Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2024 – 08:05 pm GMT

PDB ID	:	6HYS
Title	:	Crystal structure of DHX8 helicase domain bound to ADP at 2.6 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	:	2.60 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:

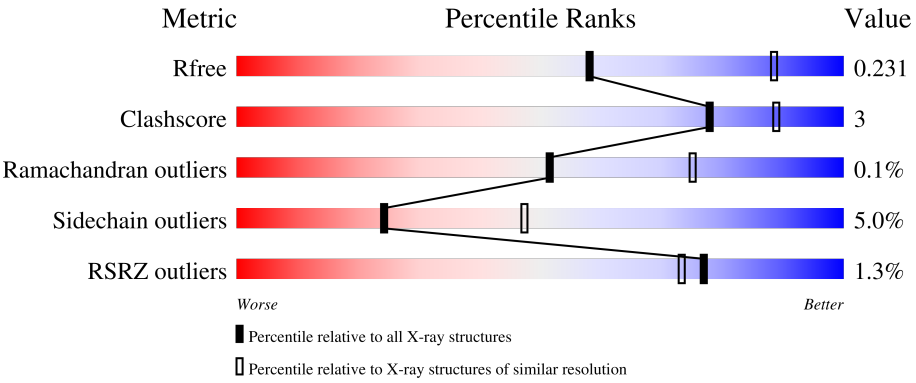
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	82% 11% • 6%
1	B	673	82% 11% • 6%
1	C	673	85% 9% • 6%
1	D	673	86% 8% • 6%

2 Entry composition (i)

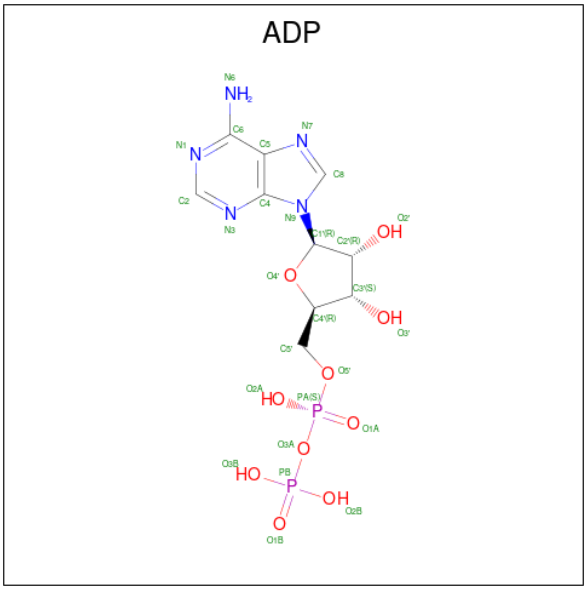
There are 7 unique types of molecules in this entry. The entry contains 19875 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1	0
			4812	3092	800	885	35			
1	B	633	Total	C	N	O	S	0	2	0
			4814	3086	796	899	33			
1	C	633	Total	C	N	O	S	0	1	0
			4726	3035	787	871	33			
1	D	632	Total	C	N	O	S	0	2	0
			4743	3038	790	881	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	1
			46	20	10	14	2		
2	B	1	Total	C	N	O	P	0	1
			46	20	10	14	2		

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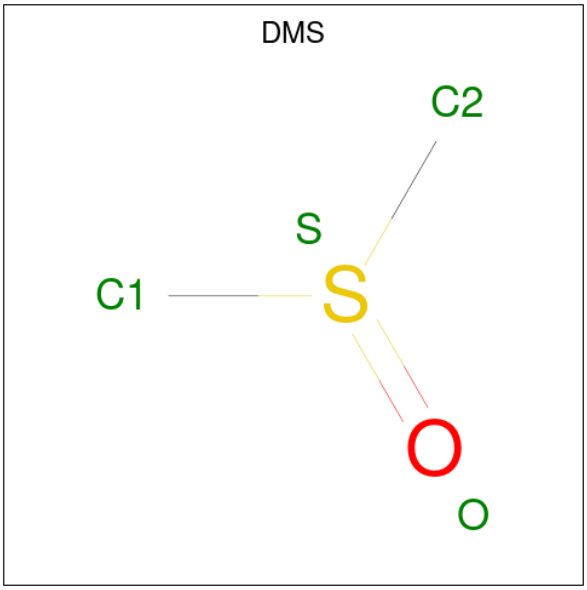
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O P 27 10 5 10 2	0	0
2	D	1	Total C N O P 46 20 10 14 2	0	1

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

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

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

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

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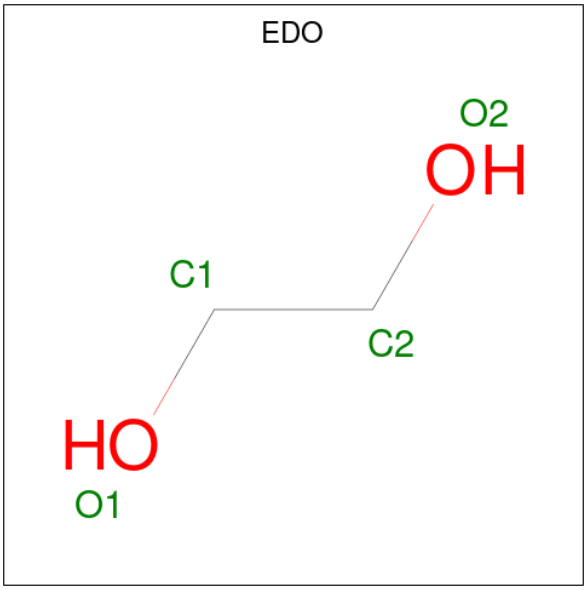
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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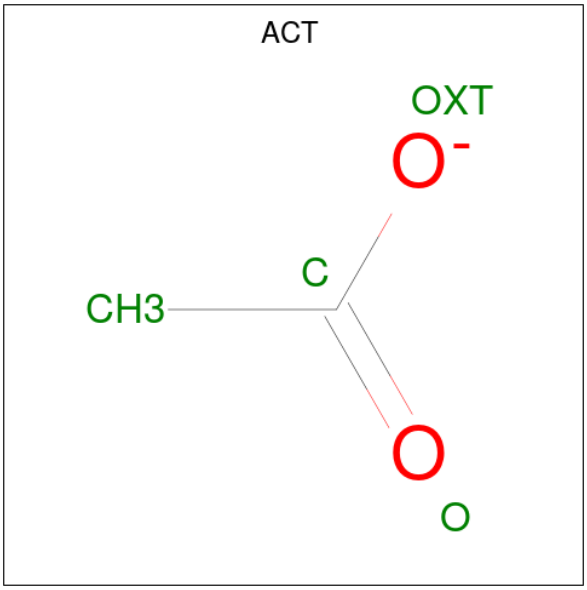
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- 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
6	D	1	Total C O 4 2 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	134	Total O 134 134	0	0
7	B	120	Total O 120 120	0	0
7	C	92	Total O 92 92	0	0

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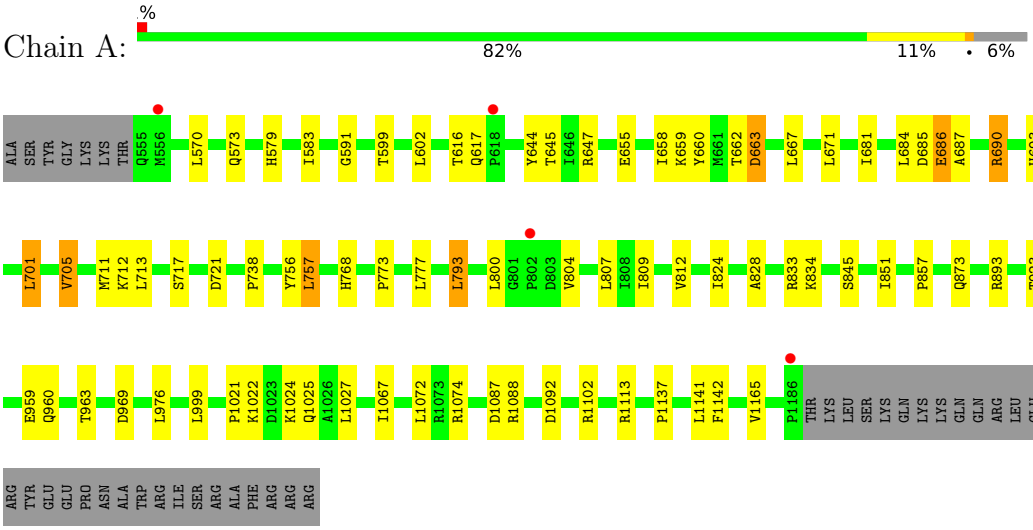
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	101	Total O 101 101	0	0

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.

