



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2026 – 01:37 pm BST

PDB ID : 28ZL / pdb_000028zl
Title : Crystal structure of human DHX8 in complex with compound 6 and ADP
Authors : Felisberto-Rodrigues, C.; Silva, S.T.N.; Le Bihan, Y.-V.; van Montfort, R.L.M.
Deposited on : 2026-03-03
Resolution : 2.69 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 : 1.8.4, CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

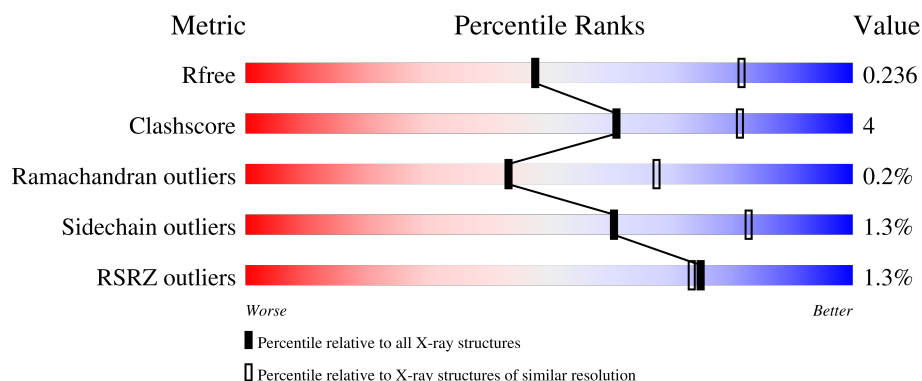
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	680	2% 83% 11% 6%
1	B	680	2% 82% 11% 6%
1	C	680	84% 9% 7%
1	D	680	2% 83% 10% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	1309	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20653 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	636	Total	C	N	O	S	0	11	2
			4996	3190	840	931	35			
1	B	637	Total	C	N	O	S	0	5	0
			4969	3188	825	921	35			
1	C	633	Total	C	N	O	S	0	1	0
			4906	3141	813	918	34			
1	D	633	Total	C	N	O	S	0	1	0
			4861	3113	813	901	34			

There are 28 discrepancies between the modelled and reference sequences:

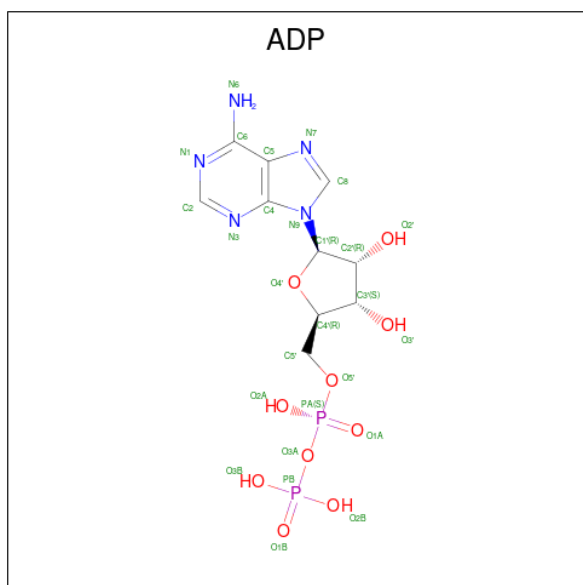
Chain	Residue	Modelled	Actual	Comment	Reference
A	547	MET	-	initiating methionine	UNP Q14562
A	1221	HIS	-	expression tag	UNP Q14562
A	1222	HIS	-	expression tag	UNP Q14562
A	1223	HIS	-	expression tag	UNP Q14562
A	1224	HIS	-	expression tag	UNP Q14562
A	1225	HIS	-	expression tag	UNP Q14562
A	1226	HIS	-	expression tag	UNP Q14562
B	547	MET	-	initiating methionine	UNP Q14562
B	1221	HIS	-	expression tag	UNP Q14562
B	1222	HIS	-	expression tag	UNP Q14562
B	1223	HIS	-	expression tag	UNP Q14562
B	1224	HIS	-	expression tag	UNP Q14562
B	1225	HIS	-	expression tag	UNP Q14562
B	1226	HIS	-	expression tag	UNP Q14562
C	547	MET	-	initiating methionine	UNP Q14562
C	1221	HIS	-	expression tag	UNP Q14562
C	1222	HIS	-	expression tag	UNP Q14562
C	1223	HIS	-	expression tag	UNP Q14562
C	1224	HIS	-	expression tag	UNP Q14562
C	1225	HIS	-	expression tag	UNP Q14562
C	1226	HIS	-	expression tag	UNP Q14562

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Chain	Residue	Modelled	Actual	Comment	Reference
D	547	MET	-	initiating methionine	UNP Q14562
D	1221	HIS	-	expression tag	UNP Q14562
D	1222	HIS	-	expression tag	UNP Q14562
D	1223	HIS	-	expression tag	UNP Q14562
D	1224	HIS	-	expression tag	UNP Q14562
D	1225	HIS	-	expression tag	UNP Q14562
D	1226	HIS	-	expression tag	UNP Q14562

- 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		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

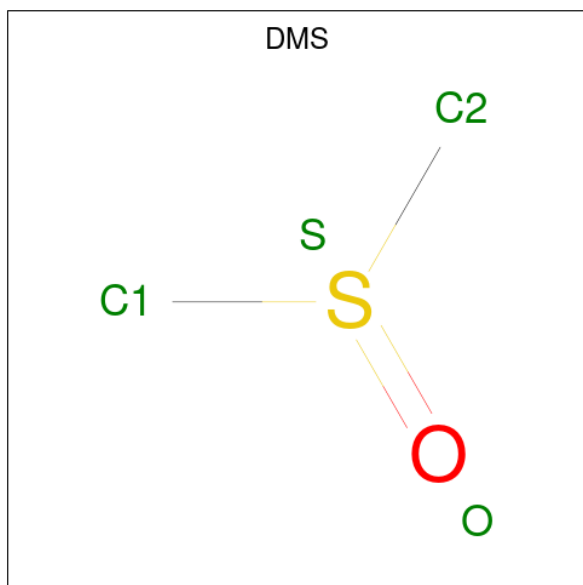
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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 DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



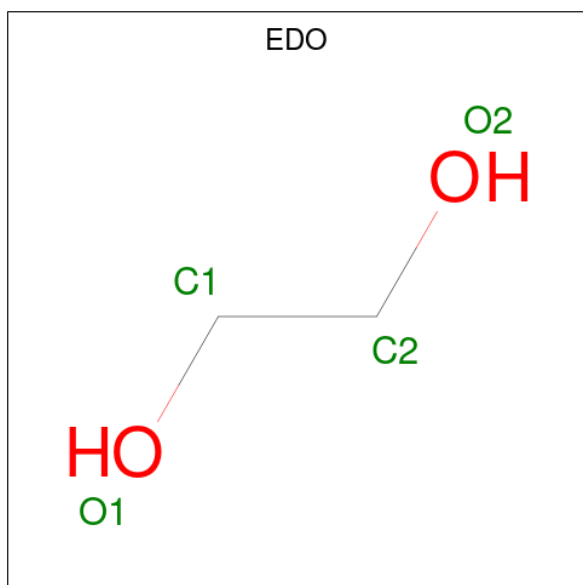
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	C	1	Total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

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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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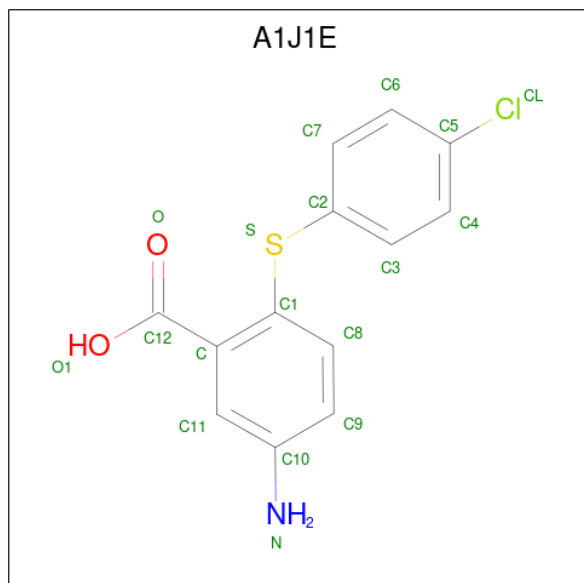
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0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

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

- Molecule 6 is 5-azanyl-2-(4-chlorophenyl)sulfanyl-benzoic acid (CCD ID: A1J1E) (formula: $C_{13}H_{10}ClNO_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	Cl	N	O	S	0	0
			18	13	1	1	2	1		
6	B	1	Total	C	Cl	N	O	S	0	0
			18	13	1	1	2	1		
6	C	1	Total	C	Cl	N	O	S	0	0
			18	13	1	1	2	1		
6	D	1	Total	C	Cl	N	O	S	0	0
			18	13	1	1	2	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	165	Total	O	0	1
			166	166		
7	B	164	Total	O	0	2
			166	166		
7	C	126	Total	O	0	0
			126	126		

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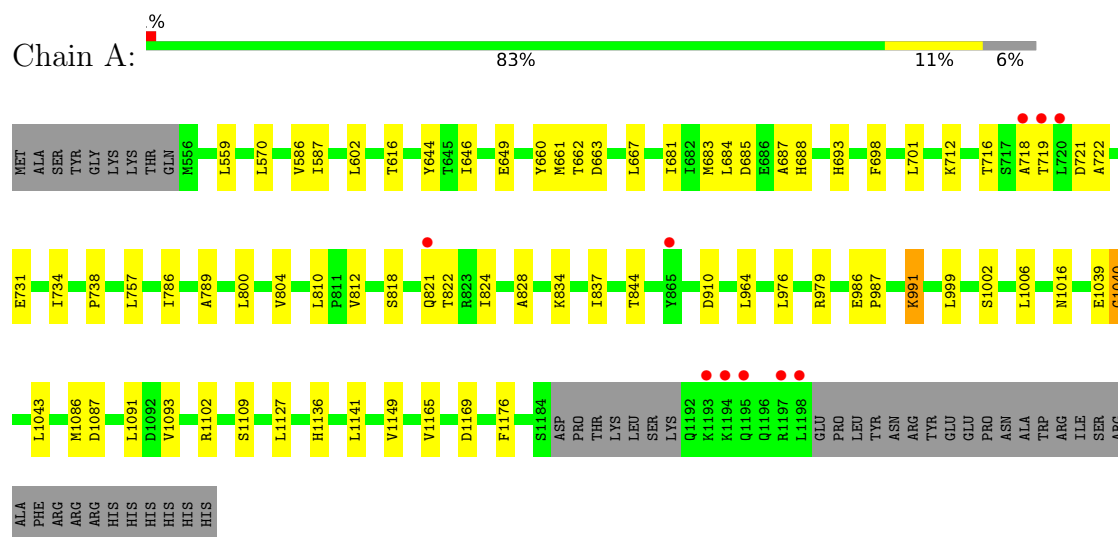
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	111	Total 111	O 111	0	0

