



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 05:35 AM UTC

PDB ID : 5NP7 / pdb_00005np7
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 ⓘ 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:

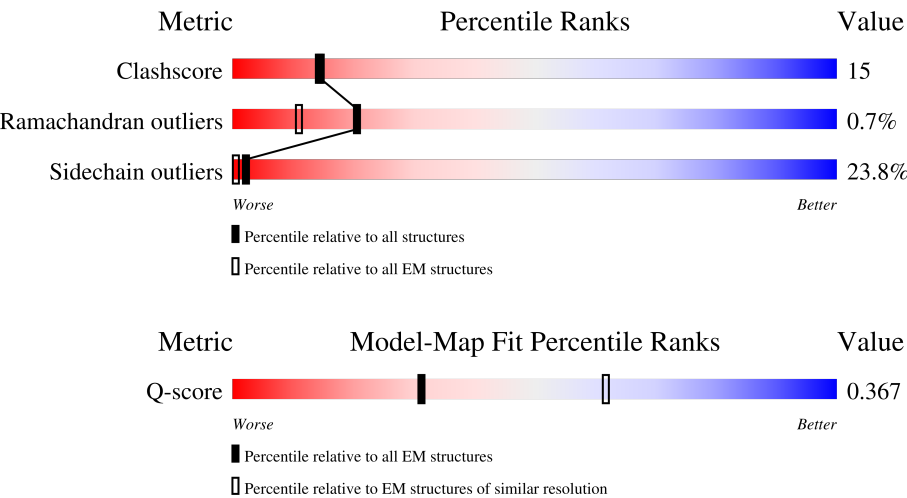
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	339	24% 57% 25% 9% 8%
1	B	339	23% 55% 26% 9% 8%
1	C	339	22% 55% 25% 11% 8%
1	D	339	22% 55% 25% 11% 8%

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Mol	Chain	Length	Quality of chain
1	E	339	23% 55% 24% 11% • 8%
1	F	339	25% 56% 24% 10% • 8%
1	G	339	24% 56% 24% 11% • 8%

2 Entry composition [i](#)

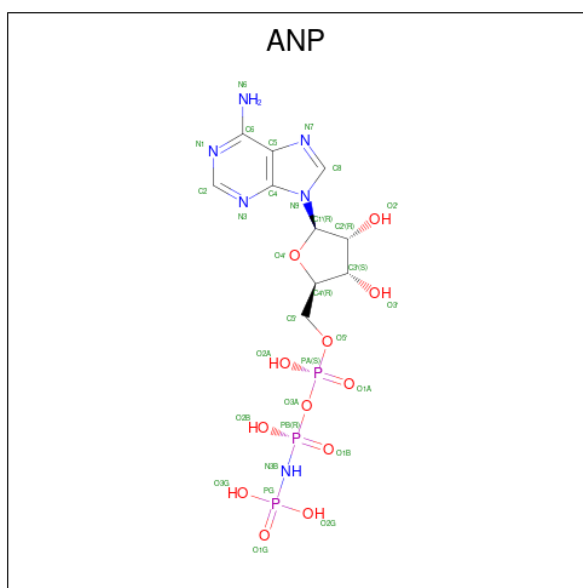
There are 2 unique types of molecules in this entry. The entry contains 16457 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

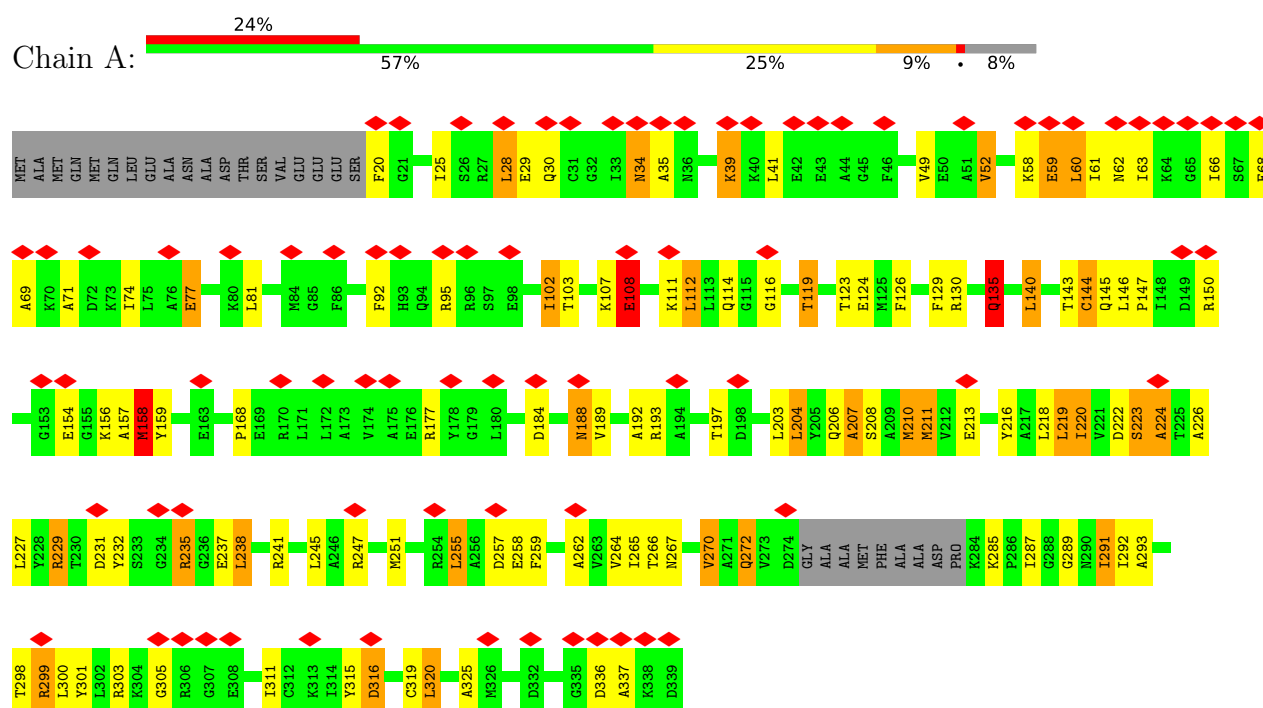


Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 31	C 10	N 6	O 12	P 3	0
2	B	1	Total 31	C 10	N 6	O 12	P 3	0
2	C	1	Total 31	C 10	N 6	O 12	P 3	0
2	D	1	Total 31	C 10	N 6	O 12	P 3	0
2	E	1	Total 31	C 10	N 6	O 12	P 3	0
2	F	1	Total 31	C 10	N 6	O 12	P 3	0
2	G	1	Total 31	C 10	N 6	O 12	P 3	0

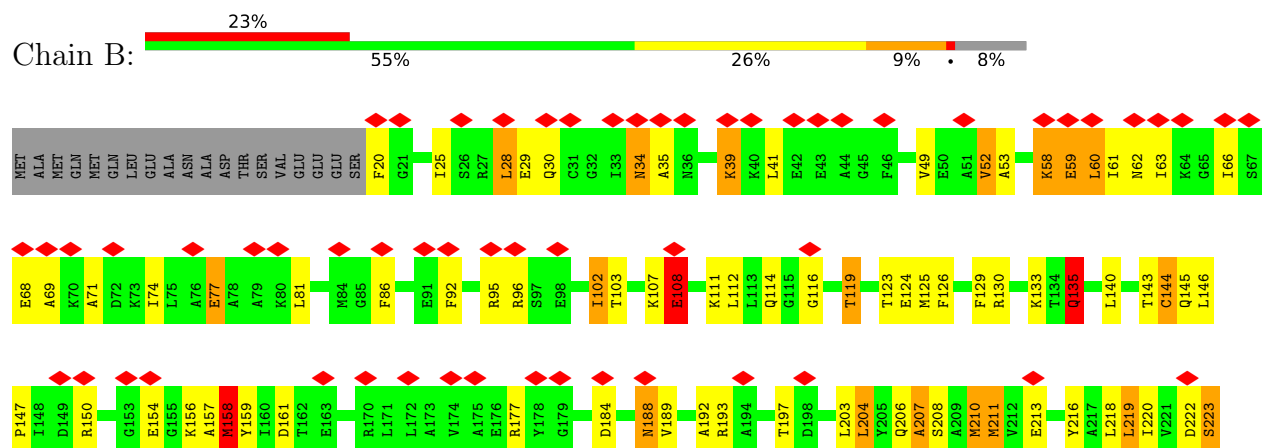
3 Residue-property plots [i](#)

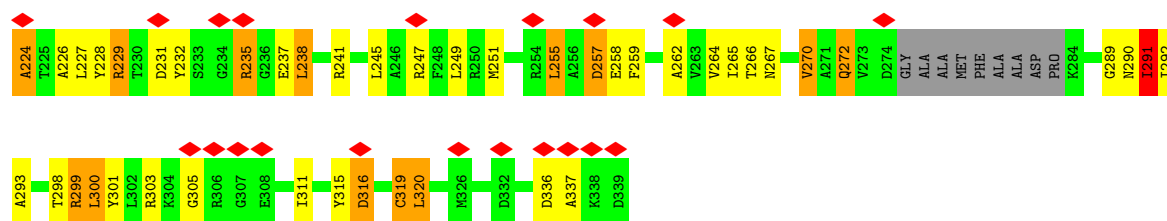
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

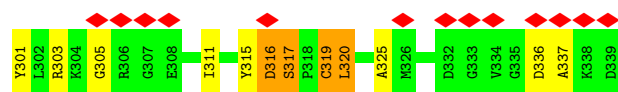
• Molecule 1: DNA repair protein RAD51 homolog 1



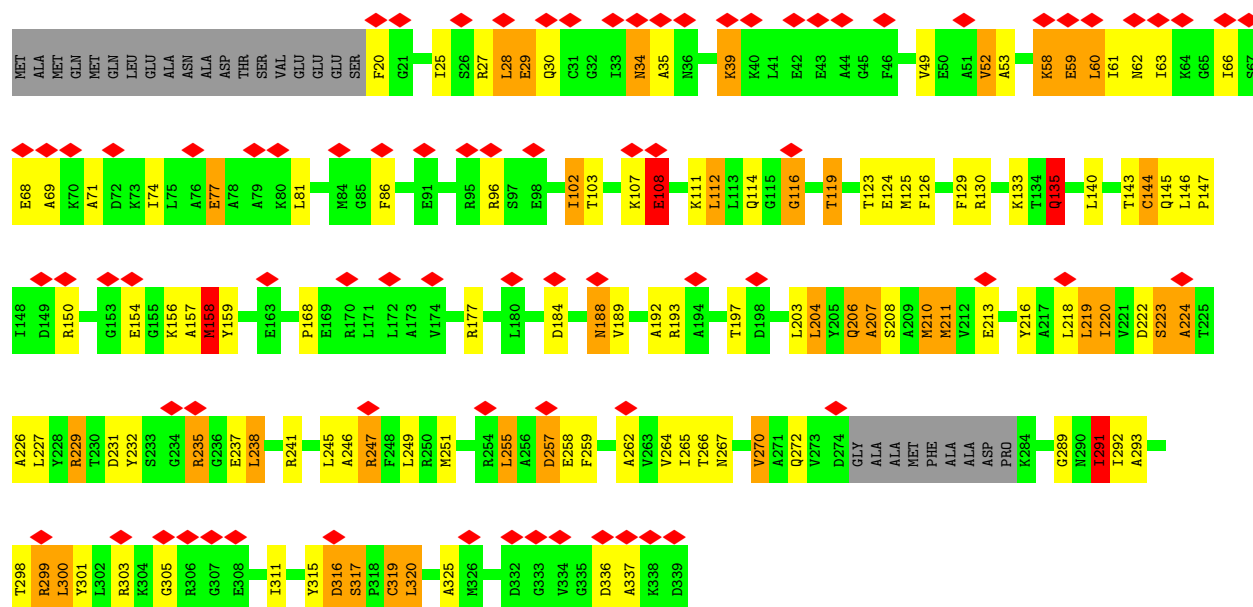
• Molecule 1: DNA repair protein RAD51 homolog 1



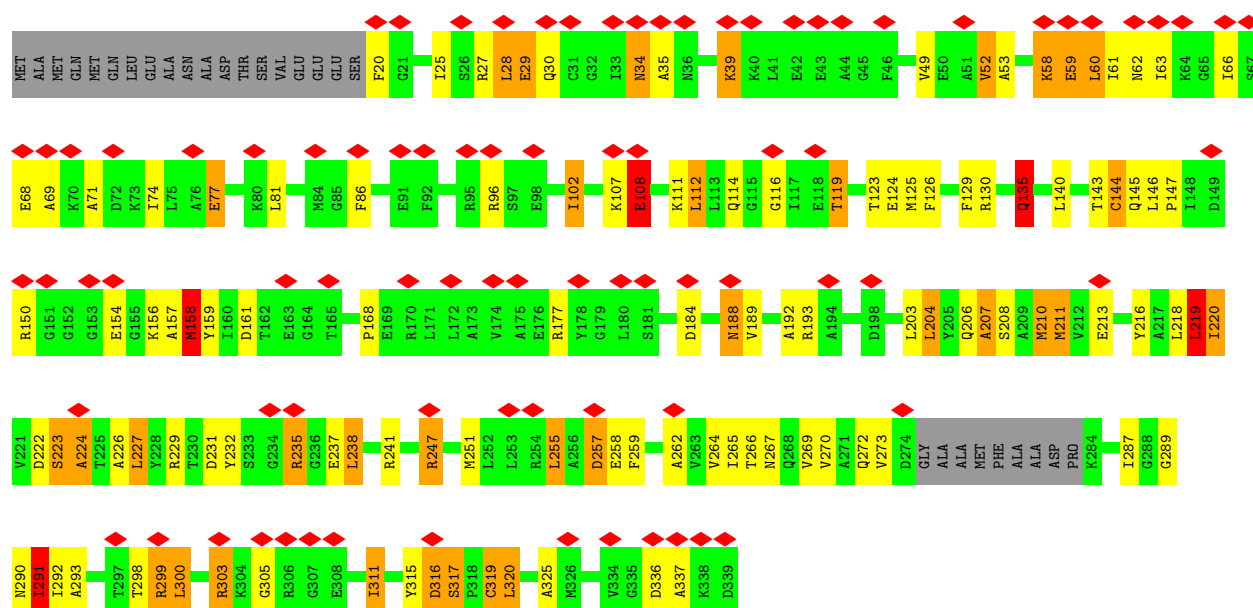




• Molecule 1: DNA repair protein RAD51 homolog 1

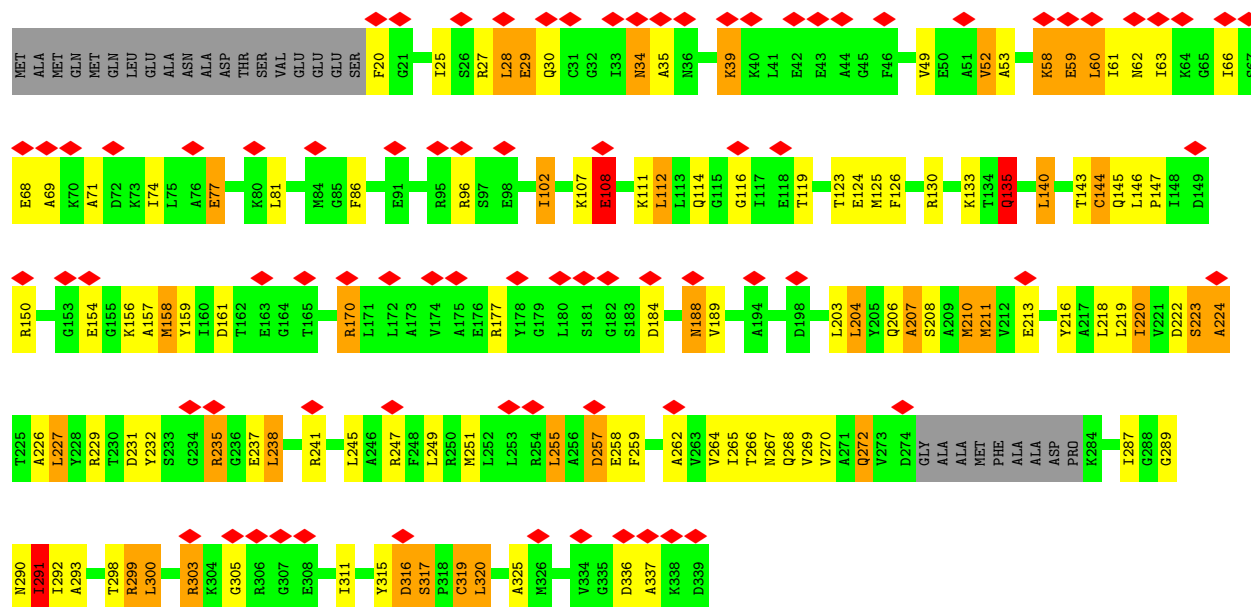


• Molecule 1: DNA repair protein RAD51 homolog 1



• Molecule 1: DNA repair protein RAD51 homolog 1

Chain G: 