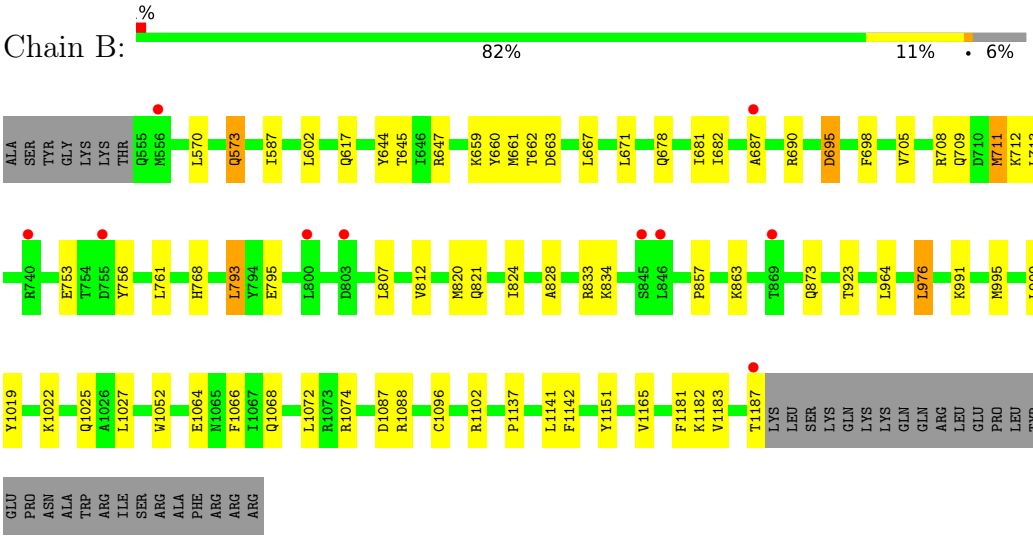
• Molecule 1: ATP-dependent RNA helicase DHX8

Chain A:



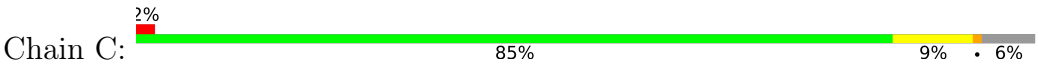
• Molecule 1: ATP-dependent RNA helicase DHX8

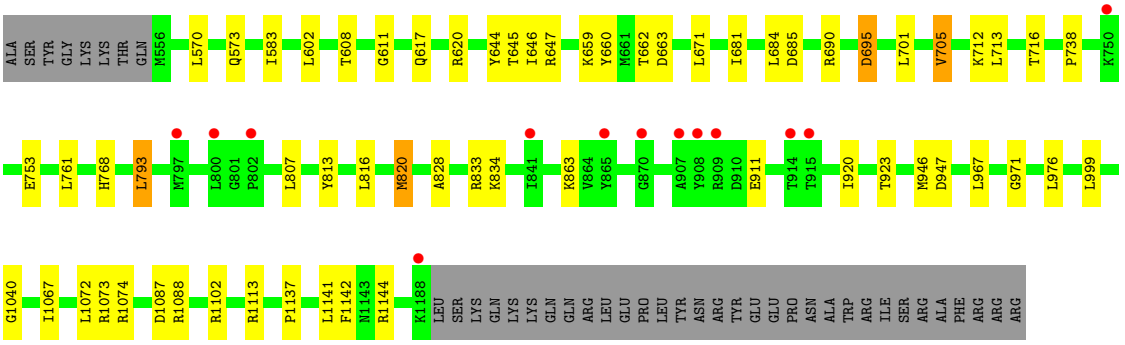
Chain B:



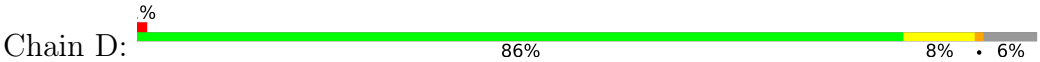
• Molecule 1: ATP-dependent RNA helicase DHX8

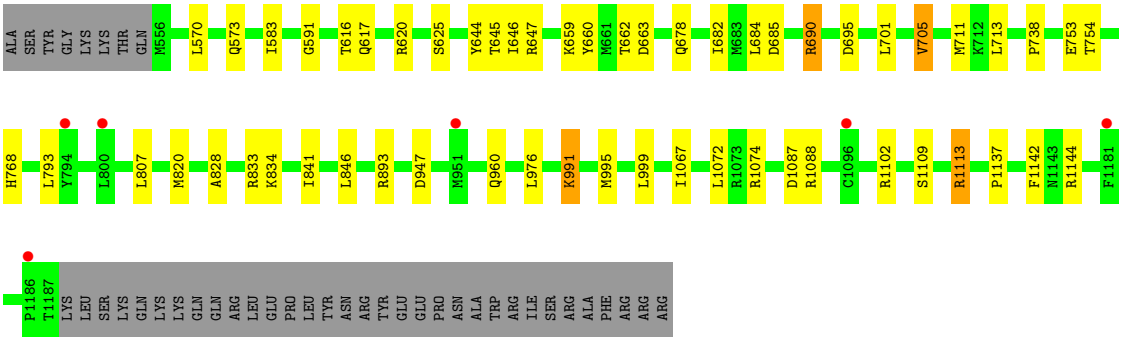
Chain C:





• Molecule 1: ATP-dependent RNA helicase DHX8





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.96Å 167.94Å 137.11Å 90.00° 92.71° 90.00°	Depositor
Resolution (Å)	37.59 – 2.60 37.59 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.59-2.60) 99.8 (37.59-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.182 , 0.214 0.194 , 0.231	Depositor DCC
R_{free} test set	4414 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	57.8	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 80.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.108 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19875	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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: EDO, ACT, MG, DMS, 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	0.52	0/4910	0.70	0/6674
1	B	0.51	0/4913	0.70	3/6676 (0.0%)
1	C	0.50	0/4825	0.68	0/6565
1	D	0.50	0/4842	0.68	0/6578
All	All	0.51	0/19490	0.69	3/26493 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1182	LYS	C-N-CA	6.16	137.10	121.70
1	B	1181	PHE	C-N-CA	5.76	136.11	121.70
1	B	1182	LYS	N-CA-C	-5.14	97.12	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	4812	0	4607	34	0
1	B	4814	0	4542	32	0
1	C	4726	0	4384	26	0
1	D	4743	0	4423	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	46	0	24	0	0
2	B	46	0	24	0	0
2	C	27	0	12	0	0
2	D	46	0	24	1	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	32	0	48	0	0
4	B	32	0	48	0	0
4	C	36	0	54	0	0
4	D	28	0	42	0	0
5	A	8	0	12	0	0
5	B	4	0	6	0	0
5	C	4	0	6	0	0
5	D	8	0	12	0	0
6	A	4	0	3	0	0
6	B	4	0	3	0	0
6	D	4	0	3	0	0
7	A	134	0	0	2	0
7	B	120	0	0	0	0
7	C	92	0	0	1	0
7	D	101	0	0	0	0
All	All	19875	0	18277	111	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 3.