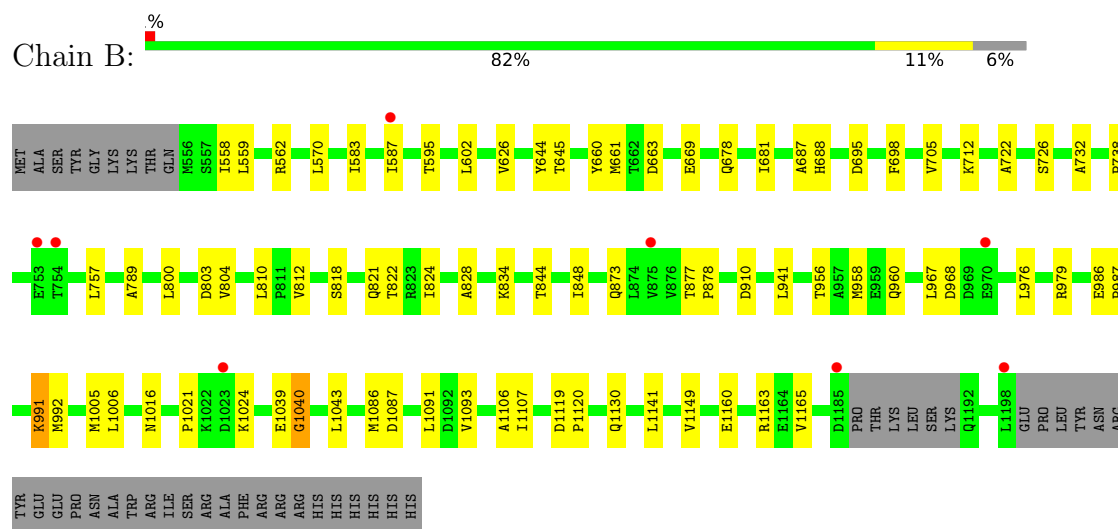
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

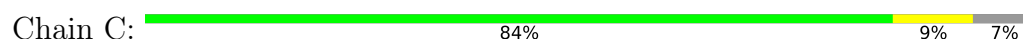
• Molecule 1: ATP-dependent RNA helicase DHX8

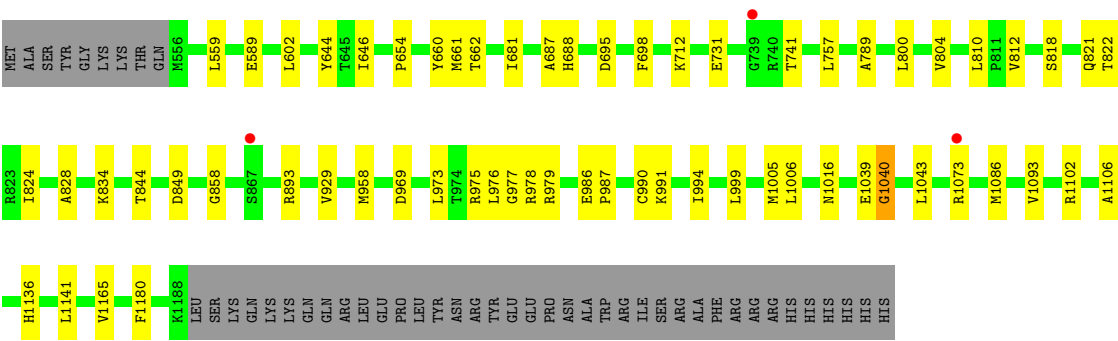


• Molecule 1: ATP-dependent RNA helicase DHX8

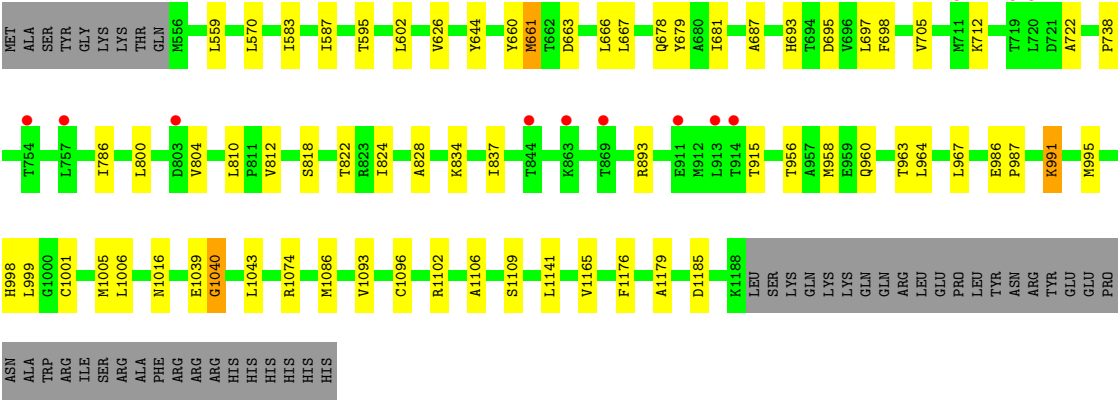
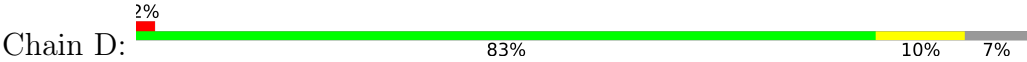


• Molecule 1: ATP-dependent RNA helicase DHX8





● Molecule 1: ATP-dependent RNA helicase DHX8



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.66Å 167.13Å 137.39Å 90.00° 92.59° 90.00°	Depositor
Resolution (Å)	137.25 – 2.69 137.25 – 2.69	Depositor EDS
% Data completeness (in resolution range)	100.0 (137.25-2.69) 100.0 (137.25-2.69)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.10.4 (26-JUL-2023)	Depositor
R, R_{free}	0.207 , 0.242 0.204 , 0.236	Depositor DCC
R_{free} test set	4015 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 73.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.107 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20653	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DMS, A1J1E, ADP, EDO