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 ⓘ

5.1 Standard geometry ⓘ

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	1.23	8/2354 (0.3%)	1.72	12/3182 (0.4%)
1	B	1.24	6/2354 (0.3%)	1.74	16/3182 (0.5%)
1	C	1.24	8/2354 (0.3%)	1.75	19/3182 (0.6%)
1	D	1.24	8/2354 (0.3%)	1.74	18/3182 (0.6%)
1	E	1.24	6/2354 (0.3%)	1.74	18/3182 (0.6%)
1	F	1.24	8/2354 (0.3%)	1.75	18/3182 (0.6%)
1	G	1.24	8/2354 (0.3%)	1.75	19/3182 (0.6%)
All	All	1.24	52/16478 (0.3%)	1.74	120/22274 (0.5%)

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	315	TYR	CA-C	7.99	1.57	1.52
1	B	315	TYR	CA-C	7.35	1.56	1.52
1	C	315	TYR	CA-C	7.20	1.56	1.52
1	D	207	ALA	CA-C	-6.90	1.44	1.52
1	E	315	TYR	CA-C	6.89	1.56	1.52
1	G	315	TYR	CA-C	6.89	1.56	1.52
1	F	315	TYR	CA-C	6.82	1.56	1.52
1	F	207	ALA	CA-C	-6.75	1.44	1.52
1	C	207	ALA	CA-C	-6.71	1.44	1.52
1	E	207	ALA	CA-C	-6.69	1.44	1.52
1	A	207	ALA	CA-C	-6.51	1.44	1.52
1	D	315	TYR	CA-C	6.50	1.56	1.52
1	B	207	ALA	CA-C	-6.41	1.45	1.52
1	F	269	VAL	N-CA	6.05	1.52	1.46
1	G	269	VAL	N-CA	6.01	1.52	1.46
1	A	219	LEU	CA-C	-6.00	1.45	1.52
1	E	219	LEU	CA-C	-5.95	1.45	1.52
1	B	305	GLY	N-CA	5.93	1.49	1.44
1	G	219	LEU	CA-C	-5.92	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	SER	C-O	-5.86	1.15	1.23
1	B	223	SER	C-O	-5.85	1.15	1.23
1	B	219	LEU	CA-C	-5.83	1.45	1.52
1	C	219	LEU	CA-C	-5.83	1.45	1.52
1	A	305	GLY	N-CA	5.78	1.49	1.44
1	D	219	LEU	CA-C	-5.74	1.45	1.52
1	D	305	GLY	N-CA	5.72	1.49	1.44
1	C	223	SER	C-O	-5.70	1.15	1.23
1	C	305	GLY	N-CA	5.67	1.49	1.44
1	F	223	SER	C-O	-5.67	1.15	1.23
1	D	223	SER	C-O	-5.66	1.15	1.23
1	G	305	GLY	N-CA	5.65	1.49	1.44
1	F	219	LEU	CA-C	-5.64	1.46	1.52
1	E	305	GLY	N-CA	5.64	1.49	1.44
1	F	305	GLY	N-CA	5.58	1.49	1.44
1	G	223	SER	C-O	-5.50	1.15	1.23
1	F	273	VAL	N-CA	5.32	1.53	1.46
1	C	269	VAL	N-CA	5.31	1.52	1.46
1	G	207	ALA	CA-C	-5.31	1.46	1.52
1	E	223	SER	C-O	-5.28	1.15	1.24
1	C	211	MET	CG-SD	-5.22	1.67	1.80
1	A	287	ILE	N-CA	5.17	1.53	1.46
1	B	211	MET	CG-SD	-5.17	1.67	1.80
1	E	211	MET	CG-SD	-5.17	1.67	1.80
1	A	211	MET	CG-SD	-5.16	1.67	1.80
1	D	211	MET	CG-SD	-5.15	1.67	1.80
1	D	269	VAL	N-CA	5.10	1.51	1.46
1	G	211	MET	CG-SD	-5.09	1.68	1.80
1	F	211	MET	CG-SD	-5.08	1.68	1.80
1	D	268	GLN	CA-C	5.04	1.59	1.53
1	C	268	GLN	CA-C	5.02	1.59	1.53
1	G	268	GLN	N-CA	5.02	1.52	1.45
1	A	285	LYS	CA-C	5.01	1.58	1.53

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	319	CYS	N-CA-C	10.49	122.68	111.03
1	F	319	CYS	N-CA-C	10.49	122.67	111.03
1	G	319	CYS	N-CA-C	10.19	122.34	111.03
1	D	319	CYS	N-CA-C	9.99	122.12	111.03
1	B	319	CYS	N-CA-C	9.95	122.07	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	319	CYS	N-CA-C	9.89	122.01	111.03
1	A	319	CYS	N-CA-C	8.51	120.24	110.97
1	E	238	LEU	N-CA-C	-7.98	103.67	113.41
1	C	238	LEU	N-CA-C	-7.92	103.75	113.41
1	D	238	LEU	N-CA-C	-7.91	103.75	113.41
1	A	238	LEU	N-CA-C	-7.62	104.12	113.41
1	G	238	LEU	N-CA-C	-7.61	104.12	113.41
1	G	135	GLN	N-CA-C	7.58	120.21	111.11
1	F	238	LEU	N-CA-C	-7.55	104.20	113.41
1	B	238	LEU	N-CA-C	-7.47	104.29	113.41
1	A	135	GLN	N-CA-C	7.34	119.92	111.11
1	D	135	GLN	N-CA-C	7.34	119.92	111.11
1	F	232	TYR	N-CA-C	7.29	118.23	108.38
1	G	232	TYR	N-CA-C	7.24	118.16	108.38
1	F	135	GLN	N-CA-C	7.23	119.78	111.11
1	C	232	TYR	N-CA-C	7.18	118.07	108.38
1	F	218	LEU	N-CA-C	7.13	121.18	109.06
1	C	135	GLN	N-CA-C	7.12	119.65	111.11
1	E	232	TYR	N-CA-C	7.10	117.96	108.38
1	E	135	GLN	N-CA-C	7.08	119.60	111.11
1	B	135	GLN	N-CA-C	7.06	119.58	111.11
1	D	232	TYR	N-CA-C	7.00	117.83	108.38
1	G	218	LEU	N-CA-C	6.91	120.81	109.06
1	B	232	TYR	N-CA-C	6.82	117.59	108.38
1	A	232	TYR	N-CA-C	6.69	117.41	108.38
1	E	218	LEU	N-CA-C	6.53	120.15	109.06
1	B	218	LEU	N-CA-C	6.49	120.08	109.06
1	A	218	LEU	N-CA-C	6.48	120.08	109.06
1	D	218	LEU	N-CA-C	6.41	119.96	109.06
1	C	218	LEU	N-CA-C	6.34	119.84	109.06
1	C	291	ILE	N-CA-C	6.17	117.66	110.62
1	F	287	ILE	N-CA-C	6.13	116.73	110.05
1	A	68	GLU	N-CA-C	6.11	118.02	111.36
1	B	291	ILE	N-CA-C	6.02	117.48	110.62
1	A	158	MET	CB-CA-C	5.96	120.62	109.71
1	F	207	ALA	CA-C-O	-5.93	114.77	121.00
1	B	68	GLU	N-CA-C	5.92	117.81	111.36
1	G	68	GLU	N-CA-C	5.91	117.80	111.36
1	D	68	GLU	N-CA-C	5.89	117.78	111.36
1	G	287	ILE	N-CA-C	5.89	116.87	110.21
1	E	68	GLU	N-CA-C	5.88	117.76	111.36
1	C	207	ALA	CA-C-O	-5.85	114.86	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	291	ILE	N-CA-C	5.84	117.28	110.62
1	B	158	MET	CB-CA-C	5.84	120.40	109.71
1	E	207	ALA	CA-C-O	-5.84	114.87	121.00
1	F	291	ILE	N-CA-C	5.83	117.27	110.62
1	E	291	ILE	N-CA-C	5.81	117.24	110.62
1	E	158	MET	CB-CA-C	5.80	120.32	109.71
1	D	207	ALA	CA-C-O	-5.78	114.93	121.00
1	B	207	ALA	CA-C-O	-5.76	114.95	121.00
1	D	158	MET	CB-CA-C	5.76	120.25	109.71
1	G	158	MET	CB-CA-C	5.72	120.18	109.71
1	A	207	ALA	CA-C-O	-5.72	115.00	121.00
1	F	68	GLU	N-CA-C	5.71	117.58	111.36
1	C	158	MET	CB-CA-C	5.70	120.14	109.71
1	C	68	GLU	N-CA-C	5.66	117.52	111.36
1	F	158	MET	CB-CA-C	5.64	120.03	109.71
1	G	207	ALA	CA-C-O	-5.61	114.93	120.82
1	G	227	LEU	CA-C-O	-5.53	114.98	120.90
1	F	227	LEU	CA-C-O	-5.42	115.09	120.90
1	G	317	SER	CA-C-N	5.42	126.62	119.84
1	G	317	SER	C-N-CA	5.42	126.62	119.84
1	B	53	ALA	CA-C-N	5.36	128.21	120.38
1	B	53	ALA	C-N-CA	5.36	128.21	120.38
1	A	108	GLU	N-CA-C	5.35	117.80	111.33
1	G	108	GLU	N-CA-C	5.35	117.80	111.33
1	F	108	GLU	N-CA-C	5.34	117.80	111.33
1	D	53	ALA	CA-C-N	5.33	128.16	120.38
1	D	53	ALA	C-N-CA	5.33	128.16	120.38
1	F	53	ALA	CA-C-N	5.33	128.16	120.38
1	F	53	ALA	C-N-CA	5.33	128.16	120.38
1	C	108	GLU	N-CA-C	5.31	117.76	111.33
1	D	108	GLU	N-CA-C	5.31	117.75	111.33
1	B	108	GLU	N-CA-C	5.30	117.74	111.33
1	E	53	ALA	CA-C-N	5.30	128.12	120.38
1	E	53	ALA	C-N-CA	5.30	128.12	120.38
1	C	197	THR	CB-CA-C	-5.27	102.61	110.88
1	B	291	ILE	O-C-N	5.26	127.05	121.89
1	C	53	ALA	CA-C-N	5.26	128.06	120.38
1	C	53	ALA	C-N-CA	5.26	128.06	120.38
1	E	108	GLU	N-CA-C	5.23	117.66	111.33
1	E	317	SER	CA-C-N	5.23	126.38	119.84
1	E	317	SER	C-N-CA	5.23	126.38	119.84
1	G	53	ALA	CA-C-N	5.22	128.00	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	53	ALA	C-N-CA	5.22	128.00	120.38
1	C	58	LYS	N-CA-C	5.21	119.96	111.37
1	A	197	THR	CB-CA-C	-5.20	102.71	110.88
1	A	291	ILE	O-C-N	5.20	127.16	121.90
1	F	317	SER	CA-C-N	5.18	126.32	119.84
1	F	317	SER	C-N-CA	5.18	126.32	119.84
1	G	140	LEU	N-CA-C	5.14	117.62	111.71
1	A	140	LEU	N-CA-C	5.13	117.61	111.71
1	D	317	SER	CA-C-N	5.13	126.25	119.84
1	D	317	SER	C-N-CA	5.13	126.25	119.84
1	D	58	LYS	N-CA-C	5.12	119.83	111.37
1	B	197	THR	CB-CA-C	-5.12	102.84	110.88
1	D	116	GLY	N-CA-C	5.12	117.49	110.58
1	G	170	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	E	197	THR	CB-CA-C	-5.10	102.87	110.88
1	G	58	LYS	N-CA-C	5.10	119.79	111.37
1	F	58	LYS	N-CA-C	5.10	119.78	111.37
1	C	228	TYR	N-CA-C	5.07	121.60	110.80
1	E	291	ILE	O-C-N	5.07	126.86	121.89
1	D	197	THR	CB-CA-C	-5.07	102.92	110.88
1	E	58	LYS	N-CA-C	5.06	119.72	111.37
1	C	311	ILE	CB-CA-C	5.06	117.96	110.77
1	F	311	ILE	CB-CA-C	5.06	118.11	110.63
1	D	140	LEU	N-CA-C	5.05	117.52	111.71
1	B	58	LYS	N-CA-C	5.04	119.68	111.37
1	C	116	GLY	N-CA-C	5.03	117.36	110.58
1	B	228	TYR	N-CA-C	5.00	121.46	110.80
1	C	317	SER	CA-C-N	5.00	126.10	119.84
1	C	317	SER	C-N-CA	5.00	126.10	119.84
1	E	116	GLY	N-CA-C	5.00	117.33	110.58
1	D	228	TYR	N-CA-C	5.00	121.45	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	71	0
1	B	2320	0	2268	73	0
1	C	2320	0	2268	78	0
1	D	2320	0	2268	78	0
1	E	2320	0	2268	78	0
1	F	2320	0	2268	71	0
1	G	2320	0	2268	75	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	495	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (495) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:LEU:O	1:D:231:ASP:OD1	1.81	0.98
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: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: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:B:135:GLN:HA	1:B:135:GLN:NE2	1.99	0.74
1:G:135:GLN:HA	1:G:135:GLN:NE2	1.99	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:135:GLN:HA	1:A:135:GLN:NE2	1.99	0.73
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:255:LEU:HA	1:G:258:GLU:HG2	1.82	0.61
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:F:207:ALA:C	1:F:211:MET:SD	2.85	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:G:207:ALA:C	1:G:211:MET:SD	2.85	0.59
1:C:208:SER:HA	1:C:211:MET:SD	2.42	0.59
1:A:207:ALA:C	1:A:211:MET:SD	2.85	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:207:ALA:C	1:E:211:MET:SD	2.85	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:B:207:ALA:C	1:B:211:MET:SD	2.85	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: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:E:129:PHE:HB3	1:F:293:ALA:HB1	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:258:GLU:HG3	1:B:259:PHE:N	2.19	0.56
1:A:303:ARG:HD2	1:A:311:ILE:HB	1.87	0.56
1:E:210:MET:HA	1:E:210:MET:HE2	1.87	0.56
1:C:210:MET:HA	1:C:210:MET:HE2	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:C:207:ALA:C	1:C:211:MET:SD	2.85	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:C:258:GLU:HG3	1:C:259:PHE:N	2.19	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:D:207:ALA:C	1:D:211:MET:SD	2.85	0.55
1:C:223:SER:O	1:C:226:ALA:N	2.34	0.55
1:B:210:MET:HE2	1:B:210:MET:HA	1.87	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:D:210:MET:HE2	1:D:210:MET:HA	1.87	0.55
1:A:210:MET:HE2	1:A:210:MET:HA	1.88	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:F:210:MET:HE2	1:F:210:MET:HA	1.88	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:E:258:GLU:HG3	1:E:259:PHE:N	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:210:MET:HE2	1:G:210:MET:HA	1.88	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:223:SER:O	1:C:224:ALA:C	2.55	0.50
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:B:223:SER:O	1:B:224:ALA:C	2.54	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: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:D:223:SER:O	1:D:224:ALA:C	2.55	0.50
1:E:114:GLN:HG2	1:E:320:LEU:HD23	1.94	0.50
1:E:223:SER:O	1:E:224:ALA:C	2.55	0.50
1:F:223:SER:O	1:F:224:ALA:C	2.55	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:G:223:SER:O	1:G:224:ALA:C	2.55	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: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:A:223:SER:O	1:A:224:ALA:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:34:ASN:OD1	1:B:34:ASN:N	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
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:B:227:LEU:C	1:B:231:ASP:OD1	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:211:MET:HE2	1:C:255:LEU:HD21	1.97	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
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:D:193:ARG:HH21	1:E:257:ASP:CG	2.24	0.46
1:E:211:MET:HE2	1:E:255:LEU:HD21	1.98	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: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:A:193:ARG:HH21	1:B:257:ASP:CG	2.25	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:G:245:LEU:HD21	1:G:292:ILE:HG23	1.98	0.45
1:F:208:SER:CA	1:F:211:MET:SD	3.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:211:MET:HE2	1:F:255:LEU:HD21	1.99	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: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:B:211:MET:HE2	1:B:255:LEU:HD21	1.99	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
1:D:211:MET:HE2	1:D:255:LEU:HD21	2.00	0.44
1:E:227:LEU:C	1:E:231:ASP:OD1	2.57	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
1:A:211:MET:HE2	1:A:255:LEU:HD21	1.99	0.44
1:E:193:ARG:HH21	1:F:257:ASP:CG	2.26	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:C:193:ARG:HH21	1:D:257:ASP:CG	2.26	0.43
1:D:272:GLN:O	1:D:272:GLN:NE2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:227:LEU:C	1:F:231:ASP:OD1	2.56	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: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:D:227:LEU:C	1:D:231:ASP:OD1	2.57	0.42
1:B:193:ARG:HH21	1:C:257:ASP:CG	2.27	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:D:247:ARG:HG3	1:D:247:ARG:HH11	1.84	0.42
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:HA	1:A:210:MET:CE	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:G:227:LEU:C	1:G:231:ASP:OD1	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:C	1:A:231:ASP:OD1	2.56	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: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
2:E:600:ANP:H8	1:F:317:SER:O	2.21	0.41
1:C:210:MET:HA	1:C:210:MET:CE	2.50	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:27:ARG:C	1:F:29:GLU:H	2.29	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:27:ARG:C	1:D:29:GLU:H	2.29	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:C:227:LEU:C	1:C:231:ASP:OD1	2.56	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
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: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:D:210:MET:HA	1:D:210:MET:CE	2.50	0.41
1:E:108:GLU:OE1	1:E:108:GLU:HA	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:211:MET:HE2	1:G:255:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:27:ARG:C	1:G:29:GLU:H	2.29	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:C:27:ARG:C	1:C:29:GLU:H	2.29	0.40
1:F:193:ARG:HH21	1:G:257:ASP:CG	2.29	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:E:27:ARG:C	1:E:29:GLU:H	2.29	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%)	18 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	307/339 (91%)	263 (86%)	42 (14%)	2 (1%)	18	54
1	C	307/339 (91%)	265 (86%)	39 (13%)	3 (1%)	12	47
1	D	307/339 (91%)	264 (86%)	41 (13%)	2 (1%)	18	54
1	E	307/339 (91%)	264 (86%)	41 (13%)	2 (1%)	18	54
1	F	307/339 (91%)	265 (86%)	40 (13%)	2 (1%)	18	54
1	G	307/339 (91%)	266 (87%)	39 (13%)	2 (1%)	18	54
All	All	2149/2373 (91%)	1850 (86%)	284 (13%)	15 (1%)	20	54

