



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:49 AM UTC

PDB ID : 5VY8 / pdb_00005vy8
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.; Kendersky, 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.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

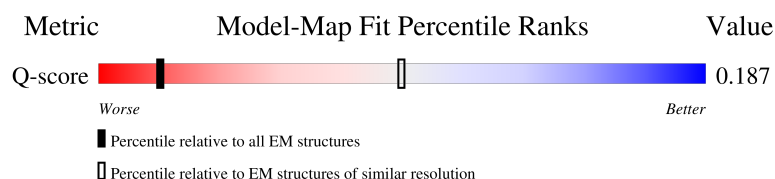
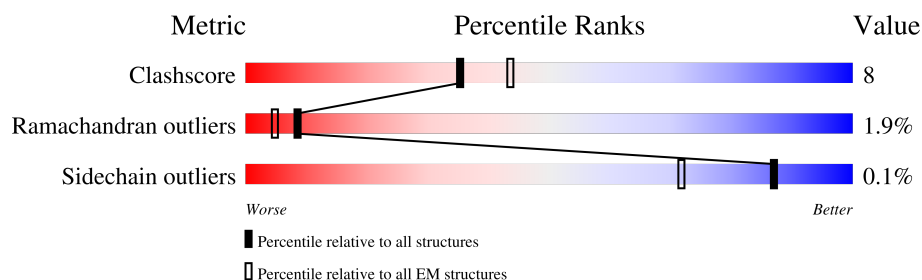
1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	513 (5.10 - 6.10)

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	908	34% 54% 7% 36%
1	B	908	11% 53% 9% 36%
1	C	908	20% 66% 11% 22%
1	D	908	15% 63% 13% 22%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	908	
1	F	908	

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	-

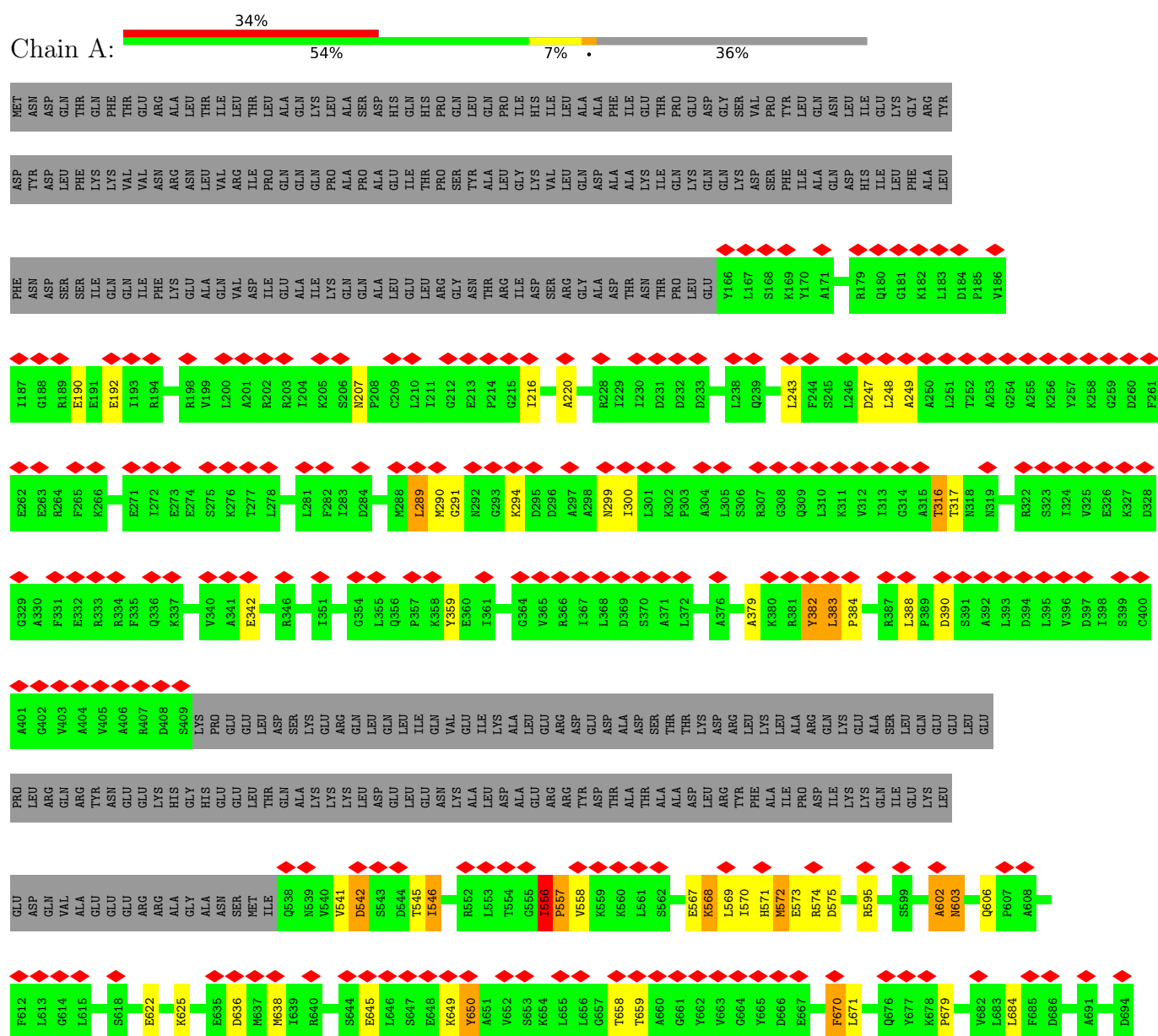
Continued from previous page...

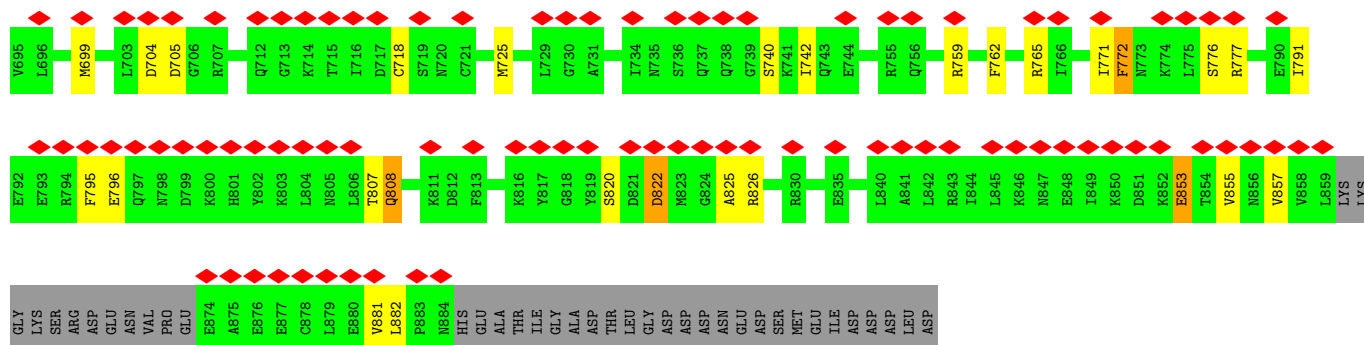
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots

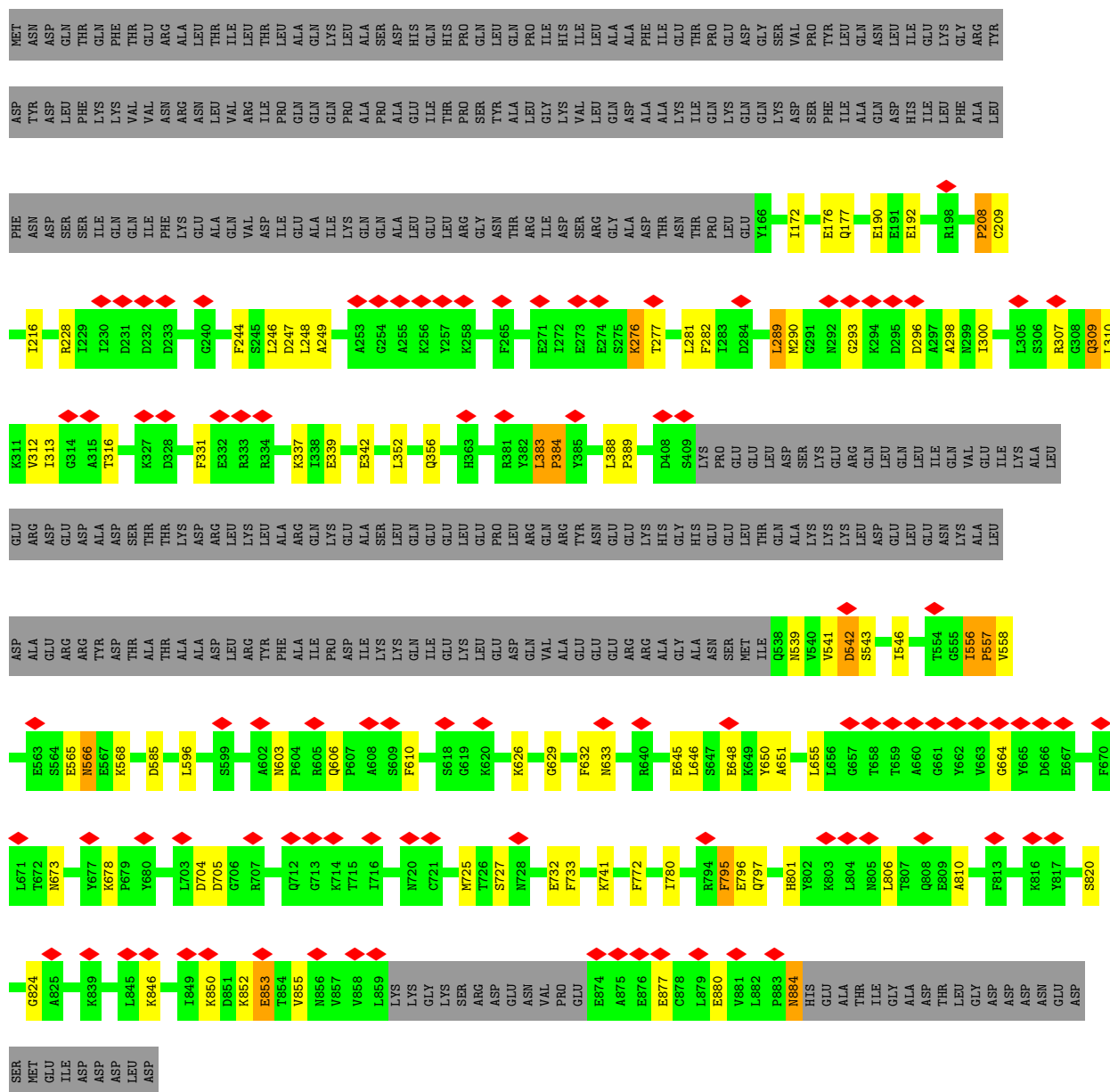
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Heat shock protein 104

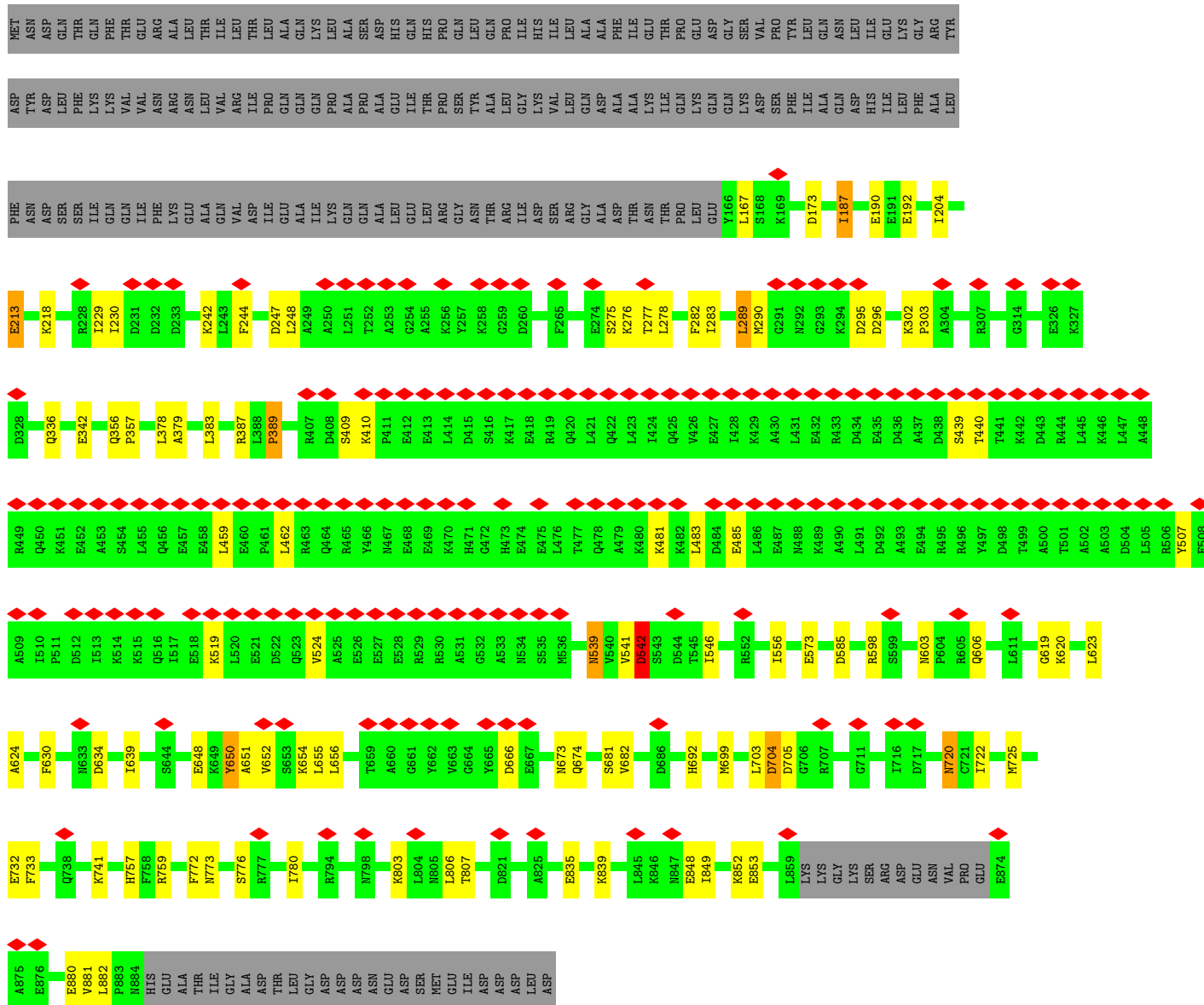




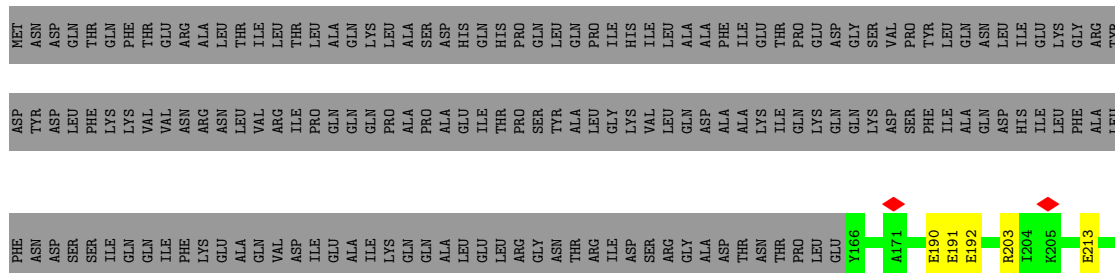
• Molecule 1: Heat shock protein 104

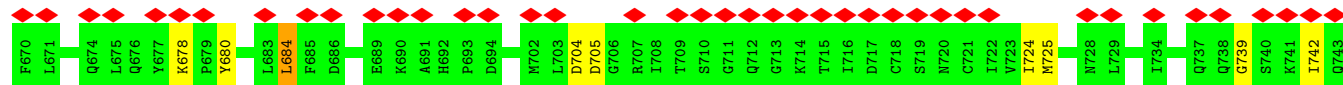


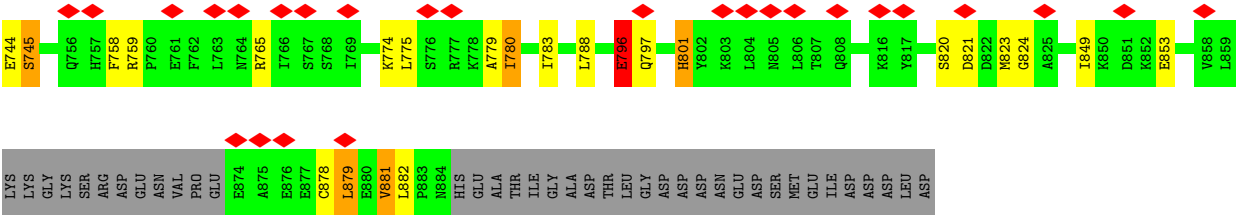
Chain C:



Chain D:







4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 ($\text{\AA}$)	256.0, 256.0, 256.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	1.13	2/4562 (0.0%)	1.32	45/6140 (0.7%)
1	B	1.27	6/4562 (0.1%)	1.33	29/6140 (0.5%)
1	C	1.31	8/5625 (0.1%)	1.32	40/7564 (0.5%)
1	D	1.36	12/5625 (0.2%)	1.37	44/7564 (0.6%)
1	E	1.27	12/5625 (0.2%)	1.35	45/7564 (0.6%)
1	F	1.16	4/4562 (0.1%)	1.33	33/6140 (0.5%)
All	All	1.26	44/30561 (0.1%)	1.34	236/41112 (0.6%)