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	0.67	0/5095	1.00	2/6911 (0.0%)
1	B	0.67	0/5067	1.01	3/6871 (0.0%)
1	C	0.66	0/5005	1.00	2/6796 (0.0%)
1	D	0.66	0/4960	1.01	3/6740 (0.0%)
All	All	0.67	0/20127	1.00	10/27318 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	910	ASP	N-CA-C	8.73	120.87	111.36
1	D	893	ARG	N-CA-C	8.58	120.41	111.14
1	A	910	ASP	N-CA-C	7.35	119.37	111.36
1	C	1180	PHE	CA-CB-CG	7.01	120.81	113.80
1	D	1040	GLY	N-CA-C	6.75	120.55	110.97
1	C	1040	GLY	N-CA-C	6.54	120.26	110.97
1	A	1040	GLY	N-CA-C	6.41	120.08	110.97
1	B	1040	GLY	N-CA-C	6.36	120.00	110.97
1	D	1185	ASP	CA-CB-CG	5.74	118.34	112.60
1	B	968	ASP	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4996	0	4881	51	0
1	B	4969	0	4884	46	0
1	C	4906	0	4777	33	0
1	D	4861	0	4710	39	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	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	16	0	24	4	0
4	B	12	0	18	1	0
4	C	8	0	12	2	0
4	D	4	0	6	1	0
5	A	40	0	60	4	0
5	B	40	0	60	3	0
5	C	20	0	30	0	0
5	D	28	0	42	0	0
6	A	18	0	0	0	0
6	B	18	0	0	0	0
6	C	18	0	0	0	0
6	D	18	0	0	0	0
7	A	166	0	0	0	0
7	B	166	0	0	0	0
7	C	126	0	0	0	0
7	D	111	0	0	0	0
All	All	20653	0	19552	166	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 (166) 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:587[A]:ILE:HD11	1:A:719[A]:THR:HA	1.36	1.04
1:B:941:LEU:H	1:B:941:LEU:HD22	1.32	0.94
1:C:849:ASP:OD1	1:C:893:ARG:NH1	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1141:LEU:HD12	1:A:1165:VAL:HG12	1.67	0.77
1:D:1141:LEU:HD12	1:D:1165:VAL:HG12	1.66	0.76
1:C:1141:LEU:HD12	1:C:1165:VAL:HG12	1.67	0.76
1:B:1141:LEU:HD12	1:B:1165:VAL:HG12	1.67	0.75
1:B:828:ALA:HB2	1:B:834:LYS:HG3	1.70	0.74
1:B:941:LEU:HD22	1:B:941:LEU:N	2.02	0.74
1:B:941:LEU:H	1:B:941:LEU:CD2	2.04	0.70
1:B:688:HIS:CE1	1:B:844:THR:HG21	2.27	0.70
1:A:688:HIS:CE1	1:A:844:THR:HG21	2.27	0.70
1:A:712:LYS:NZ	5:A:1309:EDO:H12	2.07	0.68
1:D:995:MET:HE3	1:D:998:HIS:HD2	1.60	0.67
1:C:1136:HIS:CE1	4:C:1306:DMS:H12	2.30	0.67
1:A:1136:HIS:NE2	4:A:1314:DMS:H23	2.14	0.62
1:B:669:GLU:OE1	1:B:678:GLN:NE2	2.33	0.62
1:D:963:THR:HG22	1:D:1179:ALA:HB3	1.82	0.60
1:C:688:HIS:CE1	1:C:844:THR:HG21	2.36	0.60
1:C:828:ALA:HB2	1:C:834:LYS:HG3	1.84	0.59
1:A:688:HIS:HE1	1:A:844:THR:HG21	1.68	0.59
1:D:995:MET:HE3	1:D:998:HIS:CD2	2.37	0.58
1:A:1039:GLU:HB2	1:A:1043:LEU:HD12	1.85	0.58
1:A:828:ALA:HB2	1:A:834:LYS:HG3	1.85	0.58
1:D:583:ILE:HD11	1:D:705:VAL:HG21	1.85	0.58
1:A:602:LEU:HD13	1:A:681:ILE:HD13	1.86	0.57
1:C:1039:GLU:HB2	1:C:1043:LEU:HD12	1.86	0.57
1:D:1039:GLU:HB2	1:D:1043:LEU:HD12	1.86	0.57
1:A:757:LEU:HD11	1:A:789:ALA:HB2	1.86	0.57
1:B:873:GLN:NE2	1:B:1160:GLU:OE2	2.30	0.57
1:D:828:ALA:HB2	1:D:834:LYS:HG3	1.85	0.57
1:B:1039:GLU:HB2	1:B:1043:LEU:HD12	1.87	0.57
1:C:757:LEU:HD11	1:C:789:ALA:HB2	1.86	0.56
1:A:712:LYS:HZ3	5:A:1309:EDO:H12	1.68	0.56
1:B:1163:ARG:HG3	5:B:1310:EDO:H12	1.87	0.55
1:B:602:LEU:HD13	1:B:681:ILE:HD13	1.88	0.55
1:D:958:MET:HE2	4:D:1305:DMS:H12	1.89	0.55
1:D:595:THR:HG22	1:D:626:VAL:HG11	1.88	0.55
1:B:757:LEU:HD11	1:B:789:ALA:HB2	1.89	0.54
1:A:999:LEU:O	1:A:1102:ARG:HD3	2.07	0.54
1:B:688:HIS:HE1	1:B:844:THR:HG21	1.73	0.54
1:B:824:ILE:HD12	1:B:848:ILE:HD11	1.90	0.53
1:C:973:LEU:HD13	1:C:978:ARG:HG2	1.91	0.53
1:C:999:LEU:O	1:C:1102:ARG:HD3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:602:LEU:HD13	1:C:681:ILE:HD13	1.89	0.53
1:D:602:LEU:HD13	1:D:681:ILE:HD13	1.90	0.53
1:B:956:THR:HG22	1:B:960:GLN:HE21	1.74	0.53
1:A:587[A]:ILE:HD11	1:A:719[A]:THR:CA	2.25	0.52
1:B:1021:PRO:HG2	1:B:1024:LYS:HB2	1.92	0.52
1:C:973:LEU:HD22	1:C:977:GLY:HA3	1.91	0.52
1:B:992:MET:HG3	1:B:1107:ILE:HA	1.92	0.51
1:D:964:LEU:HD22	1:D:991:LYS:HG3	1.91	0.51
1:D:999:LEU:O	1:D:1102:ARG:HD3	2.11	0.50
1:A:587[A]:ILE:CD1	1:A:719[A]:THR:HA	2.25	0.50
1:A:587[B]:ILE:CG1	1:A:722[B]:ALA:HB2	2.42	0.49
1:B:558:ILE:O	1:B:562:ARG:HG3	2.11	0.49
1:D:661:MET:HE1	1:D:679:TYR:OH	2.12	0.49
1:A:1136:HIS:CD2	4:A:1314:DMS:H23	2.48	0.49
1:A:712:LYS:HZ2	5:A:1309:EDO:H12	1.78	0.48
1:C:858:GLY:HA3	4:C:1304:DMS:H13	1.95	0.48
1:B:821:GLN:O	1:B:824:ILE:HG12	2.13	0.48
1:C:821:GLN:O	1:C:824:ILE:HG12	2.13	0.48
1:D:1005:MET:HE3	1:D:1106:ALA:HB3	1.95	0.48
1:C:654:PRO:HG2	1:D:1074:ARG:HD3	1.96	0.48
1:C:1086:MET:HE3	1:C:1093:VAL:HG22	1.96	0.47
1:D:667:LEU:HD23	1:D:693:HIS:HD2	1.78	0.47
1:A:587[A]:ILE:HD12	1:A:722[A]:ALA:HB2	1.94	0.47
1:D:995:MET:CE	1:D:998:HIS:CD2	2.98	0.47
1:C:688:HIS:HE1	1:C:844:THR:HG21	1.79	0.47
1:A:718[A]:ALA:HB3	1:A:721[A]:ASP:HB2	1.98	0.46
1:A:1002:SER:HB2	1:A:1086:MET:HE1	1.97	0.46
1:A:1086:MET:HE3	1:A:1093:VAL:HG22	1.98	0.46
1:A:964:LEU:HD22	1:A:991:LYS:HG3	1.96	0.46
1:B:1086:MET:HE3	1:B:1093:VAL:HG22	1.98	0.46
1:A:646:ILE:HG22	1:A:662:THR:HG23	1.97	0.46
1:A:821:GLN:O	1:A:824:ILE:HG12	2.15	0.46
1:D:687:ALA:HB1	1:D:698:PHE:HZ	1.81	0.46
1:A:616:THR:O	1:A:685:ASP:HB3	2.15	0.45
1:A:1136:HIS:CD2	4:A:1314:DMS:C2	2.99	0.45
1:B:726:SER:OG	1:B:732:ALA:O	2.34	0.45
1:D:666:LEU:HD23	1:D:697:LEU:HD13	1.98	0.45
1:D:1086:MET:HE3	1:D:1093:VAL:HG22	1.97	0.45
1:B:687:ALA:HB1	1:B:698:PHE:HZ	1.81	0.45
1:B:1119:ASP:OD1	1:B:1120:PRO:HD2	2.17	0.45
1:B:583:ILE:HD11	1:B:705:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:877:THR:HG22	5:B:1316:EDO:H22	1.97	0.45
1:C:1073[B]:ARG:NH2	1:D:678:GLN:OE1	2.50	0.45
1:C:1005:MET:HE3	1:C:1106:ALA:HB3	1.99	0.45
1:B:644:TYR:HA	1:B:660:TYR:O	2.17	0.45
1:D:681:ILE:HG12	1:D:712:LYS:HB2	1.99	0.45
1:C:589:GLU:HG2	1:C:741:THR:CG2	2.47	0.45
1:A:687:ALA:HB1	1:A:698:PHE:HZ	1.82	0.45
1:B:976:LEU:HD21	1:B:991:LYS:HE3	1.99	0.45
1:C:644:TYR:HA	1:C:660:TYR:O	2.17	0.45
1:A:681:ILE:HG12	1:A:712:LYS:HB2	1.99	0.44
1:B:1005:MET:HE3	1:B:1106:ALA:HB3	1.99	0.44
1:C:929:VAL:HG11	1:C:958:MET:HG2	1.99	0.44
1:D:958:MET:HE3	1:D:967:LEU:HD13	1.99	0.44
1:D:995:MET:CE	1:D:998:HIS:HD2	2.28	0.44
1:D:818:SER:O	1:D:822:THR:HG23	2.17	0.44
1:C:681:ILE:HG12	1:C:712:LYS:HB2	1.98	0.44
1:A:586:VAL:HB	1:A:716[B]:THR:HG22	2.00	0.44
1:B:681:ILE:HG12	1:B:712:LYS:HB2	1.99	0.43
1:B:812:VAL:HG22	1:B:824:ILE:HG21	2.00	0.43
1:A:684:LEU:HD11	1:A:701:LEU:HD13	1.99	0.43
1:B:958:MET:HE3	1:B:967:LEU:HD13	2.00	0.43
1:C:986:GLU:HG2	1:C:987:PRO:HD2	2.01	0.43
1:A:644:TYR:HA	1:A:660:TYR:O	2.19	0.43
1:A:812:VAL:HG22	1:A:824:ILE:HG21	2.00	0.43
1:A:976:LEU:HD21	1:A:991:LYS:HE3	2.00	0.43
1:D:1109:SER:HA	1:D:1176:PHE:HB3	2.00	0.43
1:A:818:SER:O	1:A:822:THR:HG23	2.19	0.43
1:B:595:THR:HG22	1:B:626:VAL:HG11	2.01	0.43
1:A:1040:GLY:HA2	1:A:1141:LEU:HG	2.00	0.43
1:D:644:TYR:HA	1:D:660:TYR:O	2.18	0.43
1:A:800:LEU:HB3	1:A:804:VAL:HG21	2.01	0.43
1:C:1040:GLY:HA2	1:C:1141:LEU:HG	2.00	0.43
1:A:1169:ASP:HB2	4:A:1304:DMS:H11	2.01	0.42
1:C:800:LEU:HB3	1:C:804:VAL:HG21	2.00	0.42
1:B:878:PRO:HB3	4:B:1306:DMS:H21	2.01	0.42
1:C:976:LEU:HD12	1:C:994:ILE:HG21	2.01	0.42
1:D:800:LEU:HB3	1:D:804:VAL:HG21	2.01	0.42
1:D:956:THR:HG22	1:D:960:GLN:HE21	1.84	0.42
1:A:570:LEU:HD11	1:A:738:PRO:HD3	2.02	0.42
1:D:812:VAL:HG22	1:D:824:ILE:HG21	2.01	0.42
1:A:1149:VAL:HB	1:A:1165:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:645:THR:O	1:B:661:MET:HB2	2.20	0.42
1:C:687:ALA:HB1	1:C:698:PHE:HZ	1.85	0.42
1:A:683:MET:HE3	1:A:716[B]:THR:HG21	2.02	0.42
1:A:786:ILE:HG12	1:A:837:ILE:HG22	2.02	0.42
1:A:979:ARG:HD2	1:A:1091:LEU:HD21	2.01	0.42
1:A:986:GLU:HG2	1:A:987:PRO:HD2	2.02	0.42
1:B:986:GLU:HG2	1:B:987:PRO:HD2	2.01	0.42
1:C:812:VAL:HG22	1:C:824:ILE:HG21	2.02	0.42
1:A:810:LEU:HD13	1:A:824:ILE:HA	2.02	0.42
1:B:1006:LEU:HD11	1:B:1086:MET:HE2	2.02	0.42
1:A:667:LEU:HD23	1:A:693:HIS:HD2	1.84	0.42
1:B:800:LEU:HB3	1:B:804:VAL:HG21	2.01	0.42
1:B:958:MET:HE2	1:B:958:MET:HB3	1.93	0.42
1:D:963:THR:HG22	1:D:1179:ALA:CB	2.49	0.42
1:C:810:LEU:HD13	1:C:824:ILE:HA	2.01	0.41
1:C:1006:LEU:HD11	1:C:1086:MET:HE2	2.02	0.41
1:D:570:LEU:HD11	1:D:738:PRO:HD3	2.02	0.41
1:D:587[A]:ILE:HG21	1:D:722:ALA:HB2	2.02	0.41
1:B:570:LEU:HD11	1:B:738:PRO:HD3	2.02	0.41
1:C:818:SER:O	1:C:822:THR:HG23	2.21	0.41
1:D:786:ILE:HG12	1:D:837:ILE:HG22	2.02	0.41
1:D:810:LEU:HD13	1:D:824:ILE:HA	2.01	0.41
1:A:722[B]:ALA:HB1	1:A:734:ILE:HD13	2.03	0.41
1:A:1109:SER:HA	1:A:1176:PHE:HB3	2.02	0.41
1:D:1006:LEU:HD11	1:D:1086:MET:HE2	2.01	0.41
1:A:1006:LEU:HD11	1:A:1086:MET:HE2	2.02	0.41
1:B:1040:GLY:HA2	1:B:1141:LEU:HG	2.02	0.41
1:D:1001:CYS:HB3	1:D:1096:CYS:HB3	2.02	0.41
1:B:587[B]:ILE:HG21	1:B:722:ALA:HB2	2.02	0.41
1:B:979:ARG:HD2	1:B:1091:LEU:HD21	2.02	0.41
1:C:646:ILE:HG22	1:C:662:THR:HG23	2.02	0.41
1:A:712:LYS:HZ3	5:A:1309:EDO:C1	2.33	0.41
1:A:649:GLU:HG3	5:B:1305:EDO:H21	2.02	0.41
1:B:1149:VAL:HB	1:B:1165:VAL:HG13	2.03	0.41
1:B:810:LEU:HD13	1:B:824:ILE:HA	2.02	0.40
1:D:1040:GLY:HA2	1:D:1141:LEU:HG	2.01	0.40
1:A:1087:ASP:HB3	1:B:1087:ASP:HB3	2.03	0.40
1:B:818:SER:O	1:B:822:THR:HG23	2.21	0.40
1:C:990:CYS:O	1:C:994:ILE:HG12	2.21	0.40
1:D:986:GLU:HG2	1:D:987:PRO:HD2	2.03	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	643/680 (95%)	622 (97%)	20 (3%)	1 (0%)	43	68
1	B	638/680 (94%)	620 (97%)	17 (3%)	1 (0%)	43	68
1	C	632/680 (93%)	615 (97%)	16 (2%)	1 (0%)	43	68
1	D	632/680 (93%)	614 (97%)	17 (3%)	1 (0%)	43	68
All	All	2545/2720 (94%)	2471 (97%)	70 (3%)	4 (0%)	43	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1016	ASN
1	B	1016	ASN
1	C	1016	ASN
1	D	1016	ASN

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	516/603 (86%)	510 (99%)	6 (1%)	63	84
1	B	512/603 (85%)	506 (99%)	6 (1%)	63	84
1	C	505/603 (84%)	497 (98%)	8 (2%)	55	80
1	D	492/603 (82%)	486 (99%)	6 (1%)	63	84
All	All	2025/2412 (84%)	1999 (99%)	26 (1%)	61	83

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	559	LEU
1	A	661	MET
1	A	663	ASP
1	A	731	GLU
1	A	991	LYS
1	A	1127	LEU
1	B	559	LEU
1	B	663	ASP
1	B	695	ASP
1	B	803	ASP
1	B	991	LYS
1	B	1130	GLN
1	C	559	LEU
1	C	661	MET
1	C	695	ASP
1	C	731	GLU
1	C	969	ASP
1	C	975	ARG
1	C	979	ARG
1	C	991	LYS
1	D	559	LEU
1	D	661	MET
1	D	663	ASP
1	D	695	ASP
1	D	915	THR
1	D	991	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	579	HIS
1	A	688	HIS
1	A	693	HIS
1	A	706	GLN
1	A	727	GLN
1	A	886	GLN
1	A	924	ASN
1	A	938	ASN
1	A	1016	ASN
1	B	688	HIS
1	B	693	HIS

