



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 09:06 AM UTC

PDB ID : 6HYT / pdb_00006hyt
Title : Crystal structure of DHX8 helicase domain bound to ADP at 2.3 Angstrom
Authors : Felisberto-Rodrigues, C.; Thomas, J.C.; McAndrew, P.C.; Le Bihan, Y.V.;
Burke, R.; Workman, P.; van Montfort, R.L.M.
Deposited on : 2018-10-22
Resolution : 2.33 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

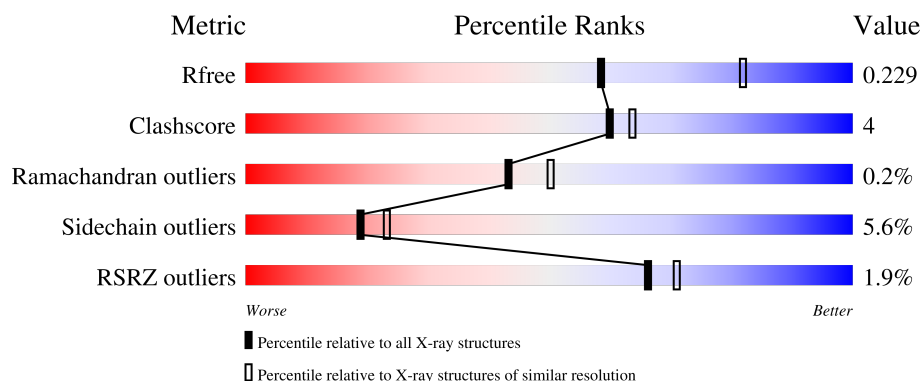
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	673	0% 77% 15% • 6%
1	B	673	0% 80% 12% • 6%
1	C	673	3% 80% 13% • 6%
1	D	673	2% 82% 10% • 6%

2 Entry composition [i](#)

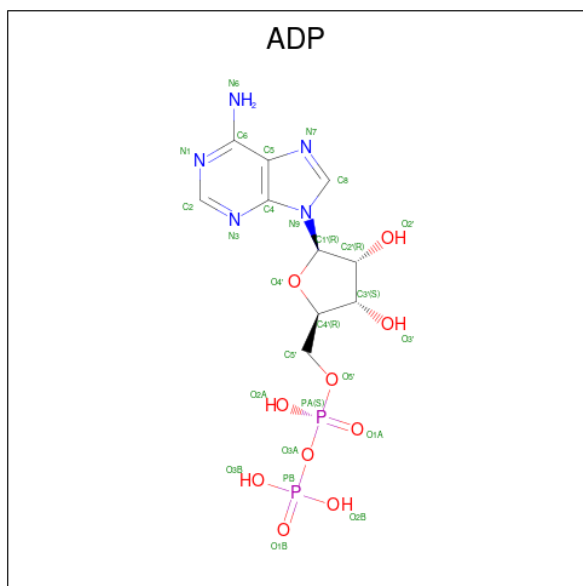
There are 8 unique types of molecules in this entry. The entry contains 20220 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 ATP-dependent RNA helicase DHX8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	632	Total	C	N	O	S	0	4	0
			4914	3146	821	912	35			
1	B	634	Total	C	N	O	S	0	4	0
			4858	3113	817	893	35			
1	C	633	Total	C	N	O	S	0	1	1
			4779	3064	789	893	33			
1	D	631	Total	C	N	O	S	0	2	1
			4808	3078	791	905	34			

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



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

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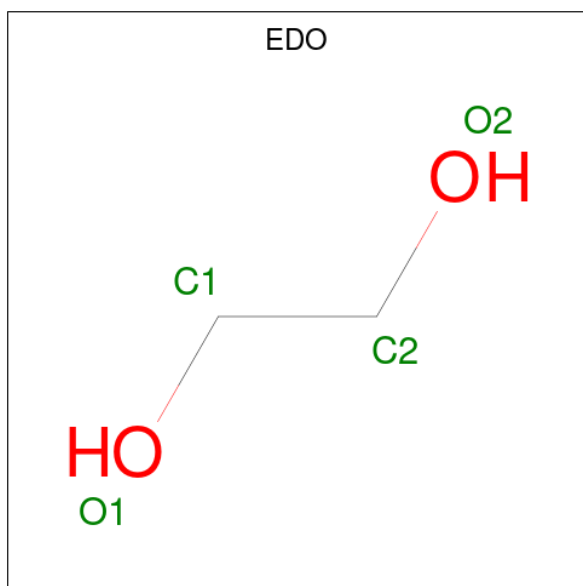
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	1
			46	20	10	14	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



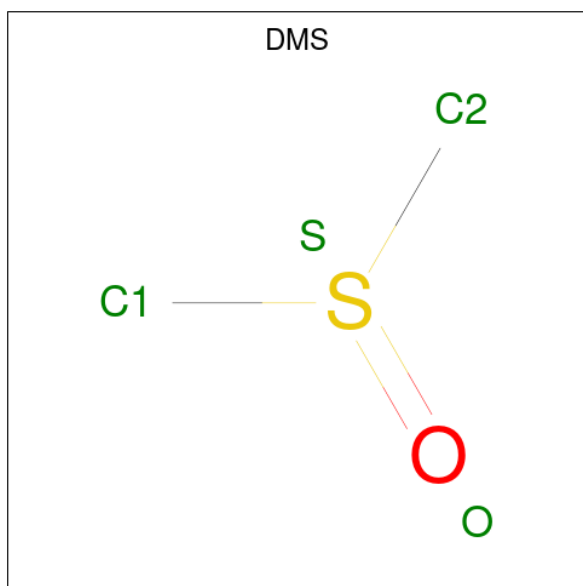
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



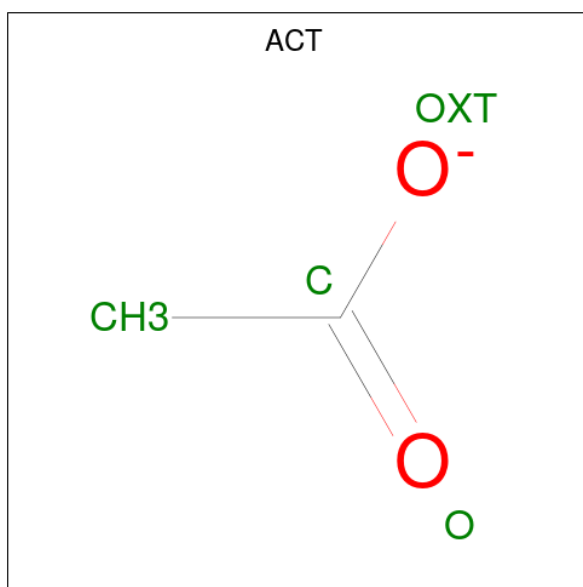
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	B	1	Total	Cl	0	0
			1	1		
7	C	1	Total	Cl	0	0
			1	1		
7	D	1	Total	Cl	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	196	Total	O	0	0
			196	196		
8	B	161	Total	O	0	0
			161	161		
8	C	121	Total	O	0	0
			121	121		

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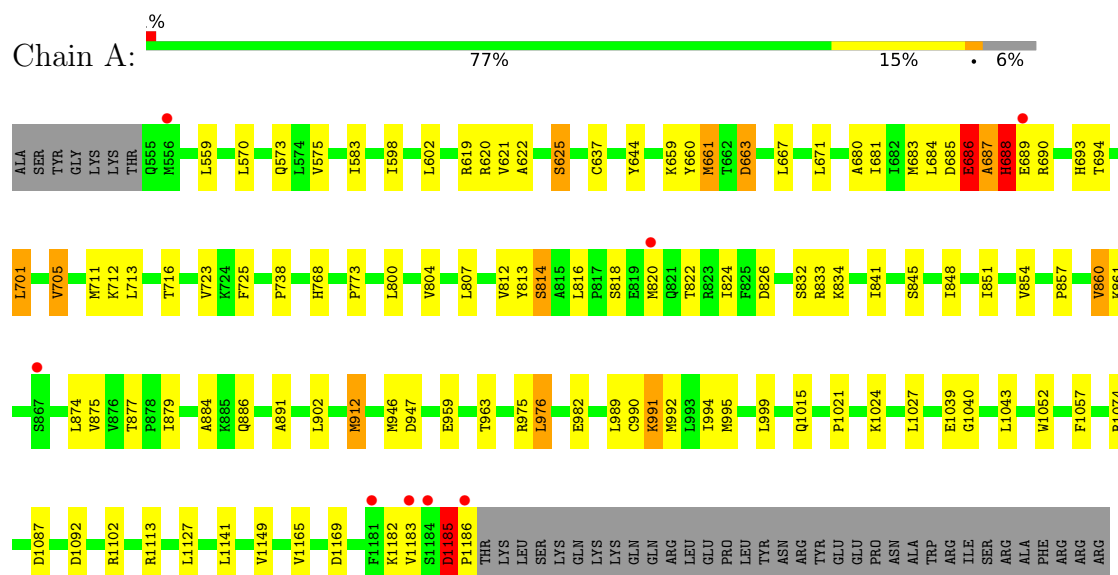
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	128	Total 128	O 128	0	0