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	788	LEU	CB-CG	-8.70	1.36	1.53
1	E	397	ASP	CB-CG	7.32	1.70	1.52
1	C	692	HIS	CB-CG	-6.77	1.40	1.50
1	D	692	HIS	CB-CG	-6.75	1.40	1.50
1	A	359	TYR	CB-CG	-6.43	1.37	1.51
1	C	780	ILE	CB-CG1	-6.32	1.40	1.53
1	E	680	TYR	CB-CG	-6.32	1.37	1.51
1	B	610	PHE	CB-CG	-6.31	1.36	1.50
1	D	630	PHE	CB-CG	-6.18	1.36	1.50
1	D	781	HIS	CB-CG	-6.17	1.41	1.50
1	F	796	GLU	CG-CD	-6.06	1.36	1.52
1	D	845	LEU	CB-CG	-6.05	1.41	1.53
1	E	216	ILE	CB-CG1	-6.02	1.41	1.53
1	D	397	ASP	CB-CG	5.93	1.66	1.52
1	E	680	TYR	CA-C	-5.88	1.45	1.52
1	C	630	PHE	CB-CG	-5.85	1.37	1.50
1	B	313	ILE	CB-CG1	-5.84	1.41	1.53
1	C	462	LEU	CB-CG	-5.78	1.41	1.53
1	C	546	ILE	CB-CG1	-5.73	1.42	1.53
1	D	230	ILE	CB-CG1	-5.62	1.42	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	882	LEU	CB-CG	-5.58	1.42	1.53
1	D	586	ALA	CA-C	-5.57	1.45	1.52
1	C	230	ILE	CB-CG1	-5.54	1.42	1.53
1	D	222	ILE	CB-CG1	-5.53	1.42	1.53
1	B	606	GLN	CG-CD	-5.51	1.38	1.52
1	E	230	ILE	CB-CG1	-5.51	1.42	1.53
1	B	244	PHE	CB-CG	-5.47	1.38	1.50
1	E	631	LEU	CB-CG	-5.42	1.42	1.53
1	B	780	ILE	CB-CG1	-5.40	1.42	1.53
1	E	362	HIS	CB-CG	-5.34	1.42	1.50
1	E	211	ILE	CB-CG1	-5.30	1.42	1.53
1	E	692	HIS	CB-CG	-5.29	1.42	1.50
1	F	780	ILE	CB-CG1	-5.27	1.43	1.53
1	E	672	THR	CA-C	-5.24	1.46	1.52
1	E	296	ASP	CB-CG	5.21	1.65	1.52
1	D	571	HIS	CB-CG	-5.17	1.43	1.50
1	D	720	ASN	CB-CG	-5.14	1.39	1.52
1	C	539	ASN	CB-CG	-5.12	1.39	1.52
1	F	742	ILE	CB-CG1	-5.11	1.43	1.53
1	D	398	ILE	CB-CG1	-5.09	1.43	1.53
1	B	313	ILE	CB-CG2	-5.08	1.35	1.52
1	D	632	PHE	CB-CG	-5.07	1.39	1.50
1	A	382	TYR	CG-CD2	-5.04	1.28	1.39
1	C	289	LEU	CA-C	-5.02	1.46	1.53

All (236) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	803	LYS	N-CA-C	-10.71	100.34	113.41
1	E	830	ARG	N-CA-C	-10.48	101.04	114.04
1	A	772	PHE	CA-CB-CG	-10.34	103.46	113.80
1	D	397	ASP	CA-CB-CG	10.24	122.84	112.60
1	E	614	GLY	N-CA-C	-9.74	100.55	112.33
1	B	606	GLN	N-CA-C	9.56	116.58	108.07
1	D	678	LYS	CA-C-N	9.10	129.34	119.87
1	D	678	LYS	C-N-CA	9.10	129.34	119.87
1	E	831	LEU	N-CA-C	-9.04	99.29	110.41
1	B	172	ILE	N-CA-C	8.95	120.63	108.11
1	C	289	LEU	N-CA-C	-8.71	99.04	110.53
1	C	733	PHE	CA-CB-CG	-8.63	105.17	113.80
1	E	685	PHE	CA-CB-CG	-8.52	105.28	113.80
1	D	746	THR	N-CA-C	-8.39	101.66	112.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	808	GLN	N-CA-C	-8.34	103.70	114.04
1	E	397	ASP	CA-CB-CG	8.11	120.71	112.60
1	C	652	VAL	N-CA-C	8.02	118.57	110.23
1	F	638	MET	N-CA-C	7.85	121.03	110.35
1	A	808	GLN	N-CA-C	-7.84	104.32	114.04
1	A	216	ILE	N-CA-C	7.78	118.58	110.72
1	F	575	ASP	CA-CB-CG	-7.72	104.88	112.60
1	D	704	ASP	N-CA-C	-7.71	100.15	110.55
1	E	723	VAL	N-CA-C	7.70	118.89	108.11
1	A	556	ILE	N-CA-C	7.67	125.45	108.88
1	F	678	LYS	CA-C-N	7.59	128.28	119.47
1	F	678	LYS	C-N-CA	7.59	128.28	119.47
1	D	256	LYS	N-CA-C	-7.53	105.00	114.56
1	A	603	ASN	CA-C-N	7.40	127.07	119.82
1	A	603	ASN	C-N-CA	7.40	127.07	119.82
1	A	882	LEU	CA-C-N	7.39	127.31	119.85
1	A	882	LEU	C-N-CA	7.39	127.31	119.85
1	A	383	LEU	CA-C-N	7.36	127.07	119.56
1	A	383	LEU	C-N-CA	7.36	127.07	119.56
1	B	606	GLN	CA-C-N	7.28	127.24	120.03
1	B	606	GLN	C-N-CA	7.28	127.24	120.03
1	D	681	SER	N-CA-C	7.17	117.99	107.88
1	C	848	GLU	N-CA-C	-7.17	104.14	113.17
1	B	342	GLU	CA-C-N	7.16	127.61	120.52
1	B	342	GLU	C-N-CA	7.16	127.61	120.52
1	B	795	PHE	CA-CB-CG	7.14	120.94	113.80
1	E	307	ARG	N-CA-C	-7.05	103.59	111.28
1	C	213	GLU	CA-C-N	7.03	126.99	120.03
1	C	213	GLU	C-N-CA	7.03	126.99	120.03
1	B	877	GLU	N-CA-C	-6.97	104.24	112.89
1	F	229	ILE	N-CA-C	-6.93	100.64	109.30
1	B	603	ASN	CA-C-N	6.91	126.59	119.82
1	B	603	ASN	C-N-CA	6.91	126.59	119.82
1	B	632	PHE	CA-CB-CG	-6.88	106.92	113.80
1	D	796	GLU	N-CA-C	6.86	119.78	111.82
1	C	603	ASN	CA-C-N	6.85	126.53	119.82
1	C	603	ASN	C-N-CA	6.85	126.53	119.82
1	B	282	PHE	N-CA-C	6.81	119.78	109.23
1	E	383	LEU	CA-C-N	6.76	126.39	119.56
1	E	383	LEU	C-N-CA	6.76	126.39	119.56
1	C	342	GLU	CA-C-N	6.75	126.71	120.03
1	C	342	GLU	C-N-CA	6.75	126.71	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	849	ILE	N-CA-CB	-6.69	103.05	111.41
1	A	388	LEU	N-CA-C	6.68	121.94	113.25
1	B	673	ASN	N-CA-C	-6.68	103.81	112.23
1	D	654	LYS	N-CA-C	-6.66	101.57	110.55
1	B	312	VAL	N-CA-C	6.65	117.42	108.11
1	E	335	PHE	N-CA-C	6.62	120.24	109.59
1	D	632	PHE	CA-CB-CG	-6.57	107.23	113.80
1	B	281	LEU	CA-C-N	-6.55	111.49	122.29
1	B	281	LEU	C-N-CA	-6.55	111.49	122.29
1	B	289	LEU	N-CA-C	-6.52	99.89	110.20
1	A	606	GLN	CA-C-N	6.50	126.46	120.03
1	A	606	GLN	C-N-CA	6.50	126.46	120.03
1	D	603	ASN	CA-C-N	6.48	126.17	119.82
1	D	603	ASN	C-N-CA	6.48	126.17	119.82
1	C	882	LEU	CA-C-N	6.46	126.84	119.92
1	C	882	LEU	C-N-CA	6.46	126.84	119.92
1	B	678	LYS	CA-C-N	6.44	126.57	119.87
1	B	678	LYS	C-N-CA	6.44	126.57	119.87
1	D	537	ILE	N-CA-C	-6.38	107.28	113.53
1	F	641	VAL	N-CA-C	6.38	117.04	108.11
1	E	363	HIS	CA-CB-CG	-6.36	107.44	113.80
1	B	646	LEU	N-CA-C	6.35	119.08	109.23
1	C	275	SER	N-CA-C	6.35	118.72	109.07
1	A	575	ASP	CA-CB-CG	-6.30	106.30	112.60
1	B	546	ILE	CB-CA-C	-6.28	103.80	112.02
1	E	705	ASP	N-CA-C	-6.27	102.75	111.52
1	C	722	ILE	CA-C-N	-6.18	114.89	123.10
1	C	722	ILE	C-N-CA	-6.18	114.89	123.10
1	A	882	LEU	CB-CA-C	6.16	118.04	108.61
1	A	382	TYR	CA-C-N	-6.16	115.70	123.15
1	A	382	TYR	C-N-CA	-6.16	115.70	123.15
1	C	524	VAL	N-CA-C	-6.14	104.52	110.72
1	F	853	GLU	N-CA-C	6.14	118.82	110.35
1	A	622	GLU	N-CA-C	-6.08	104.73	111.36
1	E	187	ILE	N-CA-C	6.08	116.62	108.11
1	E	728	ASN	CA-C-N	6.07	128.69	120.38
1	E	728	ASN	C-N-CA	6.07	128.69	120.38
1	A	740	SER	N-CA-C	-6.04	104.81	111.82
1	C	546	ILE	CB-CA-C	-6.00	104.17	112.04
1	E	203	ARG	CA-C-N	-6.00	117.09	122.97
1	E	203	ARG	C-N-CA	-6.00	117.09	122.97
1	C	459	LEU	N-CA-C	6.00	117.49	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	568	LYS	N-CA-C	-5.99	104.33	111.69
1	D	882	LEU	CA-C-N	5.99	127.38	120.98
1	D	882	LEU	C-N-CA	5.99	127.38	120.98
1	E	235	PRO	N-CA-C	-5.99	101.79	111.19
1	D	289	LEU	N-CA-C	-5.97	101.64	110.48
1	A	557	PRO	N-CA-C	5.95	124.72	112.47
1	C	204	ILE	CB-CA-C	-5.94	106.66	111.71
1	D	278	LEU	CA-C-N	-5.93	113.47	121.66
1	D	278	LEU	C-N-CA	-5.93	113.47	121.66
1	A	243	LEU	N-CA-C	5.93	118.90	109.24
1	F	383	LEU	CA-C-N	5.92	125.60	119.56
1	F	383	LEU	C-N-CA	5.92	125.60	119.56
1	D	388	LEU	N-CA-C	5.92	120.94	113.25
1	E	556	ILE	CA-C-N	5.91	125.88	120.21
1	E	556	ILE	C-N-CA	5.91	125.88	120.21
1	F	821	ASP	CA-CB-CG	-5.90	106.70	112.60
1	D	234	VAL	CA-C-N	5.88	125.89	119.89
1	D	234	VAL	C-N-CA	5.88	125.89	119.89
1	A	289	LEU	N-CA-C	-5.87	101.31	110.42
1	C	757	HIS	CA-CB-CG	-5.87	107.93	113.80
1	B	727	SER	N-CA-C	5.85	117.42	108.52
1	F	342	GLU	CA-C-N	5.85	125.76	119.85
1	F	342	GLU	C-N-CA	5.85	125.76	119.85
1	F	801	HIS	CA-CB-CG	-5.83	107.97	113.80
1	F	606	GLN	CA-C-N	5.83	125.80	120.03
1	F	606	GLN	C-N-CA	5.83	125.80	120.03
1	E	544	ASP	N-CA-C	5.80	118.35	111.33
1	D	680	TYR	N-CA-C	-5.79	98.85	108.34
1	F	289	LEU	N-CA-C	-5.78	101.91	110.46
1	A	855	VAL	N-CA-C	5.76	116.78	108.48
1	D	797	GLN	N-CA-C	5.74	117.69	109.14
1	E	614	GLY	CA-C-O	-5.72	118.00	122.52
1	C	606	GLN	CA-C-N	5.71	125.69	120.03
1	C	606	GLN	C-N-CA	5.71	125.69	120.03
1	B	884	ASN	CA-CB-CG	-5.71	106.89	112.60
1	F	879	LEU	N-CA-C	5.69	122.92	110.80
1	C	704	ASP	N-CA-C	-5.69	100.98	109.96
1	E	284	ASP	CA-CB-CG	-5.68	106.92	112.60
1	E	848	GLU	N-CA-C	-5.67	103.88	112.04
1	D	530	ARG	N-CA-C	5.66	117.00	108.46
1	D	567	GLU	N-CA-C	-5.65	105.12	111.28
1	B	733	PHE	N-CA-C	-5.64	106.07	113.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	733	PHE	CA-CB-CG	-5.64	108.16	113.80
1	F	603	ASN	CA-C-N	5.61	126.86	119.84
1	F	603	ASN	C-N-CA	5.61	126.86	119.84
1	D	621	THR	N-CA-C	-5.58	106.31	113.23
1	E	678	LYS	CA-C-N	5.58	125.94	119.47
1	E	678	LYS	C-N-CA	5.58	125.94	119.47
1	A	546	ILE	N-CA-C	5.58	115.78	110.42
1	D	622	GLU	N-CA-C	-5.58	105.28	111.36
1	E	230	ILE	CB-CA-C	-5.58	104.83	111.97
1	A	556	ILE	CA-C-N	5.57	126.81	119.84
1	A	556	ILE	C-N-CA	5.57	126.81	119.84
1	B	655	LEU	CB-CA-C	-5.57	110.13	116.54
1	F	257	TYR	N-CA-C	5.55	115.87	108.38
1	C	282	PHE	N-CA-C	5.55	117.70	108.99
1	C	187	ILE	N-CA-C	5.54	115.86	108.11
1	D	752	GLY	N-CA-C	-5.52	106.10	112.50
1	C	244	PHE	N-CA-C	5.51	117.89	108.90
1	C	383	LEU	CA-C-N	5.51	125.22	119.82
1	C	383	LEU	C-N-CA	5.51	125.22	119.82
1	E	175	THR	N-CA-C	-5.51	105.29	112.23
1	C	542	ASP	CA-CB-CG	5.50	118.10	112.60
1	B	855	VAL	N-CA-C	5.49	115.77	107.75
1	F	279	ILE	N-CA-C	5.49	116.17	109.30
1	C	229	ILE	CA-C-N	5.48	127.97	120.46
1	C	229	ILE	C-N-CA	5.48	127.97	120.46
1	F	556	ILE	CA-C-N	5.48	125.31	119.28
1	F	556	ILE	C-N-CA	5.48	125.31	119.28
1	D	566	ASN	CA-CB-CG	-5.48	107.12	112.60
1	F	739	GLY	N-CA-C	-5.45	104.74	112.81
1	E	452	GLU	N-CA-C	-5.44	105.35	111.28
1	A	857	VAL	CA-C-N	-5.44	115.69	122.48
1	A	857	VAL	C-N-CA	-5.44	115.69	122.48
1	C	848	GLU	CA-C-N	5.41	130.02	122.93
1	C	848	GLU	C-N-CA	5.41	130.02	122.93
1	D	795	PHE	CA-CB-CG	-5.38	108.42	113.80
1	D	392	ALA	N-CA-C	-5.36	105.52	111.36
1	F	724	ILE	N-CA-C	5.35	115.56	107.75
1	A	759	ARG	CA-C-N	5.35	125.68	119.47
1	A	759	ARG	C-N-CA	5.35	125.68	119.47
1	D	383	LEU	CA-C-N	5.35	126.53	119.84
1	D	383	LEU	C-N-CA	5.35	126.53	119.84
1	F	882	LEU	CA-C-N	5.34	125.64	119.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	882	LEU	C-N-CA	5.34	125.64	119.92
1	A	822	ASP	CA-CB-CG	5.33	117.93	112.60
1	D	641	VAL	N-CA-C	5.33	115.53	107.75
1	E	686	ASP	CA-CB-CG	5.33	117.92	112.60
1	A	316	THR	N-CA-C	5.32	116.23	108.14
1	A	670	PHE	CA-CB-CG	5.32	119.12	113.80
1	B	539	ASN	N-CA-C	5.32	116.36	108.60
1	E	615	LEU	N-CA-C	5.30	118.64	110.42
1	E	606	GLN	CA-C-N	5.28	125.26	120.03
1	E	606	GLN	C-N-CA	5.28	125.26	120.03
1	A	772	PHE	CA-C-N	5.28	128.72	120.75
1	A	772	PHE	C-N-CA	5.28	128.72	120.75
1	A	762	PHE	CA-CB-CG	5.28	119.08	113.80
1	A	602	ALA	N-CA-C	-5.27	102.68	110.48
1	D	668	GLY	N-CA-C	-5.27	105.73	114.48
1	E	759	ARG	CA-C-N	5.27	125.58	119.47
1	E	759	ARG	C-N-CA	5.27	125.58	119.47
1	A	299	ASN	N-CA-C	5.25	118.78	112.38
1	D	857	VAL	CA-C-N	-5.25	116.31	122.14
1	D	857	VAL	C-N-CA	-5.25	116.31	122.14
1	F	878	CYS	CA-C-N	5.23	131.53	121.54
1	F	878	CYS	C-N-CA	5.23	131.53	121.54
1	D	398	ILE	CB-CA-C	-5.21	105.19	112.02
1	F	684	LEU	N-CA-C	5.20	117.93	109.24
1	A	300	ILE	N-CA-C	-5.20	106.73	111.67
1	D	750	VAL	CB-CA-C	-5.20	105.32	111.97
1	A	771	ILE	N-CA-C	5.19	115.33	107.80
1	E	772	PHE	CA-CB-CG	-5.19	108.61	113.80
1	B	541	VAL	CA-C-N	5.19	131.46	121.54
1	B	541	VAL	C-N-CA	5.19	131.46	121.54
1	E	829	ASN	CA-CB-CG	-5.18	107.42	112.60
1	C	692	HIS	CA-C-N	5.17	125.47	119.47
1	C	692	HIS	C-N-CA	5.17	125.47	119.47
1	C	650	TYR	N-CA-C	5.16	118.28	110.64
1	E	288	MET	N-CA-C	-5.16	105.84	111.82
1	E	313	ILE	CA-C-N	-5.16	117.88	122.47
1	E	313	ILE	C-N-CA	-5.16	117.88	122.47
1	A	342	GLU	CA-C-N	5.15	125.13	120.03
1	A	342	GLU	C-N-CA	5.15	125.13	120.03
1	F	640	ARG	N-CA-C	5.14	116.89	109.07
1	C	389	PRO	CA-C-N	-5.14	112.88	120.28
1	C	389	PRO	C-N-CA	-5.14	112.88	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	312	VAL	N-CA-C	5.14	115.52	108.12
1	D	268	VAL	CB-CA-C	-5.13	105.40	111.97
1	E	372	LEU	N-CA-C	-5.11	105.71	111.28
1	D	723	VAL	N-CA-C	5.09	115.23	108.11
1	E	232	ASP	CA-CB-CG	5.08	117.69	112.60
1	A	207	ASN	CA-C-N	5.08	126.20	120.66
1	A	207	ASN	C-N-CA	5.08	126.20	120.66
1	F	774	LYS	N-CA-C	-5.06	102.38	109.96
1	D	781	HIS	CA-CB-CG	5.05	118.85	113.80
1	C	720	ASN	CA-CB-CG	-5.03	107.57	112.60
1	E	501	THR	N-CA-C	-5.02	107.00	113.23
1	F	316	THR	N-CA-C	5.01	116.68	109.07

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	4507	0	4627	64	0
1	B	4507	0	4627	52	0
1	C	5560	0	5679	66	0
1	D	5560	0	5679	74	0
1	E	5560	0	5679	73	0
1	F	4507	0	4624	145	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	7	0
2	F	54	0	23	105	0
All	All	30525	0	31058	489	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 8.

