Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 05:46 am BST

PDB ID	:	6HYT
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 following versions of software and data (see references ⓘ) were used in the production of this report:

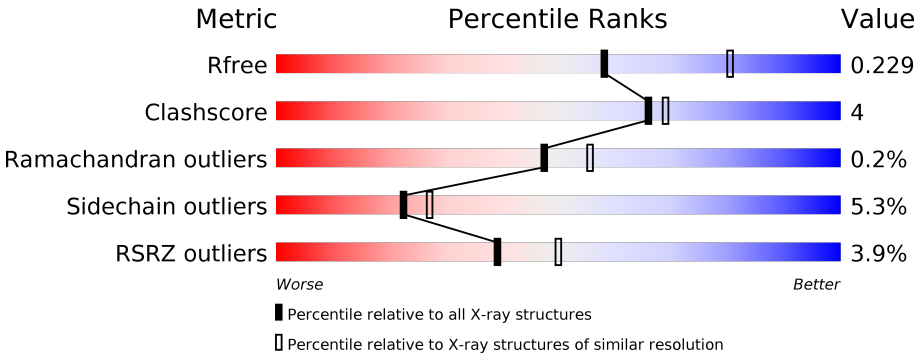
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (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 on 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 <=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	3% 80% 13% • 6%
1	B	673	3% 82% 10% • 6%
1	C	673	5% 83% 10% • 6%
1	D	673	3% 84% 9% • 6%

2 Entry composition

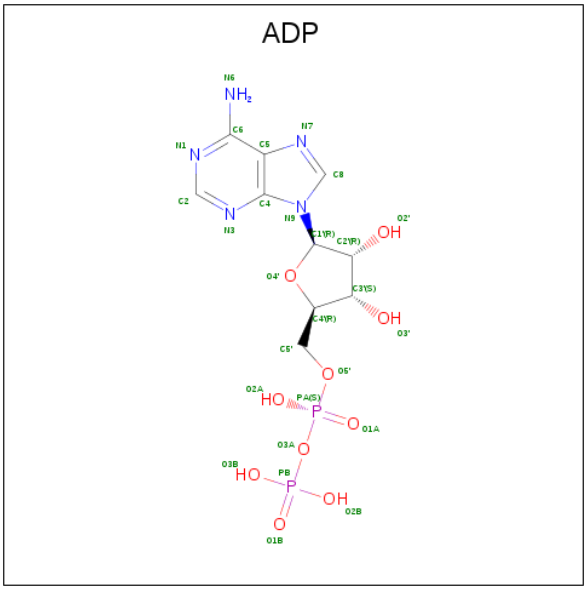
There are 8 unique types of molecules in this entry. The entry contains 20220 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: 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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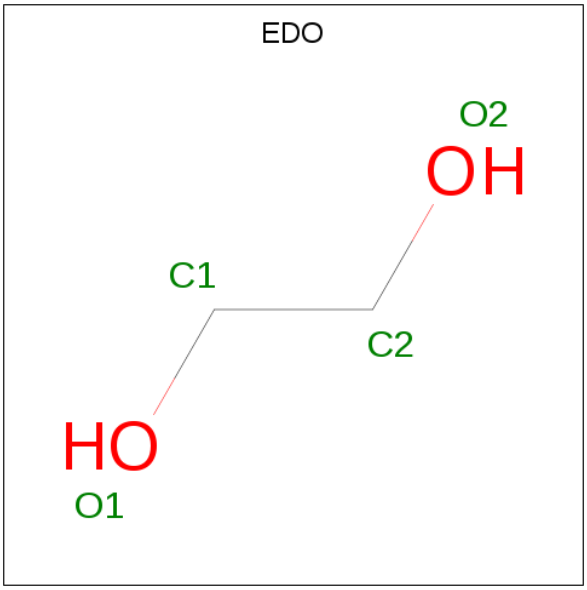
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	1
			46	20	10	14	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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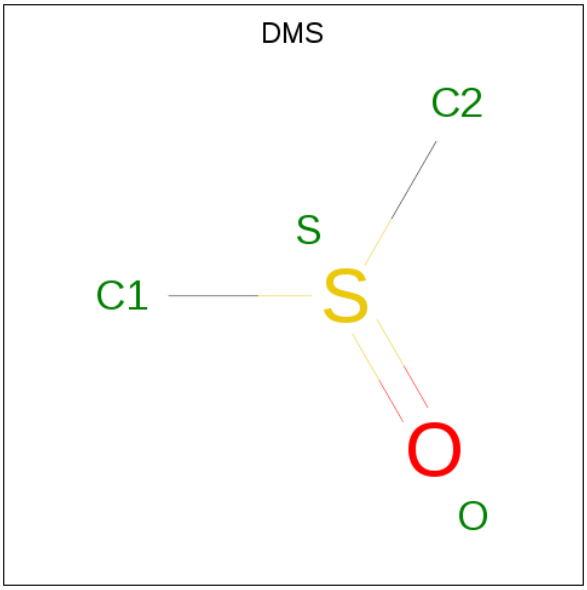
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

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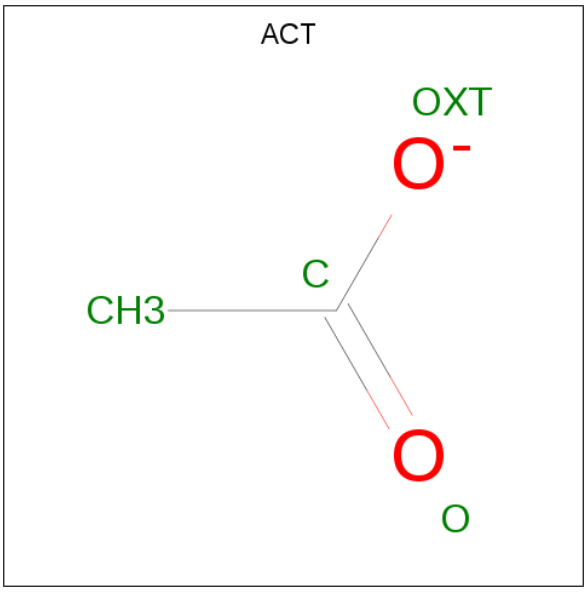
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O S 4 2 1 1	0	0
5	B	1	Total C O S 4 2 1 1	0	0
5	B	1	Total C O S 4 2 1 1	0	0
5	B	1	Total C O S 4 2 1 1	0	0
5	B	1	Total C O S 4 2 1 1	0	0
5	B	1	Total C O S 4 2 1 1	0	0
5	C	1	Total C O S 4 2 1 1	0	0
5	C	1	Total C O S 4 2 1 1	0	0
5	C	1	Total C O S 4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

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is water.