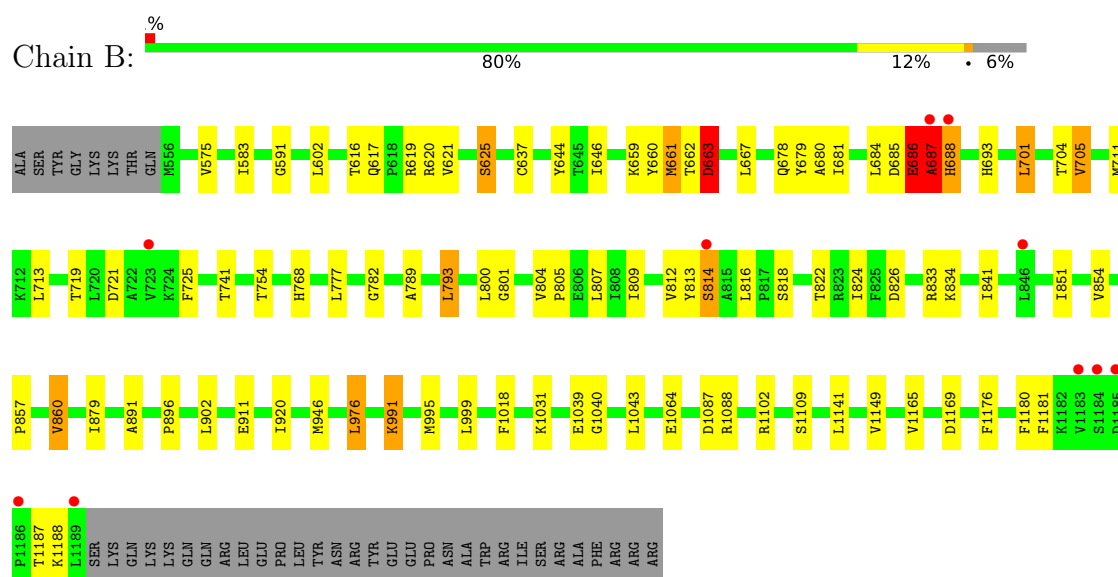
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: ATP-dependent RNA helicase DHX8

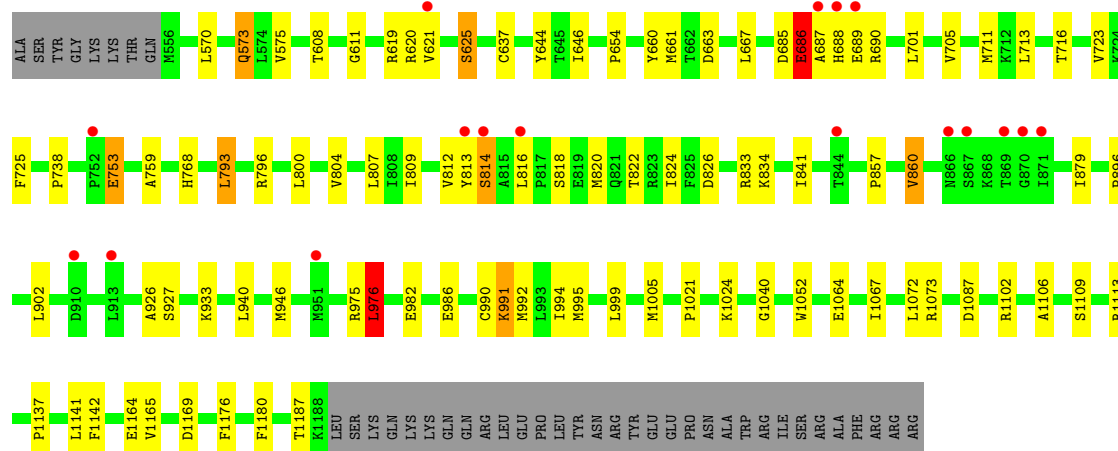


• Molecule 1: ATP-dependent RNA helicase DHX8



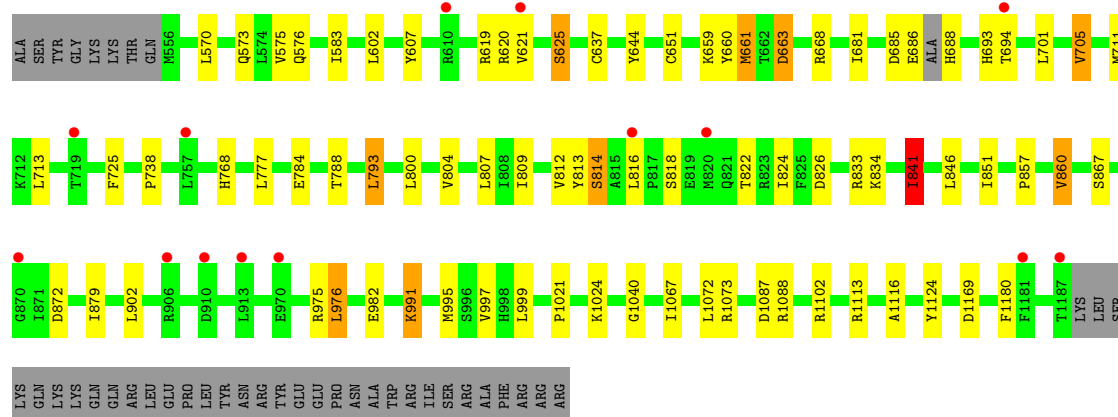
• Molecule 1: ATP-dependent RNA helicase DHX8

Chain C: 



• Molecule 1: ATP-dependent RNA helicase DHX8

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.95Å 167.58Å 137.23Å 90.00° 92.68° 90.00°	Depositor
Resolution (Å)	33.80 – 2.33 33.80 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.80-2.33) 99.4 (33.80-2.33)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.34Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.187 , 0.222 0.196 , 0.229	Depositor DCC
R_{free} test set	6422 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	54.1	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.116 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20220	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, ADP, MG, CL, ACT, DMS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.88	2/5012 (0.0%)	1.34	21/6809 (0.3%)
1	B	0.87	0/4958	1.33	17/6742 (0.3%)
1	C	0.86	2/4878 (0.0%)	1.34	23/6645 (0.3%)
1	D	0.86	0/4906	1.32	21/6676 (0.3%)
All	All	0.87	4/19754 (0.0%)	1.34	82/26872 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	912	MET	SD-CE	-6.23	1.64	1.79
1	C	946	MET	SD-CE	-5.43	1.66	1.79
1	A	820	MET	SD-CE	5.30	1.92	1.79
1	C	986	GLU	CA-C	5.07	1.58	1.53

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1180	PHE	CA-CB-CG	10.98	124.78	113.80
1	A	687	ALA	CA-C-N	8.75	133.95	120.82
1	A	687	ALA	C-N-CA	8.75	133.95	120.82
1	A	1040	GLY	N-CA-C	8.13	122.79	111.25
1	C	1180	PHE	CA-CB-CG	7.75	121.55	113.80
1	C	1040	GLY	N-CA-C	7.55	121.70	110.97
1	C	685	ASP	CA-C-N	7.30	135.49	121.54
1	C	685	ASP	C-N-CA	7.30	135.49	121.54
1	B	1040	GLY	N-CA-C	7.28	121.30	110.97
1	D	1040	GLY	N-CA-C	7.05	120.98	110.97
1	A	685	ASP	CA-C-N	6.94	134.79	121.54
1	A	685	ASP	C-N-CA	6.94	134.79	121.54
1	A	686	GLU	CA-C-N	6.76	134.46	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	686	GLU	C-N-CA	6.76	134.46	121.54
1	A	689	GLU	N-CA-C	-6.65	97.22	108.26
1	B	687	ALA	CA-C-N	6.42	133.80	121.54
1	B	687	ALA	C-N-CA	6.42	133.80	121.54
1	C	689	GLU	N-CA-C	-6.37	98.83	108.96
1	B	680	ALA	N-CA-C	-6.12	104.16	111.69
1	D	841	ILE	N-CA-CB	6.04	118.75	110.54
1	B	663	ASP	CA-CB-CG	5.99	118.59	112.60
1	D	685	ASP	CA-C-N	5.98	132.47	121.70
1	D	685	ASP	C-N-CA	5.98	132.47	121.70
1	C	686	GLU	CA-C-N	5.82	132.69	122.79
1	C	686	GLU	C-N-CA	5.82	132.69	122.79
1	B	1180	PHE	CA-CB-CG	5.79	119.59	113.80
1	C	927	SER	CA-C-N	5.75	127.99	120.28
1	C	927	SER	C-N-CA	5.75	127.99	120.28
1	B	1181	PHE	CA-C-N	5.74	132.51	121.54
1	B	1181	PHE	C-N-CA	5.74	132.51	121.54
1	B	619	ARG	CA-C-N	5.70	128.23	120.54
1	B	619	ARG	C-N-CA	5.70	128.23	120.54
1	C	663	ASP	CA-CB-CG	5.65	118.25	112.60
1	D	688	HIS	CA-C-N	5.65	129.12	121.05
1	D	688	HIS	C-N-CA	5.65	129.12	121.05
1	B	1169	ASP	N-CA-C	-5.59	100.55	109.04
1	D	841	ILE	CB-CA-C	-5.50	104.71	112.14
1	A	680	ALA	N-CA-C	-5.47	104.85	112.45
1	D	1169	ASP	N-CA-C	-5.46	101.70	109.62
1	A	688	HIS	CA-C-N	5.45	130.46	122.39
1	A	688	HIS	C-N-CA	5.45	130.46	122.39
1	A	1183	VAL	N-CA-C	5.42	114.17	106.53
1	C	976	LEU	CA-C-N	5.38	126.06	120.03
1	C	976	LEU	C-N-CA	5.38	126.06	120.03
1	A	975	ARG	CA-C-N	5.35	127.40	120.44
1	A	975	ARG	C-N-CA	5.35	127.40	120.44
1	D	663	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	841	ILE	N-CA-CB	5.33	117.80	110.54
1	A	1169	ASP	N-CA-C	-5.32	100.95	109.04
1	A	663	ASP	CA-CB-CG	5.31	117.91	112.60
1	C	1052	TRP	CA-C-N	5.29	127.37	120.28
1	C	1052	TRP	C-N-CA	5.29	127.37	120.28
1	B	782	GLY	CA-C-N	5.28	127.67	120.54
1	B	782	GLY	C-N-CA	5.28	127.67	120.54
1	B	841	ILE	N-CA-CB	5.23	117.65	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	753	GLU	CB-CG-CD	5.22	121.47	112.60
1	C	975	ARG	CA-C-N	5.20	127.20	120.44
1	C	975	ARG	C-N-CA	5.20	127.20	120.44
1	A	619	ARG	CA-C-N	5.18	127.53	120.54
1	A	619	ARG	C-N-CA	5.18	127.53	120.54
1	A	1052	TRP	CA-C-N	5.17	127.16	120.44
1	A	1052	TRP	C-N-CA	5.17	127.16	120.44
1	D	872	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	926	ALA	CA-C-N	5.14	127.12	120.44
1	C	926	ALA	C-N-CA	5.14	127.12	120.44
1	B	721	ASP	CA-CB-CG	5.13	117.73	112.60
1	D	725	PHE	CA-CB-CG	5.13	118.93	113.80
1	B	704	THR	CA-C-N	5.11	129.00	120.62
1	B	704	THR	C-N-CA	5.11	129.00	120.62
1	C	619	ARG	CA-C-N	5.10	127.07	120.44
1	C	619	ARG	C-N-CA	5.10	127.07	120.44
1	D	975	ARG	CA-C-N	5.07	127.34	120.65
1	D	975	ARG	C-N-CA	5.07	127.34	120.65
1	D	784	GLU	CA-C-N	5.07	127.02	120.44
1	D	784	GLU	C-N-CA	5.07	127.02	120.44
1	D	997	VAL	N-CA-C	-5.06	105.78	110.53
1	D	694	THR	CA-C-N	5.05	127.30	120.38
1	D	694	THR	C-N-CA	5.05	127.30	120.38
1	C	1169	ASP	N-CA-C	-5.04	102.31	109.62
1	C	841	ILE	N-CA-CB	5.03	117.39	110.54
1	D	663	ASP	CA-C-N	5.01	125.54	119.98
1	D	663	ASP	C-N-CA	5.01	125.54	119.98

