Full wwPDB EM Validation Report ⓘ

Nov 5, 2022 – 01:32 PM EDT

PDB ID	:	5VY8
EMDB ID	:	EMD-8744
Title	:	S. cerevisiae Hsp104-ADP complex
Authors	:	Gates, S.N.; Yokom, A.L.; Lin, J.-B.; Jackrel, M.E.; Rizo, A.N.; Kendsersky, N.M.; Buell, C.E.; Sweeny, E.A.; Chuang, E.; Torrente, M.P.; Mack, K.L.; Su, M.; Shorter, J.; Southworth, D.R.
Deposited on	:	2017-05-24
Resolution	:	5.60 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:

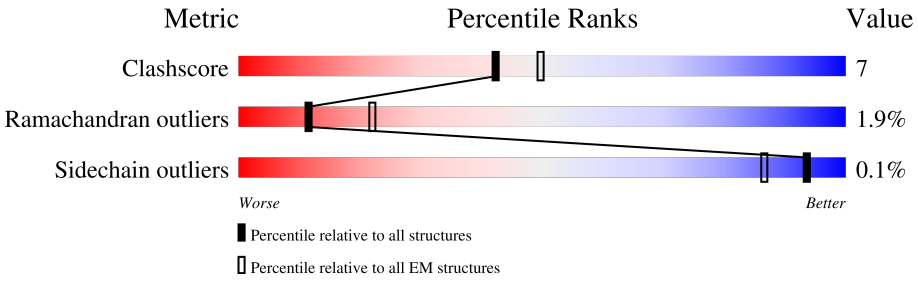
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 5.60 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	908	34% 55% 7% • 36%
1	B	908	11% 53% 9% • 36%
1	C	908	20% 67% 10% • 22%
1	D	908	15% 66% 11% • 22%
1	E	908	20% 66% 11% • 22%
1	F	908	23% 55% 8% 36%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	F	1001	-	-	X	-
2	ADP	F	1002	-	-	X	-

2 Entry composition (i)

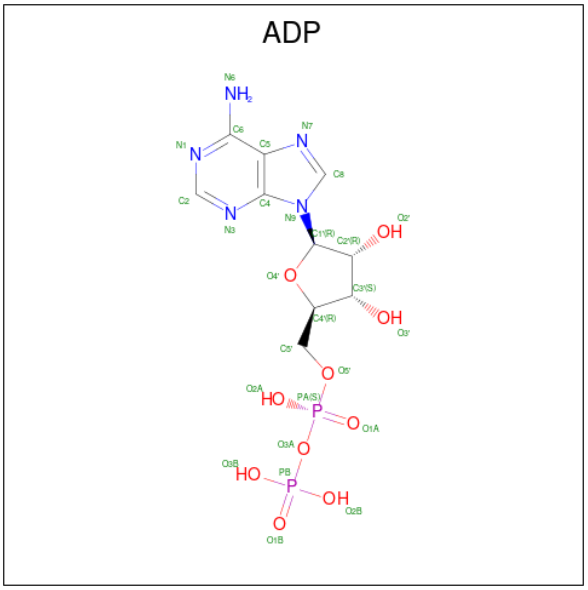
There are 2 unique types of molecules in this entry. The entry contains 30525 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Heat shock protein 104.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	577	Total	C	N	O	S	0	0
			4507	2836	789	864	18		
1	B	577	Total	C	N	O	S	0	0
			4507	2836	789	864	18		
1	C	705	Total	C	N	O	S	0	0
			5560	3479	980	1082	19		
1	D	705	Total	C	N	O	S	0	0
			5560	3479	980	1082	19		
1	E	705	Total	C	N	O	S	0	0
			5560	3479	980	1082	19		
1	F	577	Total	C	N	O	S	0	0
			4507	2836	789	864	18		

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



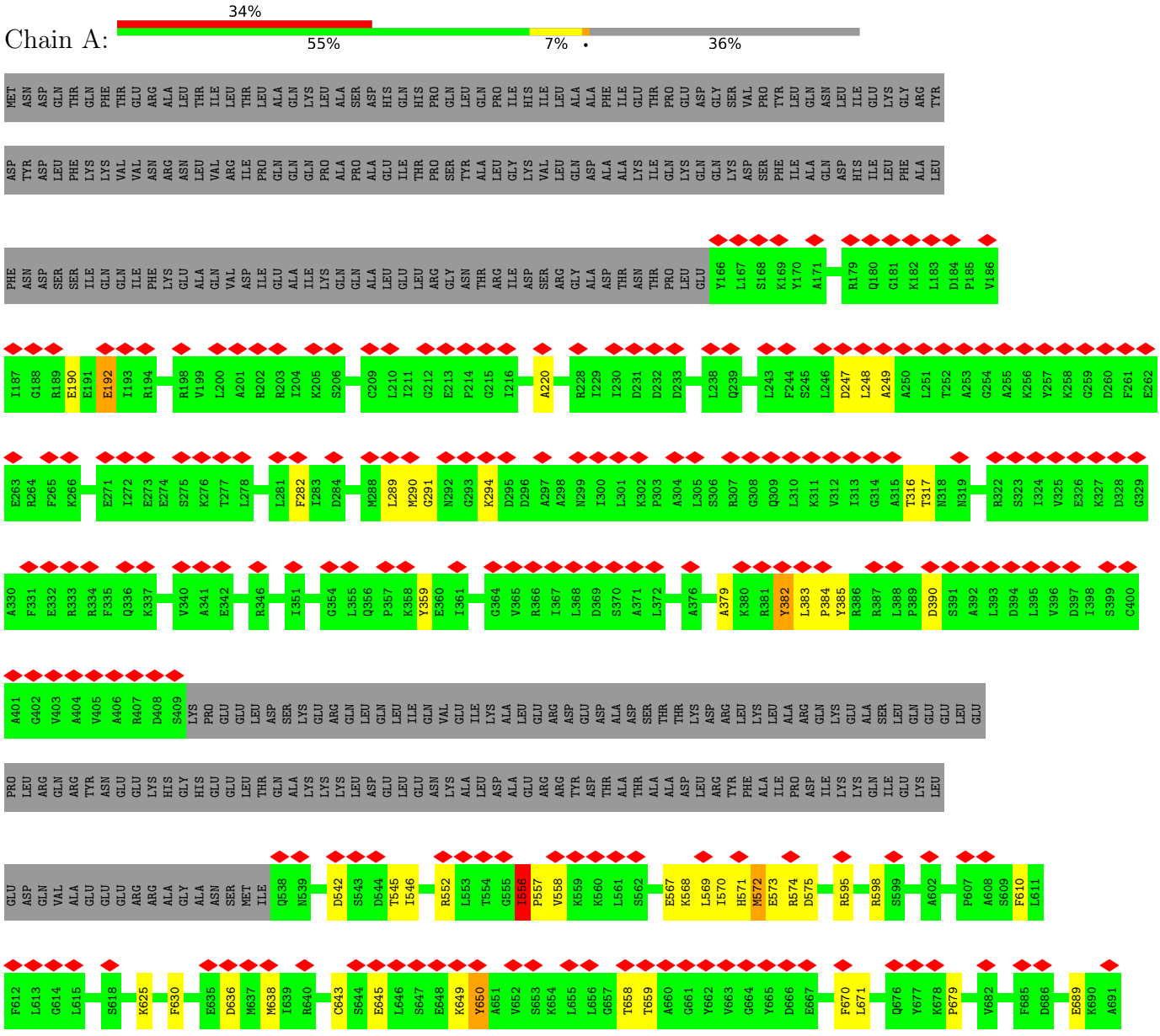
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	A	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	B	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	B	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	C	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	C	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	D	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	D	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	E	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	E	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	F	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	F	1	Total	C	N	O	P	0
			54	20	10	20	4	

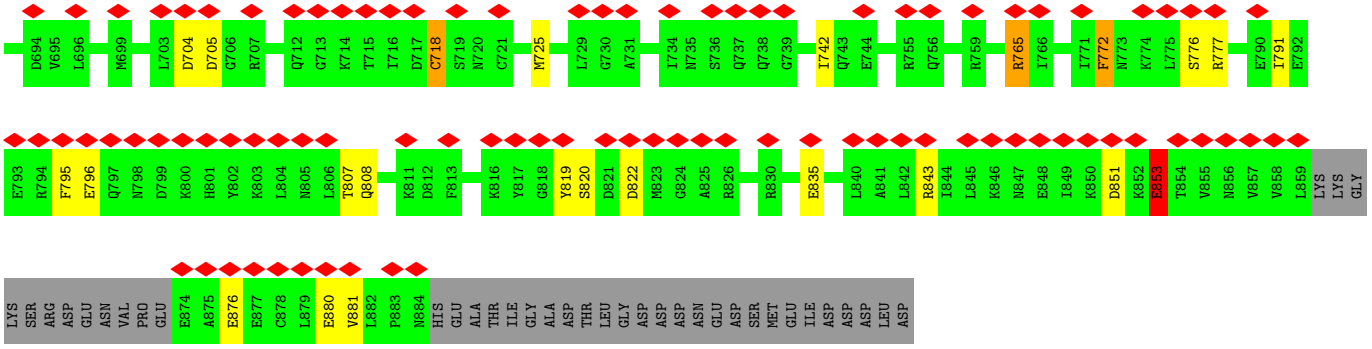
3 Residue-property plots (i)

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: Heat shock protein 104

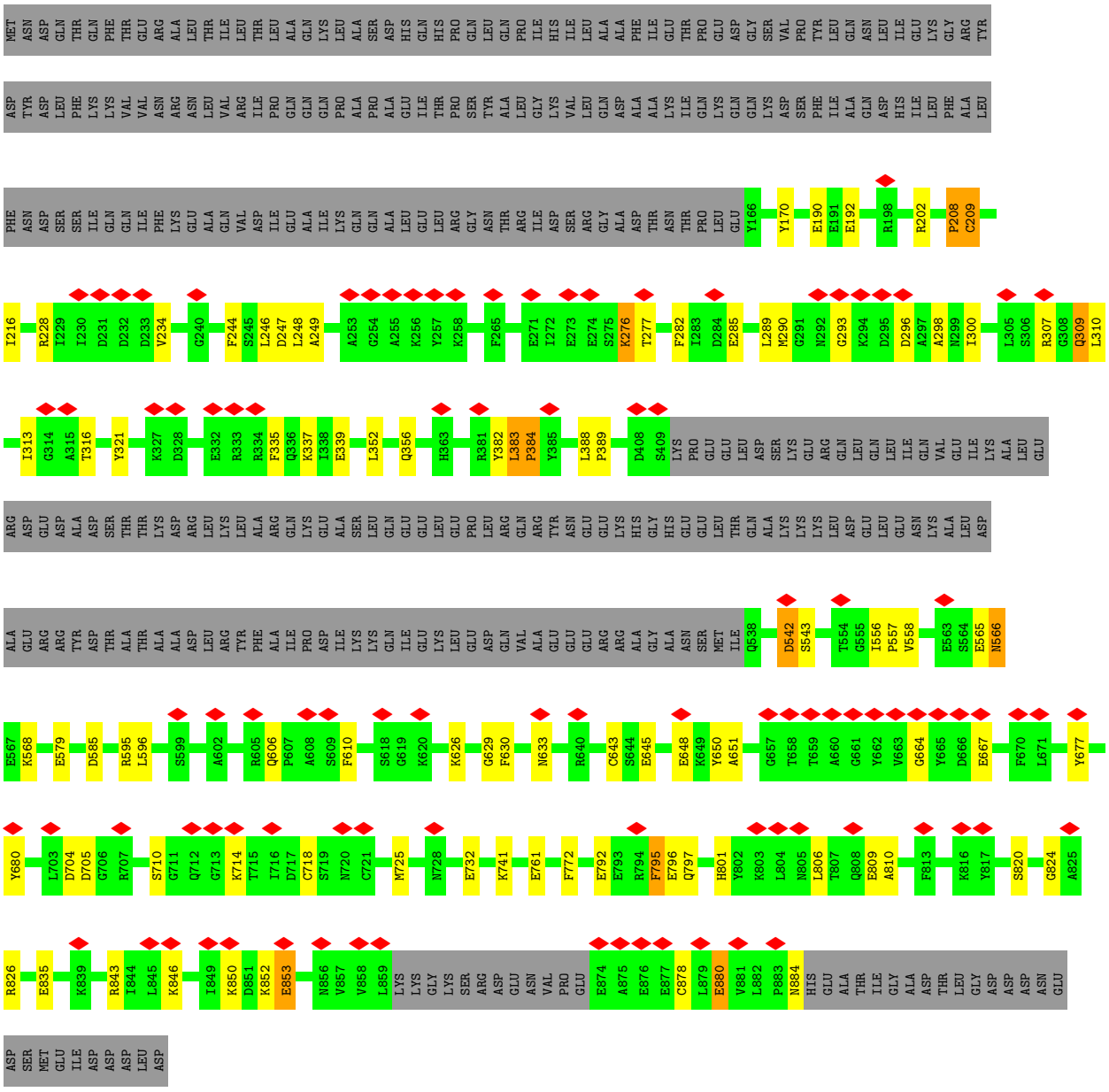
Chain A:





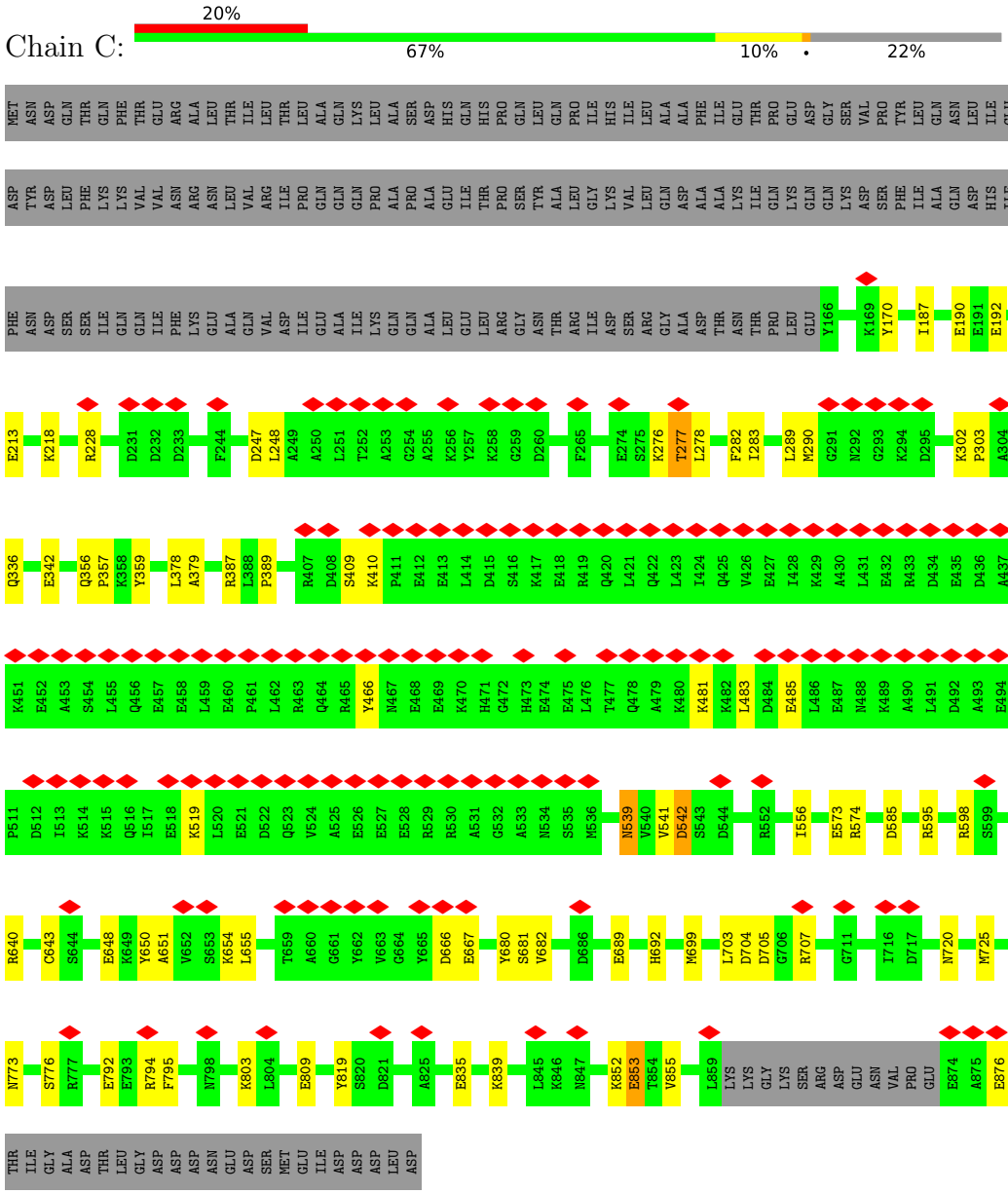
• Molecule 1: Heat shock protein 104

Chain B:



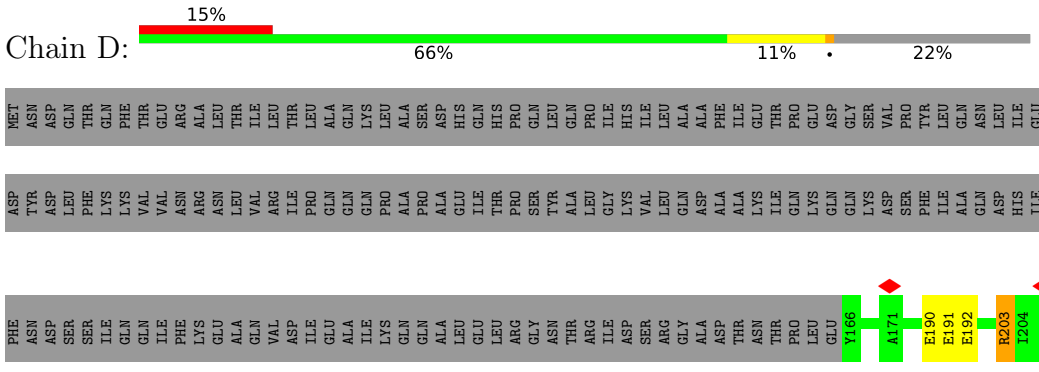
• Molecule 1: Heat shock protein 104

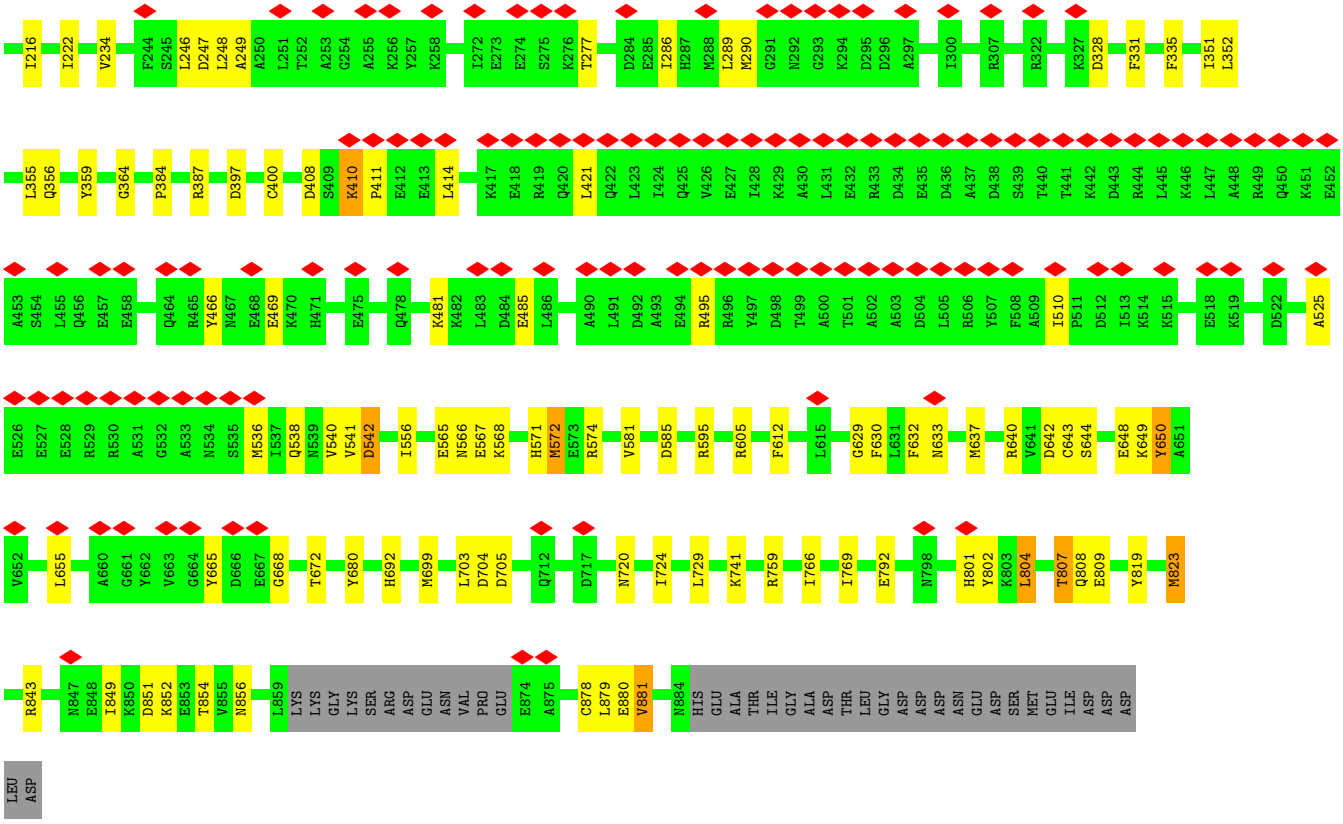
Chain C:



• Molecule 1: Heat shock protein 104

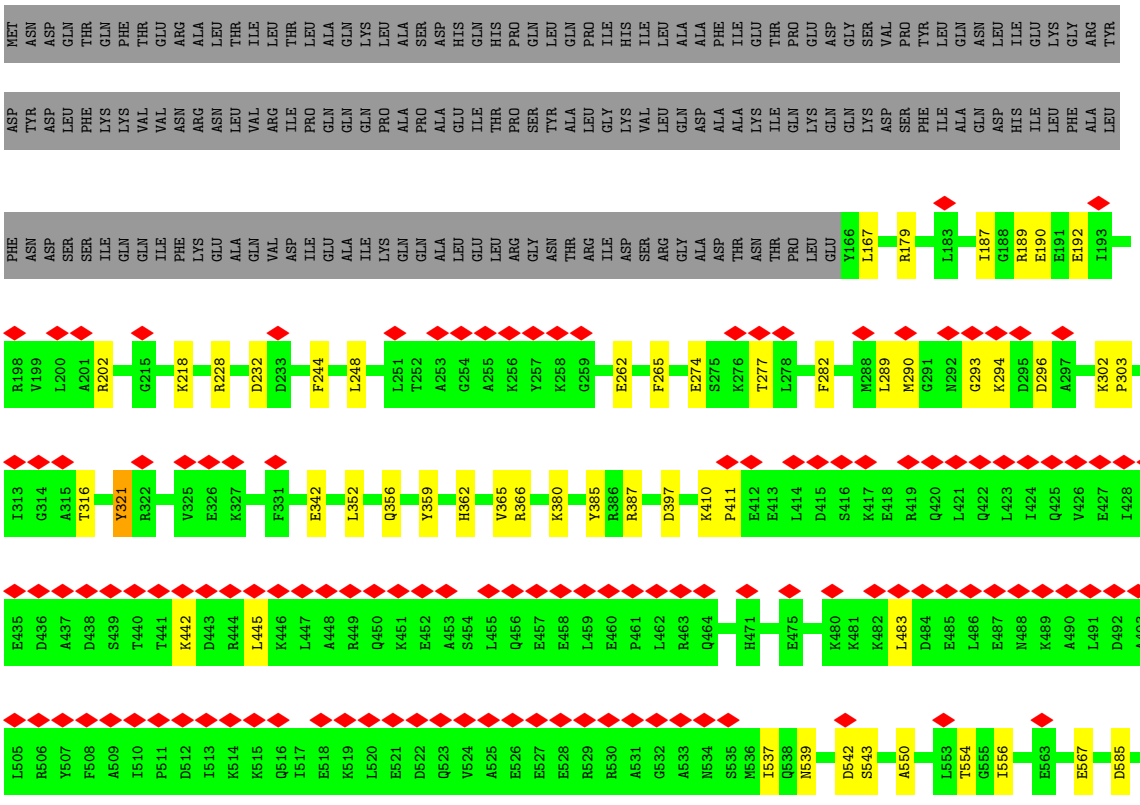
Chain D:

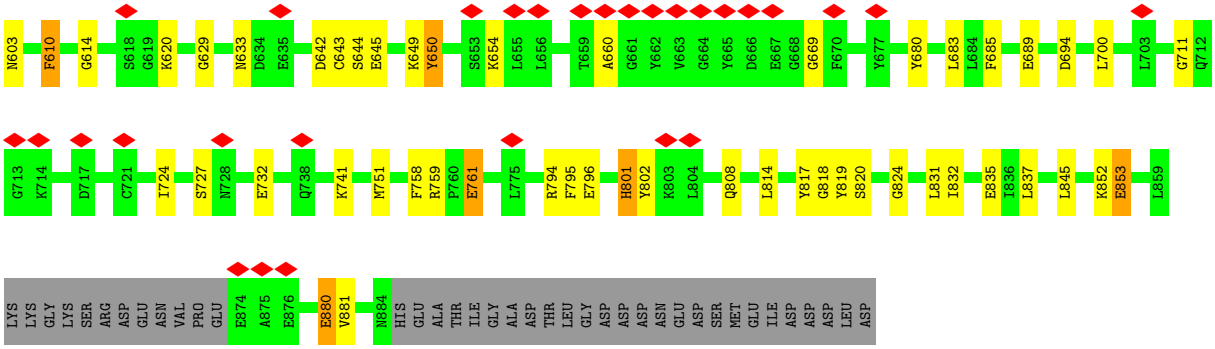




• Molecule 1: Heat shock protein 104

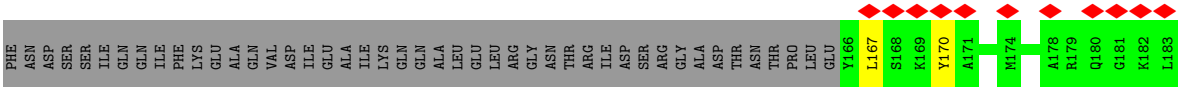
Chain E:

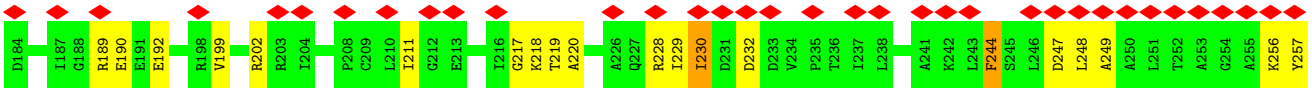


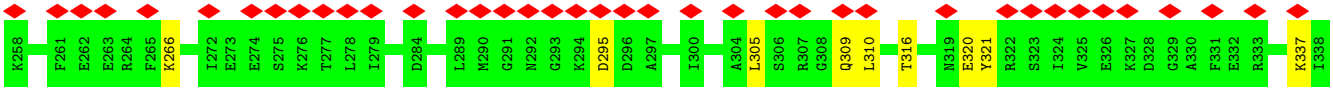


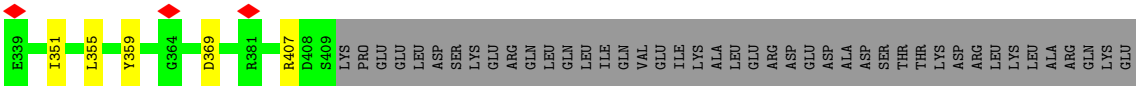
• Molecule 1: Heat shock protein 104

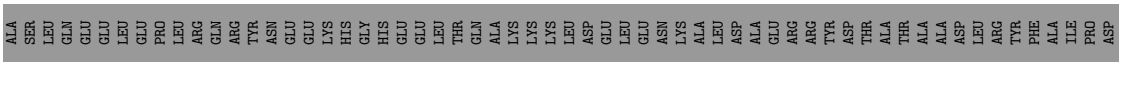
Chain F:

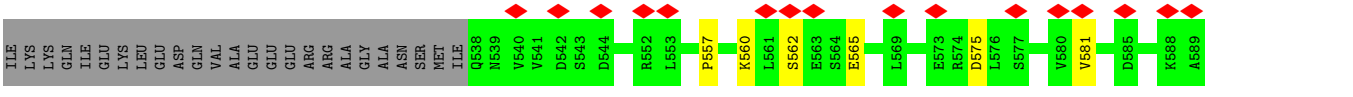


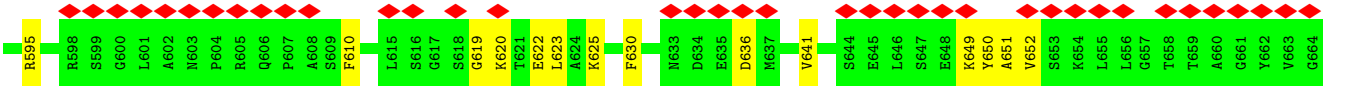


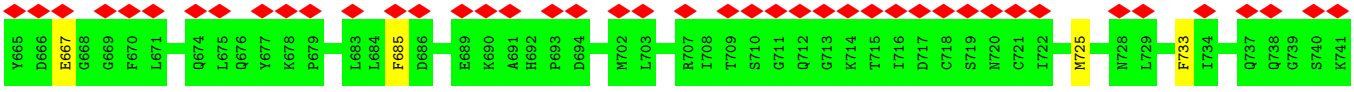


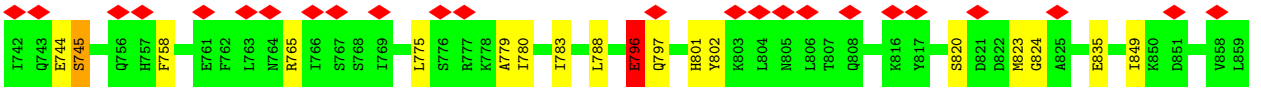


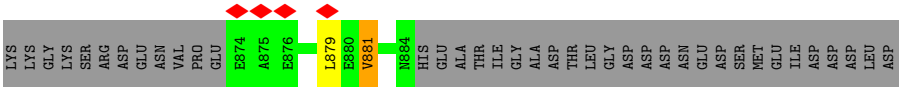











LYS
LYS
GLY
LYS
SER
ARG
ASP
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ASN
VAL
PRO
GLU
E874
A875
E876
L879
E880
V881
N884
HIS
GLU
ALA
THR
ILE
GLY
ALA
ASP
THR
LEU
GLY
ASP
ASP
ASP
ASN
GLU
ASP
SER
MET
GLU
ILE
ASP
ASP
ASP
LEU
ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	146463	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	0.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	50000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.081	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0194	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: ADP

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	1.12	17/4562 (0.4%)	0.95	10/6140 (0.2%)
1	B	1.21	25/4562 (0.5%)	0.97	11/6140 (0.2%)
1	C	1.23	23/5625 (0.4%)	0.96	11/7564 (0.1%)
1	D	1.24	16/5625 (0.3%)	0.99	13/7564 (0.2%)
1	E	1.20	24/5625 (0.4%)	0.98	12/7564 (0.2%)
1	F	1.13	18/4562 (0.4%)	0.96	8/6140 (0.1%)
All	All	1.19	123/30561 (0.4%)	0.97	65/41112 (0.2%)

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	718	CYS	CB-SG	-10.22	1.64	1.82
1	F	796	GLU	CG-CD	-10.04	1.36	1.51
1	A	359	TYR	CB-CG	-9.43	1.37	1.51
1	E	680	TYR	CB-CG	-9.27	1.37	1.51
1	B	610	PHE	CB-CG	-8.95	1.36	1.51
1	E	397	ASP	CB-CG	8.85	1.70	1.51
1	D	630	PHE	CB-CG	-8.77	1.36	1.51
1	C	630	PHE	CB-CG	-8.33	1.37	1.51
1	D	400	CYS	CB-SG	-8.30	1.68	1.82
1	A	382	TYR	CG-CD2	-7.99	1.28	1.39
1	B	244	PHE	CB-CG	-7.82	1.38	1.51
1	B	792	GLU	CD-OE1	-7.60	1.17	1.25
1	B	880	GLU	CG-CD	-7.50	1.40	1.51
1	D	632	PHE	CB-CG	-7.28	1.39	1.51
1	A	835	GLU	CD-OE1	-7.22	1.17	1.25
1	D	397	ASP	CB-CG	7.21	1.66	1.51
1	B	282	PHE	CB-CG	-7.18	1.39	1.51
1	C	282	PHE	CB-CG	-7.08	1.39	1.51
1	A	835	GLU	CG-CD	-7.01	1.41	1.51
1	C	359	TYR	CB-CG	-6.96	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	733	PHE	CB-CG	-6.92	1.39	1.51
1	C	819	TYR	CB-CG	-6.88	1.41	1.51
1	A	610	PHE	CB-CG	-6.71	1.40	1.51
1	F	244	PHE	CB-CG	-6.71	1.40	1.51
1	E	265	PHE	CB-CG	-6.65	1.40	1.51
1	C	795	PHE	CB-CG	-6.64	1.40	1.51
1	B	878	CYS	CB-SG	-6.62	1.71	1.82
1	B	880	GLU	CD-OE1	-6.60	1.18	1.25
1	E	321	TYR	CD2-CE2	-6.59	1.29	1.39
1	E	853	GLU	CD-OE2	-6.59	1.18	1.25
1	D	359	TYR	CB-CG	-6.54	1.41	1.51
1	E	321	TYR	CB-CG	-6.53	1.41	1.51
1	F	835	GLU	CD-OE1	-6.53	1.18	1.25
1	C	170	TYR	CB-CG	-6.50	1.41	1.51
1	C	331	PHE	CB-CG	-6.49	1.40	1.51
1	F	610	PHE	CB-CG	-6.46	1.40	1.51
1	E	610	PHE	CB-CG	-6.46	1.40	1.51
1	E	321	TYR	CG-CD2	-6.37	1.30	1.39
1	E	296	ASP	CB-CG	6.34	1.65	1.51
1	F	359	TYR	CB-CG	-6.32	1.42	1.51
1	E	359	TYR	CB-CG	-6.32	1.42	1.51
1	C	667	GLU	CG-CD	-6.31	1.42	1.51
1	D	469	GLU	CG-CD	-6.27	1.42	1.51
1	D	234	VAL	CB-CG1	-6.26	1.39	1.52
1	F	192	GLU	CD-OE1	-6.24	1.18	1.25
1	C	689	GLU	CD-OE1	-6.19	1.18	1.25
1	C	853	GLU	CD-OE1	-6.14	1.18	1.25
1	D	540	VAL	CB-CG1	-6.12	1.40	1.52
1	D	878	CYS	CB-SG	-6.11	1.71	1.82
1	B	234	VAL	CB-CG1	-6.09	1.40	1.52
1	F	802	TYR	CB-CG	-6.08	1.42	1.51
1	D	469	GLU	CD-OE1	-6.08	1.19	1.25
1	C	643	CYS	CB-SG	-6.05	1.72	1.82
1	C	792	GLU	CD-OE1	-6.03	1.19	1.25
1	E	680	TYR	CG-CD2	-6.03	1.31	1.39
1	D	643	CYS	CB-SG	-6.00	1.72	1.82
1	E	680	TYR	CD2-CE2	-6.00	1.30	1.39
1	A	772	PHE	CB-CG	-5.98	1.41	1.51
1	B	835	GLU	CD-OE1	-5.98	1.19	1.25
1	E	643	CYS	CB-SG	-5.96	1.72	1.81
1	D	209	CYS	CB-SG	-5.95	1.72	1.81
1	B	643	CYS	CB-SG	-5.94	1.72	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	PHE	CB-CG	-5.93	1.41	1.51
1	F	796	GLU	CD-OE2	-5.93	1.19	1.25
1	F	641	VAL	CB-CG2	-5.87	1.40	1.52
1	E	880	GLU	CD-OE2	-5.84	1.19	1.25
1	B	761	GLU	CD-OE1	-5.82	1.19	1.25
1	A	643	CYS	CB-SG	-5.76	1.72	1.81
1	E	761	GLU	CD-OE1	-5.75	1.19	1.25
1	F	685	PHE	CB-CG	-5.70	1.41	1.51
1	D	469	GLU	CD-OE2	-5.70	1.19	1.25
1	F	788	LEU	CB-CG	-5.69	1.36	1.52
1	C	855	VAL	CB-CG2	-5.68	1.41	1.52
1	A	689	GLU	CD-OE1	-5.65	1.19	1.25
1	A	192	GLU	CD-OE1	-5.65	1.19	1.25
1	A	876	GLU	CD-OE1	-5.64	1.19	1.25
1	E	385	TYR	CB-CG	-5.63	1.43	1.51
1	C	680	TYR	CB-CG	-5.62	1.43	1.51
1	F	630	PHE	CB-CG	-5.61	1.41	1.51
1	C	331	PHE	CG-CD2	-5.59	1.30	1.38
1	E	567	GLU	CD-OE2	-5.57	1.19	1.25
1	B	809	GLU	CD-OE1	-5.56	1.19	1.25
1	B	606	GLN	CG-CD	-5.55	1.38	1.51
1	A	853	GLU	CD-OE2	-5.52	1.19	1.25
1	C	853	GLU	CG-CD	-5.52	1.43	1.51
1	B	667	GLU	CD-OE1	-5.52	1.19	1.25
1	B	313	ILE	CB-CG2	-5.51	1.35	1.52
1	C	876	GLU	CD-OE2	-5.50	1.19	1.25
1	B	209	CYS	CB-SG	-5.47	1.72	1.81
1	B	795	PHE	CB-CG	-5.45	1.42	1.51
1	A	853	GLU	CG-CD	-5.43	1.43	1.51
1	E	321	TYR	CE2-CZ	-5.42	1.31	1.38
1	B	835	GLU	CD-OE2	-5.40	1.19	1.25
1	E	835	GLU	CG-CD	-5.36	1.44	1.51
1	E	689	GLU	CD-OE1	-5.36	1.19	1.25
1	F	407	ARG	CG-CD	-5.35	1.38	1.51
1	F	796	GLU	CD-OE1	-5.35	1.19	1.25
1	F	667	GLU	CD-OE1	-5.33	1.19	1.25
1	A	630	PHE	CB-CG	-5.31	1.42	1.51
1	C	209	CYS	CB-SG	-5.28	1.73	1.81
1	E	880	GLU	CD-OE1	-5.26	1.19	1.25
1	A	880	GLU	CD-OE2	-5.25	1.19	1.25
1	B	579	GLU	CD-OE1	-5.25	1.19	1.25
1	B	335	PHE	CB-CG	-5.24	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	630	PHE	CB-CG	-5.22	1.42	1.51
1	C	692	HIS	CB-CG	-5.21	1.40	1.50
1	D	692	HIS	CB-CG	-5.20	1.40	1.50
1	B	718	CYS	CB-SG	-5.18	1.73	1.81
1	C	809	GLU	CD-OE1	-5.17	1.20	1.25
1	E	244	PHE	CB-CG	-5.17	1.42	1.51
1	B	244	PHE	CG-CD2	-5.15	1.31	1.38
1	D	720	ASN	CB-CG	-5.15	1.39	1.51
1	C	342	GLU	CD-OE1	-5.15	1.20	1.25
1	E	192	GLU	CD-OE1	-5.15	1.20	1.25
1	F	758	PHE	CB-CG	-5.13	1.42	1.51
1	C	539	ASN	CB-CG	-5.13	1.39	1.51
1	E	282	PHE	CB-CG	-5.13	1.42	1.51
1	F	320	GLU	CD-OE1	-5.11	1.20	1.25
1	B	680	TYR	CB-CG	-5.08	1.44	1.51
1	D	203	ARG	CG-CD	-5.08	1.39	1.51
1	C	667	GLU	CD-OE1	-5.08	1.20	1.25
1	B	285	GLU	CD-OE1	-5.06	1.20	1.25
1	A	851	ASP	CB-CG	5.02	1.62	1.51