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Mol	Chain	Res	Type
1	B	886	GLN
1	B	924	ASN
1	B	938	ASN
1	B	960	GLN
1	B	1016	ASN
1	B	1037	GLN
1	C	576	GLN
1	C	886	GLN
1	C	924	ASN
1	C	960	GLN
1	C	1016	ASN
1	C	1059	ASN
1	D	579	HIS
1	D	693	HIS
1	D	727	GLN
1	D	938	ASN
1	D	998	HIS
1	D	1016	ASN
1	D	1143	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 54 ligands modelled in this entry, 4 are monoatomic - leaving 50 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	DMS	B	1314	-	3,3,3	0.76	0	3,3,3	0.48	0
5	EDO	B	1308	-	3,3,3	0.37	0	2,2,2	0.08	0
5	EDO	A	1306	-	3,3,3	0.19	0	2,2,2	0.46	0
5	EDO	C	1308	-	3,3,3	0.25	0	2,2,2	0.29	0
4	DMS	B	1311	-	3,3,3	0.71	0	3,3,3	0.41	0
5	EDO	B	1307	-	3,3,3	0.25	0	2,2,2	0.24	0
5	EDO	B	1316	-	3,3,3	0.33	0	2,2,2	0.24	0
5	EDO	D	1307	-	3,3,3	0.28	0	2,2,2	0.25	0
2	ADP	C	1301	3	27,29,29	0.79	1 (3%)	42,45,45	0.72	2 (4%)
5	EDO	D	1311	-	3,3,3	0.21	0	2,2,2	0.36	0
5	EDO	A	1309	-	3,3,3	0.34	0	2,2,2	0.16	0
5	EDO	B	1305	-	3,3,3	0.19	0	2,2,2	0.35	0
5	EDO	C	1305	-	3,3,3	0.18	0	2,2,2	0.37	0
4	DMS	A	1303	-	3,3,3	0.72	0	3,3,3	0.33	0
5	EDO	B	1313	-	3,3,3	0.38	0	2,2,2	0.11	0
5	EDO	D	1306	-	3,3,3	0.24	0	2,2,2	0.13	0
4	DMS	B	1306	-	3,3,3	0.57	0	3,3,3	0.30	0
5	EDO	A	1311	-	3,3,3	0.57	0	2,2,2	0.26	0
5	EDO	A	1317	-	3,3,3	0.18	0	2,2,2	0.34	0
4	DMS	D	1305	-	3,3,3	0.67	0	3,3,3	0.32	0
5	EDO	B	1310	-	3,3,3	0.23	0	2,2,2	0.29	0
2	ADP	B	1301	3	27,29,29	0.85	2 (7%)	42,45,45	0.58	0
6	A1J1E	B	1312	-	19,19,19	0.20	0	26,26,26	0.36	0
5	EDO	C	1307	-	3,3,3	0.31	0	2,2,2	0.27	0
6	A1J1E	D	1310	-	19,19,19	0.23	0	26,26,26	0.27	0
5	EDO	A	1313	-	3,3,3	0.38	0	2,2,2	0.34	0
2	ADP	D	1301	3	27,29,29	0.92	2 (7%)	42,45,45	0.57	1 (2%)
5	EDO	B	1304	-	3,3,3	0.25	0	2,2,2	0.34	0
4	DMS	A	1314	-	3,3,3	0.64	0	3,3,3	0.35	0
4	DMS	A	1308	-	3,3,3	0.63	0	3,3,3	0.49	0
5	EDO	B	1315	-	3,3,3	0.26	0	2,2,2	0.27	0
4	DMS	C	1306	-	3,3,3	0.72	0	3,3,3	0.52	0
5	EDO	B	1309	-	3,3,3	0.32	0	2,2,2	0.15	0
5	EDO	C	1303	-	3,3,3	0.30	0	2,2,2	0.12	0
5	EDO	A	1305	-	3,3,3	0.31	0	2,2,2	0.03	0
5	EDO	D	1304	-	3,3,3	0.28	0	2,2,2	0.21	0
5	EDO	A	1310	-	3,3,3	0.24	0	2,2,2	0.19	0
4	DMS	A	1304	-	3,3,3	0.65	0	3,3,3	0.34	0
6	A1J1E	A	1312	-	19,19,19	0.22	0	26,26,26	0.28	0
6	A1J1E	C	1309	-	19,19,19	0.21	0	26,26,26	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	C	1310	-	3,3,3	0.28	0	2,2,2	0.21	0
5	EDO	D	1308	-	3,3,3	0.23	0	2,2,2	0.34	0
5	EDO	A	1307	-	3,3,3	0.28	0	2,2,2	0.26	0
5	EDO	D	1303	-	3,3,3	0.38	0	2,2,2	0.05	0
5	EDO	B	1303	-	3,3,3	0.20	0	2,2,2	0.18	0
5	EDO	A	1315	-	3,3,3	0.29	0	2,2,2	0.17	0
5	EDO	D	1309	-	3,3,3	0.19	0	2,2,2	0.43	0
5	EDO	A	1316	-	3,3,3	0.32	0	2,2,2	0.10	0
4	DMS	C	1304	-	3,3,3	0.56	0	3,3,3	0.46	0
2	ADP	A	1301	3	27,29,29	0.89	2 (7%)	42,45,45	0.60	1 (2%)

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
5	EDO	B	1308	-	-	0/1/1/1	-
5	EDO	A	1306	-	-	1/1/1/1	-
5	EDO	C	1308	-	-	1/1/1/1	-
5	EDO	B	1307	-	-	0/1/1/1	-
5	EDO	B	1316	-	-	1/1/1/1	-
5	EDO	D	1307	-	-	0/1/1/1	-
2	ADP	C	1301	3	-	2/16/32/32	0/3/3/3
5	EDO	D	1311	-	-	1/1/1/1	-
5	EDO	A	1309	-	-	1/1/1/1	-
5	EDO	B	1305	-	-	1/1/1/1	-
5	EDO	C	1305	-	-	1/1/1/1	-
5	EDO	B	1313	-	-	1/1/1/1	-
5	EDO	D	1306	-	-	0/1/1/1	-
5	EDO	A	1311	-	-	0/1/1/1	-
5	EDO	A	1317	-	-	0/1/1/1	-
5	EDO	B	1310	-	-	0/1/1/1	-
2	ADP	B	1301	3	-	3/16/32/32	0/3/3/3
6	A1J1E	B	1312	-	-	4/8/8/8	0/2/2/2
5	EDO	C	1307	-	-	1/1/1/1	-
6	A1J1E	D	1310	-	-	4/8/8/8	0/2/2/2
5	EDO	A	1313	-	-	0/1/1/1	-
2	ADP	D	1301	3	-	5/16/32/32	0/3/3/3
5	EDO	B	1304	-	-	1/1/1/1	-
5	EDO	B	1315	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	1303	-	-	0/1/1/1	-
5	EDO	B	1309	-	-	1/1/1/1	-
5	EDO	A	1305	-	-	0/1/1/1	-
5	EDO	D	1304	-	-	1/1/1/1	-
5	EDO	A	1310	-	-	0/1/1/1	-
6	A1J1E	A	1312	-	-	4/8/8/8	0/2/2/2
6	A1J1E	C	1309	-	-	4/8/8/8	0/2/2/2
5	EDO	C	1310	-	-	0/1/1/1	-
5	EDO	D	1308	-	-	0/1/1/1	-
5	EDO	A	1307	-	-	0/1/1/1	-
5	EDO	D	1303	-	-	1/1/1/1	-
5	EDO	B	1303	-	-	0/1/1/1	-
5	EDO	A	1315	-	-	0/1/1/1	-
5	EDO	D	1309	-	-	0/1/1/1	-
5	EDO	A	1316	-	-	0/1/1/1	-
2	ADP	A	1301	3	-	2/16/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1301	ADP	PB-O1B	-2.88	1.41	1.50
2	A	1301	ADP	PB-O1B	-2.77	1.41	1.50
2	B	1301	ADP	PB-O1B	-2.47	1.42	1.50
2	C	1301	ADP	PB-O2B	-2.26	1.46	1.54
2	D	1301	ADP	PB-O2B	-2.22	1.46	1.54
2	A	1301	ADP	PB-O2B	-2.21	1.46	1.54
2	B	1301	ADP	PB-O2B	-2.12	1.46	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1301	ADP	PA-O3A-PB	2.68	142.02	132.83
2	C	1301	ADP	C4'-O4'-C1'	-2.41	104.16	109.47
2	D	1301	ADP	C4'-O4'-C1'	-2.26	104.48	109.47
2	A	1301	ADP	PA-O3A-PB	2.10	140.01	132.83