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

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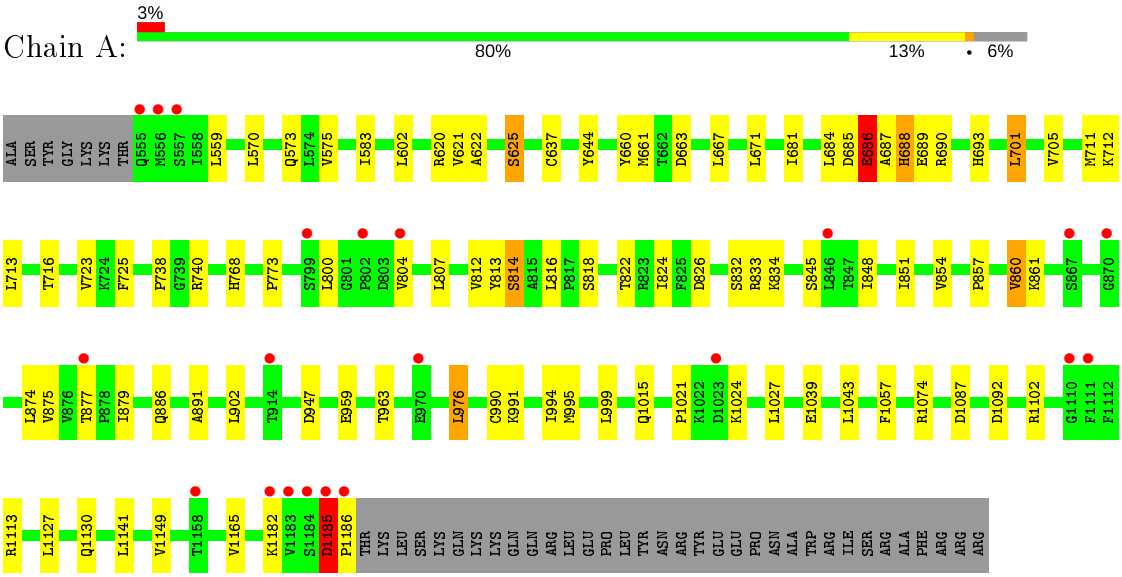
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	128	Total	O	0	0
			128	128		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

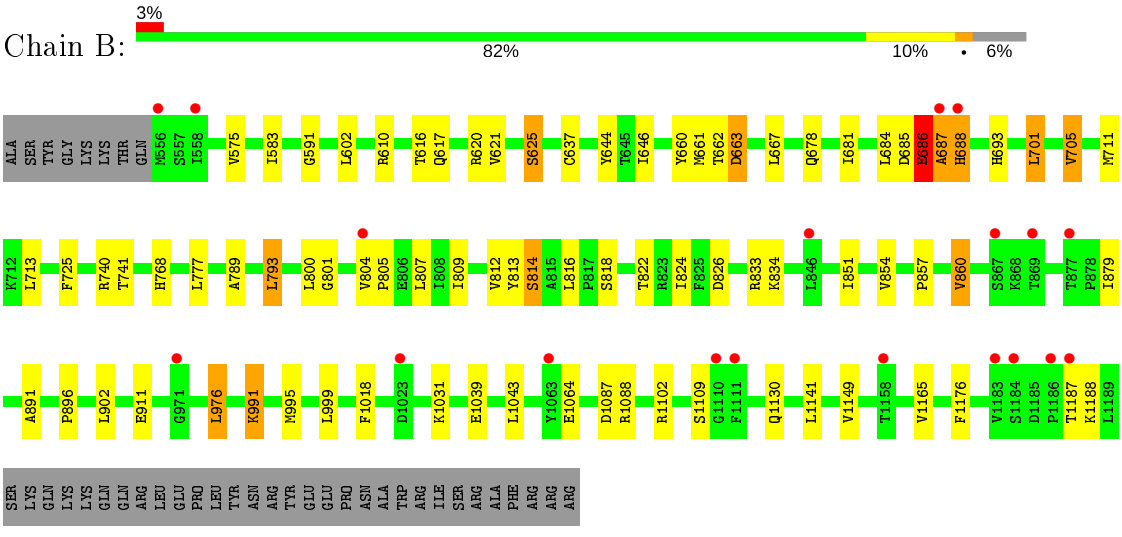
- Molecule 1: ATP-dependent RNA helicase DHX8

Chain A:



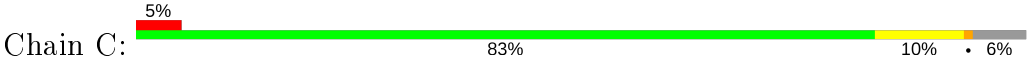
- Molecule 1: ATP-dependent RNA helicase DHX8

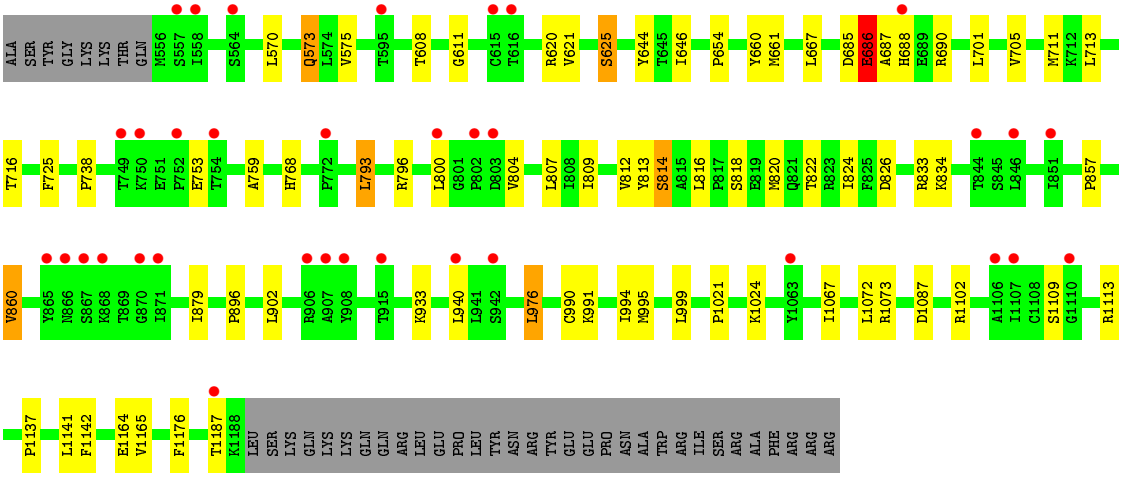
Chain B:



- Molecule 1: ATP-dependent RNA helicase DHX8

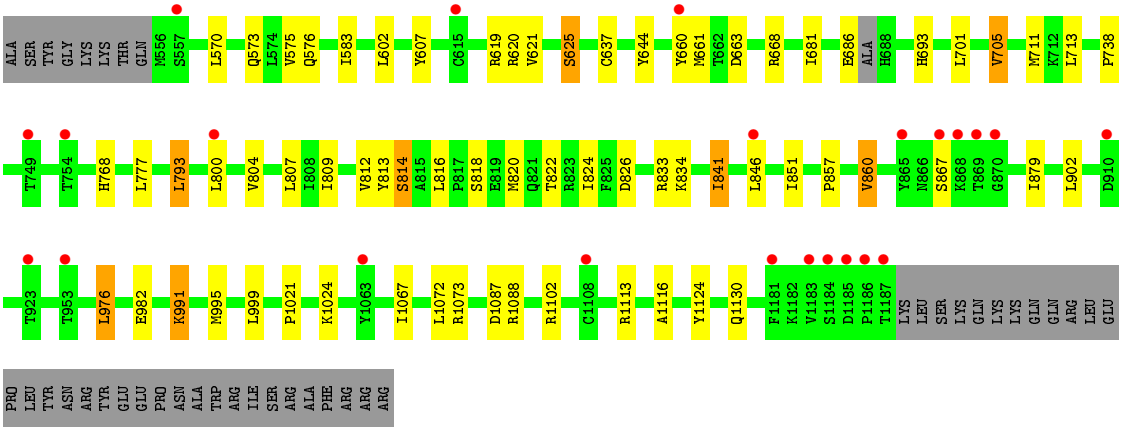
Chain C:





- Molecule 1: ATP-dependent RNA helicase DHX8

Chain D:



4 Data and refinement statistics (i)

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 33.79 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.80-2.33) 99.4 (33.79-2.33)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.31 , 57.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, ADP, CL, EDO, DMS, ACT