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	202	ARG	NE-CZ-NH2	-10.37	115.12	120.30
1	D	466	TYR	CB-CG-CD1	-10.00	115.00	121.00
1	E	202	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	B	202	ARG	NE-CZ-NH2	-9.67	115.47	120.30
1	F	595	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	B	843	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	E	189	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	D	605	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	D	640	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	C	819	TYR	CB-CG-CD2	-8.05	116.17	121.00
1	D	203	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	D	595	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	C	794	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	B	826	ARG	NE-CZ-NH2	-7.69	116.46	120.30
1	E	366	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	B	382	TYR	CB-CG-CD1	-7.50	116.50	121.00
1	C	507	TYR	CB-CG-CD2	-7.12	116.73	121.00
1	D	495	ARG	NE-CZ-NH1	-7.03	116.78	120.30
1	E	802	TYR	CB-CG-CD2	-6.87	116.88	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	707	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	D	665	TYR	CB-CG-CD2	-6.78	116.94	121.00
1	D	680	TYR	CB-CG-CD2	-6.60	117.04	121.00
1	F	189	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	A	765	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	598	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	C	574	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	F	170	TYR	CB-CG-CD1	-6.31	117.21	121.00
1	B	680	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	C	595	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	E	179	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	C	202	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	A	819	TYR	CB-CG-CD2	-5.98	117.41	121.00
1	E	397	ASP	CB-CG-OD1	5.92	123.63	118.30
1	E	680	TYR	CB-CG-CD2	-5.86	117.48	121.00
1	D	843	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	556	ILE	C-N-CD	-5.77	107.90	120.60
1	E	496	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	B	170	TYR	CB-CG-CD2	-5.71	117.58	121.00
1	D	819	TYR	CB-CG-CD1	-5.68	117.59	121.00
1	B	843	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	C	228	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	E	321	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	A	385	TYR	CB-CG-CD2	-5.64	117.61	121.00
1	C	466	TYR	CB-CG-CD1	-5.64	117.62	121.00
1	A	843	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	F	321	TYR	CB-CG-CD1	-5.39	117.76	121.00
1	A	556	ILE	N-CA-C	5.35	125.45	111.00
1	C	640	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	F	575	ASP	CB-CG-OD2	5.32	123.08	118.30
1	D	408	ASP	CB-CG-OD2	-5.31	113.53	118.30
1	C	307	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	359	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	B	610	PHE	CB-CG-CD2	-5.22	117.14	120.80
1	B	677	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	B	321	TYR	CB-CG-CD2	-5.21	117.87	121.00
1	B	595	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	F	359	TYR	CB-CG-CD2	-5.16	117.91	121.00
1	D	574	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	552	ARG	NE-CZ-NH2	5.11	122.86	120.30
1	F	407	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	D	466	TYR	CB-CG-CD2	5.09	124.05	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	575	ASP	CB-CG-OD2	5.08	122.88	118.30
1	F	257	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	E	614	GLY	N-CA-C	-5.02	100.55	113.10
1	E	758	PHE	CB-CG-CD1	-5.02	117.29	120.80

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	4507	0	4627	58	0
1	B	4507	0	4627	49	0
1	C	5560	0	5679	57	0
1	D	5560	0	5679	64	0
1	E	5560	0	5679	64	0
1	F	4507	0	4624	138	0
2	A	54	0	24	4	0
2	B	54	0	24	1	0
2	C	54	0	24	6	0
2	D	54	0	24	11	0
2	E	54	0	24	6	0
2	F	54	0	23	104	0
All	All	30525	0	31058	444	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 7.

