



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2026 – 01:41 pm BST

PDB ID : 28ZQ / pdb_000028zq
Title : Crystal structure of human DHX8 in complex with compound 43 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 : 2.20 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

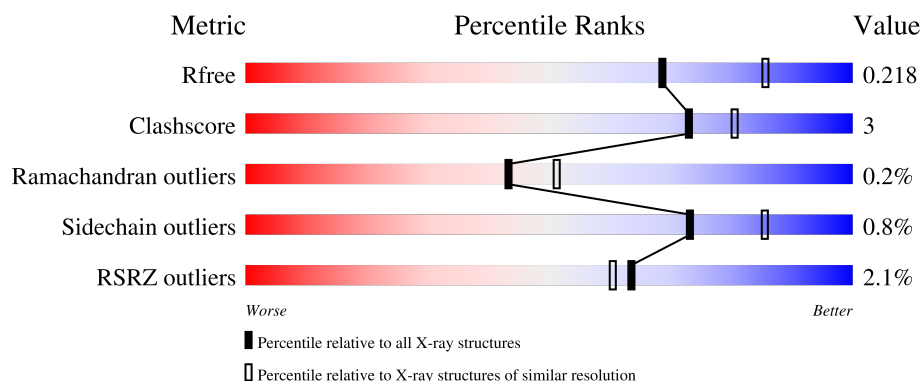
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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% 84% 9% 6%
1	B	680	% 84% 9% 6%
1	C	680	% 86% 7% 7%
1	D	680	4% 82% 11% 7%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21047 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	5	2
			4962	3177	822	928	35			
1	B	638	Total	C	N	O	S	0	10	0
			4973	3185	822	931	35			
1	C	633	Total	C	N	O	S	0	6	0
			4921	3158	807	921	35			
1	D	632	Total	C	N	O	S	0	4	0
			4832	3096	791	908	37			

There are 28 discrepancies between the modelled and reference sequences:

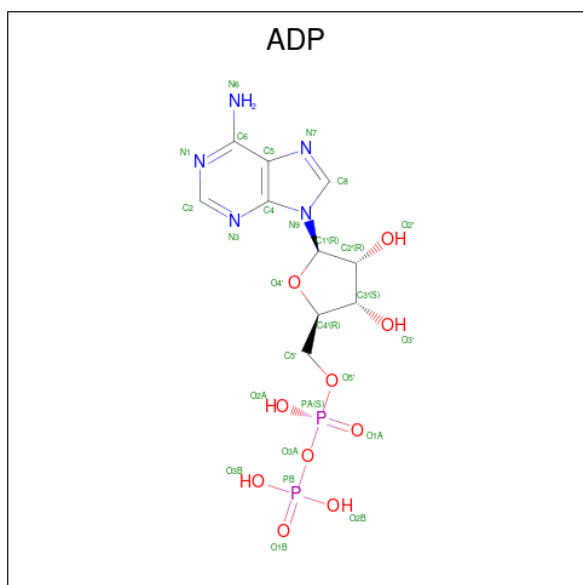
Chain	Residue	Modelled	Actual	Comment	Reference
A	547	MET	-	initiating methionine	UNP Q14562
A	1221	HIS	-	expression tag	UNP Q14562
A	1222	HIS	-	expression tag	UNP Q14562
A	1223	HIS	-	expression tag	UNP Q14562
A	1224	HIS	-	expression tag	UNP Q14562
A	1225	HIS	-	expression tag	UNP Q14562
A	1226	HIS	-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

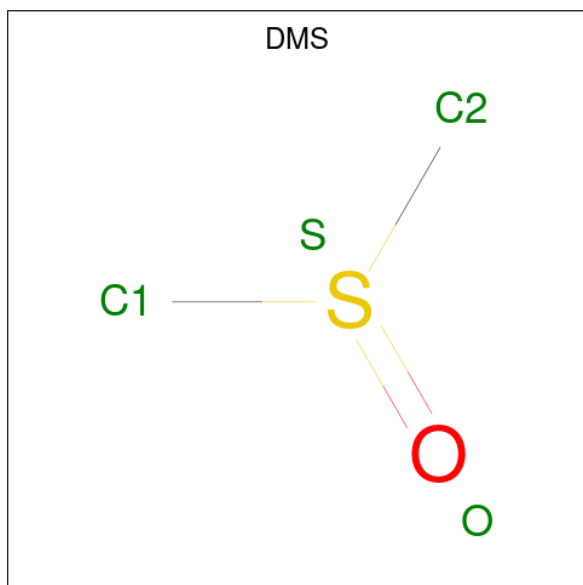
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