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	0.51	0/5012	0.71	3/6809 (0.0%)
1	B	0.50	0/4958	0.70	0/6742
1	C	0.49	0/4878	0.68	1/6645 (0.0%)
1	D	0.50	0/4906	0.68	0/6676
All	All	0.50	0/19754	0.69	4/26872 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	685	ASP	C-N-CA	5.52	135.49	121.70
1	A	685	ASP	C-N-CA	5.24	134.79	121.70
1	A	686	GLU	C-N-CA	5.10	134.46	121.70
1	A	689	GLU	N-CA-C	-5.10	97.22	111.00

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	46	0
1	B	4858	0	4686	46	0
1	C	4779	0	4534	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4808	0	4567	29	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	0	0
5	D	16	0	24	0	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	153	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 (153) 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
1:B:1141:LEU:HD12	1:B:1165:VAL:HG12	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1021:PRO:HG2	1:D:1024:LYS:HB2	1.94	0.49
1:D:812:VAL:HG22	1:D:824:ILE:HG21	1.93	0.49
1:A:1185:ASP:HB3	1:A:1186:PRO:CD	2.25	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:999:LEU:O	1:C:1102:ARG:HD3	2.13	0.48
1:C:620:ARG:HD3	1:C:814:SER:O	2.14	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: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:B:1018:PHE:HE2	4:B:1305:EDO:H12	1.79	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1109:SER:HA	1:C:1176:PHE:HB3	1.99	0.45
1:C:654:PRO:O	1:D:1073:ARG:NH1	2.50	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:1015:GLN:H	1:A:1074:ARG:HH22	1.65	0.44
1:A:818:SER:O	1:A:822:THR:HG23	2.18	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1039:GLU:HB2	1:B:1043:LEU:HD12	2.02	0.41
1:B:976:LEU:HD11	1:B:991:LYS:HE3	2.02	0.41
1:C:608:THR:HA	1:C:611:GLY:O	2.21	0.41
1:B:1109:SER:HA	1:B:1176:PHE:HB3	2.02	0.41
1:B:854:VAL:HG23	1:B:891:ALA:HB2	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: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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	41 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	635/673 (94%)	611 (96%)	21 (3%)	3 (0%)	29 31
1	C	632/673 (94%)	614 (97%)	17 (3%)	1 (0%)	47 55
1	D	629/673 (94%)	612 (97%)	17 (3%)	0	100 100
All	All	2530/2692 (94%)	2449 (97%)	75 (3%)	6 (0%)	47 55

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 (i)

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%)	477 (94%)	28 (6%)	21 25
1	B	479/596 (80%)	453 (95%)	26 (5%)	22 26
1	C	469/596 (79%)	448 (96%)	21 (4%)	27 34
1	D	475/596 (80%)	448 (94%)	27 (6%)	20 24
All	All	1928/2384 (81%)	1826 (95%)	102 (5%)	22 27

All (102) 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

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Mol	Chain	Res	Type
1	A	661	MET
1	A	667	LEU
1	A	671	LEU
1	A	686	GLU
1	A	688	HIS
1	A	701	LEU
1	A	711	MET
1	A	713	LEU
1	A	723	VAL
1	A	740	ARG
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	995	MET
1	A	1027	LEU
1	A	1092	ASP
1	A	1113	ARG
1	A	1127	LEU
1	A	1130	GLN
1	A	1185	ASP
1	B	575	VAL
1	B	610	ARG
1	B	625	SER
1	B	637	CYS
1	B	661	MET
1	B	663	ASP
1	B	667	LEU
1	B	686	GLU
1	B	688	HIS
1	B	701	LEU
1	B	705	VAL
1	B	711	MET
1	B	713	LEU
1	B	740	ARG
1	B	741	THR
1	B	793	LEU
1	B	807	LEU
1	B	814	SER
1	B	860	VAL

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Mol	Chain	Res	Type
1	B	911	GLU
1	B	976	LEU
1	B	991	LYS
1	B	995	MET
1	B	1088	ARG
1	B	1130	GLN
1	B	1187	THR
1	C	573	GLN
1	C	575	VAL
1	C	625	SER
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	793	LEU
1	C	807	LEU
1	C	814	SER
1	C	820	MET
1	C	860	VAL
1	C	976	LEU
1	C	995	MET
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	793	LEU
1	D	807	LEU

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Mol	Chain	Res	Type
1	D	814	SER
1	D	820[A]	MET
1	D	820[B]	MET
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
1	D	1130	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	862	GLN
1	B	678	GLN
1	C	688	HIS
1	D	576	GLN
1	D	1015	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 carbohydrates 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	$\#\|Z\| > 2$
4	EDO	C	1304	-	3,3,3	0.58	0	2,2,2	0.17	0
5	DMS	A	1306	-	3,3,3	0.27	0	3,3,3	0.35	0
5	DMS	B	1307	-	3,3,3	0.24	0	3,3,3	0.23	0
4	EDO	D	1304	-	3,3,3	0.54	0	2,2,2	0.36	0
4	EDO	B	1303	-	3,3,3	0.82	0	2,2,2	0.56	0
4	EDO	C	1303	-	3,3,3	0.78	0	2,2,2	0.22	0
5	DMS	D	1306	-	3,3,3	0.31	0	3,3,3	0.27	0
4	EDO	A	1304	-	3,3,3	0.47	0	2,2,2	0.45	0
5	DMS	D	1305	-	3,3,3	0.38	0	3,3,3	0.31	0
5	DMS	A	1307	-	3,3,3	0.27	0	3,3,3	0.11	0
6	ACT	A	1309	-	1,3,3	6.10	1 (100%)	0,3,3	0.00	-
4	EDO	B	1305	-	3,3,3	0.60	0	2,2,2	0.41	0
4	EDO	A	1305	-	3,3,3	0.43	0	2,2,2	0.56	0
4	EDO	B	1304	-	3,3,3	0.46	0	2,2,2	0.53	0
6	ACT	B	1313	-	1,3,3	5.29	1 (100%)	0,3,3	0.00	-
2	ADP	A	1301	3	24,29,29	0.85	1 (4%)	29,45,45	1.03	1 (3%)
5	DMS	C	1306	-	3,3,3	0.47	0	3,3,3	0.32	0
2	ADP	C	1301	3	24,29,29	0.76	0	29,45,45	1.02	3 (10%)
5	DMS	B	1306	-	3,3,3	0.25	0	3,3,3	0.31	0
5	DMS	C	1308	-	3,3,3	0.41	0	3,3,3	0.56	0
5	DMS	B	1310	-	3,3,3	0.30	0	3,3,3	0.33	0
5	DMS	B	1308	-	3,3,3	0.29	0	3,3,3	0.21	0
5	DMS	B	1311	-	3,3,3	0.24	0	3,3,3	0.15	0
4	EDO	D	1303	-	3,3,3	0.46	0	2,2,2	0.68	0
5	DMS	C	1307	-	3,3,3	0.33	0	3,3,3	0.29	0
5	DMS	B	1312	-	3,3,3	0.30	0	3,3,3	0.19	0
2	ADP	D	1301[B]	-	24,29,29	0.63	0	29,45,45	0.98	2 (6%)
5	DMS	B	1309	-	3,3,3	0.30	0	3,3,3	0.23	0
2	ADP	D	1301[A]	-	24,29,29	0.60	0	29,45,45	1.01	3 (10%)
5	DMS	D	1308	-	3,3,3	0.33	0	3,3,3	0.64	0
5	DMS	A	1308	-	3,3,3	0.33	0	3,3,3	0.30	0
4	EDO	A	1303	-	3,3,3	0.41	0	2,2,2	0.30	0
5	DMS	C	1305	-	3,3,3	0.32	0	3,3,3	0.36	0
2	ADP	B	1301	3	24,29,29	0.93	1 (4%)	29,45,45	0.90	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DMS	D	1307	-	3,3,3	0.29	0	3,3,3	0.06	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	C	1303	-	-	0/1/1/1	-
4	EDO	A	1304	-	-	0/1/1/1	-
2	ADP	C	1301	3	-	3/12/32/32	0/3/3/3
4	EDO	B	1303	-	-	1/1/1/1	-
2	ADP	D	1301[B]	-	-	5/12/32/32	0/3/3/3
4	EDO	B	1305	-	-	0/1/1/1	-
2	ADP	D	1301[A]	-	-	0/12/32/32	0/3/3/3
4	EDO	A	1305	-	-	0/1/1/1	-
4	EDO	B	1304	-	-	0/1/1/1	-
4	EDO	D	1304	-	-	0/1/1/1	-
4	EDO	A	1303	-	-	0/1/1/1	-
2	ADP	A	1301	3	-	1/12/32/32	0/3/3/3
2	ADP	B	1301	3	-	3/12/32/32	0/3/3/3
4	EDO	C	1304	-	-	1/1/1/1	-
4	EDO	D	1303	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1309	ACT	CH3-C	6.10	1.56	1.48
6	B	1313	ACT	CH3-C	5.29	1.55	1.48
2	B	1301	ADP	PB-O3B	-3.21	1.42	1.54
2	A	1301	ADP	PB-O3B	-3.09	1.42	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1301	ADP	C5-C6-N6	2.56	124.24	120.35
2	B	1301	ADP	C5-C6-N6	2.46	124.08	120.35
2	D	1301[A]	ADP	C5-C6-N6	2.26	123.78	120.35
2	D	1301[B]	ADP	C5-C6-N6	2.22	123.73	120.35
2	C	1301	ADP	C5-C6-N6	2.10	123.55	120.35
2	D	1301[B]	ADP	O3B-PB-O2B	2.10	115.65	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1301[A]	ADP	O3B-PB-O2B	2.10	115.65	107.64
2	C	1301	ADP	O4'-C1'-C2'	-2.08	103.89	106.93
2	D	1301[A]	ADP	O2A-PA-O5'	2.05	117.28	107.75
2	C	1301	ADP	O2A-PA-O5'	2.01	117.08	107.75