All (489) 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:1001:ADP:C5'	1.35	1.53
1:F:619:GLY:CA	2:F:1001:ADP:H5'2	1.40	1.51
1:F:775:LEU:HD11	2:F:1001:ADP:C2	1.41	1.50
1:A:568:LYS:HB3	1:A:572:MET:SD	1.56	1.39
1:F:622:GLU:OE1	2:F:1001:ADP:H2'	1.32	1.29
1:F:775:LEU:CD1	2:F:1001:ADP:C2	2.14	1.28
1:F:775:LEU:HD21	2:F:1001:ADP:N3	1.54	1.23
1:F:217:GLY:HA2	2:F:1002:ADP:O4'	1.08	1.21
1:F:351:ILE:CG2	2:F:1002:ADP:N6	2.04	1.21
1:F:217:GLY:CA	2:F:1002:ADP:O4'	1.89	1.20
1:F:775:LEU:HD21	2:F:1001:ADP:C2	1.79	1.18
1:F:217:GLY:HA2	2:F:1002:ADP:C1'	1.73	1.17
1:F:775:LEU:CG	2:F:1001:ADP:H2	1.56	1.17
1:F:219:THR:HB	2:F:1002:ADP:C3'	1.77	1.14
1:F:622:GLU:CD	2:F:1001:ADP:H2'	1.75	1.10
1:F:775:LEU:CG	2:F:1001:ADP:C2	2.33	1.08
1:F:351:ILE:HG23	2:F:1002:ADP:HN62	1.09	1.07
1:C:556:ILE:HG22	1:C:556:ILE:O	1.53	1.06
1:A:568:LYS:HE2	1:A:572:MET:SD	1.96	1.05
1:F:217:GLY:HA3	2:F:1002: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:1002:ADP:H3'	1.05	1.03
1:F:775:LEU:CD2	2:F:1001:ADP:C2	2.41	1.03
1:F:622:GLU:CD	2:F:1001:ADP:C2'	2.32	1.02
1:F:219:THR:CB	2:F:1002:ADP:H3'	1.88	1.02
1:F:220:ALA:HB2	2:F:1002: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:1002:ADP:HN62	1.67	1.00
1:F:355:LEU:HD11	2:F:1002:ADP:C2	1.96	1.00
1:F:220:ALA:H	2:F:1002: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:1002:ADP:H8	1.19	0.98
1:F:351:ILE:HG23	2:F:1002:ADP:N6	1.68	0.96
1:F:775:LEU:HG	2:F:1001: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:1002:ADP:C6	2.52	0.92
1:F:622:GLU:HB2	2:F:1001:ADP:H5'1	1.48	0.92
1:F:220:ALA:HB2	2:F:1002:ADP:C2'	1.99	0.92
1:F:351:ILE:HG21	2:F:1002:ADP:N6	1.85	0.91
1:E:761:GLU:OE1	1:E:761:GLU:N	2.04	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:351:ILE:HG21	2:F:1002:ADP:C6	2.05	0.90
1:F:351:ILE:CG1	2:F:1002:ADP:N6	2.35	0.89
1:F:775:LEU:CD2	2:F:1001:ADP:N3	2.35	0.88
1:F:581:VAL:HB	2:F:1001:ADP:N6	1.89	0.88
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:1002:ADP:C2'	2.06	0.85
1:F:355:LEU:HD11	2:F:1002: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:1002:ADP:N6	1.92	0.84
1:D:565:GLU:CD	1:D:565:GLU:H	1.80	0.84
1:F:351:ILE:CD1	2:F:1002:ADP:HN61	1.92	0.83
1:A:568:LYS:O	1:A:572:MET:CA	2.10	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:1002: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:1001:ADP:C2'	2.23	0.81
1:F:217:GLY:HA2	2:F:1002: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:1002:ADP:H2'	1.95	0.80
1:F:783:ILE:HD13	2:F:1001:ADP:N7	1.97	0.80
1:F:622:GLU:CD	2:F:1001:ADP:H3'	2.08	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:1001:ADP:O1A	2:F:1001:ADP:H4'	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:1001:ADP:N1	1.97	0.78
1:A:568:LYS:O	1:A:572:MET:C	2.26	0.78
1:F:217:GLY:CA	2:F:1002:ADP:C1'	2.56	0.78
1:F:622:GLU:HG3	2:F:1001:ADP:H3'	1.64	0.77
1:B:884:ASN:OD1	1:B:884:ASN:C	2.26	0.77
1:C:507:TYR:CD1	1:C:507:TYR:C	2.61	0.77
1:E:761:GLU:H	1:E:761:GLU:CD	1.91	0.77
1:E:732:GLU:N	1:E:732:GLU:OE1	2.17	0.76
1:F:351:ILE:HD13	2:F:1002:ADP:HN61	1.48	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:622:GLU:CD	2:F:1001:ADP:C3'	2.59	0.75
1:D:556:ILE:O	1:D:556:ILE:CG2	2.32	0.75
1:C:507:TYR:CD1	1:C:507:TYR:O	2.40	0.75
2:D:1001:ADP:H5'1	2:D:1001:ADP:PB	2.26	0.74
1:F:351:ILE:HG23	2:F:1002:ADP:C6	2.18	0.74
1:F:581:VAL:HB	2:F:1001:ADP:HN62	1.50	0.74
1:F:622:GLU:CB	2:F:1001:ADP:H5'1	2.18	0.73
1:F:351:ILE:HD13	2:F:1002: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:D:581:VAL:H	2:D:1002:ADP:HN62	1.36	0.72
1:F:775:LEU:HD11	2:F:1001:ADP:N3	2.03	0.72
2:D:1001:ADP:N3	2:D:1001:ADP:H2'	2.05	0.72
1:A:568:LYS:C	1:A:572:MET:H	1.96	0.72
1:F:620:LYS:N	2:F:1001:ADP:O2A	2.23	0.71
1:F:351:ILE:CG1	2:F:1002:ADP:HN61	2.03	0.71
1:E:445:LEU:C	1:E:445:LEU:HD23	2.15	0.70
1:F:217:GLY:CA	2:F:1002:ADP:C8	2.73	0.70
1:F:622:GLU:CG	2:F:1001:ADP:H3'	2.19	0.70
1:F:220:ALA:H	2:F:1002:ADP:C2'	2.03	0.70
1:F:355:LEU:HD11	2:F:1002:ADP:H2	1.57	0.69
1:F:351:ILE:CD1	2:F:1002:ADP:N6	2.55	0.69
1:D:414:LEU:HD23	1:D:414:LEU:C	2.17	0.69
1:E:732:GLU:H	1:E:732:GLU:CD	1.98	0.68
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:F:355:LEU:CD1	2:F:1002:ADP:C2	2.77	0.66
1:F:219:THR:HB	2:F:1002:ADP:O3'	1.94	0.66
1:C:598:ARG:HA	1:C:598:ARG:NE	2.10	0.66
1:D:246:LEU:C	1:D:246:LEU:HD23	2.20	0.66
1:F:775:LEU:CD2	2:F:1001:ADP:H2	1.93	0.65
1:C:387:ARG:HA	1:C:387:ARG:NE	2.11	0.65
1:C:650:TYR:C	1:C:650:TYR:CD2	2.75	0.65
1:F:167:LEU:C	1:F:167:LEU:HD23	2.23	0.64
1:F:581:VAL:CB	2:F:1001: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:1002:ADP:O4'	2.31	0.63
1:C:556:ILE:O	1:C:556:ILE:CG2	2.30	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:445:LEU:HD23	1:E:445:LEU:O	2.00	0.62
1:C:773:ASN:C	1:C:773:ASN:OD1	2.41	0.62
1:B:246:LEU:C	1:B:246:LEU:HD23	2.24	0.61
1:C:289:LEU:O	1:C:290:MET:HB2	2.00	0.61
1:F:622:GLU:OE2	2:F:1001:ADP:C2'	2.49	0.61
1:E:218:LYS:NZ	1:E:316:THR:O	2.34	0.61
1:E:645:GLU:O	1:E:645:GLU:HG3	2.00	0.60
1:F:351:ILE:CB	2:F:1002:ADP:N6	2.64	0.60
1:C:655:LEU:C	1:C:655:LEU:HD23	2.25	0.60
1:F:619:GLY:H	2:F:1001:ADP:PA	2.24	0.60
1:F:581:VAL:CG2	2:F:1001: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:1002:ADP:C2'	2.65	0.59
1:E:387:ARG:HA	1:E:387:ARG:NE	2.16	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:D:387:ARG:NE	1:D:387:ARG:HA	2.18	0.57
1:F:801:HIS:CD2	1:F:801:HIS:N	2.71	0.57
1:E:434:ASP:OD2	1:E:442:LYS:NZ	2.37	0.57
1:C:585:ASP:OD2	1:C:741:LYS:NZ	2.38	0.56
1:C:648:GLU:H	1:C:648:GLU:CD	2.05	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:1002: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:1002: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: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:C:190:GLU:CD	1:C:190:GLU:H	2.12	0.55
1:C:541:VAL:O	1:C:542:ASP:C	2.49	0.55
1:F:619:GLY:HA2	2:F:1001:ADP:C4'	2.29	0.55
1:D:668:GLY:O	1:D:672:THR:N	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:351:ILE:HG12	2:F:1002:ADP:HN61	1.65	0.55
1:E:761:GLU:N	1:E:761:GLU:CD	2.55	0.55
1:F:351:ILE:HG23	2:F:1002: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:A:568:LYS:O	1:A:572:MET:CG	2.37	0.55
1:B:820:SER:O	1:B:824:GLY:N	2.40	0.54
1:F:220:ALA:CB	2:F:1002:ADP:O2'	2.46	0.54
1:F:305:LEU:HD12	1:F:305:LEU:C	2.32	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:655:LEU:HD23	1:D:655:LEU:C	2.32	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:F:565:GLU:H	1:F:565:GLU:CD	2.16	0.54
1:C:699:MET:O	1:C:703:LEU:N	2.42	0.53
1:C:539:ASN:C	1:C:539:ASN:OD1	2.50	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:E:751:MET:HE2	1:E:751:MET:HA	1.91	0.53
1:D:759:ARG:NH1	1:E:644:SER:OG	2.41	0.53
1:A:190:GLU:H	1:A:190:GLU:CD	2.17	0.53
1:F:190:GLU:CD	1:F:190:GLU:H	2.16	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: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:B:290:MET:O	1:B:290:MET:HG2	2.09	0.52
1:D:566:ASN:O	1:D:567:GLU:C	2.50	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:1001: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:856:ASN:C	1:D:856:ASN:OD1	2.52	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:GLU:CD	1:E:190:GLU:H	2.18	0.51
1:D:421:LEU:C	1:D:421:LEU:HD23	2.34	0.51
1:D:851:ASP:OD2	1:D:852:LYS:NZ	2.44	0.51
1:E:649:LYS:O	1:E:650:TYR:C	2.54	0.51
1:E:650:TYR:O	1:E:650:TYR:CD1	2.64	0.51
1:C:483:LEU:HD13	1:C:483:LEU:C	2.36	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:1001:ADP:N7	2.70	0.51
1:B:388:LEU:HB3	1:B:389:PRO:HD3	1.93	0.50
1:F:622:GLU:OE2	2:F:1001: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:1002:ADP:HN62	2.21	0.50
1:A:382:TYR:CD1	1:A:382:TYR:C	2.89	0.50
1:A:776:SER:OG	1:A:777:ARG:N	2.45	0.50
1:A:699:MET:HE3	1:A:699:MET:O	2.12	0.50
1:B:732:GLU:OE1	1:B:732:GLU:N	2.39	0.50
1:B:565:GLU:O	1:B:566:ASN:C	2.54	0.50
1:B:650:TYR:CD1	1:B:650:TYR:C	2.86	0.50
1:D:414:LEU:C	1:D:414:LEU:CD2	2.85	0.50
1:F:775:LEU:HG	2:F:1001:ADP:C2	2.27	0.50
1:A:853:GLU:OE1	1:A:853:GLU:C	2.54	0.50
1:D:190:GLU:H	1:D:190:GLU:CD	2.17	0.50
2:D:1002:ADP:N3	2:D:1002:ADP:C2'	2.73	0.49
1:E:483:LEU:C	1:E:483:LEU:HD23	2.36	0.49
1:C:619:GLY:O	1:C:620:LYS:C	2.52	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:336:GLN:N	1:C:336:GLN:CD	2.70	0.49
1:C:387:ARG:HA	1:C:387:ARG:HE	1.78	0.49
1:D:541:VAL:O	1:D:542:ASP:C	2.56	0.49
1:D:807:THR:OG1	1:D:809:GLU:OE1	2.24	0.49
1:C:720:ASN:OD1	1:C:720:ASN:N	2.43	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:A:638:MET:SD	1:A:638:MET:C	2.96	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:772:PHE:CD1	1:C:772:PHE:N	2.80	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:598:ARG:HA	1:C:598:ARG:HE	1.78	0.48
1:E:845:LEU:C	1:E:845:LEU:HD12	2.38	0.48
1:A:704:ASP:O	1:A:705:ASP:C	2.56	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:D:649:LYS:O	1:D:650:TYR:C	2.55	0.48
1:F:649:LYS:O	1:F:650:TYR:C	2.56	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:D:729:LEU:C	1:D:729:LEU:HD23	2.38	0.48
1:E:602:ALA:O	1:E:603:ASN:C	2.54	0.48
1:E:650:TYR:O	1:E:650:TYR:HD1	1.95	0.48
1:F:581:VAL:HG23	2:F:1001:ADP:HN61	1.78	0.48
1:F:650:TYR:O	1:F:651:ALA:C	2.55	0.48
1:F:247:ASP:O	1:F:249:ALA:N	2.47	0.48
1:F:622:GLU:CG	2:F:1001:ADP:H5'1	2.43	0.48
1:F:775:LEU:CD1	2:F:1001: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:E:700:LEU:HD23	1:E:700:LEU:C	2.39	0.48
2:D:1002:ADP:N3	2:D:1002:ADP:H2'	2.29	0.48
1:F:355:LEU:CD1	2:F:1002: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:B:309:GLN:O	1:B:310:LEU:C	2.57	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:D:802:TYR:CD1	1:D:802:TYR:C	2.91	0.47
1:E:819:TYR:O	1:E:819:TYR:HD2	1.96	0.47
1:F:619:GLY:C	2:F:1001:ADP:H5'2	2.28	0.47
2:F:1002:ADP:H5'2	2:F:1002:ADP:O3B	2.14	0.47
1:F:217:GLY:CA	2:F:1002:ADP:C2'	2.86	0.47
1:A:545:THR:OG1	1:A:546:ILE:N	2.46	0.47
1:A:853:GLU:C	1:A:853:GLU:CD	2.82	0.47
1:C:378:LEU:O	1:C:379:ALA:C	2.57	0.47
1:B:704:ASP:O	1:B:705:ASP:C	2.57	0.47
1:B:806:LEU:HB3	1:B:810:ALA:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:321:TYR:C	1:E:321:TYR:CD1	2.92	0.47
1:F:228:ARG:O	1:F:232:ASP:N	2.48	0.47
1:F:619:GLY:N	2:F:1001:ADP:O2A	2.47	0.47
1:F:220:ALA:CA	2:F:1002:ADP:H2'	2.44	0.47
1:A:569:LEU:HB2	1:A:595:ARG:HE	1.79	0.47
1:E:445:LEU:C	1:E:445:LEU:CD2	2.85	0.47
1:D:704:ASP:O	1:D:705:ASP:C	2.58	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:A:658:THR:O	1:A:659:THR:C	2.57	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:A:390:ASP:OD1	1:A:390:ASP:O	2.33	0.46
1:B:190:GLU:H	1:B:190:GLU:CD	2.23	0.46
1:D:222:ILE:HD13	1:D:222:ILE:HA	1.62	0.46
1:E:794:ARG:O	1:E:795:PHE:C	2.59	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: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:218:LYS:NZ	1:F:316:THR:O	2.45	0.46
1:F:309:GLN:O	1:F:310:LEU:C	2.58	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:C:704:ASP:O	1:C:705:ASP:C	2.56	0.46
1:F:779:ALA:CB	2:F:1001:ADP:N1	2.78	0.46
1:E:167:LEU:C	1:E:167:LEU:HD12	2.40	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:D:571:HIS:O	1:D:572:MET:C	2.59	0.45
1:F:619:GLY:N	2:F:1001:ADP:PA	2.88	0.45
1:A:649:LYS:O	1:A:650:TYR:C	2.59	0.45
1:D:355:LEU:O	1:D:356:GLN:C	2.57	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:622:GLU:O	1:F:623:LEU:C	2.59	0.45
1:B:565:GLU:O	1:B:568:LYS:N	2.49	0.45
1:D:203:ARG:HG3	1:E:362:HIS:CG	2.52	0.45
1:E:365:VAL:O	1:E:365:VAL:HG23	2.17	0.45
1:E:642:ASP:OD1	1:E:642:ASP:C	2.58	0.45
1:F:779:ALA:HB1	2:F:1001:ADP:N1	2.31	0.45
2:C:1001:ADP:O1A	2:C:1001:ADP:O3B	2.35	0.45
1:D:642:ASP:C	1:D:642:ASP:OD1	2.58	0.45
1:F:581:VAL:CG2	2:F:1001:ADP:HN61	2.30	0.45
1:F:619:GLY:CA	2:F:1001: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:F:684:LEU:C	1:F:684:LEU:HD23	2.42	0.45
1:D:638:MET:HE2	1:D:638:MET:HB3	1.87	0.44
1:F:680:TYR:CD1	1:F:680:TYR:C	2.95	0.44
1:F:229:ILE:O	1:F:230:ILE:HB	2.17	0.44
1:F:622:GLU:OE2	2:F:1001:ADP:C3'	2.65	0.44
1:F:355:LEU:CD1	2:F:1002:ADP:N1	2.73	0.44
1:A:541:VAL:O	1:A:542:ASP:C	2.61	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: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:673:ASN:O	1:C:674:GLN:C	2.60	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:D:262:GLU:CD	1:D:262:GLU:H	2.25	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
1:B:316:THR:O	1:B:316:THR:HG23	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:817:TYR:N	1:E:817:TYR:CD2	2.83	0.43
1:C:190:GLU:CD	1:C:190:GLU:N	2.77	0.43
1:E:751:MET:HE2	1:E:751:MET:CA	2.48	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:374:THR:O	1:E:375:ALA:C	2.60	0.43
1:E:495:ARG:HD2	1:E:495:ARG:HA	1.72	0.43
1:F:220:ALA:CB	2:F:1002: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:B:176:GLU:O	1:B:177:GLN:C	2.60	0.43
1:D:481:LYS:NZ	1:D:485:GLU:OE2	2.47	0.43
1:E:309:GLN:O	1:E:310:LEU:C	2.61	0.43
1:E:660:ALA:N	1:E:711:GLY:O	2.51	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:634:ASP:OD1	1:C:634:ASP:C	2.60	0.43
1:C:681:SER:OG	1:C:682:VAL:N	2.52	0.43
1:D:301:LEU:O	1:D:302:LYS:C	2.57	0.43
1:D:806:LEU:O	1:D:807:THR:C	2.61	0.43
1:D:825:ALA:C	1:D:827:PRO:HD2	2.43	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: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:E:629:GLY:O	1:E:633:ASN:N	2.52	0.42
1:F:355:LEU:O	1:F:356:GLN:C	2.62	0.42
1:F:625:LYS:NZ	1:F:636:ASP:OD1	2.50	0.42
1:A:684:LEU:C	1:A:684:LEU:HD23	2.44	0.42
1:B:556:ILE:O	1:B:557:PRO:C	2.62	0.42
1:B:216:ILE:O	1:B:216:ILE:HG13	2.19	0.42
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:704:ASP:O	1:F:705:ASP:C	2.61	0.42
1:A:725:MET:SD	1:A:725:MET:N	2.92	0.42
1:B:331:PHE:CD2	1:B:331:PHE:C	2.98	0.42
1:D:792:GLU:OE2	1:D:801:HIS:N	2.52	0.42
1:E:558:VAL:O	1:E:559:LYS:C	2.62	0.42
1:A:602:ALA:O	1:A:603:ASN:C	2.59	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:B:542:ASP:OD1	1:B:543:SER:N	2.51	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:E:634:ASP:OD1	1:E:634:ASP:C	2.61	0.42
1:F:744:GLU:O	1:F:745:SER:CB	2.68	0.42
1:C:655:LEU:O	1:C:656:LEU:C	2.63	0.42
1:C:806:LEU:C	1:C:807:THR:O	2.62	0.42
1:D:410:LYS:CB	1:D:411:PRO:CD	2.97	0.42
1:F:622:GLU:OE2	2:F:1001:ADP:H3'	2.17	0.42
1:B:732:GLU:H	1:B:732:GLU:CD	2.27	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:E:539:ASN:O	1:E:540:VAL:C	2.60	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:C:283:ILE:N	1:C:283:ILE:HD12	2.35	0.41
1:C:483:LEU:HD22	1:C:483:LEU:C	2.44	0.41
2:C:1002:ADP:O2'	2:C:1002:ADP:C8	2.70	0.41
1:D:650:TYR:CD1	1:D:650:TYR:C	2.97	0.41
1:D:699:MET:O	1:D:703:LEU:N	2.53	0.41
1:F:581:VAL:CB	2:F:1001: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:A:638:MET:HE2	1:A:638:MET:HB2	1.91	0.41
1:B:626:LYS:HD3	1:B:626:LYS:HA	1.87	0.41
1:D:296:ASP:O	1:D:296:ASP:CG	2.61	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
1:F:758:PHE:O	1:F:759:ARG:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:623:LEU:O	1:C:624:ALA:C	2.62	0.41
1:E:568:LYS:O	1:E:569:LEU:C	2.62	0.41
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:590:VAL:HA	1:E:610:PHE:CZ	2.56	0.41
2:E:1001:ADP:O1A	2:E:1001:ADP:O3'	2.39	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:173:ASP:OD2	1:C:242:LYS:NZ	2.41	0.41
1:C:276:LYS:O	1:C:278:LEU:N	2.54	0.41
1:A:825:ALA:O	1:A:826:ARG:C	2.63	0.41
1:D:568:LYS:O	1:D:572:MET:N	2.53	0.41
1:E:668:GLY:O	1:E:669:GLY:C	2.63	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:543:SER:O	1:F:544:ASP:C	2.62	0.41
1:F:619:GLY:HA2	2:F:1001:ADP:PA	2.61	0.41
1:B:296:ASP:CG	1:B:296:ASP:O	2.64	0.41
1:B:596:LEU:HD23	1:B:596:LEU:HA	1.67	0.41
1:C:295:ASP:O	1:C:296:ASP:C	2.63	0.41
1:C:655:LEU:C	1:C:655:LEU:CD2	2.94	0.41
1:E:388:LEU:O	1:E:389:PRO:C	2.63	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: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:D:261:PHE:CD2	1:D:261:PHE:C	2.97	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:C:167:LEU:C	1:C:167:LEU:HD12	2.47	0.40
1:D:247:ASP:O	1:D:249:ALA:N	2.54	0.40
1:D:684:LEU:HD23	1:D:684:LEU:C	2.47	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:N	1:C:190:GLU:OE1	2.38	0.40
1:C:650:TYR:CE1	1:C:654:LYS:HB3	2.57	0.40
1:D:623:LEU:O	1:D:624:ALA:C	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	571/908 (63%)	530 (93%)	33 (6%)	8 (1%)	9	39
1	B	571/908 (63%)	516 (90%)	37 (6%)	18 (3%)	3	21
1	C	701/908 (77%)	661 (94%)	33 (5%)	7 (1%)	12	48
1	D	701/908 (77%)	642 (92%)	43 (6%)	16 (2%)	5	27
1	E	701/908 (77%)	648 (92%)	38 (5%)	15 (2%)	5	29
1	F	571/908 (63%)	528 (92%)	35 (6%)	8 (1%)	9	39
All	All	3816/5448 (70%)	3525 (92%)	219 (6%)	72 (2%)	8	31