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 ⓘ

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%)	176 (77%)	53 (23%)	1	6
1	B	229/269 (85%)	172 (75%)	57 (25%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	229/269 (85%)	173 (76%)	56 (24%)	1	5
1	D	229/269 (85%)	174 (76%)	55 (24%)	1	5
1	E	229/269 (85%)	175 (76%)	54 (24%)	1	5
1	F	229/269 (85%)	174 (76%)	55 (24%)	1	5
1	G	229/269 (85%)	177 (77%)	52 (23%)	1	6
All	All	1603/1883 (85%)	1221 (76%)	382 (24%)	2	5

All (382) 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	41	LEU
1	A	52	VAL
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	102	ILE
1	A	103	THR
1	A	107	LYS
1	A	108	GLU
1	A	111	LYS
1	A	112	LEU
1	A	119	THR
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	177	ARG
1	A	188	ASN
1	A	203	LEU

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Mol	Chain	Res	Type
1	A	204	LEU
1	A	206	GLN
1	A	210	MET
1	A	213	GLU
1	A	220	ILE
1	A	229	ARG
1	A	235	ARG
1	A	237	GLU
1	A	238	LEU
1	A	241	ARG
1	A	247	ARG
1	A	255	LEU
1	A	257	ASP
1	A	270	VAL
1	A	272	GLN
1	A	291	ILE
1	A	298	THR
1	A	299	ARG
1	A	300	LEU
1	A	301	TYR
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	41	LEU
1	B	52	VAL
1	B	58	LYS
1	B	59	GLU
1	B	60	LEU
1	B	61	ILE
1	B	77	GLU
1	B	81	LEU
1	B	102	ILE
1	B	103	THR
1	B	107	LYS
1	B	108	GLU
1	B	111	LYS

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Mol	Chain	Res	Type
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	161	ASP
1	B	177	ARG
1	B	188	ASN
1	B	203	LEU
1	B	204	LEU
1	B	206	GLN
1	B	210	MET
1	B	213	GLU
1	B	220	ILE
1	B	229	ARG
1	B	235	ARG
1	B	237	GLU
1	B	238	LEU
1	B	241	ARG
1	B	247	ARG
1	B	249	LEU
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
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

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Mol	Chain	Res	Type
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	102	ILE
1	C	103	THR
1	C	107	LYS
1	C	108	GLU
1	C	111	LYS
1	C	112	LEU
1	C	122	ILE
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	161	ASP
1	C	177	ARG
1	C	188	ASN
1	C	203	LEU
1	C	204	LEU
1	C	206	GLN
1	C	210	MET
1	C	213	GLU
1	C	219	LEU
1	C	220	ILE
1	C	229	ARG
1	C	235	ARG
1	C	237	GLU
1	C	238	LEU
1	C	241	ARG
1	C	247	ARG
1	C	255	LEU
1	C	257	ASP
1	C	270	VAL
1	C	272	GLN

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Mol	Chain	Res	Type
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	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	102	ILE
1	D	103	THR
1	D	107	LYS
1	D	108	GLU
1	D	111	LYS
1	D	112	LEU
1	D	122	ILE
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	177	ARG
1	D	188	ASN
1	D	203	LEU
1	D	204	LEU
1	D	206	GLN
1	D	210	MET

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Mol	Chain	Res	Type
1	D	213	GLU
1	D	219	LEU
1	D	220	ILE
1	D	229	ARG
1	D	235	ARG
1	D	237	GLU
1	D	238	LEU
1	D	241	ARG
1	D	247	ARG
1	D	255	LEU
1	D	257	ASP
1	D	270	VAL
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	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
1	E	102	ILE
1	E	103	THR
1	E	107	LYS
1	E	108	GLU
1	E	111	LYS
1	E	112	LEU

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Mol	Chain	Res	Type
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	177	ARG
1	E	188	ASN
1	E	203	LEU
1	E	204	LEU
1	E	206	GLN
1	E	210	MET
1	E	213	GLU
1	E	220	ILE
1	E	229	ARG
1	E	235	ARG
1	E	237	GLU
1	E	238	LEU
1	E	241	ARG
1	E	247	ARG
1	E	249	LEU
1	E	255	LEU
1	E	257	ASP
1	E	270	VAL
1	E	272	GLN
1	E	291	ILE
1	E	298	THR
1	E	299	ARG
1	E	300	LEU
1	E	301	TYR
1	E	316	ASP
1	E	319	CYS
1	E	320	LEU
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

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Mol	Chain	Res	Type
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	102	ILE
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	161	ASP
1	F	177	ARG
1	F	188	ASN
1	F	203	LEU
1	F	204	LEU
1	F	206	GLN
1	F	210	MET
1	F	213	GLU
1	F	219	LEU
1	F	220	ILE
1	F	229	ARG
1	F	235	ARG
1	F	237	GLU
1	F	238	LEU
1	F	241	ARG
1	F	247	ARG
1	F	255	LEU
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

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Mol	Chain	Res	Type
1	F	300	LEU
1	F	303	ARG
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	102	ILE
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	161	ASP
1	G	177	ARG
1	G	188	ASN
1	G	203	LEU
1	G	204	LEU
1	G	206	GLN
1	G	210	MET
1	G	213	GLU
1	G	220	ILE
1	G	229	ARG
1	G	235	ARG
1	G	237	GLU

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Mol	Chain	Res	Type
1	G	238	LEU
1	G	241	ARG
1	G	247	ARG
1	G	255	LEU
1	G	257	ASP
1	G	270	VAL
1	G	272	GLN
1	G	291	ILE
1	G	298	THR
1	G	299	ARG
1	G	300	LEU
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 (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	A	294	HIS
1	B	135	GLN
1	B	145	GLN
1	B	294	HIS
1	B	330	ASN
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
1	E	145	GLN
1	E	294	HIS
1	E	330	ASN
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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B	600	-	33,33,33	2.54	15 (45%)	45,52,52	2.14	14 (31%)
2	ANP	G	600	-	33,33,33	2.51	14 (42%)	45,52,52	2.26	18 (40%)
2	ANP	A	600	-	33,33,33	2.53	15 (45%)	45,52,52	2.14	14 (31%)
2	ANP	D	600	-	33,33,33	2.56	15 (45%)	45,52,52	2.13	14 (31%)
2	ANP	F	600	-	33,33,33	2.50	14 (42%)	45,52,52	2.14	15 (33%)
2	ANP	C	600	-	33,33,33	2.55	15 (45%)	45,52,52	2.12	14 (31%)
2	ANP	E	600	-	33,33,33	2.56	15 (45%)	45,52,52	2.14	14 (31%)

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	B	600	-	-	4/18/38/38	0/3/3/3

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

All (103) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	600	ANP	C5-C4	6.50	1.50	1.39
2	B	600	ANP	C5-C4	6.28	1.50	1.39
2	C	600	ANP	C5-C4	6.26	1.50	1.39
2	E	600	ANP	C5-C4	6.26	1.50	1.39
2	D	600	ANP	C5-C4	6.26	1.50	1.39
2	A	600	ANP	C5-C4	6.23	1.50	1.39
2	F	600	ANP	C5-C4	6.17	1.50	1.39
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	E	600	ANP	PA-O3A	4.97	1.64	1.59
2	D	600	ANP	PA-O3A	4.91	1.64	1.59
2	C	600	ANP	PA-O3A	4.83	1.64	1.59
2	B	600	ANP	PA-O3A	4.66	1.64	1.59
2	A	600	ANP	PA-O3A	4.62	1.64	1.59
2	F	600	ANP	PA-O3A	4.60	1.64	1.59
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	PG-O1G	4.41	1.52	1.46
2	G	600	ANP	PA-O3A	4.38	1.64	1.59
2	E	600	ANP	PG-O1G	4.38	1.52	1.46
2	F	600	ANP	PB-N3B	4.32	1.74	1.63
2	D	600	ANP	PG-O1G	4.31	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	ANP	PG-O1G	4.29	1.52	1.46
2	B	600	ANP	PG-O1G	4.29	1.52	1.46
2	A	600	ANP	PG-O1G	4.09	1.52	1.46
2	G	600	ANP	PG-O1G	4.08	1.52	1.46
2	D	600	ANP	PB-O3A	3.55	1.63	1.59
2	E	600	ANP	PB-O3A	3.53	1.63	1.59
2	A	600	ANP	PB-O1B	3.51	1.51	1.46
2	B	600	ANP	PB-O3A	3.45	1.63	1.59
2	F	600	ANP	PB-O1B	3.42	1.51	1.46
2	G	600	ANP	PB-O3A	3.40	1.63	1.59
2	C	600	ANP	PB-O3A	3.39	1.63	1.59
2	D	600	ANP	PB-O1B	3.34	1.51	1.46
2	A	600	ANP	PB-O3A	3.32	1.63	1.59
2	C	600	ANP	PB-O1B	3.30	1.51	1.46
2	E	600	ANP	PB-O1B	3.27	1.51	1.46
2	B	600	ANP	C5-C6	3.25	1.50	1.41
2	G	600	ANP	PB-O1B	3.22	1.51	1.46
2	G	600	ANP	C5-C6	3.20	1.49	1.41
2	A	600	ANP	C5-C6	3.20	1.49	1.41
2	B	600	ANP	PB-O1B	3.18	1.51	1.46
2	D	600	ANP	C5-C6	3.17	1.49	1.41
2	F	600	ANP	C5-C6	3.14	1.49	1.41
2	F	600	ANP	PB-O3A	3.14	1.63	1.59
2	E	600	ANP	C5-C6	3.11	1.49	1.41
2	C	600	ANP	C5-C6	3.10	1.49	1.41
2	A	600	ANP	C5-N7	-3.02	1.33	1.39
2	E	600	ANP	C5-N7	-3.01	1.33	1.39
2	D	600	ANP	C5-N7	-3.00	1.33	1.39
2	F	600	ANP	C5-N7	-3.00	1.33	1.39
2	C	600	ANP	C5-N7	-2.98	1.33	1.39
2	G	600	ANP	C4-N3	2.98	1.40	1.34
2	B	600	ANP	C5-N7	-2.95	1.33	1.39
2	G	600	ANP	C8-N7	2.68	1.36	1.31
2	F	600	ANP	PG-O3G	-2.50	1.50	1.56
2	B	600	ANP	PG-O3G	-2.49	1.50	1.56
2	B	600	ANP	C2-N1	2.49	1.38	1.33
2	D	600	ANP	C2-N1	2.49	1.38	1.33
2	C	600	ANP	PG-O3G	-2.49	1.50	1.56
2	E	600	ANP	PG-O3G	-2.49	1.50	1.56
2	E	600	ANP	C2-N1	2.48	1.38	1.33
2	F	600	ANP	C2-N1	2.45	1.38	1.33
2	A	600	ANP	C2-N1	2.45	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	ANP	C2-N1	2.44	1.38	1.33
2	D	600	ANP	PG-O3G	-2.40	1.50	1.56
2	A	600	ANP	PG-O3G	-2.40	1.50	1.56
2	A	600	ANP	C4-N3	2.36	1.38	1.34
2	F	600	ANP	C4-N3	2.35	1.38	1.34
2	C	600	ANP	C4-N3	2.33	1.38	1.34
2	D	600	ANP	C4-N3	2.33	1.38	1.34
2	G	600	ANP	PG-O3G	-2.32	1.50	1.56
2	B	600	ANP	C4-N3	2.31	1.38	1.34
2	G	600	ANP	PB-O2B	-2.31	1.50	1.56
2	E	600	ANP	C4-N3	2.25	1.38	1.34
2	B	600	ANP	PB-O2B	-2.16	1.51	1.56
2	C	600	ANP	PB-O2B	-2.15	1.51	1.56
2	G	600	ANP	C2-N1	2.14	1.37	1.33
2	E	600	ANP	PB-O2B	-2.14	1.51	1.56
2	A	600	ANP	PB-O2B	-2.14	1.51	1.56
2	F	600	ANP	PB-O2B	-2.13	1.51	1.56
2	D	600	ANP	PB-O2B	-2.11	1.51	1.56
2	B	600	ANP	C8-N7	2.11	1.35	1.31
2	A	600	ANP	C8-N7	2.08	1.35	1.31
2	C	600	ANP	C8-N7	2.06	1.35	1.31
2	E	600	ANP	C8-N7	2.05	1.35	1.31
2	F	600	ANP	C8-N7	2.04	1.35	1.31
2	A	600	ANP	C2-N3	2.04	1.37	1.33
2	D	600	ANP	C8-N7	2.03	1.35	1.31
2	G	600	ANP	C1'-N9	2.03	1.51	1.46
2	B	600	ANP	C2-N3	2.02	1.37	1.33
2	C	600	ANP	C2-N3	2.02	1.37	1.33
2	E	600	ANP	C2-N3	2.01	1.37	1.33
2	D	600	ANP	C2-N3	2.00	1.37	1.33

