Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 03:48 pm GMT

PDB ID	:	5NP7
EMDB ID	:	EMD-8183
Title	:	CryoEM structure of Human Rad51 on single-stranded DNA to 4.2A resolution.
Authors	:	Short, J.M.; Venkitaraman, A.
Deposited on	:	2017-04-13
Resolution	:	4.20 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 (i) symbol.

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

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

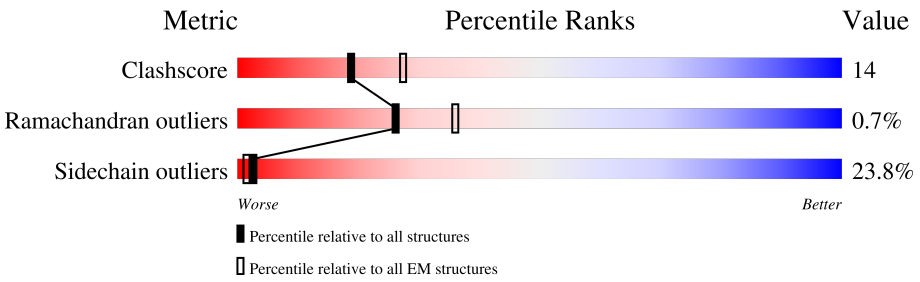
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.20 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	339	24% 57% 24% 9% • 8%
1	B	339	23% 56% 24% 10% • 8%
1	C	339	22% 56% 25% 9% • 8%
1	D	339	22% 56% 25% 9% • 8%
1	E	339	23% 55% 25% 9% • 8%
1	F	339	25% 56% 25% 9% • 8%
1	G	339	24% 57% 24% 9% • 8%

2 Entry composition (i)

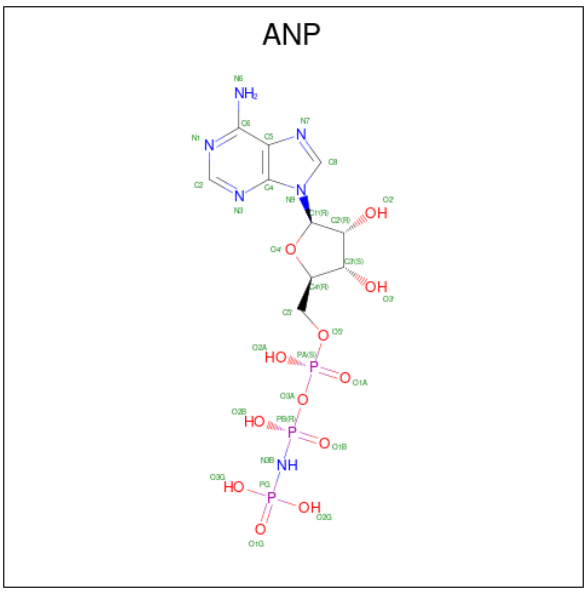
There are 2 unique types of molecules in this entry. The entry contains 16457 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S		
1	A	311	2320	1455	411	441	13	0	0
1	B	311	2320	1455	411	441	13	0	0
1	C	311	2320	1455	411	441	13	0	0
1	D	311	2320	1455	411	441	13	0	0
1	E	311	2320	1455	411	441	13	0	0
1	F	311	2320	1455	411	441	13	0	0
1	G	311	2320	1455	411	441	13	0	0

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



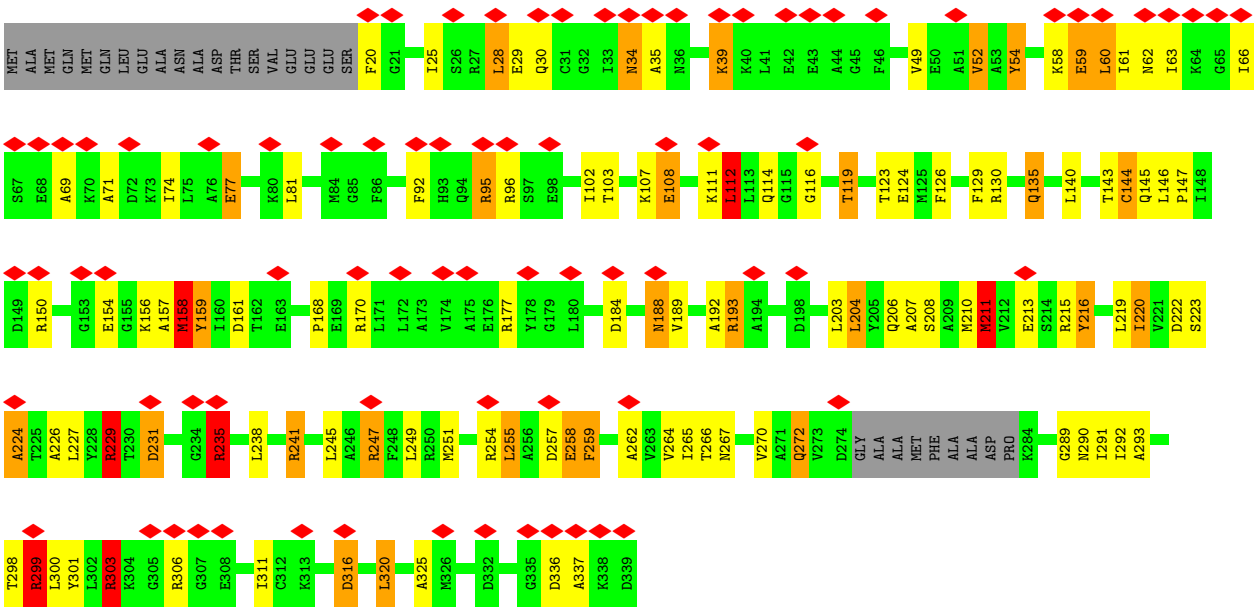
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	31	10	6	12	3	0
2	B	1	31	10	6	12	3	0
2	C	1	31	10	6	12	3	0
2	D	1	31	10	6	12	3	0
2	E	1	31	10	6	12	3	0
2	F	1	31	10	6	12	3	0
2	G	1	31	10	6	12	3	0

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.

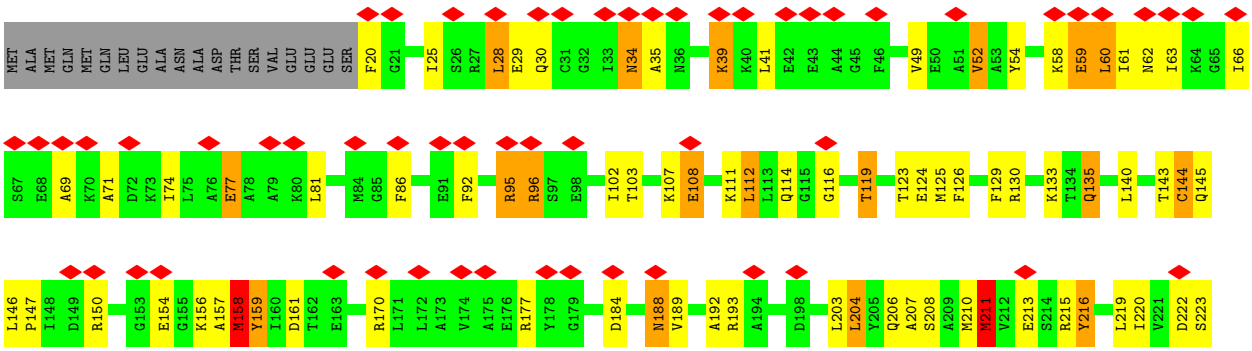
• Molecule 1: DNA repair protein RAD51 homolog 1

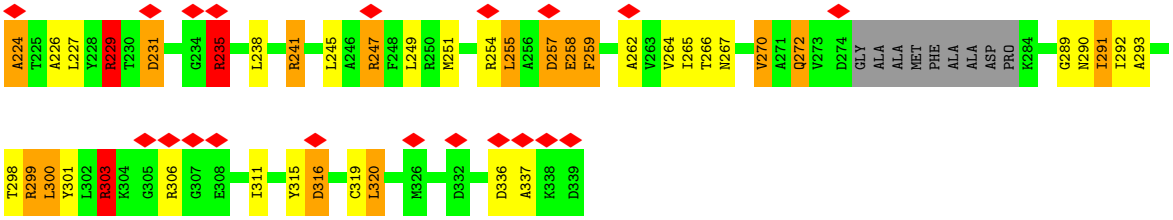
Chain A:



• Molecule 1: DNA repair protein RAD51 homolog 1

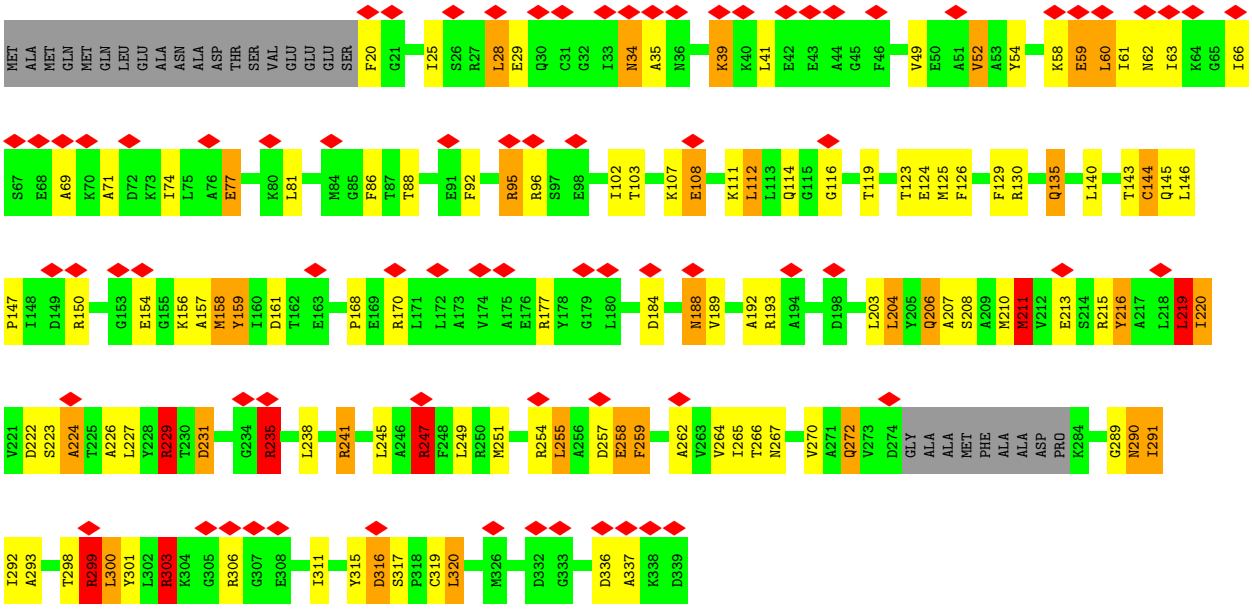
Chain B:





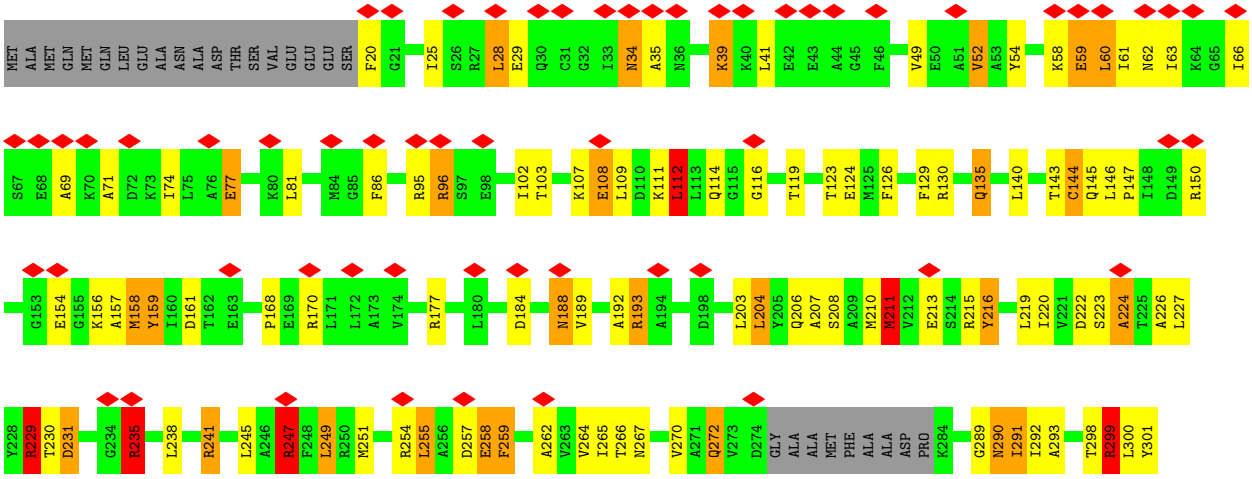
• Molecule 1: DNA repair protein RAD51 homolog 1

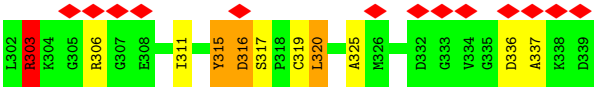
Chain C:



• Molecule 1: DNA repair protein RAD51 homolog 1

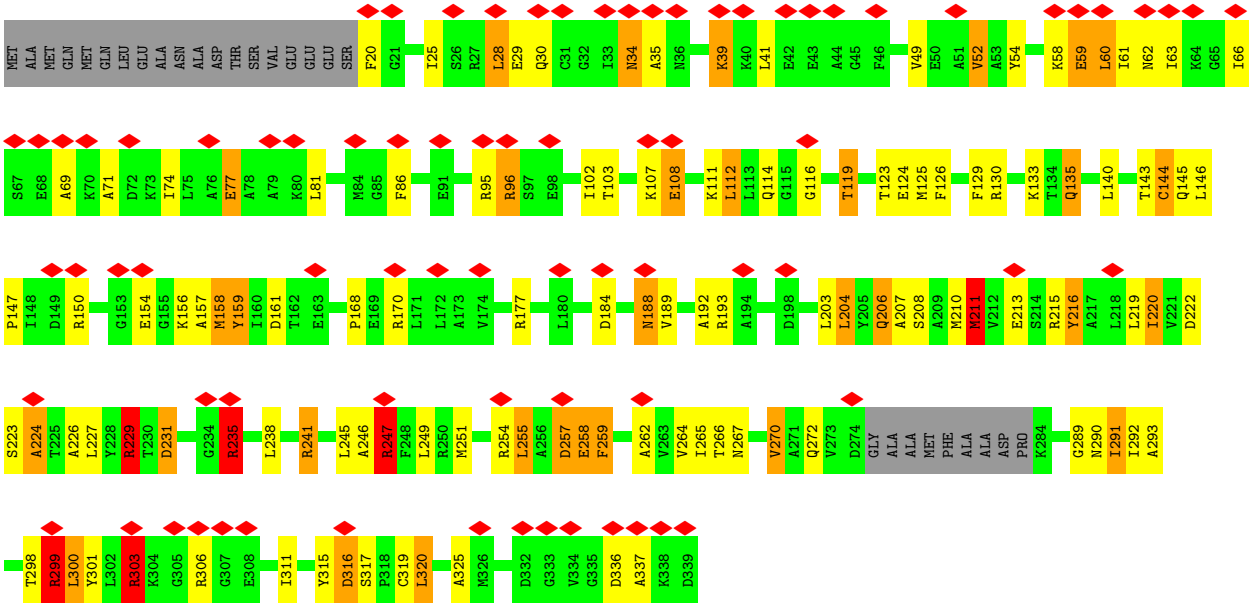
Chain D:





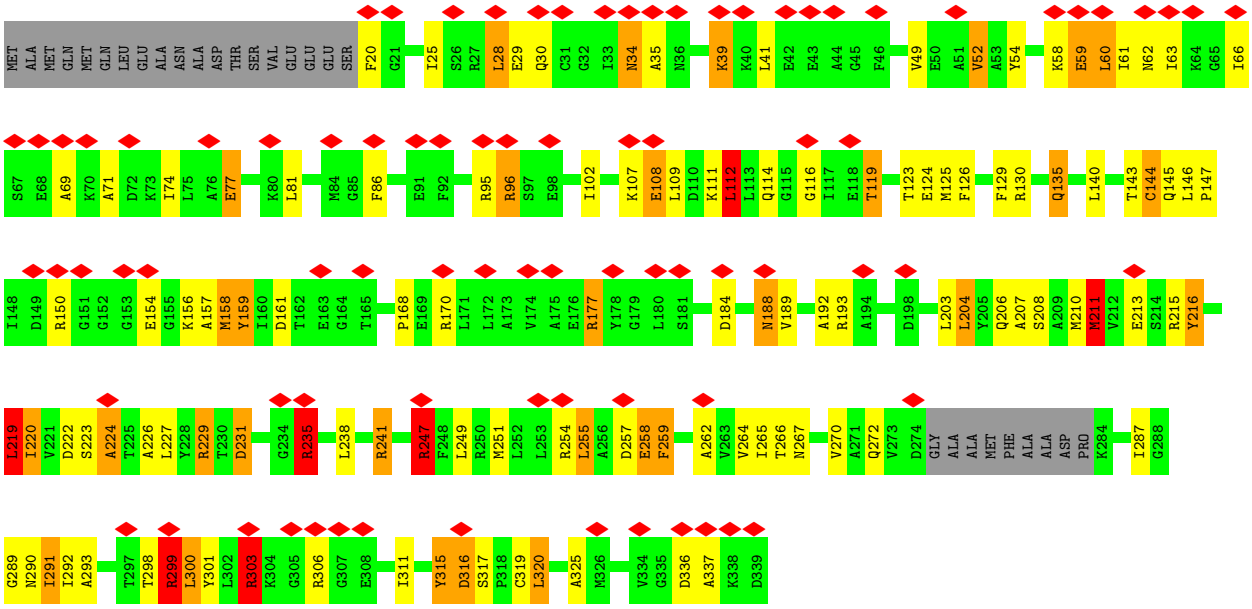
• Molecule 1: DNA repair protein RAD51 homolog 1

Chain E:



• Molecule 1: DNA repair protein RAD51 homolog 1

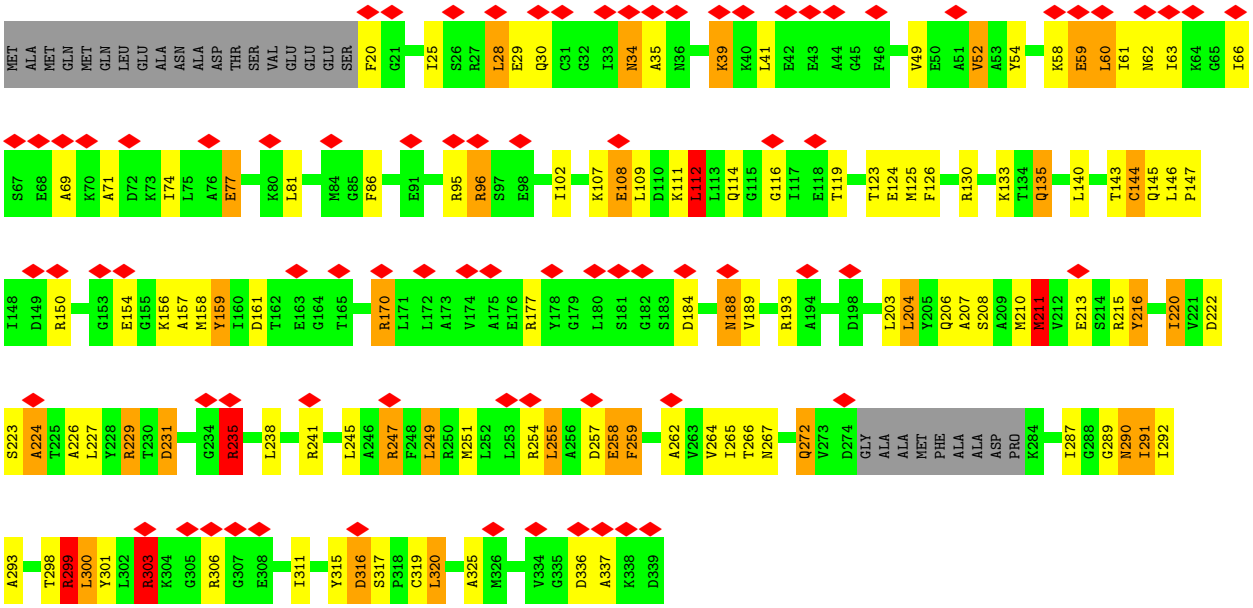
Chain F:



