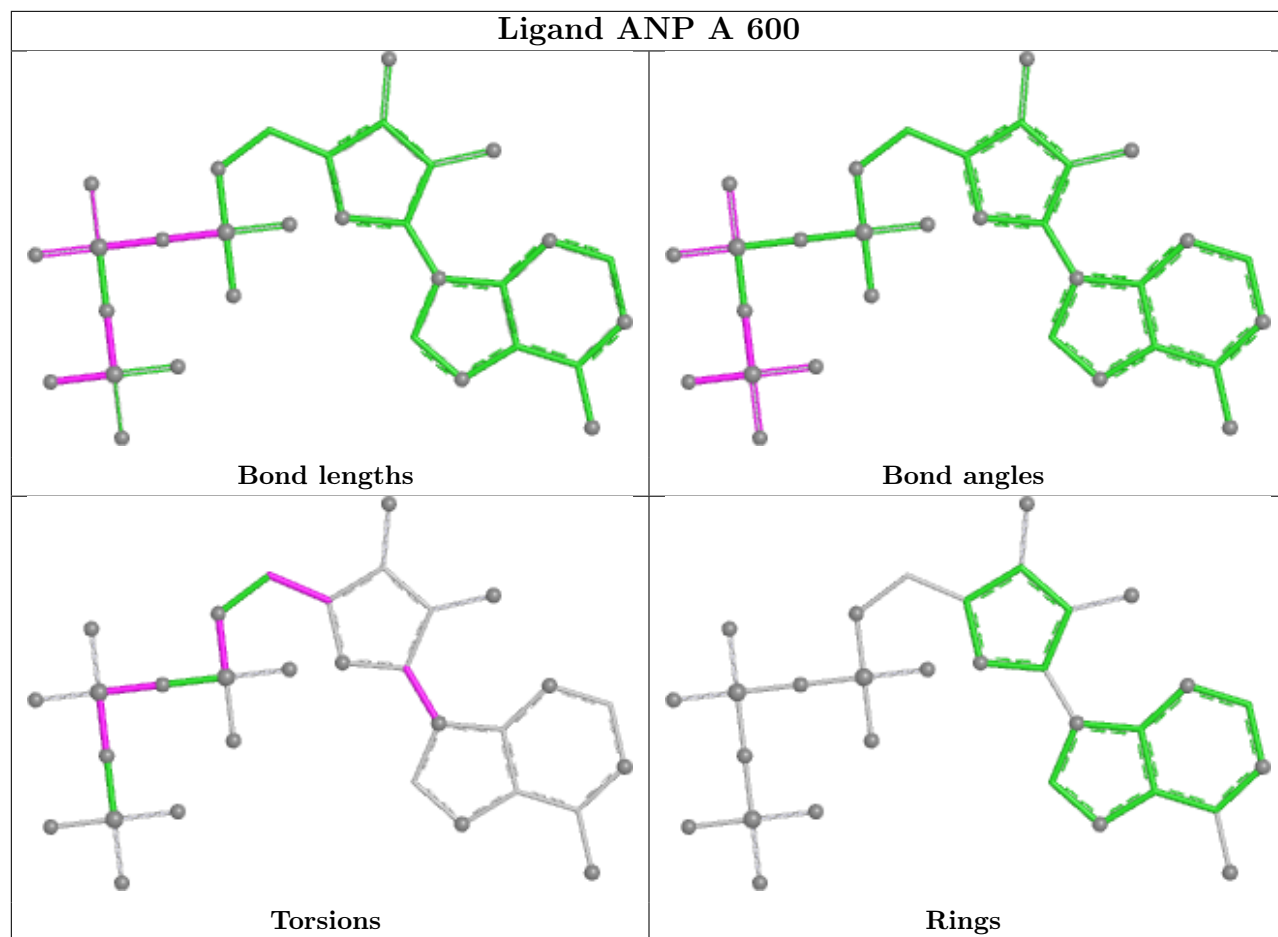


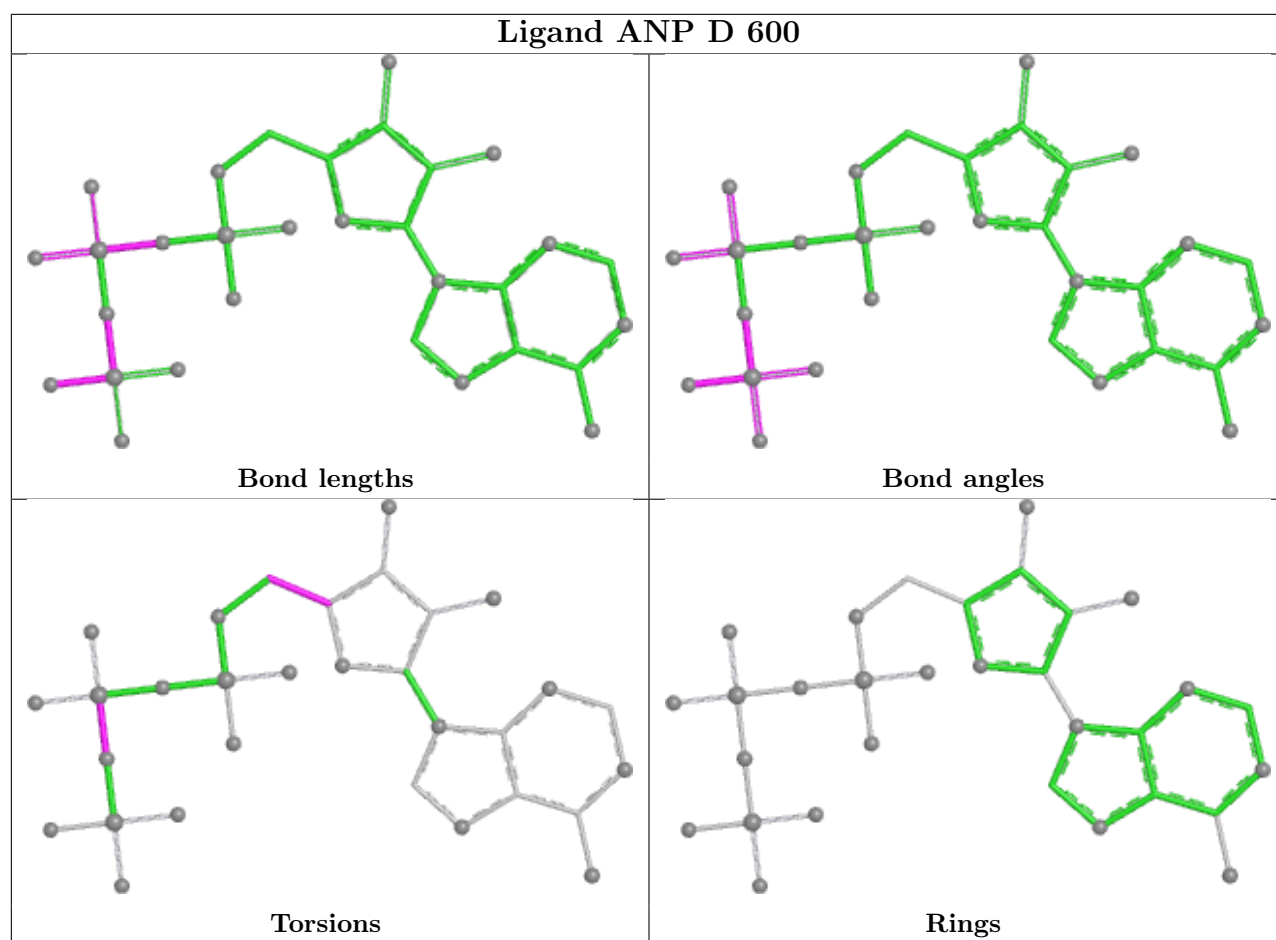












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

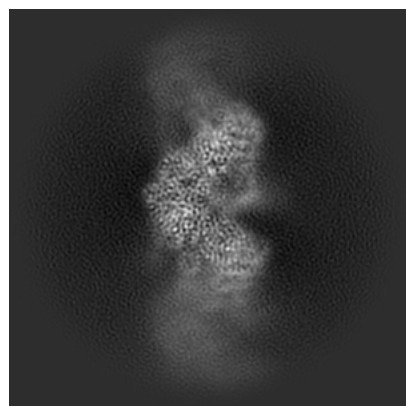
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64187. These allow visual inspection of the internal detail of the map and identification of artifacts.

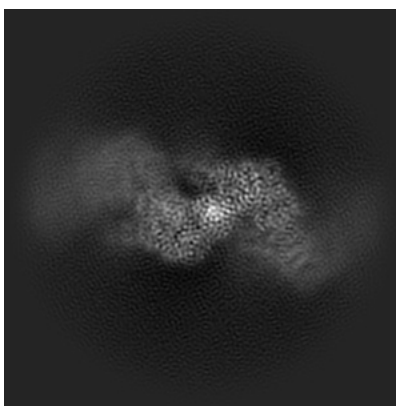