There are no chirality outliers.

All (14) 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	B	1301	ADP	C3'-C4'-C5'-O5'
2	D	1301[B]	ADP	O4'-C4'-C5'-O5'
2	B	1301	ADP	O4'-C4'-C5'-O5'
2	B	1301	ADP	PA-O3A-PB-O1B
2	A	1301	ADP	C5'-O5'-PA-O3A
2	C	1301	ADP	C5'-O5'-PA-O3A
2	D	1301[B]	ADP	C5'-O5'-PA-O3A
2	C	1301	ADP	C5'-O5'-PA-O1A
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.

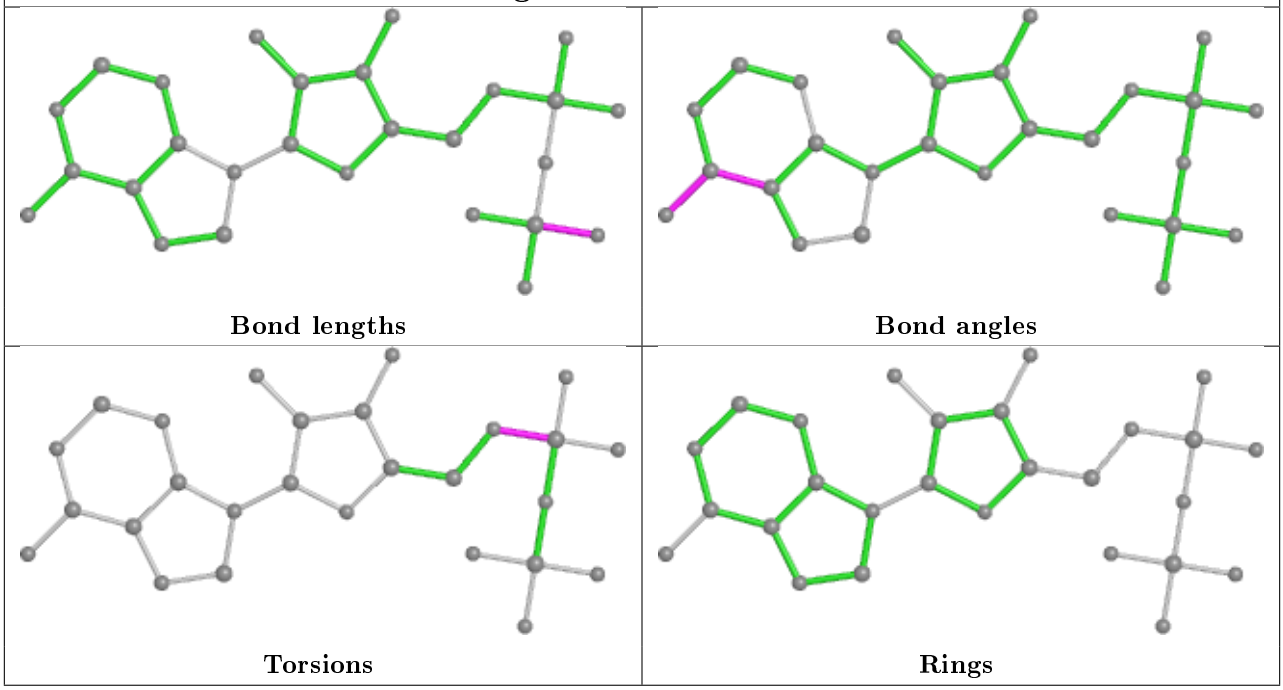
6 monomers are involved in 7 short contacts:

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

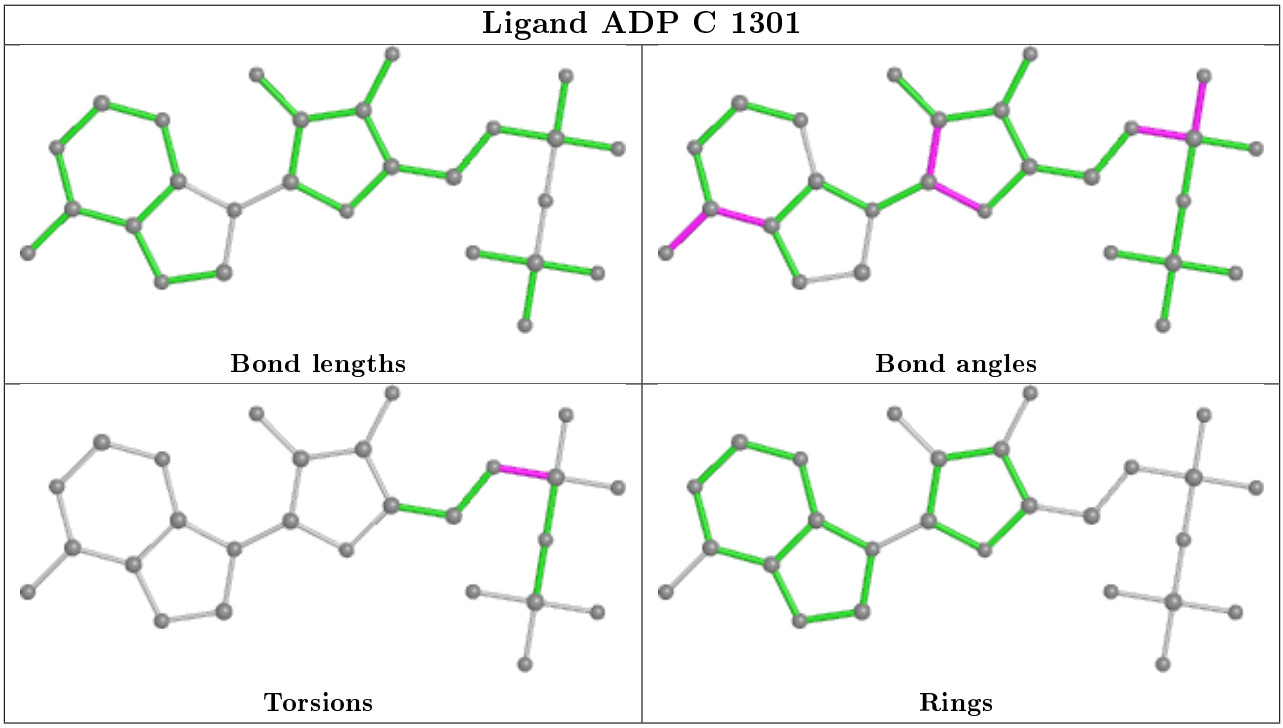
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