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	4914	0	4805	52	0
1	B	4858	0	4686	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4779	0	4534	38	0
1	D	4808	0	4567	31	0
2	A	27	0	12	0	0
2	B	27	0	12	1	0
2	C	27	0	12	0	0
2	D	46	0	24	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	12	0	18	1	0
4	B	12	0	18	4	0
4	C	8	0	12	1	0
4	D	8	0	12	0	0
5	A	12	0	18	0	0
5	B	28	0	42	0	0
5	C	16	0	24	1	0
5	D	16	0	24	2	0
6	A	4	0	3	0	0
6	B	4	0	3	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	196	0	0	0	0
8	B	161	0	0	0	0
8	C	121	0	0	0	0
8	D	128	0	0	0	0
All	All	20220	0	18826	167	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 4.

All (167) 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:A:1185:ASP:HB3	1:A:1186:PRO:HD2	1.44	0.97
1:B:687:ALA:HB1	1:B:725:PHE:HZ	1.35	0.91
1:A:583:ILE:HD11	1:A:705:VAL:HG11	1.66	0.77
1:B:687:ALA:HB1	1:B:725:PHE:CZ	2.19	0.77
1:D:583:ILE:HD11	1:D:705:VAL:HG11	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1141:LEU:HD12	1:B:1165:VAL:HG12	1.72	0.71
1:B:860:VAL:HG22	1:B:879:ILE:HG22	1.72	0.70
1:C:753:GLU:HG2	1:C:759:ALA:HB2	1.73	0.69
1:A:687:ALA:HB3	1:A:725:PHE:HZ	1.56	0.69
1:A:1141:LEU:HD12	1:A:1165:VAL:HG12	1.77	0.67
1:C:686:GLU:HB3	1:C:688:HIS:HD2	1.60	0.66
1:C:686:GLU:HA	1:C:716:THR:O	1.98	0.63
1:C:686:GLU:HB3	1:C:688:HIS:CD2	2.34	0.62
1:D:621:VAL:O	1:D:625:SER:HB2	2.00	0.62
1:A:663:ASP:HB3	1:A:693:HIS:HB3	1.82	0.61
1:C:800:LEU:HB3	1:C:804:VAL:HG21	1.83	0.60
1:A:659:LYS:HE2	1:A:661:MET:HE3	1.83	0.60
1:A:621:VAL:O	1:A:625:SER:HB2	2.00	0.60
1:A:1185:ASP:CB	1:A:1186:PRO:HD2	2.27	0.60
1:D:663:ASP:HB3	1:D:693:HIS:HB3	1.83	0.60
1:C:621:VAL:O	1:C:625:SER:HB2	2.02	0.59
1:A:800:LEU:HB3	1:A:804:VAL:HG21	1.84	0.59
1:B:621:VAL:O	1:B:625:SER:HB2	2.02	0.59
1:B:583:ILE:HD11	1:B:705:VAL:HG11	1.85	0.58
1:C:620:ARG:HG3	1:C:646:ILE:HD13	1.85	0.58
1:B:687:ALA:CB	1:B:725:PHE:CZ	2.86	0.58
1:D:602:LEU:HD13	1:D:681:ILE:HD13	1.86	0.57
1:C:1067:ILE:HG21	1:C:1072:LEU:HD11	1.85	0.57
1:D:860:VAL:HG22	1:D:879:ILE:HG22	1.87	0.56
1:C:976:LEU:HD11	1:C:991:LYS:HE3	1.86	0.56
1:A:687:ALA:HB1	1:A:690:ARG:HD3	1.87	0.56
1:A:690:ARG:NH1	1:A:946:MET:HE3	2.21	0.56
1:A:686:GLU:HA	1:A:716:THR:O	2.05	0.56
1:C:796:ARG:O	1:C:800:LEU:HD13	2.05	0.55
1:B:659:LYS:HE2	1:B:661:MET:HE3	1.88	0.54
1:A:602:LEU:HD13	1:A:681:ILE:HD13	1.90	0.54
1:B:812:VAL:HG22	1:B:824:ILE:HG21	1.91	0.52
1:A:684:LEU:HD11	1:A:701:LEU:HD13	1.92	0.51
1:A:690:ARG:HH11	1:A:946:MET:HE3	1.75	0.51
1:D:621:VAL:HG23	1:D:814:SER:HA	1.93	0.51
1:A:1149:VAL:HB	1:A:1165:VAL:HG13	1.92	0.51
1:B:621:VAL:HG23	1:B:814:SER:HA	1.93	0.51
1:D:1067:ILE:HG21	1:D:1072:LEU:HD11	1.93	0.51
1:D:768:HIS:ND1	1:D:833:ARG:HD2	2.26	0.50
1:C:621:VAL:HG23	1:C:814:SER:HA	1.93	0.50
1:C:992:MET:HE3	1:C:1005:MET:SD	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:812:VAL:HG22	1:C:824:ILE:HG21	1.92	0.50
1:A:812:VAL:HG22	1:A:824:ILE:HG21	1.93	0.50
1:D:659:LYS:HE2	1:D:661:MET:HE3	1.94	0.50
1:A:621:VAL:HG23	1:A:814:SER:HA	1.93	0.50
1:A:768:HIS:ND1	1:A:833:ARG:HD2	2.27	0.50
1:A:976:LEU:HD11	1:A:991:LYS:HE3	1.93	0.50
1:D:999:LEU:O	1:D:1102:ARG:HD3	2.11	0.49
1:C:860:VAL:HG22	1:C:879:ILE:HG22	1.92	0.49
1:C:687:ALA:HB2	1:C:725:PHE:CZ	2.47	0.49
1:A:1021:PRO:HG2	1:A:1024:LYS:HB2	1.94	0.49
1:D:812:VAL:HG22	1:D:824:ILE:HG21	1.93	0.49
1:D:1021:PRO:HG2	1:D:1024:LYS:HB2	1.94	0.49
1:A:1185:ASP:HB3	1:A:1186:PRO:CD	2.25	0.49
5:C:1308:DMS:H21	5:D:1305:DMS:H12	1.94	0.49
1:B:768:HIS:ND1	1:B:833:ARG:HD2	2.28	0.49
1:B:896:PRO:HD3	4:B:1304:EDO:H12	1.94	0.48
1:B:685:ASP:O	1:B:686:GLU:HB2	2.13	0.48
1:C:1021:PRO:HG2	1:C:1024:LYS:HB2	1.95	0.48
1:C:1164:GLU:OE1	4:C:1304:EDO:H22	2.14	0.48
1:C:620:ARG:HD3	1:C:814:SER:O	2.14	0.48
1:C:999:LEU:O	1:C:1102:ARG:HD3	2.13	0.48
1:A:1087:ASP:HB3	1:B:1087:ASP:HB3	1.96	0.48
1:C:768:HIS:ND1	1:C:833:ARG:HD2	2.27	0.48
1:A:884:ALA:HB2	1:A:912:MET:HE1	1.94	0.48
1:A:687:ALA:HB3	1:A:725:PHE:CZ	2.42	0.48
1:D:644:TYR:HA	1:D:660:TYR:O	2.13	0.48
1:A:813:TYR:O	1:A:816:LEU:HB2	2.14	0.47
1:D:620:ARG:HD3	1:D:814:SER:O	2.14	0.47
1:A:644:TYR:HA	1:A:660:TYR:O	2.14	0.47
1:B:813:TYR:O	1:B:816:LEU:HB2	2.14	0.47
1:A:999:LEU:O	1:A:1102:ARG:HD3	2.15	0.47
1:B:686:GLU:HG2	1:B:688:HIS:CD2	2.50	0.47
1:B:1018:PHE:HE2	4:B:1305:EDO:H12	1.79	0.47
1:D:619:ARG:HG3	1:D:841:ILE:HG23	1.97	0.47
1:A:686:GLU:HB3	1:A:688:HIS:CD2	2.50	0.47
1:A:773:PRO:HG3	4:A:1304:EDO:H21	1.96	0.47
1:A:620:ARG:HD3	1:A:814:SER:O	2.15	0.47
1:A:1057:PHE:HB2	1:B:678:GLN:HE22	1.80	0.47
1:B:620:ARG:HD3	1:B:814:SER:O	2.15	0.47
1:D:813:TYR:O	1:D:816:LEU:HB2	2.15	0.46
1:A:687:ALA:CB	1:A:725:PHE:HZ	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:ILE:HG22	1:B:662:THR:HG23	1.96	0.46
1:B:818:SER:O	1:B:822:THR:HG23	2.16	0.46
1:B:701:LEU:O	1:B:705:VAL:HB	2.16	0.46
1:D:818:SER:O	1:D:822:THR:HG23	2.16	0.46
1:A:860:VAL:HG22	1:A:879:ILE:HG22	1.97	0.46
1:B:860:VAL:HG22	1:B:879:ILE:CG2	2.44	0.46
1:D:651:CYS:HA	5:D:1305:DMS:H11	1.97	0.46
1:B:857:PRO:HA	1:B:902:LEU:HB2	1.97	0.46
1:C:818:SER:O	1:C:822:THR:HG23	2.16	0.45
1:C:644:TYR:HA	1:C:660:TYR:O	2.17	0.45