All (444) 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:F:619:GLY:HA2	2:F:1002:ADP:C5'	1.35	1.53
1:F:619:GLY:CA	2:F:1002:ADP:H5'2	1.40	1.51
1:F:775:LEU:HD11	2:F:1002:ADP:C2	1.41	1.50
1:A:568:LYS:HB3	1:A:572:MET:SD	1.56	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:622:GLU:OE1	2:F:1002:ADP:H2'	1.32	1.29
1:F:775:LEU:CD1	2:F:1002:ADP:C2	2.14	1.28
1:F:775:LEU:HD21	2:F:1002:ADP:N3	1.54	1.23
1:F:217:GLY:HA2	2:F:1001:ADP:O4'	1.08	1.21
1:F:351:ILE:CG2	2:F:1001:ADP:N6	2.04	1.21
1:F:217:GLY:CA	2:F:1001:ADP:O4'	1.89	1.20
1:F:775:LEU:HD21	2:F:1002:ADP:C2	1.79	1.18
1:F:217:GLY:HA2	2:F:1001:ADP:C1'	1.73	1.17
1:F:775:LEU:CG	2:F:1002:ADP:H2	1.56	1.17
1:F:219:THR:HB	2:F:1001:ADP:C3'	1.77	1.14
1:F:775:LEU:CG	2:F:1002:ADP:C2	2.33	1.08
1:F:351:ILE:HG23	2:F:1001:ADP:HN62	1.09	1.07
1:C:556:ILE:HG22	1:C:556:ILE:O	1.53	1.06
1:F:622:GLU:CD	2:F:1002:ADP:H2'	1.75	1.06
1:A:568:LYS:HE2	1:A:572:MET:SD	1.96	1.05
1:F:217:GLY:HA3	2:F:1001:ADP:C8	1.91	1.04
1:D:556:ILE:O	1:D:556:ILE:HG22	1.55	1.04
1:F:219:THR:HB	2:F:1001:ADP:H3'	1.05	1.03
1:F:775:LEU:CD2	2:F:1002:ADP:C2	2.41	1.03
1:F:219:THR:CB	2:F:1001:ADP:H3'	1.88	1.02
1:F:220:ALA:HB2	2:F:1001:ADP:O2'	1.61	1.01
1:A:568:LYS:CB	1:A:572:MET:SD	2.48	1.00
1:F:351:ILE:CG2	2:F:1001:ADP:HN62	1.67	1.00
1:F:355:LEU:HD11	2:F:1001:ADP:C2	1.96	1.00
1:F:220:ALA:H	2:F:1001:ADP:H2'	1.26	0.98
1:A:568:LYS:HD2	1:A:572:MET:HB2	1.43	0.98
1:F:217:GLY:HA3	2:F:1001:ADP:H8	1.19	0.98
1:F:622:GLU:CD	2:F:1002:ADP:C2'	2.32	0.98
1:F:351:ILE:HG23	2:F:1001:ADP:N6	1.68	0.96
1:F:775:LEU:HG	2:F:1002:ADP:H2	1.32	0.95
1:A:853:GLU:OE1	1:A:853:GLU:O	1.84	0.94
1:A:568:LYS:O	1:A:573:GLU:N	2.00	0.94
1:F:351:ILE:CG2	2:F:1001:ADP:C6	2.52	0.92
1:F:622:GLU:HB2	2:F:1002:ADP:H5'1	1.48	0.92
1:F:220:ALA:HB2	2:F:1001:ADP:C2'	1.99	0.92
1:F:351:ILE:HG21	2:F:1001:ADP:N6	1.85	0.91
1:E:761:GLU:OE1	1:E:761:GLU:N	2.04	0.90
1:F:351:ILE:HG21	2:F:1001:ADP:C6	2.05	0.90
1:F:351:ILE:CG1	2:F:1001:ADP:N6	2.35	0.89
1:F:775:LEU:CD2	2:F:1002:ADP:N3	2.35	0.88
1:F:581:VAL:HB	2:F:1002:ADP:N6	1.89	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1002:ADP:N3	2:A:1002:ADP:C2'	2.37	0.88
2:A:1002:ADP:N3	2:A:1002:ADP:H2'	1.88	0.87
1:D:565:GLU:N	1:D:565:GLU:OE1	2.07	0.87
1:D:192:GLU:N	1:D:192:GLU:OE1	2.07	0.86
1:C:573:GLU:OE1	1:C:573:GLU:N	2.08	0.86
1:D:650:TYR:O	1:D:650:TYR:CD1	2.28	0.86
1:B:339:GLU:N	1:B:339:GLU:OE1	2.08	0.85
1:F:217:GLY:HA2	2:F:1001:ADP:C2'	2.06	0.85
1:A:568:LYS:O	1:A:572:MET:CA	2.10	0.85
1:F:355:LEU:HD11	2:F:1001:ADP:N1	1.91	0.85
1:C:192:GLU:OE1	1:C:192:GLU:N	2.09	0.84
1:F:351:ILE:HG12	2:F:1001:ADP:N6	1.92	0.84
1:F:351:ILE:CD1	2:F:1001:ADP:HN61	1.92	0.83
1:C:648:GLU:OE1	1:C:648:GLU:N	2.09	0.82
1:B:192:GLU:N	1:B:192:GLU:OE1	2.11	0.82
1:F:220:ALA:CB	2:F:1001:ADP:H2'	2.10	0.81
1:A:568:LYS:O	1:A:572:MET:N	2.13	0.81
1:F:622:GLU:OE1	2:F:1002:ADP:C2'	2.23	0.81
1:F:217:GLY:HA2	2:F:1001:ADP:C4'	2.11	0.81
1:A:568:LYS:CD	1:A:572:MET:HB2	2.04	0.80
1:F:220:ALA:N	2:F:1001:ADP:H2'	1.95	0.80
1:F:783:ILE:HD13	2:F:1002:ADP:N7	1.97	0.80
1:D:565:GLU:CD	1:D:565:GLU:H	1.80	0.79
2:E:1001:ADP:H3'	2:E:1001:ADP:O1A	1.83	0.79
1:F:823:MET:O	1:F:823:MET:HG3	1.83	0.78
2:F:1002:ADP:H4'	2:F:1002:ADP:O1A	1.83	0.78
1:D:792:GLU:OE1	1:D:792:GLU:HA	1.83	0.78
1:F:775:LEU:HD11	2:F:1002:ADP:N1	1.97	0.78
1:F:217:GLY:CA	2:F:1001:ADP:C1'	2.56	0.78
1:F:622:GLU:HG3	2:F:1002:ADP:H3'	1.64	0.77
1:E:732:GLU:N	1:E:732:GLU:OE1	2.17	0.76
1:F:351:ILE:HD13	2:F:1001:ADP:HN61	1.48	0.76
1:A:570:ILE:HD11	1:B:846:LYS:HB3	1.67	0.75
2:E:1002:ADP:O1A	2:E:1002:ADP:H4'	1.83	0.75
1:D:556:ILE:O	1:D:556:ILE:CG2	2.32	0.75
1:C:507:TYR:O	1:C:507:TYR:CD1	2.40	0.75
1:F:622:GLU:CD	2:F:1002:ADP:H3'	2.08	0.75
2:D:1001:ADP:H5'1	2:D:1001:ADP:PB	2.26	0.74
1:F:351:ILE:HG23	2:F:1001:ADP:C6	2.18	0.74
1:F:581:VAL:HB	2:F:1002:ADP:HN62	1.50	0.74
1:A:568:LYS:O	1:A:572:MET:C	2.26	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:622:GLU:CB	2:F:1002:ADP:H5'1	2.18	0.73
1:F:351:ILE:HD13	2:F:1001:ADP:N6	2.03	0.73
1:F:650:TYR:O	1:F:650:TYR:CD1	2.41	0.73
2:E:1001:ADP:H3'	2:E:1001:ADP:PA	2.29	0.72
1:A:650:TYR:O	1:A:650:TYR:CD1	2.43	0.72
1:B:884:ASN:OD1	1:B:884:ASN:C	2.26	0.72
1:C:507:TYR:CD1	1:C:507:TYR:C	2.61	0.72
1:D:581:VAL:H	2:D:1002:ADP:HN62	1.36	0.72
1:F:775:LEU:HD11	2:F:1002:ADP:N3	2.03	0.72
2:D:1001:ADP:N3	2:D:1001:ADP:H2'	2.05	0.72
1:F:620:LYS:N	2:F:1002:ADP:O2A	2.23	0.71
1:F:622:GLU:CD	2:F:1002:ADP:C3'	2.59	0.71
1:F:351:ILE:CG1	2:F:1001:ADP:HN61	2.03	0.71
1:F:217:GLY:CA	2:F:1001:ADP:C8	2.73	0.70
1:F:622:GLU:CG	2:F:1002:ADP:H3'	2.19	0.70
1:F:220:ALA:H	2:F:1001:ADP:C2'	2.03	0.70
1:F:355:LEU:HD11	2:F:1001:ADP:H2	1.57	0.69
1:F:351:ILE:CD1	2:F:1001:ADP:N6	2.55	0.69
1:A:568:LYS:C	1:A:572:MET:H	1.96	0.69
2:A:1002:ADP:N3	2:A:1002:ADP:O2'	2.24	0.68
2:E:1001:ADP:O1A	2:E:1001:ADP:C3'	2.41	0.67
1:E:761:GLU:H	1:E:761:GLU:CD	1.91	0.67
1:F:355:LEU:CD1	2:F:1001:ADP:C2	2.77	0.66
1:F:219:THR:HB	2:F:1001:ADP:O3'	1.94	0.66
1:E:445:LEU:C	1:E:445:LEU:HD23	2.15	0.66
1:C:598:ARG:HA	1:C:598:ARG:NE	2.10	0.66
1:F:775:LEU:CD2	2:F:1002:ADP:H2	1.93	0.65
1:C:387:ARG:HA	1:C:387:ARG:NE	2.11	0.65
1:D:414:LEU:HD23	1:D:414:LEU:C	2.17	0.64
1:F:581:VAL:CB	2:F:1002:ADP:N6	2.60	0.63
2:C:1001:ADP:N3	2:C:1001:ADP:H2'	2.14	0.63
1:F:217:GLY:N	2:F:1001:ADP:O4'	2.31	0.63
1:C:556:ILE:O	1:C:556:ILE:CG2	2.30	0.62
1:E:732:GLU:H	1:E:732:GLU:CD	1.98	0.62
1:E:445:LEU:HD23	1:E:445:LEU:O	2.00	0.62
1:D:246:LEU:C	1:D:246:LEU:HD23	2.20	0.62
1:C:289:LEU:O	1:C:290:MET:HB2	2.00	0.61
1:E:645:GLU:O	1:E:645:GLU:HG3	2.00	0.61
1:F:622:GLU:OE2	2:F:1002:ADP:C2'	2.49	0.61
1:E:218:LYS:NZ	1:E:316:THR:O	2.34	0.61
1:F:351:ILE:CB	2:F:1001:ADP:N6	2.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:650:TYR:C	1:C:650:TYR:CD2	2.75	0.60
1:F:619:GLY:H	2:F:1002:ADP:PA	2.24	0.60
1:F:581:VAL:CG2	2:F:1002:ADP:N6	2.65	0.59
1:C:483:LEU:HD22	1:C:483:LEU:O	2.02	0.59
1:B:246:LEU:HD23	1:B:246:LEU:O	2.03	0.59
1:F:220:ALA:N	2:F:1001:ADP:C2'	2.65	0.59
1:E:387:ARG:HA	1:E:387:ARG:NE	2.16	0.59
1:F:167:LEU:C	1:F:167:LEU:HD23	2.23	0.59
1:B:307:ARG:NE	1:B:307:ARG:HA	2.18	0.59
1:A:192:GLU:OE1	1:A:192:GLU:N	2.34	0.58
1:E:808:GLN:OE1	1:E:808:GLN:N	2.29	0.58
1:A:568:LYS:C	1:A:572:MET:N	2.54	0.57
1:D:387:ARG:NE	1:D:387:ARG:HA	2.18	0.57
1:C:773:ASN:C	1:C:773:ASN:OD1	2.41	0.57
1:F:801:HIS:CD2	1:F:801:HIS:N	2.71	0.57
1:A:568:LYS:O	1:A:572:MET:CG	2.37	0.57
1:E:434:ASP:OD2	1:E:442:LYS:NZ	2.37	0.57
1:B:246:LEU:HD23	1:B:246:LEU:C	2.24	0.57
1:C:585:ASP:OD2	1:C:741:LYS:NZ	2.38	0.56
1:D:191:GLU:OE1	1:D:191:GLU:HA	2.04	0.56
2:E:1001:ADP:PA	2:E:1001:ADP:C3'	2.93	0.56
1:F:351:ILE:HG12	2:F:1001:ADP:HN62	1.68	0.56
1:F:823:MET:O	1:F:823:MET:CG	2.53	0.56
1:B:585:ASP:OD2	1:B:741:LYS:NZ	2.39	0.56
1:A:650:TYR:O	1:A:650:TYR:HD1	1.89	0.56
1:F:351:ILE:CG2	2:F:1001:ADP:N1	2.68	0.56
1:A:570:ILE:HG13	1:B:846:LYS:HG2	1.87	0.56
2:D:1001:ADP:H4'	2:D:1001:ADP:O3A	2.05	0.56
1:E:852:LYS:N	1:E:852:LYS:HD2	2.20	0.55
1:C:650:TYR:CD2	1:C:650:TYR:O	2.59	0.55
1:D:629:GLY:O	1:D:633:ASN:N	2.39	0.55
1:C:655:LEU:C	1:C:655:LEU:HD23	2.25	0.55
1:C:732:GLU:OE1	1:C:732:GLU:HA	2.05	0.55
1:A:718:CYS:SG	1:A:718:CYS:O	2.61	0.55
1:F:619:GLY:HA2	2:F:1002:ADP:C4'	2.29	0.55
1:D:668:GLY:O	1:D:672:THR:N	2.40	0.55
1:F:351:ILE:HG12	2:F:1001:ADP:HN61	1.65	0.55
1:F:351:ILE:HG23	2:F:1001:ADP:N1	2.21	0.55
1:D:351:ILE:HG21	2:D:1001:ADP:HN62	1.71	0.55
1:D:637:MET:HG3	1:D:637:MET:O	2.05	0.55
1:B:820:SER:O	1:B:824:GLY:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:220:ALA:CB	2:F:1001:ADP:O2'	2.46	0.54
1:C:852:LYS:N	1:C:852:LYS:HD2	2.22	0.54
1:A:820:SER:OG	1:A:822:ASP:OD1	2.24	0.54
1:D:585:ASP:OD2	1:D:741:LYS:NZ	2.40	0.54
1:D:414:LEU:HD23	1:D:414:LEU:O	2.07	0.54
1:D:650:TYR:O	1:D:650:TYR:HD1	1.87	0.54
1:E:820:SER:O	1:E:824:GLY:N	2.41	0.54
1:A:567:GLU:O	1:A:572:MET:N	2.40	0.54
1:C:699:MET:O	1:C:703:LEU:N	2.42	0.53
1:D:809:GLU:OE1	1:D:809:GLU:N	2.39	0.53
2:D:1001:ADP:N3	2:D:1001:ADP:C2'	2.72	0.53
1:E:685:PHE:CD1	1:E:685:PHE:N	2.75	0.53
1:D:759:ARG:NH1	1:E:644:SER:OG	2.41	0.53
1:C:655:LEU:HD23	1:C:655:LEU:O	2.09	0.53
1:A:645:GLU:OE2	1:F:266:LYS:NZ	2.43	0.52
1:B:290:MET:O	1:B:290:MET:HG2	2.09	0.52
1:E:585:ASP:OD2	1:E:741:LYS:NZ	2.43	0.52
1:A:772:PHE:CD1	1:A:772:PHE:N	2.76	0.52
1:C:648:GLU:H	1:C:648:GLU:CD	2.05	0.52
2:D:1001:ADP:H5'1	2:D:1001:ADP:O3B	2.09	0.52
1:A:570:ILE:HD11	1:B:846:LYS:CB	2.38	0.51
1:B:289:LEU:O	1:B:290:MET:HB3	2.11	0.51
1:F:780:ILE:HG22	2:F:1002:ADP:C2	2.45	0.51
2:C:1002:ADP:O1A	2:C:1002:ADP:H4'	2.10	0.51
1:A:796:GLU:O	1:A:796:GLU:HG2	2.10	0.51
1:E:620:LYS:NZ	1:E:727:SER:O	2.43	0.51
1:D:851:ASP:OD2	1:D:852:LYS:NZ	2.44	0.51
1:E:650:TYR:O	1:E:650:TYR:CD1	2.64	0.51
1:E:761:GLU:N	1:E:761:GLU:CD	2.55	0.51
2:D:1001:ADP:PB	2:D:1001:ADP:C5'	2.98	0.51
1:F:211:ILE:HG13	1:F:337:LYS:HB2	1.93	0.51
1:F:783:ILE:CD1	2:F:1002:ADP:N7	2.70	0.51
1:B:388:LEU:HB3	1:B:389:PRO:HD3	1.93	0.50
1:C:190:GLU:CD	1:C:190:GLU:H	2.12	0.50
1:C:541:VAL:O	1:C:542:ASP:C	2.49	0.50
1:F:622:GLU:OE2	2:F:1002:ADP:O2'	2.29	0.50
1:A:570:ILE:CG1	1:B:846:LYS:HG2	2.41	0.50
1:D:351:ILE:CG2	2:D:1001:ADP:HN62	2.25	0.50
1:F:351:ILE:CB	2:F:1001:ADP:HN62	2.21	0.50
1:A:776:SER:OG	1:A:777:ARG:N	2.45	0.50
1:B:732:GLU:OE1	1:B:732:GLU:N	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:305:LEU:HD12	1:F:305:LEU:C	2.32	0.50
1:C:720:ASN:OD1	1:C:720:ASN:N	2.43	0.50
1:D:655:LEU:HD23	1:D:655:LEU:C	2.32	0.50
1:F:775:LEU:HG	2:F:1002:ADP:C2	2.27	0.50
2:D:1002:ADP:N3	2:D:1002:ADP:C2'	2.73	0.49
1:D:802:TYR:CD1	1:D:804:LEU:HB2	2.47	0.49
1:D:766:ILE:O	1:D:766:ILE:HG13	2.12	0.49
1:D:849:ILE:HD12	1:D:849:ILE:N	2.28	0.49
1:C:387:ARG:HA	1:C:387:ARG:HE	1.78	0.49
1:E:819:TYR:CD2	1:E:819:TYR:O	2.66	0.49
1:F:820:SER:O	1:F:824:GLY:N	2.45	0.49
1:F:565:GLU:H	1:F:565:GLU:CD	2.16	0.49
1:C:803:LYS:H	1:C:853:GLU:HG2	1.77	0.49
1:C:187:ILE:H	2:C:1001:ADP:HN62	1.61	0.49
1:C:539:ASN:C	1:C:539:ASN:OD1	2.50	0.48
1:C:772:PHE:CD1	1:C:772:PHE:N	2.80	0.48
1:C:598:ARG:HA	1:C:598:ARG:HE	1.78	0.48
1:B:228:ARG:HA	1:B:228:ARG:NE	2.29	0.48
1:D:213:GLU:H	1:D:216:ILE:HB	1.78	0.48
1:D:289:LEU:O	1:D:290:MET:HB2	2.13	0.48
1:F:849:ILE:HG12	1:F:849:ILE:O	2.13	0.48
1:A:807:THR:OG1	1:A:808:GLN:N	2.46	0.48
1:E:650:TYR:O	1:E:650:TYR:HD1	1.95	0.48
1:F:581:VAL:HG23	2:F:1002:ADP:HN61	1.78	0.48
1:A:190:GLU:H	1:A:190:GLU:CD	2.17	0.48
1:F:247:ASP:O	1:F:249:ALA:N	2.47	0.48
1:F:622:GLU:CG	2:F:1002:ADP:H5'1	2.43	0.48
1:F:775:LEU:CD1	2:F:1002:ADP:N3	2.68	0.48
1:A:220:ALA:HB2	2:A:1001:ADP:C4	2.49	0.48
1:B:337:LYS:NZ	1:B:339:GLU:OE2	2.44	0.48
1:E:410:LYS:N	1:E:411:PRO:CD	2.77	0.48
1:D:856:ASN:C	1:D:856:ASN:OD1	2.52	0.48
2:D:1002:ADP:N3	2:D:1002:ADP:H2'	2.29	0.48
1:F:355:LEU:CD1	2:F:1001:ADP:H2	2.24	0.48
2:B:1001:ADP:H5'2	2:B:1001:ADP:O3B	2.14	0.47
1:E:550:ALA:O	1:E:554:THR:N	2.44	0.47
1:A:556:ILE:O	1:A:558:VAL:N	2.47	0.47
1:C:666:ASP:OD1	1:C:666:ASP:N	2.38	0.47
1:E:262:GLU:OE1	1:F:256:LYS:NZ	2.45	0.47
1:F:650:TYR:O	1:F:650:TYR:HD1	1.95	0.47
1:E:819:TYR:O	1:E:819:TYR:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1001:ADP:H5'2	2:F:1001:ADP:O3B	2.14	0.47
1:F:217:GLY:CA	2:F:1001:ADP:C2'	2.86	0.47
1:A:545:THR:OG1	1:A:546:ILE:N	2.46	0.47
1:C:619:GLY:O	1:C:620:LYS:C	2.52	0.47
1:B:806:LEU:HB3	1:B:810:ALA:HB3	1.97	0.47
1:F:228:ARG:O	1:F:232:ASP:N	2.48	0.47
1:F:619:GLY:N	2:F:1002:ADP:O2A	2.47	0.47
1:D:566:ASN:O	1:D:567:GLU:C	2.50	0.47
1:F:220:ALA:CA	2:F:1001:ADP:H2'	2.44	0.47
1:A:569:LEU:HB2	1:A:595:ARG:HE	1.79	0.47
1:D:879:LEU:O	1:D:881:VAL:N	2.48	0.47
1:E:724:ILE:N	1:E:724:ILE:HD12	2.30	0.47
1:D:387:ARG:HA	1:D:387:ARG:HE	1.80	0.46
1:F:557:PRO:O	1:F:560:LYS:NZ	2.42	0.46
1:D:724:ILE:N	1:D:724:ILE:HD12	2.30	0.46
1:E:190:GLU:H	1:E:190:GLU:CD	2.18	0.46
1:A:390:ASP:OD1	1:A:390:ASP:O	2.33	0.46
1:D:222:ILE:HD13	1:D:222:ILE:HA	1.62	0.46
1:D:421:LEU:C	1:D:421:LEU:HD23	2.34	0.46
1:A:568:LYS:CE	1:A:572:MET:SD	2.87	0.46
1:C:213:GLU:O	1:C:218:LYS:NZ	2.46	0.46
1:C:835:GLU:OE1	1:C:839:LYS:NZ	2.47	0.46
1:E:649:LYS:O	1:E:650:TYR:C	2.54	0.46
1:A:567:GLU:O	1:A:571:HIS:N	2.48	0.46
1:D:246:LEU:HD23	1:D:246:LEU:O	2.16	0.46
1:F:190:GLU:H	1:F:190:GLU:CD	2.16	0.46
1:A:568:LYS:O	1:A:572:MET:HG2	2.11	0.46
1:C:639:ILE:HD12	1:C:639:ILE:N	2.30	0.46
1:E:814:LEU:O	1:E:818:GLY:N	2.48	0.46
1:C:302:LYS:HB3	1:C:303:PRO:HD3	1.97	0.46
1:F:779:ALA:CB	2:F:1002:ADP:N1	2.78	0.46
1:C:483:LEU:HD13	1:C:483:LEU:C	2.36	0.46
1:C:409:SER:OG	1:C:410:LYS:N	2.48	0.46
2:C:1001:ADP:O1A	2:C:1001:ADP:H4'	2.15	0.46
1:E:683:LEU:HD12	1:E:683:LEU:N	2.31	0.46
1:F:316:THR:O	1:F:316:THR:HG23	2.15	0.46
1:A:382:TYR:CD1	1:A:382:TYR:C	2.89	0.45
1:F:619:GLY:N	2:F:1002:ADP:PA	2.88	0.45
1:C:276:LYS:C	1:C:277:THR:HG1	2.17	0.45
1:F:244:PHE:N	1:F:244:PHE:CD1	2.84	0.45
1:D:637:MET:O	1:D:637:MET:CG	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:GLU:O	1:B:566:ASN:C	2.54	0.45
1:B:565:GLU:O	1:B:568:LYS:N	2.49	0.45
1:B:650:TYR:CD1	1:B:650:TYR:C	2.86	0.45
1:D:414:LEU:C	1:D:414:LEU:CD2	2.85	0.45
1:D:203:ARG:HG3	1:E:362:HIS:CG	2.52	0.45
1:E:365:VAL:HG23	1:E:365:VAL:O	2.17	0.45
1:A:853:GLU:OE1	1:A:853:GLU:C	2.54	0.45
1:D:190:GLU:H	1:D:190:GLU:CD	2.17	0.45
1:F:779:ALA:HB1	2:F:1002:ADP:N1	2.31	0.45
2:C:1001:ADP:O1A	2:C:1001:ADP:O3B	2.35	0.45
1:E:483:LEU:C	1:E:483:LEU:HD23	2.36	0.45
1:F:581:VAL:CG2	2:F:1002:ADP:HN61	2.30	0.45
1:F:619:GLY:CA	2:F:1002:ADP:PA	3.05	0.45
1:F:881:VAL:HG12	1:F:881:VAL:O	2.16	0.45
1:E:342:GLU:OE1	1:E:380:LYS:NZ	2.50	0.45
1:E:759:ARG:HB3	1:E:761:GLU:OE1	2.16	0.45
1:B:795:PHE:O	1:B:797:GLN:N	2.50	0.45
1:B:558:VAL:O	1:B:558:VAL:HG12	2.17	0.45
1:C:336:GLN:N	1:C:336:GLN:CD	2.70	0.45
1:D:541:VAL:O	1:D:542:ASP:C	2.56	0.44
1:F:218:LYS:NZ	1:F:316:THR:O	2.45	0.44
1:F:229:ILE:O	1:F:230:ILE:HB	2.17	0.44
1:F:622:GLU:OE2	2:F:1002:ADP:C3'	2.65	0.44
1:F:355:LEU:CD1	2:F:1001:ADP:N1	2.73	0.44
1:D:328:ASP:OD2	1:D:331:PHE:N	2.51	0.44
1:D:807:THR:OG1	1:D:808:GLN:N	2.51	0.44
1:E:852:LYS:HD2	1:E:852:LYS:H	1.82	0.44
1:F:765:ARG:HA	1:F:765:ARG:NE	2.32	0.44
1:A:638:MET:SD	1:A:638:MET:C	2.96	0.44
1:E:290:MET:O	1:E:290:MET:HG2	2.18	0.44
1:A:289:LEU:O	1:A:290:MET:HB2	2.18	0.44
1:A:765:ARG:HA	1:A:765:ARG:NE	2.33	0.44
1:B:276:LYS:O	1:B:276:LYS:HG2	2.18	0.44
1:E:302:LYS:HB3	1:E:303:PRO:HD3	2.00	0.44
1:A:316:THR:OG1	1:A:317:THR:N	2.50	0.44
1:C:725:MET:SD	1:C:725:MET:N	2.90	0.44
1:C:759:ARG:NH2	1:D:644:SER:OG	2.48	0.44
1:E:795:PHE:CG	1:E:796:GLU:N	2.86	0.44
1:B:852:LYS:HD2	1:B:852:LYS:N	2.32	0.44
1:E:289:LEU:O	1:E:290:MET:HB3	2.18	0.44
1:E:410:LYS:HB2	1:E:411:PRO:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:ASP:O	1:A:705:ASP:C	2.56	0.43
1:B:316:THR:O	1:B:316:THR:HG23	2.18	0.43
1:D:649:LYS:O	1:D:650:TYR:C	2.55	0.43
1:E:817:TYR:N	1:E:817:TYR:CD2	2.83	0.43
1:F:650:TYR:O	1:F:651:ALA:C	2.55	0.43
1:D:729:LEU:C	1:D:729:LEU:HD23	2.38	0.43
1:E:602:ALA:O	1:E:603:ASN:C	2.54	0.43
1:F:649:LYS:O	1:F:650:TYR:C	2.56	0.43
1:C:519:LYS:HA	1:C:519:LYS:HD3	1.68	0.43
1:C:773:ASN:OD1	1:C:773:ASN:O	2.37	0.43
1:E:495:ARG:HD2	1:E:495:ARG:HA	1.72	0.43
1:E:845:LEU:C	1:E:845:LEU:HD12	2.38	0.43
1:F:220:ALA:CB	2:F:1001:ADP:C2'	2.71	0.43
1:B:772:PHE:CD1	1:B:772:PHE:N	2.84	0.43
1:B:383:LEU:HA	1:B:384:PRO:HD3	1.91	0.43
1:D:209:CYS:HG	1:D:335:PHE:HD2	1.64	0.43
1:F:622:GLU:OE2	2:F:1002:ADP:H3'	2.17	0.43
1:D:481:LYS:NZ	1:D:485:GLU:OE2	2.47	0.43
1:E:660:ALA:N	1:E:711:GLY:O	2.51	0.43
1:E:700:LEU:HD23	1:E:700:LEU:C	2.39	0.43
1:A:383:LEU:HD12	1:A:383:LEU:HA	1.82	0.43
1:A:384:PRO:HB3	1:A:679:PRO:CG	2.49	0.43
1:A:625:LYS:NZ	1:A:636:ASP:OD1	2.49	0.43
1:B:629:GLY:O	1:B:633:ASN:N	2.51	0.43
1:C:681:SER:OG	1:C:682:VAL:N	2.52	0.43
1:E:187:ILE:O	2:E:1001:ADP:N6	2.52	0.43
1:F:229:ILE:O	1:F:230:ILE:CB	2.67	0.43
1:B:309:GLN:O	1:B:310:LEU:C	2.57	0.43
1:C:289:LEU:O	1:C:290:MET:CB	2.63	0.43
1:D:364:GLY:O	1:D:538:GLN:NE2	2.52	0.43
1:D:648:GLU:OE2	1:E:649:LYS:NZ	2.51	0.43
1:B:247:ASP:O	1:B:249:ALA:N	2.51	0.43
1:C:356:GLN:N	1:C:357:PRO:HD2	2.34	0.43
1:E:654:LYS:NZ	1:E:694:ASP:OD2	2.36	0.43
1:D:802:TYR:CD1	1:D:802:TYR:C	2.91	0.42
1:E:629:GLY:O	1:E:633:ASN:N	2.52	0.42
1:F:625:LYS:NZ	1:F:636:ASP:OD1	2.50	0.42
1:C:378:LEU:O	1:C:379:ALA:C	2.57	0.42
1:B:216:ILE:HG13	1:B:216:ILE:O	2.19	0.42
1:B:704:ASP:O	1:B:705:ASP:C	2.57	0.42
1:E:321:TYR:CD1	1:E:321:TYR:C	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:199:VAL:O	1:F:202:ARG:HB3	2.19	0.42
1:F:849:ILE:O	1:F:849:ILE:HG23	2.18	0.42
1:B:645:GLU:O	1:B:645:GLU:HG3	2.19	0.42
1:C:247:ASP:OD1	1:C:248:LEU:N	2.51	0.42
1:E:445:LEU:C	1:E:445:LEU:CD2	2.85	0.42
1:A:725:MET:SD	1:A:725:MET:N	2.92	0.42
1:C:704:ASP:O	1:C:705:ASP:C	2.56	0.42
1:D:792:GLU:OE2	1:D:801:HIS:N	2.52	0.42
1:B:852:LYS:O	1:B:853:GLU:HB2	2.19	0.42
1:C:481:LYS:NZ	1:C:485:GLU:OE2	2.48	0.42
1:D:286:ILE:O	1:D:286:ILE:HG22	2.19	0.42
1:D:704:ASP:O	1:D:705:ASP:C	2.58	0.42
1:A:658:THR:O	1:A:659:THR:C	2.57	0.42
1:B:542:ASP:OD1	1:B:543:SER:N	2.51	0.42
1:B:710:SER:HG	1:B:714:LYS:H	1.67	0.42
1:D:769:ILE:O	1:D:769:ILE:HG23	2.19	0.42
1:E:542:ASP:OD1	1:E:543:SER:N	2.52	0.42
1:F:744:GLU:O	1:F:745:SER:CB	2.68	0.42
1:D:355:LEU:O	1:D:356:GLN:C	2.57	0.42
1:D:410:LYS:CB	1:D:411:PRO:CD	2.97	0.42
1:C:439:SER:OG	1:C:440:THR:N	2.53	0.42
1:D:352:LEU:O	1:D:356:GLN:N	2.53	0.42
1:F:725:MET:SD	1:F:725:MET:N	2.93	0.42
1:A:289:LEU:O	1:A:291:GLY:N	2.53	0.41
1:A:670:PHE:CD2	1:A:671:LEU:HG	2.56	0.41
1:A:791:ILE:O	1:A:795:PHE:N	2.53	0.41
1:B:190:GLU:H	1:B:190:GLU:CD	2.23	0.41
1:C:283:ILE:N	1:C:283:ILE:HD12	2.35	0.41
2:C:1002:ADP:O2'	2:C:1002:ADP:C8	2.70	0.41
1:D:642:ASP:C	1:D:642:ASP:OD1	2.58	0.41
1:D:699:MET:O	1:D:703:LEU:N	2.53	0.41
1:E:794:ARG:O	1:E:795:PHE:C	2.59	0.41
1:F:581:VAL:CB	2:F:1002:ADP:HN62	2.24	0.41
1:B:725:MET:SD	1:B:725:MET:N	2.93	0.41
1:E:352:LEU:O	1:E:356:GLN:N	2.53	0.41
1:B:648:GLU:OE1	1:B:648:GLU:N	2.43	0.41
1:B:626:LYS:HD3	1:B:626:LYS:HA	1.87	0.41
1:E:751:MET:HE2	1:E:751:MET:HA	2.02	0.41
1:F:309:GLN:O	1:F:310:LEU:C	2.58	0.41
1:F:369:ASP:OD1	1:F:369:ASP:N	2.53	0.41
1:F:652:VAL:O	1:F:652:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ASP:O	1:A:249:ALA:N	2.54	0.41
1:B:352:LEU:O	1:B:356:GLN:N	2.53	0.41
1:E:167:LEU:C	1:E:167:LEU:HD12	2.40	0.41
1:E:590:VAL:HA	1:E:610:PHE:CZ	2.56	0.41
1:A:379:ALA:HA	1:A:382:TYR:CE2	2.56	0.41
1:A:742:ILE:HD13	1:A:742:ILE:HA	1.91	0.41
1:C:276:LYS:O	1:C:278:LEU:N	2.54	0.41
1:C:682:VAL:HG13	1:C:682:VAL:O	2.20	0.41
1:A:649:LYS:O	1:A:650:TYR:C	2.59	0.41
1:D:568:LYS:O	1:D:572:MET:N	2.53	0.41
1:D:571:HIS:O	1:D:572:MET:C	2.59	0.41
1:E:642:ASP:C	1:E:642:ASP:OD1	2.58	0.41
1:E:831:LEU:O	1:E:832:ILE:HB	2.21	0.41
1:E:837:LEU:HD23	1:E:837:LEU:HA	1.88	0.41
1:F:619:GLY:HA2	2:F:1002:ADP:PA	2.61	0.41
1:B:596:LEU:HD23	1:B:596:LEU:HA	1.67	0.41
1:F:622:GLU:O	1:F:623:LEU:C	2.59	0.41
1:B:208:PRO:O	1:B:209:CYS:HB3	2.21	0.40
1:B:296:ASP:OD1	1:B:300:ILE:N	2.54	0.40
1:B:558:VAL:O	1:B:558:VAL:CG1	2.69	0.40
1:B:850:LYS:HE3	1:B:850:LYS:HB2	1.92	0.40
1:A:567:GLU:O	1:A:571:HIS:HB2	2.20	0.40
1:B:296:ASP:O	1:B:298:ALA:N	2.53	0.40
1:E:801:HIS:O	1:E:801:HIS:CG	2.72	0.40
1:D:247:ASP:O	1:D:249:ALA:N	2.54	0.40
1:E:228:ARG:O	1:E:232:ASP:N	2.55	0.40
1:F:796:GLU:HG3	1:F:797:GLN:N	2.36	0.40
1:A:595:ARG:HD2	1:A:595:ARG:HA	1.83	0.40
1:C:190:GLU:OE1	1:C:190:GLU:N	2.38	0.40
1:C:650:TYR:CE1	1:C:654:LYS:HB3	2.57	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	571/908 (63%)	530 (93%)	33 (6%)	8 (1%)	11 45
1	B	571/908 (63%)	516 (90%)	37 (6%)	18 (3%)	4 26
1	C	701/908 (77%)	661 (94%)	33 (5%)	7 (1%)	15 54
1	D	701/908 (77%)	642 (92%)	43 (6%)	16 (2%)	6 34
1	E	701/908 (77%)	648 (92%)	38 (5%)	15 (2%)	7 36
1	F	571/908 (63%)	528 (92%)	35 (6%)	8 (1%)	11 45
All	All	3816/5448 (70%)	3525 (92%)	219 (6%)	72 (2%)	11 38