• Molecule 1: DNA repair protein RAD51 homolog 1

Chain G:

24%
57%
24%
9%
8%


MET ALA MET GLN MET GLN LEU GLU ALA ASN ALA ASP THR SER VAL GLU GLU GLU GLU SER F20 G21 I25 S26 R27 L28 E29 Q30 C31 G32 I33 N34 A35 N36 K39 K40 L41 E42 E43 A44 G45 F46 V49 E50 A51 V52 A53 Y54 K58 E59 L60 I61 N62 I63 K64 G65 I66
S67 E68 A69 K70 A71 D72 K73 I74 L75 A76 E77 K80 L81 M84 G85 F86 E91 R95 R96 S97 E98 I102 K107 E108 L109 D110 K111 L112 L113 Q114 G115 G116 I117 E118 T119 T123 E124 M125 F126 R130 K133 T134 Q135 L140 T143 C144 Q145 L146 P147
I148 D149 R150 G153 E154 G155 K156 A157 M158 Y159 I160 D161 T162 E163 G164 T165 R170 L171 L172 A173 V174 A175 E176 R177 Y178 G179 L180 S181 G182 S183 D184 N188 V189 R193 A194 D198 L203 L204 Y205 Q206 A207 S208 A209 M210 M211 V212 E213 S214 R215 Y216 I220 V221 D222
S223 A224 T225 A226 L227 Y228 R229 T230 D231 G234 R235 L238 R241 L245 A246 R247 F248 L249 R250 M251 L252 L253 R254 L255 A256 D257 E258 F259 A262 V263 V264 I265 T266 N267 Q272 V273 D274 GLY ALA ALA MET PHE ALA ALA ASP PRO K284 I287 G288 G289 N290 I291 I292
A293 T298 R299 L300 Y301 L302 R303 K304 G305 R306 G307 E308 I311 Y315 D316 S317 P318 C319 L320 A325 M326 V334 G335 D336 A337 K338 D339

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=56.2°, rise=16.0 Å, axial sym=C1	Depositor
Number of segments used	60000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; per segment	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	Not provided	
Magnification	104477	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.511	Depositor
Minimum map value	-0.237	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	256.0, 256.0, 256.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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

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	0.99	3/2354 (0.1%)	1.39	24/3182 (0.8%)
1	B	0.99	5/2354 (0.2%)	1.39	25/3182 (0.8%)
1	C	0.99	5/2354 (0.2%)	1.41	27/3182 (0.8%)
1	D	0.99	5/2354 (0.2%)	1.40	27/3182 (0.8%)
1	E	0.99	4/2354 (0.2%)	1.40	24/3182 (0.8%)
1	F	0.99	5/2354 (0.2%)	1.40	27/3182 (0.8%)
1	G	1.00	5/2354 (0.2%)	1.40	24/3182 (0.8%)
All	All	0.99	32/16478 (0.2%)	1.40	178/22274 (0.8%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	54	TYR	CE1-CZ	6.85	1.47	1.38
1	B	54	TYR	CE1-CZ	6.36	1.46	1.38
1	G	54	TYR	CE1-CZ	5.98	1.46	1.38
1	E	54	TYR	CG-CD2	5.91	1.46	1.39
1	A	258	GLU	CG-CD	-5.83	1.43	1.51
1	C	54	TYR	CE1-CZ	5.75	1.46	1.38
1	D	258	GLU	CG-CD	-5.73	1.43	1.51
1	B	258	GLU	CG-CD	-5.71	1.43	1.51
1	G	54	TYR	CG-CD2	5.70	1.46	1.39
1	G	258	GLU	CG-CD	-5.69	1.43	1.51
1	E	258	GLU	CG-CD	-5.67	1.43	1.51
1	B	54	TYR	CG-CD2	5.67	1.46	1.39
1	D	54	TYR	CE1-CZ	5.65	1.45	1.38
1	F	258	GLU	CG-CD	-5.63	1.43	1.51
1	C	258	GLU	CG-CD	-5.63	1.43	1.51
1	D	54	TYR	CG-CD2	5.61	1.46	1.39
1	C	54	TYR	CG-CD2	5.45	1.46	1.39
1	F	54	TYR	CG-CD2	5.31	1.46	1.39
1	A	54	TYR	CG-CD1	5.27	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	315	TYR	CE1-CZ	5.25	1.45	1.38
1	F	54	TYR	CE1-CZ	5.19	1.45	1.38
1	C	211	MET	CG-SD	-5.17	1.67	1.81
1	B	211	MET	CG-SD	-5.12	1.67	1.81
1	E	211	MET	CG-SD	-5.12	1.67	1.81
1	A	211	MET	CG-SD	-5.12	1.67	1.81
1	D	211	MET	CG-SD	-5.10	1.67	1.81
1	F	315	TYR	CE1-CZ	5.06	1.45	1.38
1	G	315	TYR	CE1-CZ	5.06	1.45	1.38
1	B	315	TYR	CE1-CZ	5.05	1.45	1.38
1	G	211	MET	CG-SD	-5.05	1.68	1.81
1	C	315	TYR	CE1-CZ	5.04	1.45	1.38
1	F	211	MET	CG-SD	-5.04	1.68	1.81

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	231	ASP	CB-CG-OD2	11.79	128.91	118.30
1	A	231	ASP	CB-CG-OD2	11.42	128.58	118.30
1	B	231	ASP	CB-CG-OD2	11.37	128.53	118.30
1	D	231	ASP	CB-CG-OD2	11.12	128.31	118.30
1	F	231	ASP	CB-CG-OD2	11.10	128.29	118.30
1	C	231	ASP	CB-CG-OD2	10.97	128.17	118.30
1	E	231	ASP	CB-CG-OD2	10.88	128.09	118.30
1	D	247	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	E	247	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	F	247	ARG	NE-CZ-NH1	9.69	125.15	120.30
1	G	229	ARG	NE-CZ-NH1	9.67	125.14	120.30
1	C	247	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	G	247	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	A	193	ARG	NE-CZ-NH1	9.01	124.81	120.30
1	D	193	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	B	247	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	A	247	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	C	193	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	F	193	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	B	193	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	E	193	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	E	229	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	F	229	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	A	229	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	D	241	ARG	NE-CZ-NH1	7.99	124.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	229	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	C	241	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	D	229	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	B	241	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	E	241	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	F	254	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	B	229	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	G	254	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	D	254	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	C	254	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	B	254	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	E	254	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	254	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	G	259	PHE	CB-CG-CD2	-7.10	115.83	120.80
1	B	259	PHE	CB-CG-CD2	-7.08	115.85	120.80
1	C	259	PHE	CB-CG-CD2	-7.07	115.85	120.80
1	A	96	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	259	PHE	CB-CG-CD2	-7.01	115.89	120.80
1	G	170	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	C	219	LEU	CB-CG-CD1	7.00	122.90	111.00
1	E	259	PHE	CB-CG-CD2	-6.99	115.91	120.80
1	D	259	PHE	CB-CG-CD2	-6.98	115.91	120.80
1	A	303	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	B	303	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	F	259	PHE	CB-CG-CD2	-6.84	116.01	120.80
1	D	303	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	F	247	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	G	193	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	E	247	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	D	247	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	G	249	LEU	CB-CG-CD2	-6.63	99.74	111.00
1	E	303	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	G	247	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	G	303	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	C	303	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	C	247	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	C	249	LEU	CB-CG-CD2	-6.39	100.14	111.00
1	A	241	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	F	303	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	D	249	LEU	CB-CG-CD2	-6.31	100.27	111.00
1	C	96	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	B	249	LEU	CB-CG-CD2	-6.22	100.43	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	216	TYR	CB-CG-CD2	-6.15	117.31	121.00
1	E	249	LEU	CB-CG-CD2	-6.15	100.55	111.00
1	B	170	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	B	216	TYR	CB-CG-CD2	-6.11	117.33	121.00
1	F	249	LEU	CB-CG-CD2	-6.09	100.65	111.00
1	C	216	TYR	CB-CG-CD2	-6.08	117.35	121.00
1	D	216	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	B	249	LEU	CB-CG-CD1	6.02	121.24	111.00
1	A	249	LEU	CB-CG-CD2	-6.00	100.80	111.00
1	C	249	LEU	CB-CG-CD1	5.96	121.14	111.00
1	D	215	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	G	216	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	A	95	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	F	96	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	C	170	ARG	NE-CZ-NH2	5.89	123.24	120.30
1	F	215	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	G	96	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	216	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	E	96	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	170	ARG	NE-CZ-NH2	5.85	123.22	120.30
1	E	215	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	215	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	247	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	G	95	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	E	170	ARG	NE-CZ-NH2	5.83	123.22	120.30
1	E	95	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	D	170	ARG	NE-CZ-NH2	5.83	123.21	120.30
1	F	170	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	F	249	LEU	CB-CG-CD1	5.82	120.90	111.00
1	B	96	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	E	249	LEU	CB-CG-CD1	5.81	120.88	111.00
1	G	235	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	D	95	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	B	215	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	F	216	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	D	249	LEU	CB-CG-CD1	5.78	120.82	111.00
1	B	241	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	F	95	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	G	249	LEU	CB-CG-CD1	5.75	120.78	111.00
1	C	241	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	G	299	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	247	ARG	NE-CZ-NH2	-5.73	117.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	235	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	215	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	G	215	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	B	235	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	95	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	E	235	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	D	96	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	D	235	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	F	219	LEU	CA-CB-CG	5.56	128.09	115.30
1	A	235	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	F	235	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	95	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	229	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	D	247	ARG	CD-NE-CZ	5.48	131.27	123.60
1	D	241	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	E	299	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	F	247	ARG	CD-NE-CZ	5.46	131.24	123.60
1	B	41	LEU	CB-CG-CD2	5.46	120.27	111.00
1	A	231	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	C	41	LEU	CB-CG-CD2	5.44	120.24	111.00
1	G	287	ILE	CG1-CB-CG2	5.42	123.33	111.40
1	E	247	ARG	CD-NE-CZ	5.40	131.17	123.60
1	B	231	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	C	247	ARG	CD-NE-CZ	5.35	131.09	123.60
1	F	41	LEU	CB-CG-CD2	5.31	120.03	111.00
1	F	112	LEU	CB-CG-CD2	5.31	120.03	111.00
1	G	231	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	E	41	LEU	CB-CG-CD2	5.30	120.01	111.00
1	F	287	ILE	CG1-CB-CG2	5.30	123.06	111.40
1	A	249	LEU	CB-CG-CD1	5.29	119.99	111.00
1	G	112	LEU	CB-CG-CD2	5.29	119.99	111.00
1	F	231	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	F	299	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	D	229	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	C	112	LEU	CB-CG-CD2	5.26	119.94	111.00
1	F	241	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	299	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	D	112	LEU	CB-CG-CD2	5.25	119.92	111.00
1	D	299	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	E	229	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	G	247	ARG	CD-NE-CZ	5.19	130.87	123.60
1	G	109	LEU	CB-CG-CD1	5.18	119.81	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	109	LEU	CB-CG-CD1	5.18	119.81	111.00
1	A	112	LEU	CB-CG-CD2	5.17	119.79	111.00
1	E	216	TYR	CB-CG-CD1	5.17	124.10	121.00
1	F	306	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	G	306	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	C	219	LEU	CA-CB-CG	5.13	127.11	115.30
1	C	231	ASP	CB-CG-OD1	-5.13	113.69	118.30
1	A	247	ARG	CD-NE-CZ	5.12	130.77	123.60
1	D	41	LEU	CB-CG-CD2	5.11	119.69	111.00
1	A	158	MET	CB-CA-C	5.11	120.62	110.40
1	E	241	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	216	TYR	CB-CG-CD1	5.11	124.06	121.00
1	C	216	TYR	CB-CG-CD1	5.10	124.06	121.00
1	G	41	LEU	CB-CG-CD2	5.10	119.67	111.00
1	A	306	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	B	306	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	B	112	LEU	CB-CG-CD2	5.09	119.65	111.00
1	E	306	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	D	306	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	D	231	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	B	247	ARG	CD-NE-CZ	5.05	130.67	123.60
1	F	109	LEU	CB-CG-CD1	5.05	119.58	111.00
1	F	177	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	299	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	D	216	TYR	CB-CG-CD1	5.04	124.02	121.00
1	C	306	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	B	158	MET	CB-CA-C	5.00	120.40	110.40