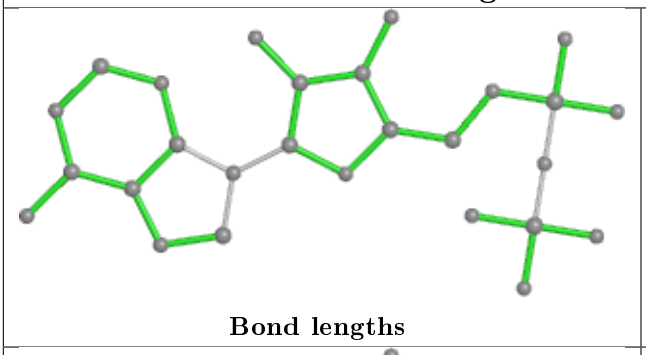
Ligand ADP A 1301



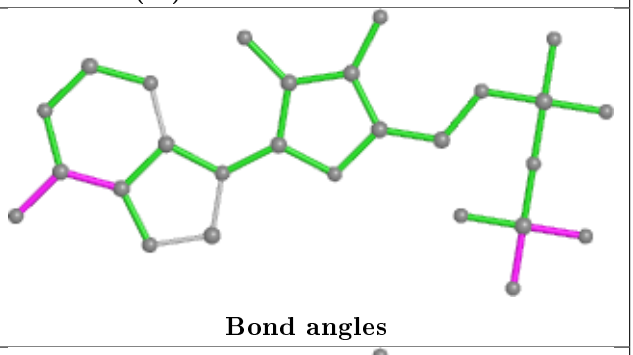
Ligand ADP C 1301



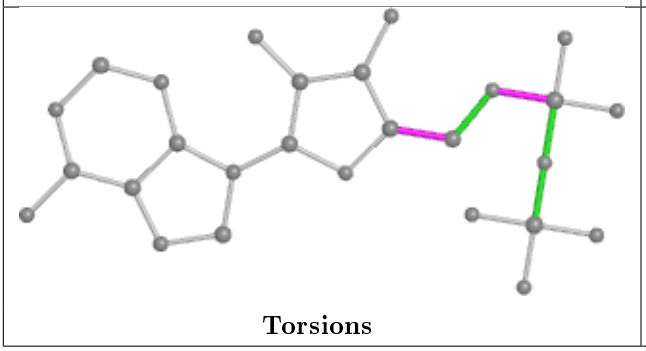
Ligand ADP D 1301 (B)



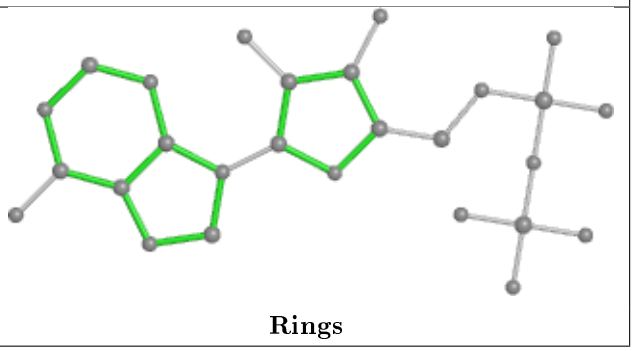
Bond lengths



Bond angles

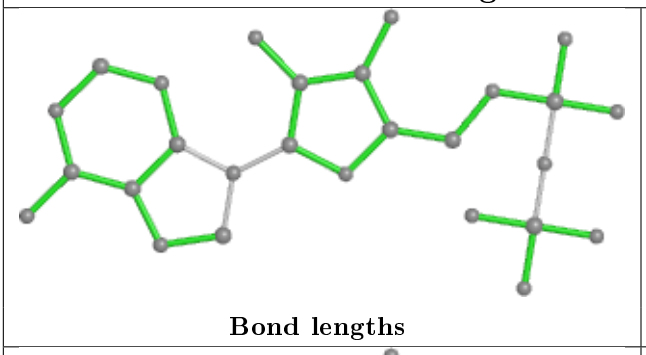


Torsions

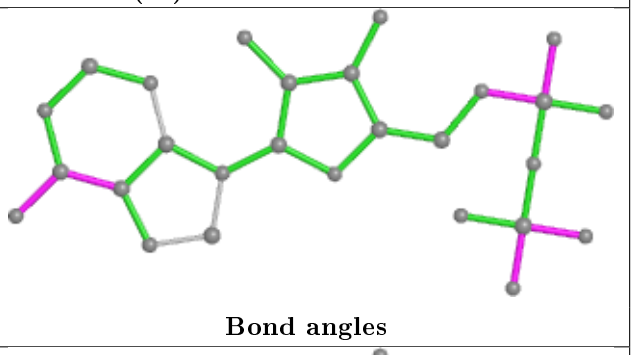


Rings

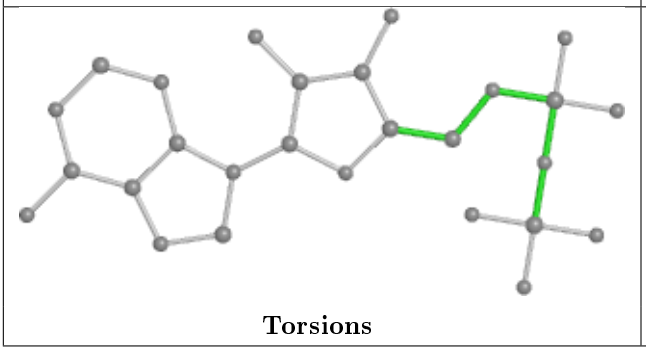
Ligand ADP D 1301 (A)