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	LEU
1	A	542	ASP
1	A	556	ILE
1	A	557	PRO
1	A	650	TYR
1	B	208	PRO
1	B	248	LEU
1	B	276	LYS
1	B	542	ASP
1	B	556	ILE
1	B	566	ASN
1	C	542	ASP
1	D	248	LEU
1	D	277	THR
1	D	410	LYS
1	D	510	ILE
1	D	542	ASP
1	F	230	ILE
1	F	248	LEU
1	F	745	SER
1	F	879	LEU
1	A	853	GLU
1	A	881	VAL
1	B	293	GLY
1	B	796	GLU
1	B	853	GLU
1	B	880	GLU

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Mol	Chain	Res	Type
1	C	277	THR
1	C	651	ALA
1	D	804	LEU
1	D	854	THR
1	E	248	LEU
1	E	274	GLU
1	E	277	THR
1	E	310	LEU
1	E	650	TYR
1	E	669	GLY
1	F	562	SER
1	B	384	PRO
1	B	557	PRO
1	B	651	ALA
1	B	664	GLY
1	B	801	HIS
1	D	650	TYR
1	E	880	GLU
1	F	796	GLU
1	C	880	GLU
1	D	525	ALA
1	D	536	MET
1	D	823	MET
1	E	293	GLY
1	E	294	LYS
1	E	539	ASN
1	E	853	GLU
1	F	295	ASP
1	A	294	LYS
1	B	277	THR
1	B	309	GLN
1	C	776	SER
1	C	881	VAL
1	D	384	PRO
1	D	572	MET
1	D	807	THR
1	D	880	GLU
1	D	881	VAL
1	E	801	HIS
1	E	881	VAL
1	B	383	LEU
1	E	537	ILE

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Mol	Chain	Res	Type
1	E	556	ILE
1	C	389	PRO
1	F	881	VAL

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	494/783 (63%)	492 (100%)	2 (0%)	91 94
1	B	494/783 (63%)	494 (100%)	0	100 100
1	C	606/783 (77%)	606 (100%)	0	100 100
1	D	606/783 (77%)	604 (100%)	2 (0%)	92 95
1	E	606/783 (77%)	606 (100%)	0	100 100
1	F	494/783 (63%)	494 (100%)	0	100 100
All	All	3300/4698 (70%)	3296 (100%)	4 (0%)	93 96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	572	MET
1	A	574	ARG
1	D	612	PHE
1	D	823	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	362	HIS
1	A	829	ASN
1	B	798	ASN

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)

12 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	ADP	E	1001	-	24,29,29	1.34	3 (12%)	29,45,45	1.84	6 (20%)
2	ADP	B	1002	-	24,29,29	1.52	5 (20%)	29,45,45	1.81	6 (20%)
2	ADP	E	1002	-	24,29,29	1.40	5 (20%)	29,45,45	1.76	5 (17%)
2	ADP	D	1001	-	24,29,29	1.35	2 (8%)	29,45,45	1.91	5 (17%)
2	ADP	A	1001	-	24,29,29	1.53	5 (20%)	29,45,45	1.91	7 (24%)
2	ADP	A	1002	-	24,29,29	1.12	1 (4%)	29,45,45	1.82	5 (17%)
2	ADP	F	1002	1	24,29,29	1.40	5 (20%)	29,45,45	1.76	5 (17%)
2	ADP	F	1001	-	24,29,29	1.33	4 (16%)	29,45,45	1.78	6 (20%)
2	ADP	C	1001	-	24,29,29	1.36	6 (25%)	29,45,45	1.56	4 (13%)
2	ADP	D	1002	-	24,29,29	1.52	5 (20%)	29,45,45	1.65	3 (10%)
2	ADP	C	1002	-	24,29,29	1.35	4 (16%)	29,45,45	1.61	7 (24%)
2	ADP	B	1001	-	24,29,29	1.32	4 (16%)	29,45,45	1.79	6 (20%)

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	ADP	E	1001	-	-	6/12/32/32	0/3/3/3
2	ADP	B	1002	-	-	5/12/32/32	0/3/3/3
2	ADP	E	1002	-	-	3/12/32/32	0/3/3/3
2	ADP	D	1001	-	-	7/12/32/32	0/3/3/3
2	ADP	A	1001	-	-	6/12/32/32	0/3/3/3
2	ADP	A	1002	-	-	4/12/32/32	0/3/3/3
2	ADP	F	1002	1	-	3/12/32/32	0/3/3/3
2	ADP	F	1001	-	-	4/12/32/32	0/3/3/3
2	ADP	C	1001	-	-	5/12/32/32	0/3/3/3
2	ADP	D	1002	-	-	3/12/32/32	0/3/3/3
2	ADP	C	1002	-	-	3/12/32/32	0/3/3/3
2	ADP	B	1001	-	-	4/12/32/32	0/3/3/3

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	ADP	O4'-C1'	3.41	1.45	1.41
2	F	1001	ADP	C2'-C1'	-3.26	1.48	1.53
2	B	1002	ADP	C5-N7	-3.25	1.27	1.39
2	F	1002	ADP	C2'-C1'	-3.22	1.48	1.53
2	E	1002	ADP	C2'-C1'	-3.20	1.48	1.53
2	B	1001	ADP	C2'-C1'	-3.17	1.48	1.53
2	B	1002	ADP	C2'-C1'	-3.13	1.49	1.53
2	D	1002	ADP	C2'-C1'	-3.02	1.49	1.53
2	D	1002	ADP	C5-N7	-2.91	1.29	1.39
2	A	1001	ADP	C2-N3	2.90	1.36	1.32
2	D	1001	ADP	C2'-C1'	-2.73	1.49	1.53
2	B	1002	ADP	C2-N3	2.63	1.36	1.32
2	C	1002	ADP	C5-N7	-2.63	1.30	1.39
2	A	1001	ADP	C2'-C1'	-2.58	1.49	1.53
2	E	1001	ADP	C2'-C1'	-2.49	1.50	1.53
2	C	1001	ADP	C5-N7	-2.46	1.30	1.39
2	C	1001	ADP	C2-N3	2.46	1.36	1.32
2	B	1001	ADP	C5-N7	-2.42	1.30	1.39
2	A	1001	ADP	C5-N7	-2.40	1.31	1.39
2	F	1001	ADP	C5-N7	-2.40	1.31	1.39
2	C	1001	ADP	C2'-C1'	-2.35	1.50	1.53
2	D	1001	ADP	C5-N7	-2.35	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1002	ADP	C2-N3	2.33	1.35	1.32
2	E	1001	ADP	C2'-C3'	-2.31	1.47	1.53
2	E	1002	ADP	PA-O2A	-2.26	1.44	1.55
2	C	1002	ADP	C2-N3	2.26	1.35	1.32
2	F	1002	ADP	PA-O2A	-2.26	1.44	1.55
2	F	1002	ADP	C5-N7	-2.25	1.31	1.39
2	E	1001	ADP	C5-N7	-2.24	1.31	1.39
2	C	1001	ADP	PA-O1A	-2.21	1.43	1.50
2	B	1001	ADP	PA-O2A	-2.21	1.45	1.55
2	F	1001	ADP	PA-O2A	-2.20	1.45	1.55
2	E	1002	ADP	C5-N7	-2.19	1.31	1.39
2	C	1001	ADP	PA-O2A	-2.15	1.45	1.55
2	A	1002	ADP	PB-O2B	2.13	1.63	1.54
2	C	1002	ADP	PA-O2A	-2.12	1.45	1.55
2	A	1001	ADP	PB-O2B	2.10	1.63	1.54
2	E	1002	ADP	PB-O2B	2.07	1.62	1.54
2	F	1002	ADP	PB-O2B	2.07	1.62	1.54
2	E	1002	ADP	PB-O3B	-2.06	1.46	1.54
2	B	1002	ADP	PB-O2B	2.05	1.62	1.54
2	B	1002	ADP	PA-O2A	-2.04	1.45	1.55
2	F	1002	ADP	PB-O3B	-2.04	1.47	1.54
2	D	1002	ADP	PB-O2B	2.03	1.62	1.54
2	D	1002	ADP	PA-O2A	-2.02	1.45	1.55
2	C	1002	ADP	PB-O2B	2.02	1.62	1.54
2	F	1001	ADP	PB-O2B	2.02	1.62	1.54
2	B	1001	ADP	PB-O2B	2.02	1.62	1.54
2	C	1001	ADP	PB-O2B	2.00	1.62	1.54

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1002	ADP	N3-C2-N1	-6.44	118.61	128.68
2	E	1002	ADP	N3-C2-N1	-6.42	118.64	128.68
2	F	1002	ADP	N3-C2-N1	-6.41	118.66	128.68
2	D	1001	ADP	N3-C2-N1	-6.25	118.91	128.68
2	D	1002	ADP	N3-C2-N1	-6.07	119.19	128.68
2	E	1001	ADP	N3-C2-N1	-6.06	119.20	128.68
2	B	1001	ADP	N3-C2-N1	-5.95	119.38	128.68
2	F	1001	ADP	N3-C2-N1	-5.93	119.41	128.68
2	C	1001	ADP	N3-C2-N1	-5.79	119.62	128.68
2	B	1002	ADP	N3-C2-N1	-5.69	119.79	128.68
2	A	1001	ADP	N3-C2-N1	-5.32	120.37	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1002	ADP	N3-C2-N1	-5.31	120.38	128.68
2	D	1001	ADP	C3'-C2'-C1'	5.30	108.95	100.98
2	A	1001	ADP	O4'-C1'-C2'	-4.59	100.22	106.93
2	B	1002	ADP	C3'-C2'-C1'	3.80	106.70	100.98
2	A	1002	ADP	C1'-N9-C4	-3.79	119.98	126.64
2	B	1001	ADP	O4'-C1'-C2'	-3.71	101.51	106.93
2	F	1001	ADP	O4'-C1'-C2'	-3.70	101.53	106.93
2	D	1002	ADP	O5'-C5'-C4'	-3.47	97.05	108.99
2	A	1001	ADP	O4'-C4'-C5'	3.32	120.31	109.37
2	F	1001	ADP	O4'-C4'-C5'	3.30	120.23	109.37
2	B	1001	ADP	O4'-C4'-C5'	3.29	120.21	109.37
2	A	1001	ADP	C5-C6-N6	-3.24	115.43	120.35
2	E	1001	ADP	C3'-C2'-C1'	-3.07	96.36	100.98
2	E	1001	ADP	O3'-C3'-C4'	3.02	119.80	111.05
2	B	1002	ADP	C5-C6-N6	-2.90	115.95	120.35
2	A	1002	ADP	C3'-C2'-C1'	2.77	105.15	100.98
2	D	1001	ADP	O5'-C5'-C4'	-2.75	99.52	108.99
2	C	1002	ADP	O5'-C5'-C4'	-2.75	99.54	108.99
2	E	1001	ADP	C1'-N9-C4	-2.72	121.86	126.64
2	B	1001	ADP	O5'-C5'-C4'	-2.72	99.62	108.99
2	F	1001	ADP	O5'-C5'-C4'	-2.71	99.65	108.99
2	A	1002	ADP	O4'-C4'-C5'	2.59	117.88	109.37
2	D	1001	ADP	O4'-C4'-C3'	2.54	110.14	105.11
2	E	1002	ADP	C1'-N9-C4	-2.51	122.23	126.64
2	F	1002	ADP	C1'-N9-C4	-2.49	122.27	126.64
2	E	1002	ADP	O5'-C5'-C4'	-2.47	100.48	108.99
2	F	1002	ADP	O5'-C5'-C4'	-2.46	100.53	108.99
2	E	1001	ADP	O5'-C5'-C4'	-2.45	100.56	108.99
2	F	1002	ADP	O4'-C1'-C2'	-2.44	103.36	106.93
2	E	1002	ADP	O4'-C1'-C2'	-2.43	103.38	106.93
2	D	1002	ADP	PA-O3A-PB	2.39	141.02	132.83
2	F	1002	ADP	C5-C6-N6	-2.35	116.78	120.35
2	A	1001	ADP	C4-C5-N7	-2.32	106.98	109.40
2	E	1002	ADP	C5-C6-N6	-2.31	116.84	120.35
2	C	1001	ADP	C4-C5-N7	-2.31	107.00	109.40
2	B	1002	ADP	O4'-C4'-C3'	2.31	109.68	105.11
2	A	1001	ADP	C5'-C4'-C3'	-2.29	106.61	115.18
2	A	1001	ADP	O5'-C5'-C4'	-2.28	101.15	108.99
2	C	1002	ADP	O4'-C4'-C3'	2.28	109.62	105.11
2	A	1002	ADP	C5'-C4'-C3'	-2.26	106.70	115.18
2	C	1002	ADP	C4-C5-N7	-2.21	107.09	109.40
2	B	1002	ADP	C5'-C4'-C3'	-2.18	107.01	115.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1001	ADP	C4-C5-N7	-2.16	107.15	109.40
2	C	1002	ADP	C3'-C2'-C1'	2.15	104.21	100.98
2	C	1001	ADP	O4'-C4'-C3'	2.14	109.34	105.11
2	B	1002	ADP	N6-C6-N1	2.13	123.00	118.57
2	C	1002	ADP	O4'-C4'-C5'	2.13	116.37	109.37
2	F	1001	ADP	C1'-N9-C4	-2.12	122.92	126.64
2	E	1001	ADP	C4-C5-N7	-2.11	107.20	109.40
2	C	1001	ADP	C5'-C4'-C3'	-2.10	107.32	115.18
2	B	1001	ADP	C1'-N9-C4	-2.09	122.97	126.64
2	B	1001	ADP	C4-C5-N7	-2.09	107.23	109.40
2	C	1002	ADP	C5'-C4'-C3'	-2.08	107.39	115.18
2	D	1001	ADP	C5-C6-N6	-2.06	117.22	120.35

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	ADP	C5'-O5'-PA-O1A
2	A	1001	ADP	C3'-C4'-C5'-O5'
2	B	1002	ADP	PA-O3A-PB-O3B
2	C	1001	ADP	PA-O3A-PB-O3B
2	C	1002	ADP	C5'-O5'-PA-O1A
2	C	1002	ADP	C5'-O5'-PA-O3A
2	D	1001	ADP	PA-O3A-PB-O3B
2	D	1001	ADP	C5'-O5'-PA-O1A
2	D	1001	ADP	C5'-O5'-PA-O3A
2	D	1001	ADP	C4'-C5'-O5'-PA
2	D	1002	ADP	O4'-C4'-C5'-O5'
2	D	1002	ADP	C3'-C4'-C5'-O5'
2	E	1001	ADP	C5'-O5'-PA-O3A
2	E	1001	ADP	C4'-C5'-O5'-PA
2	E	1001	ADP	O4'-C4'-C5'-O5'
2	B	1002	ADP	O4'-C4'-C5'-O5'
2	C	1002	ADP	C4'-C5'-O5'-PA
2	E	1002	ADP	C4'-C5'-O5'-PA
2	F	1002	ADP	C4'-C5'-O5'-PA
2	C	1001	ADP	C4'-C5'-O5'-PA
2	B	1002	ADP	C3'-C4'-C5'-O5'
2	C	1001	ADP	O4'-C4'-C5'-O5'
2	B	1001	ADP	PA-O3A-PB-O1B
2	F	1001	ADP	PA-O3A-PB-O1B
2	A	1001	ADP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	C	1001	ADP	C3'-C4'-C5'-O5'
2	D	1001	ADP	PB-O3A-PA-O5'
2	A	1001	ADP	C5'-O5'-PA-O3A
2	A	1002	ADP	C5'-O5'-PA-O3A
2	E	1002	ADP	O4'-C4'-C5'-O5'
2	F	1002	ADP	O4'-C4'-C5'-O5'
2	E	1001	ADP	PB-O3A-PA-O1A
2	A	1001	ADP	C4'-C5'-O5'-PA
2	A	1001	ADP	C5'-O5'-PA-O2A
2	A	1002	ADP	C5'-O5'-PA-O2A
2	D	1001	ADP	C5'-O5'-PA-O2A
2	E	1001	ADP	C5'-O5'-PA-O1A
2	B	1001	ADP	O4'-C4'-C5'-O5'
2	F	1001	ADP	O4'-C4'-C5'-O5'
2	B	1001	ADP	C4'-C5'-O5'-PA
2	B	1002	ADP	PA-O3A-PB-O1B
2	E	1001	ADP	PA-O3A-PB-O1B
2	F	1001	ADP	C4'-C5'-O5'-PA
2	E	1002	ADP	PB-O3A-PA-O1A
2	F	1002	ADP	PB-O3A-PA-O1A
2	D	1001	ADP	PA-O3A-PB-O1B
2	B	1001	ADP	PA-O3A-PB-O3B
2	B	1002	ADP	PA-O3A-PB-O2B
2	F	1001	ADP	PA-O3A-PB-O3B
2	A	1002	ADP	PB-O3A-PA-O1A
2	D	1002	ADP	PB-O3A-PA-O1A
2	A	1002	ADP	C5'-O5'-PA-O1A
2	C	1001	ADP	PA-O3A-PB-O1B

There are no ring outliers.