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	600	ANP	C5-C4-N3	-5.42	119.26	126.72
2	E	600	ANP	C5-C4-N3	-5.41	119.26	126.72
2	D	600	ANP	C5-C4-N3	-5.37	119.32	126.72
2	A	600	ANP	C5-C4-N3	-5.36	119.34	126.72
2	B	600	ANP	C5-C4-N3	-5.33	119.38	126.72
2	C	600	ANP	C5-C4-N3	-5.23	119.52	126.72
2	G	600	ANP	N3-C2-N1	-5.21	120.69	128.58
2	A	600	ANP	O2B-PB-O1B	4.72	120.00	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	ANP	N3-C2-N1	-4.62	121.59	128.58
2	E	600	ANP	N3-C2-N1	-4.60	121.62	128.58
2	G	600	ANP	C5-C4-N3	-4.60	120.39	126.72
2	B	600	ANP	N3-C2-N1	-4.59	121.64	128.58
2	C	600	ANP	N3-C2-N1	-4.58	121.65	128.58
2	D	600	ANP	N3-C2-N1	-4.56	121.69	128.58
2	F	600	ANP	N3-C2-N1	-4.55	121.69	128.58
2	F	600	ANP	N3-C4-N9	4.47	134.77	127.17
2	E	600	ANP	N3-C4-N9	4.45	134.73	127.17
2	A	600	ANP	N3-C4-N9	4.44	134.71	127.17
2	B	600	ANP	N3-C4-N9	4.41	134.66	127.17
2	C	600	ANP	N3-C4-N9	4.39	134.64	127.17
2	C	600	ANP	O2B-PB-O1B	4.38	119.27	109.87
2	D	600	ANP	N3-C4-N9	4.38	134.62	127.17
2	B	600	ANP	O2B-PB-O1B	4.38	119.26	109.87
2	F	600	ANP	O2B-PB-O1B	4.38	119.25	109.87
2	G	600	ANP	N3-C4-N9	4.34	134.54	127.17
2	D	600	ANP	O2B-PB-O1B	4.32	119.14	109.87
2	E	600	ANP	O2B-PB-O1B	4.32	119.14	109.87
2	G	600	ANP	O2B-PB-O1B	4.23	118.95	109.87
2	G	600	ANP	C2-N3-C4	4.04	121.69	111.83
2	G	600	ANP	O1G-PG-N3B	-4.03	105.84	111.77
2	A	600	ANP	C2-N3-C4	3.94	121.46	111.83
2	F	600	ANP	C2-N3-C4	3.94	121.45	111.83
2	E	600	ANP	C2-N3-C4	3.92	121.41	111.83
2	B	600	ANP	C2-N3-C4	3.92	121.40	111.83
2	D	600	ANP	C2-N3-C4	3.91	121.38	111.83
2	C	600	ANP	C2-N3-C4	3.85	121.22	111.83
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
2	G	600	ANP	O5'-C5'-C4'	3.58	121.17	108.99
2	B	600	ANP	O3A-PB-N3B	3.49	116.28	106.59
2	G	600	ANP	O3A-PB-N3B	3.40	116.02	106.59
2	F	600	ANP	O1G-PG-N3B	-3.34	106.86	111.77
2	A	600	ANP	O3A-PB-N3B	3.31	115.78	106.59
2	B	600	ANP	O1G-PG-N3B	-3.18	107.09	111.77
2	G	600	ANP	C2-N1-C6	3.08	123.79	118.73
2	F	600	ANP	O5'-C5'-C4'	3.01	119.25	108.99
2	D	600	ANP	O5'-C5'-C4'	2.99	119.18	108.99
2	B	600	ANP	O5'-C5'-C4'	2.99	119.16	108.99
2	C	600	ANP	O5'-C5'-C4'	2.98	119.14	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	A	600	ANP	O1G-PG-N3B	-2.95	107.42	111.77
2	E	600	ANP	O1G-PG-N3B	-2.95	107.43	111.77
2	C	600	ANP	O1G-PG-N3B	-2.92	107.47	111.77
2	A	600	ANP	O5'-C5'-C4'	2.89	118.83	108.99
2	E	600	ANP	O5'-C5'-C4'	2.86	118.72	108.99
2	B	600	ANP	C2-N1-C6	2.64	123.06	118.73
2	C	600	ANP	C2-N1-C6	2.64	123.06	118.73
2	E	600	ANP	C2-N1-C6	2.63	123.06	118.73
2	B	600	ANP	O2'-C2'-C3'	2.62	120.22	111.82
2	C	600	ANP	O2'-C2'-C3'	2.60	120.16	111.82
2	E	600	ANP	O2'-C2'-C3'	2.60	120.14	111.82
2	D	600	ANP	C2-N1-C6	2.60	122.99	118.73
2	A	600	ANP	C2-N1-C6	2.58	122.97	118.73
2	D	600	ANP	O2'-C2'-C3'	2.57	120.07	111.82
2	F	600	ANP	C2-N1-C6	2.56	122.93	118.73
2	F	600	ANP	O2'-C2'-C3'	2.52	119.91	111.82
2	A	600	ANP	O2'-C2'-C3'	2.52	119.90	111.82
2	G	600	ANP	C4-N9-C1'	-2.51	120.77	126.63
2	E	600	ANP	C3'-C2'-C1'	2.50	106.19	101.46
2	G	600	ANP	O2'-C2'-C3'	2.48	119.77	111.82
2	D	600	ANP	C3'-C2'-C1'	2.47	106.13	101.46
2	B	600	ANP	C3'-C2'-C1'	2.46	106.12	101.46
2	A	600	ANP	C3'-C2'-C1'	2.41	106.01	101.46
2	B	600	ANP	C4-C5-N7	-2.40	107.84	110.58
2	A	600	ANP	C4-C5-N7	-2.39	107.85	110.58
2	D	600	ANP	C4-C5-N7	-2.37	107.88	110.58
2	C	600	ANP	C3'-C2'-C1'	2.36	105.92	101.46
2	G	600	ANP	O4'-C1'-N9	2.36	112.61	108.09
2	E	600	ANP	C4-C5-N7	-2.34	107.91	110.58
2	A	600	ANP	O2G-PG-O3G	2.33	113.86	107.59
2	F	600	ANP	C3'-C2'-C1'	2.33	105.87	101.46
2	F	600	ANP	C4-C5-N7	-2.32	107.94	110.58
2	G	600	ANP	N6-C6-N1	2.24	123.36	118.38
2	E	600	ANP	O3'-C3'-C2'	2.23	118.97	111.82
2	C	600	ANP	C4-C5-N7	-2.22	108.05	110.58
2	D	600	ANP	O3'-C3'-C2'	2.20	118.88	111.82
2	D	600	ANP	O2G-PG-O3G	2.13	113.31	107.59
2	F	600	ANP	O2G-PG-O3G	2.12	113.30	107.59
2	G	600	ANP	C5-C6-N6	-2.12	118.03	123.29
2	A	600	ANP	O3'-C3'-C2'	2.12	118.62	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	600	ANP	O3'-C3'-C2'	2.11	118.58	111.82
2	G	600	ANP	O2G-PG-O1G	2.11	118.73	113.45
2	F	600	ANP	O2G-PG-O1G	2.06	118.62	113.45
2	G	600	ANP	C6-C5-N7	2.06	136.06	132.09
2	G	600	ANP	C1'-N9-C8	2.06	131.67	127.09
2	F	600	ANP	O3'-C3'-C2'	2.05	118.39	111.82
2	B	600	ANP	O3'-C3'-C2'	2.05	118.38	111.82
2	C	600	ANP	O2G-PG-O3G	2.04	113.07	107.59
2	B	600	ANP	O2G-PG-O3G	2.02	113.03	107.59
2	C	600	ANP	O3'-C3'-C2'	2.02	118.29	111.82
2	E	600	ANP	O2G-PG-O3G	2.01	112.98	107.59

There are no chirality outliers.

All (34) 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	A	600	ANP	C2'-C1'-N9-C8
2	B	600	ANP	C2'-C1'-N9-C8
2	D	600	ANP	C2'-C1'-N9-C8
2	E	600	ANP	C2'-C1'-N9-C8
2	F	600	ANP	C2'-C1'-N9-C8
2	C	600	ANP	C2'-C1'-N9-C8
2	G	600	ANP	C3'-C4'-C5'-O5'
2	G	600	ANP	C2'-C1'-N9-C8
2	E	600	ANP	C5'-O5'-PA-O1A
2	A	600	ANP	C2'-C1'-N9-C4
2	B	600	ANP	C2'-C1'-N9-C4
2	C	600	ANP	C2'-C1'-N9-C4
2	D	600	ANP	C2'-C1'-N9-C4
2	E	600	ANP	C2'-C1'-N9-C4
2	F	600	ANP	C2'-C1'-N9-C4
2	G	600	ANP	C2'-C1'-N9-C4
2	B	600	ANP	O4'-C1'-N9-C8
2	D	600	ANP	O4'-C1'-N9-C8

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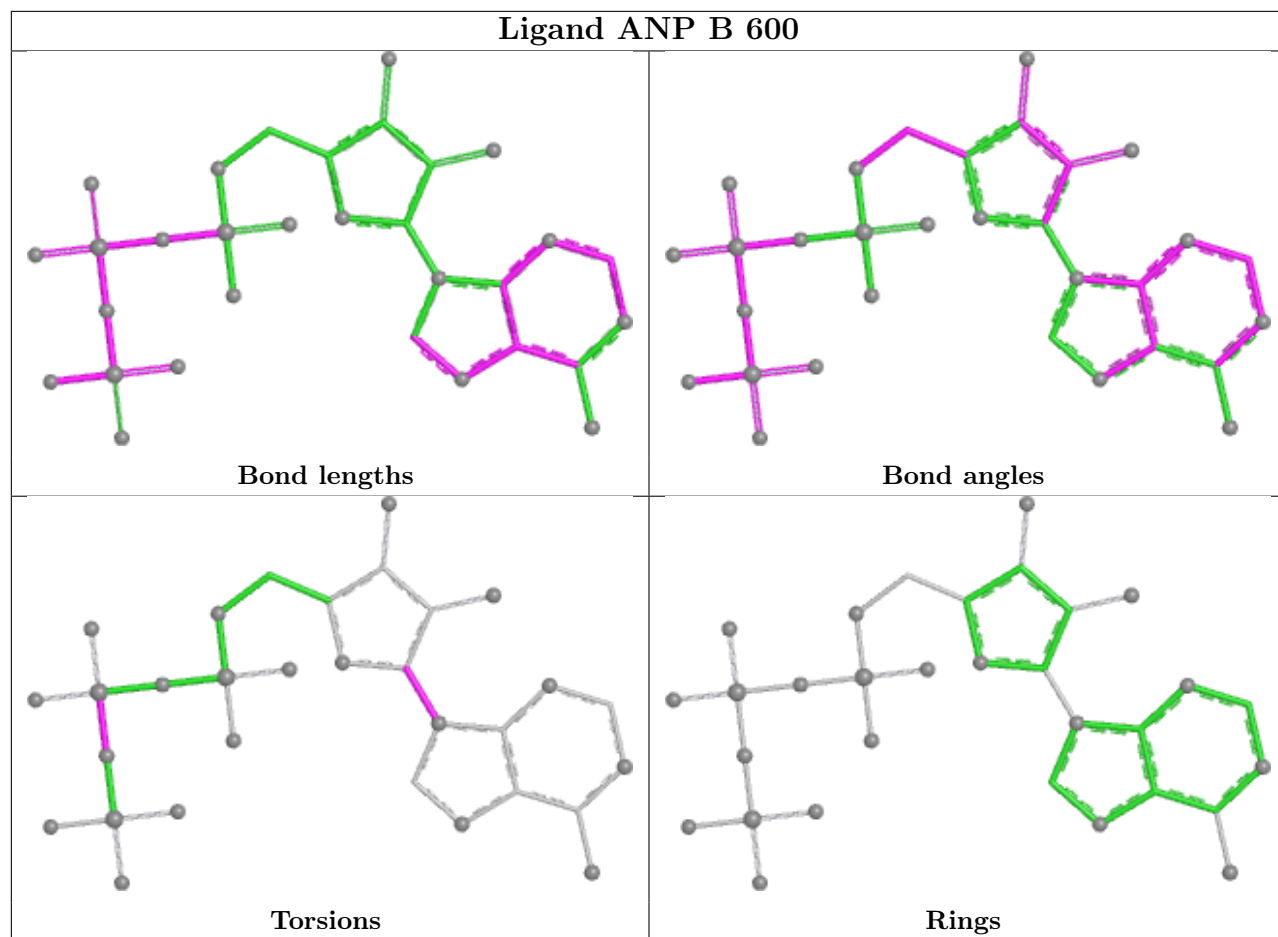
Mol	Chain	Res	Type	Atoms
2	E	600	ANP	O4'-C1'-N9-C8
2	F	600	ANP	O4'-C1'-N9-C8
2	G	600	ANP	O4'-C1'-N9-C8
2	F	600	ANP	O4'-C4'-C5'-O5'
2	A	600	ANP	O4'-C1'-N9-C8
2	C	600	ANP	O4'-C1'-N9-C8
2	A	600	ANP	O4'-C4'-C5'-O5'
2	D	600	ANP	O4'-C4'-C5'-O5'