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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		

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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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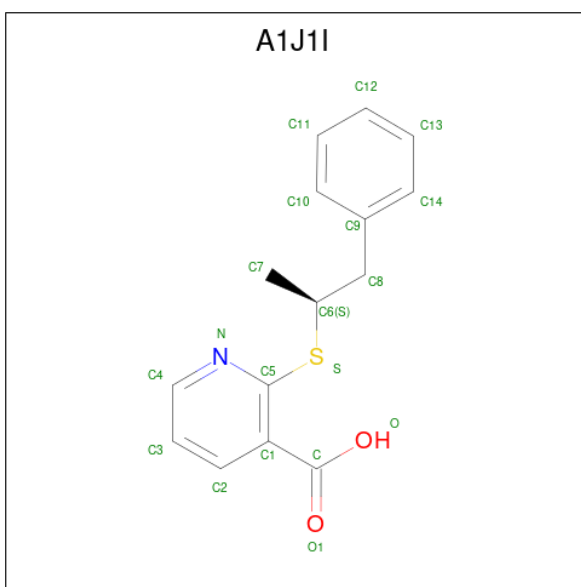
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0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

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

- Molecule 6 is 2-[(2S)-1-phenylpropan-2-yl]sulfanylpuridine-3-carboxylic acid (CCD ID: A1J1I) (formula: C₁₅H₁₅NO₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			19	15	1	2	1		
6	B	1	Total	C	N	O	S	0	0
			19	15	1	2	1		
6	C	1	Total	C	N	O	S	0	0
			19	15	1	2	1		
6	D	1	Total	C	N	O	S	0	0
			19	15	1	2	1		

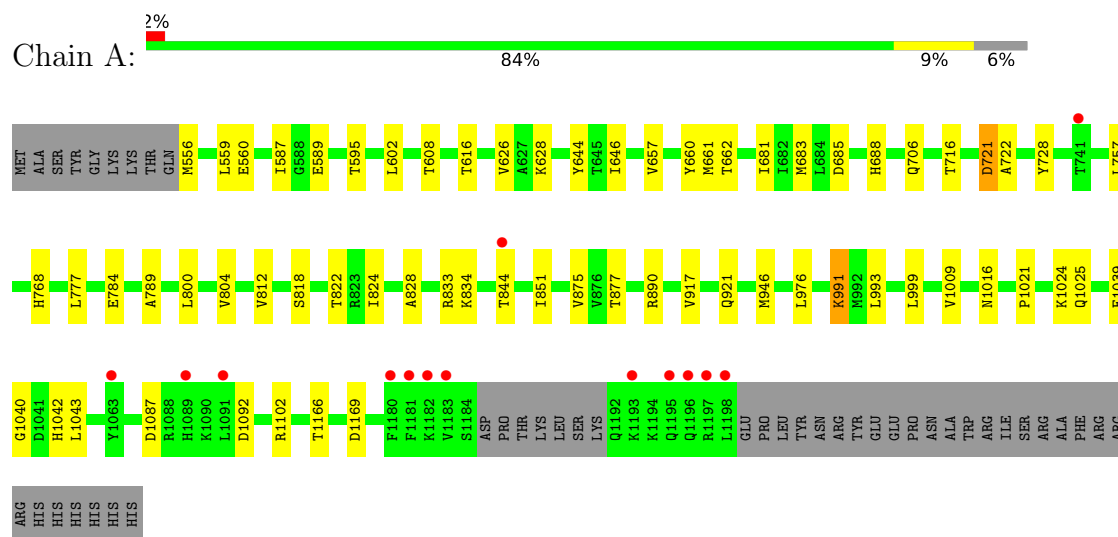
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	262	Total	O	0	2
			264	264		
7	B	242	Total	O	0	3
			245	245		
7	C	253	Total	O	0	3
			256	256		
7	D	191	Total	O	0	3
			194	194		