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	2320	0	2268	68	0
1	B	2320	0	2268	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2320	0	2268	72	0
1	D	2320	0	2268	73	0
1	E	2320	0	2268	74	0
1	F	2320	0	2268	65	0
1	G	2320	0	2268	70	0
2	A	31	0	13	0	0
2	B	31	0	13	1	0
2	C	31	0	13	1	0
2	D	31	0	13	1	0
2	E	31	0	13	1	0
2	F	31	0	13	1	0
2	G	31	0	13	0	0
All	All	16457	0	15967	467	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 (467) 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:D:207:ALA:O	1:D:211:MET:SD	2.06	1.13
1:C:207:ALA:O	1:C:211:MET:SD	2.06	1.13
1:F:207:ALA:O	1:F:211:MET:SD	2.06	1.13
1:A:207:ALA:O	1:A:211:MET:SD	2.06	1.12
1:B:207:ALA:O	1:B:211:MET:SD	2.06	1.12
1:E:207:ALA:O	1:E:211:MET:SD	2.06	1.12
1:G:207:ALA:O	1:G:211:MET:SD	2.06	1.12
1:A:223:SER:HB3	1:A:226:ALA:HB3	1.37	1.07
1:D:223:SER:HB3	1:D:226:ALA:HB3	1.37	1.06
1:E:223:SER:HB3	1:E:226:ALA:HB3	1.37	1.06
1:C:223:SER:HB3	1:C:226:ALA:HB3	1.37	1.05
1:F:223:SER:HB3	1:F:226:ALA:HB3	1.37	1.05
1:G:223:SER:HB3	1:G:226:ALA:HB3	1.38	1.05
1:B:223:SER:HB3	1:B:226:ALA:HB3	1.37	1.04
1:G:227:LEU:O	1:G:231:ASP:OD1	1.79	1.00
1:F:227:LEU:O	1:F:231:ASP:OD1	1.80	1.00
1:A:227:LEU:O	1:A:231:ASP:OD1	1.80	0.99
1:C:227:LEU:O	1:C:231:ASP:OD1	1.81	0.99
1:E:227:LEU:O	1:E:231:ASP:OD1	1.81	0.98
1:B:227:LEU:O	1:B:231:ASP:OD1	1.81	0.98
1:D:227:LEU:O	1:D:231:ASP:OD1	1.81	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:184:ASP:O	1:G:188:ASN:OD1	1.90	0.90
1:F:184:ASP:O	1:F:188:ASN:OD1	1.91	0.89
1:E:184:ASP:O	1:E:188:ASN:OD1	1.91	0.89
1:D:184:ASP:O	1:D:188:ASN:OD1	1.91	0.89
1:C:184:ASP:O	1:C:188:ASN:OD1	1.91	0.89
1:B:184:ASP:O	1:B:188:ASN:OD1	1.91	0.87
1:A:184:ASP:O	1:A:188:ASN:OD1	1.91	0.87
1:E:140:LEU:HA	1:E:143:THR:HG22	1.59	0.85
1:E:135:GLN:HE21	1:E:135:GLN:HA	1.41	0.85
1:F:140:LEU:HA	1:F:143:THR:HG22	1.59	0.85
1:D:135:GLN:HE21	1:D:135:GLN:HA	1.42	0.84
1:A:140:LEU:HA	1:A:143:THR:HG22	1.59	0.84
1:G:140:LEU:HA	1:G:143:THR:HG22	1.60	0.84
1:A:135:GLN:HA	1:A:135:GLN:HE21	1.40	0.83
1:D:140:LEU:HA	1:D:143:THR:HG22	1.59	0.83
1:C:135:GLN:HE21	1:C:135:GLN:HA	1.40	0.83
1:F:135:GLN:HE21	1:F:135:GLN:HA	1.41	0.83
1:B:140:LEU:HA	1:B:143:THR:HG22	1.60	0.82
1:G:135:GLN:HE21	1:G:135:GLN:HA	1.44	0.82
1:B:135:GLN:HA	1:B:135:GLN:HE21	1.42	0.81
1:C:140:LEU:HA	1:C:143:THR:HG22	1.61	0.81
1:G:223:SER:H	1:G:266:THR:HB	1.47	0.79
1:E:223:SER:H	1:E:266:THR:HB	1.48	0.78
1:C:135:GLN:HA	1:C:135:GLN:NE2	1.99	0.78
1:A:135:GLN:HA	1:A:135:GLN:NE2	1.99	0.78
1:B:135:GLN:HA	1:B:135:GLN:NE2	1.99	0.78
1:B:223:SER:H	1:B:266:THR:HB	1.50	0.77
1:F:135:GLN:HA	1:F:135:GLN:NE2	1.99	0.77
1:E:135:GLN:HA	1:E:135:GLN:NE2	1.99	0.77
1:F:140:LEU:HA	1:F:143:THR:CG2	2.15	0.77
1:D:135:GLN:HA	1:D:135:GLN:NE2	2.00	0.76
1:E:140:LEU:HA	1:E:143:THR:CG2	2.15	0.76
1:B:140:LEU:HA	1:B:143:THR:CG2	2.15	0.76
1:C:223:SER:H	1:C:266:THR:HB	1.49	0.76
1:F:223:SER:H	1:F:266:THR:HB	1.49	0.76
1:A:140:LEU:HA	1:A:143:THR:CG2	2.16	0.76
1:D:223:SER:H	1:D:266:THR:HB	1.50	0.76
1:G:135:GLN:HA	1:G:135:GLN:NE2	1.99	0.76
1:G:140:LEU:HA	1:G:143:THR:CG2	2.16	0.75
1:D:140:LEU:HA	1:D:143:THR:CG2	2.16	0.74
1:C:140:LEU:HA	1:C:143:THR:CG2	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:SER:H	1:A:266:THR:HB	1.53	0.72
1:C:229:ARG:HH22	1:C:270:VAL:HG23	1.56	0.71
1:D:229:ARG:HH22	1:D:270:VAL:HG23	1.57	0.69
1:B:229:ARG:HH22	1:B:270:VAL:HG23	1.59	0.68
1:D:145:GLN:HE22	1:D:156:LYS:HA	1.58	0.68
1:E:145:GLN:HE22	1:E:156:LYS:HA	1.58	0.68
1:G:204:LEU:HD12	1:G:251:MET:HG2	1.76	0.67
1:C:145:GLN:HE22	1:C:156:LYS:HA	1.60	0.67
1:F:145:GLN:HE22	1:F:156:LYS:HA	1.60	0.67
1:E:204:LEU:HD12	1:E:251:MET:HG2	1.77	0.66
1:D:192:ALA:HB2	1:E:86:PHE:H	1.61	0.65
1:C:192:ALA:HB2	1:D:86:PHE:H	1.61	0.65
1:B:145:GLN:HE22	1:B:156:LYS:HA	1.61	0.65
1:E:192:ALA:HB2	1:F:86:PHE:H	1.61	0.65
1:F:192:ALA:HB2	1:G:86:PHE:H	1.61	0.65
1:B:192:ALA:HB2	1:C:86:PHE:H	1.61	0.65
1:F:204:LEU:HD12	1:F:251:MET:HG2	1.78	0.65
1:E:210:MET:HB3	1:E:216:TYR:OH	1.97	0.65
1:A:145:GLN:HE22	1:A:156:LYS:HA	1.62	0.64
1:B:204:LEU:HD12	1:B:251:MET:HG2	1.79	0.64
1:C:204:LEU:HD12	1:C:251:MET:HG2	1.79	0.64
1:E:229:ARG:HH22	1:E:270:VAL:HG23	1.63	0.64
1:A:192:ALA:HB2	1:B:86:PHE:H	1.61	0.64
1:E:299:ARG:HB2	1:E:316:ASP:H	1.63	0.64
1:G:145:GLN:HE22	1:G:156:LYS:HA	1.61	0.64
1:C:210:MET:HB3	1:C:216:TYR:OH	1.98	0.64
1:D:204:LEU:HD12	1:D:251:MET:HG2	1.79	0.64
1:F:210:MET:HB3	1:F:216:TYR:OH	1.98	0.63
1:D:210:MET:HB3	1:D:216:TYR:OH	1.98	0.63
1:G:210:MET:HB3	1:G:216:TYR:OH	1.98	0.63
1:B:210:MET:HB3	1:B:216:TYR:OH	1.98	0.63
1:A:210:MET:HB3	1:A:216:TYR:OH	1.98	0.62
1:G:208:SER:HA	1:G:211:MET:SD	2.40	0.62
1:F:299:ARG:HB2	1:F:316:ASP:H	1.64	0.61
1:B:299:ARG:HB2	1:B:316:ASP:H	1.63	0.61
1:A:204:LEU:HD12	1:A:251:MET:HG2	1.80	0.61
1:F:211:MET:SD	1:F:211:MET:N	2.69	0.61
1:A:255:LEU:HA	1:A:258:GLU:HG2	1.81	0.61
1:D:255:LEU:HA	1:D:258:GLU:HG2	1.83	0.61
1:E:211:MET:SD	1:E:211:MET:N	2.69	0.61
1:G:255:LEU:HA	1:G:258:GLU:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:299:ARG:HB2	1:G:316:ASP:H	1.65	0.61
1:D:299:ARG:HB2	1:D:316:ASP:H	1.65	0.61
1:D:223:SER:O	1:D:226:ALA:N	2.33	0.60
1:A:208:SER:HA	1:A:211:MET:SD	2.42	0.60
1:E:223:SER:O	1:E:226:ALA:N	2.33	0.60
1:G:289:GLY:O	1:G:292:ILE:HD11	2.01	0.60
1:E:208:SER:HA	1:E:211:MET:SD	2.41	0.60
1:D:208:SER:HA	1:D:211:MET:SD	2.41	0.60
1:A:223:SER:O	1:A:226:ALA:N	2.33	0.60
1:C:255:LEU:HA	1:C:258:GLU:HG2	1.83	0.60
1:C:299:ARG:HB2	1:C:316:ASP:H	1.65	0.60
1:B:255:LEU:HA	1:B:258:GLU:HG2	1.83	0.60
1:E:124:GLU:HB2	1:E:265:ILE:O	2.01	0.60
1:B:208:SER:HA	1:B:211:MET:SD	2.42	0.59
1:G:124:GLU:HB2	1:G:265:ILE:O	2.02	0.59
1:C:208:SER:HA	1:C:211:MET:SD	2.42	0.59
1:F:255:LEU:HA	1:F:258:GLU:HG2	1.83	0.59
1:F:208:SER:HA	1:F:211:MET:SD	2.42	0.59
1:E:255:LEU:HA	1:E:258:GLU:HG2	1.83	0.59
1:B:124:GLU:HB2	1:B:265:ILE:O	2.04	0.58
1:D:211:MET:SD	1:D:211:MET:N	2.69	0.58
1:G:223:SER:O	1:G:226:ALA:N	2.35	0.58
1:B:223:SER:O	1:B:226:ALA:N	2.34	0.58
1:C:258:GLU:HG3	1:C:259:PHE:N	2.19	0.58
1:D:124:GLU:HB2	1:D:265:ILE:O	2.03	0.58
1:G:211:MET:SD	1:G:211:MET:N	2.69	0.57
1:C:211:MET:HG3	1:C:259:PHE:CE2	2.40	0.57
1:C:235:ARG:H	1:C:235:ARG:HE	1.53	0.57
1:B:235:ARG:H	1:B:235:ARG:HE	1.51	0.57
1:D:235:ARG:HE	1:D:235:ARG:H	1.53	0.57
1:F:258:GLU:HG3	1:F:259:PHE:N	2.19	0.57
1:G:235:ARG:H	1:G:235:ARG:HE	1.50	0.57
1:G:258:GLU:HG3	1:G:259:PHE:N	2.19	0.57
1:B:258:GLU:HG3	1:B:259:PHE:N	2.19	0.57
1:E:129:PHE:HB3	1:F:293:ALA:HB1	1.86	0.57
1:E:258:GLU:HG3	1:E:259:PHE:N	2.20	0.57
1:A:211:MET:HG3	1:A:259:PHE:CE2	2.39	0.57
1:D:211:MET:HG3	1:D:259:PHE:CE2	2.40	0.57
1:D:289:GLY:O	1:D:292:ILE:HD11	2.05	0.57
1:E:211:MET:HG3	1:E:259:PHE:CE2	2.40	0.57
1:D:258:GLU:HG3	1:D:259:PHE:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ARG:HD2	1:A:311:ILE:HB	1.87	0.56
1:C:289:GLY:O	1:C:292:ILE:HD11	2.05	0.56
1:B:303:ARG:HD2	1:B:311:ILE:HB	1.88	0.56
1:F:289:GLY:O	1:F:292:ILE:HD11	2.06	0.56
1:B:289:GLY:O	1:B:292:ILE:HD11	2.05	0.56
1:C:114:GLN:HG2	1:C:320:LEU:HD23	1.88	0.56
1:F:223:SER:O	1:F:226:ALA:N	2.34	0.56
1:F:235:ARG:H	1:F:235:ARG:HE	1.51	0.56
1:B:129:PHE:HB3	1:C:293:ALA:HB1	1.88	0.56
1:A:211:MET:SD	1:A:211:MET:N	2.69	0.56
1:A:258:GLU:HG3	1:A:259:PHE:N	2.20	0.55
1:F:211:MET:HG3	1:F:259:PHE:CE2	2.42	0.55
1:C:223:SER:O	1:C:226:ALA:N	2.34	0.55
1:E:235:ARG:H	1:E:235:ARG:HE	1.54	0.55
1:G:114:GLN:HG2	1:G:320:LEU:HD23	1.88	0.55
1:C:129:PHE:HB3	1:D:293:ALA:HB1	1.88	0.55
1:F:123:THR:O	1:F:264:VAL:HA	2.07	0.55
1:F:124:GLU:HB2	1:F:265:ILE:O	2.06	0.55
1:G:207:ALA:C	1:G:211:MET:SD	2.85	0.55
1:A:207:ALA:C	1:A:211:MET:SD	2.85	0.55
1:C:211:MET:SD	1:C:211:MET:N	2.69	0.55
1:E:303:ARG:HD2	1:E:311:ILE:HB	1.89	0.55
1:D:129:PHE:HB3	1:E:293:ALA:HB1	1.88	0.55
1:D:158:MET:SD	1:D:219:LEU:HG	2.47	0.55
1:B:211:MET:HG3	1:B:259:PHE:CE2	2.43	0.54
1:B:123:THR:O	1:B:264:VAL:HA	2.07	0.54
1:A:123:THR:O	1:A:264:VAL:HA	2.08	0.54
1:A:299:ARG:HB2	1:A:316:ASP:H	1.72	0.54
1:F:114:GLN:HG2	1:F:320:LEU:HD23	1.89	0.54
1:E:289:GLY:O	1:E:292:ILE:HD11	2.07	0.54
1:B:211:MET:SD	1:B:211:MET:N	2.69	0.54
1:E:123:THR:O	1:E:264:VAL:HA	2.08	0.54
1:F:188:ASN:OD1	1:F:188:ASN:N	2.41	0.54
1:C:158:MET:SD	1:C:219:LEU:HG	2.48	0.54
1:A:124:GLU:HB2	1:A:265:ILE:O	2.08	0.54
1:B:207:ALA:C	1:B:211:MET:SD	2.85	0.54
1:G:188:ASN:OD1	1:G:188:ASN:N	2.40	0.54
1:A:235:ARG:H	1:A:235:ARG:HE	1.54	0.53
1:E:188:ASN:OD1	1:E:188:ASN:N	2.41	0.53
1:F:60:LEU:O	1:F:63:ILE:HG12	2.08	0.53
1:A:129:PHE:HB3	1:B:293:ALA:HB1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASN:OD1	1:A:188:ASN:N	2.41	0.53
1:C:124:GLU:HB2	1:C:265:ILE:O	2.08	0.53
1:A:289:GLY:O	1:A:292:ILE:HD11	2.08	0.53
1:B:114:GLN:HG2	1:B:320:LEU:HD23	1.91	0.53
1:E:158:MET:SD	1:E:219:LEU:HG	2.48	0.53
1:B:188:ASN:OD1	1:B:188:ASN:N	2.41	0.52
1:C:211:MET:CG	1:C:259:PHE:CE2	2.93	0.52
1:A:119:THR:HB	1:A:262:ALA:HB2	1.90	0.52
1:G:211:MET:HG3	1:G:259:PHE:CE2	2.44	0.52
1:C:188:ASN:OD1	1:C:188:ASN:N	2.41	0.52
1:G:123:THR:O	1:G:264:VAL:HA	2.10	0.52
1:C:123:THR:O	1:C:264:VAL:HA	2.08	0.52
1:D:188:ASN:OD1	1:D:188:ASN:N	2.41	0.52
1:A:158:MET:SD	1:A:219:LEU:HG	2.50	0.52
1:E:60:LEU:O	1:E:63:ILE:HG12	2.10	0.52
1:D:102:ILE:O	1:D:116:GLY:HA3	2.09	0.52
1:B:102:ILE:O	1:B:116:GLY:HA3	2.10	0.51
1:A:157:ALA:HB3	1:A:189:VAL:HG22	1.93	0.51
1:C:60:LEU:O	1:C:63:ILE:HG12	2.10	0.51
1:C:207:ALA:C	1:C:211:MET:SD	2.85	0.51
1:D:159:TYR:HE1	1:D:222:ASP:HB2	1.76	0.51
1:G:159:TYR:HE1	1:G:222:ASP:HB2	1.76	0.51
1:A:114:GLN:HG2	1:A:320:LEU:HD23	1.93	0.51
1:E:211:MET:CG	1:E:259:PHE:CE2	2.93	0.51
1:A:211:MET:CG	1:A:259:PHE:CE2	2.94	0.51
1:B:158:MET:SD	1:B:219:LEU:HG	2.50	0.51
1:C:303:ARG:HD2	1:C:311:ILE:HB	1.93	0.51
1:D:303:ARG:HD2	1:D:311:ILE:HB	1.93	0.51
1:B:211:MET:CG	1:B:259:PHE:CE2	2.94	0.51
1:D:211:MET:CG	1:D:259:PHE:CE2	2.94	0.51
1:G:60:LEU:O	1:G:63:ILE:HG12	2.10	0.51
1:C:159:TYR:HE1	1:C:222:ASP:HB2	1.75	0.51
1:D:207:ALA:C	1:D:211:MET:SD	2.85	0.51
1:B:60:LEU:O	1:B:63:ILE:HG12	2.11	0.51
1:D:114:GLN:HG2	1:D:320:LEU:HD23	1.92	0.51
1:D:60:LEU:O	1:D:63:ILE:HG12	2.11	0.50
1:F:303:ARG:HD2	1:F:311:ILE:HB	1.93	0.50
1:F:129:PHE:HB3	1:G:293:ALA:HB1	1.93	0.50
1:A:60:LEU:O	1:A:63:ILE:HG12	2.12	0.50
1:D:123:THR:O	1:D:264:VAL:HA	2.12	0.50
1:E:207:ALA:C	1:E:211:MET:SD	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:ILE:O	1:E:116:GLY:HA3	2.11	0.50
1:E:119:THR:HB	1:E:262:ALA:HB2	1.93	0.50
1:F:211:MET:CG	1:F:259:PHE:CE2	2.95	0.50
1:A:102:ILE:O	1:A:116:GLY:HA3	2.12	0.50
1:C:102:ILE:O	1:C:116:GLY:HA3	2.12	0.50
1:D:157:ALA:HB3	1:D:189:VAL:HG22	1.94	0.50
1:E:114:GLN:HG2	1:E:320:LEU:HD23	1.94	0.50
1:F:207:ALA:C	1:F:211:MET:SD	2.85	0.50
1:B:157:ALA:HB3	1:B:189:VAL:HG22	1.94	0.49
1:A:235:ARG:HE	1:A:235:ARG:N	2.10	0.49
1:E:144:CYS:SG	1:E:157:ALA:HB2	2.53	0.49
1:G:235:ARG:HE	1:G:235:ARG:N	2.10	0.49
1:B:235:ARG:HE	1:B:235:ARG:N	2.10	0.49
1:G:211:MET:CG	1:G:259:PHE:CE2	2.96	0.49
1:D:157:ALA:O	1:D:189:VAL:HA	2.13	0.49
1:A:49:VAL:HA	1:A:52:VAL:HG12	1.95	0.49
1:B:229:ARG:CZ	1:C:291:ILE:HD11	2.43	0.49
1:F:157:ALA:HB3	1:F:189:VAL:HG22	1.95	0.49
1:C:235:ARG:HE	1:C:235:ARG:N	2.10	0.49
1:E:157:ALA:HB3	1:E:189:VAL:HG22	1.94	0.49
1:B:34:ASN:OD1	1:B:34:ASN:N	2.46	0.48
1:C:34:ASN:N	1:C:34:ASN:OD1	2.46	0.48
1:D:66:ILE:HG22	1:D:69:ALA:H	1.77	0.48
1:D:144:CYS:SG	1:D:157:ALA:HB2	2.53	0.48
1:F:235:ARG:HE	1:F:235:ARG:N	2.10	0.48
1:G:157:ALA:O	1:G:189:VAL:HA	2.13	0.48
1:G:303:ARG:HD2	1:G:311:ILE:HB	1.95	0.48
1:F:119:THR:HB	1:F:262:ALA:HB2	1.94	0.48
1:G:144:CYS:SG	1:G:157:ALA:HB2	2.53	0.48
1:D:235:ARG:HE	1:D:235:ARG:N	2.10	0.48
1:E:34:ASN:N	1:E:34:ASN:OD1	2.46	0.48
1:E:157:ALA:O	1:E:189:VAL:HA	2.13	0.48
1:A:66:ILE:HG22	1:A:69:ALA:H	1.77	0.48
1:A:124:GLU:OE1	1:A:299:ARG:HD3	2.14	0.48
1:F:159:TYR:HE1	1:F:222:ASP:HB2	1.79	0.48
1:G:34:ASN:OD1	1:G:34:ASN:N	2.46	0.48
1:A:293:ALA:HA	1:A:299:ARG:HH12	1.79	0.48
1:B:119:THR:HB	1:B:262:ALA:HB2	1.96	0.48
1:D:34:ASN:OD1	1:D:34:ASN:N	2.46	0.48
1:B:159:TYR:HE1	1:B:222:ASP:HB2	1.78	0.48
1:A:272:GLN:O	1:A:272:GLN:NE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:CYS:SG	1:B:157:ALA:HB2	2.54	0.48
1:E:66:ILE:HG22	1:E:69:ALA:H	1.78	0.48
1:F:35:ALA:O	1:F:39:LYS:HB2	2.14	0.48
1:D:126:PHE:HB3	1:D:267:ASN:HB3	1.95	0.47
1:F:102:ILE:O	1:F:116:GLY:HA3	2.13	0.47
1:F:147:PRO:HG2	1:F:150:ARG:HB2	1.96	0.47
1:G:35:ALA:O	1:G:39:LYS:HB2	2.14	0.47
1:G:102:ILE:O	1:G:116:GLY:HA3	2.13	0.47
1:C:157:ALA:HB3	1:C:189:VAL:HG22	1.95	0.47
1:D:119:THR:HB	1:D:262:ALA:HB2	1.95	0.47
1:A:35:ALA:O	1:A:39:LYS:HB2	2.15	0.47
1:E:235:ARG:HE	1:E:235:ARG:N	2.11	0.47
1:A:34:ASN:N	1:A:34:ASN:OD1	2.46	0.47
1:A:144:CYS:SG	1:A:157:ALA:HB2	2.54	0.47
1:A:157:ALA:O	1:A:189:VAL:HA	2.13	0.47
1:C:35:ALA:O	1:C:39:LYS:HB2	2.14	0.47
1:E:35:ALA:O	1:E:39:LYS:HB2	2.14	0.47
1:F:66:ILE:HG22	1:F:69:ALA:H	1.78	0.47
1:B:157:ALA:O	1:B:189:VAL:HA	2.14	0.47
1:F:144:CYS:SG	1:F:157:ALA:HB2	2.54	0.47
1:G:66:ILE:HG22	1:G:69:ALA:H	1.78	0.47
1:A:147:PRO:HG2	1:A:150:ARG:HB2	1.97	0.47
1:B:35:ALA:O	1:B:39:LYS:HB2	2.14	0.47
1:C:144:CYS:SG	1:C:157:ALA:HB2	2.54	0.47
1:G:147:PRO:HG2	1:G:150:ARG:HB2	1.97	0.47
1:C:66:ILE:HG22	1:C:69:ALA:H	1.78	0.47
1:C:157:ALA:O	1:C:189:VAL:HA	2.14	0.47
1:C:229:ARG:CZ	1:D:291:ILE:HD11	2.45	0.47
1:D:35:ALA:O	1:D:39:LYS:HB2	2.14	0.47
1:F:34:ASN:N	1:F:34:ASN:OD1	2.47	0.47
1:G:157:ALA:HB3	1:G:189:VAL:HG22	1.96	0.47
1:G:208:SER:CA	1:G:211:MET:SD	3.03	0.47
1:B:126:PHE:HB3	1:B:267:ASN:HB3	1.95	0.47
1:D:147:PRO:HG2	1:D:150:ARG:HB2	1.97	0.47
1:B:66:ILE:HG22	1:B:69:ALA:H	1.79	0.47
1:C:147:PRO:HG2	1:C:150:ARG:HB2	1.97	0.47
1:A:229:ARG:HH22	1:A:270:VAL:HG23	1.80	0.46
1:E:147:PRO:HG2	1:E:150:ARG:HB2	1.98	0.46
1:A:28:LEU:HD13	1:A:77:GLU:HB2	1.98	0.46
1:A:208:SER:CA	1:A:211:MET:SD	3.04	0.46
1:E:126:PHE:HB3	1:E:267:ASN:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:PHE:HB3	1:A:267:ASN:HB3	1.96	0.46
1:E:208:SER:CA	1:E:211:MET:SD	3.04	0.46
1:B:147:PRO:HG2	1:B:150:ARG:HB2	1.98	0.46
1:C:223:SER:O	1:C:224:ALA:C	2.55	0.46
1:C:126:PHE:HB3	1:C:267:ASN:HB3	1.97	0.46
1:D:208:SER:CA	1:D:211:MET:SD	3.04	0.46
1:F:158:MET:SD	1:F:219:LEU:HG	2.56	0.46
1:C:208:SER:CA	1:C:211:MET:SD	3.04	0.46
1:D:28:LEU:HD13	1:D:77:GLU:HB2	1.97	0.46
1:G:119:THR:HB	1:G:262:ALA:HB2	1.98	0.46
1:B:223:SER:O	1:B:224:ALA:C	2.54	0.45
1:F:125:MET:HB3	1:F:300:LEU:HD12	1.98	0.45
1:G:290:ASN:O	1:G:293:ALA:HB3	2.16	0.45
1:G:28:LEU:HD13	1:G:77:GLU:HB2	1.98	0.45
1:G:126:PHE:HB3	1:G:267:ASN:HB3	1.96	0.45
1:B:71:ALA:O	1:B:74:ILE:HG22	2.16	0.45
1:D:223:SER:O	1:D:224:ALA:C	2.55	0.45
1:G:245:LEU:HD21	1:G:292:ILE:HG23	1.98	0.45
1:E:223:SER:O	1:E:224:ALA:C	2.55	0.45
1:F:208:SER:CA	1:F:211:MET:SD	3.04	0.45
1:F:223:SER:O	1:F:224:ALA:C	2.55	0.45
1:B:245:LEU:HD21	1:B:292:ILE:HG23	1.98	0.45
1:C:28:LEU:HD13	1:C:77:GLU:HB2	1.98	0.45
1:D:245:LEU:HD21	1:D:292:ILE:HG23	1.99	0.45
1:E:159:TYR:HE1	1:E:222:ASP:HB2	1.81	0.45
1:F:126:PHE:HB3	1:F:267:ASN:HB3	1.98	0.45
1:A:71:ALA:O	1:A:74:ILE:HG22	2.17	0.45
1:B:208:SER:CA	1:B:211:MET:SD	3.04	0.45
1:C:71:ALA:O	1:C:74:ILE:HG22	2.17	0.45
1:E:49:VAL:HA	1:E:52:VAL:HG12	1.99	0.45
1:G:223:SER:O	1:G:224:ALA:C	2.55	0.44
1:D:59:GLU:HA	1:D:62:ASN:ND2	2.33	0.44
1:C:49:VAL:HA	1:C:52:VAL:HG12	2.00	0.44
1:D:71:ALA:O	1:D:74:ILE:HG22	2.17	0.44
1:E:71:ALA:O	1:E:74:ILE:HG22	2.17	0.44
1:A:229:ARG:NH2	1:A:270:VAL:HG23	2.32	0.44
1:C:272:GLN:O	1:C:272:GLN:NE2	2.49	0.44
1:B:272:GLN:O	1:B:272:GLN:NE2	2.49	0.44
1:D:49:VAL:HA	1:D:52:VAL:HG12	2.00	0.44
1:D:291:ILE:HD12	1:D:291:ILE:HA	1.85	0.44
1:E:133:LYS:HE2	1:E:133:LYS:HB2	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:SER:O	1:A:224:ALA:C	2.55	0.44
1:E:247:ARG:HG3	1:E:247:ARG:HH11	1.83	0.44
1:F:71:ALA:O	1:F:74:ILE:HG22	2.18	0.44
2:D:600:ANP:H8	1:E:317:SER:O	2.18	0.43
1:B:49:VAL:HA	1:B:52:VAL:HG12	2.00	0.43
1:B:59:GLU:HA	1:B:62:ASN:ND2	2.33	0.43
1:E:28:LEU:HD13	1:E:77:GLU:HB2	1.99	0.43
1:F:49:VAL:HA	1:F:52:VAL:HG12	2.00	0.43
1:B:291:ILE:HD12	1:B:291:ILE:HA	1.73	0.43
1:F:157:ALA:O	1:F:189:VAL:HA	2.18	0.43
1:G:49:VAL:HA	1:G:52:VAL:HG12	2.00	0.43
1:C:220:ILE:H	1:C:220:ILE:HG12	1.74	0.43
1:F:28:LEU:HD13	1:F:77:GLU:HB2	1.99	0.43
1:C:119:THR:HB	1:C:262:ALA:HB2	1.99	0.43
1:E:59:GLU:HA	1:E:62:ASN:ND2	2.33	0.43
1:G:59:GLU:HA	1:G:62:ASN:ND2	2.33	0.43
1:G:133:LYS:HE2	1:G:133:LYS:HB2	1.83	0.43
1:G:291:ILE:HD12	1:G:291:ILE:HA	1.75	0.43
1:A:245:LEU:HD21	1:A:292:ILE:HG23	2.01	0.43
1:C:59:GLU:HA	1:C:62:ASN:ND2	2.33	0.43
1:D:272:GLN:O	1:D:272:GLN:NE2	2.50	0.43
1:E:125:MET:HB3	1:E:300:LEU:HD12	1.99	0.43
1:F:59:GLU:HA	1:F:62:ASN:ND2	2.33	0.43
1:G:71:ALA:O	1:G:74:ILE:HG22	2.18	0.43
1:A:59:GLU:HA	1:A:62:ASN:ND2	2.34	0.43
1:A:293:ALA:HA	1:A:299:ARG:NH1	2.33	0.43
1:G:258:GLU:HG3	1:G:259:PHE:H	1.84	0.43
1:D:112:LEU:HG	1:D:325:ALA:HB2	2.00	0.42
1:B:28:LEU:HD13	1:B:77:GLU:HB2	2.01	0.42
1:C:210:MET:CE	1:C:210:MET:HA	2.50	0.42
1:E:245:LEU:HD21	1:E:292:ILE:HG23	2.01	0.42
1:A:220:ILE:H	1:A:220:ILE:HG12	1.74	0.42
1:B:258:GLU:HG3	1:B:259:PHE:H	1.85	0.42
1:F:168:PRO:HD2	1:G:96:ARG:HD3	2.01	0.42
1:G:124:GLU:OE1	1:G:299:ARG:HD3	2.20	0.42
1:A:229:ARG:CZ	1:B:291:ILE:HD11	2.49	0.42
1:A:292:ILE:HD12	1:A:293:ALA:N	2.35	0.42
2:C:600:ANP:H8	1:D:317:SER:O	2.19	0.42
1:F:247:ARG:HG3	1:F:247:ARG:HH11	1.83	0.42
1:B:210:MET:HA	1:B:210:MET:CE	2.50	0.42
1:D:247:ARG:HG3	1:D:247:ARG:HH11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:LEU:HG	1:E:325:ALA:HB2	2.01	0.42
2:F:600:ANP:H8	1:G:317:SER:O	2.20	0.42
1:A:112:LEU:HG	1:A:325:ALA:HB2	2.01	0.42
1:A:210:MET:CE	1:A:210:MET:HA	2.50	0.42
1:B:133:LYS:HE2	1:B:133:LYS:HB2	1.85	0.42
1:C:245:LEU:HD21	1:C:292:ILE:HG23	2.01	0.42
1:E:220:ILE:H	1:E:220:ILE:HG12	1.73	0.42
1:A:159:TYR:HE1	1:A:222:ASP:HB2	1.85	0.42
1:G:292:ILE:HD12	1:G:293:ALA:N	2.35	0.42
1:C:168:PRO:HD2	1:D:96:ARG:HD3	2.02	0.42
1:D:229:ARG:CZ	1:E:291:ILE:HD11	2.50	0.42
1:B:211:MET:HG2	1:B:259:PHE:CE2	2.55	0.41
1:C:291:ILE:HD12	1:C:291:ILE:HA	1.83	0.41
1:E:168:PRO:HD2	1:F:96:ARG:HD3	2.02	0.41
1:G:59:GLU:HA	1:G:62:ASN:HD21	1.85	0.41
1:G:125:MET:HB3	1:G:300:LEU:HD12	2.01	0.41
1:D:168:PRO:HD2	1:E:96:ARG:HD3	2.02	0.41
1:E:258:GLU:HG3	1:E:259:PHE:H	1.85	0.41
1:F:108:GLU:OE1	1:F:108:GLU:HA	2.21	0.41
1:B:30:GLN:OE1	1:B:30:GLN:HA	2.21	0.41
1:D:249:LEU:HD21	1:D:292:ILE:HA	2.03	0.41
1:D:210:MET:HA	1:D:210:MET:CE	2.50	0.41
1:E:30:GLN:OE1	1:E:30:GLN:HA	2.21	0.41
1:F:220:ILE:H	1:F:220:ILE:HG12	1.74	0.41
1:G:108:GLU:HA	1:G:108:GLU:OE1	2.21	0.41
1:G:210:MET:HA	1:G:210:MET:CE	2.50	0.41
1:E:210:MET:HA	1:E:210:MET:CE	2.50	0.41
2:E:600:ANP:H8	1:F:317:SER:O	2.21	0.41
1:C:247:ARG:HH11	1:C:247:ARG:HG3	1.86	0.41
1:D:258:GLU:HG3	1:D:259:PHE:H	1.85	0.41
1:F:59:GLU:HA	1:F:62:ASN:HD21	1.86	0.41
1:F:258:GLU:HG3	1:F:259:PHE:H	1.85	0.41
1:C:159:TYR:CE1	1:C:222:ASP:HB2	2.55	0.41
1:D:193:ARG:HH21	1:E:257:ASP:CG	2.24	0.41
1:G:220:ILE:H	1:G:220:ILE:HG12	1.75	0.41
1:A:30:GLN:OE1	1:A:30:GLN:HA	2.21	0.41
1:B:108:GLU:HA	1:B:108:GLU:OE1	2.21	0.41
2:B:600:ANP:H8	1:C:317:SER:O	2.21	0.41
1:C:125:MET:HB3	1:C:300:LEU:HD12	2.02	0.41
1:D:293:ALA:HA	1:D:299:ARG:NH1	2.36	0.41
1:E:59:GLU:HA	1:E:62:ASN:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:LEU:HG	1:G:325:ALA:HB2	2.01	0.41
1:A:59:GLU:HA	1:A:62:ASN:HD21	1.86	0.41
1:A:193:ARG:HH21	1:B:257:ASP:CG	2.25	0.41
1:C:206:GLN:OE1	1:C:206:GLN:HA	2.21	0.41
1:C:211:MET:HG2	1:C:259:PHE:CE2	2.56	0.41
1:E:108:GLU:HA	1:E:108:GLU:OE1	2.21	0.41
1:E:206:GLN:OE1	1:E:206:GLN:HA	2.21	0.41
1:F:30:GLN:OE1	1:F:30:GLN:HA	2.21	0.41
1:F:112:LEU:HG	1:F:325:ALA:HB2	2.01	0.41
1:G:30:GLN:OE1	1:G:30:GLN:HA	2.21	0.41
1:G:170:ARG:HH21	1:G:170:ARG:HA	1.85	0.41
1:G:249:LEU:HD21	1:G:292:ILE:HA	2.02	0.41
1:B:59:GLU:HA	1:B:62:ASN:HD21	1.86	0.41
1:C:290:ASN:O	1:C:293:ALA:HB3	2.22	0.41
1:D:59:GLU:HA	1:D:62:ASN:HD21	1.85	0.41
1:D:108:GLU:OE1	1:D:108:GLU:HA	2.21	0.41
1:G:293:ALA:HA	1:G:299:ARG:NH1	2.36	0.41
1:A:92:PHE:O	1:A:95:ARG:HB2	2.21	0.40
1:A:108:GLU:OE1	1:A:108:GLU:HA	2.21	0.40
1:C:108:GLU:OE1	1:C:108:GLU:HA	2.21	0.40
1:D:292:ILE:HD12	1:D:293:ALA:N	2.36	0.40
1:E:292:ILE:H	1:E:292:ILE:HG13	1.68	0.40
1:G:227:LEU:HD12	1:G:227:LEU:HA	2.01	0.40
1:B:125:MET:HB3	1:B:300:LEU:HD12	2.02	0.40
1:B:92:PHE:O	1:B:95:ARG:HB2	2.22	0.40
1:C:92:PHE:O	1:C:95:ARG:HB2	2.22	0.40
1:C:292:ILE:HD12	1:C:293:ALA:N	2.35	0.40
1:F:210:MET:HA	1:F:210:MET:CE	2.51	0.40
1:G:272:GLN:O	1:G:272:GLN:NE2	2.55	0.40
1:A:168:PRO:HD2	1:B:96:ARG:HD3	2.02	0.40
1:D:290:ASN:O	1:D:293:ALA:HB3	2.22	0.40
1:B:293:ALA:HA	1:B:299:ARG:NH1	2.37	0.40
1:C:59:GLU:HA	1:C:62:ASN:HD21	1.86	0.40
1:D:230:THR:HG22	1:E:246:ALA:HB1	2.04	0.40
1:E:229:ARG:CZ	1:F:291:ILE:HD11	2.51	0.40
1:E:293:ALA:HA	1:E:299:ARG:NH1	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	307/339 (91%)	263 (86%)	42 (14%)	2 (1%)	22	62
1	B	307/339 (91%)	263 (86%)	42 (14%)	2 (1%)	22	62
1	C	307/339 (91%)	265 (86%)	39 (13%)	3 (1%)	15	54
1	D	307/339 (91%)	264 (86%)	41 (13%)	2 (1%)	22	62
1	E	307/339 (91%)	264 (86%)	41 (13%)	2 (1%)	22	62
1	F	307/339 (91%)	265 (86%)	40 (13%)	2 (1%)	22	62
1	G	307/339 (91%)	266 (87%)	39 (13%)	2 (1%)	22	62
All	All	2149/2373 (91%)	1850 (86%)	284 (13%)	15 (1%)	26	62