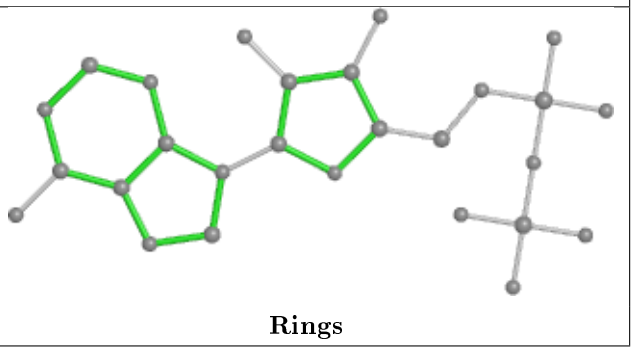
Bond lengths



Bond angles

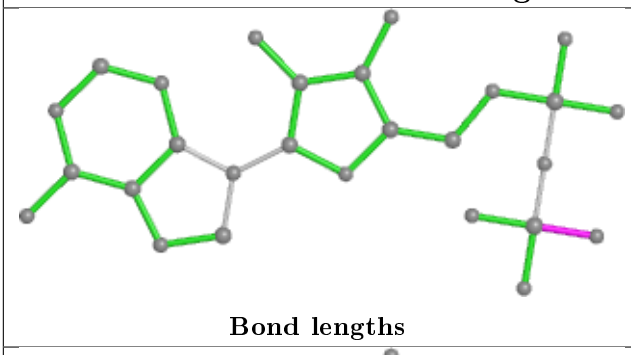


Torsions

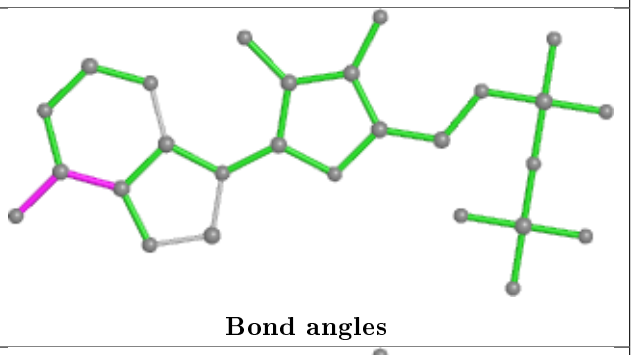


Rings

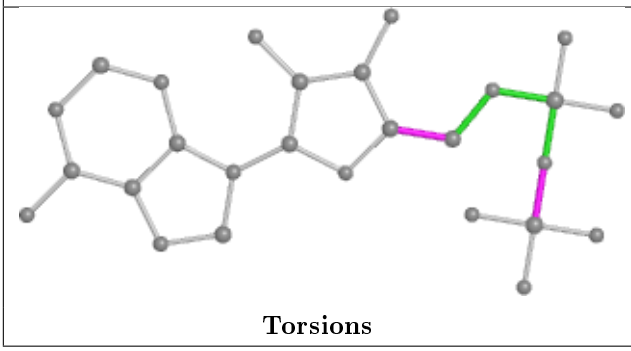
Ligand ADP B 1301



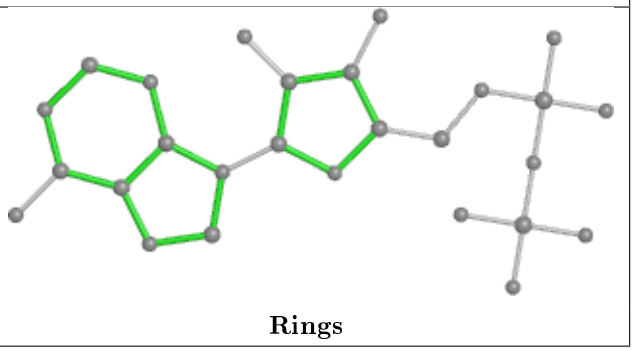
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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%)	0.12	21 (3%)	46	57	39, 59, 89, 110	0
1	B	634/673 (94%)	0.11	19 (2%)	50	60	38, 64, 93, 128	0
1	C	633/673 (94%)	0.24	35 (5%)	25	34	44, 68, 99, 121	0
1	D	631/673 (93%)	0.15	23 (3%)	42	53	45, 66, 94, 120	0
All	All	2530/2692 (93%)	0.15	98 (3%)	39	50	38, 64, 94, 128	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	556	MET	7.5
1	C	870	GLY	6.9
1	C	868	LYS	5.5
1	A	555	GLN	5.3
1	C	867	SER	4.4
1	D	1187	THR	4.3
1	D	1185	ASP	4.0
1	B	869	THR	3.9
1	C	1187	THR	3.9
1	A	1182	LYS	3.8
1	B	1187	THR	3.7
1	D	867	SER	3.6
1	B	556	MET	3.6
1	C	865	TYR	3.6
1	D	1186	PRO	3.6
1	C	802	PRO	3.5
1	C	846	LEU	3.4
1	B	867	SER	3.4
1	A	1186	PRO	3.4
1	C	906	ARG	3.4
1	A	867	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	1183	VAL	3.3
1	A	804	VAL	3.2
1	A	799	SER	3.2
1	C	615	CYS	3.1
1	B	1183	VAL	3.0
1	C	749	THR	3.0
1	C	754	THR	3.0
1	A	1185	ASP	3.0
1	C	688	HIS	3.0
1	A	1110	GLY	2.9
1	D	754	THR	2.8
1	C	907	ALA	2.8
1	B	1023	ASP	2.8
1	A	1184	SER	2.8
1	D	615	CYS	2.8
1	D	1063	TYR	2.8
1	D	870	GLY	2.7
1	B	1186	PRO	2.7
1	D	846	LEU	2.7
1	D	868	LYS	2.6
1	A	802	PRO	2.6
1	C	1107	ILE	2.6
1	A	914	THR	2.6
1	D	865	TYR	2.6
1	B	877	THR	2.6
1	C	942	SER	2.6
1	D	1183	VAL	2.6
1	B	558	ILE	2.6
1	A	870	GLY	2.5
1	C	908	TYR	2.5
1	A	1023	ASP	2.5
1	A	1111	PHE	2.5
1	C	557	SER	2.5
1	B	1184	SER	2.4
1	B	846	LEU	2.4
1	B	804	VAL	2.4
1	C	915	THR	2.4
1	C	851	ILE	2.4
1	C	752	PRO	2.4
1	D	953	THR	2.4
1	A	557	SER	2.4
1	B	1110	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	803	ASP	2.4
1	C	800	LEU	2.4
1	D	923	THR	2.4
1	C	871	ILE	2.3
1	B	971	GLY	2.3
1	B	687	ALA	2.3
1	A	1158	THR	2.3
1	C	1106	ALA	2.3
1	D	869	THR	2.3
1	C	866	ASN	2.3
1	C	940	LEU	2.3
1	C	1063	TYR	2.3
1	D	660	TYR	2.3
1	D	1184	SER	2.3
1	C	844	THR	2.2
1	B	1111	PHE	2.2
1	D	800	LEU	2.2
1	C	558	ILE	2.2
1	C	616	THR	2.1
1	C	772	PRO	2.1
1	C	1110	GLY	2.1
1	B	1063	TYR	2.1
1	A	846	LEU	2.1
1	D	749	THR	2.1
1	B	688	HIS	2.1
1	D	557	SER	2.1
1	B	1158	THR	2.1
1	C	750	LYS	2.1
1	D	1108	CYS	2.1
1	D	1181	PHE	2.1
1	A	877	THR	2.0
1	D	910	ASP	2.0
1	A	970	GLU	2.0
1	C	564	SER	2.0
1	C	595	THR	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 carbohydrates 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, 95^{th} 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
4	EDO	B	1303	4/4	0.69	0.28	63,64,65,66	0
5	DMS	D	1306	4/4	0.74	0.32	124,125,125,126	0
6	ACT	A	1309	4/4	0.74	0.21	76,77,77,77	0
5	DMS	B	1310	4/4	0.74	0.19	131,132,132,132	0
5	DMS	B	1309	4/4	0.79	0.36	136,137,137,138	0
5	DMS	B	1311	4/4	0.81	0.27	116,117,117,117	0
3	MG	C	1302	1/1	0.84	0.15	72,72,72,72	0
7	CL	A	1310	1/1	0.85	0.10	91,91,91,91	0
7	CL	D	1309	1/1	0.87	0.09	101,101,101,101	0
4	EDO	C	1303	4/4	0.87	0.23	59,63,65,65	0
7	CL	B	1314	1/1	0.87	0.14	107,107,107,107	0
5	DMS	A	1306	4/4	0.88	0.27	97,99,99,100	0
5	DMS	C	1308	4/4	0.88	0.28	109,110,111,111	0
7	CL	C	1309	1/1	0.88	0.19	91,91,91,91	0
4	EDO	D	1304	4/4	0.88	0.26	83,84,86,88	0
4	EDO	B	1304	4/4	0.89	0.28	74,74,76,78	0
5	DMS	A	1308	4/4	0.89	0.22	108,109,110,110	0
5	DMS	B	1312	4/4	0.90	0.20	104,105,105,106	0
3	MG	A	1302	1/1	0.90	0.14	63,63,63,63	0
5	DMS	B	1307	4/4	0.91	0.18	113,113,114,114	0
6	ACT	B	1313	4/4	0.91	0.14	76,77,78,78	0
4	EDO	A	1303	4/4	0.91	0.23	55,58,59,61	0
4	EDO	B	1305	4/4	0.92	0.22	71,71,72,75	0
5	DMS	D	1308	4/4	0.92	0.18	124,125,125,125	0
5	DMS	C	1305	4/4	0.92	0.15	116,116,116,116	0
5	DMS	B	1306	4/4	0.93	0.15	111,112,113,113	0
5	DMS	A	1307	4/4	0.93	0.29	116,116,117,118	0
5	DMS	C	1306	4/4	0.93	0.52	93,94,95,96	0
5	DMS	D	1307	4/4	0.93	0.18	99,102,102,102	0
4	EDO	C	1304	4/4	0.94	0.16	72,72,72,74	0
4	EDO	D	1303	4/4	0.94	0.16	69,69,70,71	0
5	DMS	D	1305	4/4	0.94	0.20	106,107,108,108	0