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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%)	84	83
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%)	606 (100%)	0	100	100
1	E	606/783 (77%)	606 (100%)	0	100	100
1	F	494/783 (63%)	493 (100%)	1 (0%)	87	86
All	All	3300/4698 (70%)	3297 (100%)	3 (0%)	87	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	572	MET
1	A	574	ARG
1	F	560	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	319	ASN
1	A	362	HIS
1	A	606	GLN
1	A	833	GLN
1	B	781	HIS
1	B	808	GLN
1	C	420	GLN
1	C	516	GLN
1	C	571	HIS
1	C	781	HIS
1	D	363	HIS
1	D	420	GLN
1	D	566	ASN
1	D	738	GLN
1	D	743	GLN
1	D	847	ASN
1	E	674	GLN
1	F	781	HIS
1	F	808	GLN

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 oligosaccharides 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	B	1001	-	28,29,29	1.59	7 (25%)	43,45,45	2.69	14 (32%)
2	ADP	D	1001	-	28,29,29	1.62	6 (21%)	43,45,45	2.57	14 (32%)
2	ADP	C	1001	-	28,29,29	1.92	7 (25%)	43,45,45	2.39	11 (25%)
2	ADP	D	1002	-	28,29,29	1.80	6 (21%)	43,45,45	2.55	13 (30%)
2	ADP	A	1002	-	28,29,29	1.48	4 (14%)	43,45,45	2.64	18 (41%)
2	ADP	E	1001	-	28,29,29	1.63	6 (21%)	43,45,45	2.68	18 (41%)
2	ADP	F	1001	-	28,29,29	1.67	7 (25%)	43,45,45	2.35	12 (27%)
2	ADP	C	1002	-	28,29,29	1.63	6 (21%)	43,45,45	2.65	15 (34%)
2	ADP	F	1002	-	28,29,29	1.59	7 (25%)	43,45,45	2.69	14 (32%)
2	ADP	B	1002	-	28,29,29	1.84	6 (21%)	43,45,45	2.43	18 (41%)
2	ADP	E	1002	-	28,29,29	1.67	7 (25%)	43,45,45	2.36	12 (27%)
2	ADP	A	1001	-	28,29,29	1.54	4 (14%)	43,45,45	3.00	16 (37%)

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	B	1001	-	-	4/16/32/32	0/3/3/3
2	ADP	D	1001	-	-	9/16/32/32	0/3/3/3
2	ADP	C	1001	-	-	7/16/32/32	0/3/3/3
2	ADP	D	1002	-	-	6/16/32/32	0/3/3/3
2	ADP	A	1002	-	-	6/16/32/32	0/3/3/3
2	ADP	E	1001	-	-	9/16/32/32	0/3/3/3
2	ADP	F	1001	-	-	5/16/32/32	0/3/3/3
2	ADP	C	1002	-	-	5/16/32/32	0/3/3/3
2	ADP	F	1002	-	-	4/16/32/32	0/3/3/3
2	ADP	B	1002	-	-	7/16/32/32	0/3/3/3
2	ADP	E	1002	-	-	5/16/32/32	0/3/3/3
2	ADP	A	1001	-	-	6/16/32/32	0/3/3/3

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	ADP	PA-O3A	-6.25	1.52	1.59
2	B	1002	ADP	C5-N7	-6.10	1.27	1.39
2	D	1002	ADP	C5-N7	-5.44	1.29	1.39
2	C	1002	ADP	C5-N7	-4.87	1.30	1.39
2	C	1001	ADP	C5-N7	-4.54	1.30	1.39
2	B	1001	ADP	C5-N7	-4.47	1.30	1.39
2	A	1001	ADP	C5-N7	-4.42	1.31	1.39
2	F	1002	ADP	C5-N7	-4.41	1.31	1.39
2	D	1001	ADP	C5-N7	-4.31	1.31	1.39
2	F	1001	ADP	C5-N7	-4.11	1.31	1.39
2	E	1001	ADP	C5-N7	-4.09	1.31	1.39
2	E	1002	ADP	C5-N7	-3.99	1.31	1.39
2	E	1002	ADP	PA-O3A	-3.66	1.55	1.59
2	F	1001	ADP	PA-O3A	-3.64	1.55	1.59
2	B	1002	ADP	C8-N9	-3.61	1.31	1.37
2	E	1001	ADP	C4-N9	-3.56	1.30	1.37
2	E	1002	ADP	C4-N9	-3.54	1.30	1.37
2	F	1001	ADP	C4-N9	-3.54	1.30	1.37
2	B	1001	ADP	PA-O3A	-3.52	1.55	1.59
2	A	1002	ADP	C5-N7	-3.51	1.32	1.39
2	F	1002	ADP	PA-O3A	-3.50	1.55	1.59
2	D	1002	ADP	PA-O3A	-3.29	1.55	1.59
2	A	1002	ADP	C4-N9	-3.26	1.30	1.37
2	D	1001	ADP	PA-O3A	-3.18	1.56	1.59
2	C	1002	ADP	C8-N9	-3.09	1.32	1.37
2	B	1002	ADP	PA-O3A	-3.07	1.56	1.59
2	D	1001	ADP	C4-N9	-3.06	1.31	1.37
2	D	1002	ADP	C8-N9	-3.02	1.32	1.37
2	E	1001	ADP	PA-O3A	-2.96	1.56	1.59
2	D	1002	ADP	C4-N9	-2.94	1.31	1.37
2	F	1002	ADP	C4-N9	-2.81	1.31	1.37
2	B	1001	ADP	C4-N9	-2.81	1.31	1.37
2	C	1001	ADP	C8-N9	-2.73	1.32	1.37
2	C	1002	ADP	PA-O3A	-2.71	1.56	1.59
2	E	1002	ADP	C8-N9	-2.63	1.33	1.37
2	F	1001	ADP	C8-N9	-2.60	1.33	1.37
2	E	1001	ADP	C8-N9	-2.52	1.33	1.37
2	A	1001	ADP	PA-O3A	-2.50	1.56	1.59
2	C	1001	ADP	C4-N9	-2.48	1.32	1.37
2	F	1002	ADP	C8-N9	-2.47	1.33	1.37
2	C	1002	ADP	C4-N9	-2.45	1.32	1.37
2	B	1002	ADP	C4-N9	-2.44	1.32	1.37
2	B	1001	ADP	C8-N9	-2.44	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1002	ADP	PA-O3A	-2.36	1.57	1.59
2	E	1001	ADP	C2'-C3'	-2.35	1.47	1.53
2	E	1002	ADP	PA-O2A	-2.29	1.44	1.55
2	F	1001	ADP	PA-O2A	-2.29	1.44	1.55
2	B	1001	ADP	PA-O2A	-2.24	1.45	1.55
2	C	1001	ADP	PA-O1A	-2.24	1.43	1.50
2	F	1002	ADP	PA-O2A	-2.23	1.45	1.55
2	A	1002	ADP	PB-O2B	2.22	1.63	1.54
2	A	1001	ADP	PB-O2B	2.19	1.63	1.54
2	C	1001	ADP	PA-O2A	-2.18	1.45	1.55
2	E	1002	ADP	PB-O2B	2.16	1.62	1.54
2	F	1001	ADP	PB-O2B	2.16	1.62	1.54
2	C	1002	ADP	PA-O2A	-2.15	1.45	1.55
2	A	1001	ADP	C8-N9	-2.14	1.33	1.37
2	B	1002	ADP	PB-O2B	2.13	1.62	1.54
2	D	1002	ADP	PB-O2B	2.12	1.62	1.54
2	E	1002	ADP	PB-O3B	-2.12	1.46	1.54
2	C	1002	ADP	PB-O2B	2.11	1.62	1.54
2	F	1002	ADP	PB-O2B	2.11	1.62	1.54
2	B	1001	ADP	PB-O2B	2.10	1.62	1.54
2	F	1001	ADP	PB-O3B	-2.10	1.47	1.54
2	D	1001	ADP	C8-N9	-2.09	1.34	1.37
2	C	1001	ADP	PB-O2B	2.09	1.62	1.54
2	B	1002	ADP	PA-O2A	-2.08	1.45	1.55
2	D	1002	ADP	PA-O2A	-2.05	1.45	1.55
2	D	1001	ADP	PB-O2B	2.05	1.62	1.54
2	E	1001	ADP	PB-O3B	-2.04	1.47	1.54
2	F	1002	ADP	PB-O3B	-2.02	1.47	1.54
2	D	1001	ADP	PB-O3B	-2.02	1.47	1.54
2	B	1001	ADP	PB-O3B	-2.01	1.47	1.54