1:A:622:ALA:HB2	1:A:845:SER:OG	2.17	0.45
1:C:1141:LEU:HD12	1:C:1165:VAL:HG12	1.97	0.45
1:A:875:VAL:HG12	1:A:877:THR:HG23	1.97	0.45
1:A:826:ASP:O	1:A:834:LYS:HE2	2.15	0.45
1:B:684:LEU:HD11	1:B:701:LEU:HD13	1.98	0.45
1:B:999:LEU:O	1:B:1102:ARG:HD3	2.16	0.45
1:C:990:CYS:O	1:C:994:ILE:HD12	2.17	0.45
1:A:857:PRO:HA	1:A:902:LEU:HB2	1.97	0.45
1:B:644:TYR:HA	1:B:660:TYR:O	2.17	0.45
1:B:793:LEU:HD13	1:B:809:ILE:HG12	1.99	0.45
1:D:793:LEU:HD13	1:D:809:ILE:HG12	1.99	0.45
1:C:654:PRO:O	1:D:1073:ARG:NH1	2.50	0.45
1:C:1109:SER:HA	1:C:1176:PHE:HB3	1.99	0.45
1:C:1005:MET:HE3	1:C:1106:ALA:HB3	1.99	0.45
4:B:1303:EDO:H21	1:C:896:PRO:HD3	1.98	0.44
1:D:857:PRO:HA	1:D:902:LEU:HB2	1.99	0.44
1:A:690:ARG:HG2	1:A:947:ASP:OD2	2.18	0.44
1:B:602:LEU:HD13	1:B:681:ILE:HD13	1.97	0.44
1:A:959:GLU:O	1:A:963:THR:HG23	2.17	0.44
1:C:1137:PRO:HA	1:C:1142:PHE:CG	2.53	0.44
1:A:848:ILE:HB	1:A:851:ILE:HD12	2.00	0.44
1:C:857:PRO:HA	1:C:902:LEU:HB2	2.00	0.44
1:D:800:LEU:HB3	1:D:804:VAL:HG21	1.98	0.44
1:B:789:ALA:O	1:B:793:LEU:HB2	2.17	0.44
1:A:818:SER:O	1:A:822:THR:HG23	2.18	0.44
1:A:1015:GLN:H	1:A:1074:ARG:HH22	1.65	0.44
1:B:685:ASP:O	1:B:686:GLU:CB	2.66	0.43
1:D:777:LEU:HB2	1:D:851:ILE:HD13	1.99	0.43
1:B:800:LEU:HB3	1:B:804:VAL:HG11	1.99	0.43
1:D:841:ILE:HD13	1:D:846:LEU:HD12	2.01	0.43
1:A:598:ILE:HB	1:A:683[B]:MET:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1149:VAL:HB	1:B:1165:VAL:HG13	2.00	0.43
1:D:826:ASP:O	1:D:834:LYS:HE2	2.19	0.43
1:A:681:ILE:HG12	1:A:712:LYS:HB2	2.01	0.43
1:B:777:LEU:HB2	1:B:851:ILE:HD13	1.99	0.43
1:A:861:LYS:HE3	1:A:874:LEU:HD13	2.00	0.43
1:B:591:GLY:HA2	2:B:1301:ADP:H5'1	2.01	0.42
1:B:826:ASP:O	1:B:834:LYS:HE2	2.19	0.42
1:B:1031:LYS:HD2	1:B:1064:GLU:O	2.19	0.42
1:D:607:TYR:CG	1:D:681:ILE:HD11	2.54	0.42
1:A:570:LEU:HD11	1:A:738:PRO:HD3	2.02	0.42
1:C:933:LYS:HE2	1:C:940:LEU:HD21	2.00	0.42
1:B:617:GLN:O	1:B:662:THR:HA	2.19	0.42
1:C:826:ASP:O	1:C:834:LYS:HE2	2.19	0.42
1:C:813:TYR:O	1:C:816:LEU:HB2	2.20	0.42
1:B:663:ASP:HB2	1:B:693:HIS:HB3	2.01	0.41
1:C:793:LEU:HD13	1:C:809:ILE:HG12	2.02	0.41
1:C:1087:ASP:HB3	1:D:1087:ASP:HB3	2.01	0.41
1:A:622:ALA:CB	1:A:845:SER:OG	2.68	0.41
1:B:801:GLY:O	1:B:804:VAL:HG22	2.20	0.41
1:D:1116:ALA:HB1	1:D:1124:TYR:HB3	2.02	0.41
1:B:616:THR:O	1:B:685:ASP:HB3	2.20	0.41
1:B:976:LEU:HD11	1:B:991:LYS:HE3	2.02	0.41
1:B:1039:GLU:HB2	1:B:1043:LEU:HD12	2.02	0.41
1:C:608:THR:HA	1:C:611:GLY:O	2.21	0.41
1:B:725:PHE:CE1	1:B:946[B]:MET:HE1	2.56	0.41
1:B:854:VAL:HG23	1:B:891:ALA:HB2	2.02	0.41
1:B:1109:SER:HA	1:B:1176:PHE:HB3	2.02	0.41
1:B:621:VAL:CG2	1:B:814:SER:HA	2.51	0.41
1:B:805:PRO:HB2	4:B:1303:EDO:H11	2.02	0.41
1:A:990:CYS:O	1:A:994:ILE:HD12	2.20	0.41
1:C:570:LEU:HD22	1:C:573:GLN:HG3	2.02	0.41
1:D:570:LEU:HD11	1:D:738:PRO:HD3	2.02	0.41
1:D:621:VAL:CG2	1:D:814:SER:HA	2.50	0.41
1:D:976:LEU:HD11	1:D:991:LYS:HE3	2.02	0.41
1:A:989:LEU:HD23	1:A:992:MET:HE2	2.03	0.40
1:A:1039[B]:GLU:HB2	1:A:1043:LEU:HD12	2.03	0.40
1:C:570:LEU:HD11	1:C:738:PRO:HD3	2.03	0.40
1:A:854:VAL:HG23	1:A:891:ALA:HB2	2.03	0.40
1:B:661:MET:HE1	1:B:679:TYR:OH	2.21	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 X-ray entries followed by that with respect to entries of similar resolution.

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	634/673 (94%)	612 (96%)	20 (3%)	2 (0%)	36	41
1	B	635/673 (94%)	611 (96%)	21 (3%)	3 (0%)	24	26
1	C	632/673 (94%)	614 (97%)	17 (3%)	1 (0%)	43	50
1	D	629/673 (94%)	612 (97%)	17 (3%)	0	100	100
All	All	2530/2692 (94%)	2449 (97%)	75 (3%)	6 (0%)	43	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	687	ALA
1	A	1185	ASP
1	B	686	GLU
1	A	1182	LYS
1	B	1188	LYS
1	C	686	GLU

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	505/596 (85%)	475 (94%)	30 (6%)	18	21
1	B	479/596 (80%)	453 (95%)	26 (5%)	20	24
1	C	469/596 (79%)	443 (94%)	26 (6%)	19	23
1	D	475/596 (80%)	450 (95%)	25 (5%)	20	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1928/2384 (81%)	1821 (94%)	107 (6%)	19	23

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	559	LEU
1	A	573	GLN
1	A	575	VAL
1	A	625	SER
1	A	637	CYS
1	A	661	MET
1	A	667	LEU
1	A	671	LEU
1	A	686	GLU
1	A	688	HIS
1	A	694	THR
1	A	701	LEU
1	A	705	VAL
1	A	711	MET
1	A	713	LEU
1	A	723	VAL
1	A	807	LEU
1	A	814	SER
1	A	832	SER
1	A	860	VAL
1	A	886	GLN
1	A	976	LEU
1	A	982	GLU
1	A	991	LYS
1	A	995	MET
1	A	1027	LEU
1	A	1092	ASP
1	A	1113	ARG
1	A	1127	LEU
1	A	1185	ASP
1	B	575	VAL
1	B	625	SER
1	B	637	CYS
1	B	661	MET
1	B	663	ASP
1	B	667	LEU
1	B	686	GLU

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Mol	Chain	Res	Type
1	B	688	HIS
1	B	701	LEU
1	B	705	VAL
1	B	711	MET
1	B	713	LEU
1	B	719	THR
1	B	741	THR
1	B	754	THR
1	B	793	LEU
1	B	807	LEU
1	B	814	SER
1	B	860	VAL
1	B	911	GLU
1	B	920	ILE
1	B	976	LEU
1	B	991	LYS
1	B	995	MET
1	B	1088	ARG
1	B	1187	THR
1	C	573	GLN
1	C	575	VAL
1	C	625	SER
1	C	637	CYS
1	C	661	MET
1	C	667	LEU
1	C	686	GLU
1	C	690	ARG
1	C	701	LEU
1	C	705	VAL
1	C	711	MET
1	C	713	LEU
1	C	723	VAL
1	C	793	LEU
1	C	807	LEU
1	C	814	SER
1	C	820	MET
1	C	860	VAL
1	C	976	LEU
1	C	982	GLU
1	C	991	LYS
1	C	995	MET
1	C	1064	GLU