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

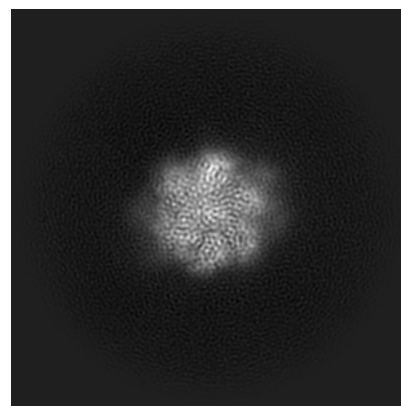
6.1.1 Primary map



X

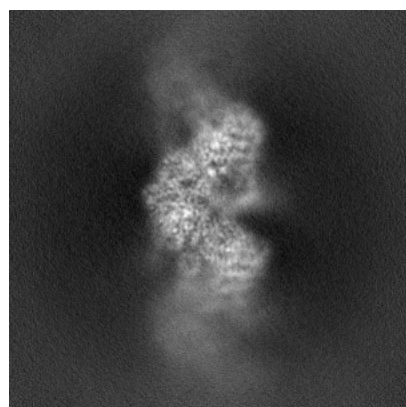


Y

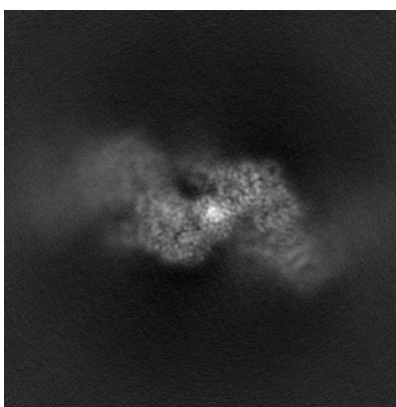


Z

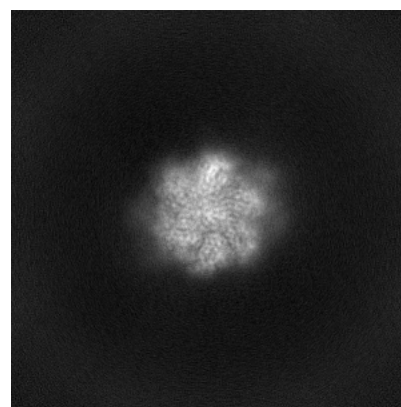
6.1.2 Raw map



X



Y

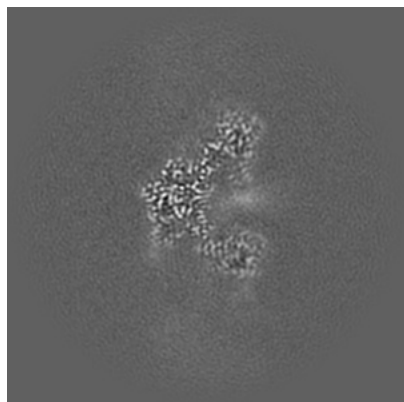


Z

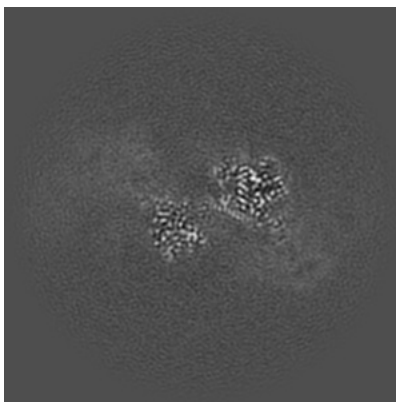
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