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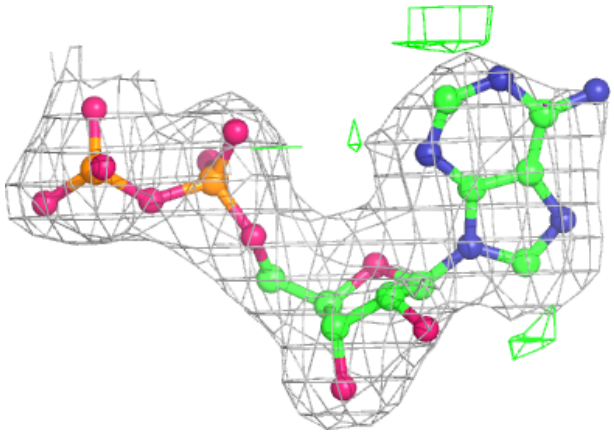
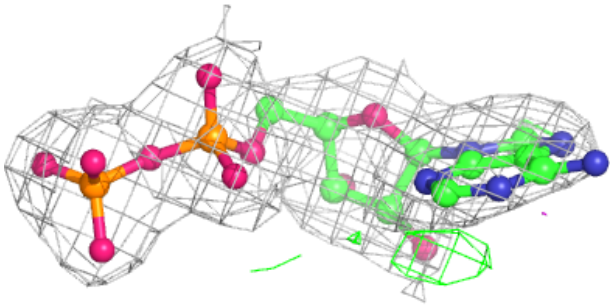
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	1305	4/4	0.94	0.15	78,78,79,80	0
3	MG	B	1302	1/1	0.94	0.12	64,64,64,64	0
5	DMS	C	1307	4/4	0.95	0.14	99,100,100,100	0
4	EDO	A	1304	4/4	0.95	0.26	78,78,78,79	0
2	ADP	C	1301	27/27	0.95	0.21	49,62,67,68	27
5	DMS	B	1308	4/4	0.96	0.35	101,101,101,102	0
2	ADP	A	1301	27/27	0.96	0.20	45,54,61,66	27
2	ADP	D	1301[A]	27/27	0.97	0.14	53,58,61,62	19
2	ADP	D	1301[B]	27/27	0.97	0.14	57,73,74,76	19
2	ADP	B	1301	27/27	0.97	0.20	50,66,72,75	27
3	MG	D	1302	1/1	0.97	0.18	65,65,65,65	0

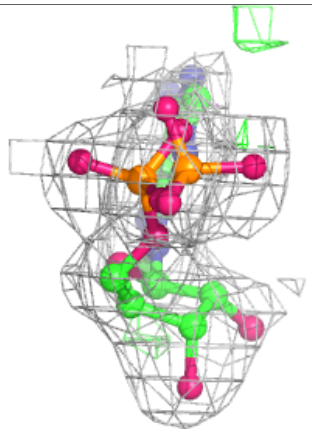
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