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Mol	Chain	Res	Type
1	C	1073	ARG
1	C	1113	ARG
1	C	1187	THR
1	D	573	GLN
1	D	575	VAL
1	D	576	GLN
1	D	625	SER
1	D	637	CYS
1	D	661	MET
1	D	668	ARG
1	D	686	GLU
1	D	701	LEU
1	D	705	VAL
1	D	711	MET
1	D	713	LEU
1	D	788	THR
1	D	793	LEU
1	D	807	LEU
1	D	814	SER
1	D	841	ILE
1	D	860	VAL
1	D	867	SER
1	D	976	LEU
1	D	982	GLU
1	D	991	LYS
1	D	995	MET
1	D	1088	ARG
1	D	1113	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	561	GLN
1	A	600	GLN
1	A	886	GLN
1	A	1089	HIS
1	B	561	GLN
1	B	600	GLN
1	B	678	GLN
1	B	709	GLN
1	B	886	GLN
1	B	916	ASN

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Mol	Chain	Res	Type
1	B	1152	HIS
1	C	600	GLN
1	C	688	HIS
1	C	706	GLN
1	C	862	GLN
1	C	916	ASN
1	C	1089	HIS
1	C	1152	HIS
1	D	576	GLN
1	D	600	GLN
1	D	862	GLN
1	D	886	GLN
1	D	916	ASN
1	D	1015	GLN
1	D	1089	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 8 are monoatomic - leaving 35 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	B	1301	3	28,29,29	0.77	1 (3%)	43,45,45	0.62	0
5	DMS	B	1312	-	3,3,3	0.30	0	3,3,3	0.18	0
5	DMS	A	1306	-	3,3,3	0.27	0	3,3,3	0.35	0
5	DMS	B	1311	-	3,3,3	0.25	0	3,3,3	0.15	0
5	DMS	D	1306	-	3,3,3	0.31	0	3,3,3	0.26	0
5	DMS	C	1308	-	3,3,3	0.43	0	3,3,3	0.56	0
5	DMS	A	1307	-	3,3,3	0.27	0	3,3,3	0.11	0
5	DMS	A	1308	-	3,3,3	0.33	0	3,3,3	0.30	0
4	EDO	D	1303	-	3,3,3	0.43	0	2,2,2	0.70	0
5	DMS	D	1307	-	3,3,3	0.29	0	3,3,3	0.07	0
2	ADP	D	1301[A]	-	28,29,29	0.35	0	43,45,45	0.71	2 (4%)
5	DMS	C	1306	-	3,3,3	0.49	0	3,3,3	0.33	0
4	EDO	B	1305	-	3,3,3	0.53	0	2,2,2	0.45	0
5	DMS	B	1310	-	3,3,3	0.31	0	3,3,3	0.33	0
4	EDO	A	1304	-	3,3,3	0.42	0	2,2,2	0.49	0
4	EDO	C	1303	-	3,3,3	0.69	0	2,2,2	0.26	0
4	EDO	C	1304	-	3,3,3	0.53	0	2,2,2	0.23	0
5	DMS	D	1305	-	3,3,3	0.39	0	3,3,3	0.31	0
5	DMS	B	1307	-	3,3,3	0.24	0	3,3,3	0.23	0
6	ACT	A	1309	-	3,3,3	1.32	0	3,3,3	0.88	0
2	ADP	C	1301	3	28,29,29	0.52	0	43,45,45	0.86	3 (6%)
2	ADP	A	1301	3	28,29,29	0.67	1 (3%)	43,45,45	0.70	0
5	DMS	C	1307	-	3,3,3	0.33	0	3,3,3	0.29	0
4	EDO	A	1303	-	3,3,3	0.38	0	2,2,2	0.33	0
5	DMS	B	1306	-	3,3,3	0.25	0	3,3,3	0.31	0
4	EDO	D	1304	-	3,3,3	0.48	0	2,2,2	0.41	0
6	ACT	B	1313	-	3,3,3	1.20	0	3,3,3	1.08	0
2	ADP	D	1301[B]	-	28,29,29	0.36	0	43,45,45	0.71	1 (2%)
5	DMS	B	1308	-	3,3,3	0.30	0	3,3,3	0.21	0
5	DMS	B	1309	-	3,3,3	0.31	0	3,3,3	0.23	0
5	DMS	C	1305	-	3,3,3	0.32	0	3,3,3	0.36	0
4	EDO	B	1304	-	3,3,3	0.41	0	2,2,2	0.56	0
4	EDO	B	1303	-	3,3,3	0.75	0	2,2,2	0.53	0
5	DMS	D	1308	-	3,3,3	0.34	0	3,3,3	0.65	0
4	EDO	A	1305	-	3,3,3	0.38	0	2,2,2	0.59	0

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
4	EDO	A	1304	-	-	0/1/1/1	-
4	EDO	C	1303	-	-	0/1/1/1	-
2	ADP	B	1301	3	-	3/16/32/32	0/3/3/3
4	EDO	B	1303	-	-	1/1/1/1	-
4	EDO	C	1304	-	-	1/1/1/1	-
4	EDO	D	1303	-	-	0/1/1/1	-
2	ADP	D	1301[A]	-	-	0/16/32/32	0/3/3/3
2	ADP	C	1301	3	-	3/16/32/32	0/3/3/3
2	ADP	A	1301	3	-	0/16/32/32	0/3/3/3
4	EDO	A	1303	-	-	0/1/1/1	-
4	EDO	B	1304	-	-	0/1/1/1	-
4	EDO	D	1304	-	-	0/1/1/1	-
4	EDO	B	1305	-	-	0/1/1/1	-
2	ADP	D	1301[B]	-	-	5/16/32/32	0/3/3/3
4	EDO	A	1305	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1301	ADP	PB-O3B	-3.32	1.42	1.54
2	A	1301	ADP	PB-O3B	-3.20	1.42	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1301	ADP	C4'-O4'-C1'	-2.35	104.28	109.47
2	D	1301[A]	ADP	O2A-PA-O5'	2.14	117.28	107.57
2	C	1301	ADP	O2A-PA-O5'	2.10	117.08	107.57
2	D	1301[A]	ADP	O3B-PB-O2B	2.09	115.65	107.80
2	D	1301[B]	ADP	O3B-PB-O2B	2.09	115.65	107.80
2	C	1301	ADP	O4'-C1'-N9	2.01	111.95	108.09

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1301	ADP	C5'-O5'-PA-O2A
2	D	1301[B]	ADP	C5'-O5'-PA-O1A
2	D	1301[B]	ADP	C5'-O5'-PA-O2A
2	D	1301[B]	ADP	C5'-O5'-PA-O3A
2	B	1301	ADP	C3'-C4'-C5'-O5'