All (111) 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:1141:LEU:HD12	1:A:1165:VAL:HG12	1.60	0.82
1:D:625:SER:HB3	2:D:1301[B]:ADP:HN62	1.55	0.71
1:B:690:ARG:HH11	1:B:695:ASP:CG	1.96	0.69
1:C:583:ILE:HD11	1:C:705:VAL:HG11	1.73	0.69
1:D:583:ILE:HD11	1:D:705:VAL:HG11	1.76	0.67
1:A:583:ILE:HD11	1:A:705:VAL:HG11	1.77	0.66
1:C:685:ASP:HA	1:C:716:THR:OG1	1.96	0.66
1:C:620:ARG:HG3	1:C:646:ILE:HD13	1.79	0.65
1:A:681:ILE:HG12	1:A:712:LYS:HB2	1.80	0.62
1:C:690:ARG:CZ	1:C:946:MET:HE2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:863:LYS:HB3	1:C:923:THR:HG22	1.87	0.57
1:D:620:ARG:HG3	1:D:646:ILE:HD12	1.87	0.56
1:B:1151:TYR:HB3	1:B:1165:VAL:HG12	1.88	0.56
1:C:602:LEU:HD13	1:C:681:ILE:HD13	1.88	0.56
1:B:602:LEU:HD13	1:B:681:ILE:HD13	1.88	0.55
1:A:959:GLU:O	1:A:963:THR:HG23	2.06	0.55
1:C:820:MET:HG2	7:C:1481:HOH:O	2.07	0.55
1:D:1067:ILE:HG21	1:D:1072:LEU:HD11	1.88	0.55
1:A:1067:ILE:HG21	1:A:1072:LEU:HD11	1.90	0.54
1:B:682:ILE:HD12	1:B:711:MET:CE	2.37	0.54
1:A:800:LEU:HB3	1:A:804:VAL:HG21	1.90	0.53
1:A:756:TYR:HB2	1:A:857:PRO:HB3	1.90	0.53
1:A:570:LEU:HD11	1:A:738:PRO:HD3	1.91	0.53
1:C:681:ILE:HG12	1:C:712:LYS:HB2	1.91	0.52
1:B:1022:LYS:HA	1:B:1025:GLN:HE21	1.74	0.52
1:B:708:ARG:HB3	1:B:711:MET:HB3	1.91	0.52
1:A:690:ARG:HH12	1:A:947:ASP:HB2	1.75	0.52
1:A:1021:PRO:HG2	1:A:1024:LYS:HB2	1.93	0.51
1:B:812:VAL:HG22	1:B:824:ILE:HG21	1.92	0.51
1:C:828:ALA:HB2	1:C:834:LYS:HG3	1.92	0.51
1:B:682:ILE:HD12	1:B:711:MET:HE1	1.92	0.51
1:B:964:LEU:HD22	1:B:991:LYS:HG3	1.92	0.51
1:D:841:ILE:HG23	1:D:846:LEU:HD12	1.93	0.51
1:A:645:THR:OG1	1:A:659:LYS:HE3	2.12	0.50
1:A:828:ALA:HB2	1:A:834:LYS:HG3	1.94	0.50
1:A:812:VAL:HG22	1:A:824:ILE:HG21	1.94	0.49
1:B:1141:LEU:HD12	1:B:1165:VAL:HG23	1.93	0.49
1:B:687:ALA:HB1	1:B:698:PHE:HZ	1.77	0.49
1:D:828:ALA:HB2	1:D:834:LYS:HG3	1.94	0.49
1:B:1019:TYR:HB2	1:B:1068:GLN:HG3	1.94	0.48
1:B:681:ILE:HG12	1:B:712:LYS:HB2	1.94	0.48
1:C:690:ARG:HH21	1:C:695:ASP:CG	2.17	0.48
1:C:690:ARG:HH22	1:C:947:ASP:HB2	1.77	0.48
1:A:644:TYR:HA	1:A:660:TYR:O	2.14	0.48
1:A:956:THR:HG22	1:A:960:GLN:HE21	1.78	0.48
1:A:1022:LYS:HA	1:A:1025:GLN:HE21	1.79	0.48
1:C:1067:ILE:HG21	1:C:1072:LEU:HD11	1.95	0.48
1:B:587:ILE:HA	1:B:717:SER:O	2.14	0.48
1:C:617:GLN:O	1:C:662:THR:HA	2.14	0.48
1:A:663:ASP:HB2	1:A:693:HIS:HB3	1.96	0.47
1:B:828:ALA:HB2	1:B:834:LYS:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:644:TYR:HA	1:C:660:TYR:O	2.14	0.47
1:D:617:GLN:O	1:D:662:THR:HA	2.14	0.47
1:B:644:TYR:HA	1:B:660:TYR:O	2.14	0.47
1:D:991:LYS:HD2	1:D:1109:SER:O	2.14	0.47
1:C:967:LEU:HD22	1:C:971:GLY:O	2.14	0.46
1:D:644:TYR:HA	1:D:660:TYR:O	2.15	0.46
1:A:579:HIS:HB2	7:A:1421:HOH:O	2.15	0.46
1:C:1137:PRO:HA	1:C:1142:PHE:CG	2.51	0.46
1:B:976:LEU:HD11	1:B:991:LYS:HE3	1.98	0.46
1:B:999:LEU:O	1:B:1102:ARG:HD3	2.16	0.46
1:B:617:GLN:O	1:B:662:THR:HA	2.16	0.46
1:A:793:LEU:HD13	1:A:809:ILE:HG12	1.97	0.45
1:B:1027:LEU:HD23	1:B:1066:PHE:CE1	2.51	0.45
1:A:686:GLU:OE2	1:A:845:SER:HA	2.17	0.45
1:B:863:LYS:HB3	1:B:923:THR:HG22	1.99	0.45
1:C:761:LEU:HD22	1:C:793:LEU:HG	1.99	0.45
1:A:684:LEU:HD11	1:A:701:LEU:HD13	1.98	0.45
1:A:768:HIS:ND1	1:A:833:ARG:HD2	2.32	0.45
1:B:1052:TRP:CG	1:B:1072:LEU:HD13	2.53	0.44
1:D:682:ILE:HB	1:D:711:MET:CE	2.47	0.44
1:B:690:ARG:NH1	1:B:695:ASP:OD2	2.51	0.44
1:B:1137:PRO:HA	1:B:1142:PHE:CG	2.52	0.44
1:D:645:THR:OG1	1:D:659:LYS:HE3	2.17	0.44
1:C:1040:GLY:HA2	1:C:1141:LEU:HG	1.99	0.44
1:D:591:GLY:HA3	1:D:893:ARG:HE	1.82	0.44
1:D:1137:PRO:HA	1:D:1142:PHE:CG	2.53	0.44
1:A:617:GLN:O	1:A:662:THR:HA	2.17	0.44
1:D:616:THR:O	1:D:685:ASP:HB3	2.18	0.44
1:A:687:ALA:HB1	1:A:698:PHE:HZ	1.82	0.44
1:A:655:GLU:HG3	7:A:1427:HOH:O	2.18	0.43
1:A:999:LEU:O	1:A:1102:ARG:HD3	2.16	0.43
1:B:645:THR:OG1	1:B:659:LYS:HE3	2.16	0.43
1:C:999:LEU:O	1:C:1102:ARG:HD3	2.18	0.43
1:B:1001:CYS:HB3	1:B:1096:CYS:HB3	1.99	0.43
1:A:599:THR:HB	1:A:658:ILE:HG12	2.01	0.43
1:B:570:LEU:HA	1:B:573:GLN:HE21	1.83	0.43
1:C:645:THR:OG1	1:C:659:LYS:HE3	2.17	0.43
1:A:602:LEU:HD13	1:A:681:ILE:HD13	1.99	0.43
1:A:1087:ASP:HB3	1:B:1087:ASP:HB3	2.01	0.43
1:C:813:TYR:O	1:C:816:LEU:HB2	2.18	0.43
1:B:768:HIS:ND1	1:B:833:ARG:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1137:PRO:HA	1:A:1142:PHE:CG	2.54	0.42
1:C:768:HIS:ND1	1:C:833:ARG:HD2	2.33	0.42
1:A:777:LEU:HB2	1:A:851:ILE:HD13	2.01	0.42
1:D:690:ARG:NH2	1:D:947:ASP:OD2	2.51	0.42
1:D:768:HIS:ND1	1:D:833:ARG:HD2	2.34	0.42
1:D:999:LEU:O	1:D:1102:ARG:HD3	2.19	0.42
1:D:684:LEU:HD11	1:D:701:LEU:HD13	2.02	0.41
1:C:608:THR:HA	1:C:611:GLY:O	2.20	0.41
1:B:756:TYR:HB2	1:B:857:PRO:HB3	2.03	0.41
1:A:591:GLY:HA3	1:A:893:ARG:HE	1.85	0.41
1:C:570:LEU:HD11	1:C:738:PRO:HD3	2.03	0.41
1:B:821:GLN:O	1:B:824:ILE:HG12	2.21	0.41
1:C:1087:ASP:HB3	1:D:1087:ASP:HB3	2.02	0.41
1:D:570:LEU:HD11	1:D:738:PRO:CD	2.51	0.41
1:B:761:LEU:HD22	1:B:793:LEU:HG	2.03	0.41
1:A:616:THR:O	1:A:685:ASP:HB3	2.21	0.40
1:D:960:GLN:HG2	1:D:1113:ARG:CZ	2.51	0.40
1:A:757:LEU:HD23	1:A:757:LEU:HA	1.94	0.40
1:C:684:LEU:HD11	1:C:701:LEU:HD13	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	631/673 (94%)	608 (96%)	22 (4%)	1 (0%)	47	71
1	B	633/673 (94%)	607 (96%)	25 (4%)	1 (0%)	47	71
1	C	632/673 (94%)	611 (97%)	21 (3%)	0	100	100
1	D	632/673 (94%)	609 (96%)	23 (4%)	0	100	100
All	All	2528/2692 (94%)	2435 (96%)	91 (4%)	2 (0%)	51	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1183	VAL
1	A	690	ARG

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	468/596 (78%)	442 (94%)	26 (6%)	21	42
1	B	466/596 (78%)	439 (94%)	27 (6%)	20	40
1	C	435/596 (73%)	416 (96%)	19 (4%)	28	53
1	D	452/596 (76%)	432 (96%)	20 (4%)	28	53
All	All	1821/2384 (76%)	1729 (95%)	92 (5%)	24	46

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	573	GLN
1	A	647	ARG
1	A	663	ASP
1	A	667	LEU
1	A	671	LEU
1	A	686	GLU
1	A	695	ASP
1	A	701	LEU
1	A	705	VAL
1	A	711	MET
1	A	713	LEU
1	A	717	SER
1	A	721	ASP
1	A	757	LEU
1	A	773	PRO
1	A	793	LEU
1	A	807	LEU
1	A	873	GLN

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Mol	Chain	Res	Type
1	A	923	THR
1	A	969	ASP
1	A	976	LEU
1	A	1027	LEU
1	A	1074	ARG
1	A	1088	ARG
1	A	1092	ASP
1	A	1113	ARG
1	B	573	GLN
1	B	647	ARG
1	B	661	MET
1	B	663	ASP
1	B	667	LEU
1	B	671	LEU
1	B	678	GLN
1	B	695	ASP
1	B	705	VAL
1	B	709	GLN
1	B	711	MET
1	B	713	LEU
1	B	721	ASP
1	B	753	GLU
1	B	793	LEU
1	B	795[A]	GLU
1	B	795[B]	GLU
1	B	807	LEU
1	B	820	MET
1	B	873	GLN
1	B	976	LEU
1	B	995	MET
1	B	1002	SER
1	B	1064	GLU
1	B	1074	ARG
1	B	1088	ARG
1	B	1187	THR
1	C	573	GLN
1	C	647	ARG
1	C	663	ASP
1	C	671	LEU
1	C	695	ASP
1	C	705	VAL
1	C	713	LEU

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Mol	Chain	Res	Type
1	C	753	GLU
1	C	793	LEU
1	C	807	LEU
1	C	820	MET
1	C	911	GLU
1	C	920	ILE
1	C	976	LEU
1	C	1073	ARG
1	C	1074	ARG
1	C	1088	ARG
1	C	1113	ARG
1	C	1144	ARG
1	D	573	GLN
1	D	647	ARG
1	D	663	ASP
1	D	678	GLN
1	D	690	ARG
1	D	695	ASP
1	D	705	VAL
1	D	713	LEU
1	D	753	GLU
1	D	754	THR
1	D	793	LEU
1	D	807	LEU
1	D	820	MET
1	D	976	LEU
1	D	991	LYS
1	D	995	MET
1	D	1074	ARG
1	D	1088	ARG
1	D	1113	ARG
1	D	1144	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	916	ASN
1	A	924	ASN
1	A	960	GLN
1	B	573	GLN
1	B	688	HIS
1	B	916	ASN