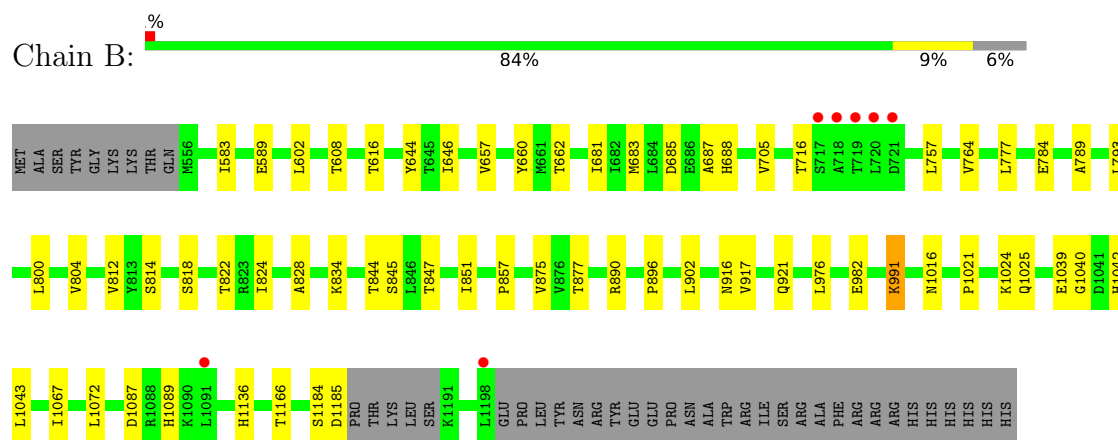
3 Residue-property plots [i](#)

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

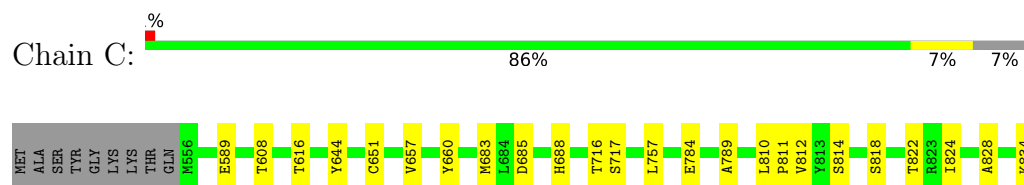
• Molecule 1: ATP-dependent RNA helicase DHX8