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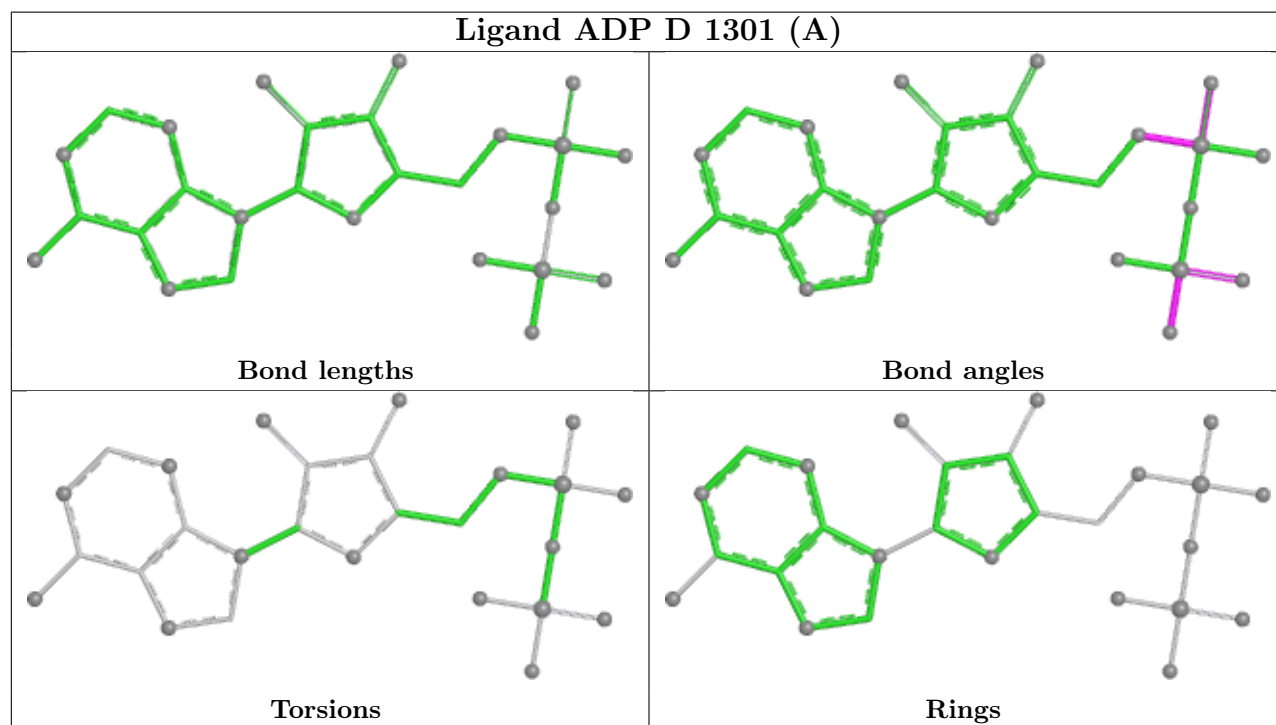
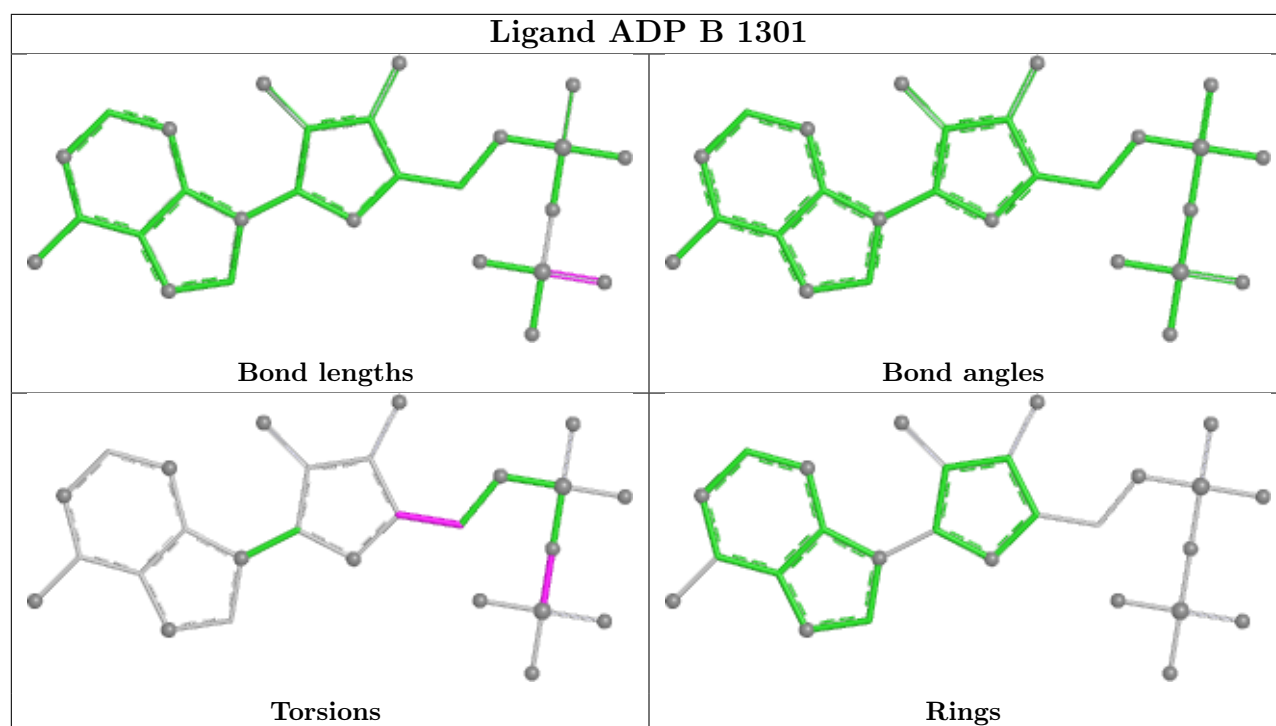
Mol	Chain	Res	Type	Atoms
2	B	1301	ADP	O4'-C4'-C5'-O5'
2	D	1301[B]	ADP	O4'-C4'-C5'-O5'
2	B	1301	ADP	PA-O3A-PB-O1B
2	C	1301	ADP	C5'-O5'-PA-O1A
2	C	1301	ADP	C5'-O5'-PA-O3A
4	C	1304	EDO	O1-C1-C2-O2
2	D	1301[B]	ADP	C3'-C4'-C5'-O5'
4	B	1303	EDO	O1-C1-C2-O2

There are no ring outliers.

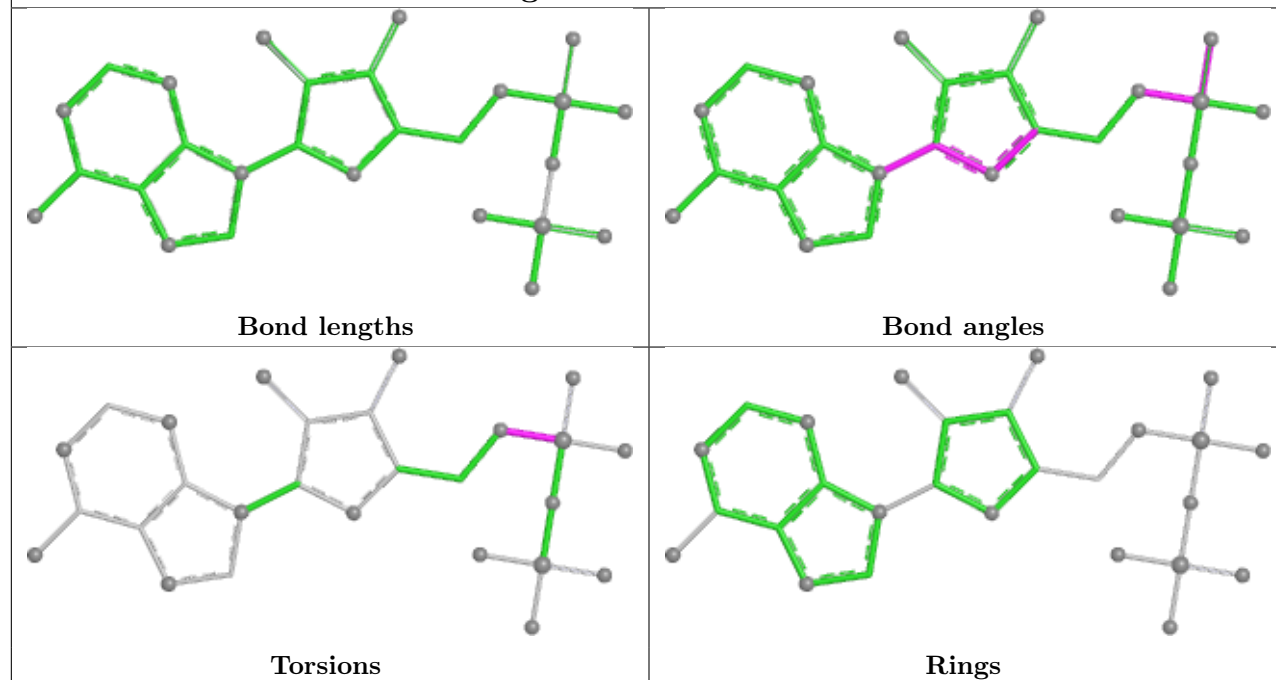
8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1301	ADP	1	0
5	C	1308	DMS	1	0
4	B	1305	EDO	1	0
4	A	1304	EDO	1	0
4	C	1304	EDO	1	0
5	D	1305	DMS	2	0
4	B	1304	EDO	1	0
4	B	1303	EDO	2	0

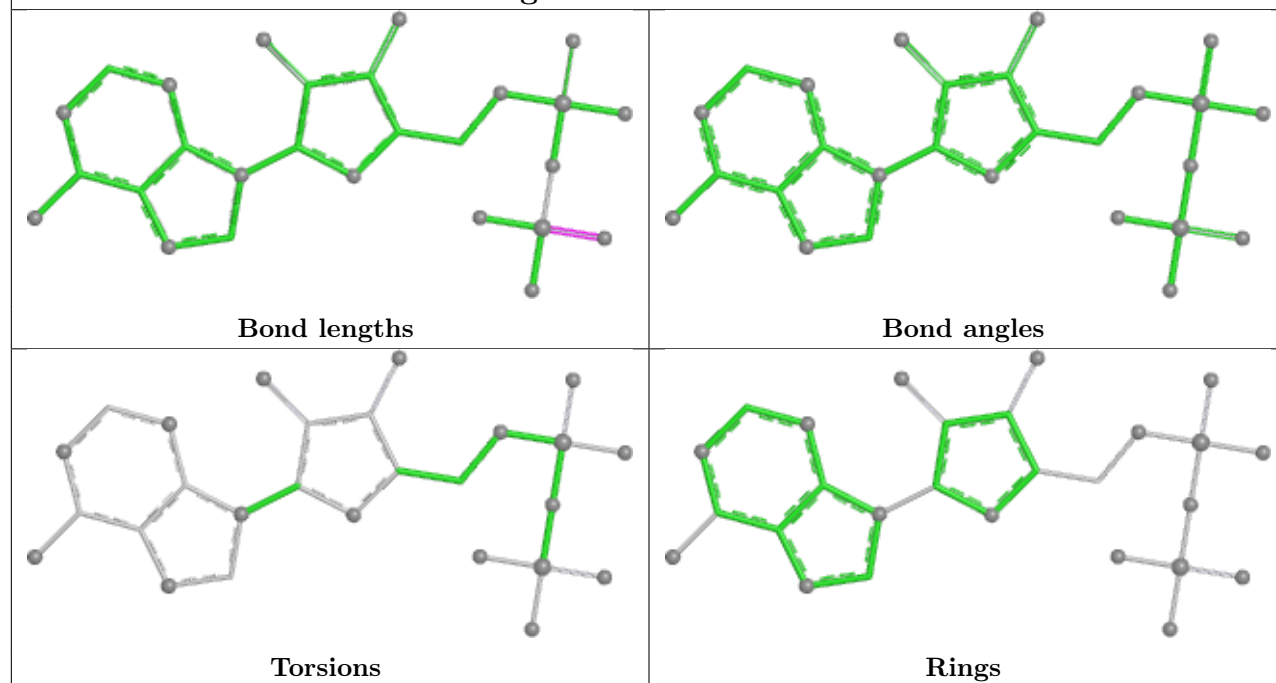
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