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	ADP	O4'-C1'-N9	10.31	127.88	108.09
2	A	1002	ADP	O4'-C1'-N9	8.38	124.19	108.09
2	E	1001	ADP	O4'-C1'-N9	8.05	123.55	108.09
2	B	1001	ADP	O4'-C1'-N9	7.69	122.86	108.09
2	F	1002	ADP	O4'-C1'-N9	7.67	122.82	108.09
2	C	1002	ADP	O4'-C1'-N9	7.45	122.40	108.09
2	C	1002	ADP	C5-C4-N3	-7.34	116.61	126.72
2	A	1001	ADP	C5-C4-N3	-7.33	116.63	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1002	ADP	C5-C4-N3	-7.21	116.79	126.72
2	C	1001	ADP	C5-C4-N3	-6.79	117.36	126.72
2	D	1002	ADP	C5-C4-N3	-6.79	117.37	126.72
2	D	1002	ADP	O4'-C1'-N9	6.78	121.11	108.09
2	A	1002	ADP	N3-C2-N1	-6.59	118.61	128.58
2	D	1001	ADP	O4'-C1'-N9	6.59	120.74	108.09
2	E	1002	ADP	N3-C2-N1	-6.56	118.64	128.58
2	F	1001	ADP	N3-C2-N1	-6.55	118.66	128.58
2	D	1001	ADP	C5-C4-N3	-6.51	117.76	126.72
2	D	1001	ADP	N3-C2-N1	-6.39	118.91	128.58
2	D	1002	ADP	N3-C2-N1	-6.21	119.19	128.58
2	E	1001	ADP	N3-C2-N1	-6.20	119.20	128.58
2	F	1002	ADP	C5-C4-N3	-6.16	118.23	126.72
2	B	1001	ADP	C5-C4-N3	-6.14	118.26	126.72
2	B	1001	ADP	N3-C2-N1	-6.08	119.38	128.58
2	F	1002	ADP	N3-C2-N1	-6.06	119.41	128.58
2	B	1002	ADP	N3-C4-N9	5.98	137.34	127.17
2	C	1001	ADP	N3-C2-N1	-5.92	119.62	128.58
2	E	1002	ADP	C5-C4-N3	-5.83	118.68	126.72
2	B	1002	ADP	N3-C2-N1	-5.81	119.79	128.58
2	F	1001	ADP	C5-C4-N3	-5.79	118.75	126.72
2	E	1001	ADP	C5-C4-N3	-5.69	118.88	126.72
2	A	1002	ADP	C5-C4-N3	-5.69	118.89	126.72
2	F	1002	ADP	C4'-O4'-C1'	-5.68	96.92	109.47
2	B	1001	ADP	C4'-O4'-C1'	-5.68	96.93	109.47
2	A	1001	ADP	N3-C4-N9	5.67	136.81	127.17
2	C	1002	ADP	N3-C4-N9	5.64	136.77	127.17
2	A	1001	ADP	N3-C2-N1	-5.43	120.37	128.58
2	C	1002	ADP	N3-C2-N1	-5.42	120.38	128.58
2	D	1002	ADP	N3-C4-N9	5.31	136.20	127.17
2	C	1001	ADP	O4'-C1'-N9	5.19	118.05	108.09
2	D	1001	ADP	C2-N3-C4	5.17	124.46	111.83
2	C	1001	ADP	N3-C4-N9	5.13	135.89	127.17
2	A	1002	ADP	C2-N3-C4	5.02	124.08	111.83
2	E	1002	ADP	C2-N3-C4	4.93	123.87	111.83
2	F	1001	ADP	C2-N3-C4	4.92	123.85	111.83
2	A	1001	ADP	C2-N3-C4	4.85	123.69	111.83
2	C	1002	ADP	C2-N3-C4	4.82	123.59	111.83
2	D	1002	ADP	C2-N3-C4	4.72	123.36	111.83
2	F	1002	ADP	N3-C4-N9	4.60	134.99	127.17
2	C	1001	ADP	C2-N3-C4	4.59	123.04	111.83
2	B	1001	ADP	N3-C4-N9	4.59	134.97	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1002	ADP	C2'-C1'-N9	-4.58	101.92	113.30
2	E	1001	ADP	C2-N3-C4	4.53	122.89	111.83
2	D	1001	ADP	N3-C4-N9	4.52	134.85	127.17
2	B	1001	ADP	C2-N3-C4	4.50	122.83	111.83
2	B	1002	ADP	C2-N3-C4	4.49	122.80	111.83
2	F	1002	ADP	C2-N3-C4	4.49	122.79	111.83
2	F	1001	ADP	N3-C4-N9	4.41	134.67	127.17
2	E	1002	ADP	N3-C4-N9	4.41	134.66	127.17
2	E	1002	ADP	O4'-C1'-N9	4.33	116.41	108.09
2	F	1001	ADP	O4'-C1'-N9	4.29	116.33	108.09
2	E	1001	ADP	N3-C4-N9	4.19	134.29	127.17
2	E	1001	ADP	N9-C8-N7	-4.07	108.17	113.94
2	A	1001	ADP	C4'-O4'-C1'	-4.06	100.50	109.47
2	D	1001	ADP	C3'-C2'-C1'	3.96	108.95	101.46
2	A	1001	ADP	C5-N7-C8	3.94	109.65	103.45
2	F	1001	ADP	N9-C8-N7	-3.90	108.41	113.94
2	E	1002	ADP	N9-C8-N7	-3.85	108.48	113.94
2	C	1001	ADP	O2A-PA-O3A	3.69	117.25	107.27
2	D	1002	ADP	C4'-O4'-C1'	-3.67	101.36	109.47
2	B	1002	ADP	O4'-C1'-N9	3.66	115.12	108.09
2	B	1001	ADP	N9-C8-N7	-3.63	108.78	113.94
2	F	1002	ADP	N9-C8-N7	-3.62	108.80	113.94
2	D	1002	ADP	C5-N7-C8	3.57	109.07	103.45
2	D	1002	ADP	O5'-C5'-C4'	-3.51	97.05	108.99
2	A	1002	ADP	N3-C4-N9	3.50	133.11	127.17
2	A	1001	ADP	C2'-C1'-N9	-3.46	104.71	113.30
2	A	1001	ADP	O4'-C4'-C5'	3.43	120.31	109.33
2	F	1001	ADP	C4-N9-C8	3.40	109.31	105.74
2	A	1002	ADP	C2'-C1'-N9	-3.40	104.86	113.30
2	F	1002	ADP	O4'-C4'-C5'	3.40	120.23	109.33
2	D	1001	ADP	N9-C8-N7	-3.40	109.12	113.94
2	B	1001	ADP	O4'-C4'-C5'	3.40	120.21	109.33
2	D	1002	ADP	N9-C8-N7	-3.39	109.12	113.94
2	E	1001	ADP	C4-N9-C8	3.39	109.30	105.74
2	E	1002	ADP	C4-N9-C8	3.38	109.29	105.74
2	E	1001	ADP	C4'-O4'-C1'	-3.37	102.02	109.47
2	F	1002	ADP	C5-N7-C8	3.37	108.75	103.45
2	B	1001	ADP	C5-N7-C8	3.36	108.73	103.45
2	C	1001	ADP	C5-N7-C8	3.34	108.69	103.45
2	A	1002	ADP	N9-C8-N7	-3.32	109.22	113.94
2	A	1001	ADP	N9-C8-N7	-3.30	109.25	113.94
2	C	1002	ADP	C5-N7-C8	3.29	108.61	103.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	ADP	O2A-PA-O3A	3.26	116.07	107.27
2	B	1002	ADP	C5-N7-C8	3.25	108.56	103.45
2	F	1002	ADP	O2A-PA-O3A	3.24	116.03	107.27
2	E	1001	ADP	C5-N7-C8	3.20	108.48	103.45
2	A	1001	ADP	C5-C6-N6	-3.17	115.43	123.29
2	A	1001	ADP	C4-C5-N7	-3.15	106.98	110.58
2	C	1001	ADP	C4-C5-N7	-3.14	107.00	110.58
2	A	1002	ADP	O2A-PA-O3A	3.08	115.59	107.27
2	F	1001	ADP	C5-N7-C8	3.06	108.25	103.45
2	C	1002	ADP	C4-C5-N7	-3.05	107.09	110.58
2	E	1001	ADP	O3'-C3'-C4'	3.03	119.80	111.08
2	E	1002	ADP	C5-N7-C8	3.03	108.21	103.45
2	D	1001	ADP	C5-N7-C8	3.02	108.19	103.45
2	F	1002	ADP	C4-C5-N7	-3.00	107.15	110.58
2	A	1001	ADP	O4'-C1'-C2'	-2.99	100.22	106.62
2	D	1001	ADP	O2A-PA-O3A	2.97	115.31	107.27
2	B	1002	ADP	C5-C6-N6	-2.96	115.95	123.29
2	E	1001	ADP	C4-C5-N7	-2.96	107.20	110.58
2	B	1001	ADP	C4-C5-N7	-2.94	107.23	110.58
2	E	1001	ADP	C2'-C1'-N9	-2.93	106.02	113.30
2	C	1001	ADP	N9-C8-N7	-2.90	109.82	113.94
2	E	1001	ADP	O2A-PA-O3A	2.89	115.09	107.27
2	A	1002	ADP	C4-N9-C1'	-2.84	119.98	126.63
2	D	1002	ADP	C4-C5-N7	-2.84	107.33	110.58
2	C	1002	ADP	N9-C8-N7	-2.83	109.93	113.94
2	D	1001	ADP	C2'-C1'-N9	-2.82	106.29	113.30
2	A	1002	ADP	C4-C5-N7	-2.82	107.36	110.58
2	E	1002	ADP	C4-C5-N7	-2.81	107.37	110.58
2	D	1001	ADP	O5'-C5'-C4'	-2.78	99.52	108.99
2	C	1002	ADP	O5'-C5'-C4'	-2.78	99.54	108.99
2	B	1002	ADP	C3'-C2'-C1'	2.77	106.70	101.46
2	B	1001	ADP	O5'-C5'-C4'	-2.75	99.62	108.99
2	F	1002	ADP	O5'-C5'-C4'	-2.74	99.65	108.99
2	F	1001	ADP	C4-C5-N7	-2.74	107.45	110.58
2	D	1001	ADP	C4-C5-N7	-2.72	107.48	110.58
2	E	1001	ADP	C3'-C2'-C1'	-2.70	96.36	101.46
2	A	1002	ADP	O4'-C4'-C5'	2.67	117.88	109.33
2	B	1002	ADP	N9-C8-N7	-2.65	110.18	113.94
2	F	1001	ADP	C5-C6-N6	-2.63	116.78	123.29
2	F	1002	ADP	C4-N9-C8	2.61	108.48	105.74
2	E	1002	ADP	C5-C6-N6	-2.60	116.84	123.29
2	B	1001	ADP	C4-N9-C8	2.59	108.46	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1002	ADP	C5-N7-C8	2.53	107.43	103.45
2	D	1001	ADP	O4'-C4'-C3'	2.51	110.14	105.15
2	E	1002	ADP	O5'-C5'-C4'	-2.50	100.48	108.99
2	A	1001	ADP	O2A-PA-O3A	2.50	114.03	107.27
2	F	1001	ADP	O5'-C5'-C4'	-2.49	100.53	108.99
2	E	1001	ADP	O5'-C5'-C4'	-2.48	100.56	108.99
2	B	1002	ADP	O2A-PA-O3A	2.47	113.94	107.27
2	D	1001	ADP	C5-C6-N6	-2.45	117.22	123.29
2	D	1002	ADP	O2A-PA-O3A	2.42	113.83	107.27
2	A	1001	ADP	C5'-C4'-C3'	-2.39	106.61	115.21
2	B	1001	ADP	O4'-C1'-C2'	-2.39	101.51	106.62
2	B	1002	ADP	C4-C5-N7	-2.38	107.86	110.58
2	F	1002	ADP	O4'-C1'-C2'	-2.38	101.53	106.62
2	A	1002	ADP	C5'-C4'-C3'	-2.36	106.70	115.21
2	A	1002	ADP	C6-C5-N7	2.35	136.62	132.09
2	A	1002	ADP	C4'-O4'-C1'	-2.31	104.37	109.47
2	A	1001	ADP	O5'-C5'-C4'	-2.30	101.15	108.99
2	B	1002	ADP	C2'-C1'-N9	-2.28	107.64	113.30
2	B	1002	ADP	O4'-C4'-C3'	2.28	109.68	105.15
2	B	1002	ADP	C5'-C4'-C3'	-2.28	107.01	115.21
2	E	1001	ADP	C5-C6-N6	-2.25	117.71	123.29
2	C	1002	ADP	O4'-C4'-C3'	2.25	109.62	105.15
2	A	1002	ADP	C1'-N9-C8	2.23	132.04	127.09
2	D	1002	ADP	C4-N9-C8	2.20	108.05	105.74
2	C	1002	ADP	O4'-C4'-C5'	2.20	116.37	109.33
2	C	1001	ADP	C5'-C4'-C3'	-2.19	107.32	115.21
2	C	1002	ADP	C5'-C4'-C3'	-2.17	107.39	115.21
2	E	1002	ADP	C2'-C1'-N9	-2.16	107.93	113.30
2	D	1002	ADP	C5-C6-N1	2.15	122.97	117.51
2	C	1002	ADP	O2A-PA-O3A	2.15	113.07	107.27
2	F	1001	ADP	C2'-C1'-N9	-2.14	107.98	113.30
2	A	1002	ADP	C4-N9-C8	2.13	107.97	105.74
2	C	1001	ADP	O4'-C4'-C3'	2.11	109.34	105.15
2	B	1002	ADP	C6-C5-C4	2.10	120.04	117.18
2	E	1001	ADP	C5'-C4'-C3'	-2.09	107.70	115.21
2	B	1002	ADP	N6-C6-N1	2.08	123.00	118.38
2	C	1002	ADP	C5-C6-N6	-2.07	118.17	123.29
2	E	1001	ADP	C4-N9-C1'	-2.04	121.86	126.63
2	B	1002	ADP	O4'-C4'-C5'	2.02	115.82	109.33
2	B	1002	ADP	O5'-C5'-C4'	-2.01	102.14	108.99
2	A	1002	ADP	C5-C4-N9	2.01	108.00	105.81

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	ADP	C5'-O5'-PA-O1A
2	A	1001	ADP	C5'-O5'-PA-O3A
2	A	1002	ADP	C5'-O5'-PA-O2A
2	A	1002	ADP	C2'-C1'-N9-C4
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	C	1002	ADP	C2'-C1'-N9-C8
2	D	1001	ADP	PA-O3A-PB-O3B
2	D	1001	ADP	C5'-O5'-PA-O1A
2	D	1001	ADP	C4'-C5'-O5'-PA
2	D	1002	ADP	O4'-C4'-C5'-O5'
2	E	1001	ADP	C5'-O5'-PA-O3A
2	E	1001	ADP	C4'-C5'-O5'-PA
2	E	1002	ADP	C2'-C1'-N9-C8
2	F	1001	ADP	C2'-C1'-N9-C8
2	A	1001	ADP	C3'-C4'-C5'-O5'
2	B	1002	ADP	O4'-C4'-C5'-O5'
2	D	1002	ADP	C3'-C4'-C5'-O5'
2	C	1002	ADP	C4'-C5'-O5'-PA
2	E	1002	ADP	C4'-C5'-O5'-PA
2	F	1001	ADP	C4'-C5'-O5'-PA
2	A	1002	ADP	C2'-C1'-N9-C8
2	C	1002	ADP	C2'-C1'-N9-C4
2	D	1002	ADP	C2'-C1'-N9-C4
2	E	1002	ADP	C2'-C1'-N9-C4
2	F	1001	ADP	C2'-C1'-N9-C4
2	C	1001	ADP	C4'-C5'-O5'-PA
2	B	1002	ADP	C3'-C4'-C5'-O5'
2	D	1002	ADP	C2'-C1'-N9-C8
2	C	1001	ADP	O4'-C4'-C5'-O5'
2	E	1001	ADP	O4'-C4'-C5'-O5'
2	C	1001	ADP	C2'-C1'-N9-C4
2	B	1001	ADP	PA-O3A-PB-O1B
2	F	1002	ADP	PA-O3A-PB-O1B
2	C	1001	ADP	C2'-C1'-N9-C8
2	C	1001	ADP	C3'-C4'-C5'-O5'
2	A	1001	ADP	O4'-C4'-C5'-O5'
2	D	1001	ADP	PB-O3A-PA-O5'
2	E	1001	ADP	PB-O3A-PA-O1A
2	A	1001	ADP	C5'-O5'-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1002	ADP	C5'-O5'-PA-O3A
2	D	1001	ADP	C5'-O5'-PA-O2A
2	D	1001	ADP	C5'-O5'-PA-O3A
2	E	1001	ADP	C5'-O5'-PA-O1A
2	A	1001	ADP	C4'-C5'-O5'-PA
2	B	1002	ADP	C2'-C1'-N9-C4
2	D	1001	ADP	C2'-C1'-N9-C4
2	B	1002	ADP	C2'-C1'-N9-C8
2	D	1001	ADP	C2'-C1'-N9-C8
2	B	1002	ADP	PA-O3A-PB-O1B
2	E	1001	ADP	PA-O3A-PB-O1B
2	E	1002	ADP	O4'-C4'-C5'-O5'
2	F	1001	ADP	O4'-C4'-C5'-O5'
2	E	1002	ADP	PB-O3A-PA-O1A
2	F	1001	ADP	PB-O3A-PA-O1A
2	B	1001	ADP	O4'-C4'-C5'-O5'
2	F	1002	ADP	O4'-C4'-C5'-O5'
2	E	1001	ADP	C2'-C1'-N9-C8
2	B	1001	ADP	C4'-C5'-O5'-PA
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	1002	ADP	PA-O3A-PB-O3B
2	F	1002	ADP	C4'-C5'-O5'-PA
2	A	1002	ADP	PB-O3A-PA-O1A
2	D	1002	ADP	PB-O3A-PA-O1A
2	C	1001	ADP	PA-O3A-PB-O1B
2	E	1001	ADP	O4'-C1'-N9-C8
2	A	1002	ADP	PB-O3A-PA-O2A
2	D	1002	ADP	PB-O3A-PA-O2A
2	E	1001	ADP	PB-O3A-PA-O2A

There are no ring outliers.

11 monomers are involved in 134 short contacts:

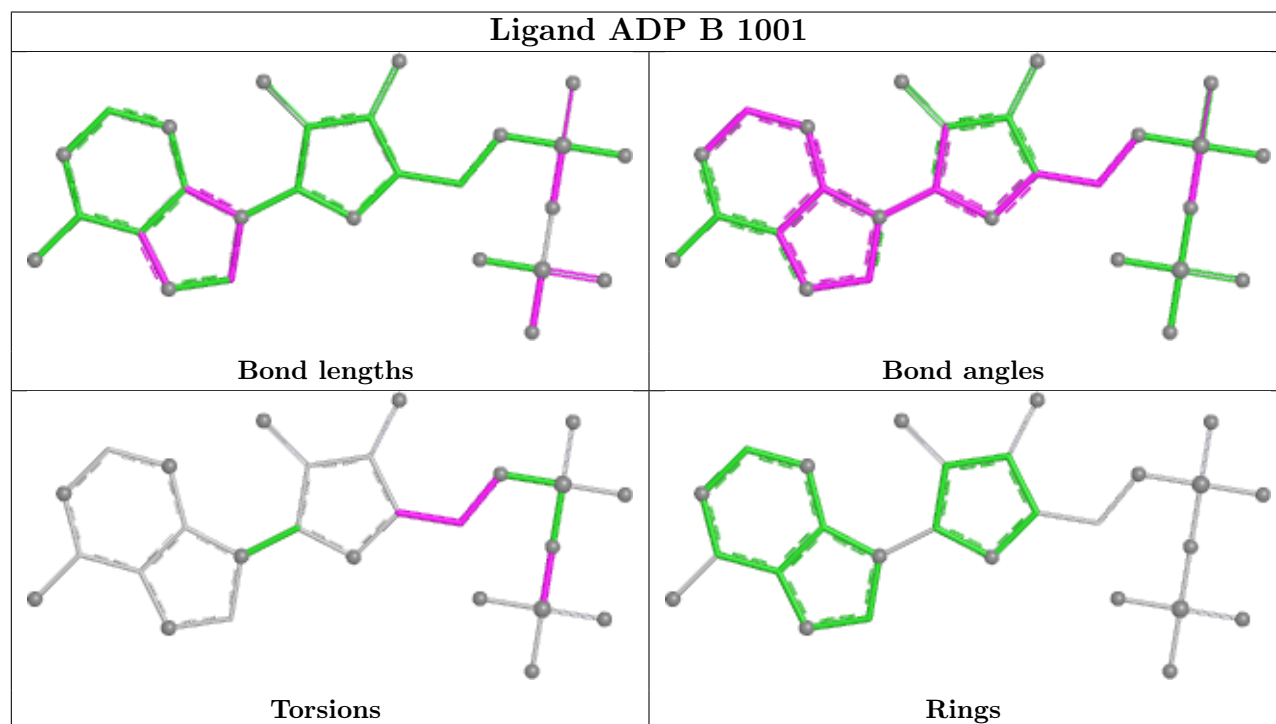
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	ADP	1	0
2	D	1001	ADP	8	0
2	C	1001	ADP	4	0
2	D	1002	ADP	3	0
2	A	1002	ADP	3	0
2	E	1001	ADP	6	0