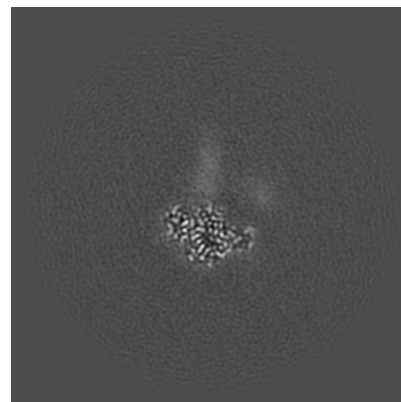
6.2.1 Primary map



X Index: 192

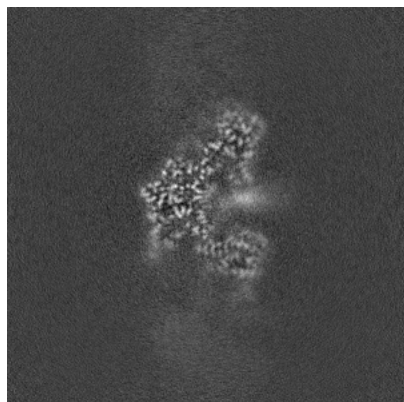


Y Index: 192

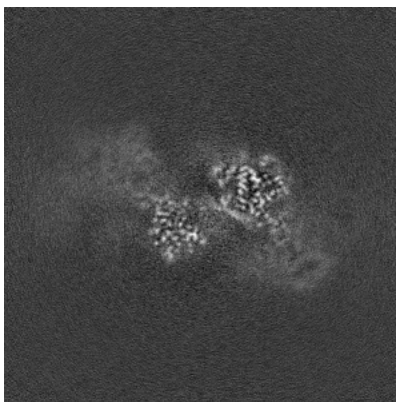


Z Index: 192

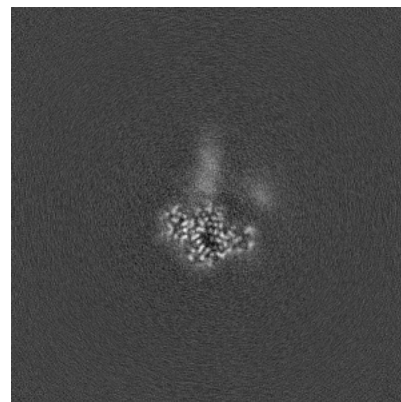
6.2.2 Raw map



X Index: 192



Y Index: 192

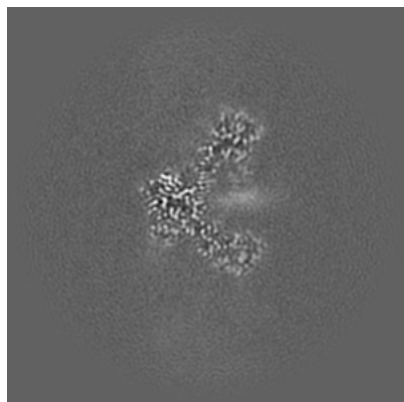


Z Index: 192

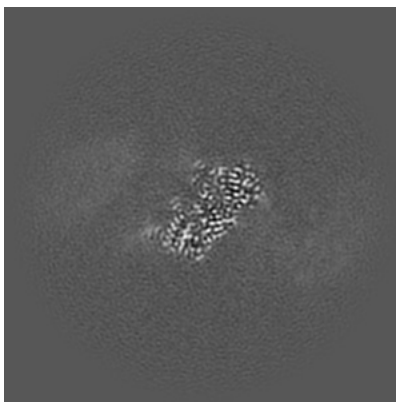
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

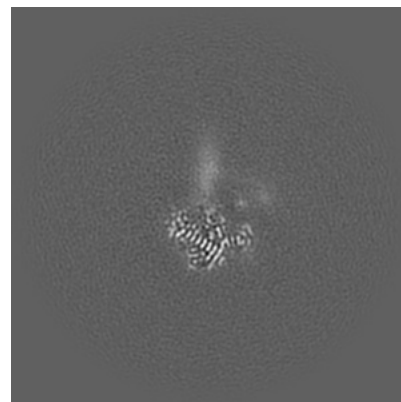
6.3.1 Primary map



X Index: 188

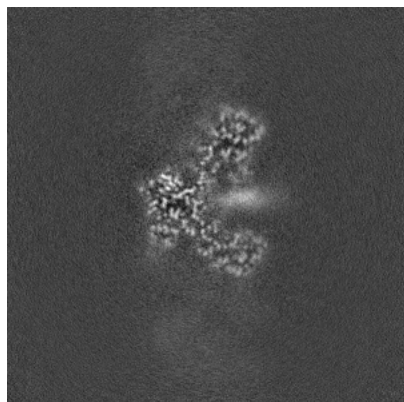


Y Index: 164

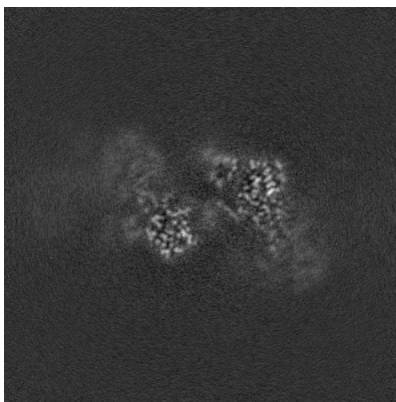


Z Index: 197

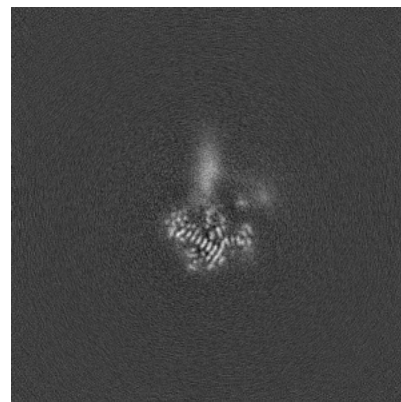
6.3.2 Raw map



X Index: 188



Y Index: 199

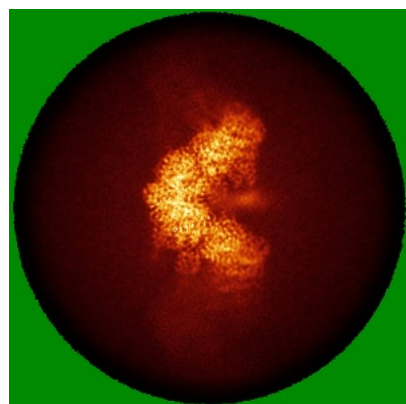


Z Index: 197

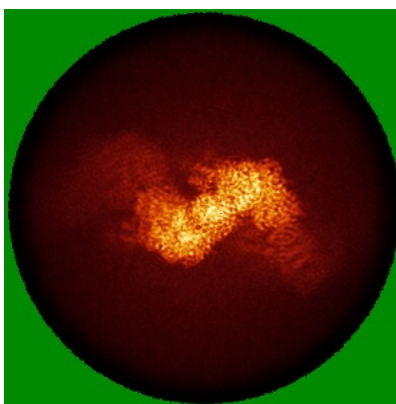
The images above show the largest variance slices of the map in three orthogonal directions.