11 monomers are involved in 132 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1001	ADP	5	0
2	E	1002	ADP	1	0
2	D	1001	ADP	8	0
2	A	1001	ADP	1	0
2	A	1002	ADP	3	0
2	F	1002	ADP	51	0
2	F	1001	ADP	53	0
2	C	1001	ADP	4	0
2	D	1002	ADP	3	0

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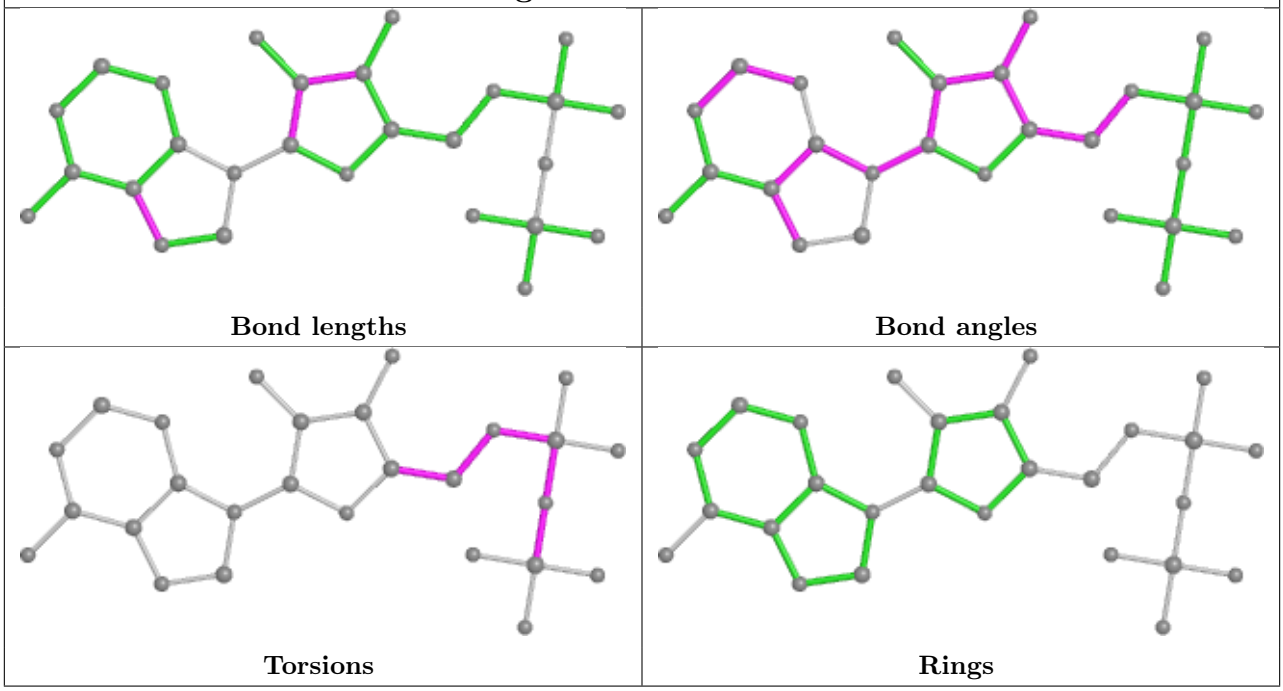
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1002	ADP	2	0
2	B	1001	ADP	1	0

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 ADP E 1001



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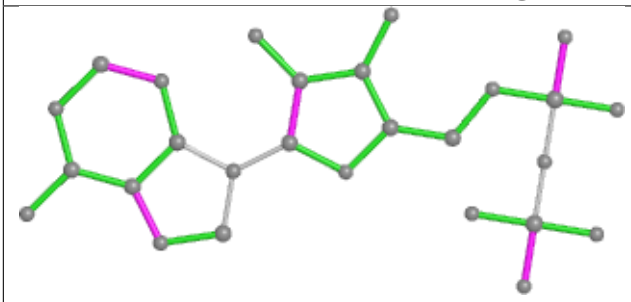
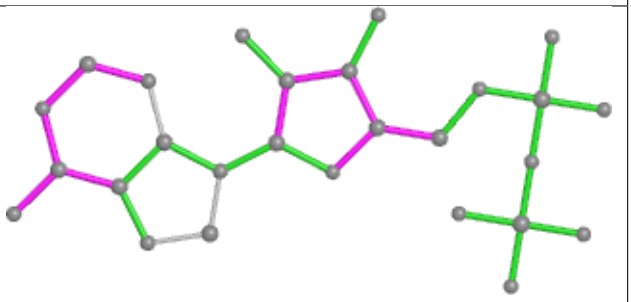
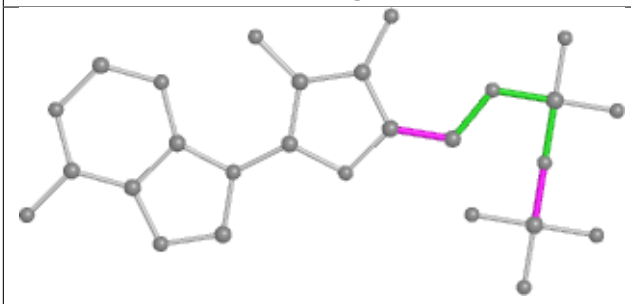
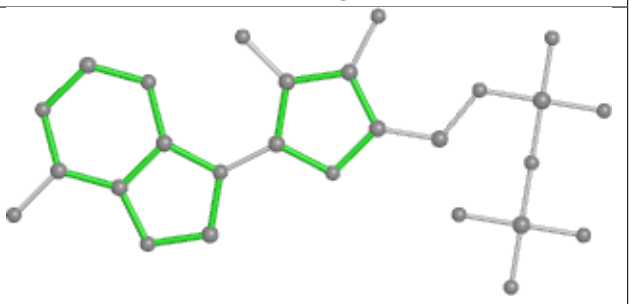
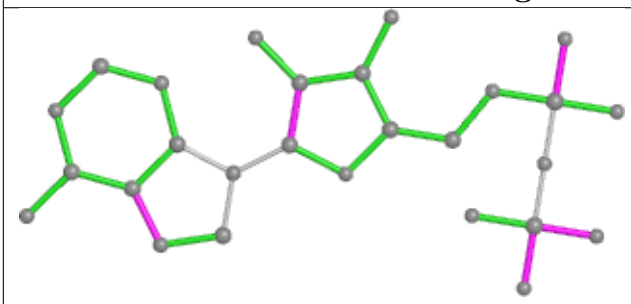
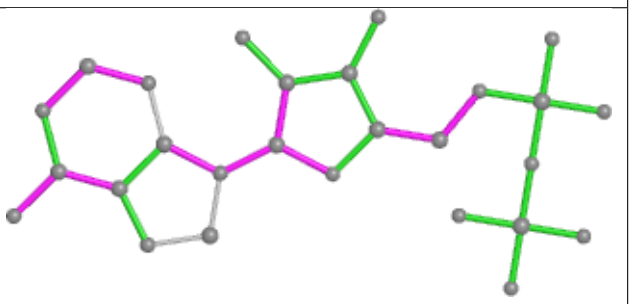
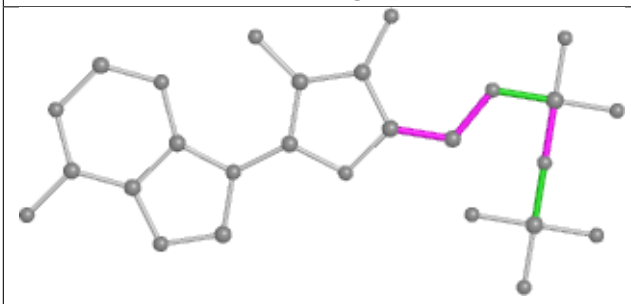
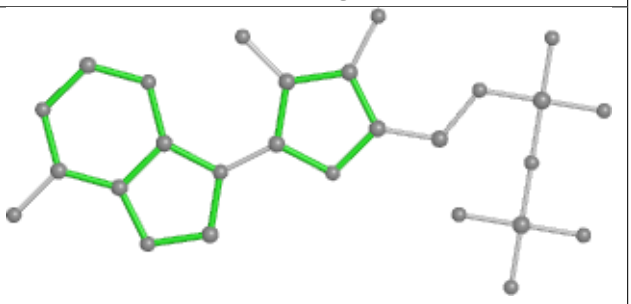
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP E 1002	
 Bond lengths	 Bond angles
 Torsions	 Rings

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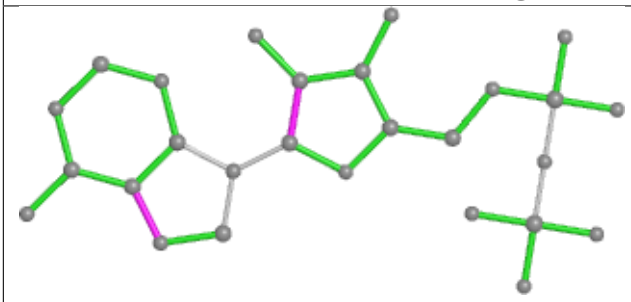
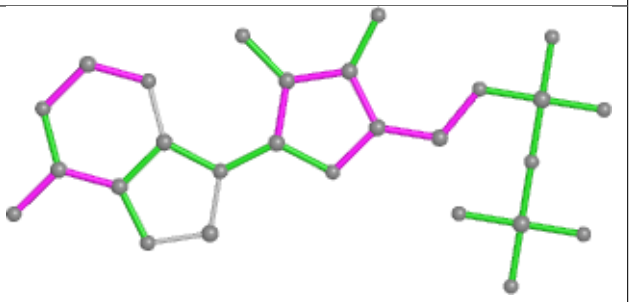
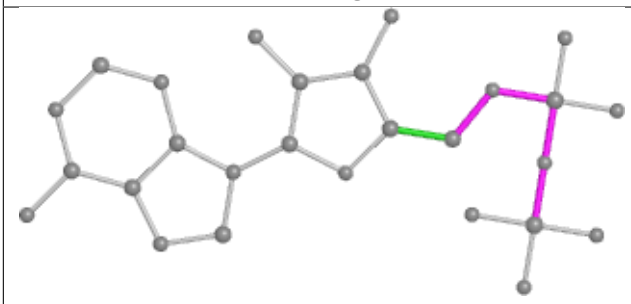
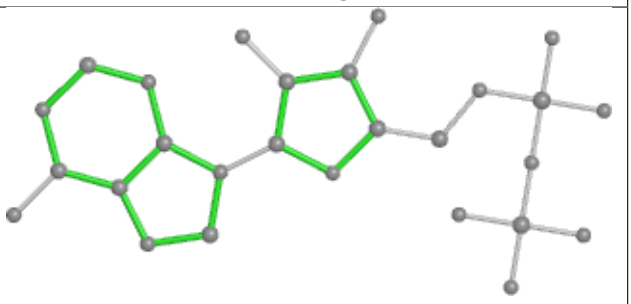
 Bond lengths	 Bond angles
 Torsions	 Rings

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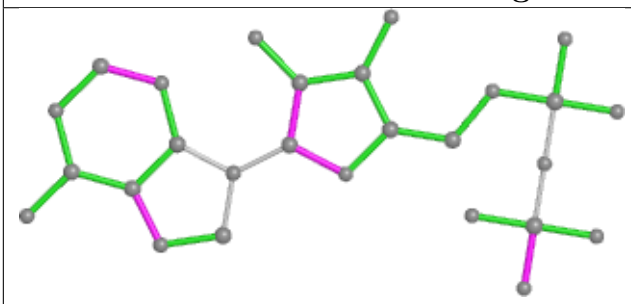
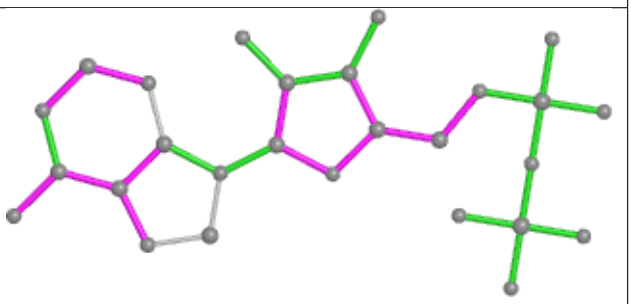
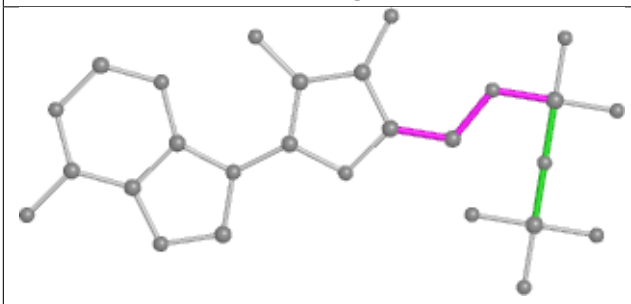
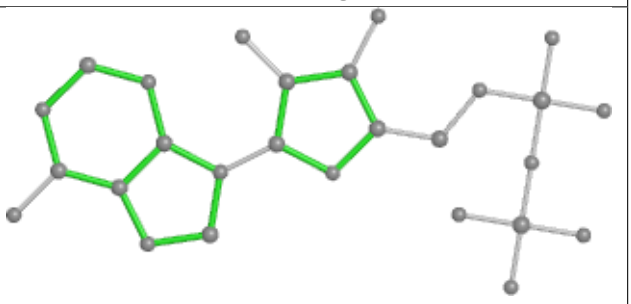
 Bond lengths	 Bond angles
 Torsions	 Rings

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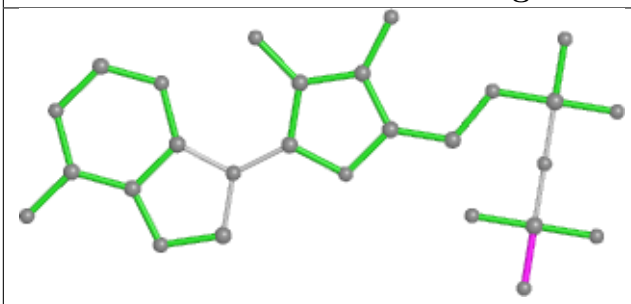
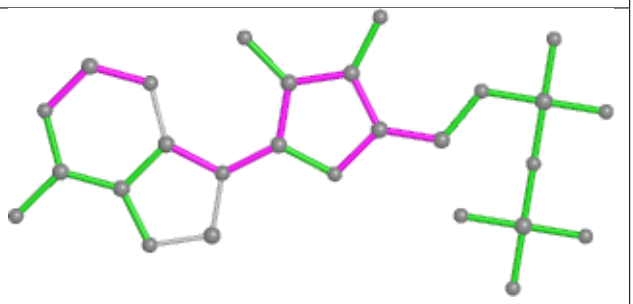


Bond lengths



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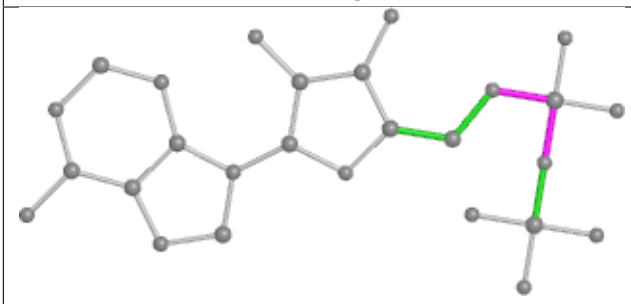
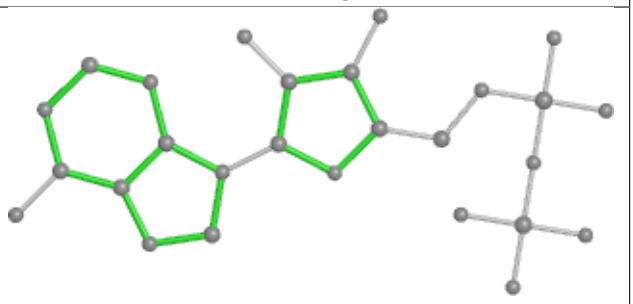


Torsions



Rings

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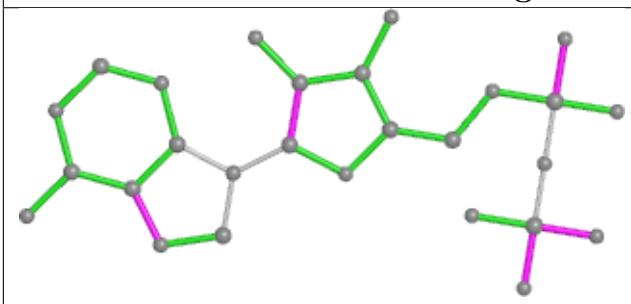

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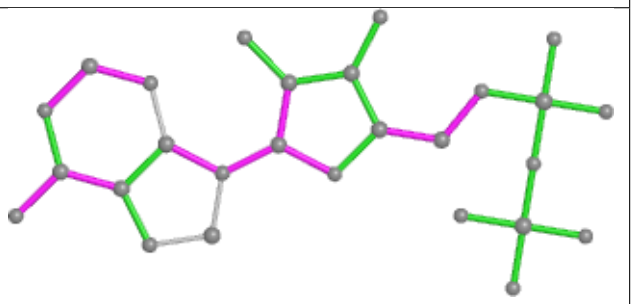
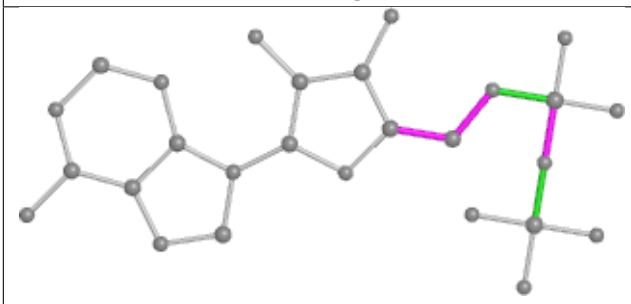


Bond angles



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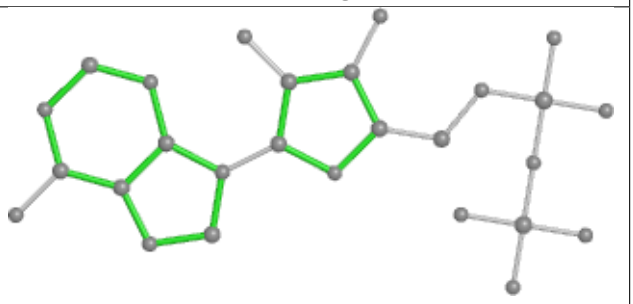