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Mol	Chain	Res	Type
1	B	1025	GLN
1	C	883	GLN
1	C	916	ASN
1	D	881	GLN
1	D	1068	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 52 ligands modelled in this entry, 4 are monoatomic - leaving 48 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	A	1301[A]	-	24,29,29	0.63	0	29,45,45	0.83	1 (3%)
4	DMS	C	1306	-	3,3,3	0.31	0	3,3,3	0.37	0
4	DMS	A	1307	-	3,3,3	0.27	0	3,3,3	0.56	0
4	DMS	C	1309	-	3,3,3	0.33	0	3,3,3	0.45	0
4	DMS	C	1310	-	3,3,3	0.34	0	3,3,3	0.39	0
4	DMS	A	1311	-	3,3,3	0.31	0	3,3,3	0.22	0
4	DMS	B	1303	-	3,3,3	0.29	0	3,3,3	0.24	0
4	DMS	D	1308	-	3,3,3	0.30	0	3,3,3	0.24	0
4	DMS	B	1304	-	3,3,3	0.32	0	3,3,3	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	DMS	C	1312	-	3,3,3	0.33	0	3,3,3	0.25	0
4	DMS	D	1309	-	3,3,3	0.33	0	3,3,3	0.25	0
6	ACT	A	1308	-	3,3,3	1.35	0	3,3,3	1.06	0
4	DMS	A	1310	-	3,3,3	0.25	0	3,3,3	0.23	0
5	EDO	D	1303	-	3,3,3	0.70	0	2,2,2	0.30	0
4	DMS	B	1305	-	3,3,3	0.23	0	3,3,3	0.28	0
4	DMS	C	1307	-	3,3,3	0.29	0	3,3,3	0.15	0
4	DMS	B	1311	-	3,3,3	0.25	0	3,3,3	0.16	0
4	DMS	A	1303	-	3,3,3	0.28	0	3,3,3	0.15	0
5	EDO	A	1304	-	3,3,3	0.73	0	2,2,2	0.07	0
4	DMS	C	1305	-	3,3,3	0.29	0	3,3,3	0.31	0
4	DMS	B	1308	-	3,3,3	0.27	0	3,3,3	0.28	0
6	ACT	D	1312	-	3,3,3	1.03	0	3,3,3	1.28	0
2	ADP	C	1301	3	24,29,29	0.71	0	29,45,45	1.05	2 (6%)
5	EDO	A	1305	-	3,3,3	0.62	0	2,2,2	0.27	0
4	DMS	C	1308	-	3,3,3	0.27	0	3,3,3	0.31	0
4	DMS	D	1305	-	3,3,3	0.27	0	3,3,3	0.18	0
5	EDO	B	1306	-	3,3,3	0.61	0	2,2,2	0.31	0
4	DMS	C	1311	-	3,3,3	0.32	0	3,3,3	0.35	0
5	EDO	D	1304	-	3,3,3	0.46	0	2,2,2	0.65	0
2	ADP	D	1301[B]	-	24,29,29	0.64	0	29,45,45	1.02	2 (6%)
4	DMS	B	1307	-	3,3,3	0.24	0	3,3,3	0.42	0
2	ADP	B	1301[B]	-	24,29,29	0.62	0	29,45,45	0.88	1 (3%)
5	EDO	C	1303	-	3,3,3	0.65	0	2,2,2	0.14	0
2	ADP	D	1301[A]	-	24,29,29	0.62	0	29,45,45	0.99	2 (6%)
2	ADP	B	1301[A]	-	24,29,29	0.62	0	29,45,45	0.83	1 (3%)
4	DMS	A	1309	-	3,3,3	0.28	0	3,3,3	0.36	0
4	DMS	A	1313	-	3,3,3	0.28	0	3,3,3	0.32	0
4	DMS	D	1311	-	3,3,3	0.33	0	3,3,3	0.45	0
4	DMS	C	1304	-	3,3,3	0.31	0	3,3,3	0.27	0
4	DMS	D	1306	-	3,3,3	0.20	0	3,3,3	0.26	0
4	DMS	D	1310	-	3,3,3	0.33	0	3,3,3	0.07	0
4	DMS	A	1306	-	3,3,3	0.31	0	3,3,3	0.27	0
6	ACT	B	1309	-	3,3,3	1.19	0	3,3,3	0.97	0
4	DMS	B	1310	-	3,3,3	0.26	0	3,3,3	0.28	0
2	ADP	A	1301[B]	-	24,29,29	0.63	0	29,45,45	0.91	1 (3%)
4	DMS	A	1312	-	3,3,3	0.26	0	3,3,3	0.42	0
4	DMS	B	1312	-	3,3,3	0.32	0	3,3,3	0.30	0
4	DMS	D	1307	-	3,3,3	0.38	0	3,3,3	0.32	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
2	ADP	A	1301[A]	-	-	2/12/32/32	0/3/3/3
5	EDO	A	1305	-	-	0/1/1/1	-
5	EDO	B	1306	-	-	1/1/1/1	-
5	EDO	D	1303	-	-	0/1/1/1	-
5	EDO	D	1304	-	-	0/1/1/1	-
2	ADP	D	1301[B]	-	-	3/12/32/32	0/3/3/3
2	ADP	B	1301[B]	-	-	2/12/32/32	0/3/3/3
5	EDO	C	1303	-	-	0/1/1/1	-
2	ADP	D	1301[A]	-	-	0/12/32/32	0/3/3/3
5	EDO	A	1304	-	-	0/1/1/1	-
2	ADP	A	1301[B]	-	-	5/12/32/32	0/3/3/3
2	ADP	B	1301[A]	-	-	5/12/32/32	0/3/3/3
2	ADP	C	1301	3	-	3/12/32/32	0/3/3/3

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1301	ADP	O3B-PB-O2B	2.55	117.37	107.64
2	B	1301[B]	ADP	C5-C6-N6	2.44	124.06	120.35
2	A	1301[A]	ADP	C5-C6-N6	2.38	123.97	120.35
2	D	1301[A]	ADP	C5-C6-N6	2.20	123.70	120.35
2	C	1301	ADP	C5-C6-N6	2.13	123.59	120.35
2	D	1301[B]	ADP	C5-C6-N6	2.12	123.57	120.35
2	A	1301[B]	ADP	C5-C6-N6	2.06	123.49	120.35
2	B	1301[A]	ADP	C5-C6-N6	2.05	123.46	120.35
2	D	1301[A]	ADP	O3B-PB-O2B	2.04	115.44	107.64
2	D	1301[B]	ADP	O3B-PB-O2B	2.04	115.44	107.64

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301[B]	ADP	C5'-O5'-PA-O1A
2	B	1301[A]	ADP	PA-O3A-PB-O3B
2	B	1301[B]	ADP	PA-O3A-PB-O3B
2	C	1301	ADP	C5'-O5'-PA-O2A
2	D	1301[B]	ADP	C5'-O5'-PA-O2A

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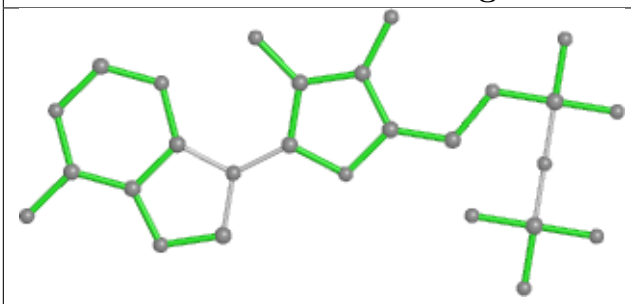
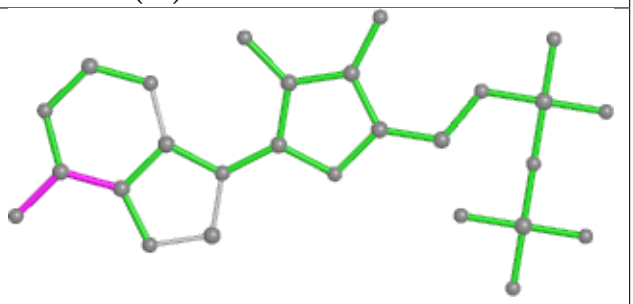
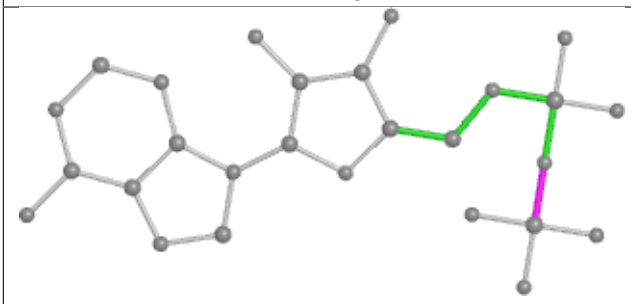
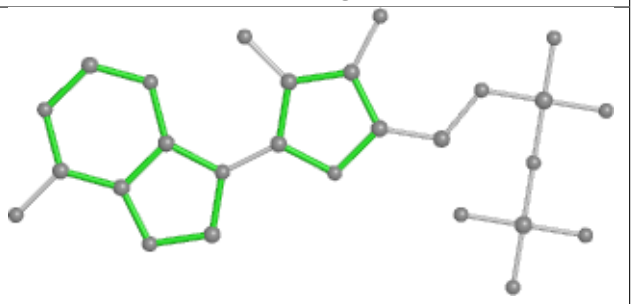
Mol	Chain	Res	Type	Atoms
2	A	1301[A]	ADP	PA-O3A-PB-O1B
2	A	1301[B]	ADP	PA-O3A-PB-O1B
2	A	1301[A]	ADP	PA-O3A-PB-O3B
2	A	1301[B]	ADP	PA-O3A-PB-O3B
2	A	1301[B]	ADP	C5'-O5'-PA-O3A
2	B	1301[A]	ADP	C5'-O5'-PA-O3A
2	C	1301	ADP	C5'-O5'-PA-O3A
2	D	1301[B]	ADP	C5'-O5'-PA-O3A
2	A	1301[B]	ADP	C5'-O5'-PA-O2A
2	B	1301[A]	ADP	C5'-O5'-PA-O2A
2	C	1301	ADP	C5'-O5'-PA-O1A
2	D	1301[B]	ADP	C5'-O5'-PA-O1A
2	B	1301[A]	ADP	PA-O3A-PB-O1B
2	B	1301[B]	ADP	PA-O3A-PB-O1B
5	B	1306	EDO	O1-C1-C2-O2
2	B	1301[A]	ADP	C5'-O5'-PA-O1A