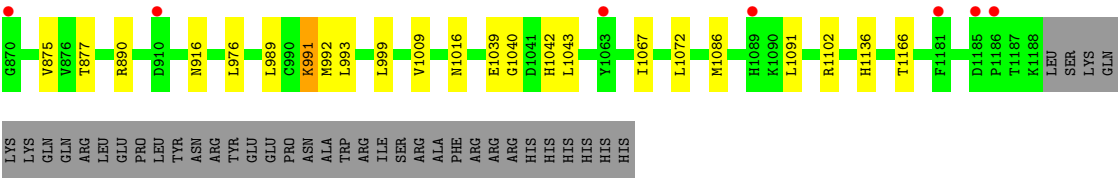


• Molecule 1: ATP-dependent RNA helicase DHX8

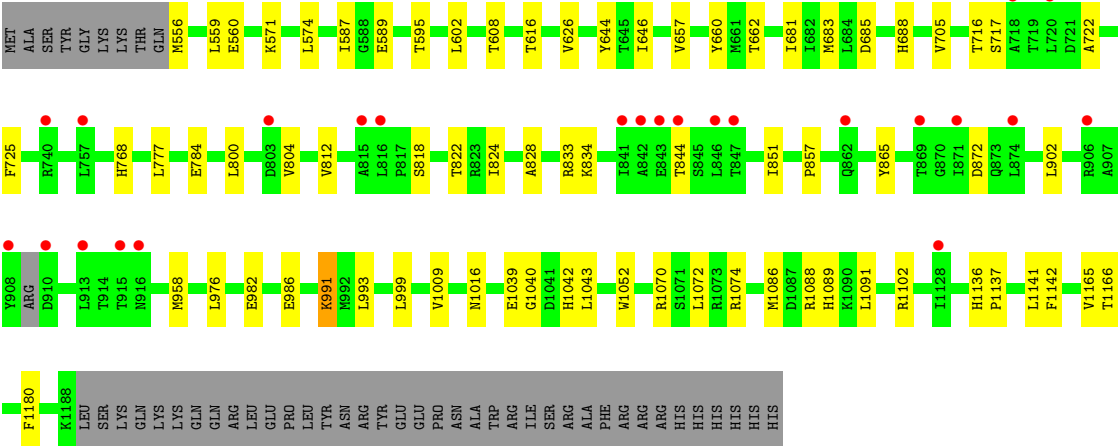
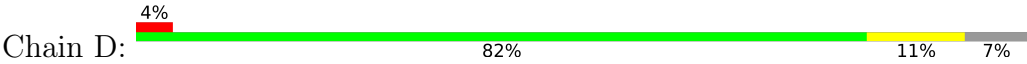


• Molecule 1: ATP-dependent RNA helicase DHX8





● 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	66.24Å 168.24Å 136.79Å 90.00° 92.49° 90.00°	Depositor
Resolution (Å)	31.90 – 2.20 31.90 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (31.90-2.20) 99.3 (31.90-2.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.10.4 (26-JUL-2023)	Depositor
R, R_{free}	0.202 , 0.229 0.196 , 0.218	Depositor DCC
R_{free} test set	7466 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.085 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21047	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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: A1J1I, EDO, ADP, MG, DMS

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.71	0/5063	0.99	5/6868 (0.1%)
1	B	0.70	0/5070	0.98	5/6880 (0.1%)
1	C	0.70	0/5023	0.98	3/6820 (0.0%)
1	D	0.68	1/4929 (0.0%)	0.99	2/6693 (0.0%)
All	All	0.70	1/20085 (0.0%)	0.99	15/27261 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	986	GLU	CA-C	5.30	1.58	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1040	GLY	N-CA-C	8.36	122.20	111.25
1	A	1040	GLY	N-CA-C	8.28	122.09	111.25
1	B	1040	GLY	N-CA-C	8.21	122.27	111.52
1	D	1040	GLY	N-CA-C	7.86	121.82	111.52
1	A	721	ASP	CA-C-N	7.14	130.18	120.54
1	A	721	ASP	C-N-CA	7.14	130.18	120.54
1	D	1180	PHE	CA-CB-CG	7.09	120.89	113.80
1	A	1025	GLN	N-CA-C	6.59	118.12	111.07
1	B	1025	GLN	N-CA-C	6.24	117.74	111.07
1	B	1184	SER	N-CA-C	6.24	118.16	111.36
1	B	814	SER	N-CA-C	5.28	116.72	111.07
1	A	1169	ASP	N-CA-C	-5.17	102.13	109.62
1	B	845	SER	N-CA-C	5.15	119.61	112.45
1	C	814	SER	N-CA-C	5.13	116.56	111.07
1	C	717	SER	N-CA-C	5.06	117.55	109.81