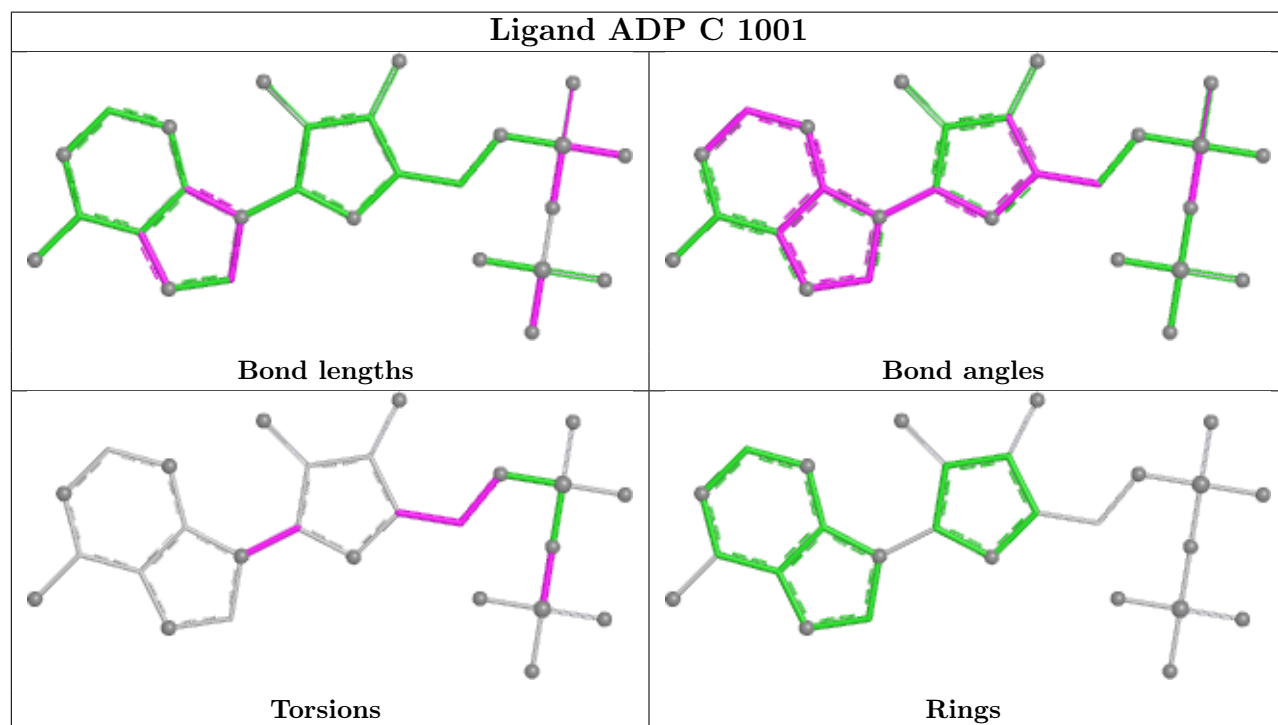
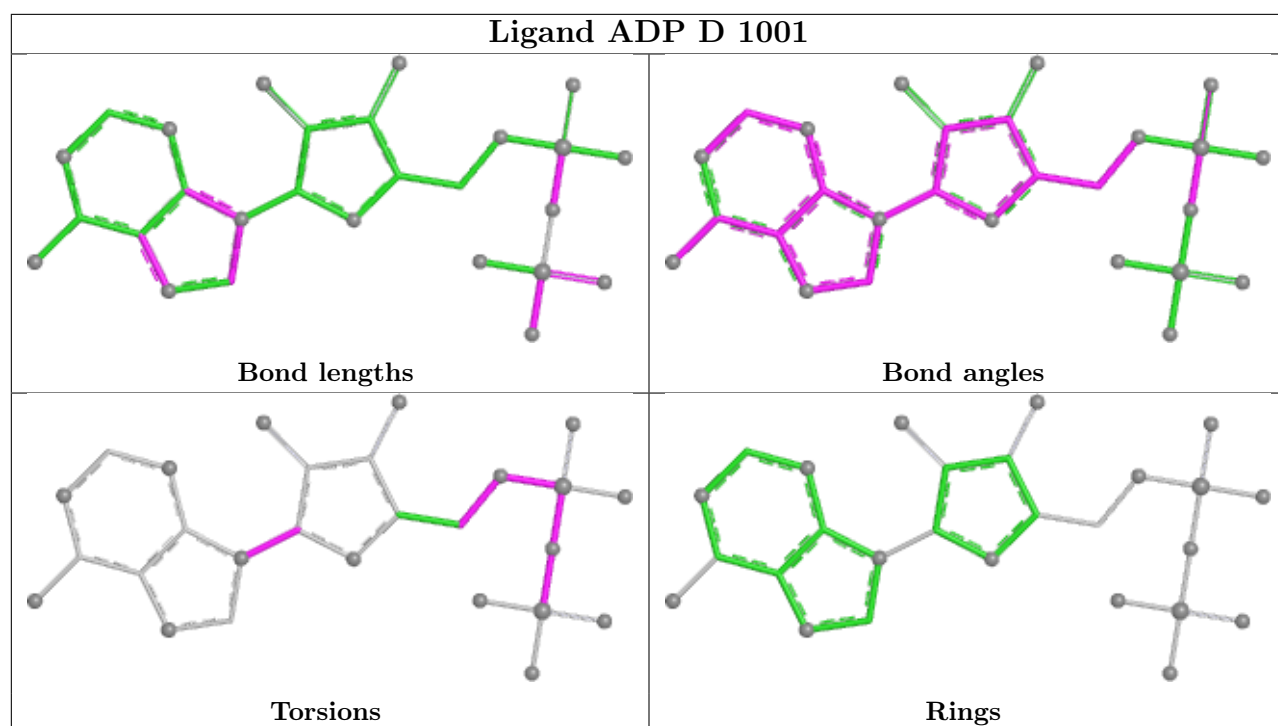
Continued on next page...

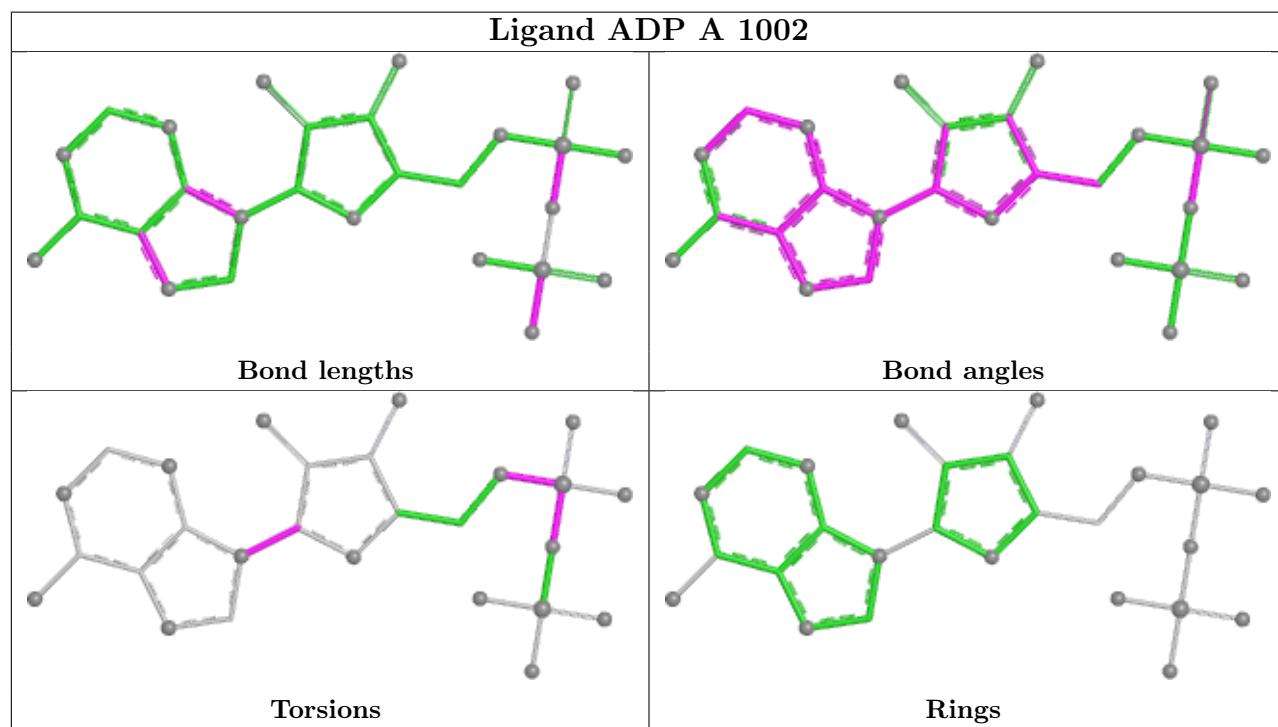
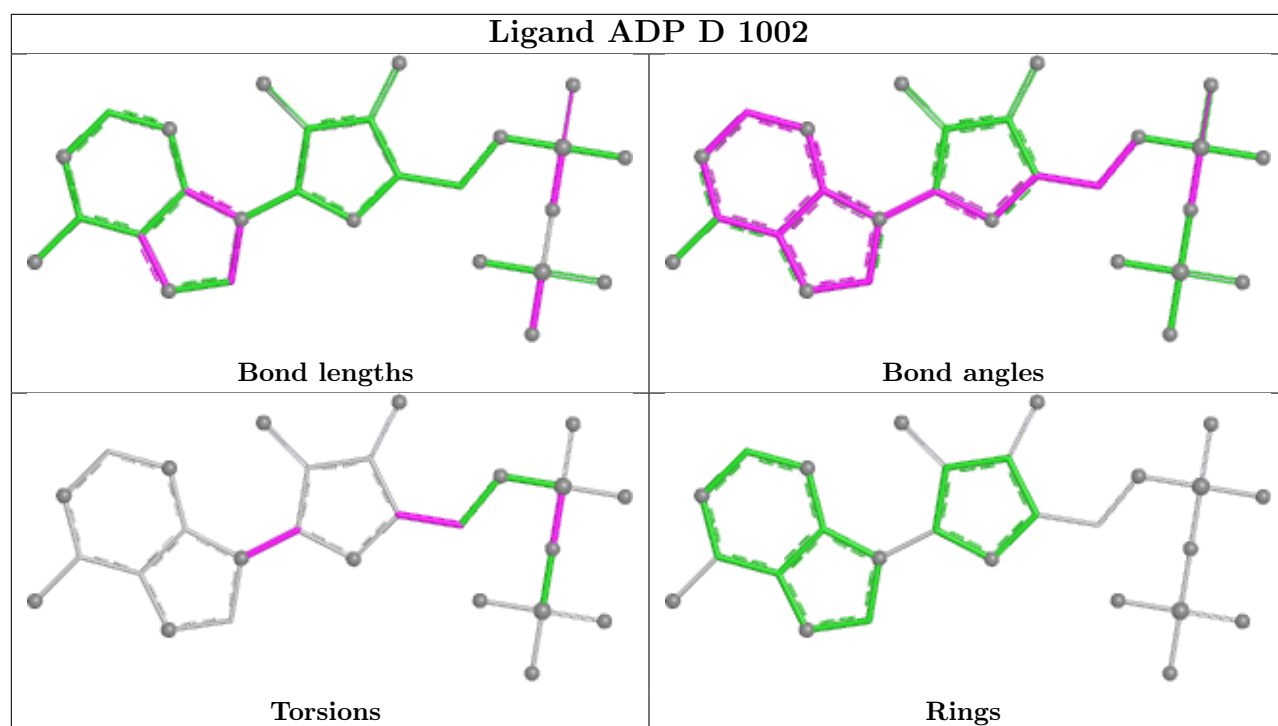
Continued from previous page...

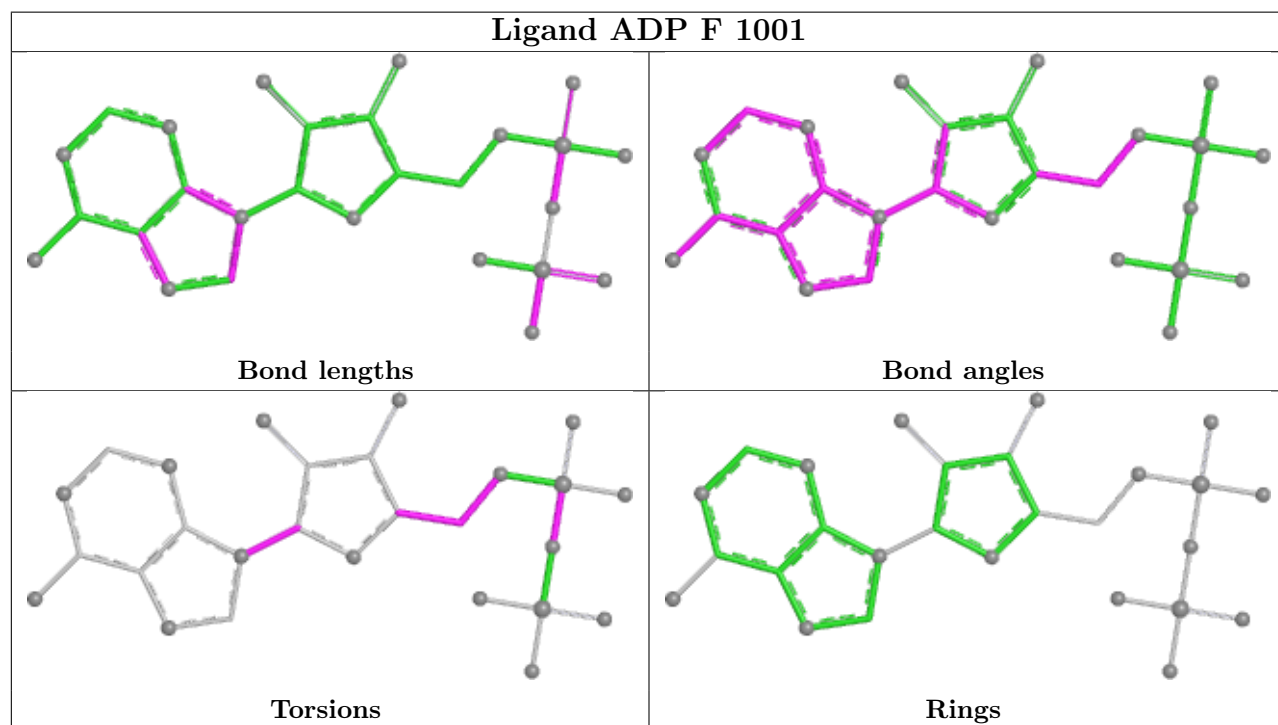
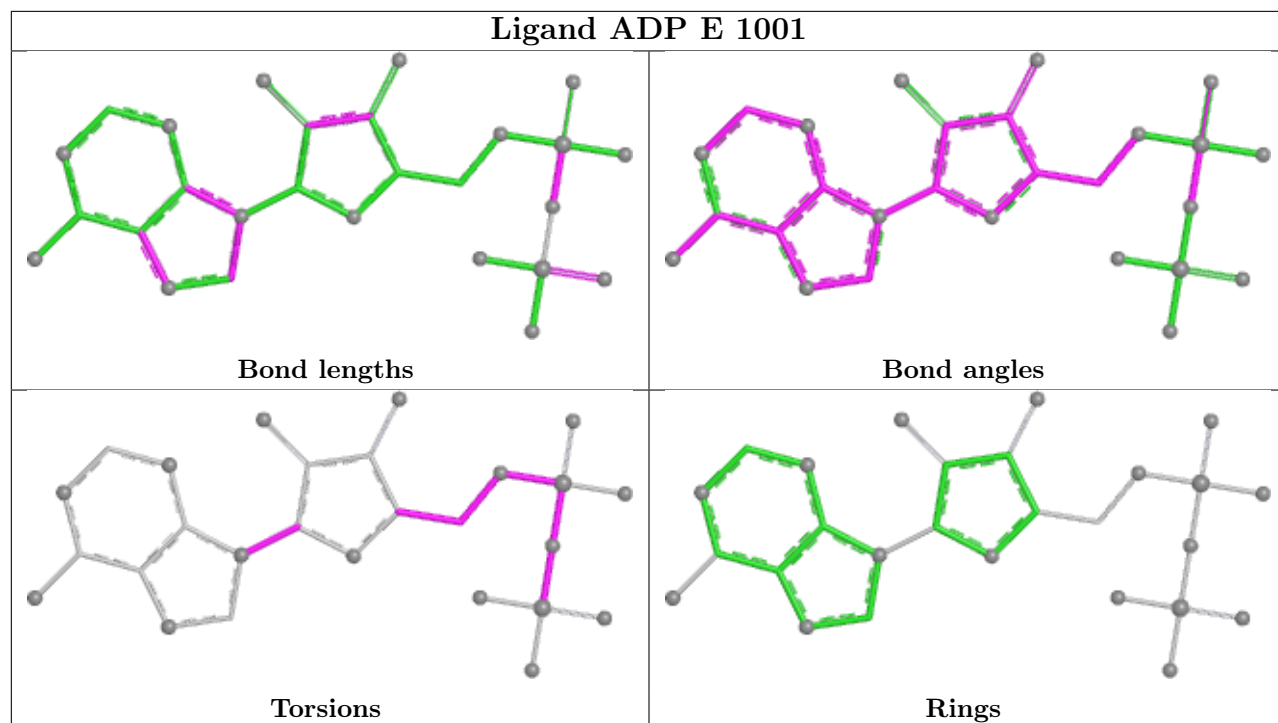
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1001	ADP	52	0
2	C	1002	ADP	2	0
2	F	1002	ADP	53	0
2	E	1002	ADP	1	0
2	A	1001	ADP	1	0