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

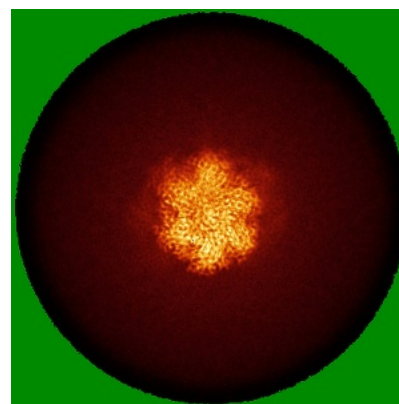
6.4.1 Primary map



X

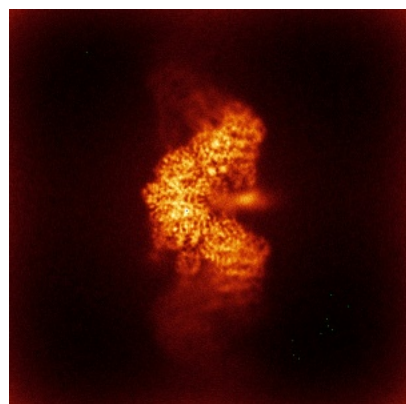


Y

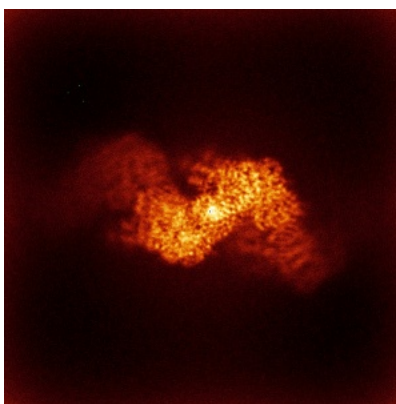


Z

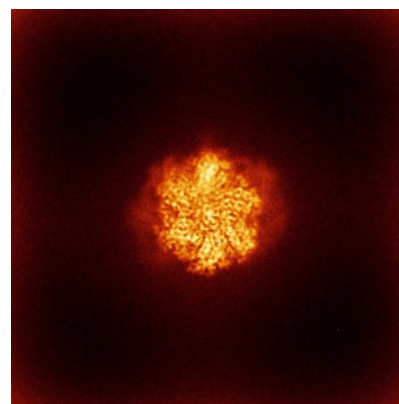
6.4.2 Raw map



X



Y

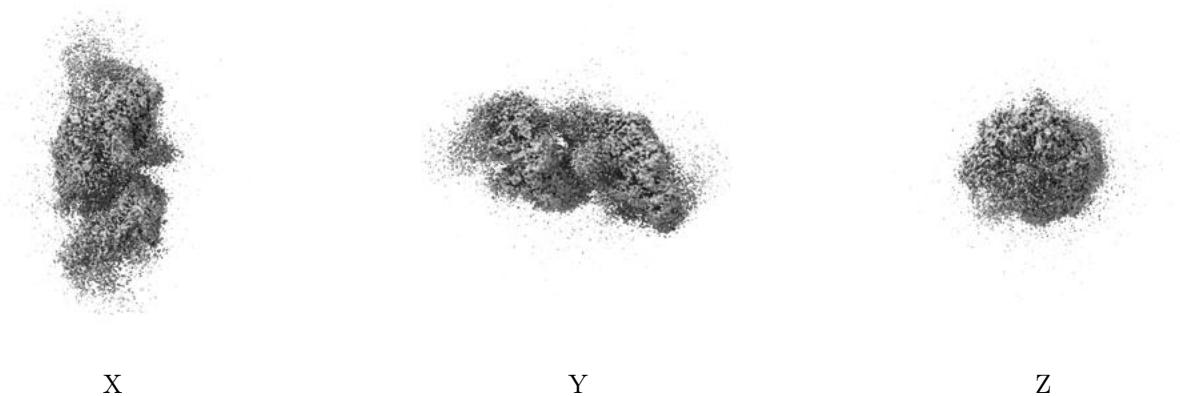


Z

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.

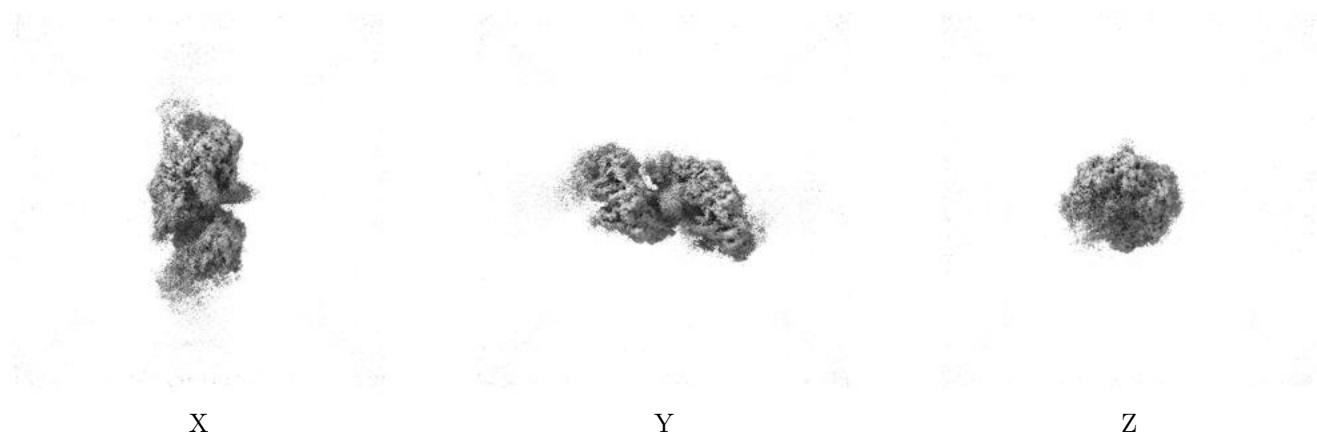
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. 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.