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	ALA
1	A	337	ALA
1	B	224	ALA
1	B	337	ALA
1	C	224	ALA
1	C	337	ALA
1	D	224	ALA
1	D	337	ALA
1	E	224	ALA
1	E	337	ALA
1	F	224	ALA
1	F	337	ALA
1	G	224	ALA
1	G	337	ALA
1	C	88	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	229/269 (85%)	175 (76%)	54 (24%)	1	5
1	B	229/269 (85%)	174 (76%)	55 (24%)	0	5
1	C	229/269 (85%)	175 (76%)	54 (24%)	1	5
1	D	229/269 (85%)	175 (76%)	54 (24%)	1	5
1	E	229/269 (85%)	173 (76%)	56 (24%)	0	4
1	F	229/269 (85%)	173 (76%)	56 (24%)	0	4
1	G	229/269 (85%)	177 (77%)	52 (23%)	1	6
All	All	1603/1883 (85%)	1222 (76%)	381 (24%)	2	5

All (381) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	PHE
1	A	25	ILE
1	A	28	LEU
1	A	29	GLU
1	A	34	ASN
1	A	39	LYS
1	A	52	VAL
1	A	54	TYR
1	A	58	LYS
1	A	59	GLU
1	A	60	LEU
1	A	61	ILE
1	A	77	GLU
1	A	81	LEU
1	A	103	THR
1	A	107	LYS
1	A	108	GLU
1	A	111	LYS
1	A	112	LEU
1	A	119	THR

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Mol	Chain	Res	Type
1	A	130	ARG
1	A	135	GLN
1	A	144	CYS
1	A	146	LEU
1	A	154	GLU
1	A	158	MET
1	A	159	TYR
1	A	161	ASP
1	A	177	ARG
1	A	188	ASN
1	A	203	LEU
1	A	204	LEU
1	A	206	GLN
1	A	211	MET
1	A	213	GLU
1	A	220	ILE
1	A	229	ARG
1	A	235	ARG
1	A	238	LEU
1	A	241	ARG
1	A	247	ARG
1	A	255	LEU
1	A	257	ASP
1	A	272	GLN
1	A	290	ASN
1	A	291	ILE
1	A	298	THR
1	A	299	ARG
1	A	300	LEU
1	A	301	TYR
1	A	303	ARG
1	A	316	ASP
1	A	320	LEU
1	A	336	ASP
1	B	20	PHE
1	B	25	ILE
1	B	28	LEU
1	B	29	GLU
1	B	34	ASN
1	B	39	LYS
1	B	52	VAL
1	B	58	LYS

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Mol	Chain	Res	Type
1	B	59	GLU
1	B	60	LEU
1	B	61	ILE
1	B	77	GLU
1	B	81	LEU
1	B	103	THR
1	B	107	LYS
1	B	108	GLU
1	B	111	LYS
1	B	112	LEU
1	B	119	THR
1	B	130	ARG
1	B	135	GLN
1	B	144	CYS
1	B	146	LEU
1	B	154	GLU
1	B	158	MET
1	B	159	TYR
1	B	161	ASP
1	B	177	ARG
1	B	188	ASN
1	B	203	LEU
1	B	204	LEU
1	B	206	GLN
1	B	211	MET
1	B	213	GLU
1	B	220	ILE
1	B	229	ARG
1	B	235	ARG
1	B	238	LEU
1	B	241	ARG
1	B	247	ARG
1	B	255	LEU
1	B	257	ASP
1	B	270	VAL
1	B	272	GLN
1	B	290	ASN
1	B	291	ILE
1	B	298	THR
1	B	299	ARG
1	B	300	LEU
1	B	301	TYR

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Mol	Chain	Res	Type
1	B	303	ARG
1	B	316	ASP
1	B	319	CYS
1	B	320	LEU
1	B	336	ASP
1	C	20	PHE
1	C	25	ILE
1	C	28	LEU
1	C	29	GLU
1	C	34	ASN
1	C	39	LYS
1	C	52	VAL
1	C	58	LYS
1	C	59	GLU
1	C	60	LEU
1	C	61	ILE
1	C	77	GLU
1	C	81	LEU
1	C	103	THR
1	C	107	LYS
1	C	108	GLU
1	C	111	LYS
1	C	112	LEU
1	C	130	ARG
1	C	135	GLN
1	C	144	CYS
1	C	146	LEU
1	C	154	GLU
1	C	158	MET
1	C	159	TYR
1	C	161	ASP
1	C	177	ARG
1	C	188	ASN
1	C	203	LEU
1	C	204	LEU
1	C	206	GLN
1	C	211	MET
1	C	213	GLU
1	C	219	LEU
1	C	220	ILE
1	C	229	ARG
1	C	235	ARG

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Mol	Chain	Res	Type
1	C	238	LEU
1	C	241	ARG
1	C	247	ARG
1	C	255	LEU
1	C	257	ASP
1	C	272	GLN
1	C	290	ASN
1	C	291	ILE
1	C	298	THR
1	C	299	ARG
1	C	300	LEU
1	C	301	TYR
1	C	303	ARG
1	C	316	ASP
1	C	319	CYS
1	C	320	LEU
1	C	336	ASP
1	D	20	PHE
1	D	25	ILE
1	D	28	LEU
1	D	29	GLU
1	D	34	ASN
1	D	39	LYS
1	D	52	VAL
1	D	58	LYS
1	D	59	GLU
1	D	60	LEU
1	D	61	ILE
1	D	77	GLU
1	D	81	LEU
1	D	103	THR
1	D	107	LYS
1	D	108	GLU
1	D	111	LYS
1	D	112	LEU
1	D	130	ARG
1	D	135	GLN
1	D	144	CYS
1	D	146	LEU
1	D	154	GLU
1	D	158	MET
1	D	159	TYR

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Mol	Chain	Res	Type
1	D	161	ASP
1	D	177	ARG
1	D	188	ASN
1	D	203	LEU
1	D	204	LEU
1	D	206	GLN
1	D	211	MET
1	D	213	GLU
1	D	220	ILE
1	D	229	ARG
1	D	235	ARG
1	D	238	LEU
1	D	241	ARG
1	D	247	ARG
1	D	255	LEU
1	D	257	ASP
1	D	272	GLN
1	D	290	ASN
1	D	291	ILE
1	D	298	THR
1	D	299	ARG
1	D	300	LEU
1	D	301	TYR
1	D	303	ARG
1	D	315	TYR
1	D	316	ASP
1	D	319	CYS
1	D	320	LEU
1	D	336	ASP
1	E	20	PHE
1	E	25	ILE
1	E	28	LEU
1	E	29	GLU
1	E	34	ASN
1	E	39	LYS
1	E	52	VAL
1	E	58	LYS
1	E	59	GLU
1	E	60	LEU
1	E	61	ILE
1	E	77	GLU
1	E	81	LEU