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	4962	0	4863	34	0
1	B	4973	0	4819	33	0
1	C	4921	0	4784	25	0
1	D	4832	0	4642	36	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	20	0	30	0	0
4	B	20	0	30	2	0
4	C	4	0	6	1	0
4	D	16	0	24	3	0
5	A	52	0	78	2	0
5	B	32	0	48	0	0
5	C	40	0	60	1	0
5	D	28	0	42	2	0
6	A	19	0	0	0	0
6	B	19	0	0	0	0
6	C	19	0	0	0	0
6	D	19	0	0	0	0
7	A	264	0	0	2	0
7	B	245	0	0	1	0
7	C	256	0	0	1	0
7	D	194	0	0	0	0
All	All	21047	0	19474	128	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 (128) 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:688:HIS:CE1	1:A:844:THR:HG21	2.18	0.79
1:A:688:HIS:HE1	1:A:844:THR:HG21	1.48	0.75
1:D:688:HIS:CE1	1:D:844:THR:HG21	2.23	0.73
1:A:587[B]:ILE:CG1	1:A:722:ALA:HB2	2.19	0.72
1:D:688:HIS:HE1	1:D:844:THR:HG21	1.57	0.69
1:B:688:HIS:CE1	1:B:844:THR:HG21	2.28	0.69
1:C:688:HIS:CE1	1:C:844:THR:HG21	2.29	0.67
1:C:1039[A]:GLU:HB2	1:C:1043:LEU:HD12	1.80	0.63
1:B:683:MET:HE3	1:B:716[B]:THR:HG21	1.81	0.61
1:B:1039[A]:GLU:HB2	1:B:1043:LEU:HD12	1.82	0.61
1:A:1039[A]:GLU:HB2	1:A:1043:LEU:HD12	1.81	0.60
1:B:896:PRO:HD3	5:D:1304:EDO:H11	1.84	0.60
5:A:1307:EDO:H12	5:A:1320:EDO:H12	1.83	0.59
1:A:683:MET:HE3	1:A:716:THR:HG21	1.85	0.59
1:C:688:HIS:HE1	1:C:844:THR:HG21	1.69	0.58
1:B:916:ASN:HB2	7:B:1489:HOH:O	2.04	0.57
1:C:1086:MET:HG3	1:C:1091:LEU:HB2	1.88	0.56
1:C:999:LEU:O	1:C:1102:ARG:HD3	2.05	0.56
1:D:999:LEU:O	1:D:1102:ARG:HD3	2.06	0.55
1:B:688:HIS:HE1	1:B:844:THR:HG21	1.68	0.55
1:A:595:THR:HG22	1:A:626:VAL:HG11	1.88	0.55
1:D:1039:GLU:HB2	1:D:1043:LEU:HD12	1.88	0.55
1:D:958:MET:HE2	4:D:1305:DMS:H21	1.88	0.54
1:D:1086:MET:HG3	1:D:1091:LEU:HB2	1.88	0.53
1:C:757:LEU:HD11	1:C:789:ALA:HB2	1.91	0.52
1:B:1136:HIS:CE1	4:B:1316:DMS:H12	2.45	0.52
1:D:683:MET:HE3	1:D:716:THR:HG21	1.91	0.52
1:A:828:ALA:HB2	1:A:834:LYS:HG3	1.92	0.52
1:C:828:ALA:HB2	1:C:834:LYS:HG3	1.93	0.51
1:D:587:ILE:HG21	1:D:722:ALA:HB2	1.92	0.51
1:D:976:LEU:HD21	1:D:991:LYS:HE3	1.93	0.51
1:C:784:GLU:H	1:C:784:GLU:CD	2.19	0.50
1:A:976:LEU:HD21	1:A:991:LYS:HE3	1.93	0.50
1:A:757:LEU:HD11	1:A:789:ALA:HB2	1.93	0.50
1:A:644:TYR:HA	1:A:660:TYR:O	2.12	0.50
1:C:976:LEU:HD21	1:C:991:LYS:HE3	1.94	0.50
1:B:784:GLU:CD	1:B:784:GLU:H	2.20	0.49
1:A:818:SER:O	1:A:822:THR:HG23	2.12	0.49