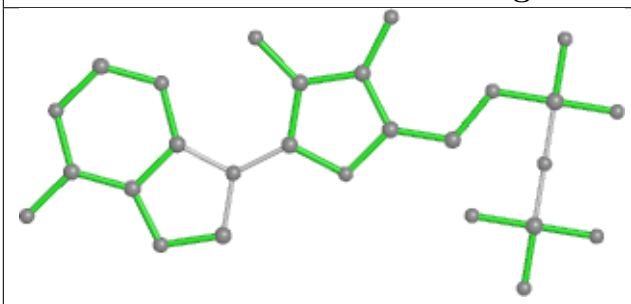
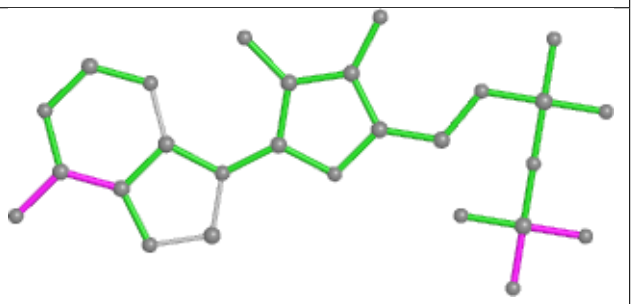
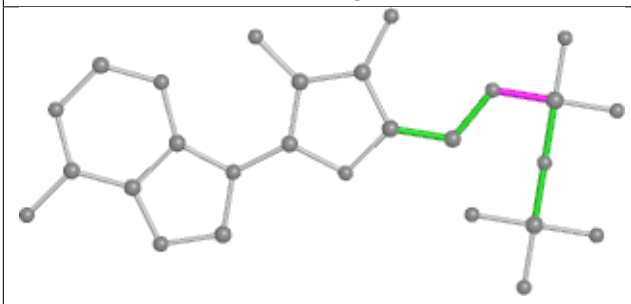
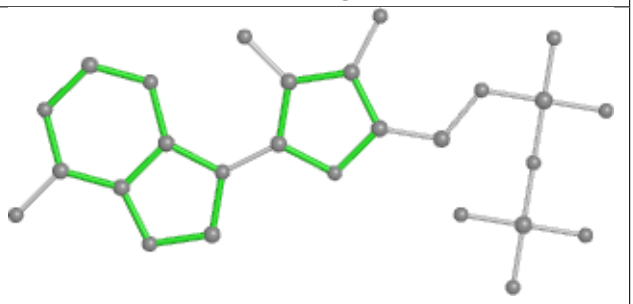
There are no ring outliers.

1 monomer is involved in 1 short contact:

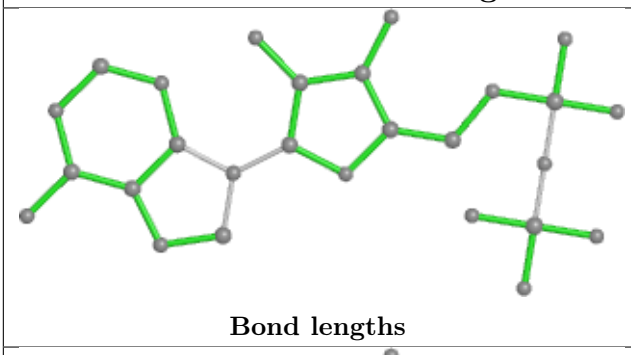
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1301[B]	ADP	1	0

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.

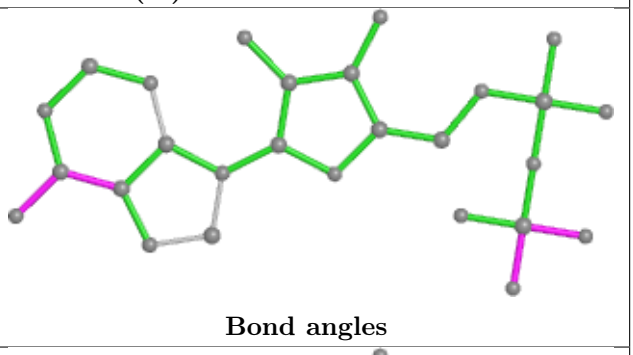
Ligand ADP A 1301 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP C 1301	
 Bond lengths	 Bond angles
 Torsions	 Rings

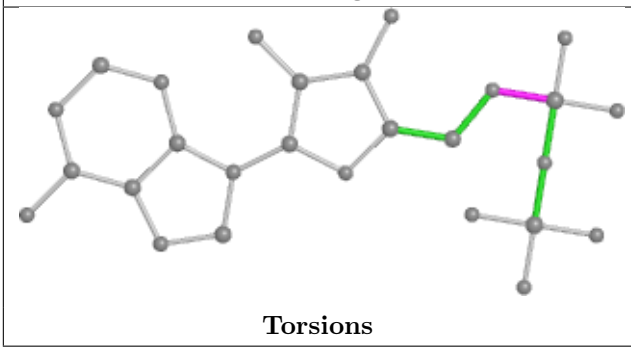
Ligand ADP D 1301 (B)



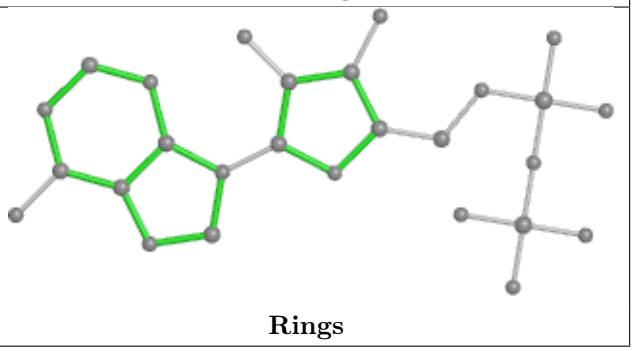
Bond lengths



Bond angles

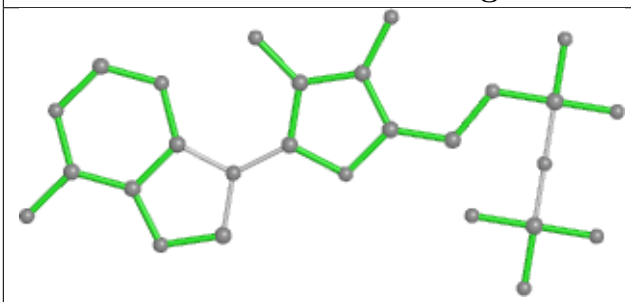


Torsions

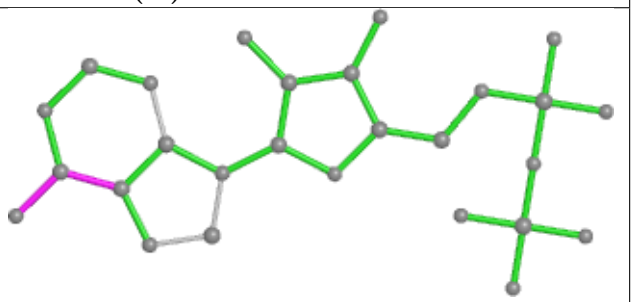


Rings

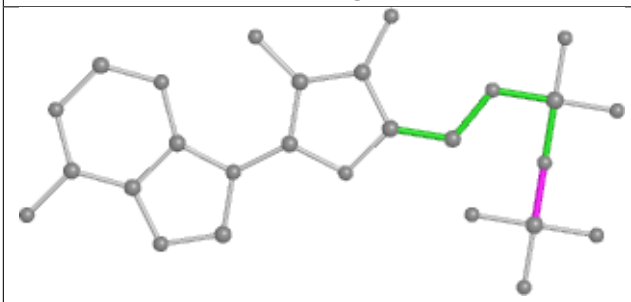
Ligand ADP B 1301 (B)