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Mol	Chain	Res	Type
1	E	103	THR
1	E	107	LYS
1	E	108	GLU
1	E	111	LYS
1	E	112	LEU
1	E	119	THR
1	E	130	ARG
1	E	135	GLN
1	E	144	CYS
1	E	146	LEU
1	E	154	GLU
1	E	158	MET
1	E	159	TYR
1	E	161	ASP
1	E	177	ARG
1	E	188	ASN
1	E	203	LEU
1	E	204	LEU
1	E	206	GLN
1	E	211	MET
1	E	213	GLU
1	E	220	ILE
1	E	229	ARG
1	E	235	ARG
1	E	238	LEU
1	E	241	ARG
1	E	247	ARG
1	E	255	LEU
1	E	257	ASP
1	E	270	VAL
1	E	272	GLN
1	E	290	ASN
1	E	291	ILE
1	E	298	THR
1	E	299	ARG
1	E	300	LEU
1	E	301	TYR
1	E	303	ARG
1	E	315	TYR
1	E	316	ASP
1	E	319	CYS
1	E	320	LEU

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Mol	Chain	Res	Type
1	E	336	ASP
1	F	20	PHE
1	F	25	ILE
1	F	28	LEU
1	F	29	GLU
1	F	34	ASN
1	F	39	LYS
1	F	52	VAL
1	F	58	LYS
1	F	59	GLU
1	F	60	LEU
1	F	61	ILE
1	F	77	GLU
1	F	81	LEU
1	F	107	LYS
1	F	108	GLU
1	F	111	LYS
1	F	112	LEU
1	F	119	THR
1	F	130	ARG
1	F	135	GLN
1	F	144	CYS
1	F	146	LEU
1	F	154	GLU
1	F	158	MET
1	F	159	TYR
1	F	161	ASP
1	F	177	ARG
1	F	188	ASN
1	F	203	LEU
1	F	204	LEU
1	F	206	GLN
1	F	211	MET
1	F	213	GLU
1	F	219	LEU
1	F	220	ILE
1	F	229	ARG
1	F	235	ARG
1	F	238	LEU
1	F	241	ARG
1	F	247	ARG
1	F	255	LEU

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Mol	Chain	Res	Type
1	F	257	ASP
1	F	270	VAL
1	F	272	GLN
1	F	290	ASN
1	F	291	ILE
1	F	298	THR
1	F	299	ARG
1	F	300	LEU
1	F	301	TYR
1	F	303	ARG
1	F	315	TYR
1	F	316	ASP
1	F	319	CYS
1	F	320	LEU
1	F	336	ASP
1	G	20	PHE
1	G	25	ILE
1	G	28	LEU
1	G	29	GLU
1	G	34	ASN
1	G	39	LYS
1	G	52	VAL
1	G	58	LYS
1	G	59	GLU
1	G	60	LEU
1	G	61	ILE
1	G	77	GLU
1	G	81	LEU
1	G	107	LYS
1	G	108	GLU
1	G	111	LYS
1	G	112	LEU
1	G	130	ARG
1	G	135	GLN
1	G	144	CYS
1	G	146	LEU
1	G	154	GLU
1	G	158	MET
1	G	159	TYR
1	G	161	ASP
1	G	177	ARG
1	G	188	ASN

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Mol	Chain	Res	Type
1	G	203	LEU
1	G	204	LEU
1	G	206	GLN
1	G	211	MET
1	G	213	GLU
1	G	220	ILE
1	G	229	ARG
1	G	235	ARG
1	G	238	LEU
1	G	241	ARG
1	G	247	ARG
1	G	255	LEU
1	G	257	ASP
1	G	272	GLN
1	G	290	ASN
1	G	291	ILE
1	G	298	THR
1	G	299	ARG
1	G	300	LEU
1	G	301	TYR
1	G	303	ARG
1	G	316	ASP
1	G	319	CYS
1	G	320	LEU
1	G	336	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	145	GLN
1	A	294	HIS
1	B	135	GLN
1	B	145	GLN
1	B	294	HIS
1	C	135	GLN
1	C	145	GLN
1	C	294	HIS
1	D	135	GLN
1	D	145	GLN
1	D	294	HIS
1	E	135	GLN

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Mol	Chain	Res	Type
1	E	145	GLN
1	E	294	HIS
1	F	135	GLN
1	F	145	GLN
1	F	294	HIS
1	G	135	GLN
1	G	145	GLN
1	G	294	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

7 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	ANP	D	600	-	29,33,33	2.25	12 (41%)	31,52,52	2.12	11 (35%)
2	ANP	B	600	-	29,33,33	2.24	12 (41%)	31,52,52	2.14	11 (35%)
2	ANP	G	600	-	29,33,33	2.23	12 (41%)	31,52,52	2.28	13 (41%)
2	ANP	F	600	-	29,33,33	2.20	11 (37%)	31,52,52	2.10	12 (38%)
2	ANP	C	600	-	29,33,33	2.24	11 (37%)	31,52,52	2.12	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ANP	A	600	-	29,33,33	2.24	12 (41%)	31,52,52	2.13	11 (35%)
2	ANP	E	600	-	29,33,33	2.26	12 (41%)	31,52,52	2.12	11 (35%)

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
2	ANP	D	600	-	-	2/14/38/38	0/3/3/3
2	ANP	B	600	-	-	2/14/38/38	0/3/3/3
2	ANP	G	600	-	-	3/14/38/38	0/3/3/3
2	ANP	F	600	-	-	2/14/38/38	0/3/3/3
2	ANP	C	600	-	-	2/14/38/38	0/3/3/3
2	ANP	A	600	-	-	2/14/38/38	0/3/3/3
2	ANP	E	600	-	-	3/14/38/38	0/3/3/3

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	ANP	PG-N3B	5.33	1.77	1.63
2	C	600	ANP	PG-N3B	5.31	1.77	1.63
2	B	600	ANP	PG-N3B	5.29	1.77	1.63
2	E	600	ANP	PG-N3B	5.29	1.77	1.63
2	A	600	ANP	PG-N3B	5.22	1.77	1.63
2	G	600	ANP	PG-N3B	5.20	1.77	1.63
2	F	600	ANP	PG-N3B	5.09	1.76	1.63
2	D	600	ANP	PB-N3B	4.53	1.75	1.63
2	C	600	ANP	PB-N3B	4.53	1.75	1.63
2	E	600	ANP	PB-N3B	4.52	1.75	1.63
2	A	600	ANP	PB-N3B	4.51	1.75	1.63
2	B	600	ANP	PB-N3B	4.49	1.75	1.63
2	G	600	ANP	PB-N3B	4.41	1.74	1.63
2	F	600	ANP	PB-N3B	4.32	1.74	1.63
2	F	600	ANP	PG-O1G	4.22	1.52	1.46
2	E	600	ANP	PG-O1G	4.20	1.52	1.46
2	D	600	ANP	PG-O1G	4.13	1.52	1.46
2	C	600	ANP	PG-O1G	4.11	1.52	1.46
2	B	600	ANP	PG-O1G	4.11	1.52	1.46
2	A	600	ANP	PG-O1G	3.92	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	600	ANP	PG-O1G	3.91	1.52	1.46
2	G	600	ANP	C5-C4	3.69	1.50	1.40
2	B	600	ANP	C5-C4	3.53	1.50	1.40
2	C	600	ANP	C5-C4	3.53	1.50	1.40
2	E	600	ANP	C5-C4	3.52	1.50	1.40
2	D	600	ANP	C5-C4	3.52	1.50	1.40
2	D	600	ANP	PB-O3A	3.51	1.63	1.59
2	A	600	ANP	C5-C4	3.50	1.50	1.40
2	E	600	ANP	PB-O3A	3.49	1.63	1.59
2	F	600	ANP	C5-C4	3.46	1.50	1.40
2	B	600	ANP	PB-O3A	3.41	1.63	1.59
2	A	600	ANP	C2-N3	3.38	1.37	1.32
2	A	600	ANP	PB-O1B	3.37	1.51	1.46
2	B	600	ANP	C2-N3	3.37	1.37	1.32
2	C	600	ANP	C2-N3	3.37	1.37	1.32
2	G	600	ANP	PB-O3A	3.36	1.63	1.59
2	E	600	ANP	C2-N3	3.36	1.37	1.32
2	C	600	ANP	PB-O3A	3.36	1.63	1.59
2	D	600	ANP	C2-N3	3.35	1.37	1.32
2	F	600	ANP	PB-O1B	3.29	1.51	1.46
2	A	600	ANP	PB-O3A	3.28	1.63	1.59
2	F	600	ANP	C2-N3	3.26	1.37	1.32
2	D	600	ANP	PB-O1B	3.21	1.51	1.46
2	C	600	ANP	PB-O1B	3.17	1.51	1.46
2	G	600	ANP	C4-N3	3.15	1.40	1.35
2	E	600	ANP	PB-O1B	3.14	1.51	1.46
2	F	600	ANP	PB-O3A	3.10	1.63	1.59
2	G	600	ANP	PB-O1B	3.09	1.51	1.46
2	B	600	ANP	PB-O1B	3.06	1.51	1.46
2	G	600	ANP	C2-N3	2.70	1.36	1.32
2	F	600	ANP	PG-O3G	-2.44	1.50	1.56
2	B	600	ANP	PG-O3G	-2.44	1.50	1.56
2	C	600	ANP	PG-O3G	-2.44	1.50	1.56
2	E	600	ANP	PG-O3G	-2.43	1.50	1.56
2	B	600	ANP	C2-N1	2.40	1.38	1.33
2	D	600	ANP	C2-N1	2.40	1.38	1.33
2	E	600	ANP	C2-N1	2.38	1.38	1.33
2	F	600	ANP	C2-N1	2.36	1.38	1.33
2	A	600	ANP	C2-N1	2.35	1.38	1.33
2	D	600	ANP	PG-O3G	-2.35	1.50	1.56
2	C	600	ANP	C2-N1	2.35	1.38	1.33
2	A	600	ANP	PG-O3G	-2.35	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	ANP	C4-N3	2.30	1.38	1.35
2	F	600	ANP	C4-N3	2.29	1.38	1.35
2	G	600	ANP	O4'-C1'	2.28	1.44	1.41
2	G	600	ANP	PG-O3G	-2.27	1.50	1.56
2	C	600	ANP	C4-N3	2.27	1.38	1.35
2	G	600	ANP	PB-O2B	-2.26	1.50	1.56
2	D	600	ANP	C4-N3	2.26	1.38	1.35
2	B	600	ANP	C4-N3	2.24	1.38	1.35
2	A	600	ANP	O4'-C1'	2.19	1.44	1.41
2	E	600	ANP	O4'-C1'	2.18	1.44	1.41
2	E	600	ANP	C4-N3	2.15	1.38	1.35
2	B	600	ANP	PB-O2B	-2.11	1.51	1.56
2	C	600	ANP	PB-O2B	-2.10	1.51	1.56
2	B	600	ANP	O4'-C1'	2.10	1.44	1.41
2	E	600	ANP	PB-O2B	-2.09	1.51	1.56
2	A	600	ANP	PB-O2B	-2.09	1.51	1.56
2	F	600	ANP	PB-O2B	-2.08	1.51	1.56
2	D	600	ANP	PB-O2B	-2.06	1.51	1.56
2	G	600	ANP	C2-N1	2.06	1.37	1.33
2	D	600	ANP	O4'-C1'	2.03	1.43	1.41

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	600	ANP	N3-C2-N1	-5.11	120.69	128.68
2	A	600	ANP	O2B-PB-O1B	4.81	120.00	109.92
2	A	600	ANP	N3-C2-N1	-4.53	121.59	128.68
2	E	600	ANP	N3-C2-N1	-4.51	121.62	128.68
2	B	600	ANP	N3-C2-N1	-4.50	121.64	128.68
2	C	600	ANP	N3-C2-N1	-4.50	121.65	128.68
2	D	600	ANP	N3-C2-N1	-4.47	121.69	128.68
2	F	600	ANP	N3-C2-N1	-4.47	121.69	128.68
2	C	600	ANP	O2B-PB-O1B	4.46	119.27	109.92
2	B	600	ANP	O2B-PB-O1B	4.45	119.26	109.92
2	F	600	ANP	O2B-PB-O1B	4.45	119.25	109.92
2	D	600	ANP	O2B-PB-O1B	4.40	119.14	109.92
2	E	600	ANP	O2B-PB-O1B	4.40	119.14	109.92
2	G	600	ANP	O2B-PB-O1B	4.31	118.95	109.92
2	G	600	ANP	O1G-PG-N3B	-4.03	105.84	111.77
2	E	600	ANP	O3A-PB-N3B	3.72	116.92	106.59
2	D	600	ANP	O3A-PB-N3B	3.67	116.76	106.59
2	C	600	ANP	O3A-PB-N3B	3.59	116.54	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	600	ANP	O5'-C5'-C4'	3.54	121.17	108.99
2	B	600	ANP	O3A-PB-N3B	3.49	116.28	106.59
2	E	600	ANP	C3'-C2'-C1'	3.46	106.19	100.98
2	D	600	ANP	C3'-C2'-C1'	3.42	106.13	100.98
2	B	600	ANP	C3'-C2'-C1'	3.41	106.12	100.98
2	G	600	ANP	O3A-PB-N3B	3.40	116.02	106.59
2	B	600	ANP	PB-O3A-PA	-3.37	120.73	132.62
2	A	600	ANP	C3'-C2'-C1'	3.34	106.01	100.98
2	G	600	ANP	C1'-N9-C4	-3.34	120.77	126.64
2	F	600	ANP	O1G-PG-N3B	-3.34	106.86	111.77
2	F	600	ANP	PB-O3A-PA	-3.32	120.92	132.62
2	A	600	ANP	O3A-PB-N3B	3.31	115.78	106.59
2	G	600	ANP	PB-O3A-PA	-3.31	120.97	132.62
2	D	600	ANP	PB-O3A-PA	-3.30	120.99	132.62
2	C	600	ANP	PB-O3A-PA	-3.28	121.06	132.62
2	C	600	ANP	C3'-C2'-C1'	3.28	105.92	100.98
2	A	600	ANP	PB-O3A-PA	-3.28	121.08	132.62
2	F	600	ANP	C3'-C2'-C1'	3.25	105.87	100.98
2	E	600	ANP	PB-O3A-PA	-3.24	121.20	132.62
2	B	600	ANP	O1G-PG-N3B	-3.18	107.09	111.77
2	F	600	ANP	O5'-C5'-C4'	2.98	119.25	108.99
2	F	600	ANP	O3A-PB-N3B	2.97	114.83	106.59
2	D	600	ANP	O1G-PG-N3B	-2.96	107.40	111.77
2	D	600	ANP	O5'-C5'-C4'	2.96	119.18	108.99
2	A	600	ANP	O1G-PG-N3B	-2.95	107.42	111.77
2	B	600	ANP	O5'-C5'-C4'	2.95	119.16	108.99
2	C	600	ANP	O5'-C5'-C4'	2.95	119.14	108.99
2	E	600	ANP	O1G-PG-N3B	-2.95	107.43	111.77
2	G	600	ANP	C2-N1-C6	2.95	123.79	118.75
2	C	600	ANP	O1G-PG-N3B	-2.92	107.47	111.77
2	A	600	ANP	O5'-C5'-C4'	2.86	118.83	108.99
2	E	600	ANP	O5'-C5'-C4'	2.83	118.72	108.99
2	G	600	ANP	C3'-C2'-C1'	2.76	105.13	100.98
2	B	600	ANP	O2'-C2'-C3'	2.60	120.22	111.82
2	C	600	ANP	O2'-C2'-C3'	2.58	120.16	111.82
2	E	600	ANP	O2'-C2'-C3'	2.57	120.14	111.82
2	D	600	ANP	O2'-C2'-C3'	2.55	120.07	111.82
2	B	600	ANP	C2-N1-C6	2.52	123.06	118.75
2	C	600	ANP	C2-N1-C6	2.52	123.06	118.75
2	E	600	ANP	C2-N1-C6	2.52	123.06	118.75
2	F	600	ANP	O2'-C2'-C3'	2.50	119.91	111.82
2	A	600	ANP	O2'-C2'-C3'	2.50	119.90	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	600	ANP	C2-N1-C6	2.48	122.99	118.75
2	A	600	ANP	C2-N1-C6	2.46	122.97	118.75
2	G	600	ANP	O2'-C2'-C3'	2.46	119.77	111.82
2	F	600	ANP	C2-N1-C6	2.44	122.93	118.75
2	A	600	ANP	O2G-PG-O3G	2.34	113.86	107.64
2	G	600	ANP	N6-C6-N1	2.30	123.36	118.57
2	E	600	ANP	O3'-C3'-C2'	2.21	118.97	111.82
2	D	600	ANP	O3'-C3'-C2'	2.18	118.88	111.82
2	D	600	ANP	O2G-PG-O3G	2.13	113.31	107.64
2	F	600	ANP	O2G-PG-O3G	2.13	113.30	107.64
2	A	600	ANP	O3'-C3'-C2'	2.10	118.62	111.82
2	G	600	ANP	O2G-PG-O1G	2.10	118.73	113.45
2	G	600	ANP	O3'-C3'-C2'	2.09	118.58	111.82
2	F	600	ANP	O2G-PG-O1G	2.05	118.62	113.45
2	C	600	ANP	O2G-PG-O3G	2.04	113.07	107.64
2	F	600	ANP	O3'-C3'-C2'	2.03	118.39	111.82
2	B	600	ANP	O3'-C3'-C2'	2.03	118.38	111.82
2	B	600	ANP	O2G-PG-O3G	2.02	113.03	107.64
2	E	600	ANP	O2G-PG-O3G	2.01	112.98	107.64

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	ANP	PG-N3B-PB-O1B
2	B	600	ANP	PG-N3B-PB-O1B
2	C	600	ANP	PG-N3B-PB-O1B
2	D	600	ANP	PG-N3B-PB-O1B
2	E	600	ANP	PG-N3B-PB-O1B
2	F	600	ANP	PG-N3B-PB-O1B
2	G	600	ANP	PG-N3B-PB-O1B
2	G	600	ANP	O4'-C4'-C5'-O5'
2	G	600	ANP	C3'-C4'-C5'-O5'
2	F	600	ANP	O4'-C4'-C5'-O5'
2	A	600	ANP	O4'-C4'-C5'-O5'
2	D	600	ANP	O4'-C4'-C5'-O5'
2	B	600	ANP	O4'-C4'-C5'-O5'
2	C	600	ANP	O4'-C4'-C5'-O5'
2	E	600	ANP	O4'-C4'-C5'-O5'
2	E	600	ANP	C5'-O5'-PA-O1A