Rings

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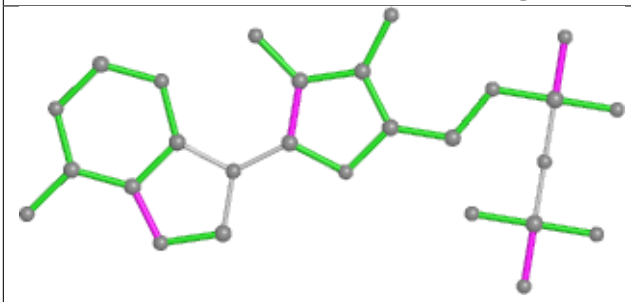
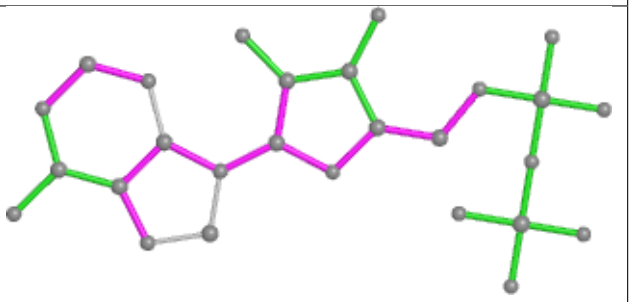
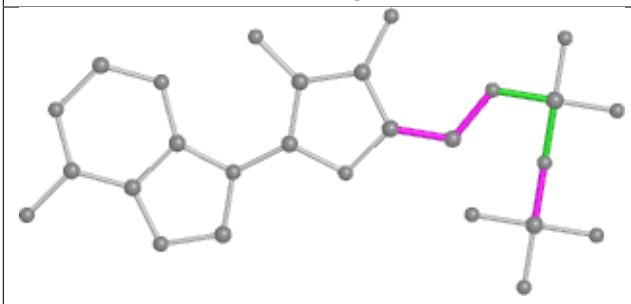
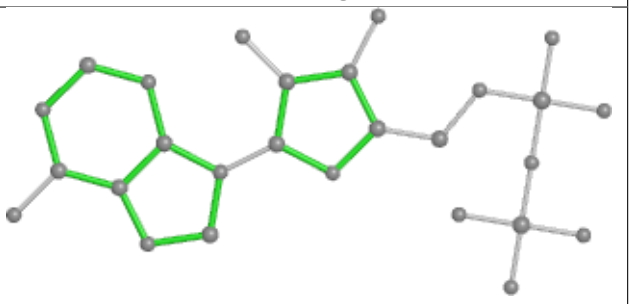
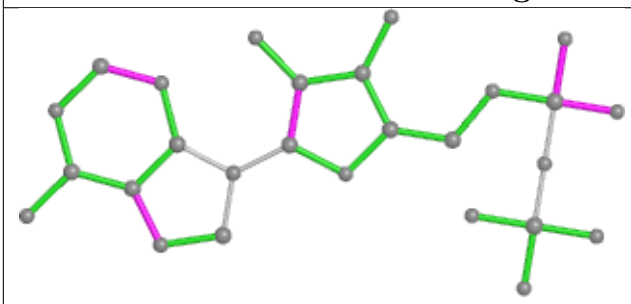
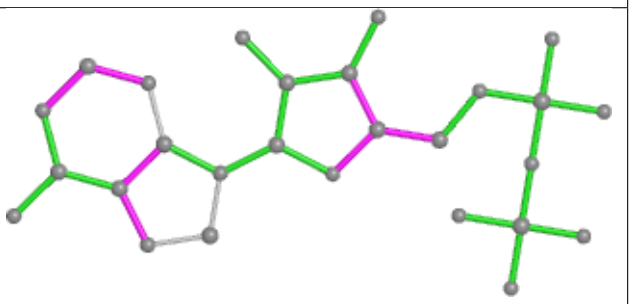
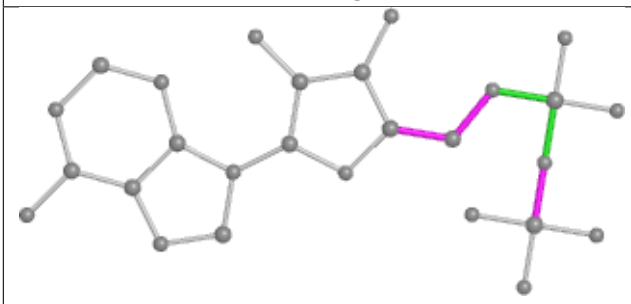
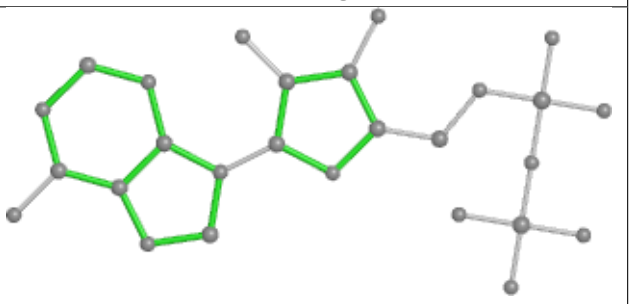
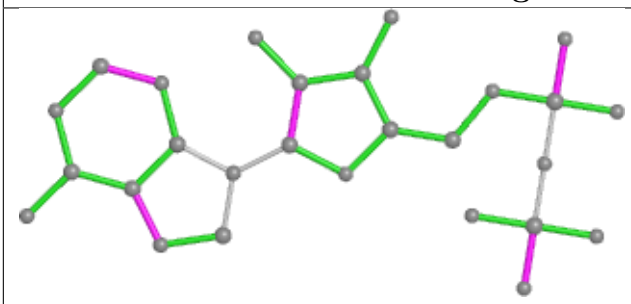
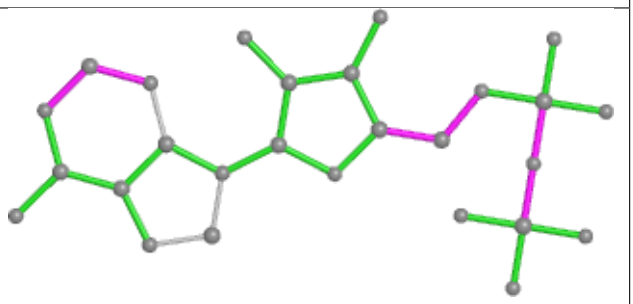
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP C 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

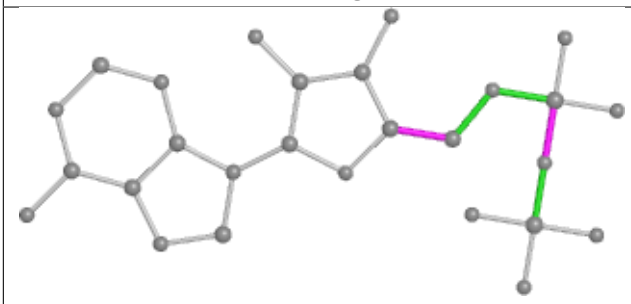
Ligand ADP D 1002



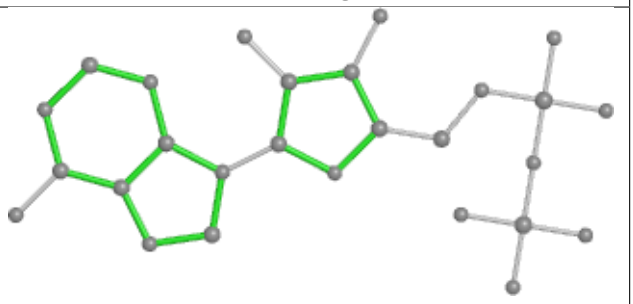
Bond lengths



Bond angles



Torsions



Rings

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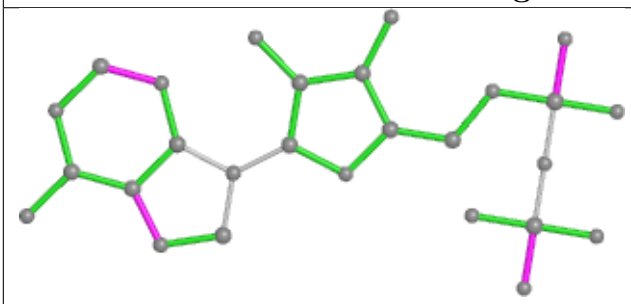

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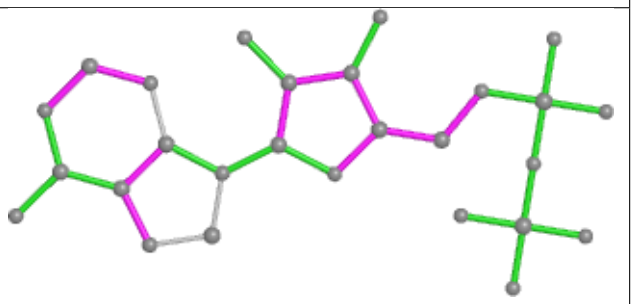
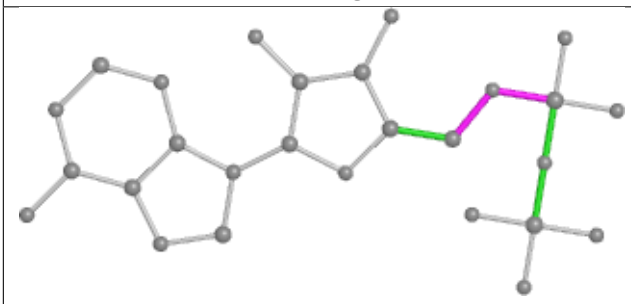
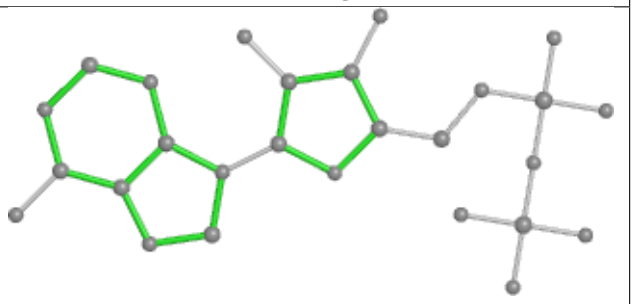


Bond angles

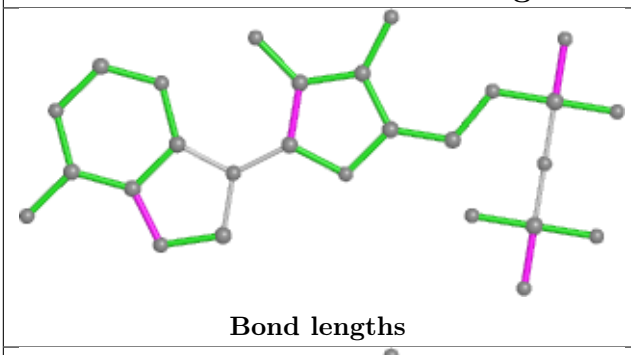


Torsions

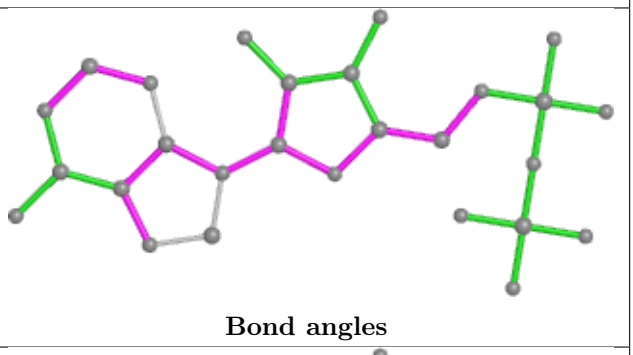


Rings

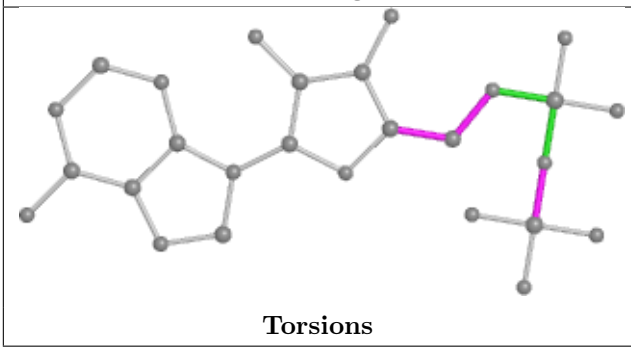
Ligand ADP B 1001



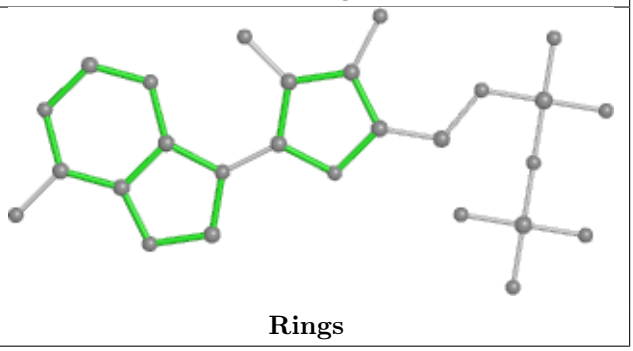
Bond lengths



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.

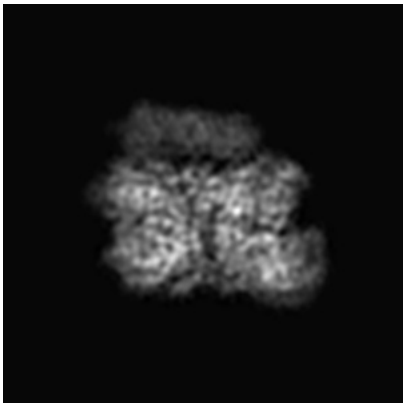
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8744. These allow visual inspection of the internal detail of the map and identification of artifacts.

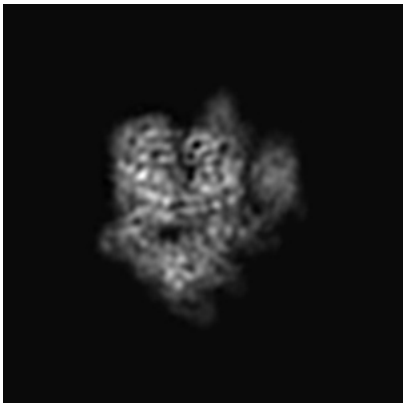
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

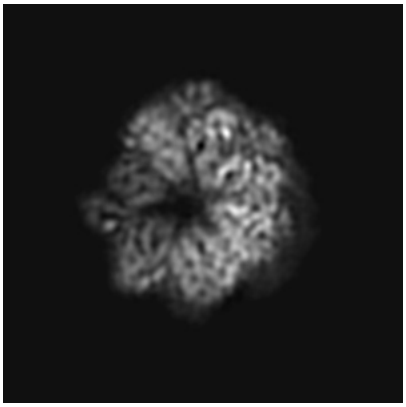
6.1.1 Primary map



X



Y

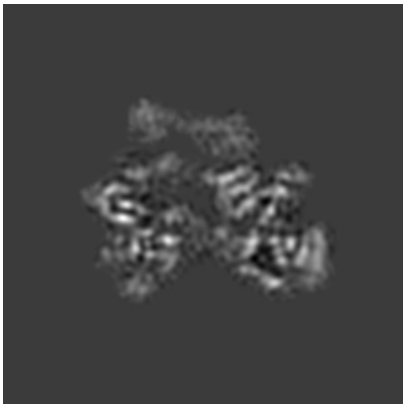


Z

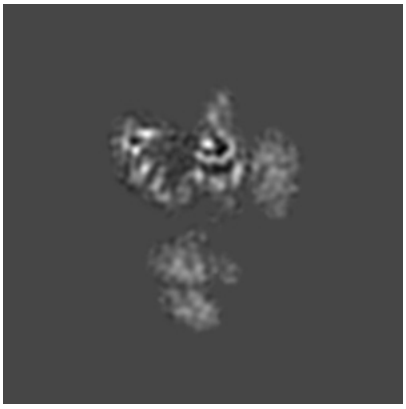
The images above show the map projected in three orthogonal directions.

6.2 Central slices

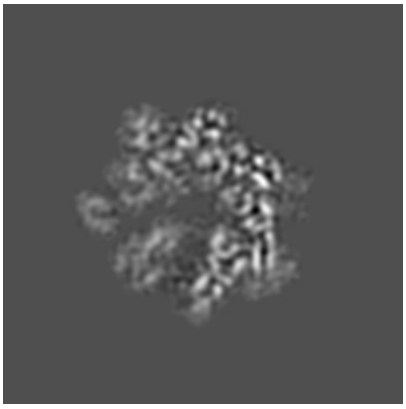
6.2.1 Primary map



X Index: 128



Y Index: 128

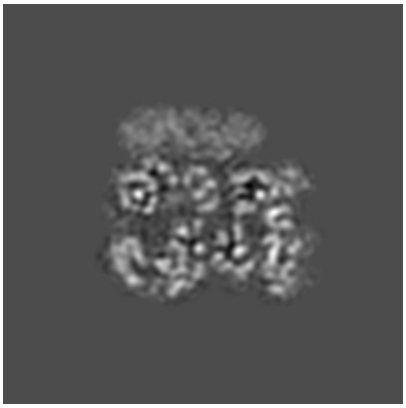


Z Index: 128

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: 143

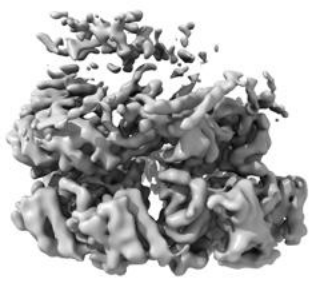
Y Index: 151

Z Index: 90

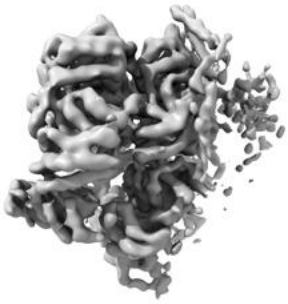
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

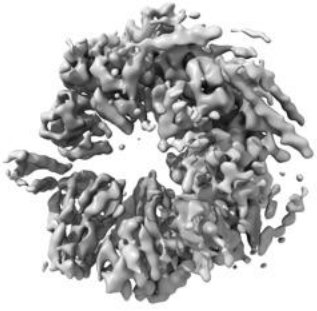
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0194. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