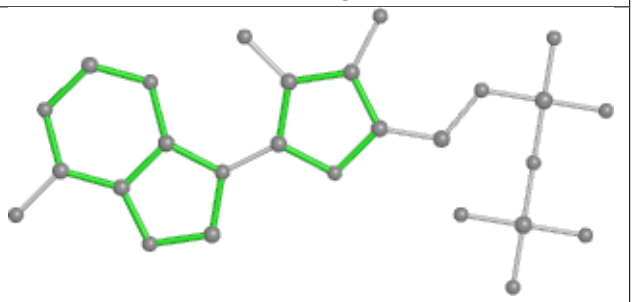
Bond lengths



Bond angles

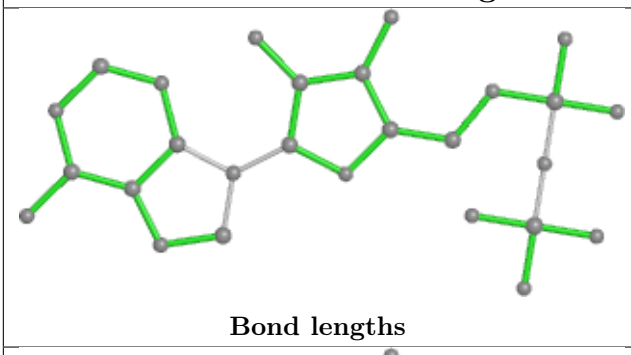


Torsions

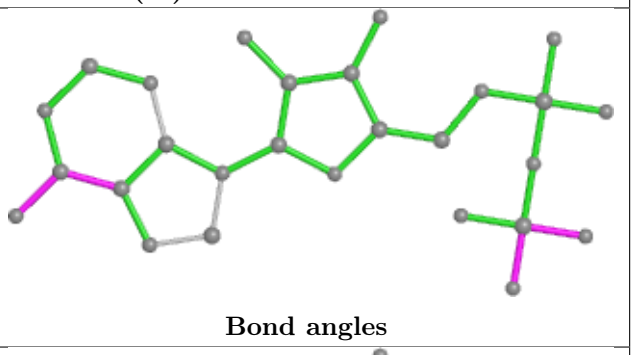


Rings

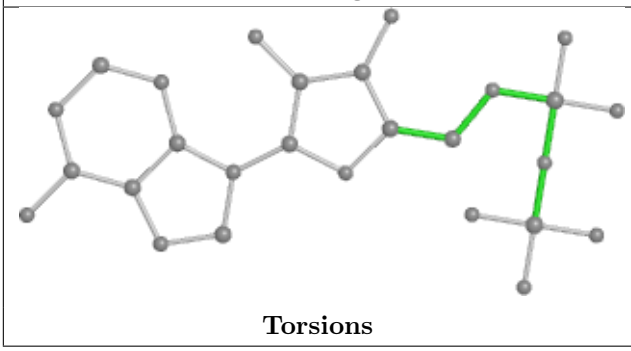
Ligand ADP D 1301 (A)



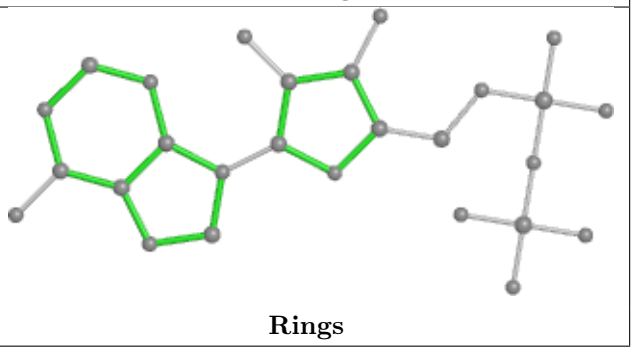
Bond lengths



Bond angles

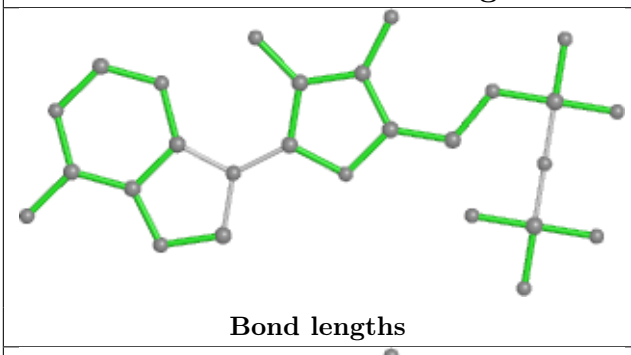


Torsions

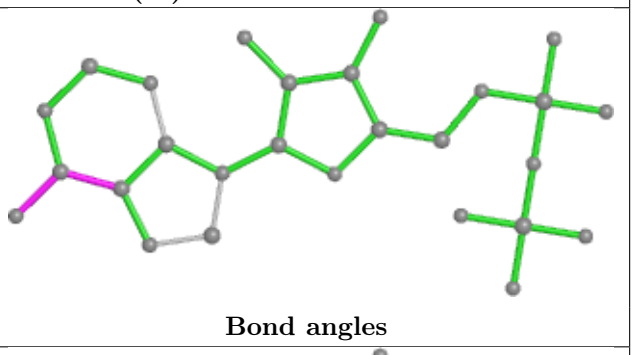


Rings

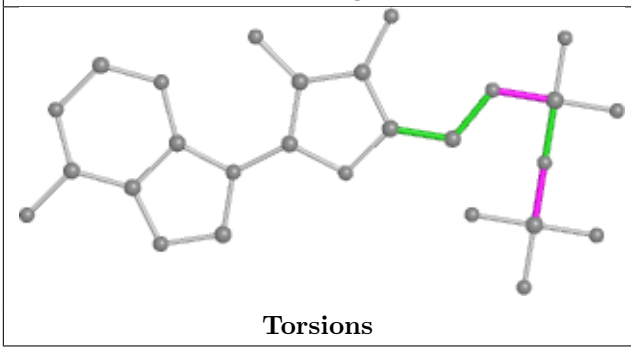
Ligand ADP B 1301 (A)



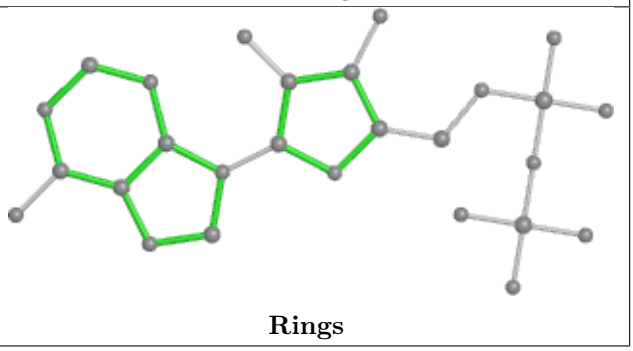
Bond lengths



Bond angles

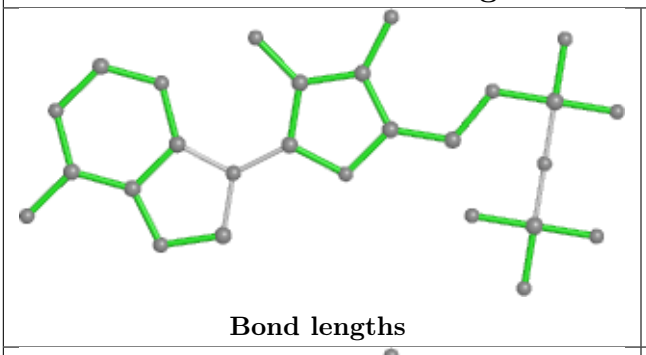


Torsions

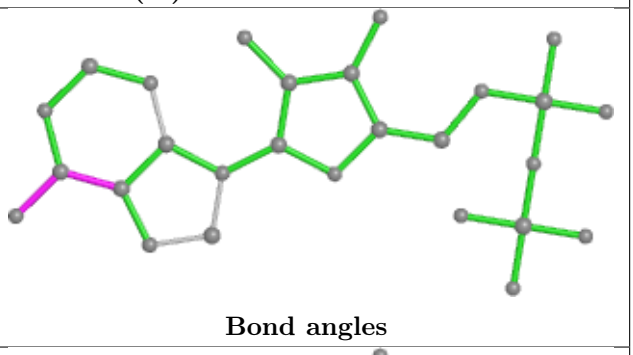


Rings

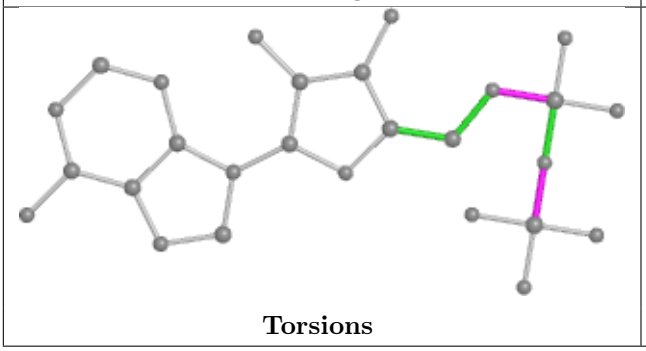
Ligand ADP A 1301 (B)