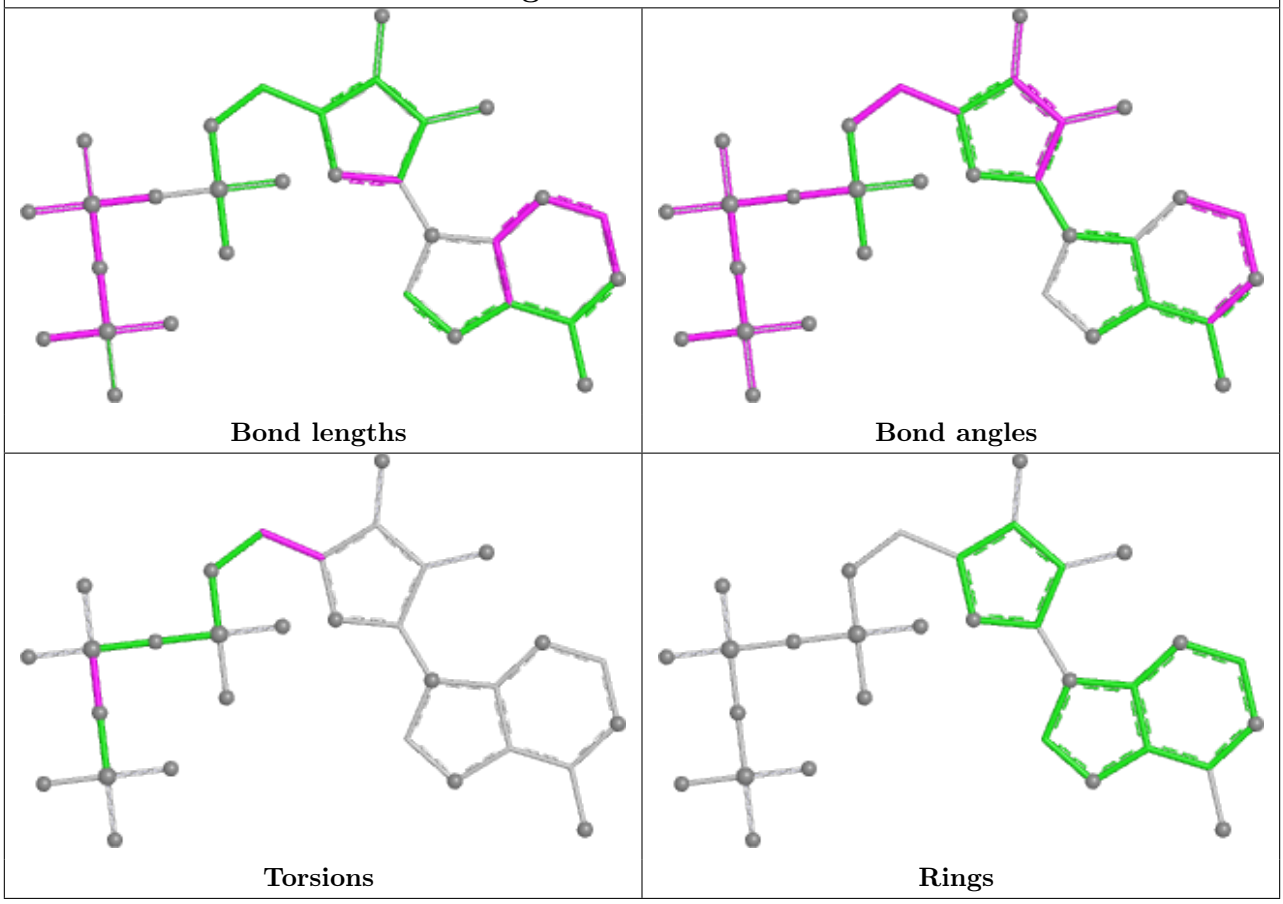
There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	600	ANP	1	0
2	B	600	ANP	1	0
2	F	600	ANP	1	0
2	C	600	ANP	1	0
2	E	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ANP D 600



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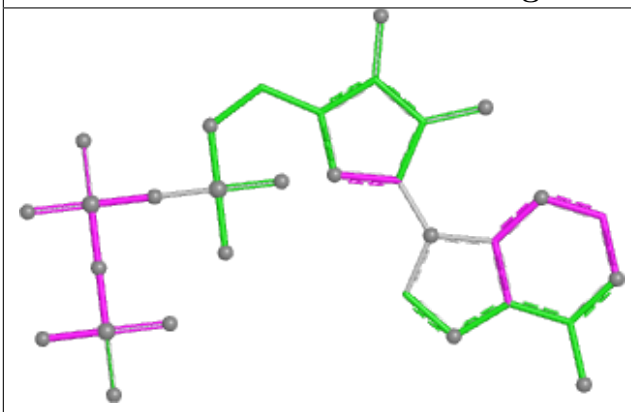
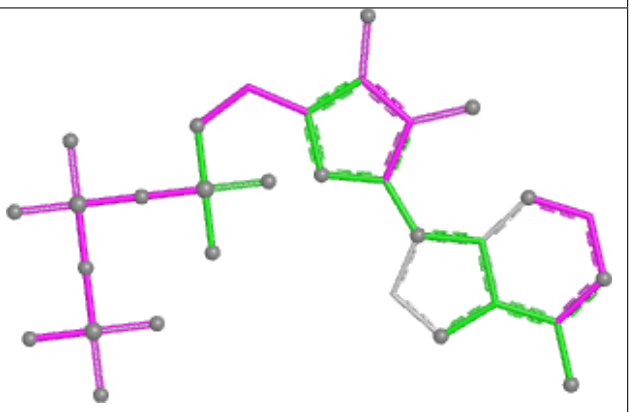
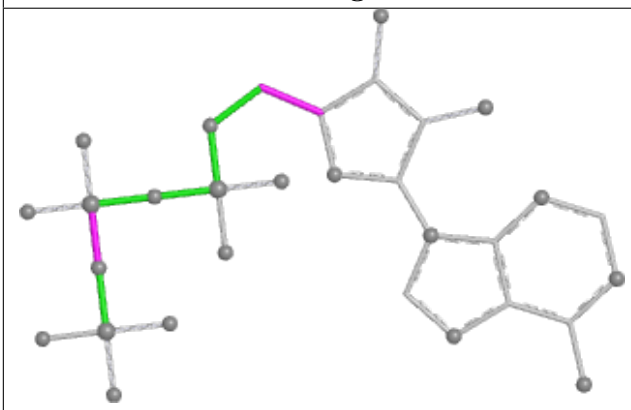
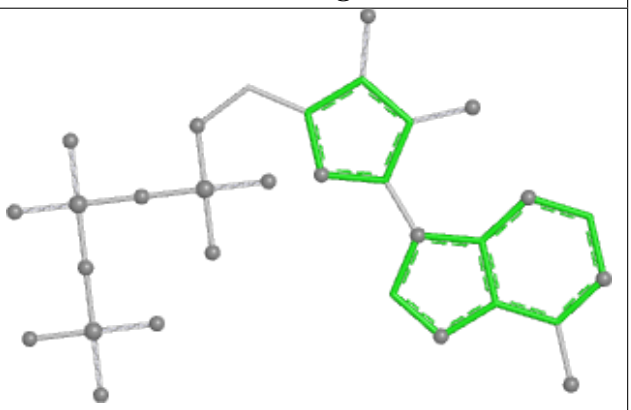
 Bond lengths	 Bond angles
 Torsions	 Rings

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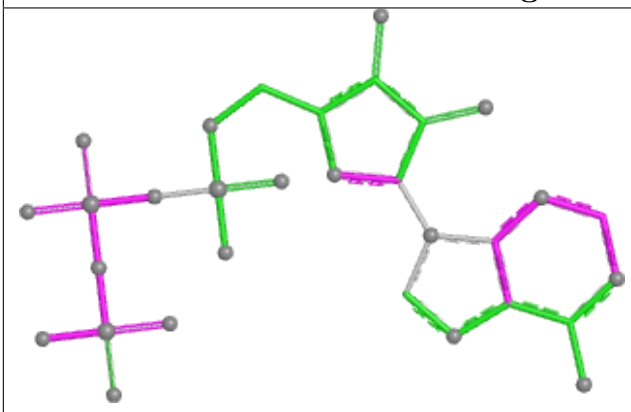
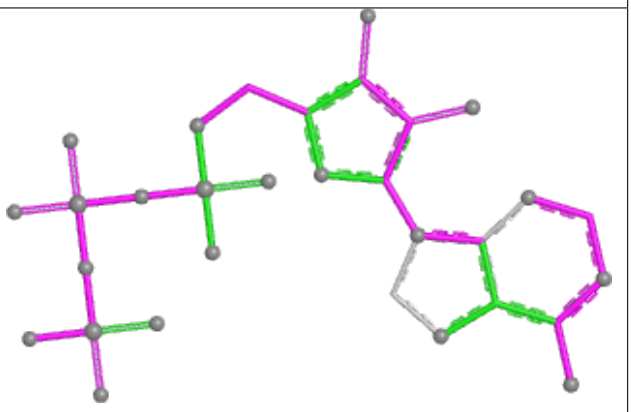
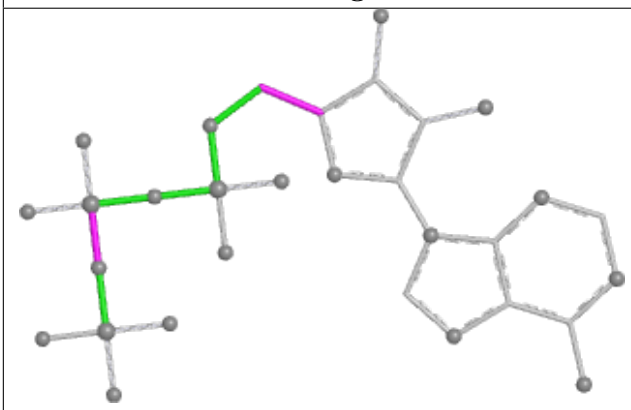
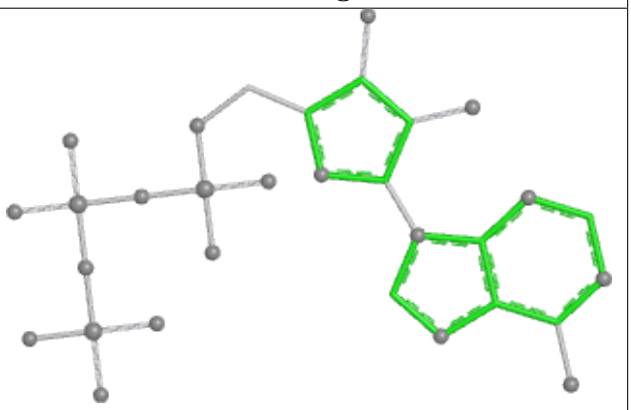
 Bond lengths	 Bond angles
 Torsions	 Rings

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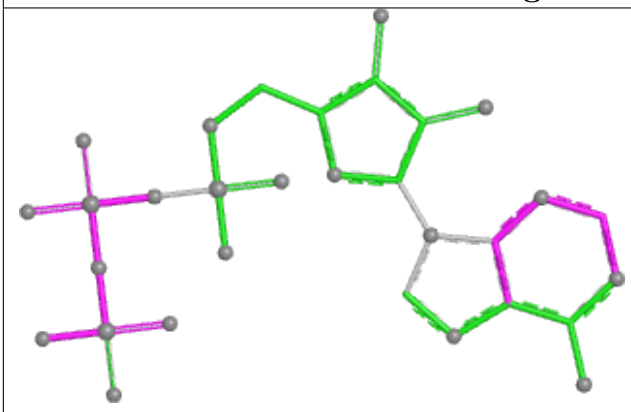
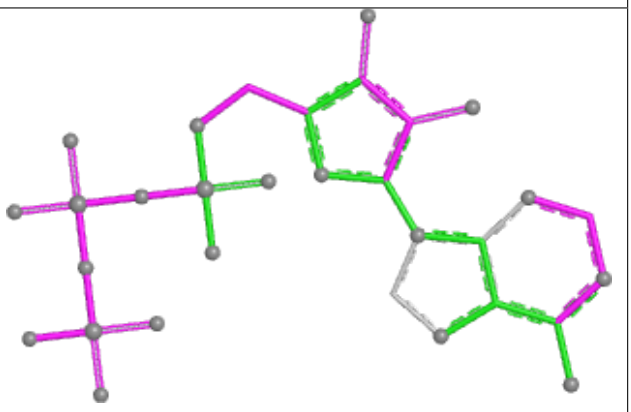
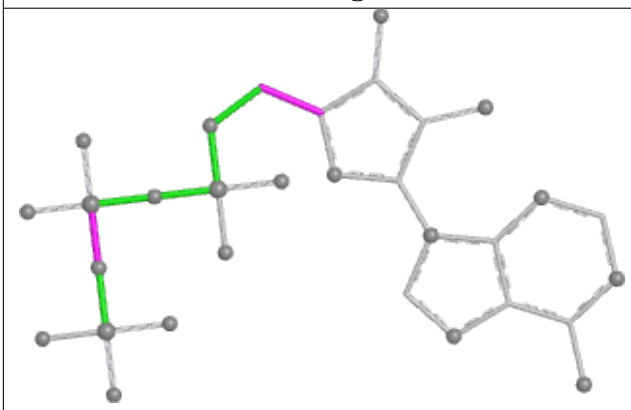
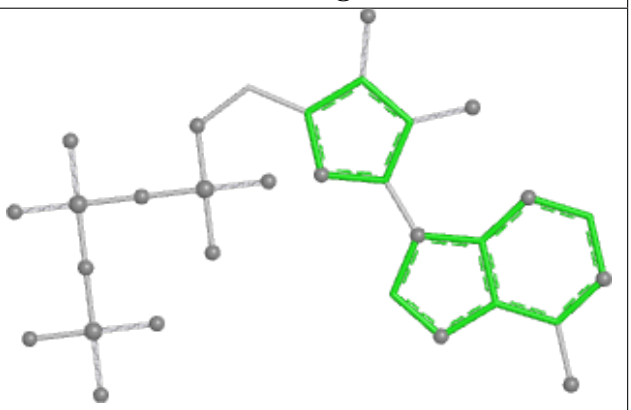
 Bond lengths	 Bond angles
 Torsions	 Rings

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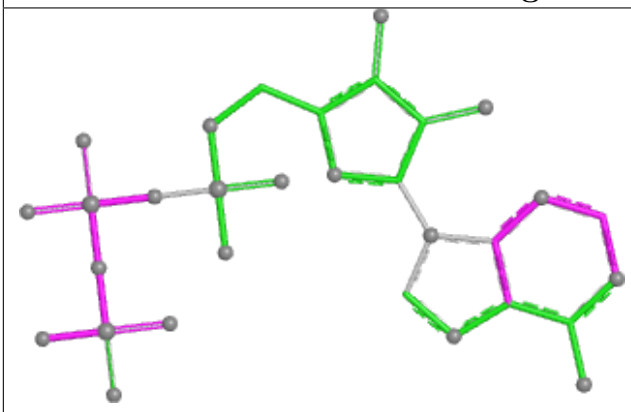
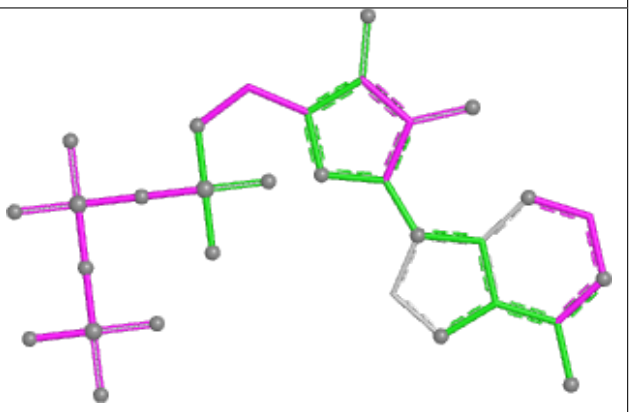
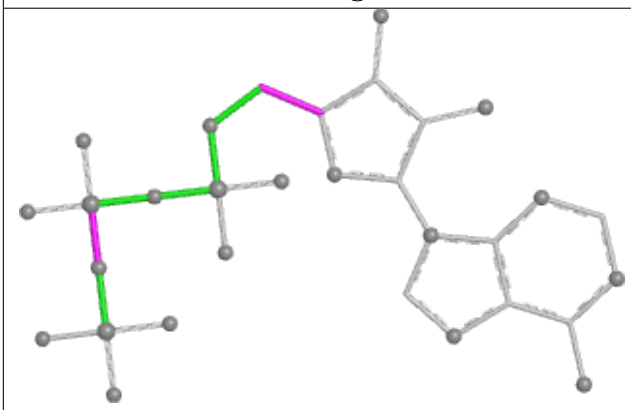
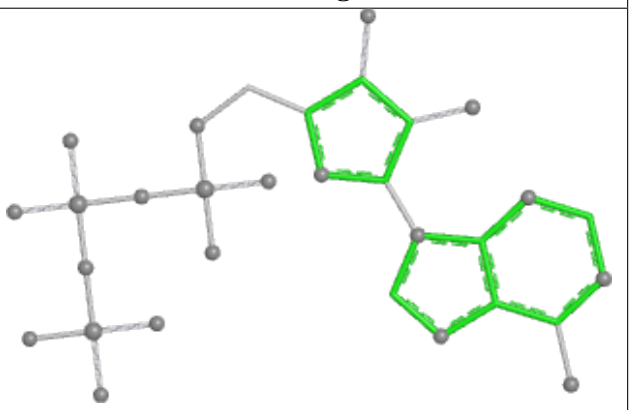
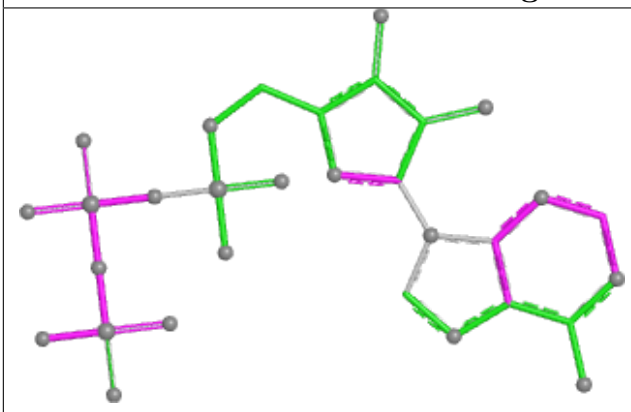
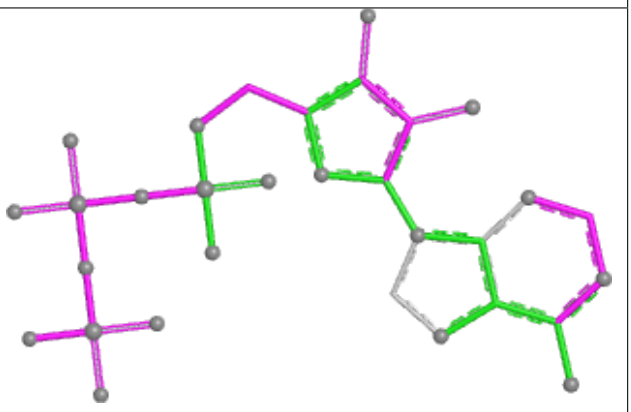
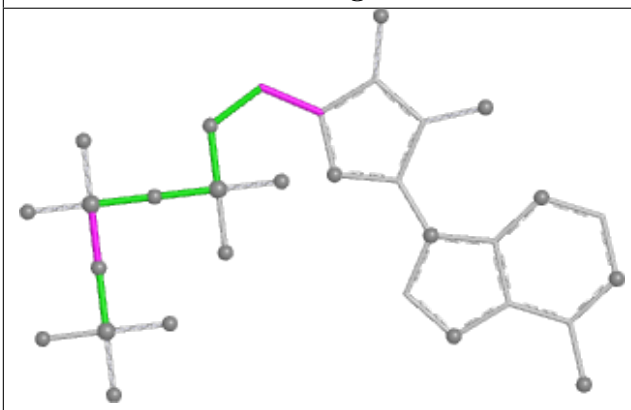
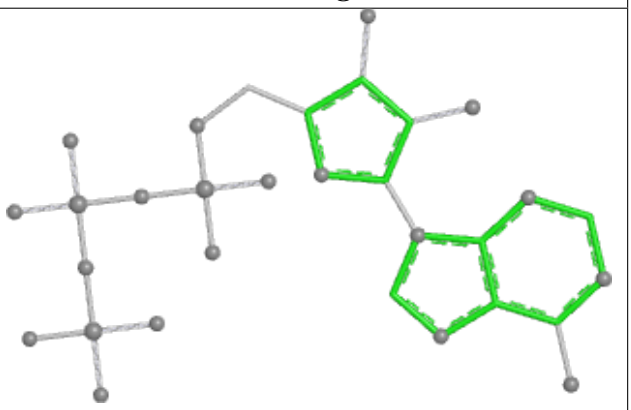
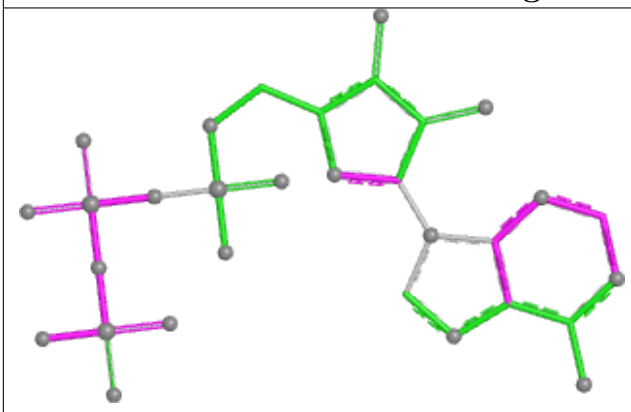
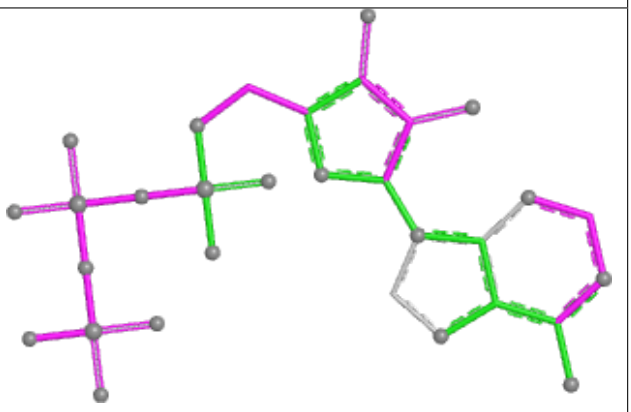
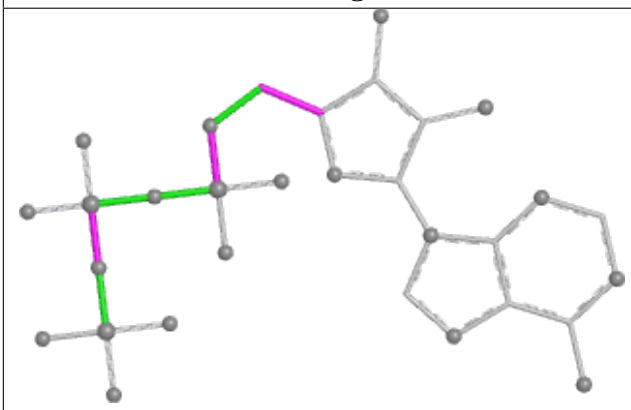
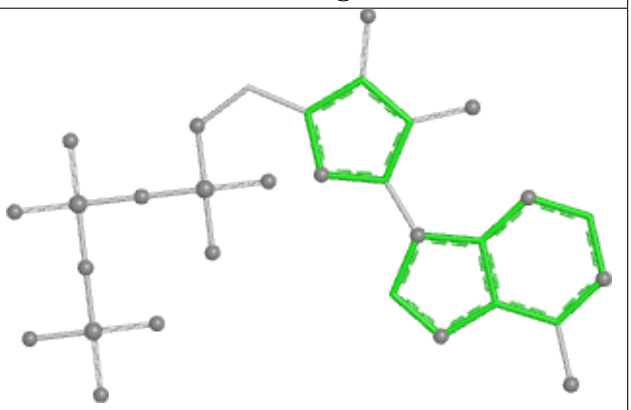
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ANP A 600	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ANP E 600	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