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1301	ADP	C5'-O5'-PA-O1A

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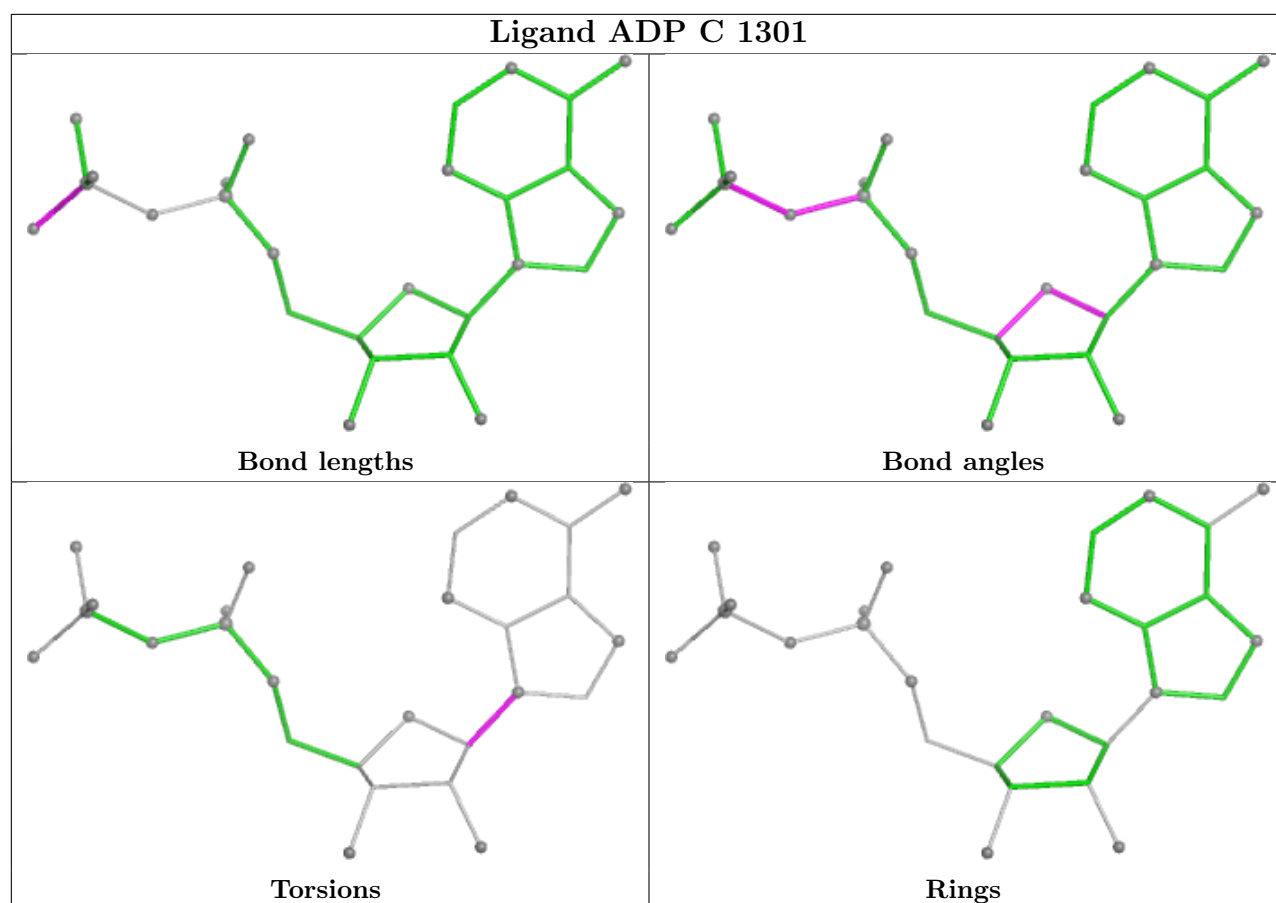
Mol	Chain	Res	Type	Atoms
2	B	1301	ADP	O4'-C1'-N9-C4
5	A	1309	EDO	O1-C1-C2-O2
5	B	1304	EDO	O1-C1-C2-O2
5	B	1305	EDO	O1-C1-C2-O2
5	C	1307	EDO	O1-C1-C2-O2
5	D	1304	EDO	O1-C1-C2-O2
5	B	1316	EDO	O1-C1-C2-O2
5	D	1311	EDO	O1-C1-C2-O2
6	B	1312	A1J1E	C1-C-C12-O1
2	B	1301	ADP	O4'-C1'-N9-C8
2	C	1301	ADP	O4'-C1'-N9-C4
6	C	1309	A1J1E	C1-C-C12-O1
5	A	1306	EDO	O1-C1-C2-O2
5	C	1308	EDO	O1-C1-C2-O2
2	A	1301	ADP	O4'-C1'-N9-C4
2	B	1301	ADP	C5'-O5'-PA-O3A
2	D	1301	ADP	C5'-O5'-PA-O3A
6	B	1312	A1J1E	C11-C-C12-O1
6	A	1312	A1J1E	C1-C-C12-O1
6	B	1312	A1J1E	C1-C-C12-O
6	C	1309	A1J1E	C1-C-C12-O
2	D	1301	ADP	C5'-O5'-PA-O2A
6	B	1312	A1J1E	C11-C-C12-O
6	C	1309	A1J1E	C11-C-C12-O
6	A	1312	A1J1E	C11-C-C12-O
2	A	1301	ADP	O4'-C1'-N9-C8
2	C	1301	ADP	O4'-C1'-N9-C8
6	D	1310	A1J1E	C11-C-C12-O
6	A	1312	A1J1E	C1-C-C12-O
6	D	1310	A1J1E	C1-C-C12-O1
6	D	1310	A1J1E	C11-C-C12-O1
6	C	1309	A1J1E	C11-C-C12-O1
6	A	1312	A1J1E	C11-C-C12-O1
2	D	1301	ADP	O4'-C4'-C5'-O5'
5	B	1309	EDO	O1-C1-C2-O2
5	D	1303	EDO	O1-C1-C2-O2
6	D	1310	A1J1E	C1-C-C12-O
5	C	1305	EDO	O1-C1-C2-O2
2	D	1301	ADP	O4'-C1'-N9-C8
5	B	1313	EDO	O1-C1-C2-O2

There are no ring outliers.

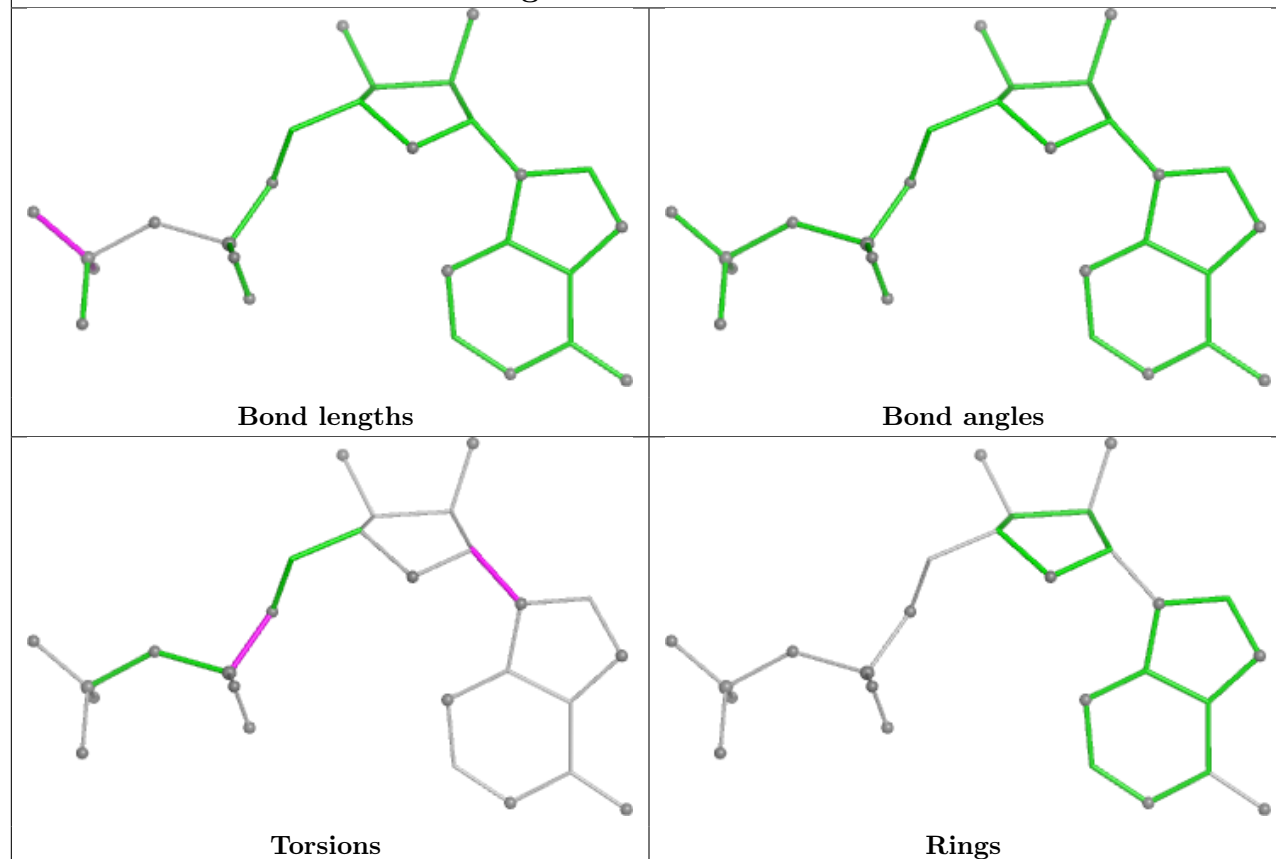
10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1316	EDO	1	0
5	A	1309	EDO	4	0
5	B	1305	EDO	1	0
4	B	1306	DMS	1	0
4	D	1305	DMS	1	0
5	B	1310	EDO	1	0
4	A	1314	DMS	3	0
4	C	1306	DMS	1	0
4	A	1304	DMS	1	0
4	C	1304	DMS	1	0

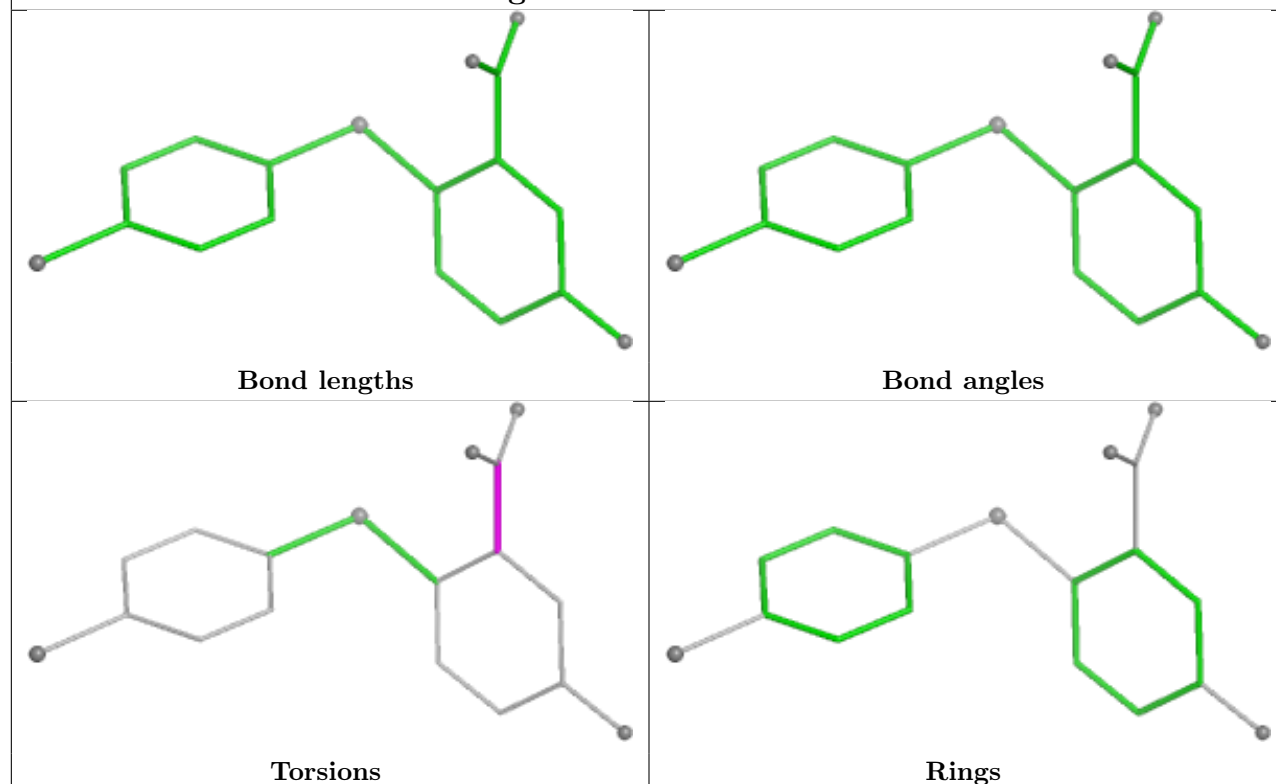
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