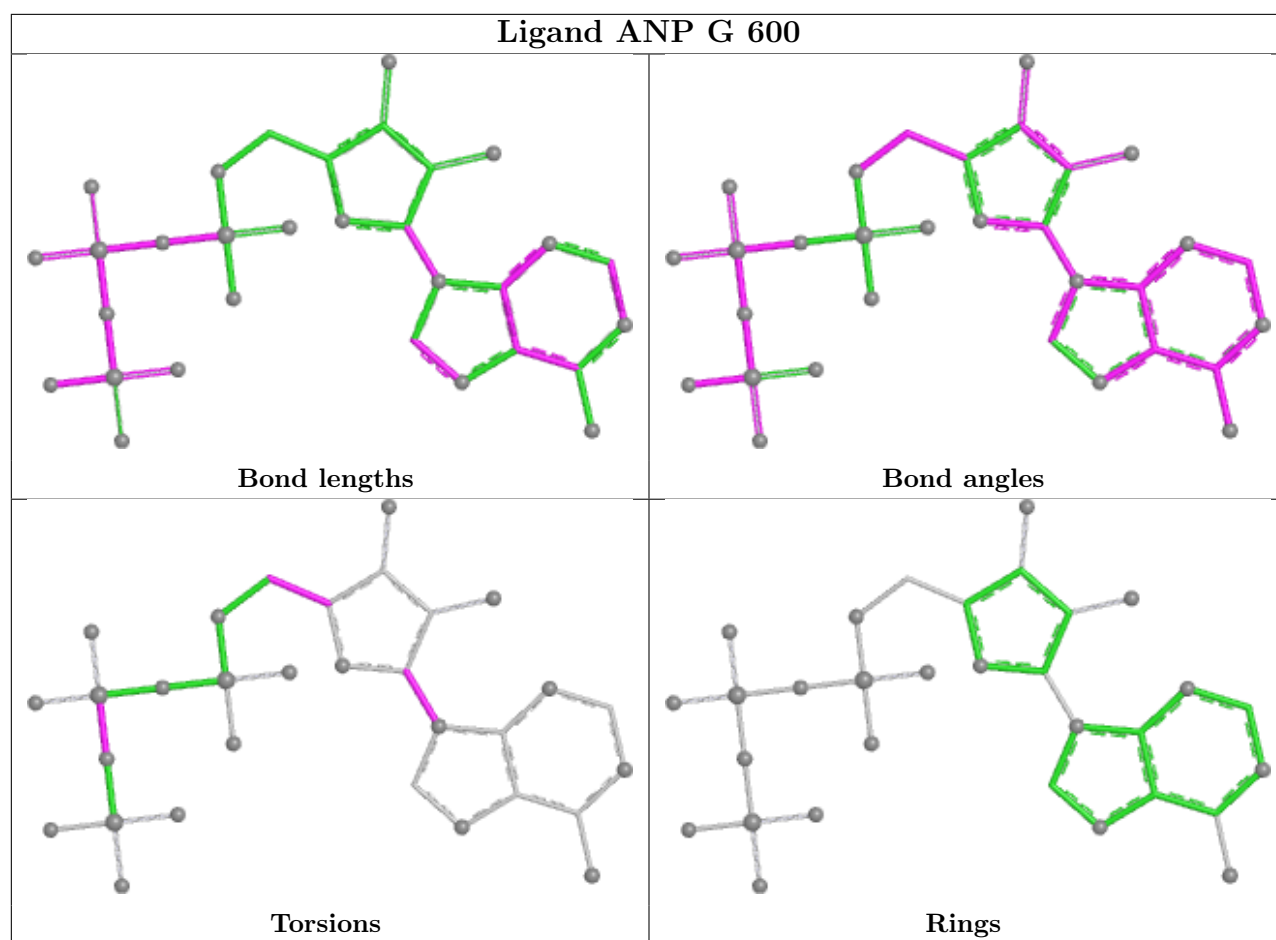
There are no ring outliers.

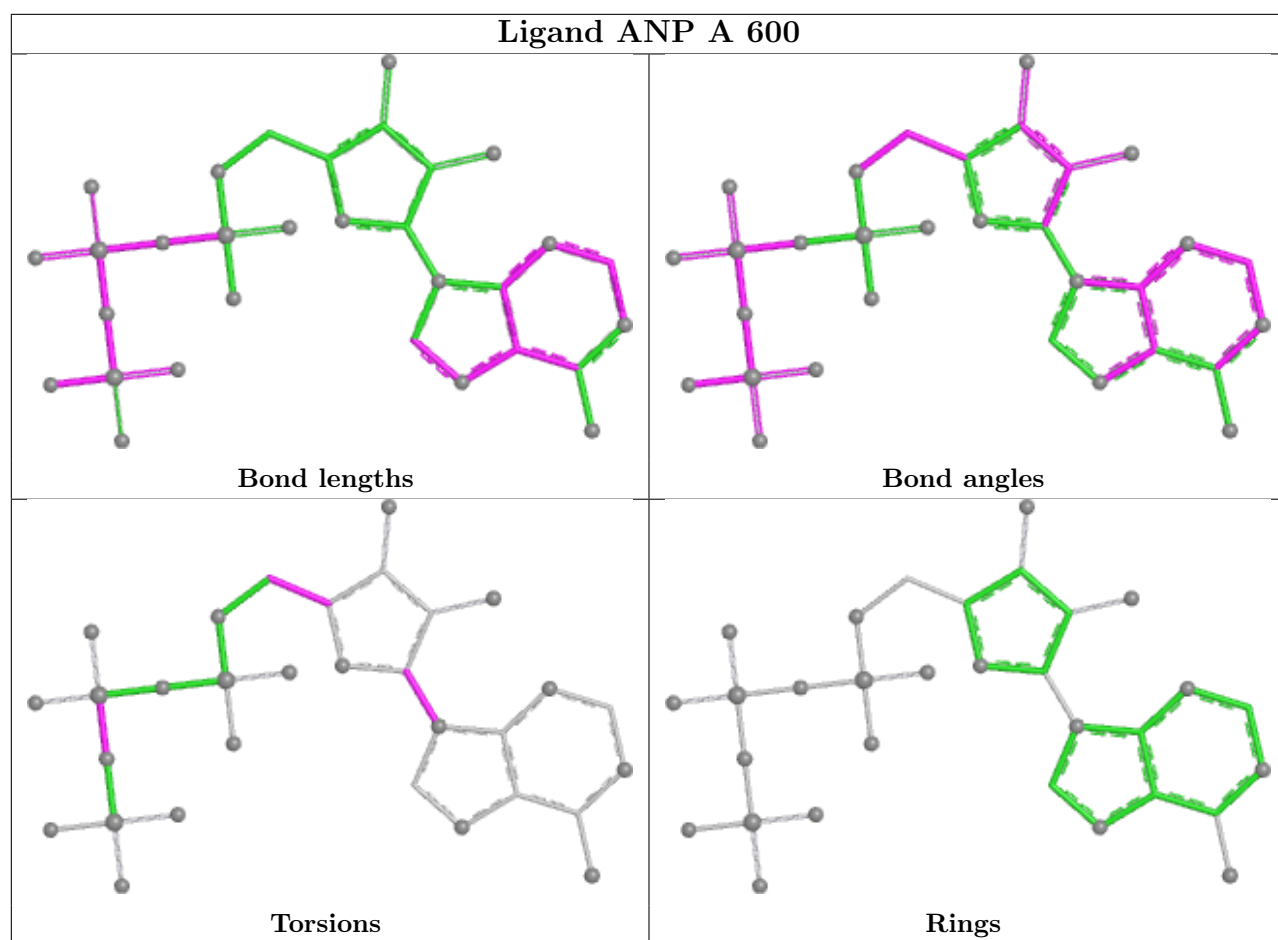
5 monomers are involved in 5 short contacts:

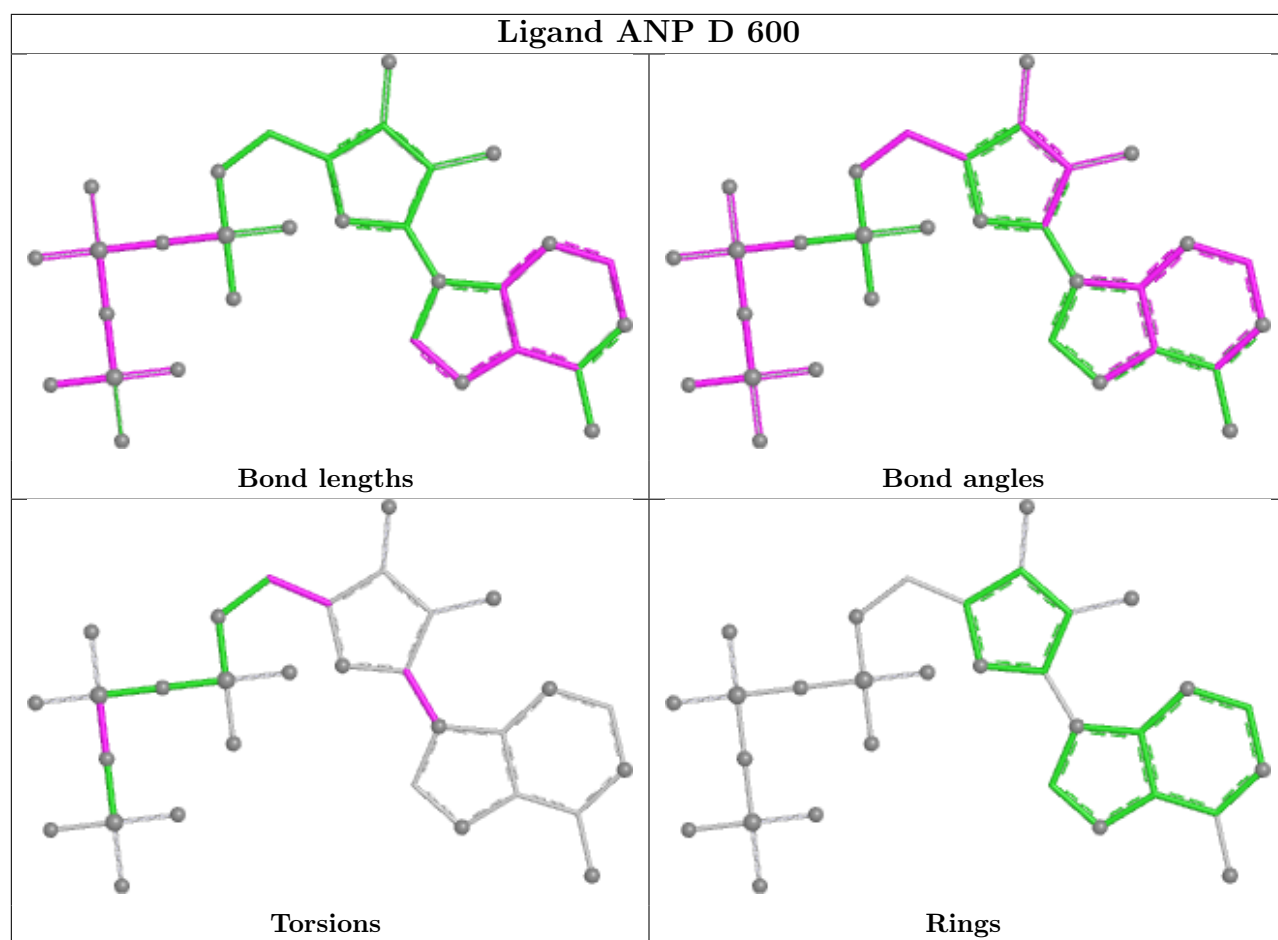
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	ANP	1	0
2	D	600	ANP	1	0
2	F	600	ANP	1	0
2	C	600	ANP	1	0
2	E	600	ANP	1	0

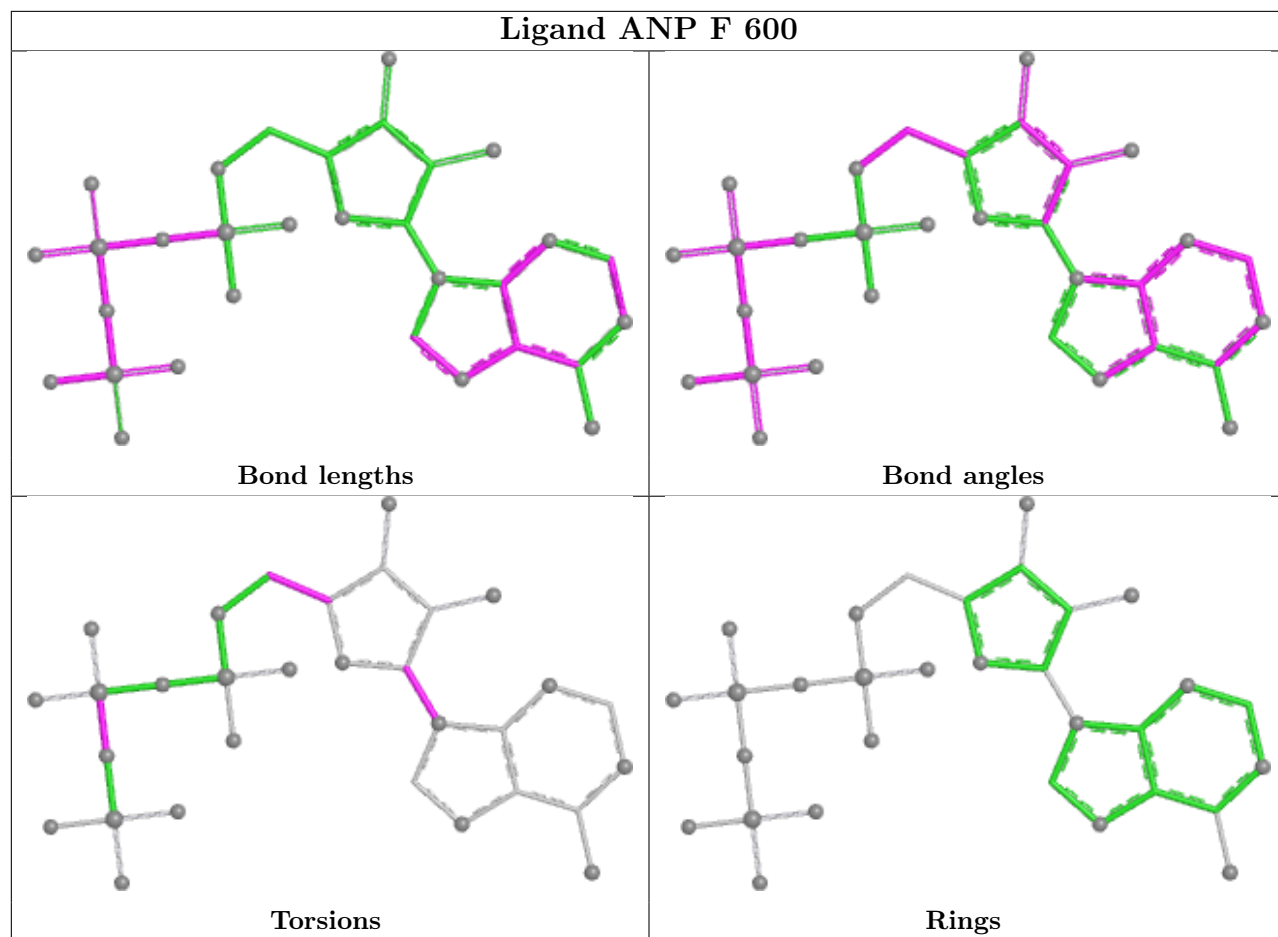
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