1:A:616:THR:O	1:A:685:ASP:HB3	2.13	0.49
1:D:784:GLU:H	1:D:784:GLU:CD	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:TYR:HA	1:B:660:TYR:O	2.12	0.49
1:D:556:MET:HE2	1:D:560:GLU:HB3	1.93	0.49
1:D:777:LEU:HB2	1:D:851:ILE:HD13	1.94	0.49
1:D:818:SER:O	1:D:822:THR:HG23	2.13	0.49
1:A:777:LEU:HB2	1:A:851:ILE:HD13	1.94	0.49
1:C:1042:HIS:ND1	1:C:1166:THR:OG1	2.45	0.48
1:B:757:LEU:HD11	1:B:789:ALA:HB2	1.95	0.48
1:C:644:TYR:HA	1:C:660:TYR:O	2.13	0.48
1:D:1136:HIS:CE1	4:D:1313:DMS:H12	2.48	0.48
1:A:999:LEU:O	1:A:1102:ARG:HD3	2.14	0.48
1:A:1021:PRO:HG2	1:A:1024:LYS:HB2	1.95	0.48
1:C:683:MET:HE3	1:C:716:THR:HG21	1.94	0.48
1:C:818:SER:O	1:C:822:THR:HG23	2.13	0.48
1:B:777:LEU:HB2	1:B:851:ILE:HD13	1.94	0.48
1:D:644:TYR:HA	1:D:660:TYR:O	2.13	0.48
1:B:687:ALA:HB3	1:B:716[A]:THR:O	2.13	0.48
1:B:583:ILE:HD11	1:B:705:VAL:HG21	1.95	0.48
1:B:875:VAL:HG13	1:B:877:THR:HG23	1.96	0.48
1:C:608:THR:HB	1:C:657:VAL:HB	1.96	0.48
1:B:828:ALA:HB2	1:B:834:LYS:HG3	1.96	0.47
1:C:1136:HIS:CD2	4:C:1305:DMS:H12	2.49	0.47
1:A:1042:HIS:ND1	1:A:1166:THR:OG1	2.45	0.47
1:B:982:GLU:OE1	1:B:1089:HIS:CG	2.67	0.47
1:B:818:SER:O	1:B:822:THR:HG23	2.14	0.47
1:D:616:THR:O	1:D:685:ASP:HB3	2.15	0.47
1:B:917:VAL:CG1	1:B:921:GLN:HB2	2.45	0.47
1:C:1067:ILE:HG21	1:C:1072:LEU:HD11	1.95	0.47
1:B:616:THR:O	1:B:685:ASP:HB3	2.15	0.47
1:D:608:THR:HB	1:D:657:VAL:HB	1.97	0.47
1:D:571:LYS:HZ2	5:D:1311:EDO:C2	2.29	0.46
1:C:890:ARG:NE	1:C:890:ARG:HA	2.30	0.46
1:A:608:THR:HB	1:A:657:VAL:HB	1.97	0.46
1:C:651:CYS:HA	5:C:1304:EDO:H22	1.98	0.46
1:D:1042:HIS:ND1	1:D:1166:THR:OG1	2.48	0.46
1:B:608:THR:HB	1:B:657:VAL:HB	1.98	0.46
1:A:784:GLU:H	1:A:784:GLU:CD	2.23	0.45
1:D:646:ILE:HG22	1:D:662:THR:HG23	1.99	0.45
1:A:628:LYS:NZ	7:A:1406:HOH:O	2.50	0.45
1:A:728:TYR:CG	1:A:946:MET:HE2	2.51	0.45
1:A:646:ILE:HG22	1:A:662:THR:HG23	1.99	0.45
1:C:616:THR:O	1:C:685:ASP:HB3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1136:HIS:CD2	4:D:1313:DMS:H23	2.52	0.44
1:D:828:ALA:HB2	1:D:834:LYS:HG3	1.98	0.44
1:A:890:ARG:NE	1:A:890:ARG:HA	2.32	0.44
1:D:595:THR:HG22	1:D:626:VAL:HG11	1.99	0.44
1:B:1042:HIS:ND1	1:B:1166:THR:OG1	2.45	0.44
1:D:812:VAL:HG22	1:D:824:ILE:HG21	2.00	0.44
1:D:768:HIS:HA	1:D:833:ARG:NE	2.33	0.43
1:D:1070:ARG:O	1:D:1074:ARG:HG3	2.18	0.43