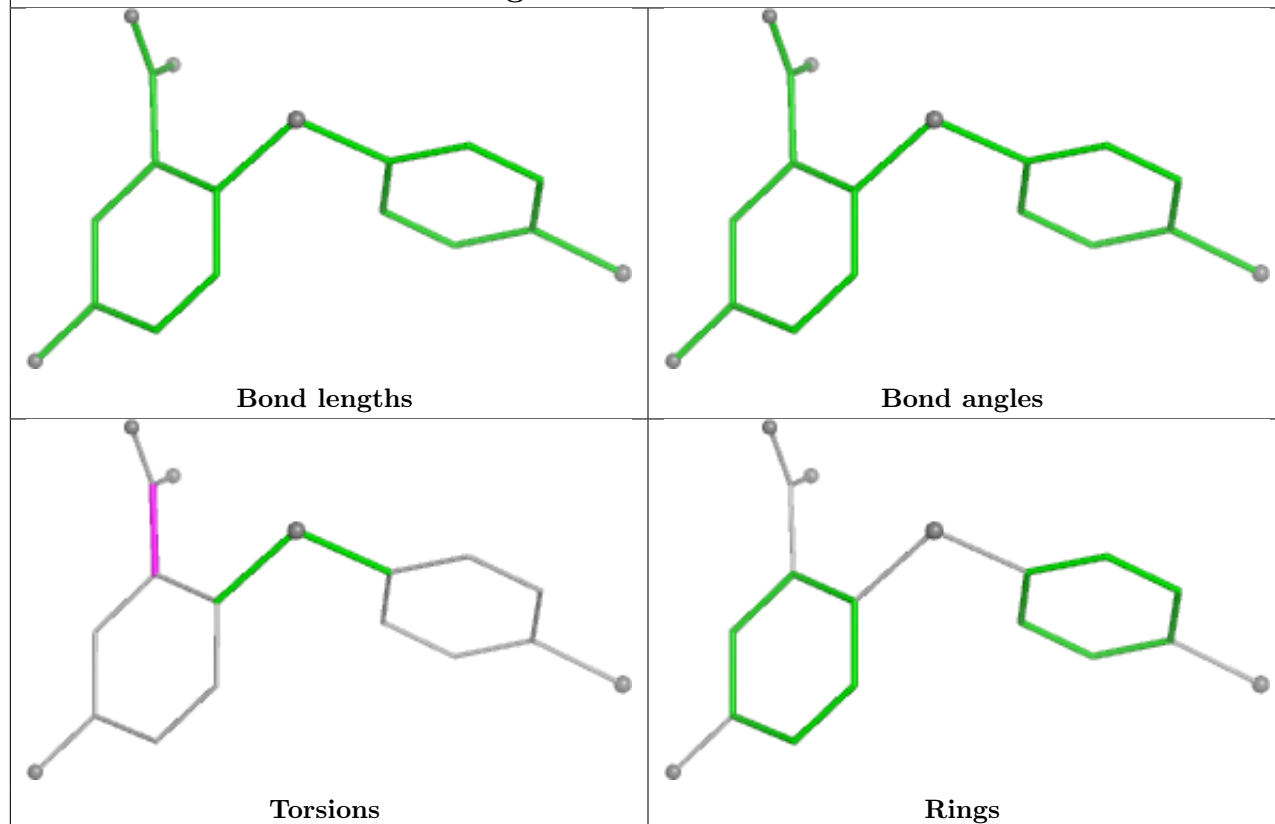
Ligand ADP B 1301



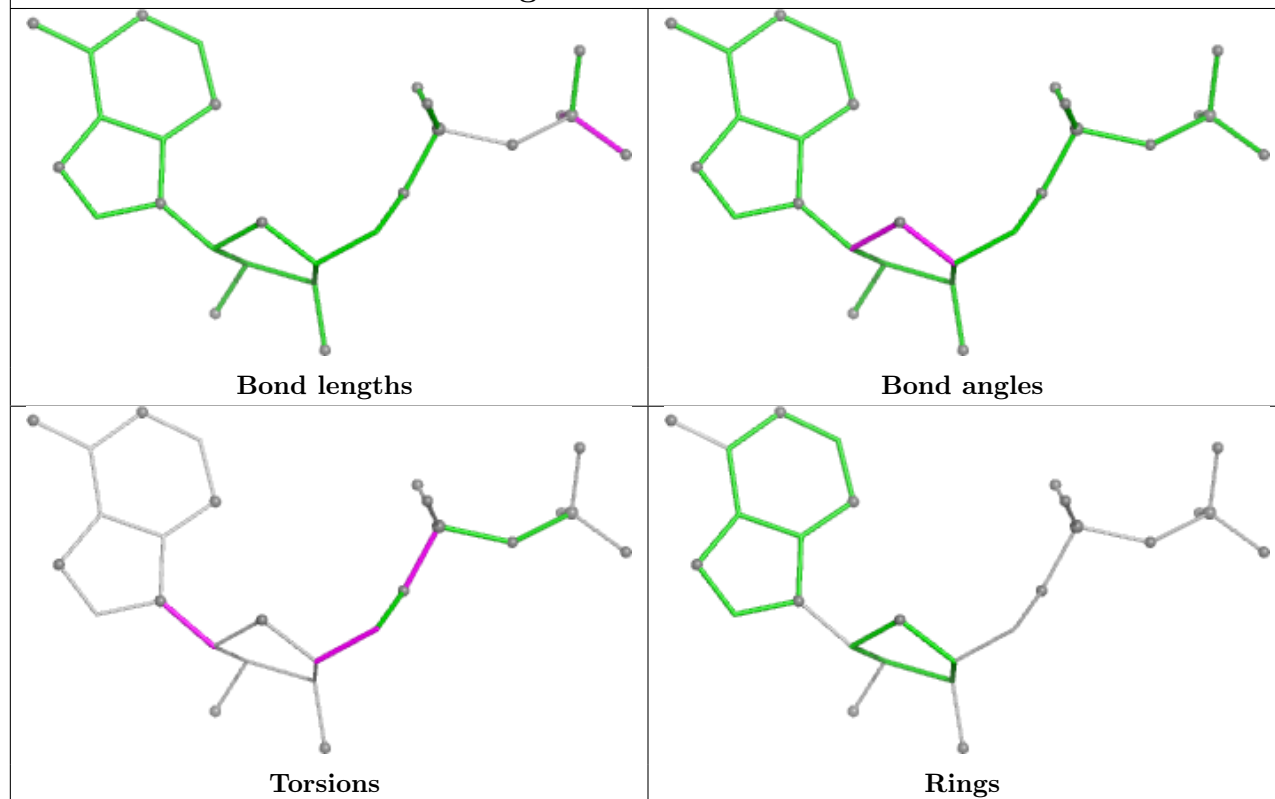
Ligand A1J1E B 1312



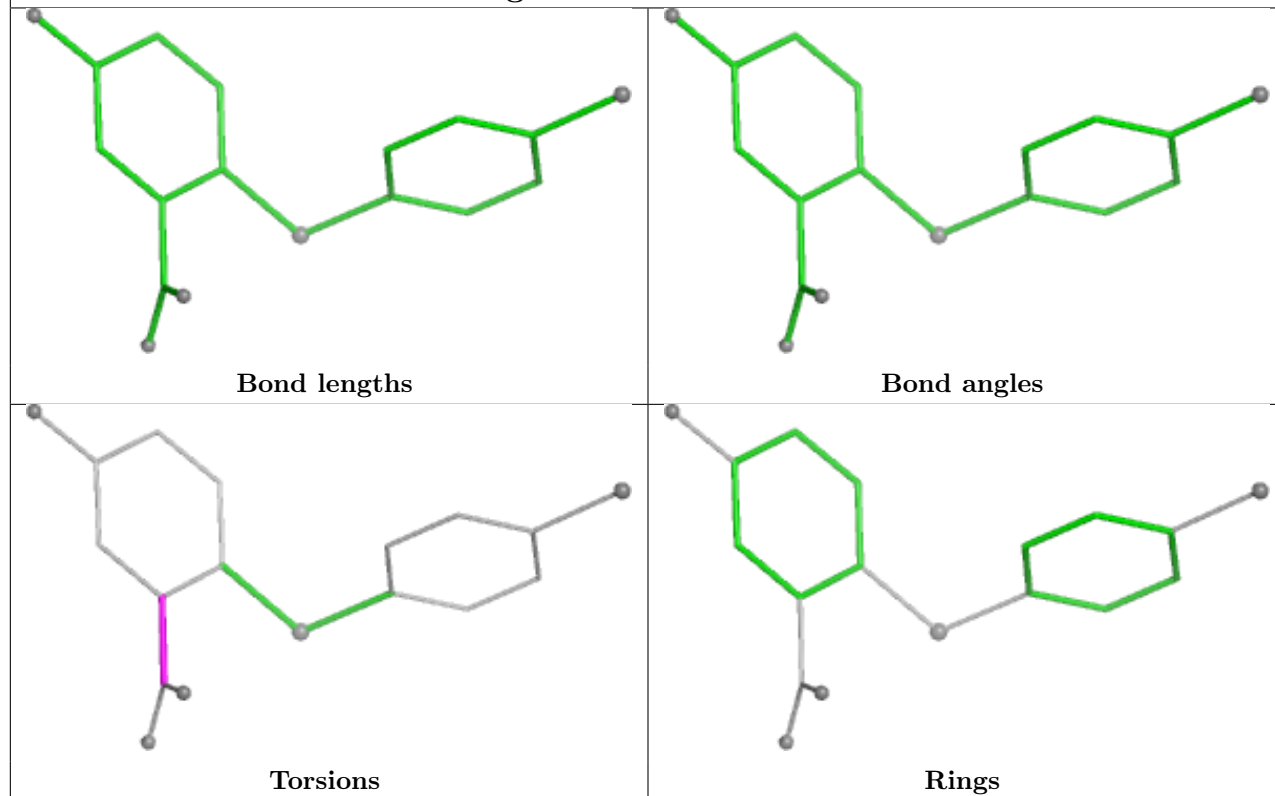
Ligand A1J1E D 1310



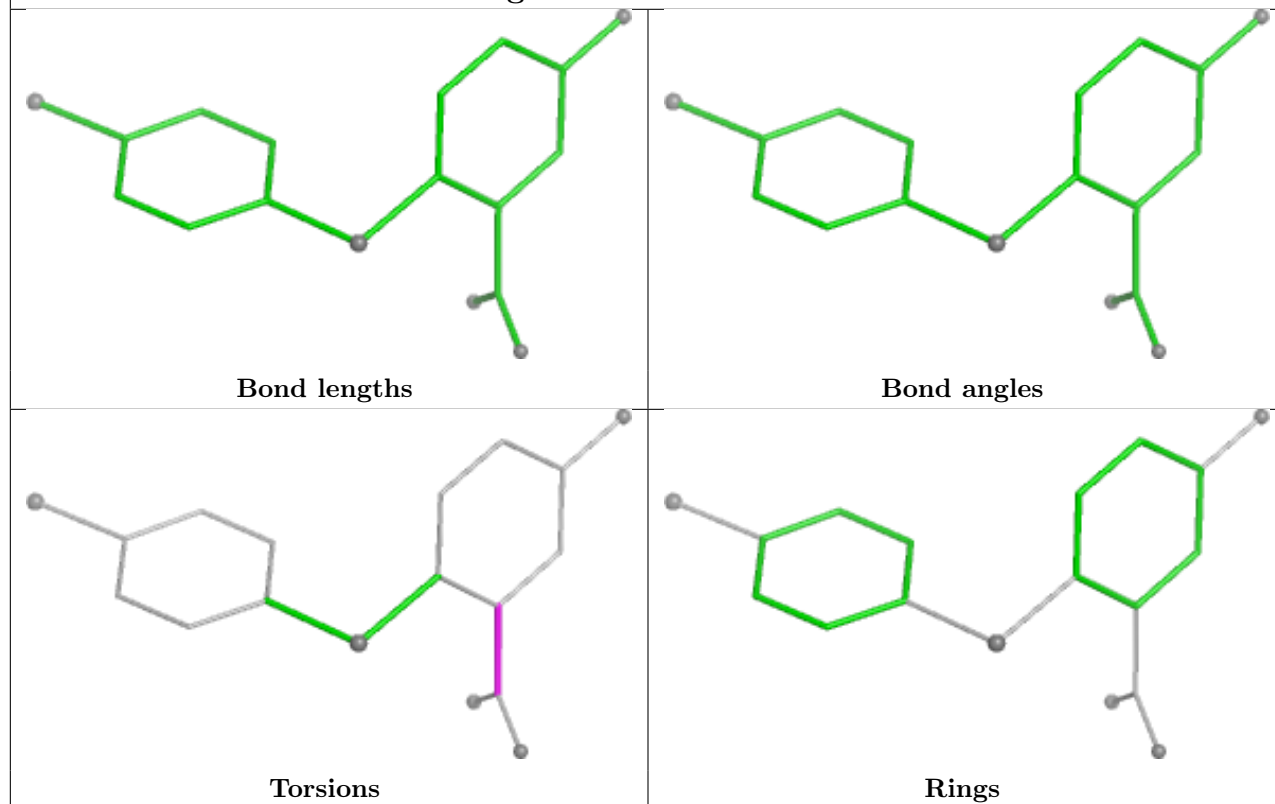
Ligand ADP D 1301

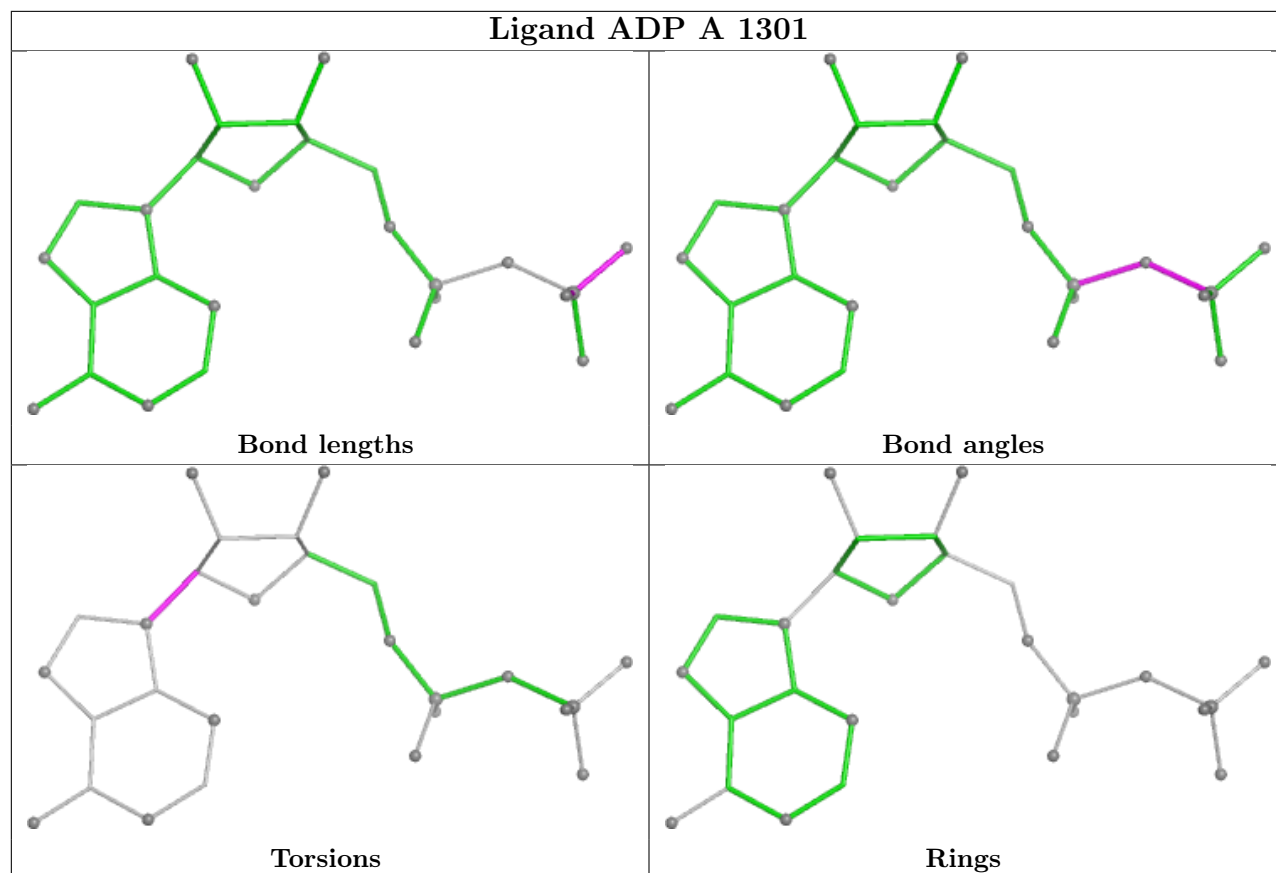


Ligand A1J1E A 1312



Ligand A1J1E C 1309





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

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, 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	636/680 (93%)	0.11	10 (1%) 70 68	20, 50, 72, 92	11 (1%)
1	B	637/680 (93%)	0.09	8 (1%) 75 73	20, 52, 70, 82	5 (0%)
1	C	633/680 (93%)	0.11	3 (0%) 87 86	23, 54, 74, 91	1 (0%)
1	D	633/680 (93%)	0.25	12 (1%) 66 63	28, 58, 81, 92	2 (0%)
All	All	2539/2720 (93%)	0.14	33 (1%) 75 73	20, 53, 75, 92	19 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	719[A]	THR	6.8
1	A	1198	LEU	6.5
1	A	720[A]	LEU	5.4
1	B	587[A]	ILE	3.9
1	A	1193	LYS	3.6
1	C	1073[A]	ARG	3.5
1	A	1195	GLN	3.4
1	B	1198	LEU	3.1
1	B	875[A]	VAL	3.0
1	D	803	ASP	3.0
1	D	913	LEU	3.0
1	A	718[A]	ALA	2.9
1	D	914	THR	2.8
1	B	1185	ASP	2.8
1	B	754	THR	2.7
1	D	754	THR	2.5
1	D	863	LYS	2.4
1	D	844	THR	2.4
1	B	753	GLU	2.4
1	A	1197	ARG	2.4
1	B	970	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	867	SER	2.4
1	D	711	MET	2.4
1	A	1194	LYS	2.3
1	D	911	GLU	2.2
1	D	869	THR	2.2
1	D	719	THR	2.1
1	C	739	GLY	2.1
1	A	821	GLN	2.1
1	B	1023	ASP	2.0
1	A	865	TYR	2.0
1	D	720	LEU	2.0
1	D	757	LEU	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
5	EDO	A	1311	4/4	0.71	0.20	59,59,59,60	0
5	EDO	B	1316	4/4	0.71	0.20	74,74,74,74	0
4	DMS	B	1314	4/4	0.74	0.26	83,83,83,83	0
5	EDO	B	1309	4/4	0.76	0.18	66,66,66,66	0
4	DMS	A	1308	4/4	0.76	0.20	113,113,113,113	0
4	DMS	C	1304	4/4	0.77	0.30	117,117,117,117	0
5	EDO	A	1309	4/4	0.78	0.17	58,58,59,59	0
3	MG	D	1302	1/1	0.79	0.17	48,48,48,48	0
5	EDO	B	1315	4/4	0.79	0.21	82,82,82,82	0
5	EDO	A	1313	4/4	0.79	0.22	73,73,73,73	0
3	MG	B	1302	1/1	0.80	0.15	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DMS	A	1303	4/4	0.81	0.26	97,97,97,97	0