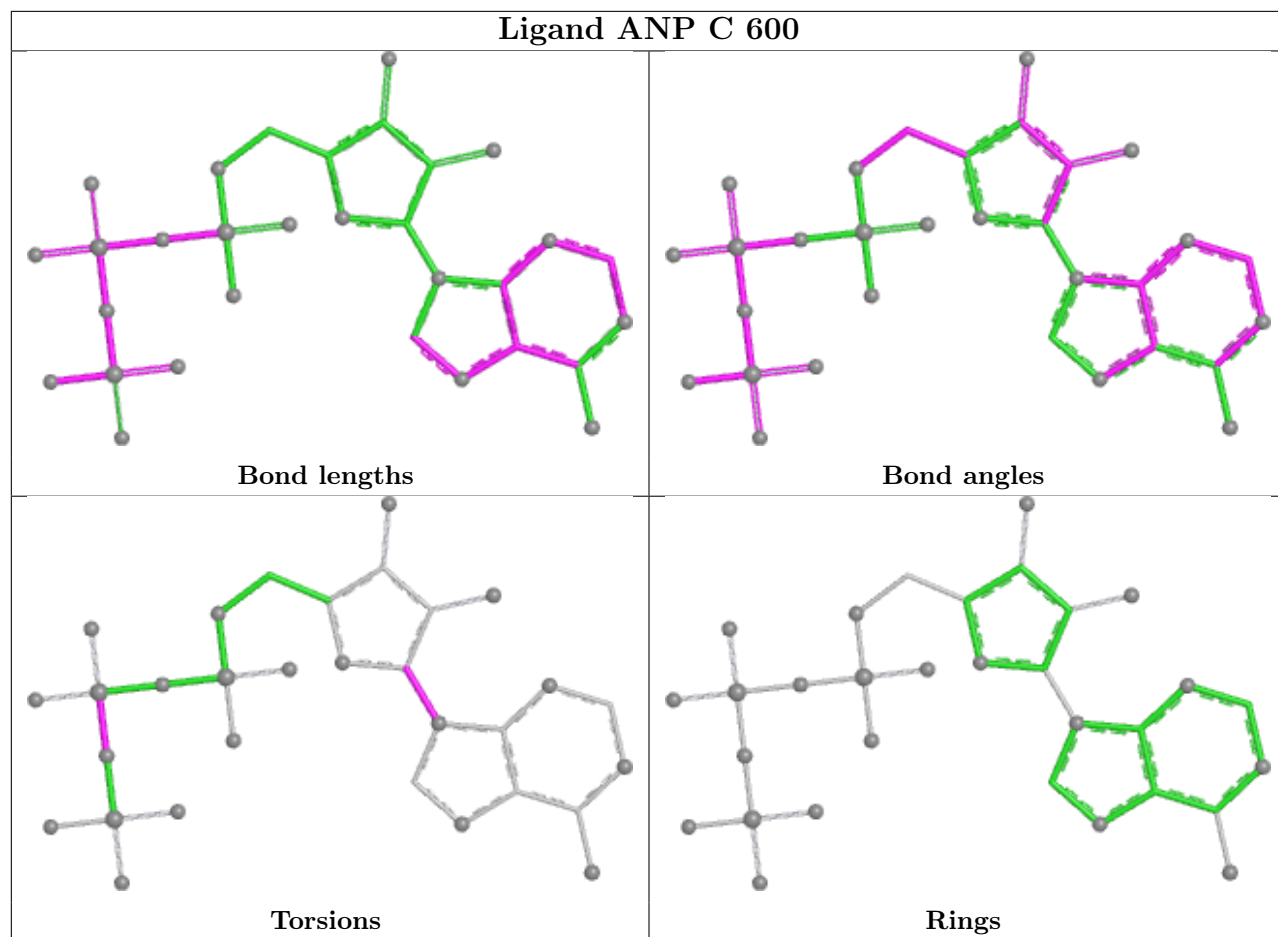


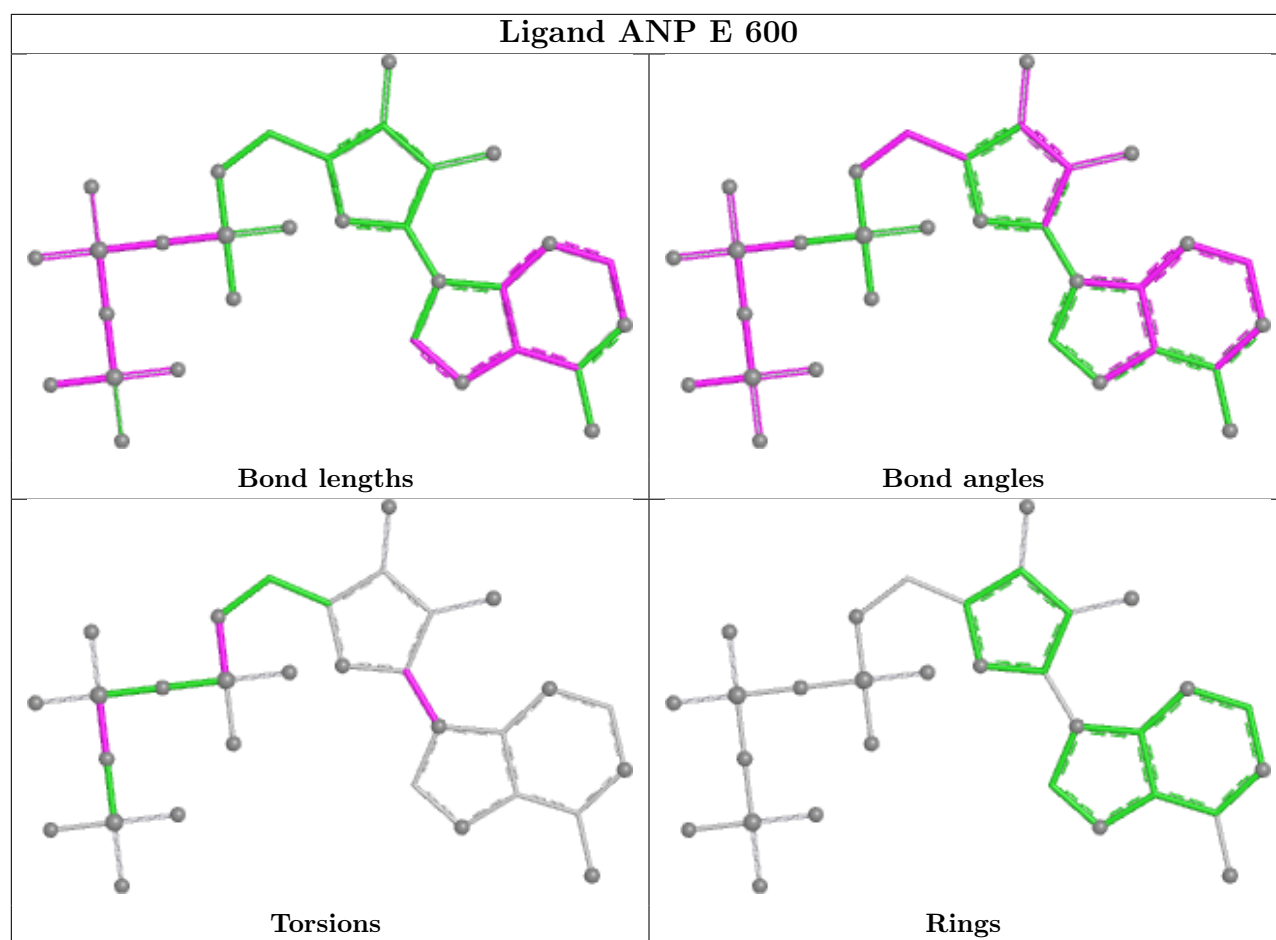












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

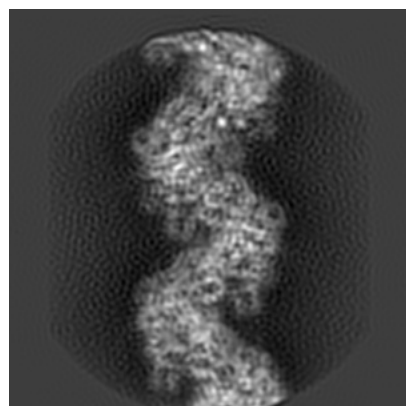
6 Map visualisation [i](#)

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

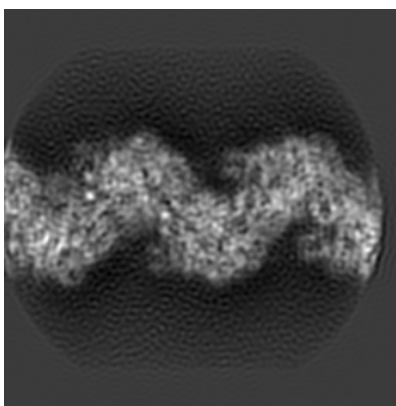
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

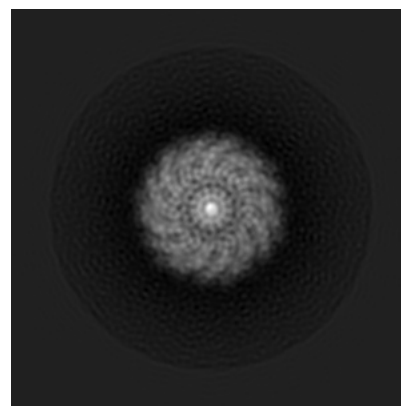
6.1.1 Primary map



X

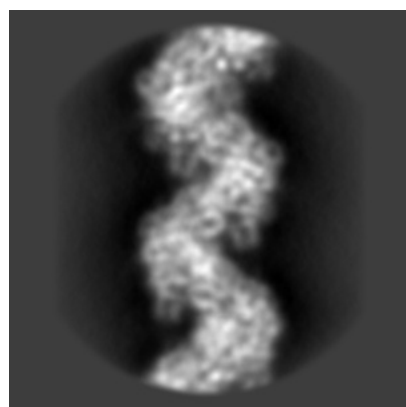


Y

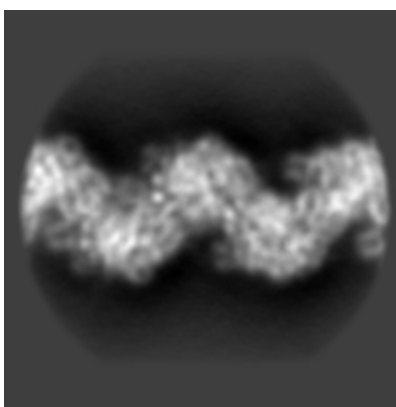


Z

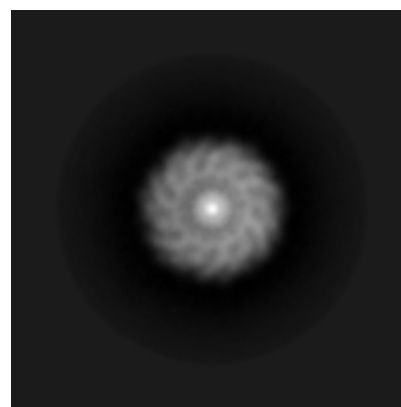
6.1.2 Raw map



X



Y

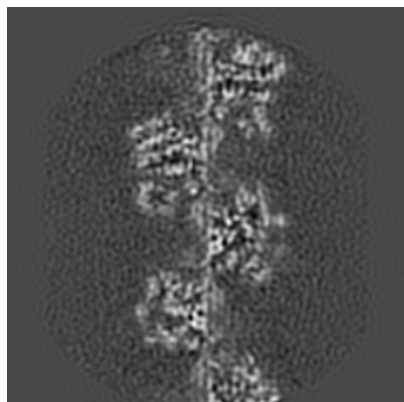


Z

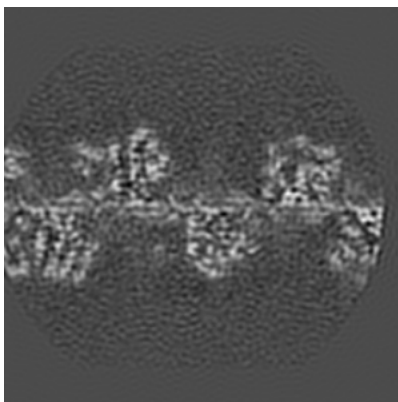
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

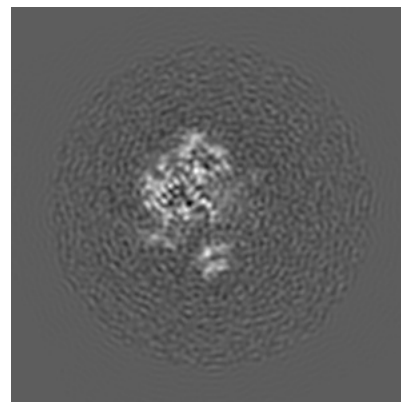
6.2.1 Primary map



X Index: 128

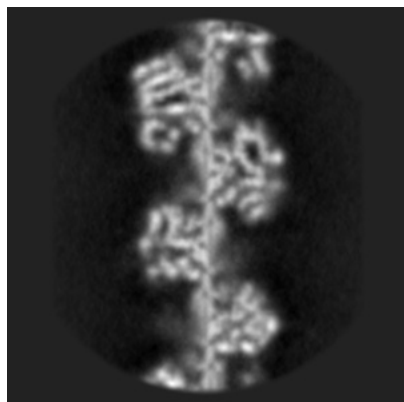


Y Index: 128

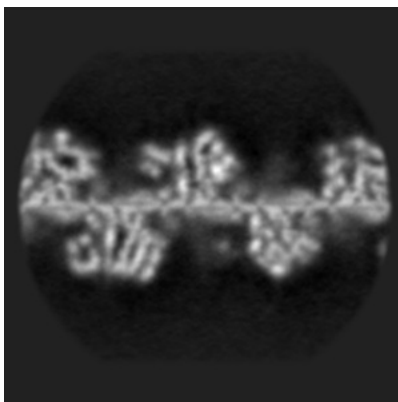


Z Index: 128

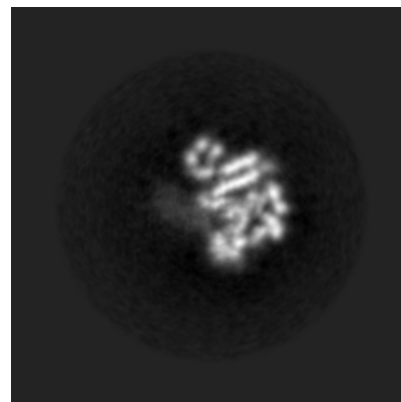
6.2.2 Raw map



X Index: 100



Y Index: 100

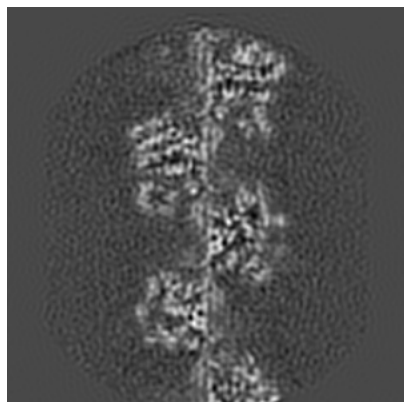


Z Index: 100

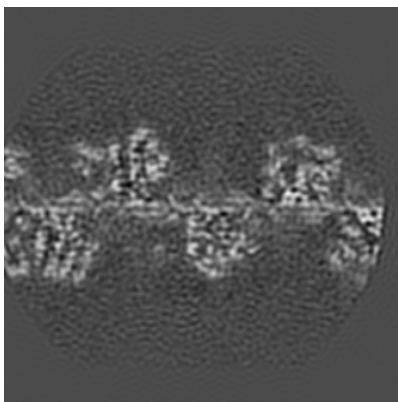
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

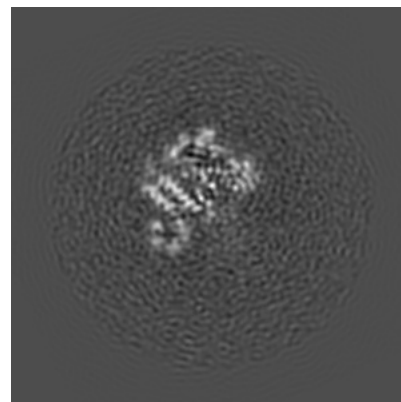
6.3.1 Primary map



X Index: 128

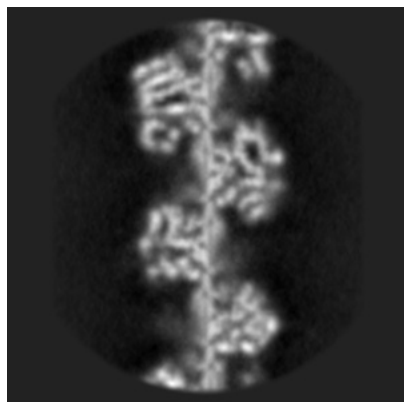


Y Index: 128

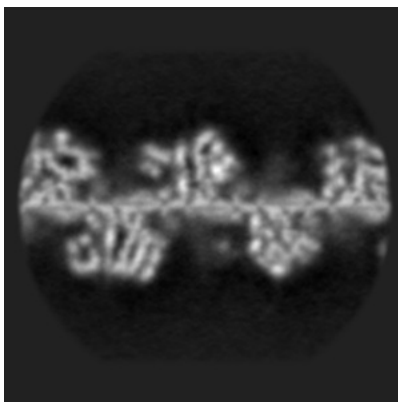


Z Index: 118

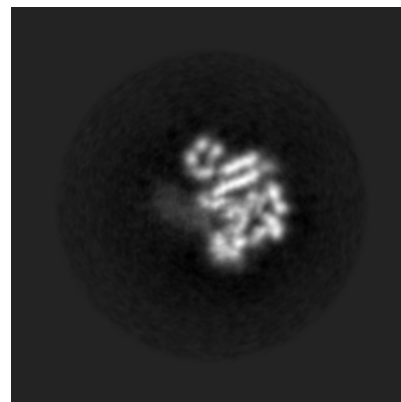
6.3.2 Raw map



X Index: 100



Y Index: 100

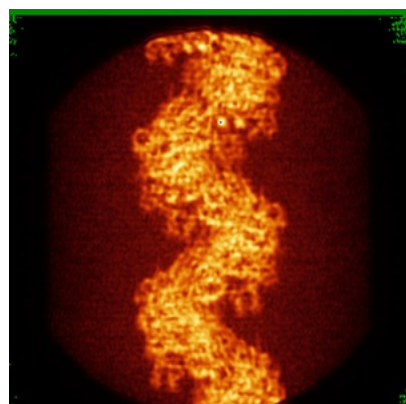


Z Index: 100

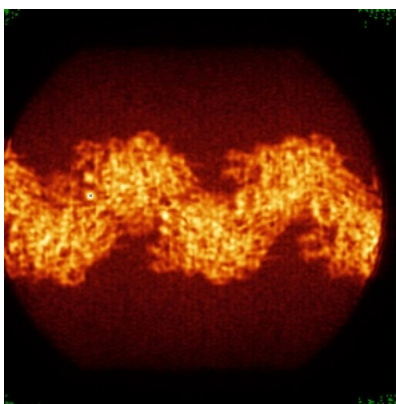
The images above show the largest variance slices of the map in three orthogonal directions.