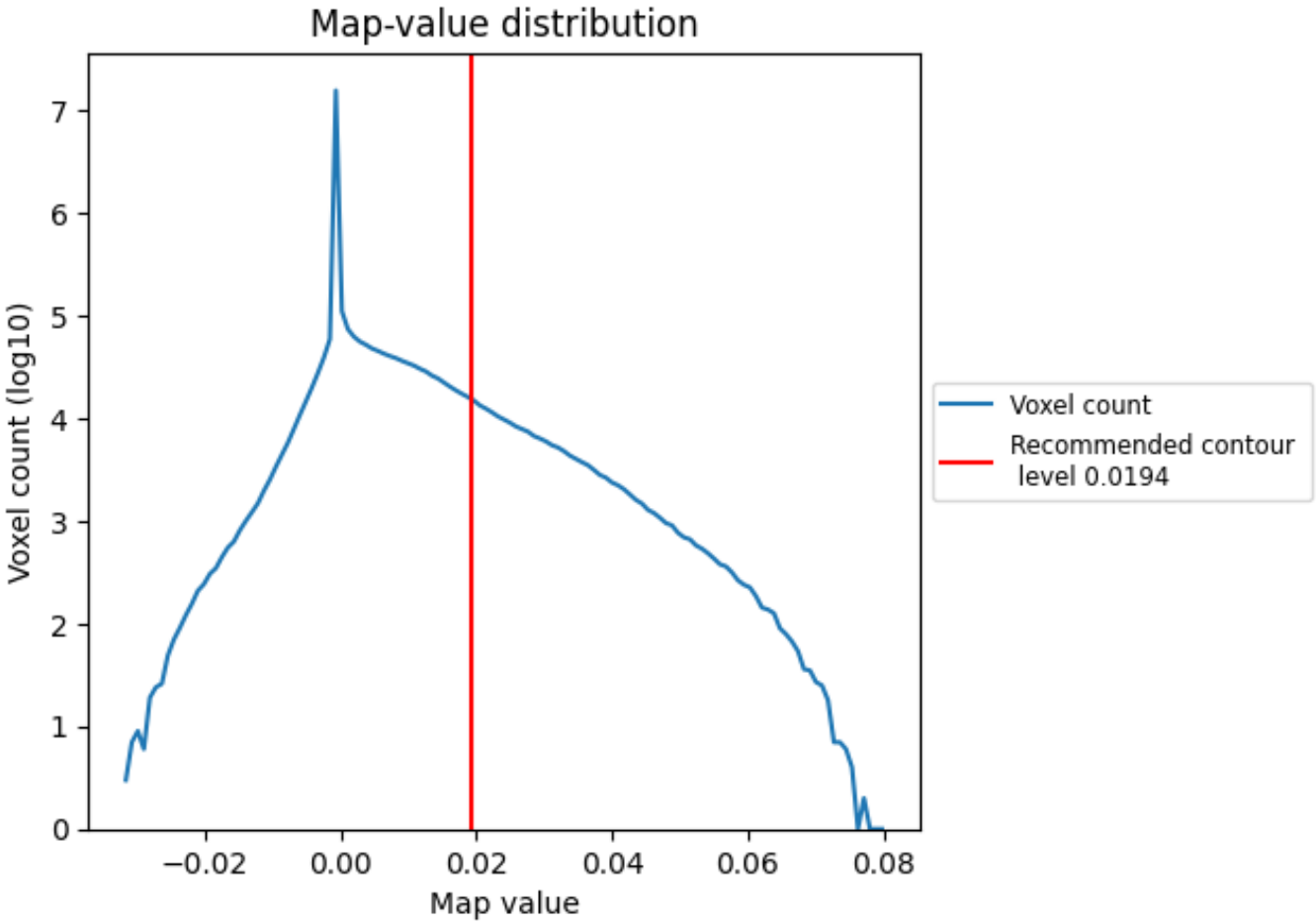
6.5 Mask visualisation (i)

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

7 Map analysis

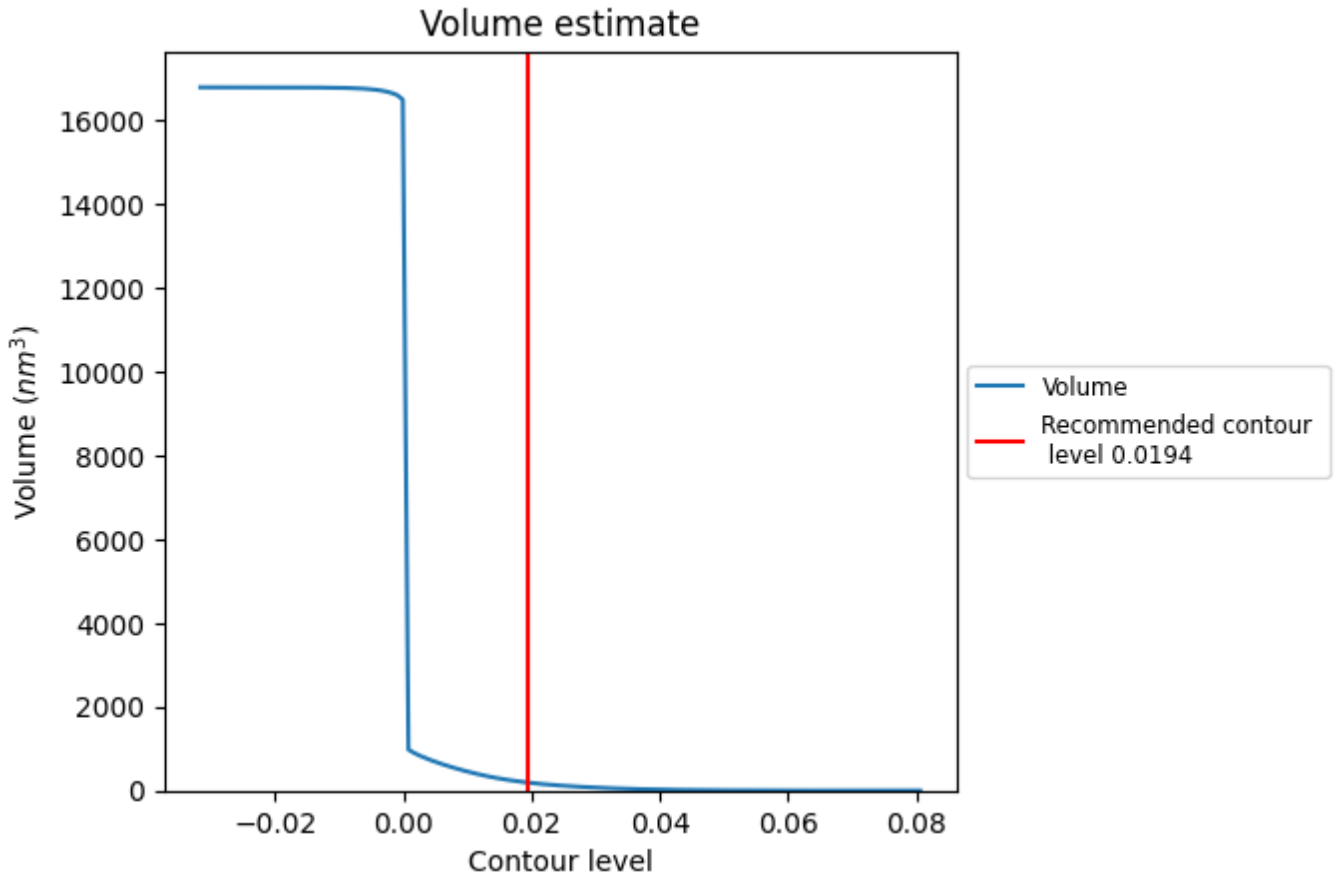
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

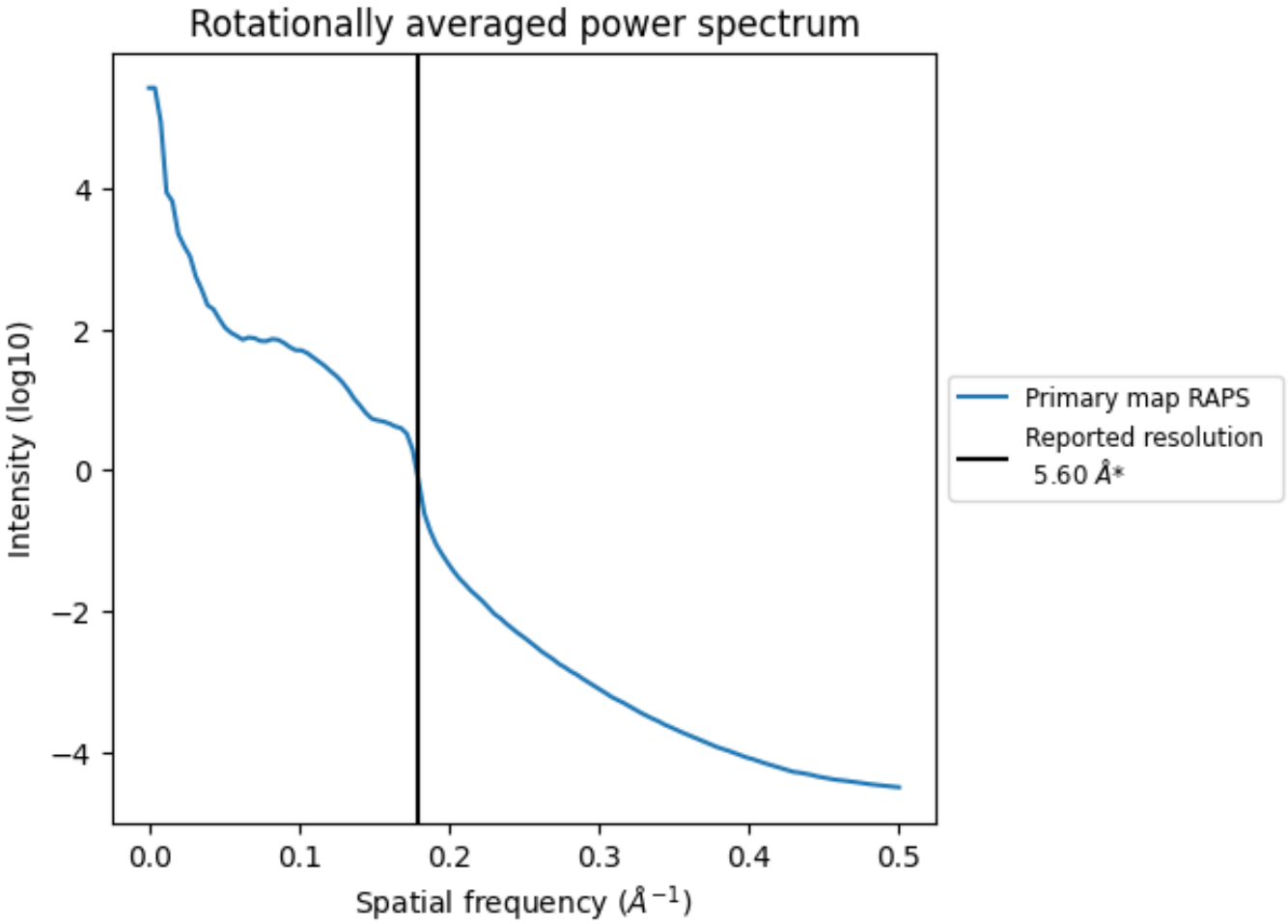
7.2 Volume estimate



The volume at the recommended contour level is 191 nm^3; this corresponds to an approximate mass of 173 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 0.179 $Å^{-1}$

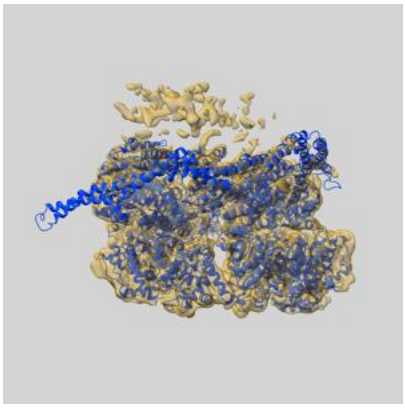
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

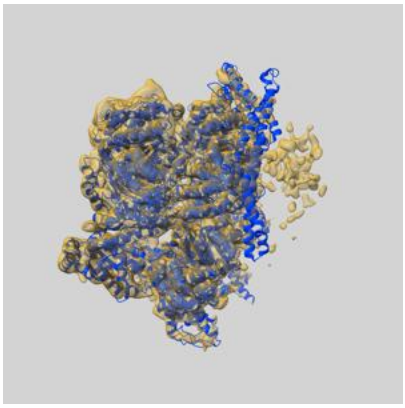
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8744 and PDB model 5VY8. Per-residue inclusion information can be found in section 3 on page 6.

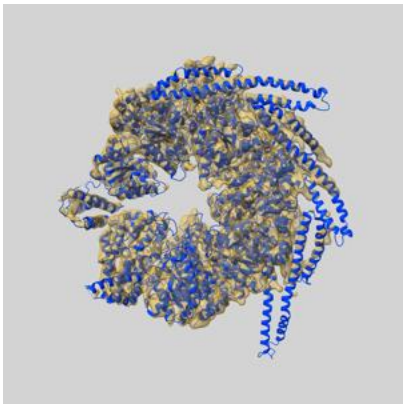
9.1 Map-model overlay



X



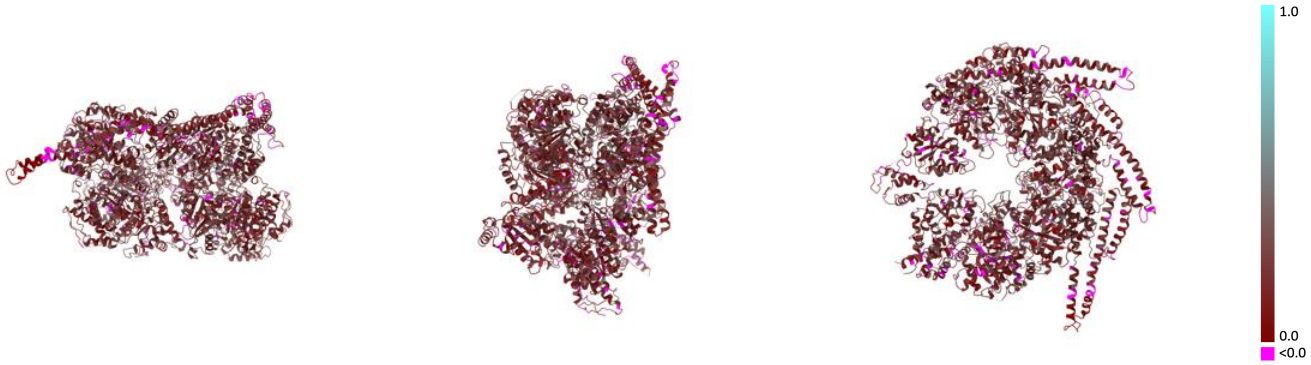
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0194 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.

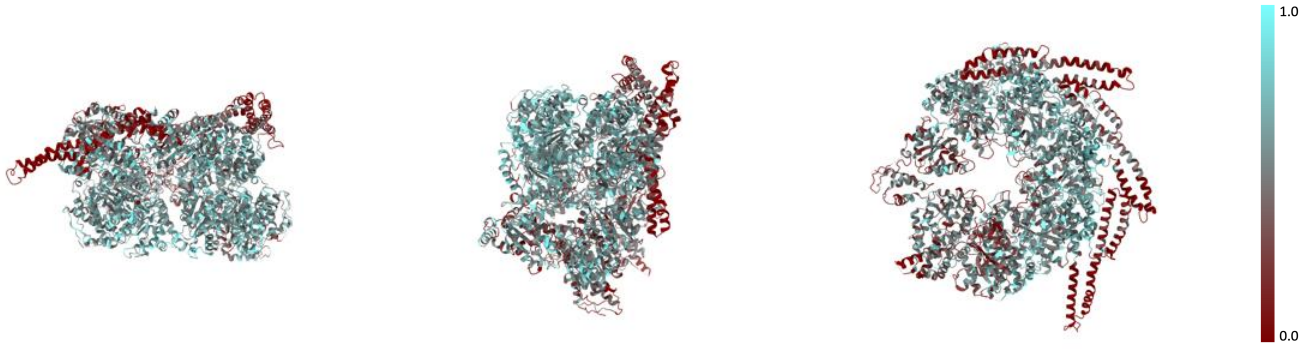
9.2 Q-score mapped to coordinate model (i)



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.

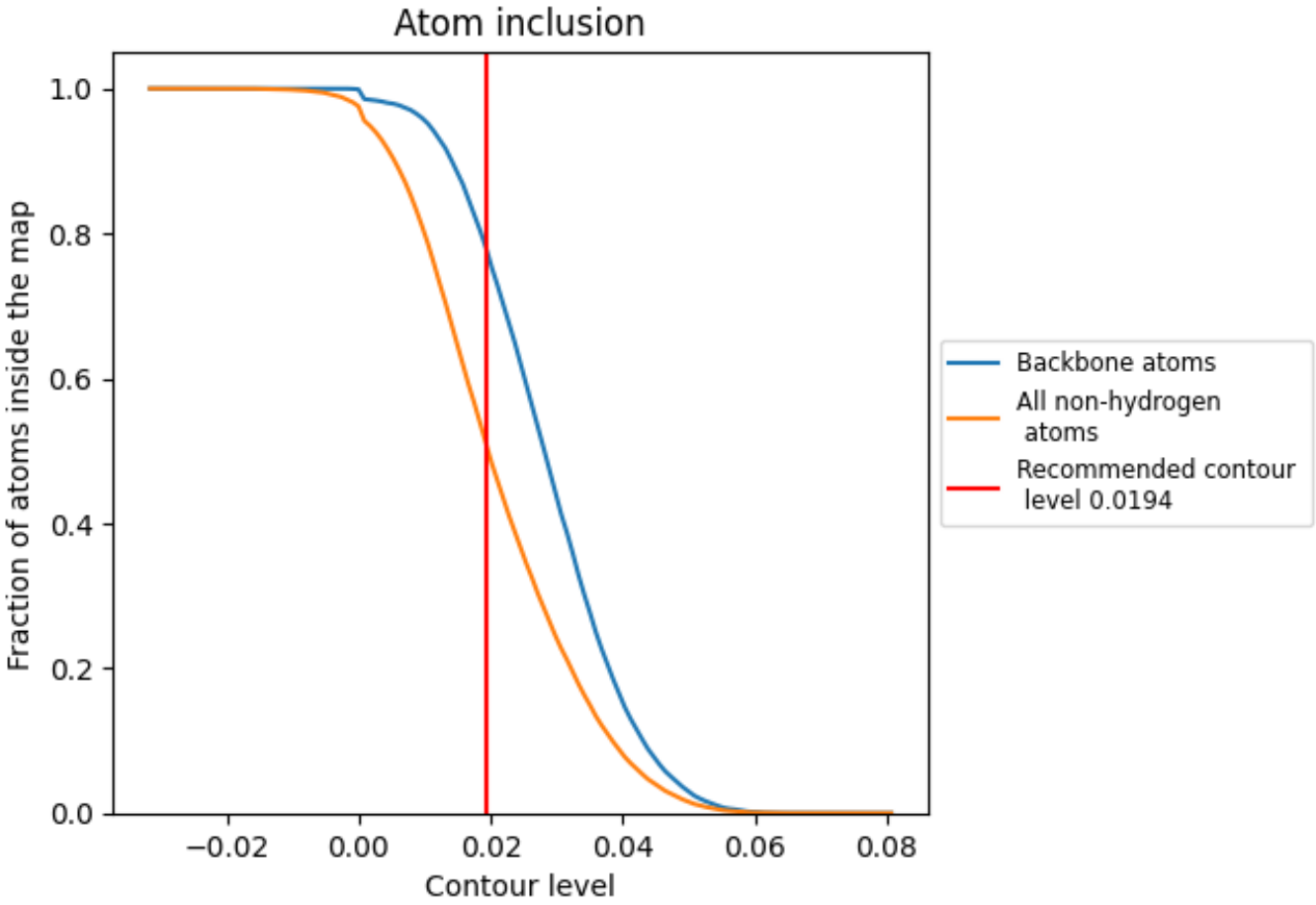
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0194).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 51% 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 (0.0194) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5059	0.1870
A	0.3742	0.1790
B	0.5688	0.1970
C	0.5200	0.1900
D	0.5660	0.1930
E	0.5254	0.1910
F	0.4598	0.1660