5	EDO	D	1308	4/4	0.81	0.25	76,76,77,77	0
5	EDO	D	1307	4/4	0.82	0.17	80,80,80,80	0
5	EDO	D	1309	4/4	0.83	0.14	72,72,72,73	0
5	EDO	A	1316	4/4	0.84	0.17	59,59,59,59	0
5	EDO	B	1310	4/4	0.84	0.17	72,72,72,72	0
5	EDO	B	1313	4/4	0.84	0.13	61,61,61,61	0
5	EDO	B	1308	4/4	0.84	0.14	54,54,54,55	0
3	MG	A	1302	1/1	0.85	0.20	44,44,44,44	0
4	DMS	B	1311	4/4	0.86	0.21	98,98,98,98	0
5	EDO	D	1311	4/4	0.86	0.15	60,60,60,60	0
5	EDO	A	1306	4/4	0.87	0.19	59,59,59,59	0
5	EDO	B	1307	4/4	0.87	0.13	70,70,70,70	0
3	MG	C	1302	1/1	0.87	0.17	42,42,42,42	0
4	DMS	D	1305	4/4	0.88	0.19	71,71,71,71	4
5	EDO	C	1307	4/4	0.88	0.17	65,65,66,66	0
5	EDO	C	1310	4/4	0.89	0.14	77,77,77,77	0
4	DMS	A	1314	4/4	0.89	0.23	107,107,107,107	0
4	DMS	C	1306	4/4	0.89	0.19	93,93,93,93	0
5	EDO	A	1317	4/4	0.89	0.14	67,68,68,68	0
5	EDO	B	1305	4/4	0.89	0.16	46,47,47,47	0
5	EDO	C	1308	4/4	0.90	0.11	57,57,58,58	0
5	EDO	D	1303	4/4	0.90	0.12	56,56,57,57	0
5	EDO	B	1304	4/4	0.91	0.16	61,61,61,61	0
5	EDO	C	1305	4/4	0.91	0.16	66,66,66,66	0
4	DMS	B	1306	4/4	0.91	0.17	85,85,85,85	0
5	EDO	D	1304	4/4	0.91	0.12	60,60,61,61	0
6	A1J1E	A	1312	18/18	0.91	0.11	44,48,54,56	18
5	EDO	C	1303	4/4	0.92	0.14	61,61,62,62	0
4	DMS	A	1304	4/4	0.92	0.17	63,63,63,63	4
6	A1J1E	B	1312	18/18	0.92	0.11	46,48,52,54	18
6	A1J1E	C	1309	18/18	0.92	0.10	45,49,52,53	0
6	A1J1E	D	1310	18/18	0.92	0.11	60,62,66,67	0
2	ADP	B	1301	27/27	0.93	0.11	42,48,50,50	0
5	EDO	A	1315	4/4	0.93	0.10	65,66,66,66	0
2	ADP	A	1301	27/27	0.94	0.10	41,46,46,47	27
2	ADP	C	1301	27/27	0.94	0.10	44,51,52,52	0
2	ADP	D	1301	27/27	0.94	0.09	43,52,54,54	27
5	EDO	A	1307	4/4	0.95	0.09	49,49,50,50	0
5	EDO	B	1303	4/4	0.95	0.12	66,66,66,66	0
5	EDO	A	1310	4/4	0.96	0.08	64,64,64,64	0
5	EDO	D	1306	4/4	0.96	0.08	57,57,58,58	0

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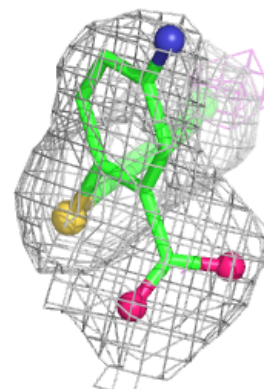
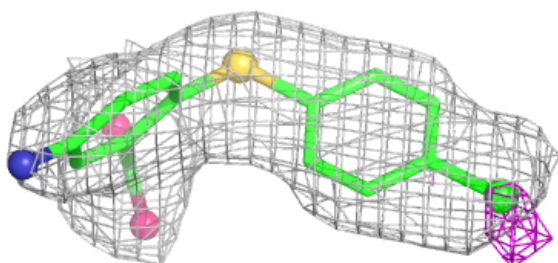
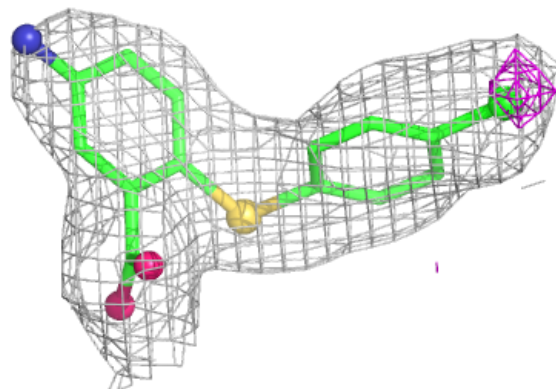
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	A	1305	4/4	0.97	0.06	29,30,30,30	4

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.