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

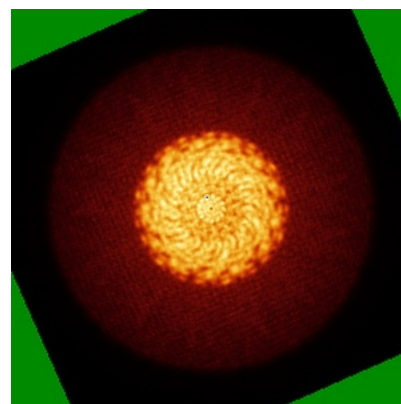
6.4.1 Primary map



X



Y

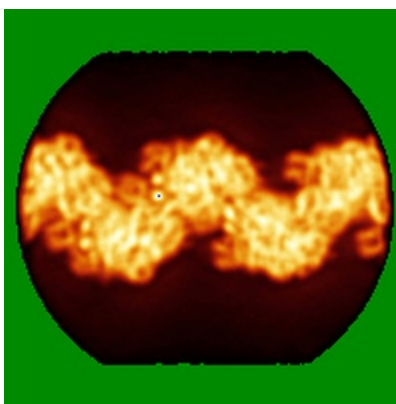


Z

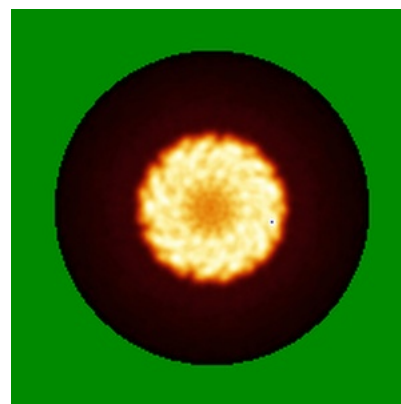
6.4.2 Raw map



X



Y

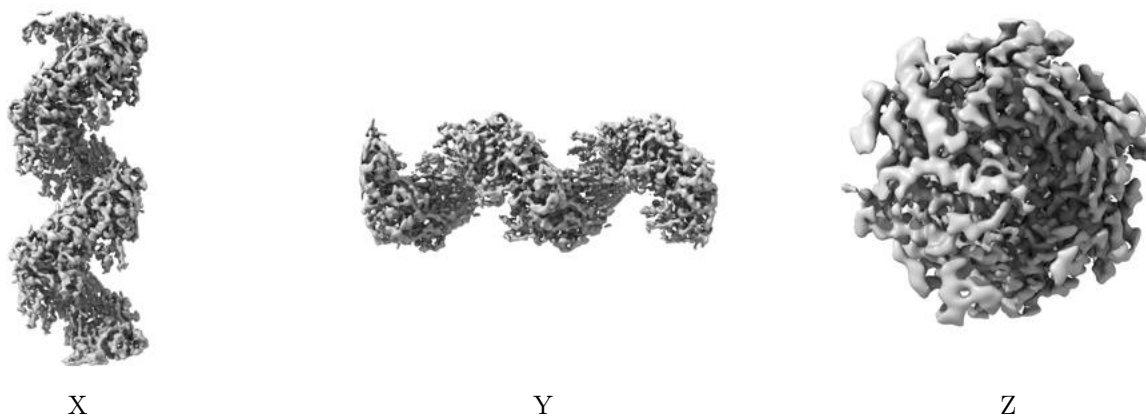


Z

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.

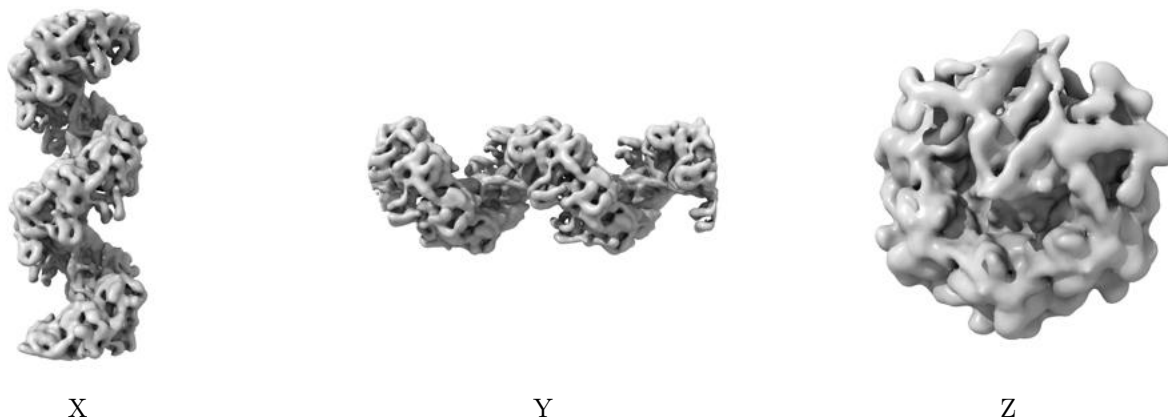
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. 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.

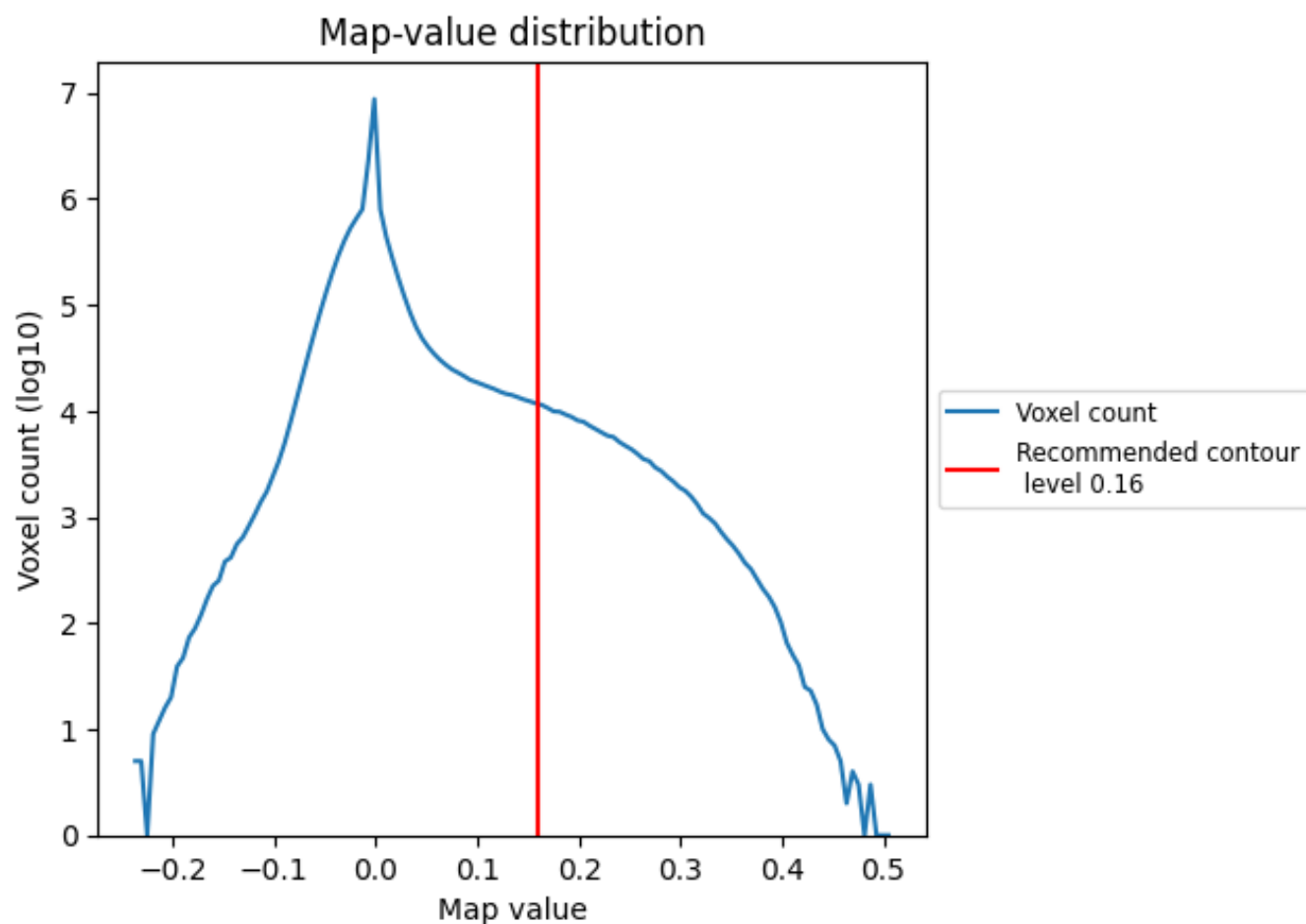
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

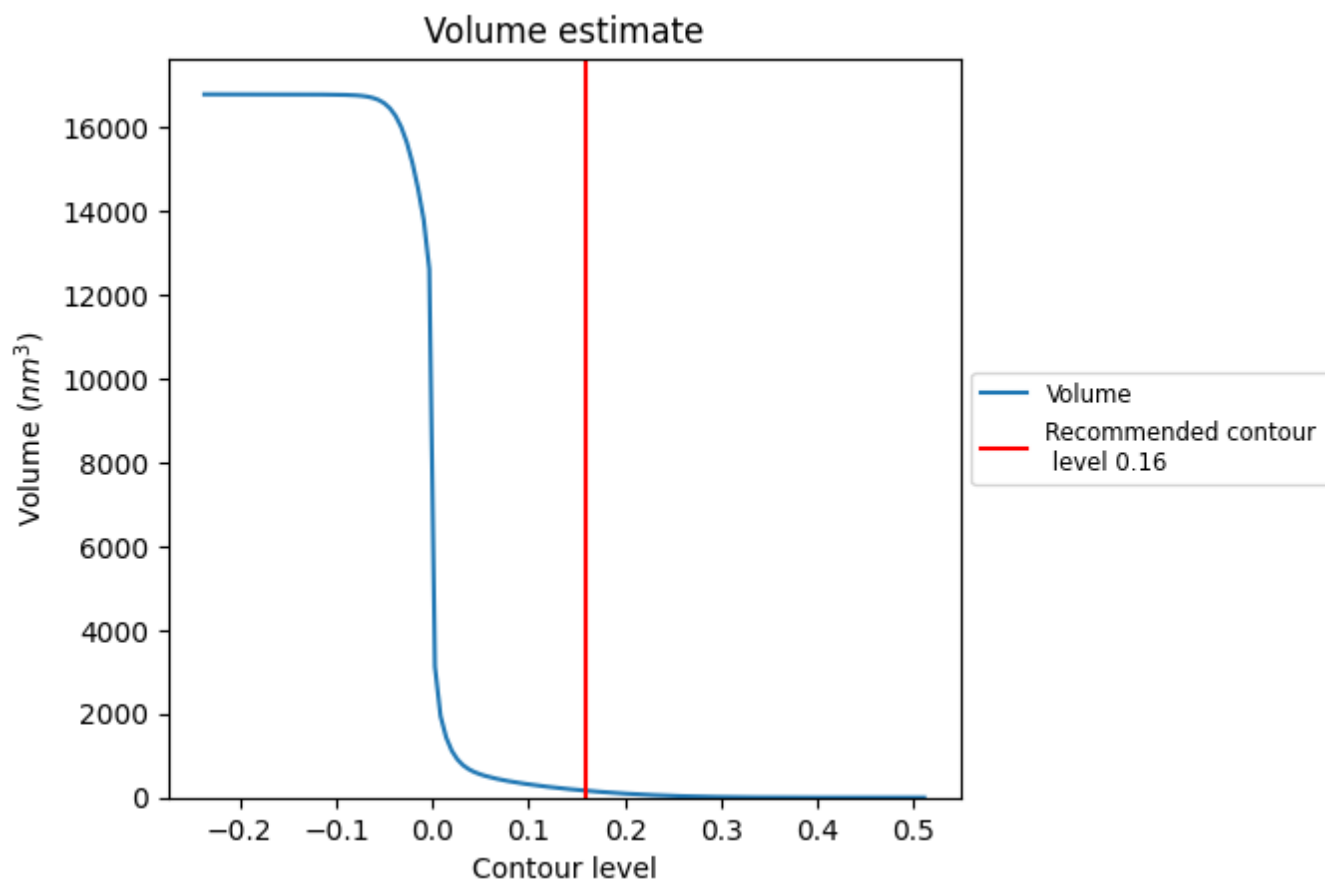
This section contains the results of statistical analysis of the map.

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.