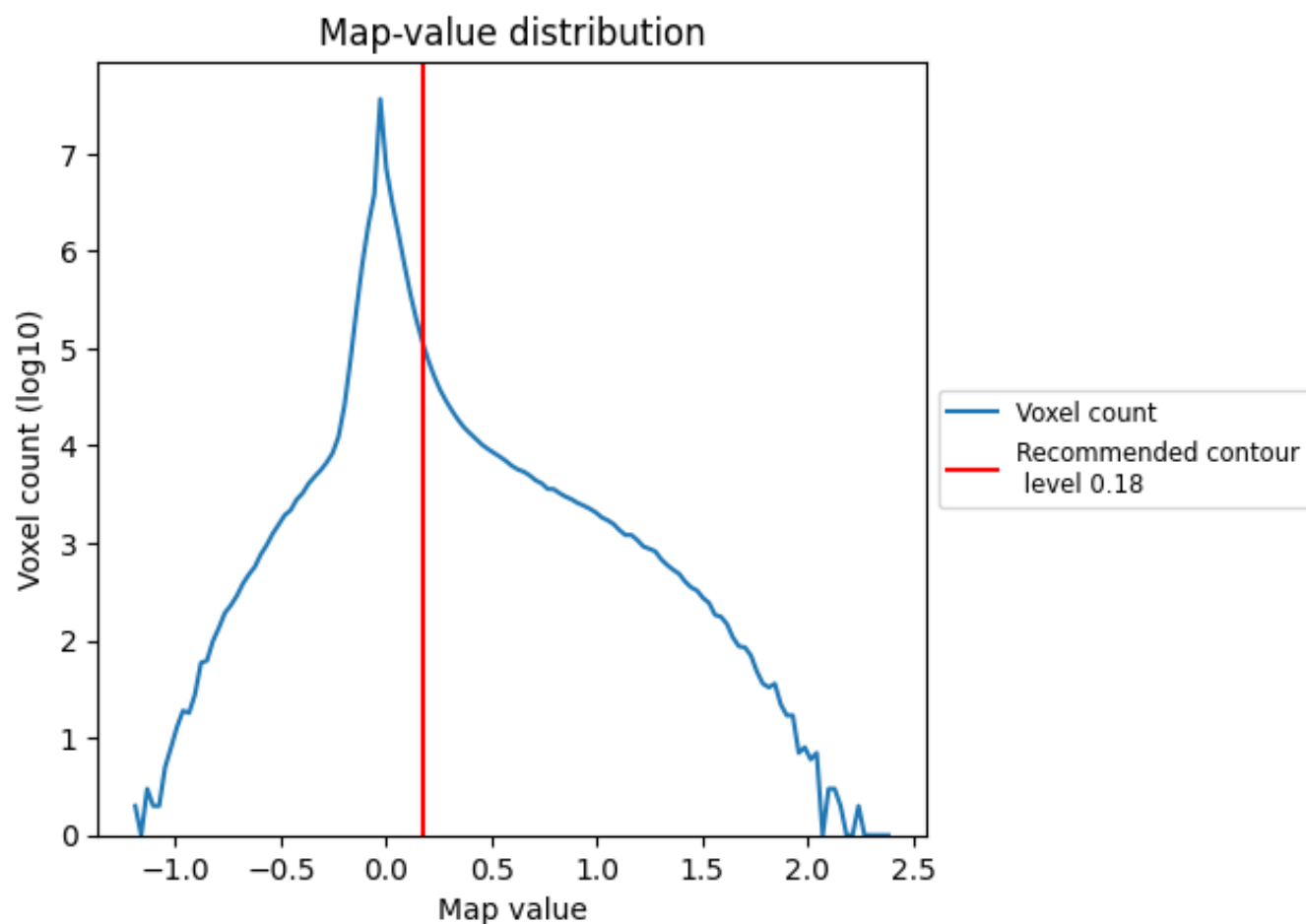
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

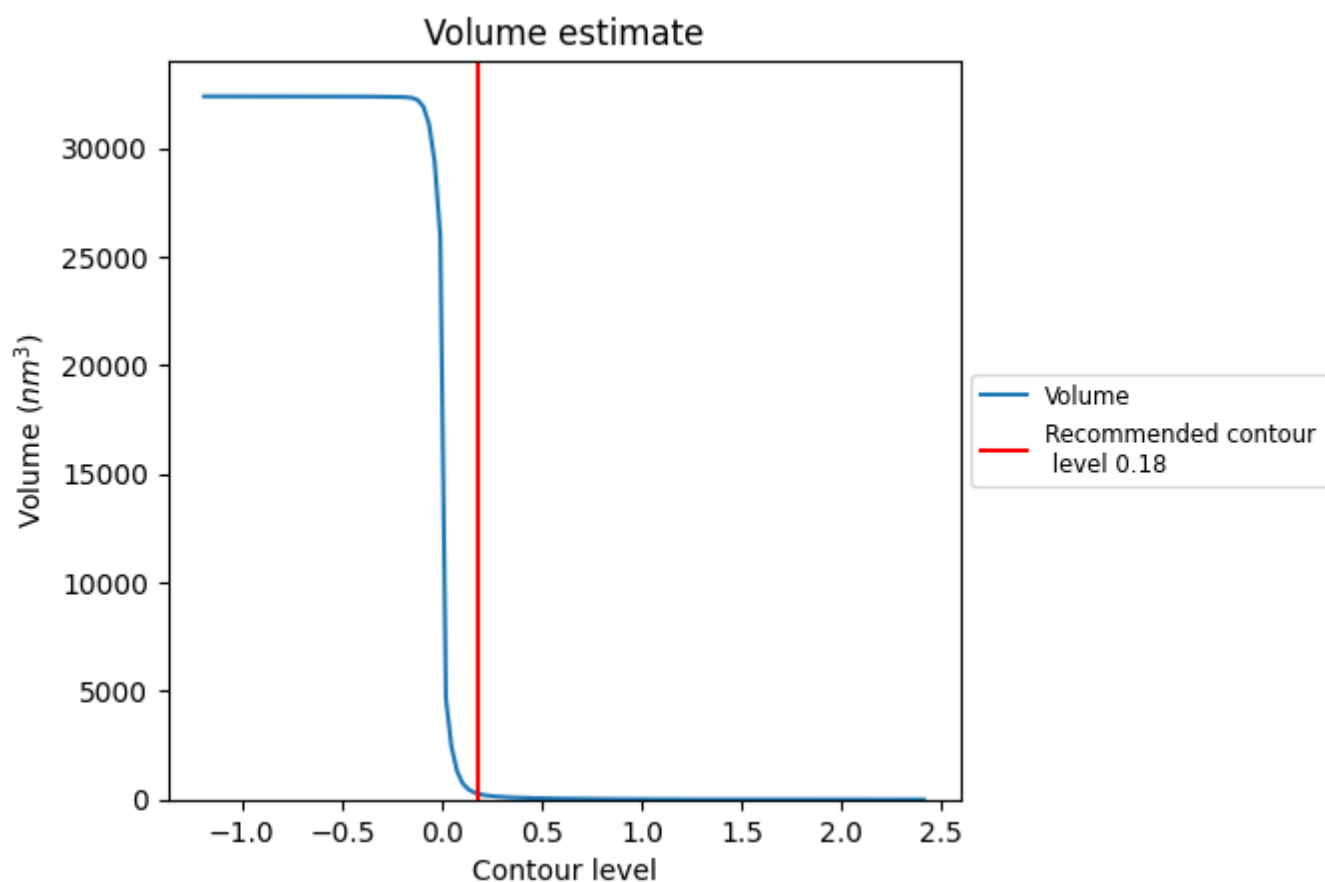
This section contains the results of statistical analysis of the map.