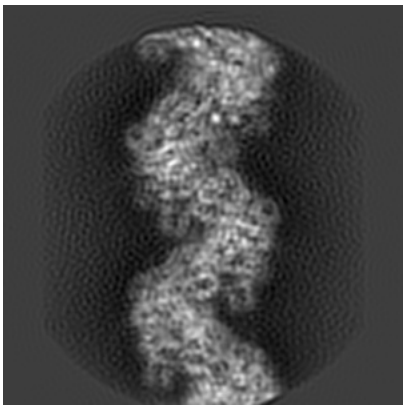
6 Map visualisation (i)

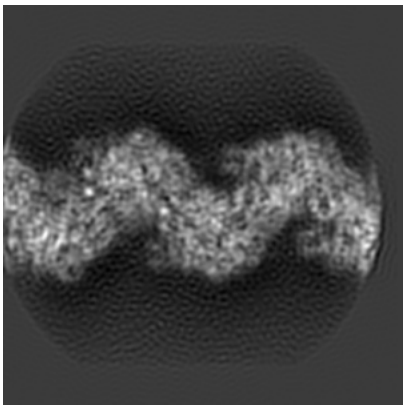
This section contains visualisations of the EMDB entry EMD-8183. These allow visual inspection of the internal detail of the map and identification of artifacts.

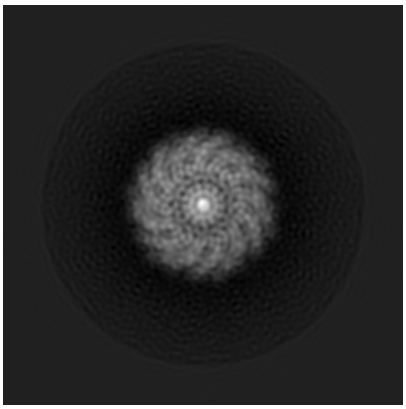
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

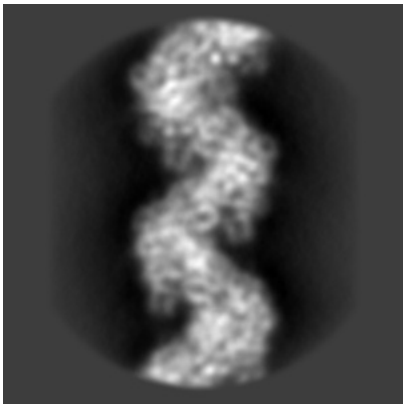
6.1.1 Primary map

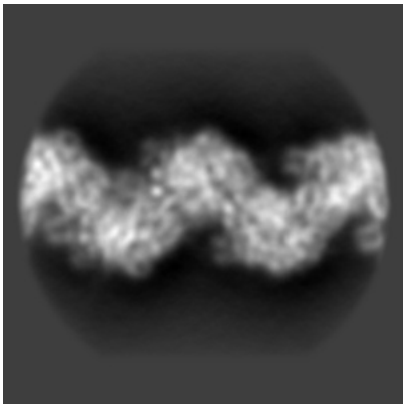

X

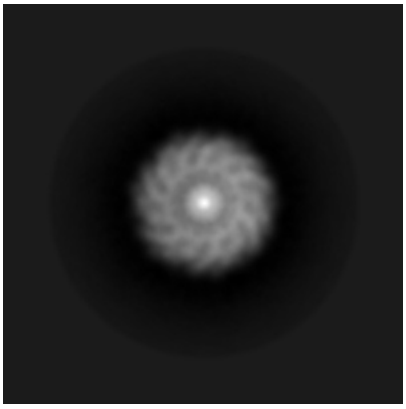

Y


Z

6.1.2 Raw map


X

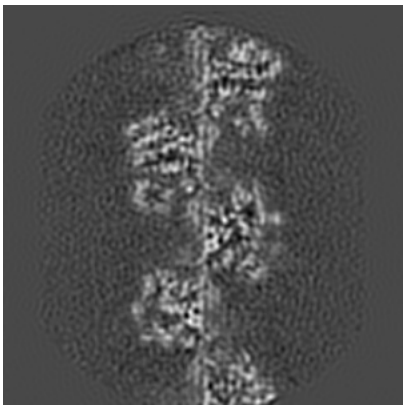

Y

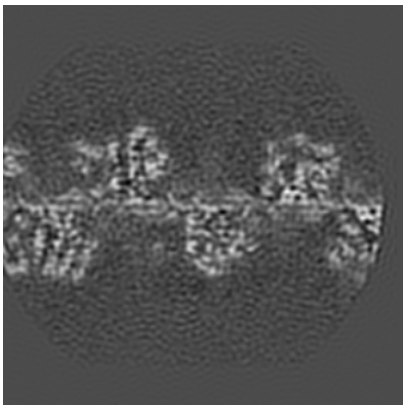

Z

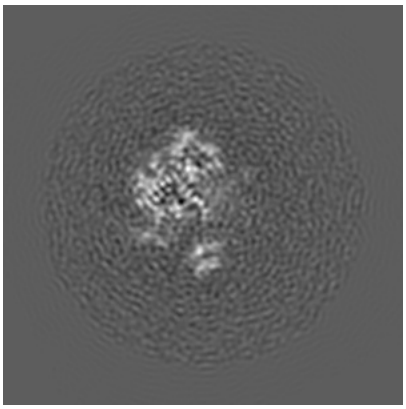
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

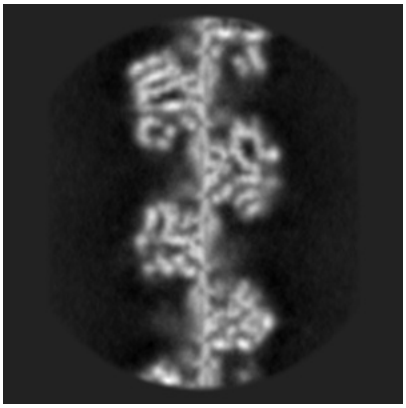
6.2.1 Primary map

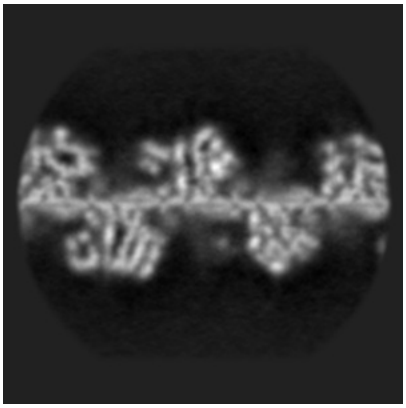

X Index: 128

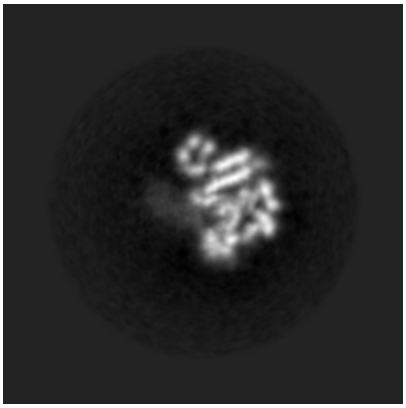

Y Index: 128


Z Index: 128

6.2.2 Raw map


X Index: 100

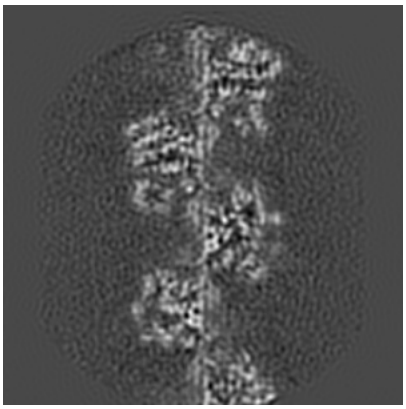

Y Index: 100

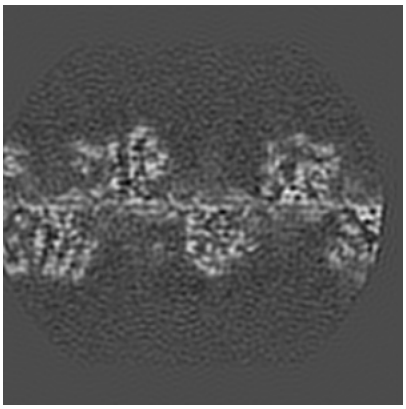

Z Index: 100

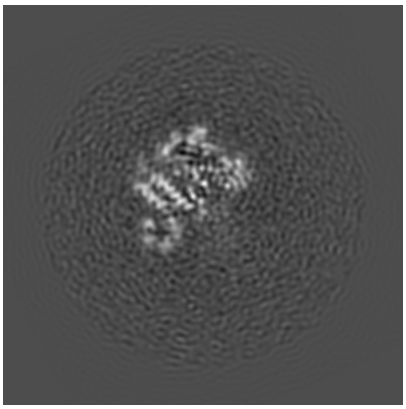
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

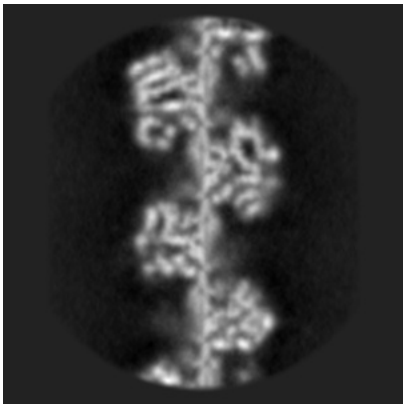
6.3.1 Primary map

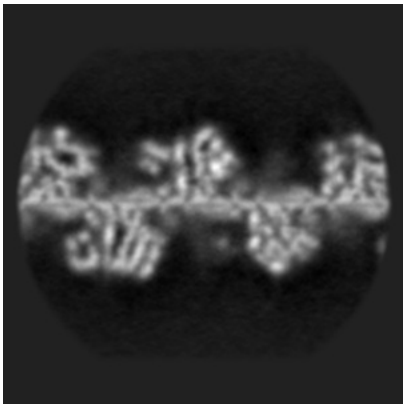

X Index: 128

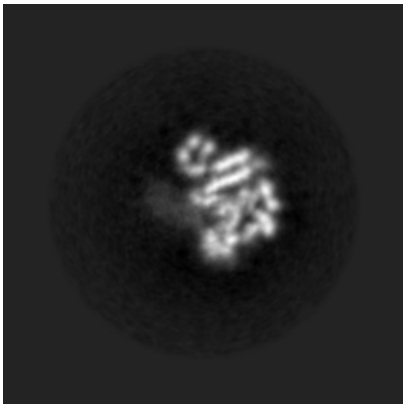

Y Index: 128


Z Index: 118

6.3.2 Raw map


X Index: 100

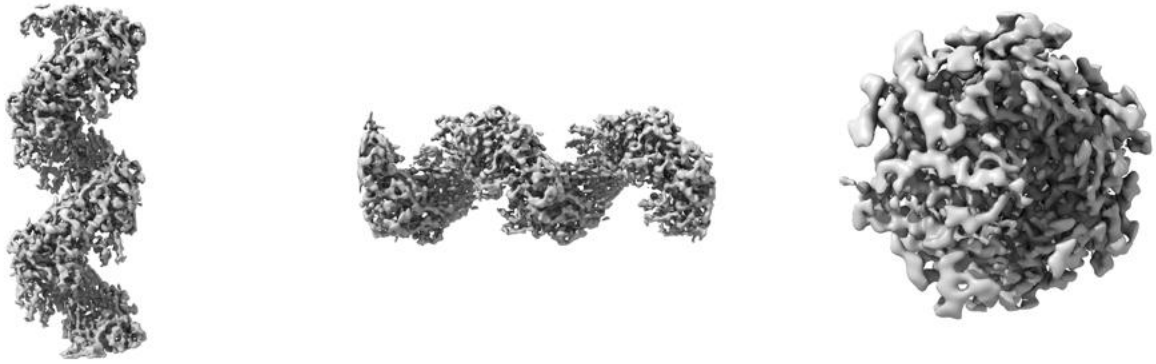

Y Index: 100


Z Index: 100

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

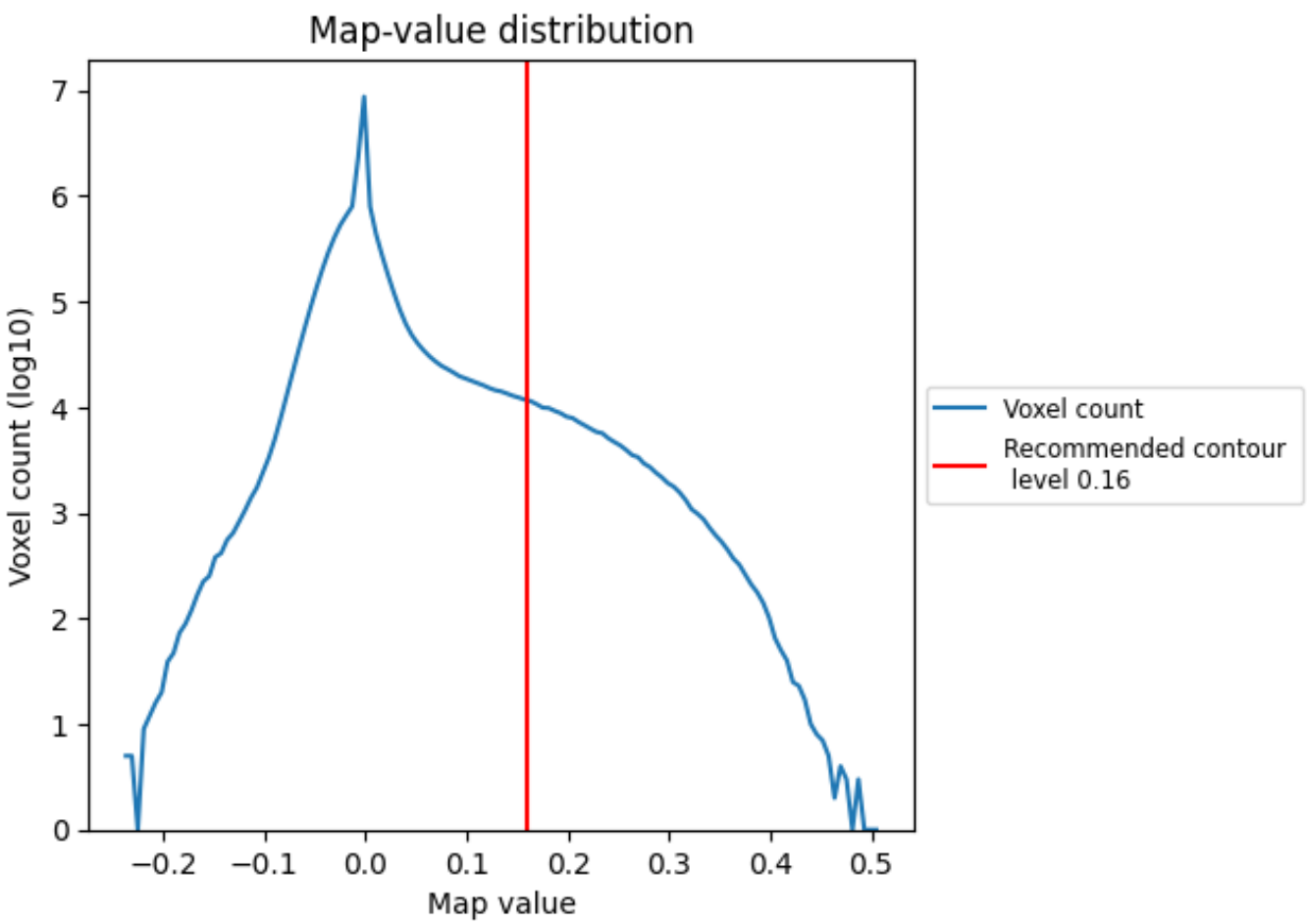
6.5 Mask visualisation (i)