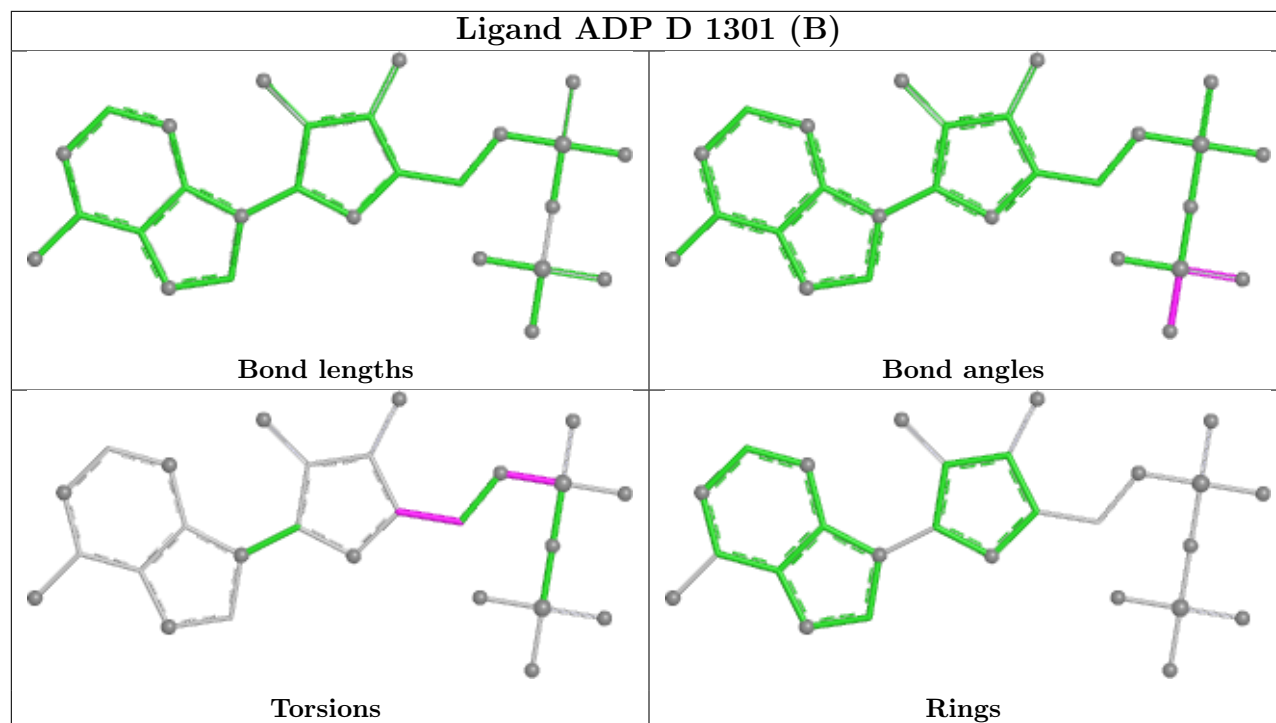


Ligand ADP C 1301



Ligand ADP A 1301





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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	632/673 (93%)	0.06	8 (1%) 75 79	23, 59, 89, 110	4 (0%)
1	B	634/673 (94%)	0.16	10 (1%) 70 75	28, 64, 93, 128	3 (0%)
1	C	633/673 (94%)	0.25	17 (2%) 56 62	42, 68, 99, 121	1 (0%)
1	D	631/673 (93%)	0.19	14 (2%) 62 67	34, 66, 94, 120	2 (0%)
All	All	2530/2692 (93%)	0.16	49 (1%) 66 71	23, 64, 94, 128	10 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1183	VAL	5.0
1	B	1184	SER	3.7
1	A	1186	PRO	3.5
1	D	1187	THR	3.3
1	C	621	VAL	3.3
1	B	1186	PRO	3.2
1	C	844	THR	3.2
1	B	687	ALA	3.1
1	B	1189	LEU	3.1
1	C	869	THR	3.0
1	A	1183	VAL	3.0
1	C	688	HIS	2.9
1	C	871	ILE	2.8
1	A	867	SER	2.8
1	C	870	GLY	2.8
1	C	813	TYR	2.8
1	C	867	SER	2.8
1	C	866	ASN	2.7
1	C	687	ALA	2.6
1	B	688	HIS	2.6
1	C	913	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	906	ARG	2.5
1	D	1181	PHE	2.5
1	A	556	MET	2.5
1	A	1184	SER	2.4
1	B	1185	ASP	2.4
1	D	910	ASP	2.4
1	D	820[A]	MET	2.4
1	B	723	VAL	2.3
1	C	910	ASP	2.3
1	C	814	SER	2.3
1	A	1181	PHE	2.2
1	D	870	GLY	2.2
1	B	846	LEU	2.2
1	D	816	LEU	2.2
1	D	719	THR	2.2
1	D	610	ARG	2.1
1	C	816	LEU	2.1
1	D	913	LEU	2.1
1	D	970	GLU	2.1
1	D	694	THR	2.1
1	C	951	MET	2.1
1	C	752	PRO	2.1
1	A	689	GLU	2.1
1	B	814	SER	2.0
1	A	820	MET	2.0
1	C	689	GLU	2.0
1	D	757	LEU	2.0
1	D	621	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

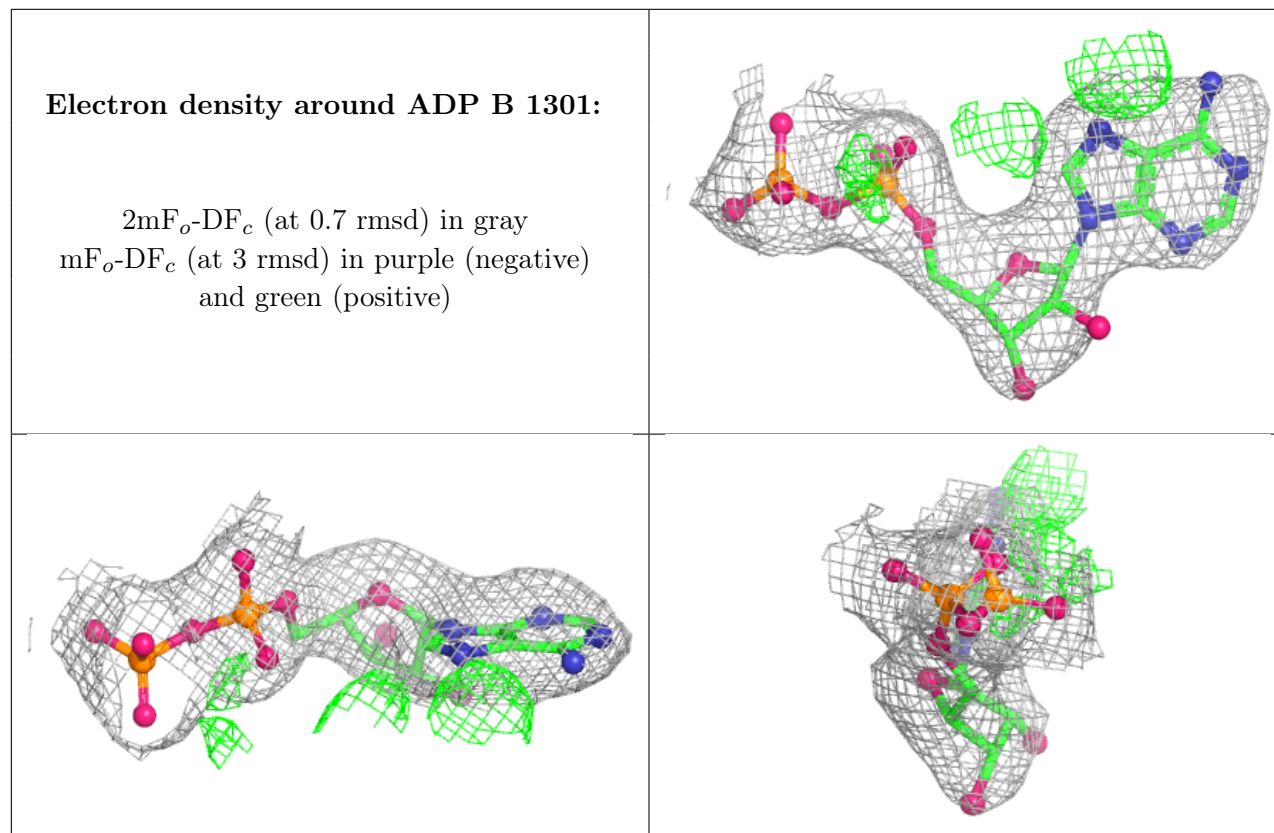
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	ACT	A	1309	4/4	0.69	0.23	76,77,77,77	0
5	DMS	D	1306	4/4	0.72	0.26	124,125,125,126	0
5	DMS	B	1312	4/4	0.73	0.24	104,105,105,106	0
5	DMS	B	1309	4/4	0.74	0.26	136,137,137,138	0
5	DMS	B	1308	4/4	0.76	0.19	101,101,101,102	0
4	EDO	B	1303	4/4	0.76	0.20	63,64,65,66	0
5	DMS	B	1310	4/4	0.76	0.25	131,132,132,132	0
5	DMS	A	1308	4/4	0.78	0.21	108,109,110,110	0
5	DMS	C	1305	4/4	0.78	0.21	116,116,116,116	0
5	DMS	C	1308	4/4	0.80	0.26	109,110,111,111	0
5	DMS	C	1306	4/4	0.81	0.16	93,94,95,96	0
5	DMS	A	1306	4/4	0.82	0.18	97,99,99,100	0
5	DMS	C	1307	4/4	0.83	0.22	99,100,100,100	0
5	DMS	A	1307	4/4	0.83	0.19	116,116,117,118	0
5	DMS	B	1306	4/4	0.83	0.22	111,112,113,113	0
5	DMS	B	1307	4/4	0.83	0.27	113,113,114,114	0
4	EDO	A	1305	4/4	0.84	0.19	78,78,79,80	0
5	DMS	D	1307	4/4	0.85	0.15	99,102,102,102	0
4	EDO	D	1304	4/4	0.85	0.23	83,84,86,88	0
7	CL	A	1310	1/1	0.85	0.16	91,91,91,91	0
6	ACT	B	1313	4/4	0.86	0.15	76,77,78,78	0
5	DMS	D	1308	4/4	0.87	0.17	124,125,125,125	0
4	EDO	C	1303	4/4	0.87	0.15	59,63,65,65	0
5	DMS	B	1311	4/4	0.89	0.18	116,117,117,117	0
5	DMS	D	1305	4/4	0.89	0.20	106,107,108,108	0
7	CL	B	1314	1/1	0.89	0.12	107,107,107,107	0
4	EDO	A	1304	4/4	0.90	0.18	78,78,78,79	0
4	EDO	B	1304	4/4	0.91	0.16	74,74,76,78	0
4	EDO	D	1303	4/4	0.92	0.15	69,69,70,71	0
4	EDO	C	1304	4/4	0.92	0.14	72,72,72,74	0
7	CL	C	1309	1/1	0.92	0.13	91,91,91,91	0
4	EDO	B	1305	4/4	0.94	0.12	71,71,72,75	0
7	CL	D	1309	1/1	0.94	0.13	101,101,101,101	0
2	ADP	B	1301	27/27	0.95	0.10	50,66,72,75	27
2	ADP	C	1301	27/27	0.95	0.09	49,62,67,68	27
4	EDO	A	1303	4/4	0.95	0.10	55,58,59,61	0
2	ADP	A	1301	27/27	0.95	0.09	45,54,61,66	27
3	MG	C	1302	1/1	0.96	0.04	72,72,72,72	0
2	ADP	D	1301[B]	27/27	0.97	0.07	57,73,74,76	19
2	ADP	D	1301[A]	27/27	0.97	0.07	53,58,61,62	19
3	MG	A	1302	1/1	0.98	0.04	63,63,63,63	0