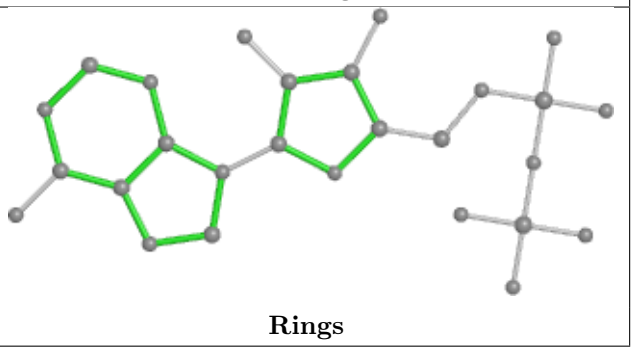
Bond lengths



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%)	-0.29	4 (0%)	89	88	38, 62, 89, 127	0
1	B	633/673 (94%)	-0.24	10 (1%)	72	68	40, 63, 89, 113	0
1	C	633/673 (94%)	-0.15	13 (2%)	63	58	43, 70, 101, 123	0
1	D	632/673 (93%)	-0.31	6 (0%)	84	82	45, 66, 91, 128	0
All	All	2530/2692 (93%)	-0.25	33 (1%)	77	73	38, 65, 93, 128	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1186	PRO	4.3
1	C	907	ALA	3.7
1	C	914	THR	3.6
1	B	800	LEU	3.4
1	C	915	THR	3.4
1	C	908	TYR	3.2
1	C	802	PRO	3.1
1	B	869	THR	3.0
1	B	556	MET	2.9
1	C	750	LYS	2.8
1	B	845	SER	2.8
1	C	865	TYR	2.8
1	B	803	ASP	2.7
1	A	802	PRO	2.7
1	D	1186	PRO	2.7
1	C	841	ILE	2.7
1	C	800	LEU	2.6
1	D	1096	CYS	2.6
1	A	556	MET	2.5
1	D	800	LEU	2.5
1	B	1187	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	846	LEU	2.3
1	D	951	MET	2.3
1	A	618	PRO	2.2
1	B	740	ARG	2.2
1	B	755	ASP	2.1
1	D	794	TYR	2.1
1	C	1188	LYS	2.1
1	B	687	ALA	2.1
1	C	797	MET	2.1
1	C	909	ARG	2.1
1	C	870	GLY	2.0
1	D	1181	PHE	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 monosaccharides 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
5	EDO	D	1303	4/4	0.44	0.39	82,83,84,84	0
5	EDO	C	1303	4/4	0.78	0.28	69,71,71,73	0
4	DMS	C	1306	4/4	0.80	0.32	121,122,122,122	0
4	DMS	B	1311	4/4	0.81	0.37	131,131,132,132	0
4	DMS	C	1310	4/4	0.82	0.42	121,122,122,123	0
4	DMS	A	1307	4/4	0.82	0.30	125,125,125,126	0
4	DMS	A	1311	4/4	0.82	0.45	125,125,126,126	0
6	ACT	D	1312	4/4	0.82	0.31	81,82,82,82	0
5	EDO	D	1304	4/4	0.84	0.27	77,78,79,81	0
6	ACT	A	1308	4/4	0.84	0.20	71,74,75,76	0
4	DMS	D	1311	4/4	0.84	0.28	122,123,123,124	0

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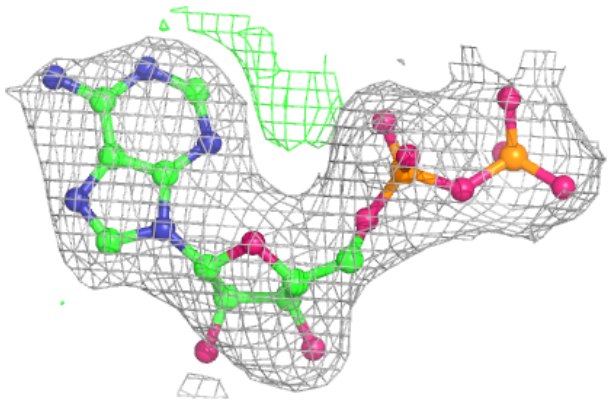
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	B	1306	4/4	0.87	0.32	74,75,75,78	0
4	DMS	D	1310	4/4	0.87	0.46	110,111,111,112	0
4	DMS	A	1313	4/4	0.88	0.23	115,115,115,115	0
4	DMS	A	1309	4/4	0.88	0.28	105,105,106,108	0
4	DMS	B	1303	4/4	0.89	0.14	95,97,98,98	0
5	EDO	A	1305	4/4	0.89	0.27	60,61,63,64	0
4	DMS	C	1312	4/4	0.89	0.28	105,106,107,108	0
4	DMS	B	1307	4/4	0.89	0.22	111,112,113,113	0
5	EDO	A	1304	4/4	0.90	0.21	62,65,66,67	0
4	DMS	C	1307	4/4	0.90	0.28	127,128,128,128	0
4	DMS	B	1305	4/4	0.90	0.34	109,109,110,110	0
4	DMS	B	1312	4/4	0.90	0.29	145,145,146,146	0
4	DMS	D	1307	4/4	0.90	0.17	108,109,110,110	0
4	DMS	D	1309	4/4	0.90	0.34	118,118,118,119	0
4	DMS	C	1304	4/4	0.90	0.20	108,109,109,109	0
6	ACT	B	1309	4/4	0.90	0.24	79,81,82,82	0
4	DMS	B	1308	4/4	0.90	0.21	133,134,134,134	0
4	DMS	A	1310	4/4	0.91	0.44	114,114,114,114	0
4	DMS	B	1310	4/4	0.91	0.38	126,126,126,126	0
4	DMS	C	1305	4/4	0.93	0.19	127,128,128,128	0
4	DMS	C	1311	4/4	0.93	0.20	110,110,111,111	0
4	DMS	A	1306	4/4	0.94	0.27	115,115,115,116	0
4	DMS	B	1304	4/4	0.94	0.24	108,108,109,109	0
4	DMS	A	1312	4/4	0.94	0.48	128,129,129,129	0
4	DMS	D	1306	4/4	0.94	0.16	104,104,104,105	0
4	DMS	A	1303	4/4	0.94	0.21	121,121,121,122	0
4	DMS	D	1308	4/4	0.94	0.30	129,129,129,130	0
4	DMS	D	1305	4/4	0.95	0.18	94,95,96,96	0
3	MG	D	1302	1/1	0.95	0.11	64,64,64,64	0
4	DMS	C	1308	4/4	0.96	0.24	105,105,105,106	0
4	DMS	C	1309	4/4	0.96	0.14	114,115,116,116	0
2	ADP	C	1301	27/27	0.96	0.12	60,79,84,90	0
2	ADP	B	1301[B]	27/27	0.97	0.17	47,57,59,63	19
2	ADP	A	1301[A]	27/27	0.97	0.16	42,48,59,65	19
2	ADP	D	1301[A]	27/27	0.97	0.15	48,58,64,67	19
2	ADP	D	1301[B]	27/27	0.97	0.15	50,63,69,73	19
3	MG	A	1302	1/1	0.97	0.19	76,76,76,76	0
3	MG	B	1302	1/1	0.97	0.17	47,47,47,47	0
2	ADP	A	1301[B]	27/27	0.97	0.16	48,64,67,70	19
2	ADP	B	1301[A]	27/27	0.97	0.17	47,69,75,78	19
3	MG	C	1302	1/1	0.98	0.05	65,65,65,65	0

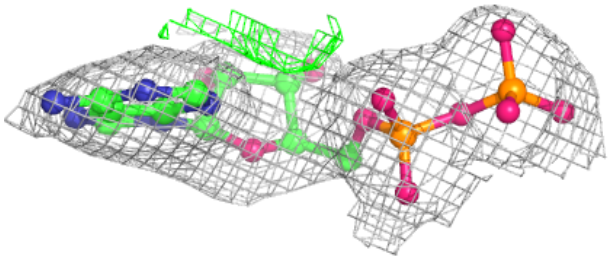
The following is a graphical depiction of the model fit to experimental electron density of all

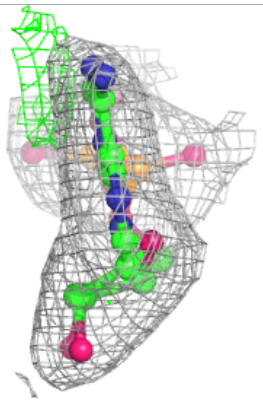
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

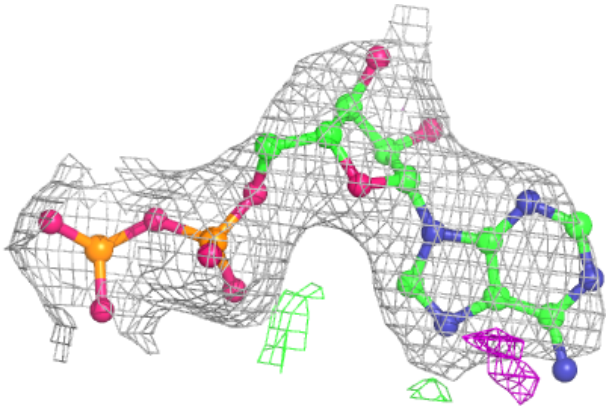


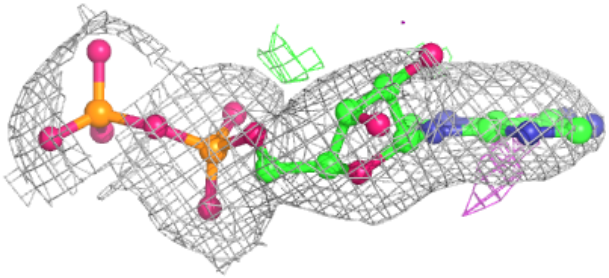


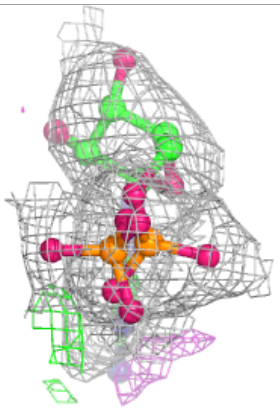


Electron density around ADP B 1301 (B):