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.

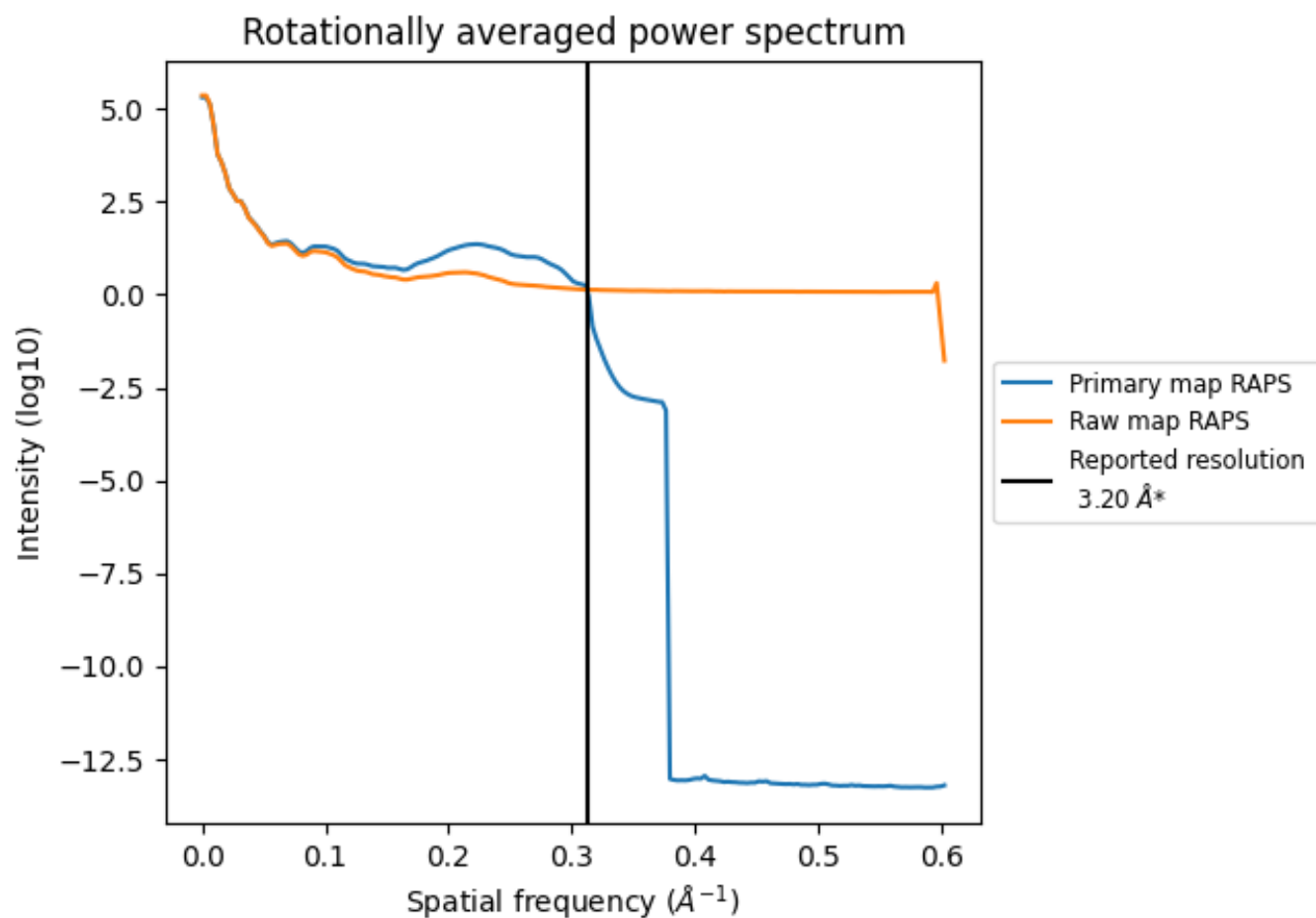
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 274 nm^3 ; this corresponds to an approximate mass of 248 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 ⓘ