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

7 Map analysis (i)

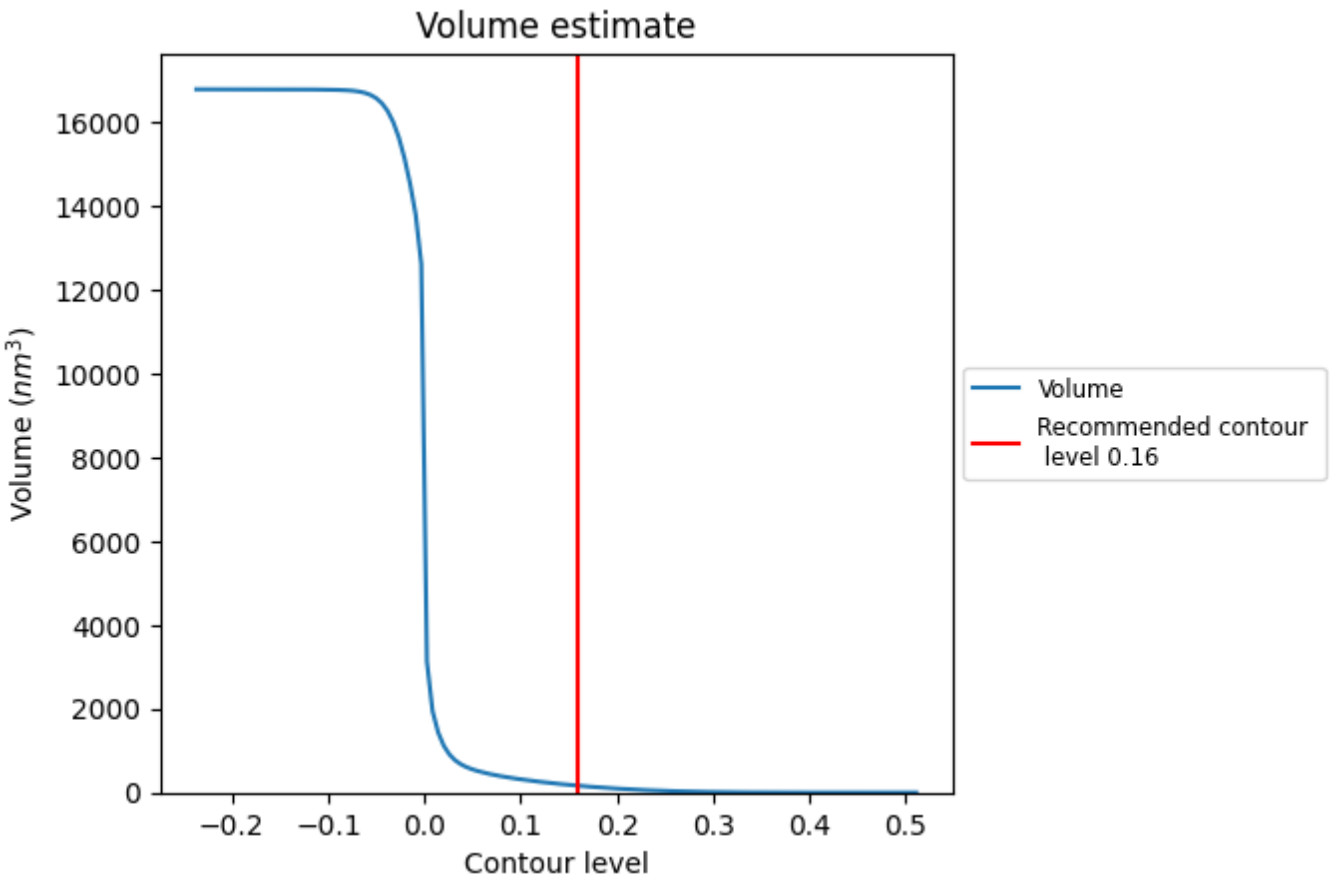
This section contains the results of statistical analysis of the map.

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.

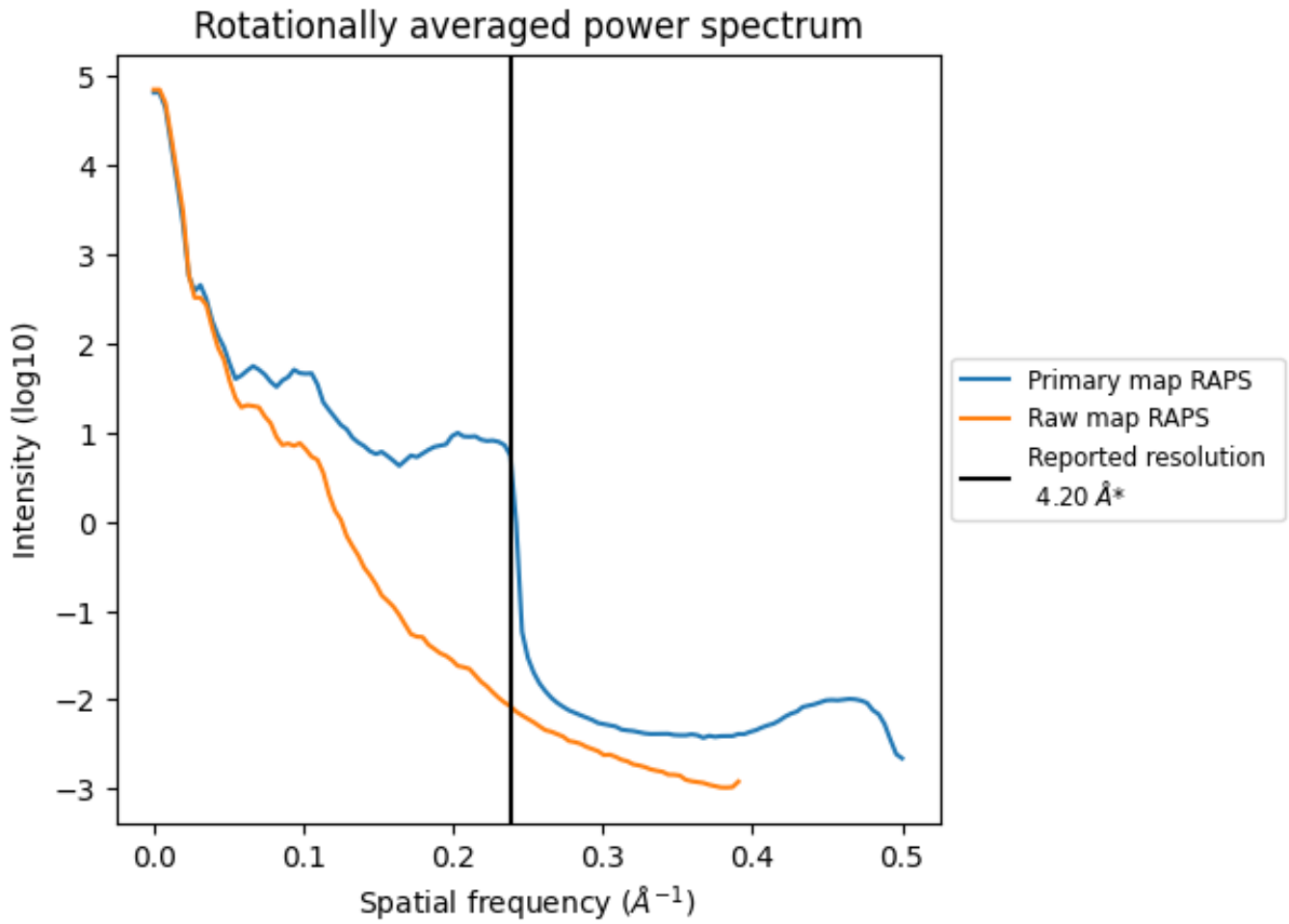
7.2 Volume estimate (i)



The volume at the recommended contour level is 164 nm^3; this corresponds to an approximate mass of 148 kDa.

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

7.3 Rotationally averaged power spectrum (i)

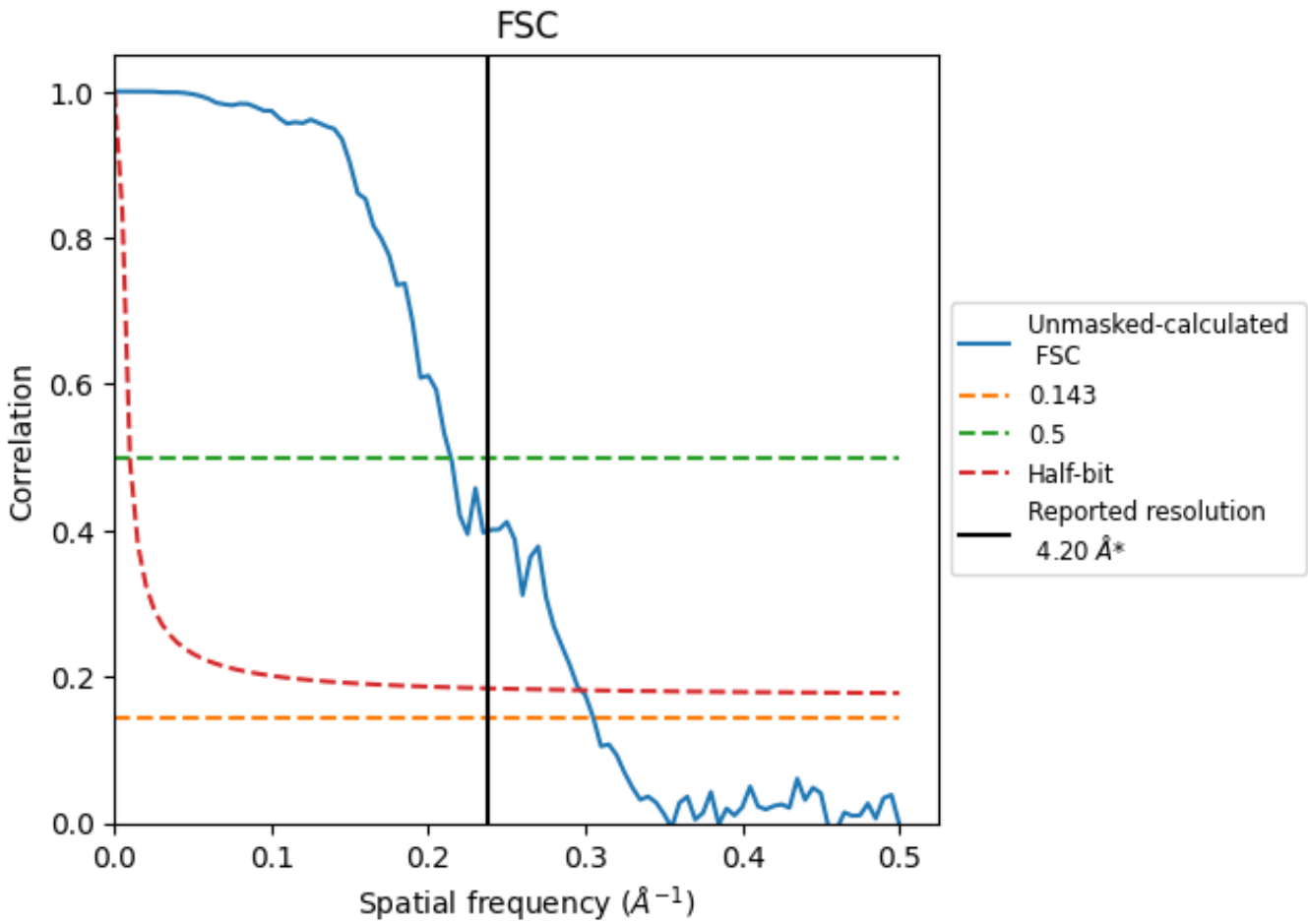


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

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 0.238 Å^{-1}

8.2 Resolution estimates (i)

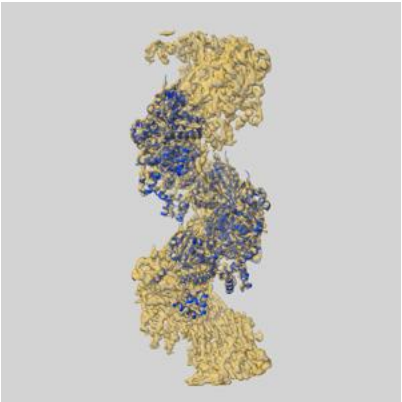
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.28	4.67	3.37

*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 3.28 differs from the reported value 4.2 by more than 10 %

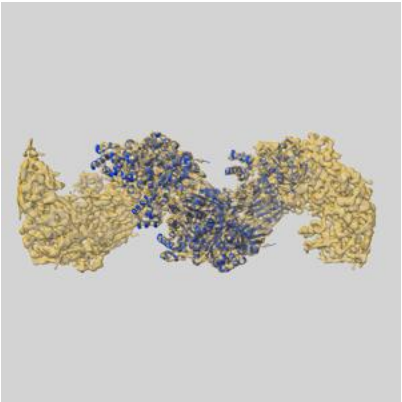
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8183 and PDB model 5NP7. Per-residue inclusion information can be found in section 3 on page 5.

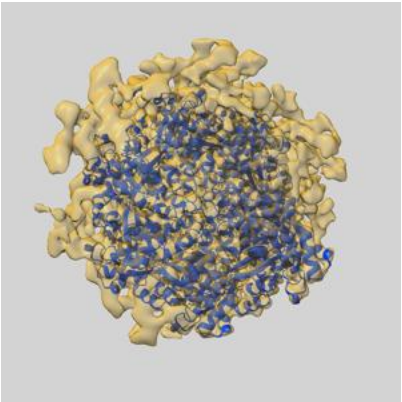
9.1 Map-model overlay (i)



X



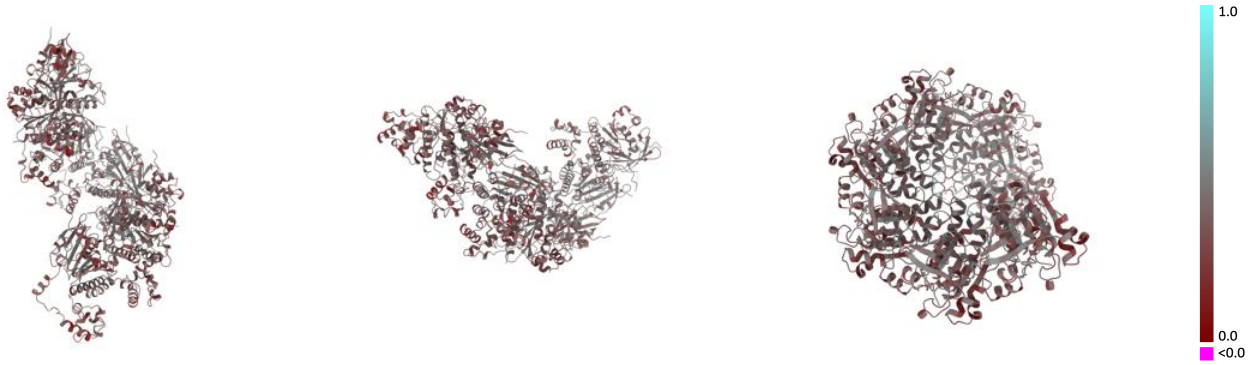
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

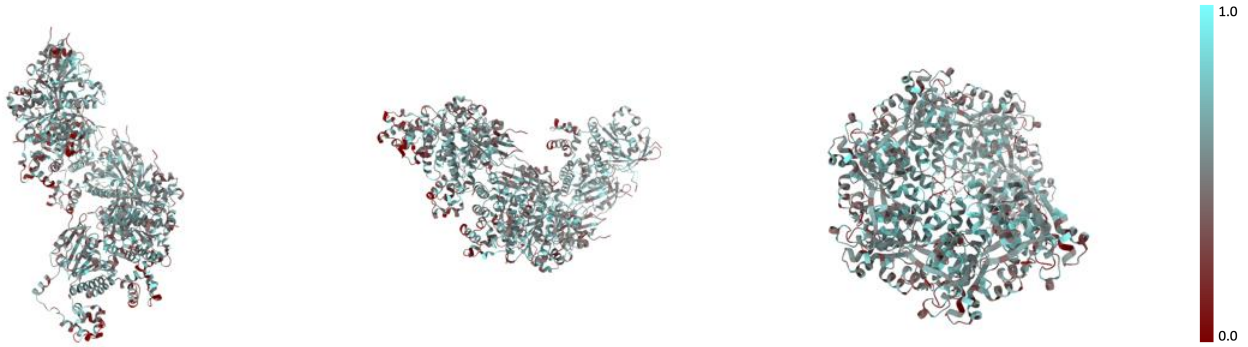
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

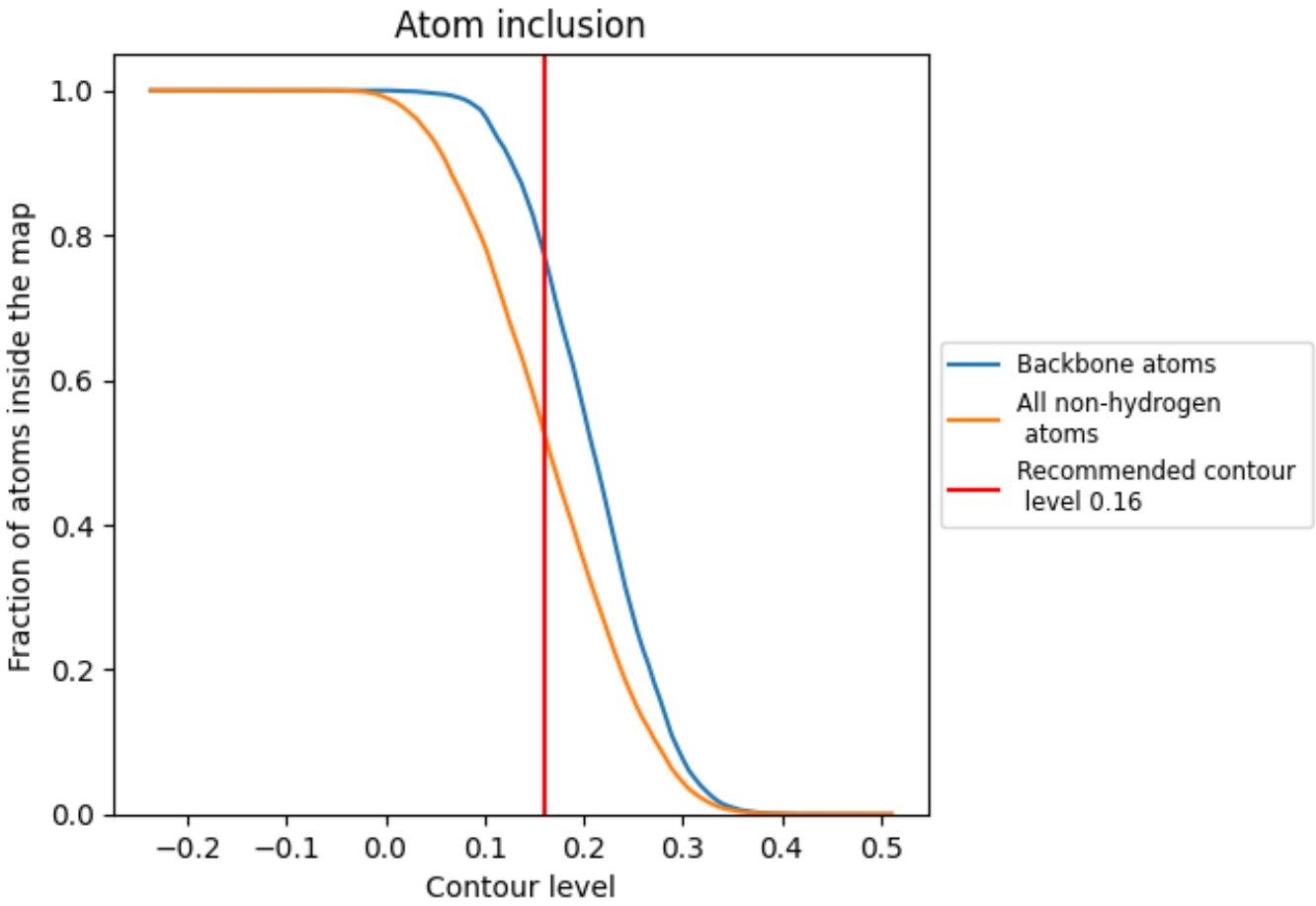
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.16).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5275	0.3670
A	0.5271	0.3630
B	0.5241	0.3700
C	0.5306	0.3710
D	0.5341	0.3710
E	0.5297	0.3690
F	0.5228	0.3640
G	0.5241	0.3630