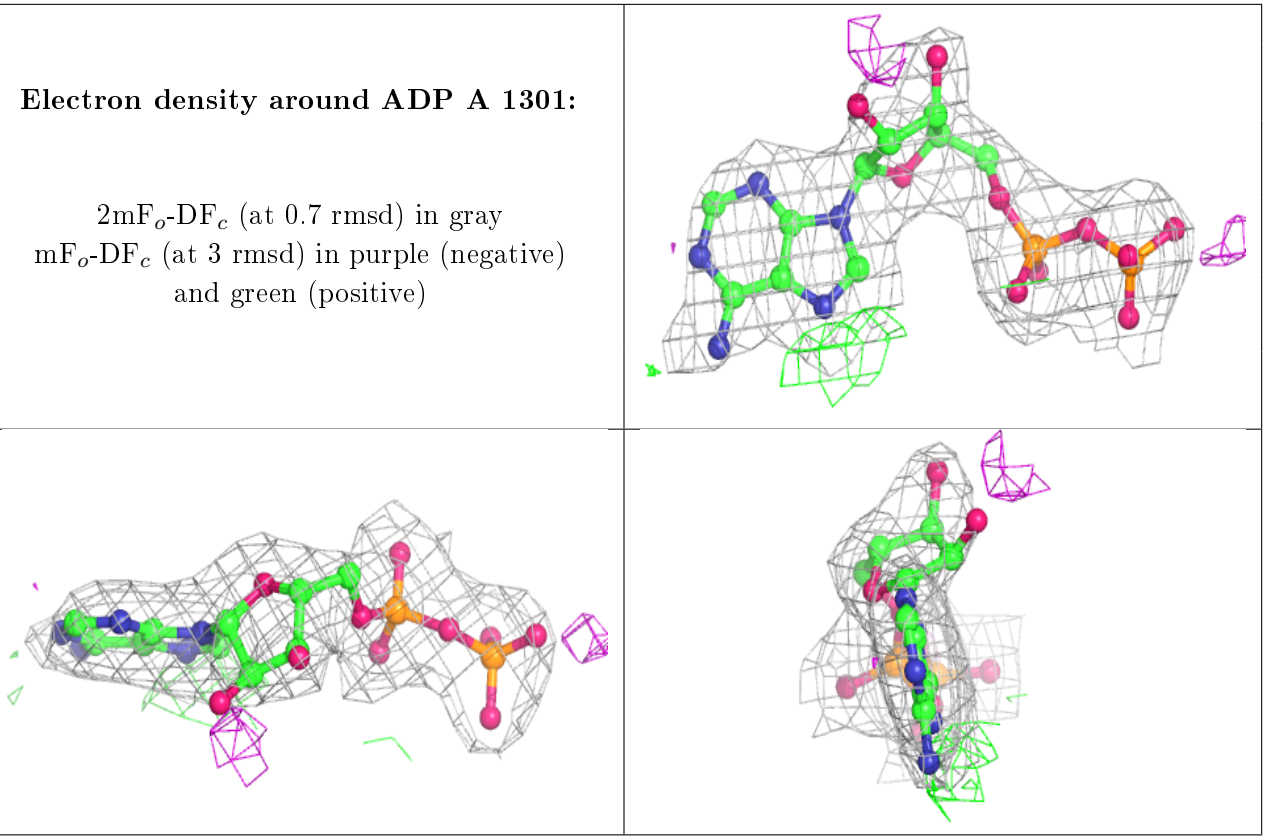






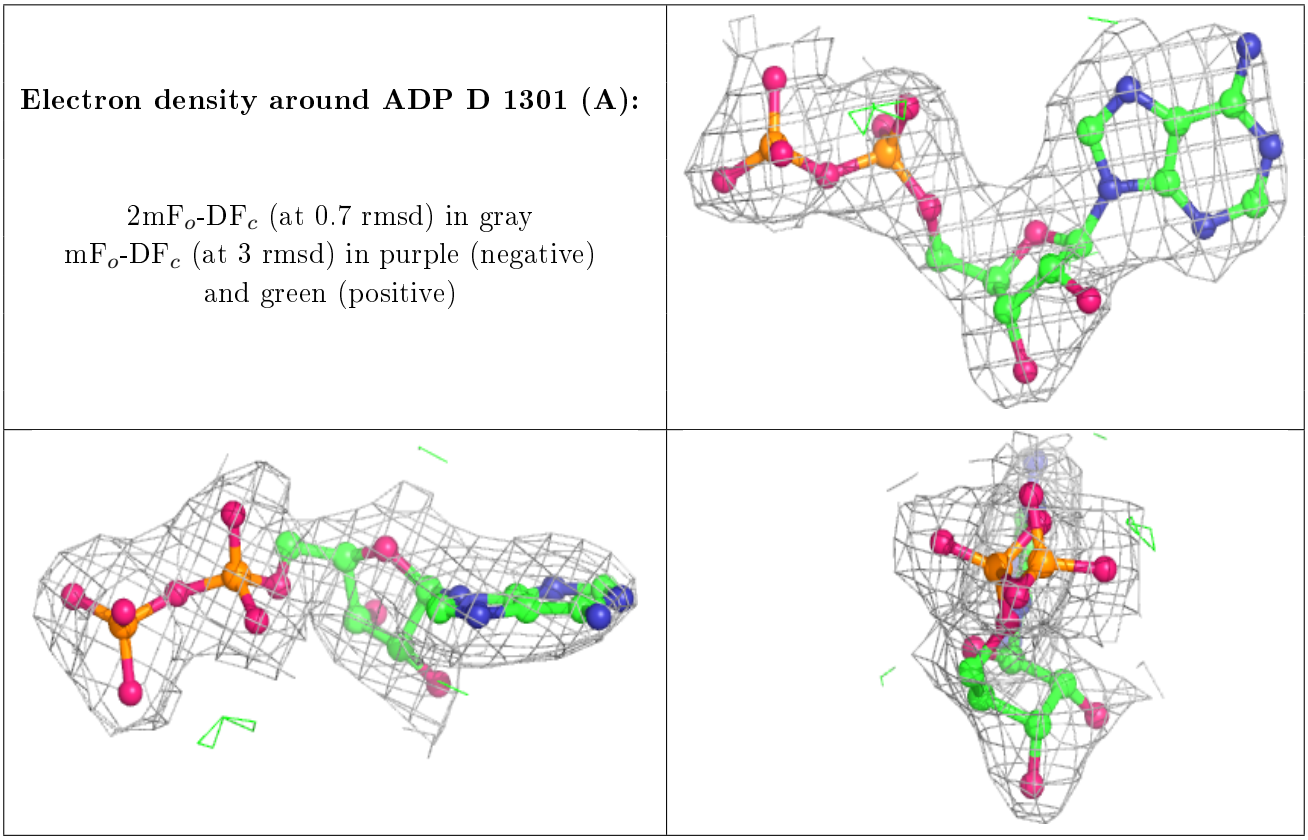
Electron density around ADP A 1301:

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



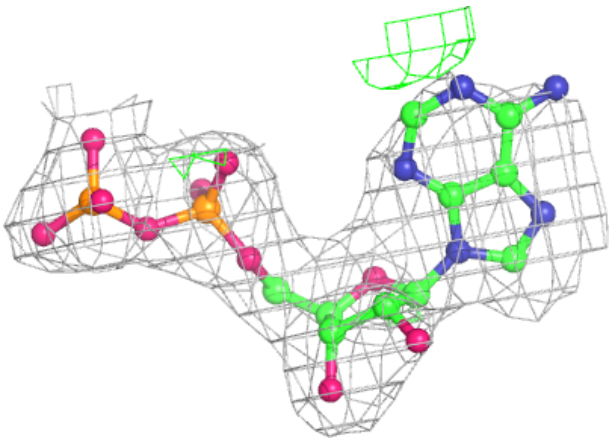
Electron density around ADP D 1301 (A):

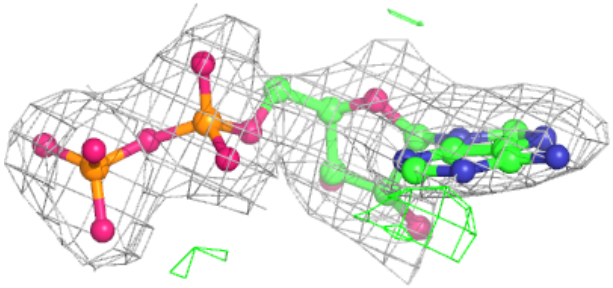
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

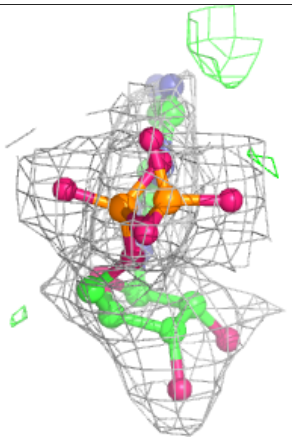


Electron density around ADP D 1301 (B):

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

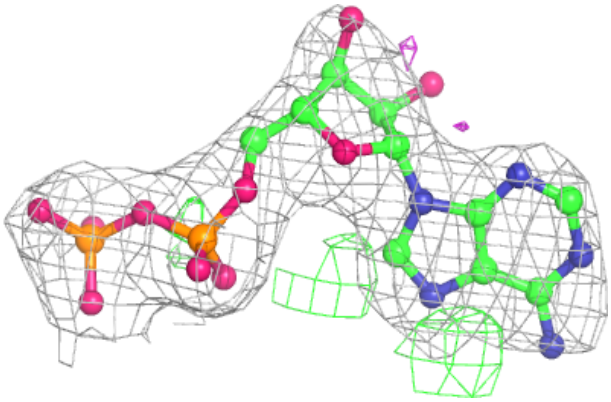


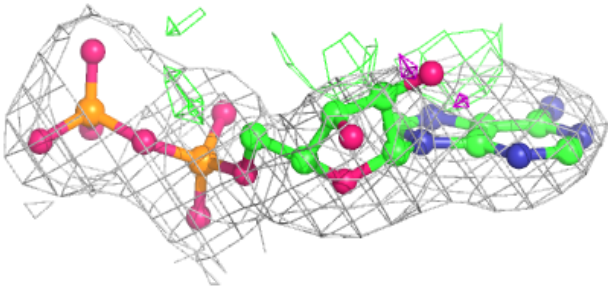


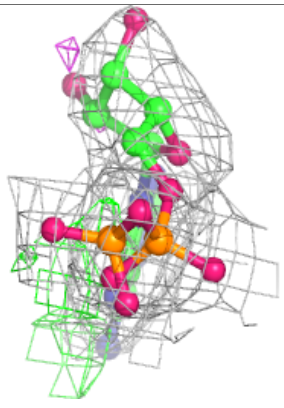


Electron density around ADP B 1301:

$2mF_o$-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.