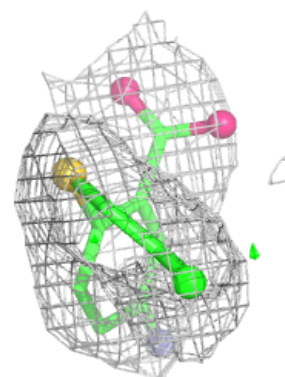
Electron density around A1J1E A 1312:

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

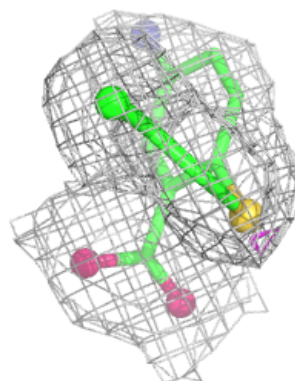
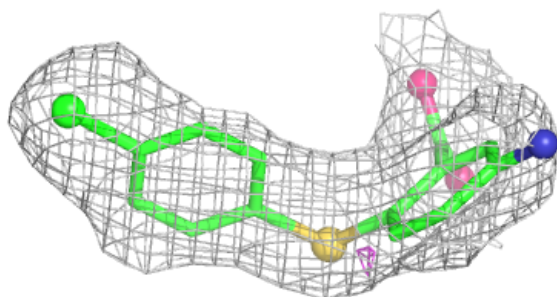
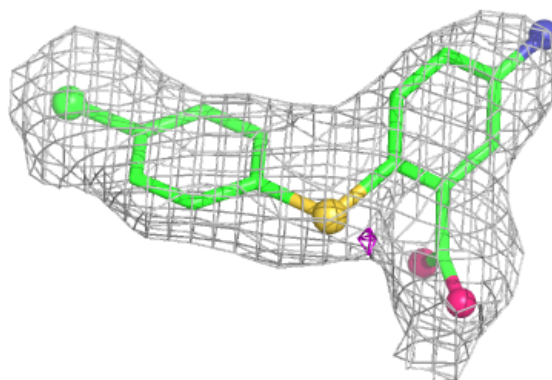


Electron density around A1J1E B 1312:

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

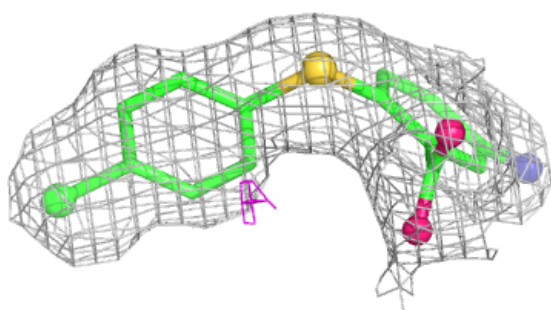
**Electron density around A1J1E C 1309:**

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and green (positive)



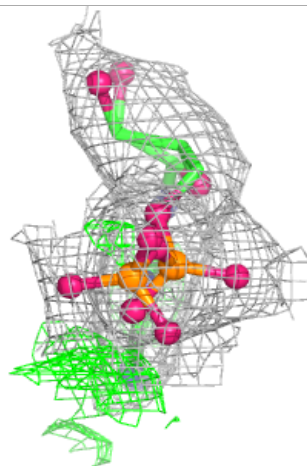
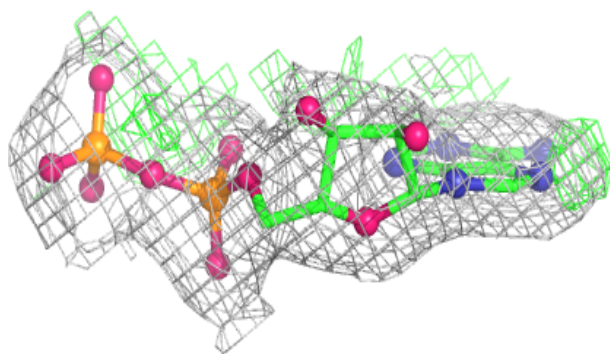
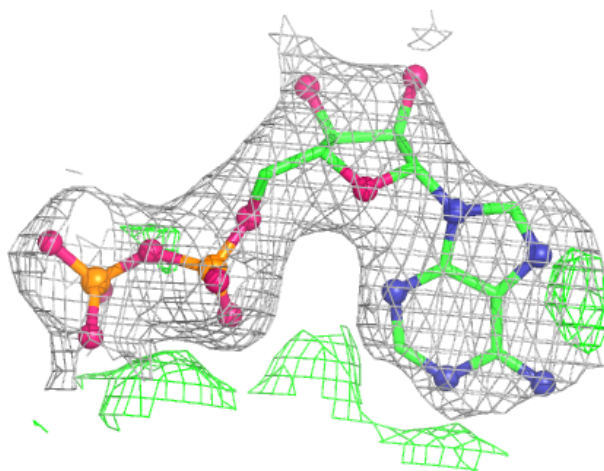
Electron density around A1J1E D 1310:

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



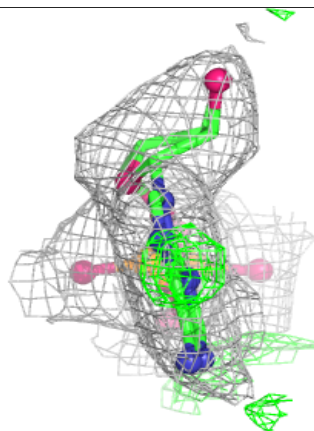
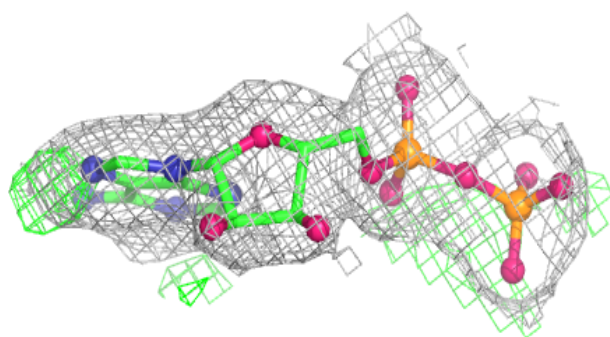
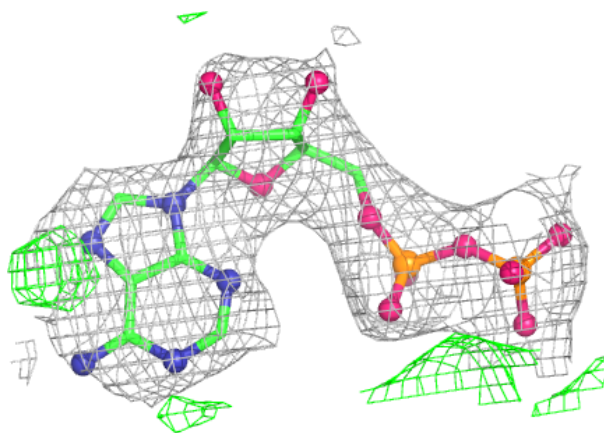
Electron density around ADP B 1301:

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



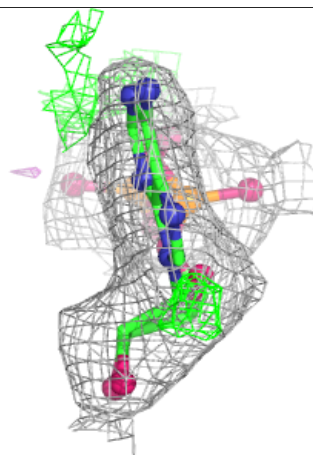
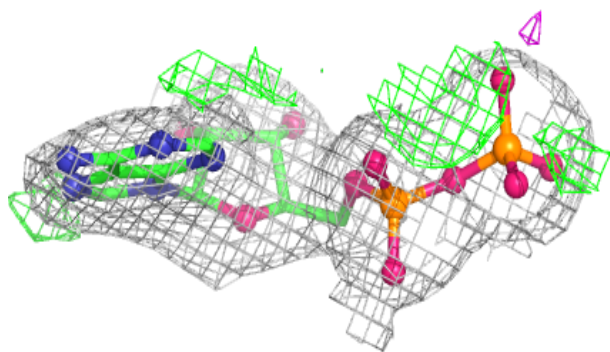
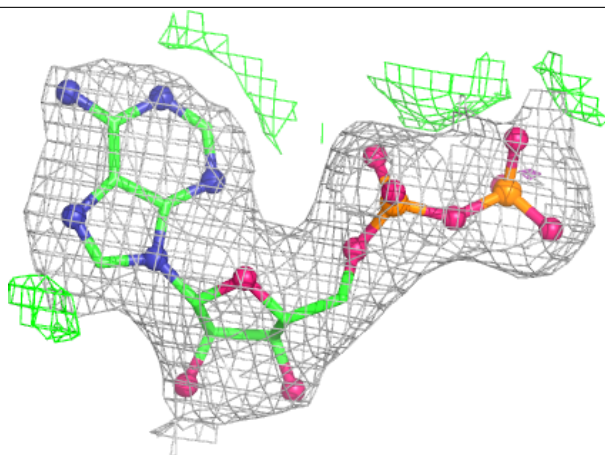
Electron density around ADP A 1301:

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



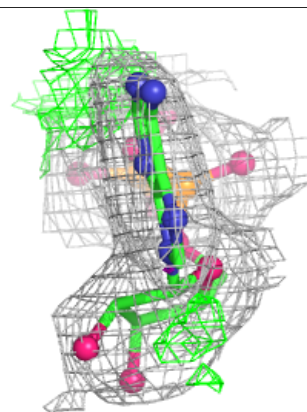
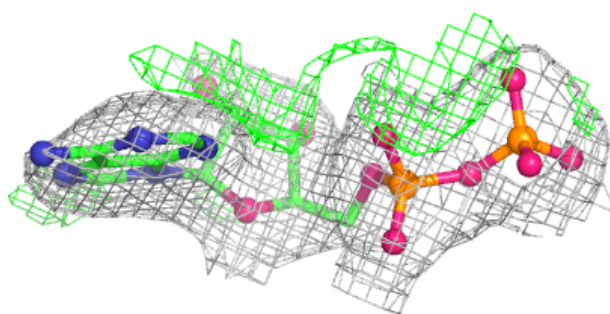
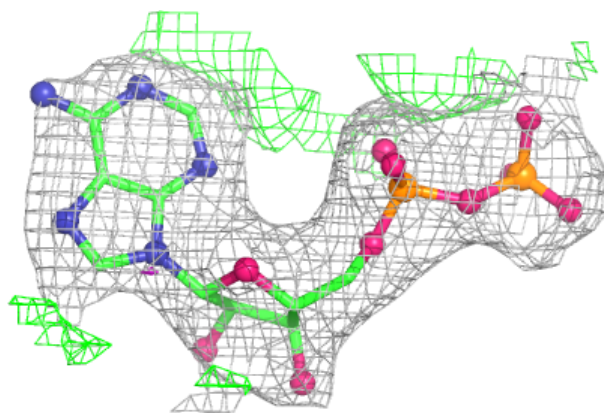
Electron density around ADP C 1301:

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



Electron density around ADP D 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 ⓘ

There are no such residues in this entry.