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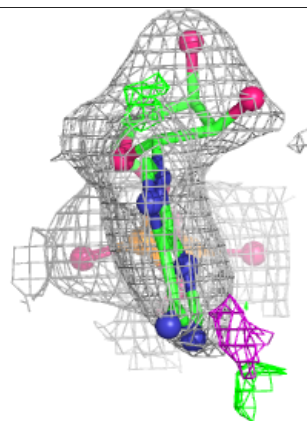
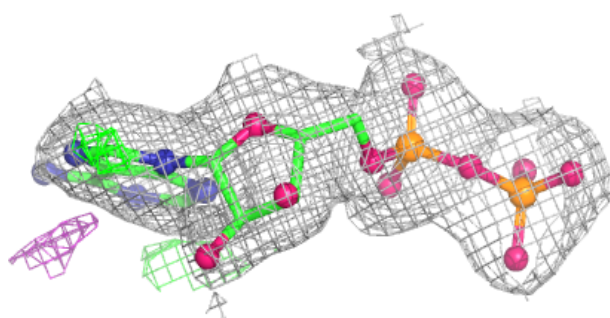
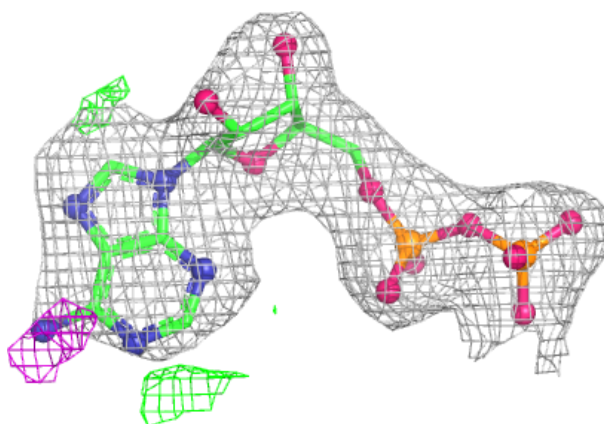
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	D	1302	1/1	0.98	0.04	65,65,65,65	0
3	MG	B	1302	1/1	0.98	0.04	64,64,64,64	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

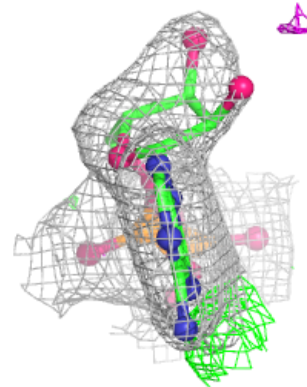
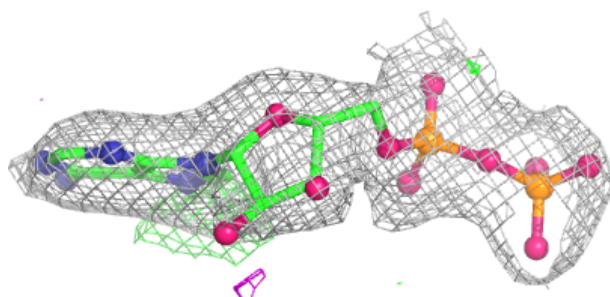
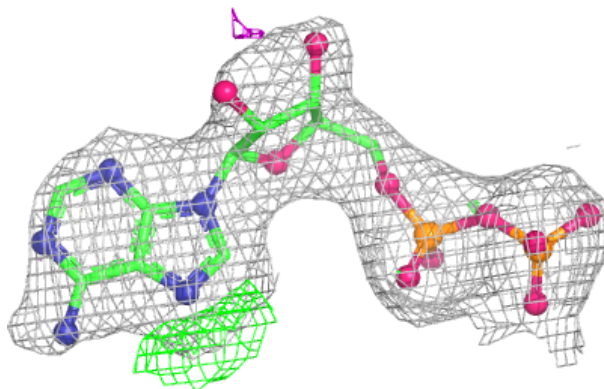


Electron density around ADP C 1301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

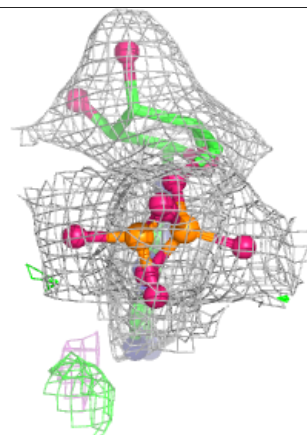
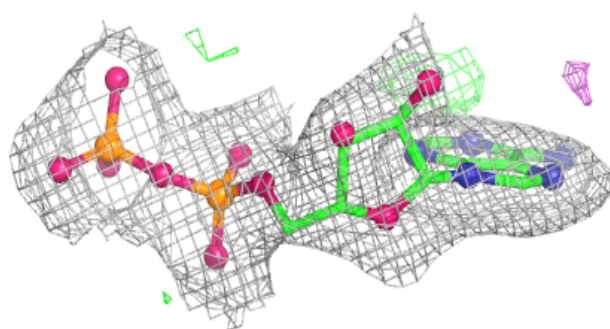
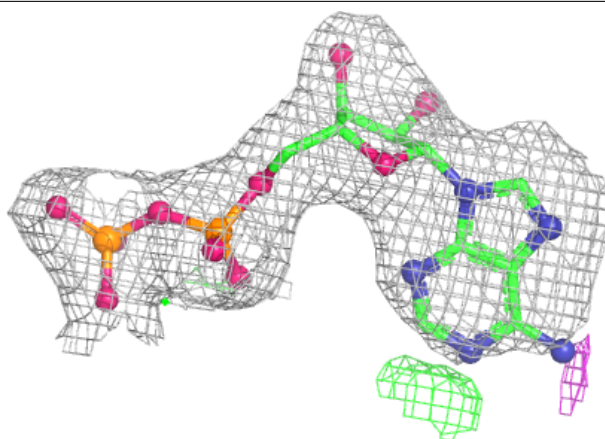
**Electron density around ADP A 1301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

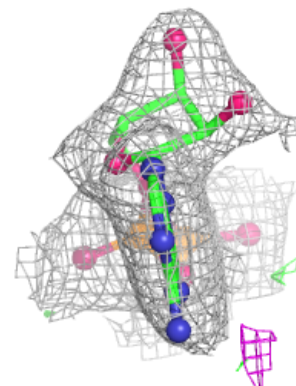
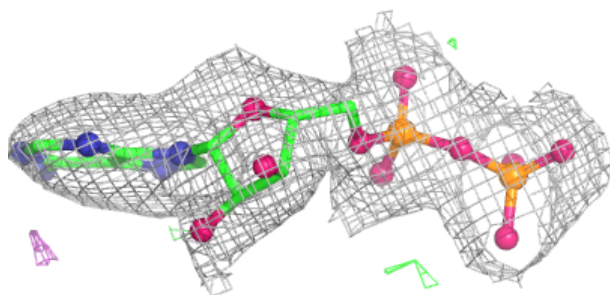
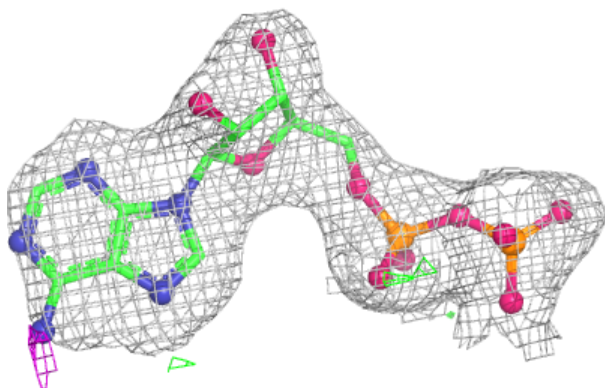


Electron density around ADP D 1301 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP D 1301 (A):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.