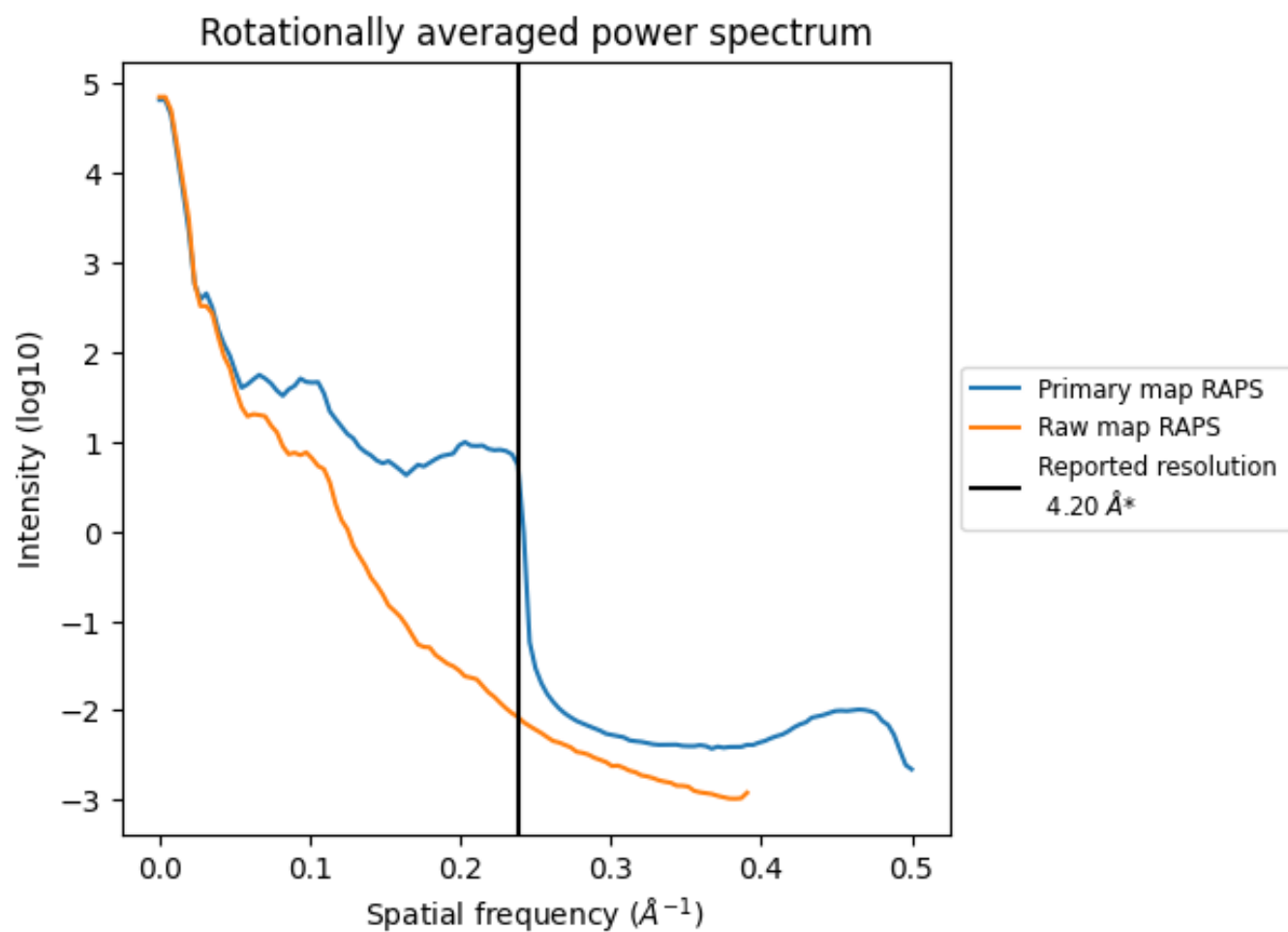
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 164 nm³; 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 ⓘ

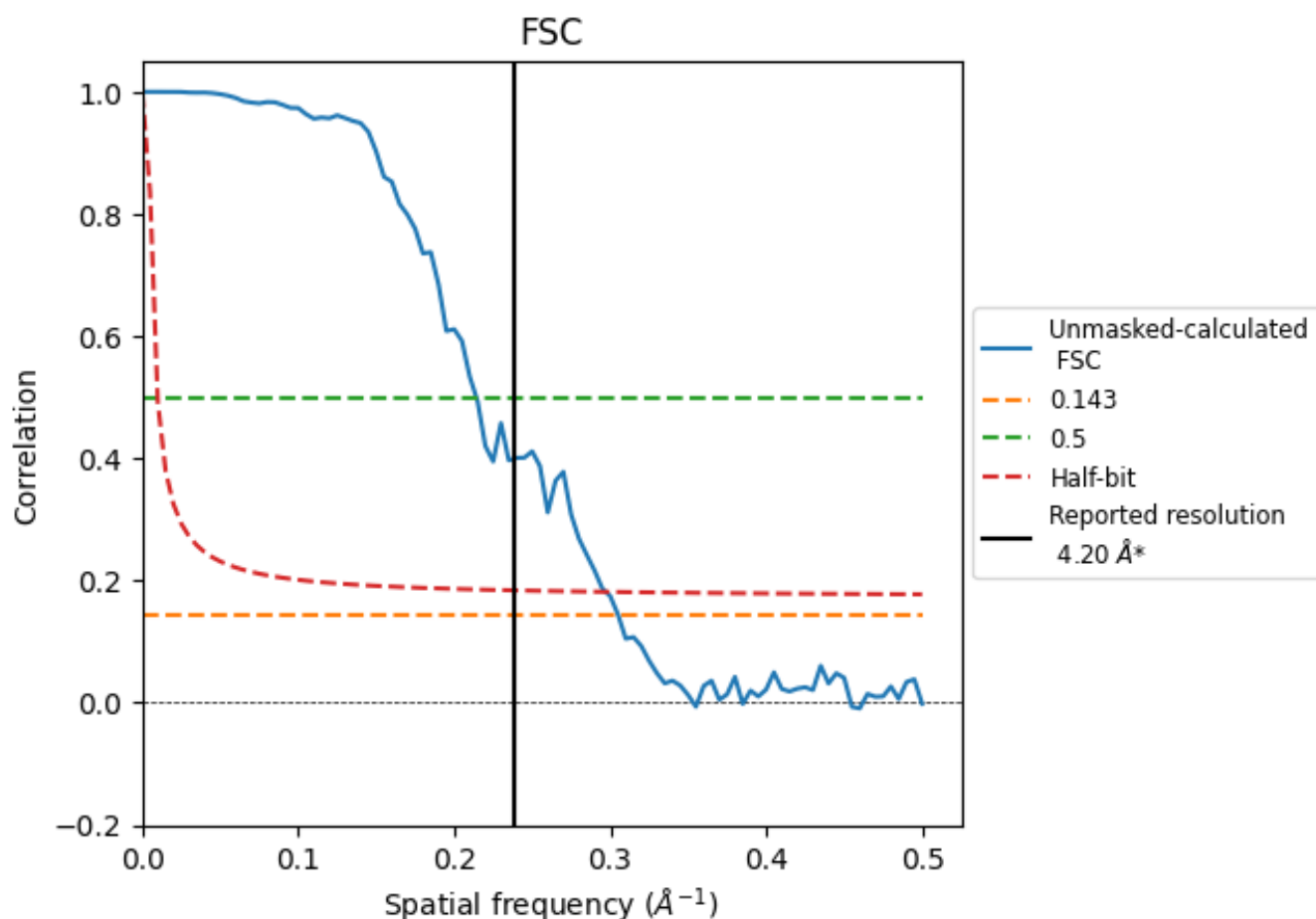


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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

8.2 Resolution estimates [i](#)

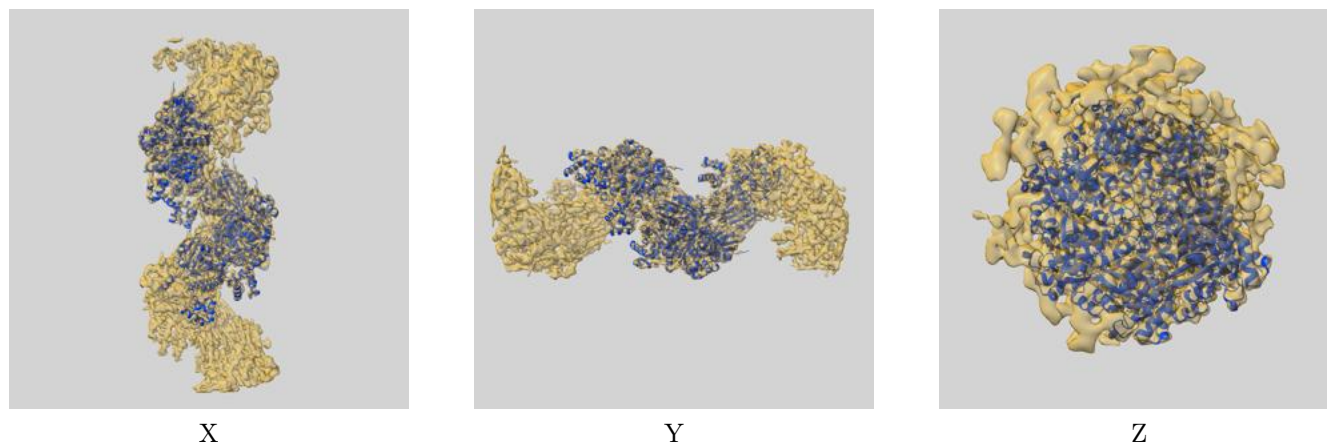
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.28	4.67	3.37

*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](#)

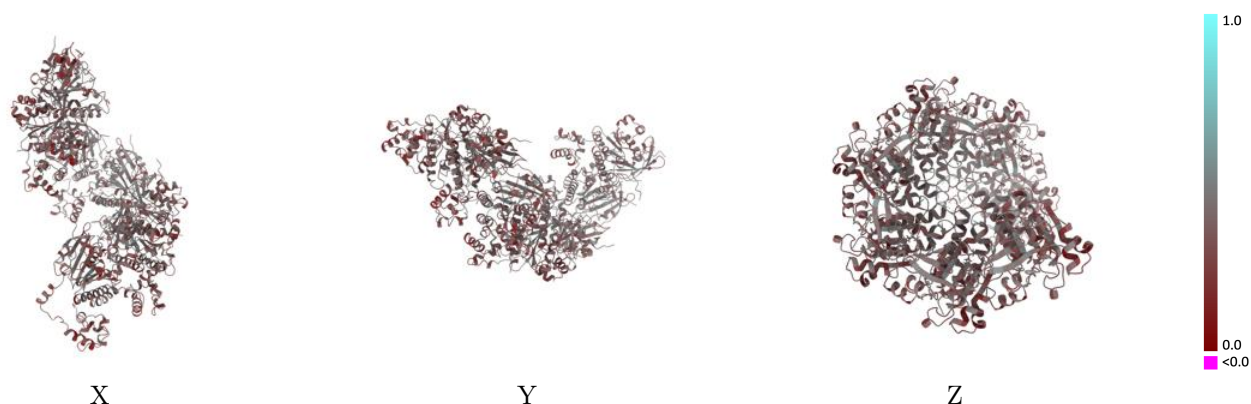
This section contains information regarding the fit between EMDB map EMD-8183 and PDB model 5NP7. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



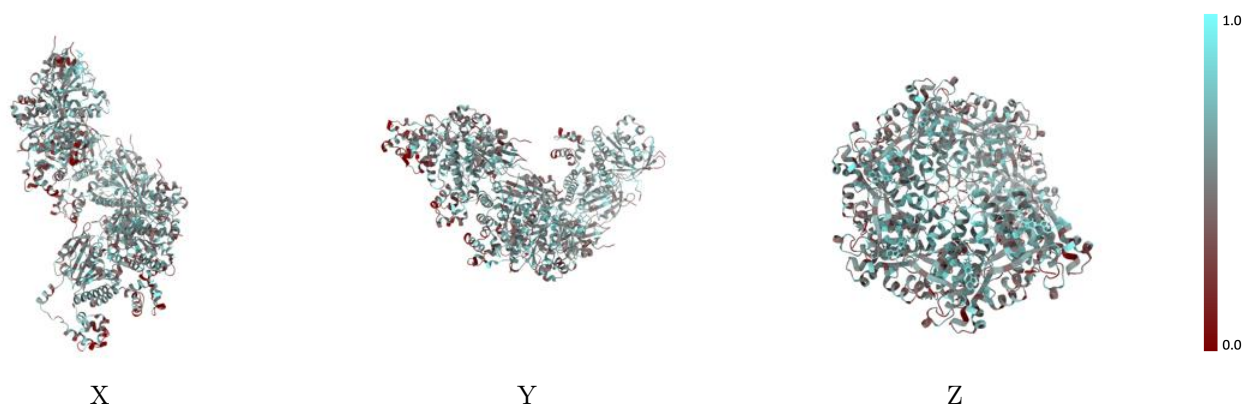
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



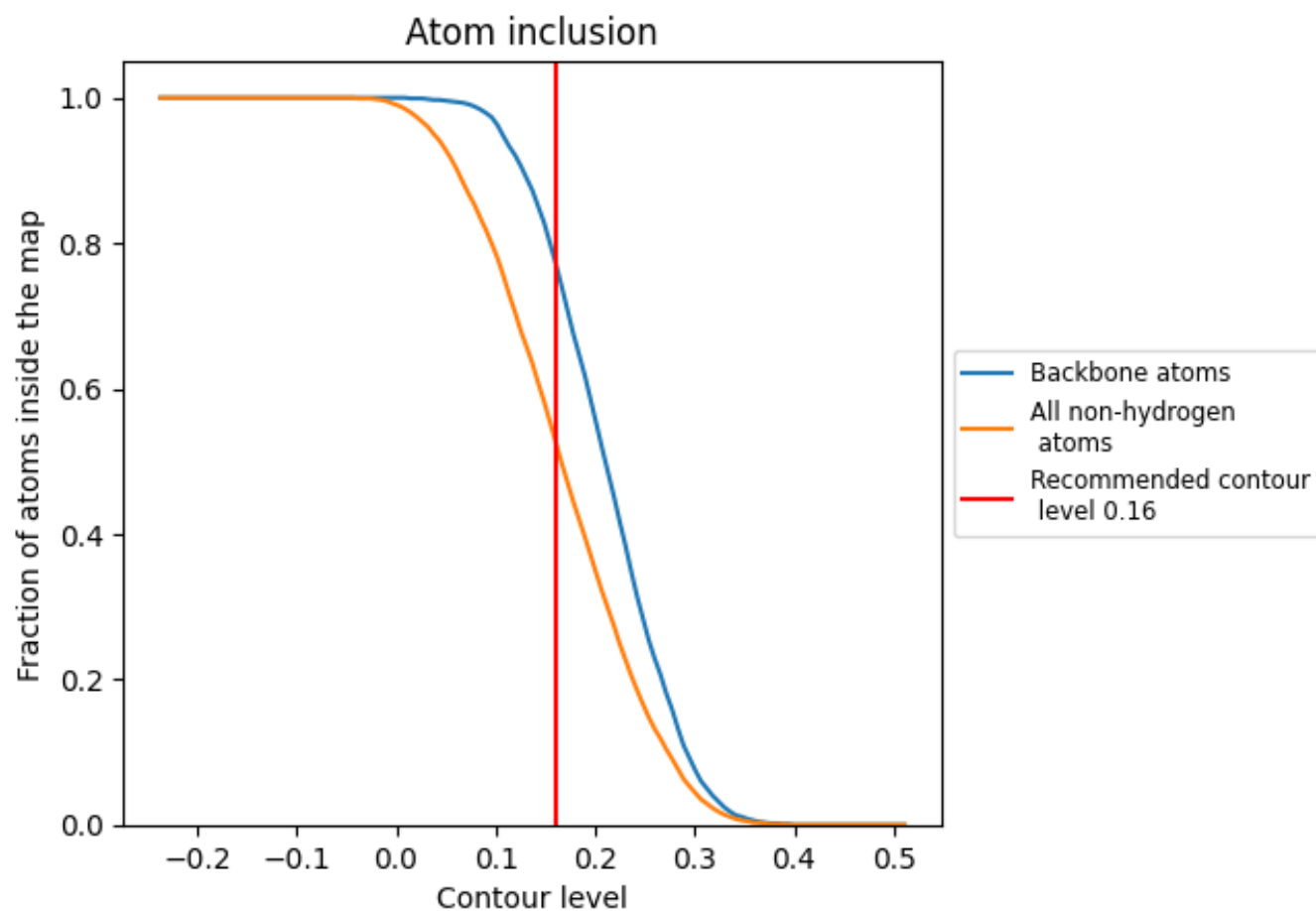
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

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 ⓘ

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	0.5280	0.3670
A	0.5270	0.3630
B	0.5240	0.3700
C	0.5310	0.3710
D	0.5340	0.3710
E	0.5300	0.3690
F	0.5230	0.3640
G	0.5240	0.3630

1.0

0.0

<0.0