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

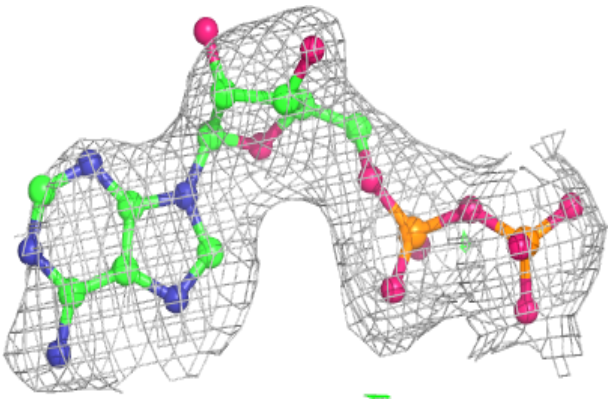


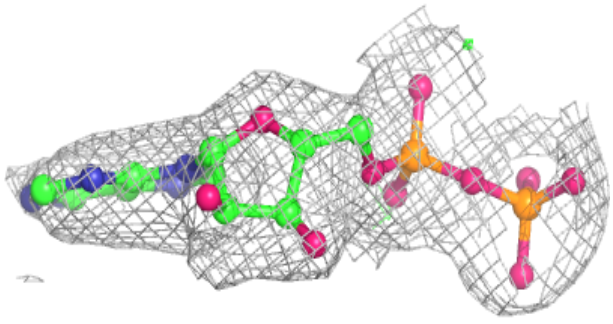


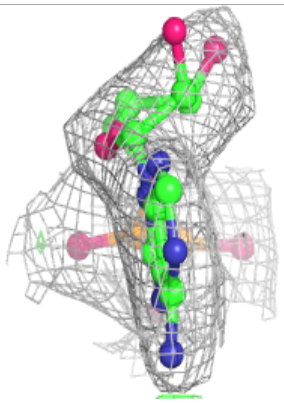


Electron density around ADP A 1301 (A):

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

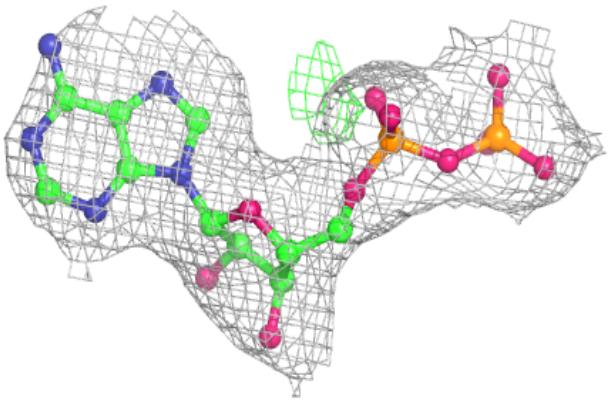


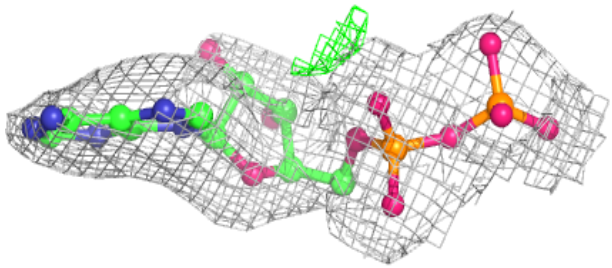


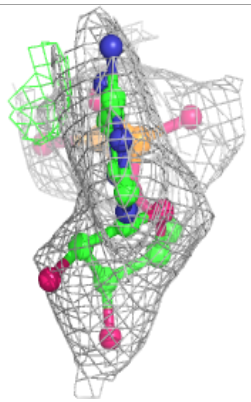


Electron density around ADP D 1301 (A):

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

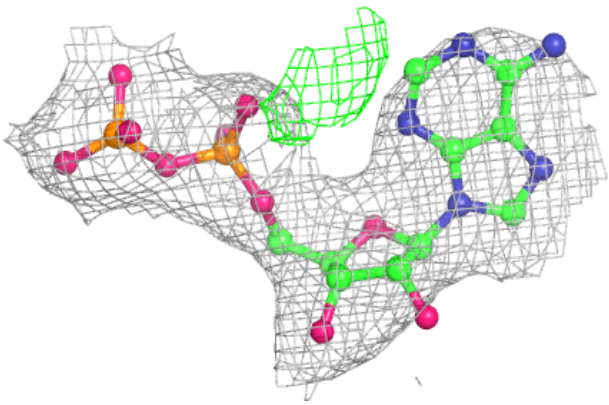


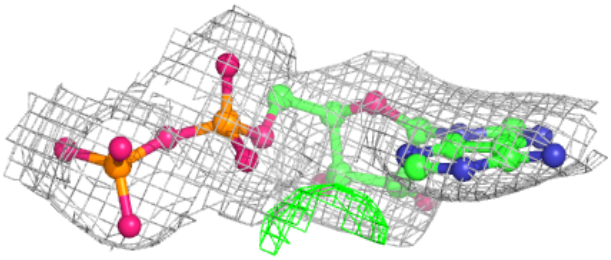


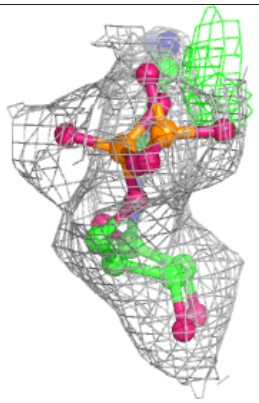


Electron density around ADP D 1301 (B):

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

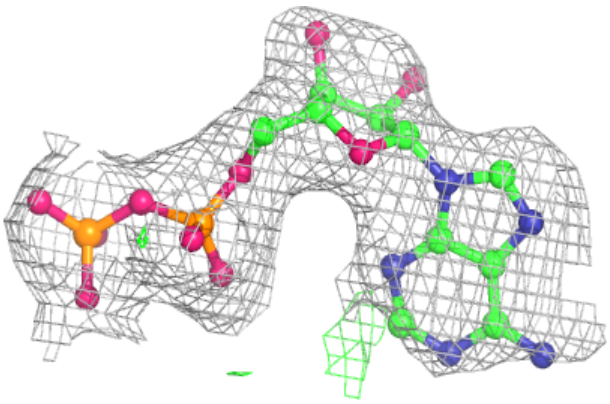


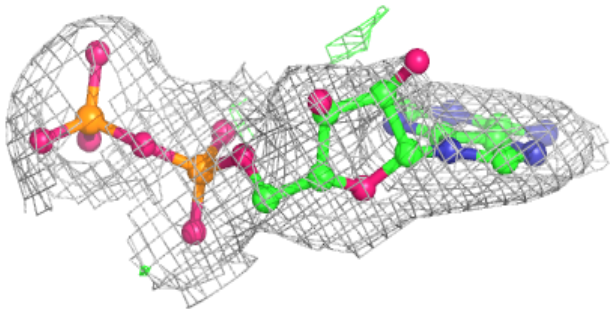


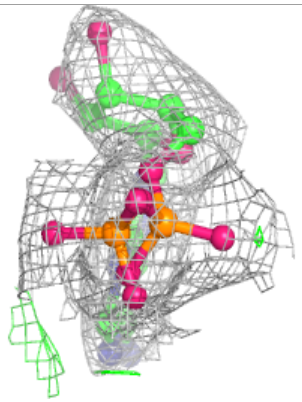


Electron density around ADP A 1301 (B):

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

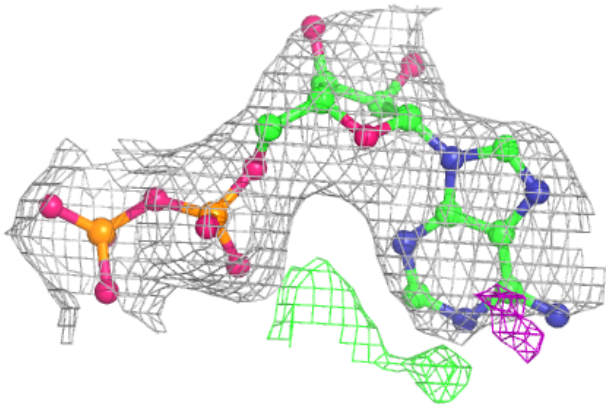


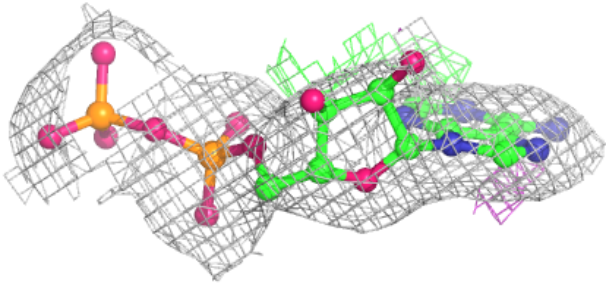


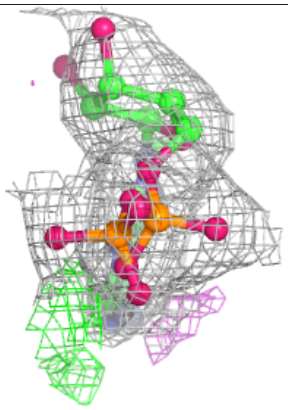


Electron density around ADP B 1301 (A):

$2mF_o$-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.