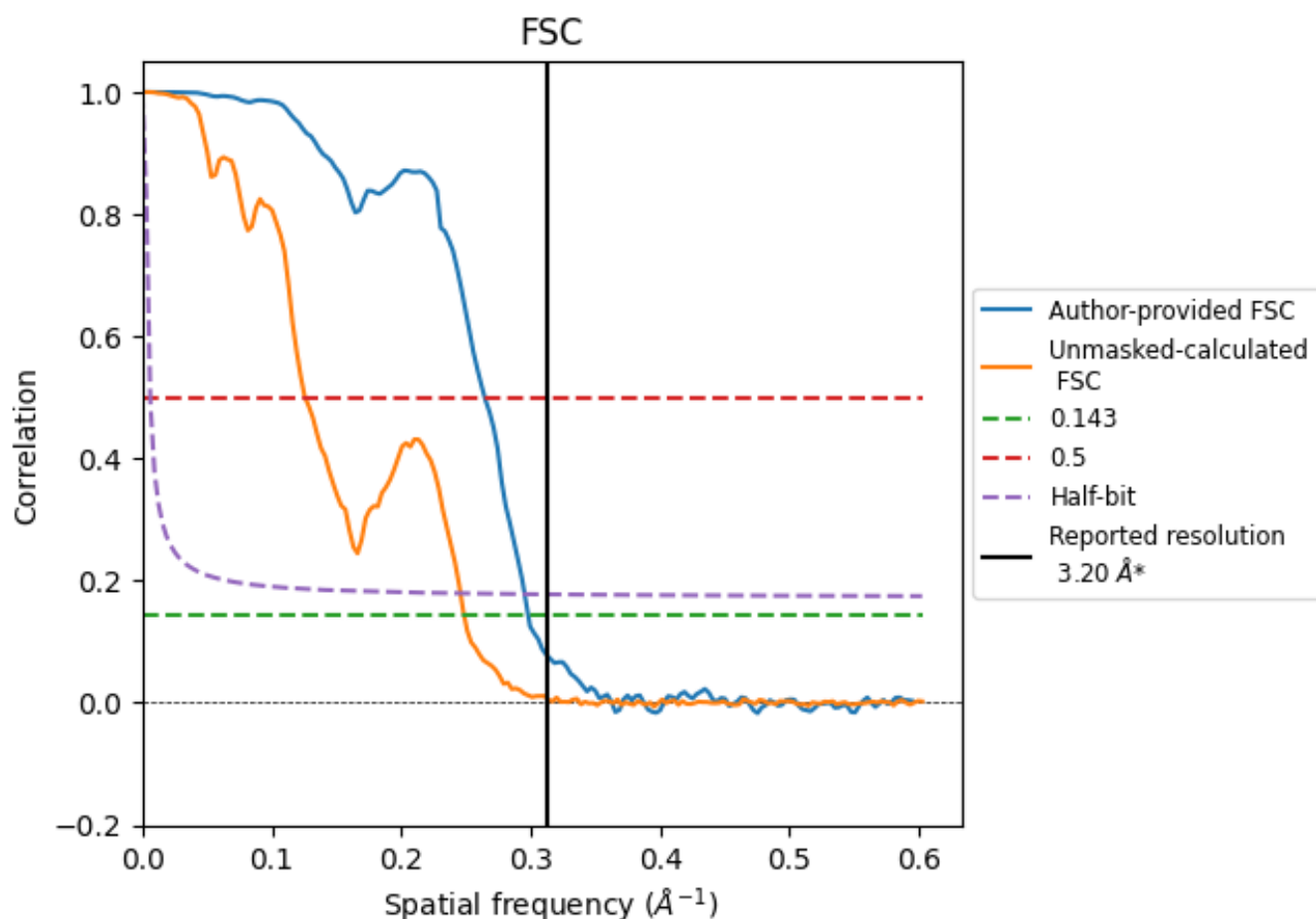


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

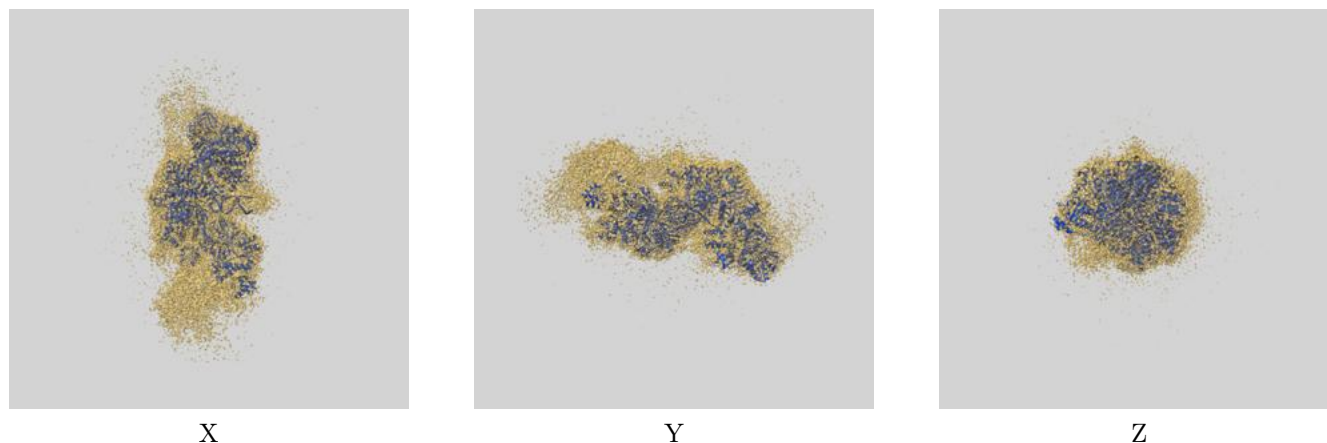
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.35	3.78	3.39
Unmasked-calculated*	4.02	7.95	4.07

*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 4.02 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

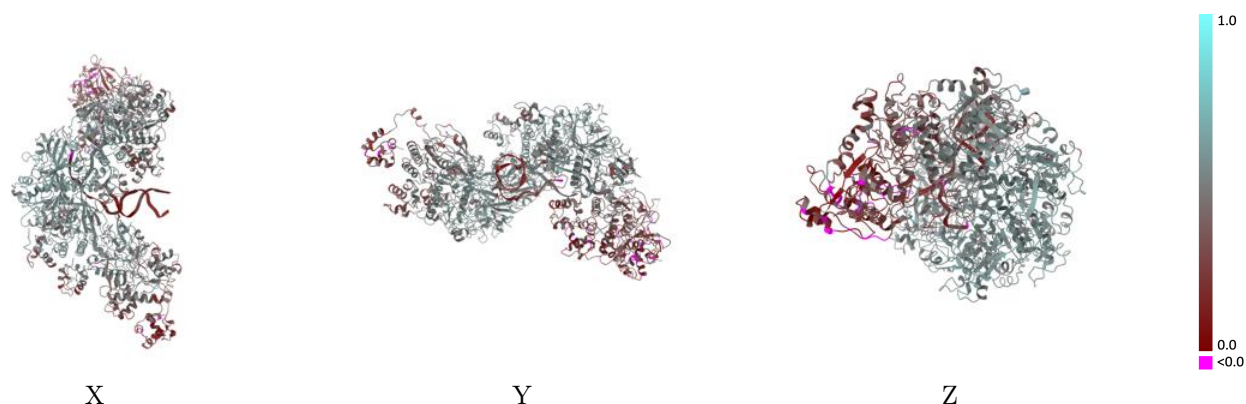
This section contains information regarding the fit between EMDB map EMD-64187 and PDB model 9UI8. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