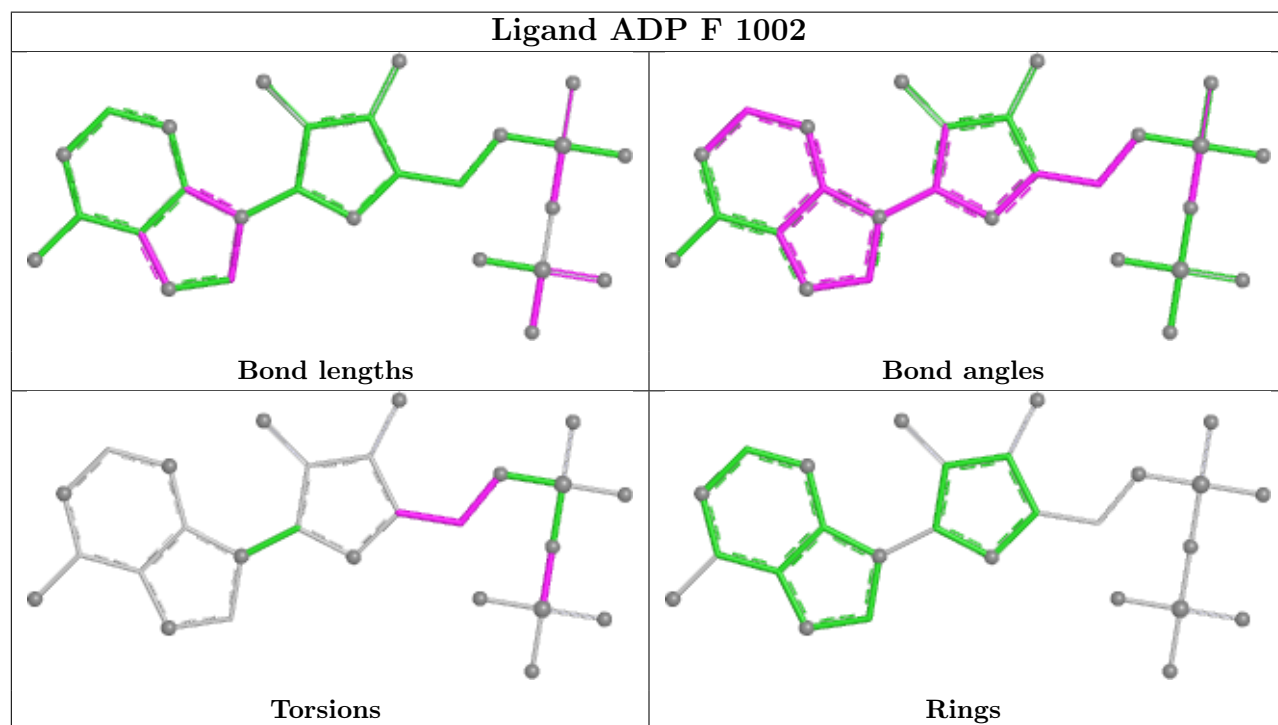
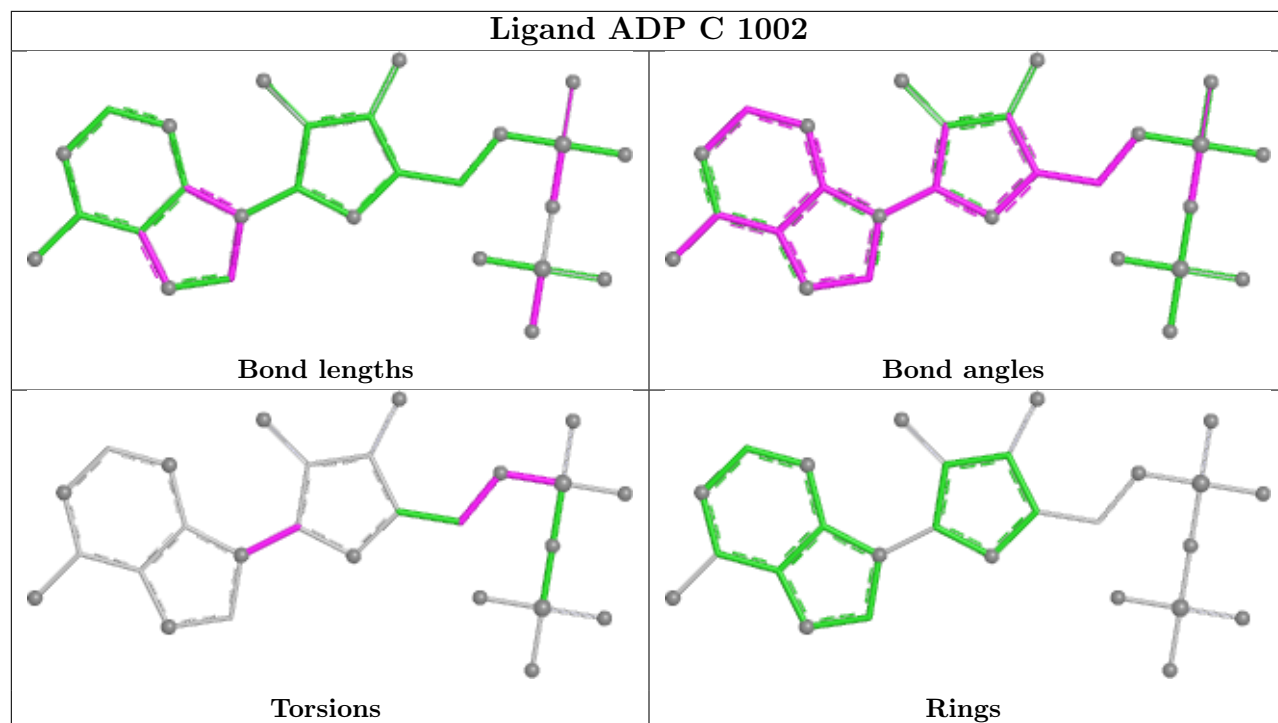
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

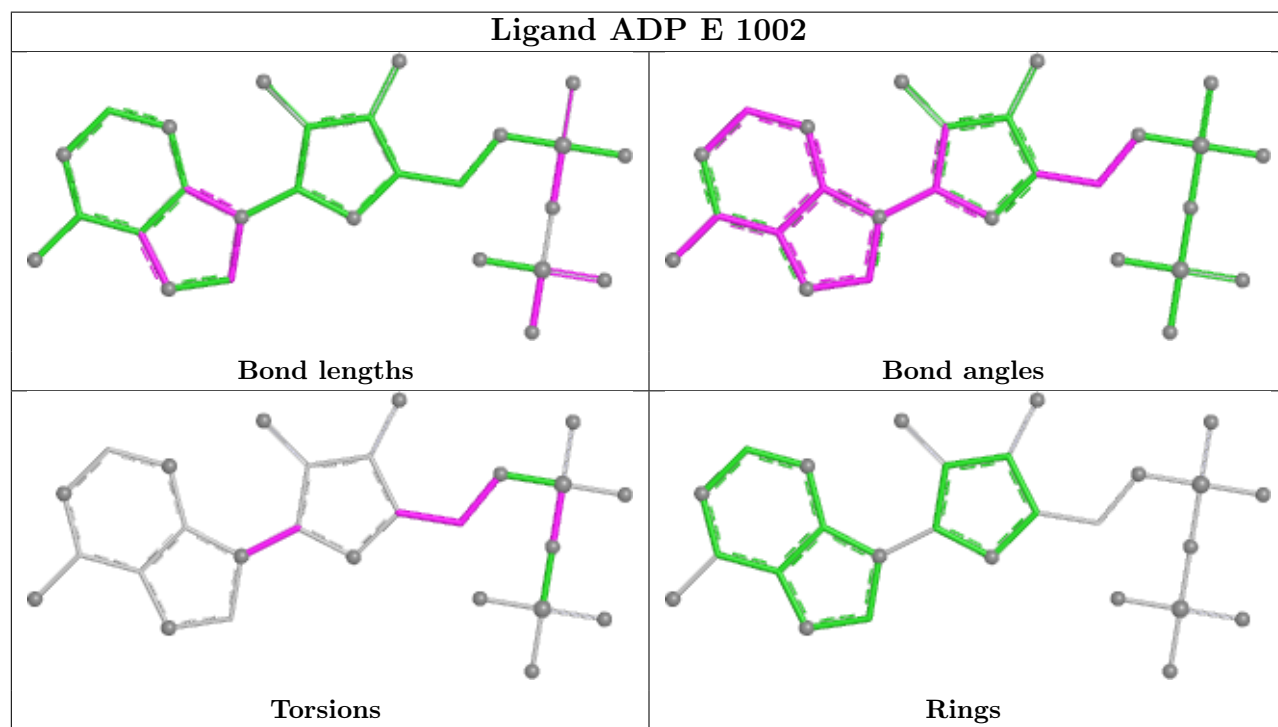
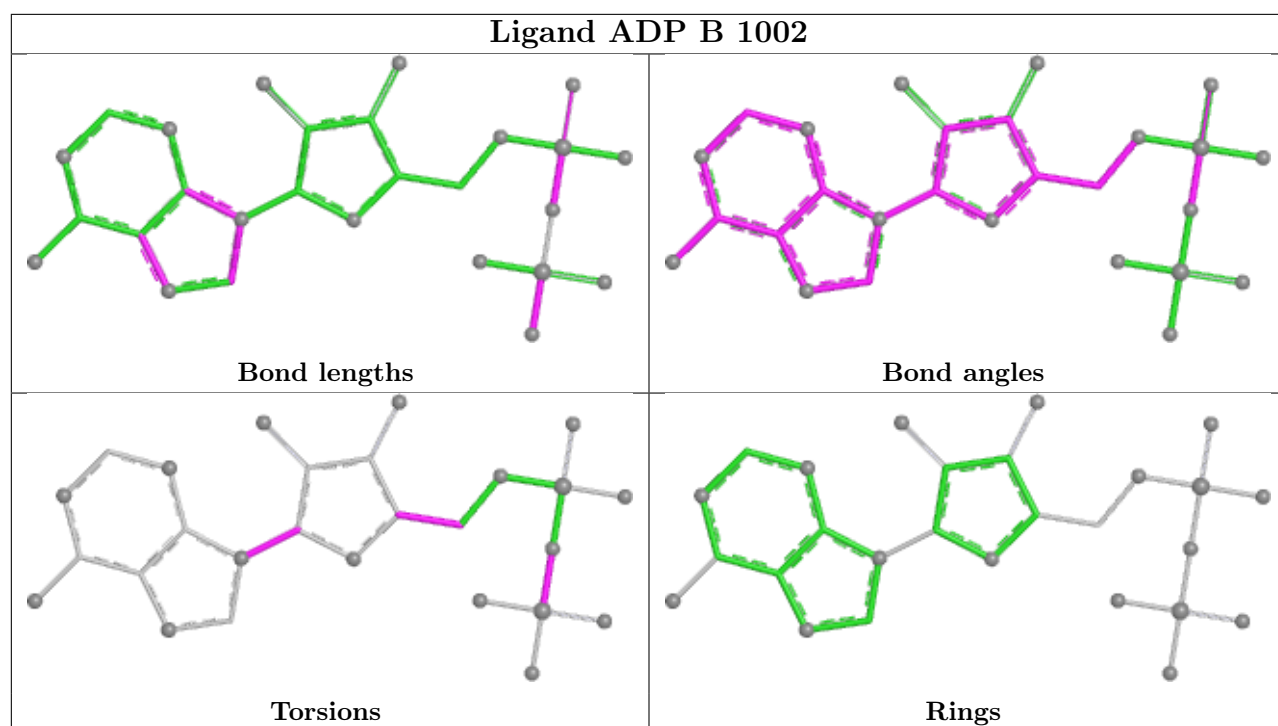


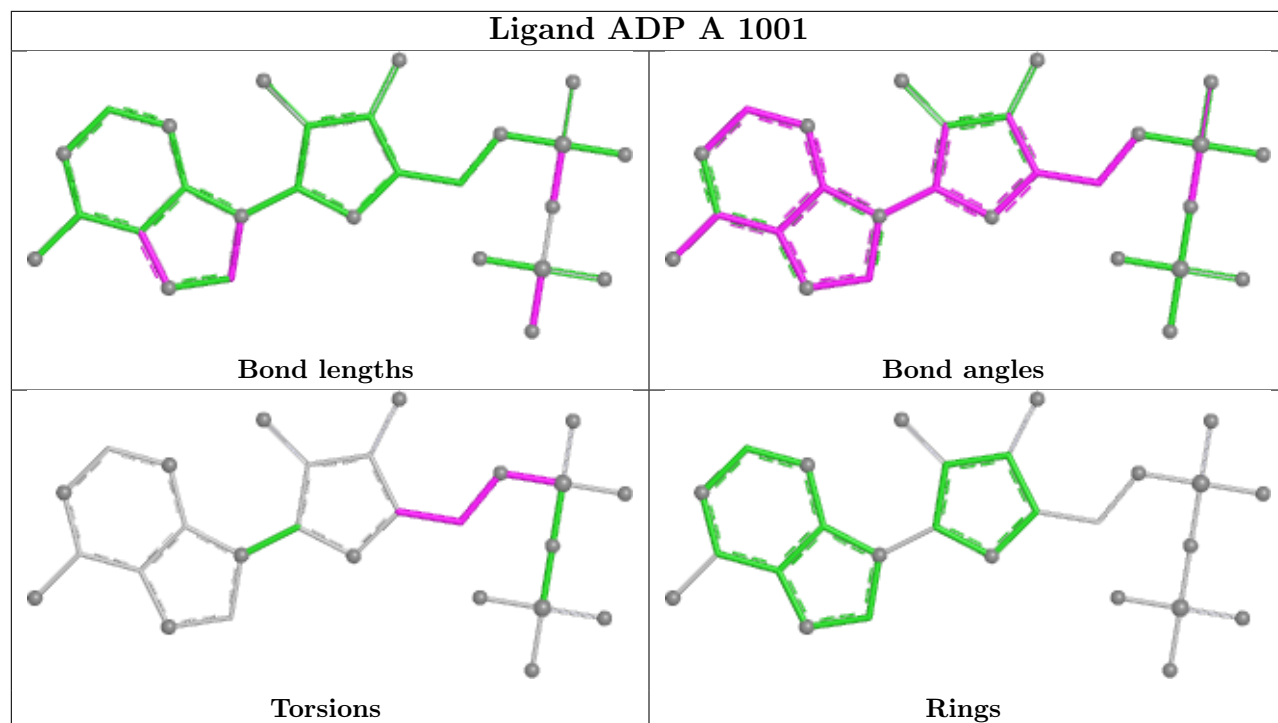












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

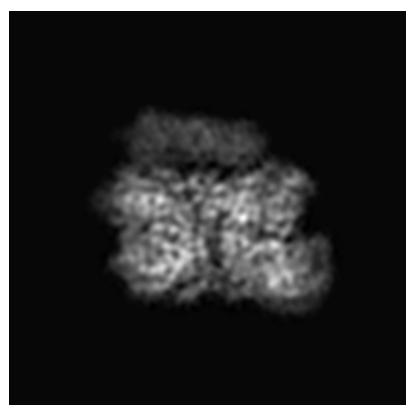
6 Map visualisation [i](#)

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

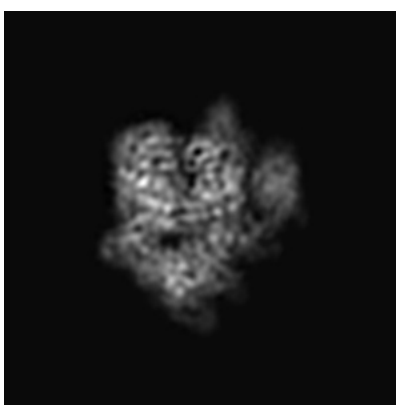
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

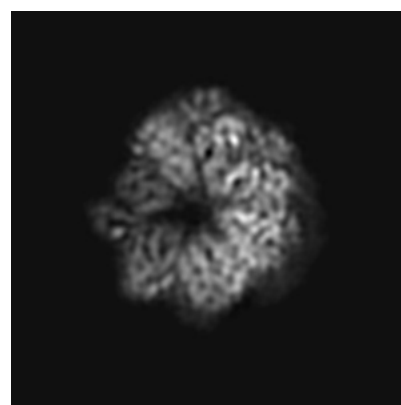
6.1.1 Primary map



X



Y



Z

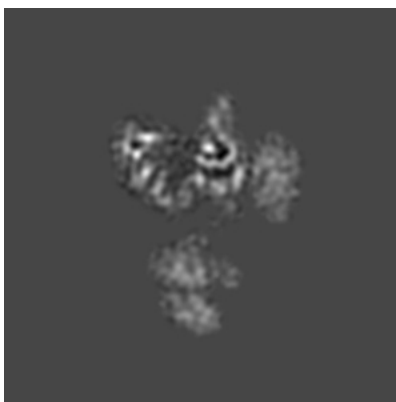
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

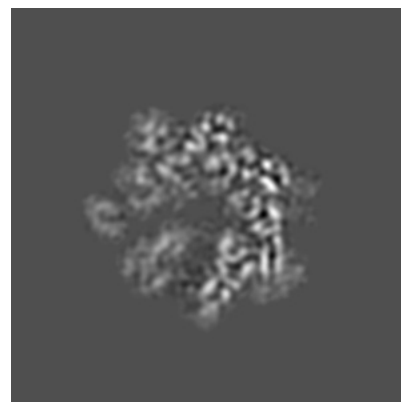
6.2.1 Primary map



X Index: 128



Y Index: 128



Z Index: 128

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

6.3 Largest variance slices [i](#)

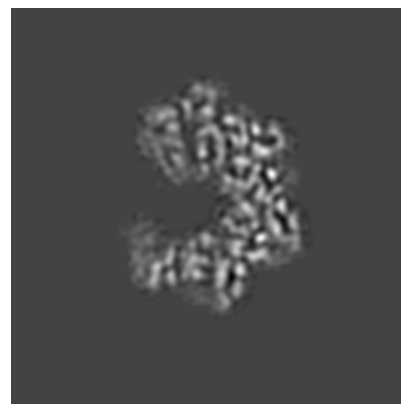
6.3.1 Primary map



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

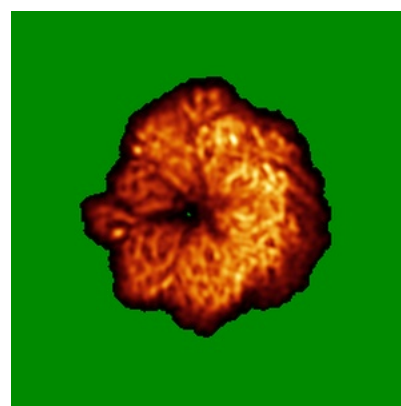
6.4.1 Primary map



X



Y



Z

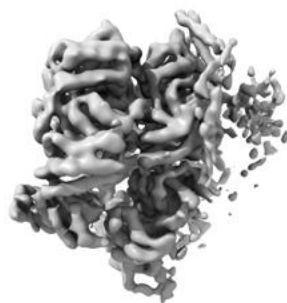
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

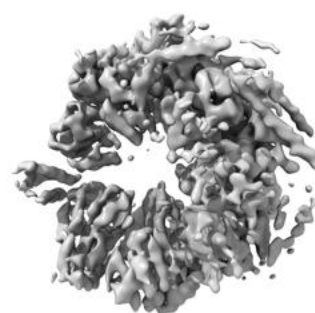
6.5.1 Primary map



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.