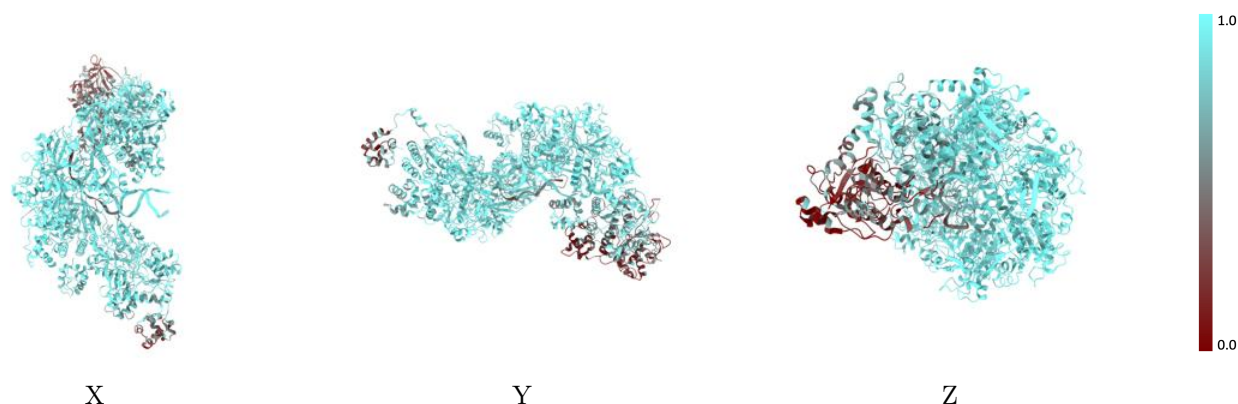
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



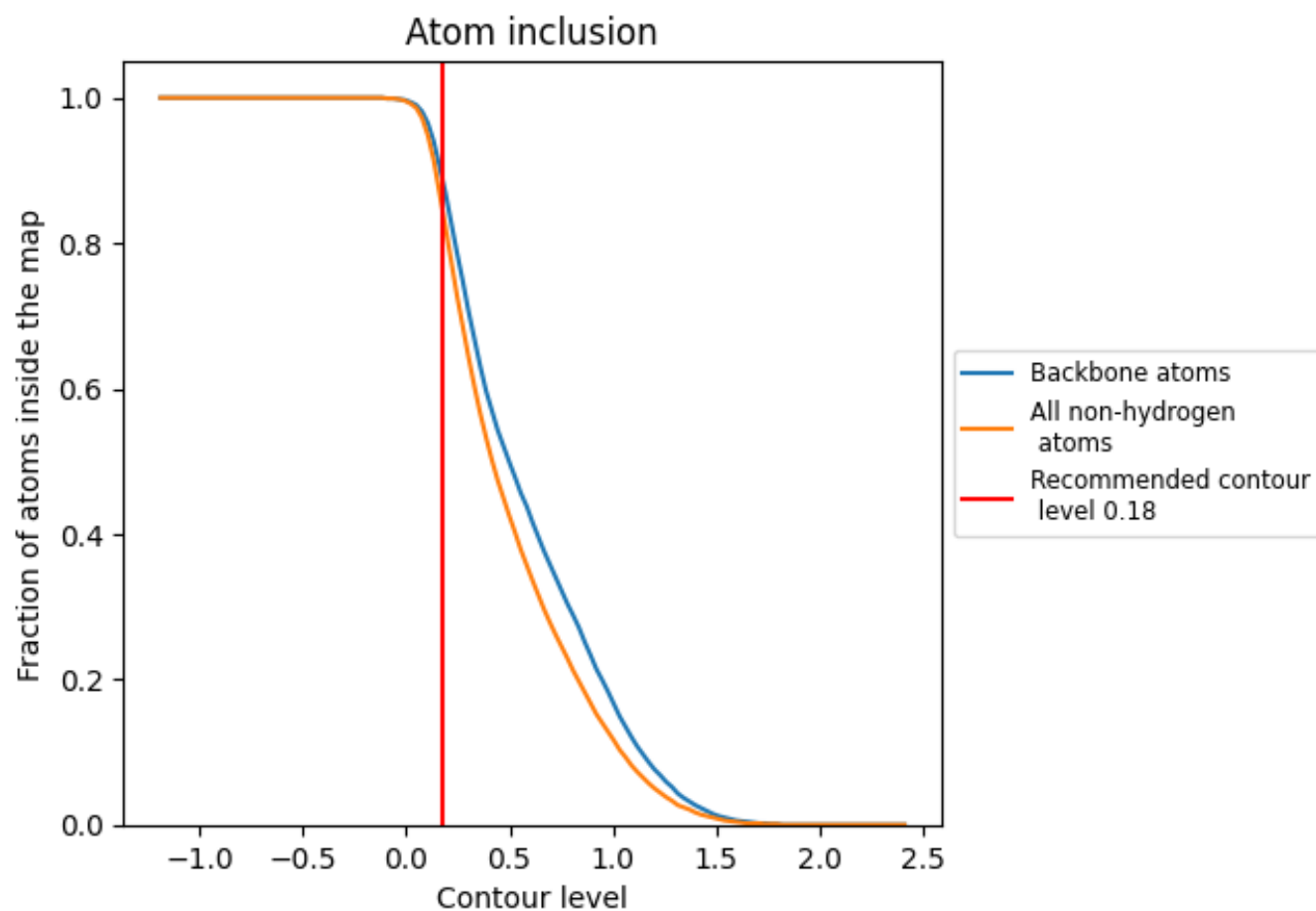
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 84% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8380	0.4490
A	0.3250	0.2230
B	0.7820	0.3600
C	0.9350	0.4990
D	0.9500	0.5360
E	0.9450	0.5340
F	0.9550	0.5350
G	0.9450	0.5210
H	0.9030	0.4910
I	0.7910	0.4030
L	0.9220	0.4760
T	0.9060	0.2830
U	0.6810	0.1970