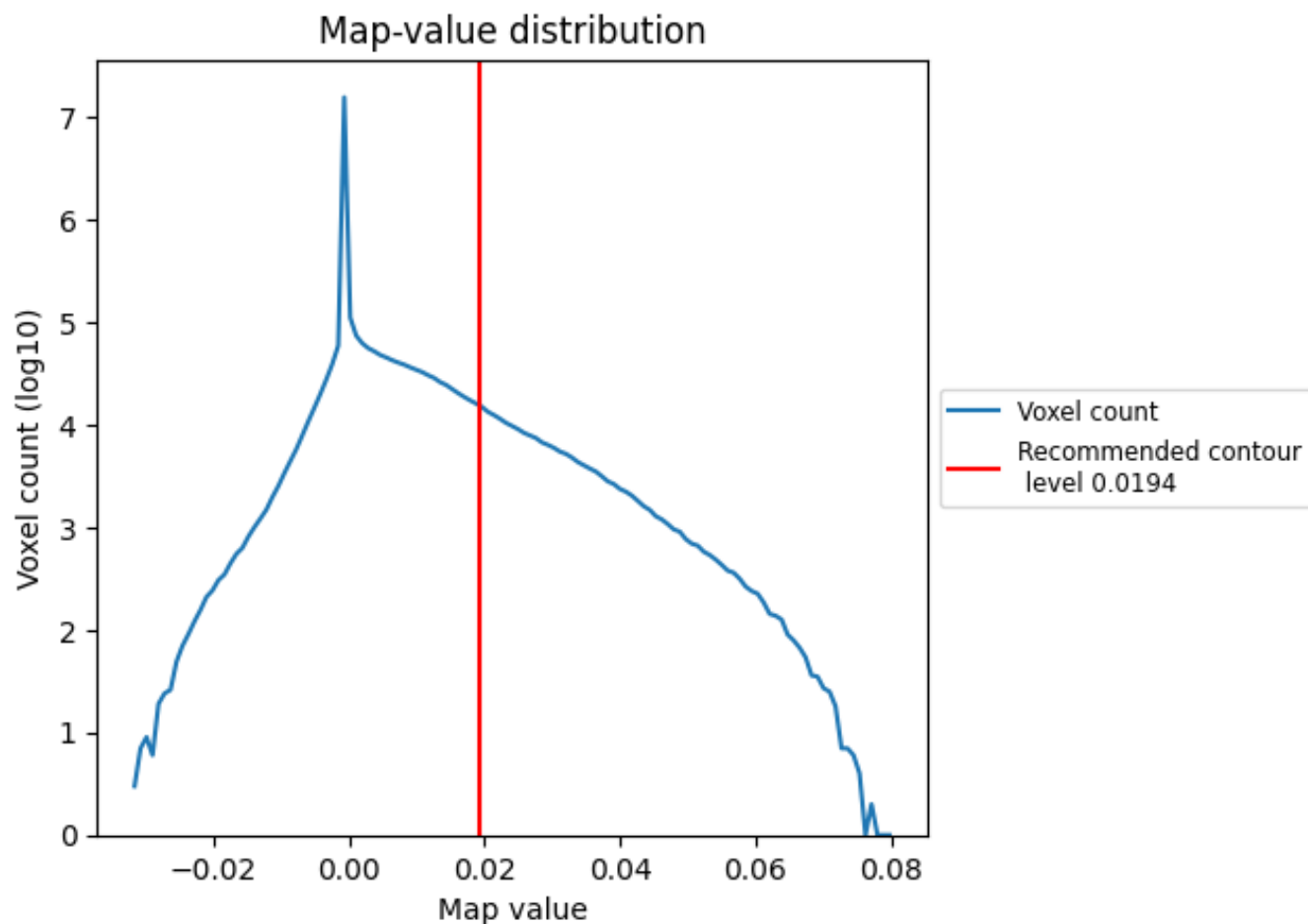
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

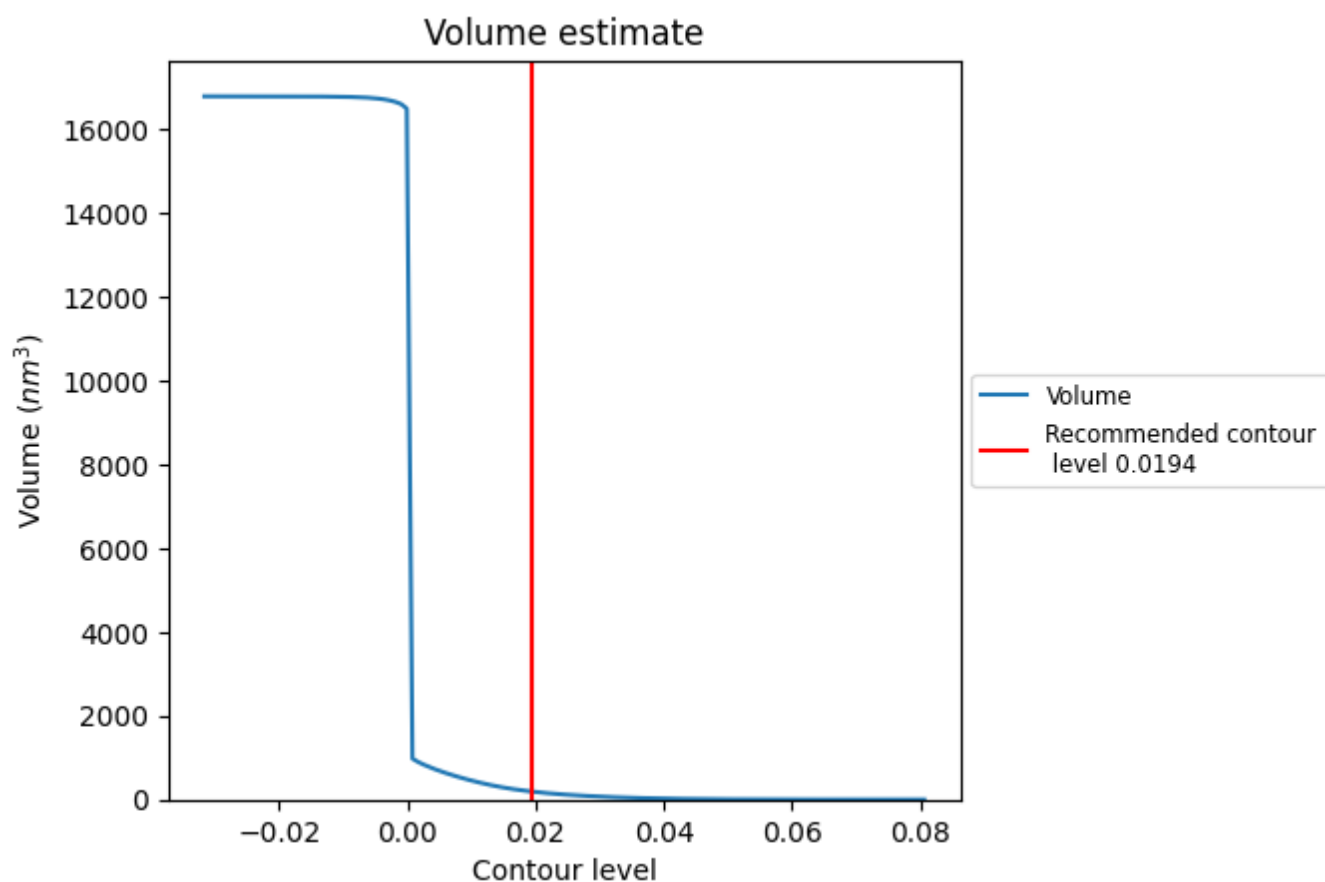
This section contains the results of statistical analysis of the map.

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.

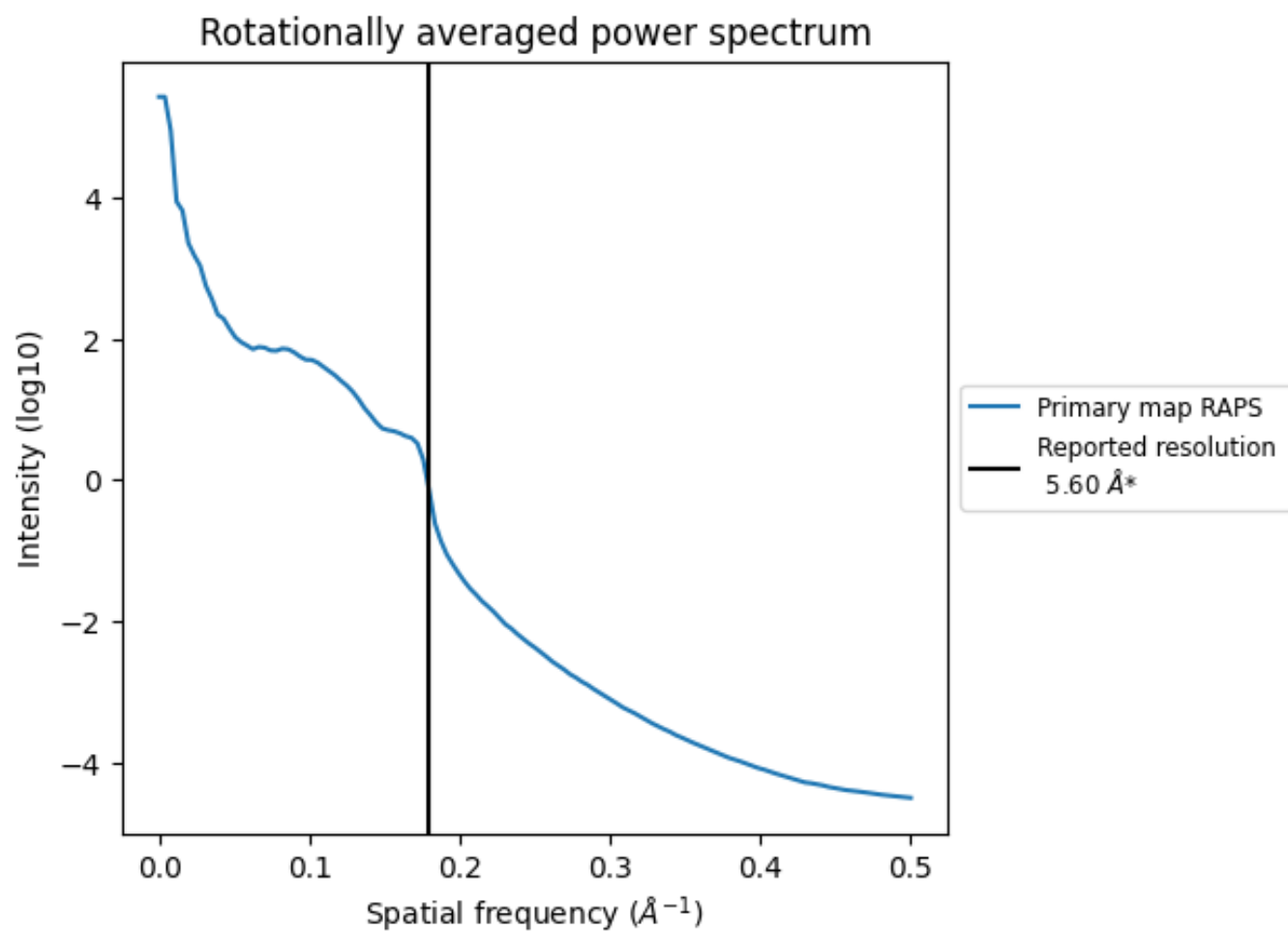
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 191 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.179 Å⁻¹

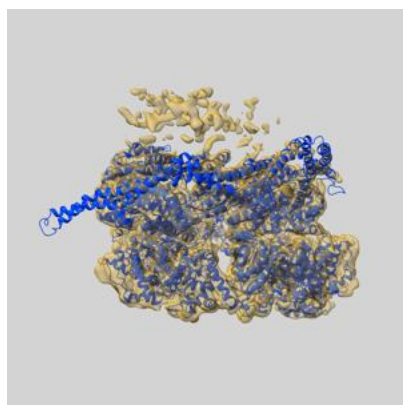
8 Fourier-Shell correlation

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

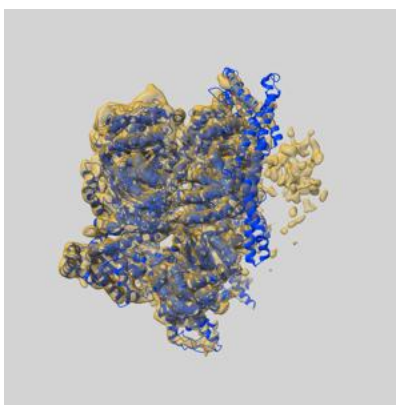
9 Map-model fit [i](#)

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](#).

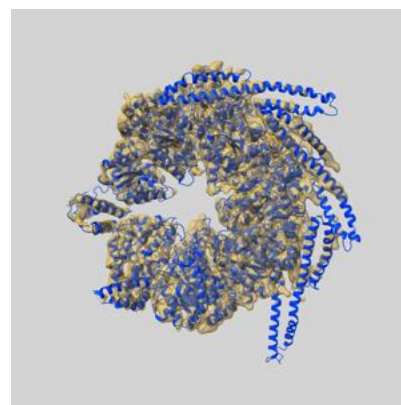
9.1 Map-model overlay [i](#)



X



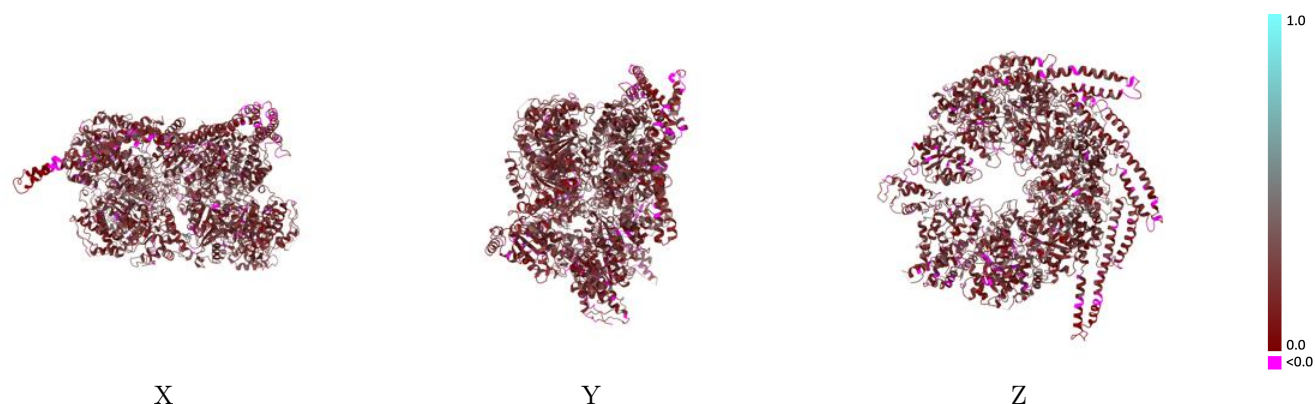
Y



Z

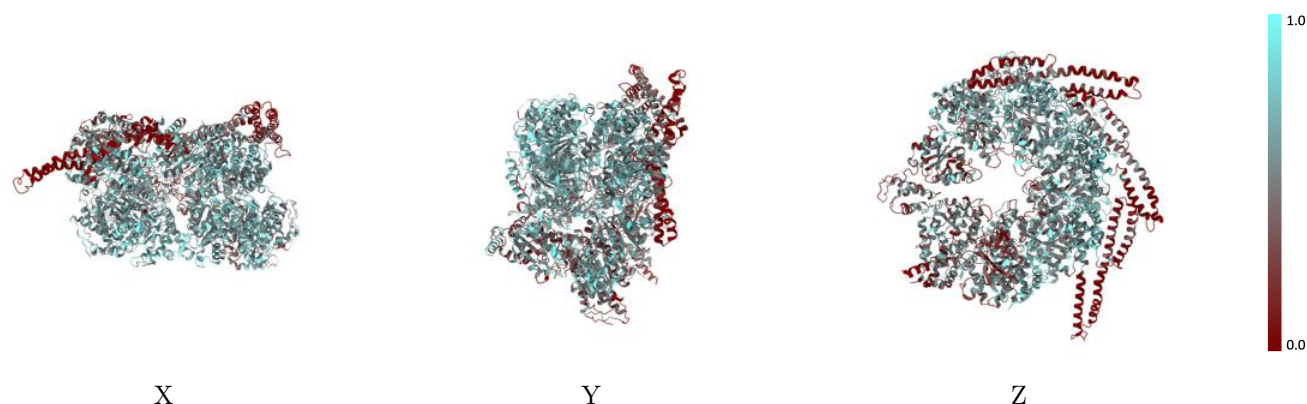
The images above show the 3D surface view of the map at the recommended contour level 0.0194 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



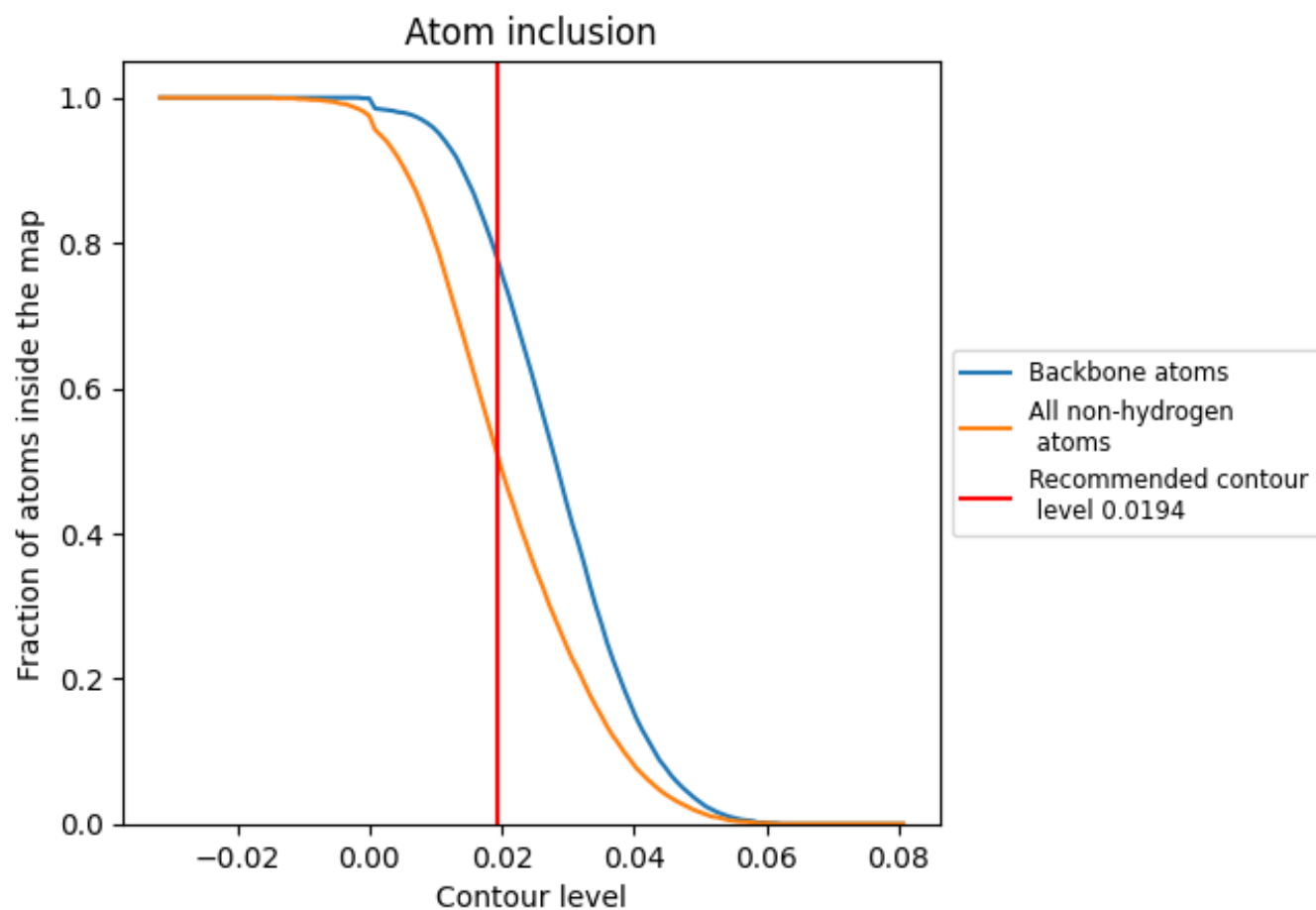
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0194).

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	0.5060	0.1870
A	0.3740	0.1790
B	0.5690	0.1970
C	0.5200	0.1900
D	0.5660	0.1930
E	0.5250	0.1910
F	0.4600	0.1660

1.0

0.0

<0.0