1:D:1052:TRP:CG	1:D:1072:LEU:HD13	2.53	0.43
1:A:602:LEU:HD13	1:A:681:ILE:HD13	2.00	0.43
1:B:1136:HIS:NE2	4:B:1316:DMS:H12	2.33	0.43
1:A:1039[A]:GLU:HG2	7:A:1404:HOH:O	2.17	0.43
1:B:847:THR:HG23	1:B:890:ARG:HH12	1.84	0.43
1:B:1021:PRO:HG2	1:B:1024:LYS:HB2	2.01	0.43
1:C:875[A]:VAL:HG13	1:C:877:THR:HG23	2.00	0.43
1:C:993:LEU:HG	1:C:1009:VAL:HG21	1.99	0.43
1:A:875:VAL:HG13	1:A:877:THR:HG23	1.99	0.42
1:B:800:LEU:HB3	1:B:804:VAL:HG21	2.01	0.42
1:D:800:LEU:HB3	1:D:804:VAL:HG21	2.00	0.42
1:A:917:VAL:CG1	1:A:921:GLN:HB2	2.49	0.42
1:C:812:VAL:HG22	1:C:824:ILE:HG21	2.01	0.42
1:B:602:LEU:HD13	1:B:681:ILE:HD13	2.00	0.42
1:D:865:TYR:HD1	1:D:872:ASP:HB3	1.85	0.42
1:D:1137:PRO:HA	1:D:1142:PHE:CG	2.55	0.42
1:A:800:LEU:HB3	1:A:804:VAL:HG21	2.01	0.42
1:B:857:PRO:HA	1:B:902:LEU:HB2	2.01	0.42
1:A:993:LEU:HG	1:A:1009:VAL:HG21	2.01	0.42
1:B:764:VAL:HG11	1:B:793:LEU:HD21	2.02	0.42
1:B:1067:ILE:HG21	1:B:1072:LEU:HD11	2.01	0.41
1:D:993:LEU:HG	1:D:1009:VAL:HG21	2.02	0.41
1:D:857:PRO:HA	1:D:902:LEU:HB2	2.02	0.41
1:B:646:ILE:HG22	1:B:662:THR:HG23	2.01	0.41
1:B:976:LEU:HD21	1:B:991:LYS:HE3	2.02	0.41
1:D:602:LEU:HD13	1:D:681:ILE:HD13	2.01	0.41
1:C:916:ASN:HB2	7:C:1553:HOH:O	2.20	0.41
1:B:812:VAL:HG22	1:B:824:ILE:HG21	2.02	0.41
1:C:989:LEU:HD23	1:C:992:MET:HE2	2.02	0.41
1:A:812:VAL:HG22	1:A:824:ILE:HG21	2.03	0.41
1:A:1087:ASP:HB3	1:B:1087:ASP:HB3	2.02	0.41
1:A:556:MET:HG2	1:A:560:GLU:HB3	2.03	0.41
1:A:768:HIS:HA	1:A:833:ARG:NE	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:THR:HA	1:A:661:MET:O	2.21	0.40
1:D:717:SER:HB2	1:D:725:PHE:CD2	2.57	0.40
1:D:982:GLU:OE1	1:D:1089:HIS:NE2	2.54	0.40
1:D:1141:LEU:HD12	1:D:1165:VAL:HG12	2.03	0.40
1:A:706:GLN:HG2	5:A:1308:EDO:H12	2.02	0.40
1:C:810:LEU:HA	1:C:811:PRO:HD2	2.02	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	637/680 (94%)	621 (98%)	15 (2%)	1 (0%)	43	51
1	B	644/680 (95%)	630 (98%)	13 (2%)	1 (0%)	43	51
1	C	637/680 (94%)	622 (98%)	14 (2%)	1 (0%)	43	51
1	D	632/680 (93%)	619 (98%)	12 (2%)	1 (0%)	43	51
All	All	2550/2720 (94%)	2492 (98%)	54 (2%)	4 (0%)	43	51

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 [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	516/603 (86%)	511 (99%)	5 (1%)	68	81
1	B	506/603 (84%)	503 (99%)	3 (1%)	78	89
1	C	507/603 (84%)	505 (100%)	2 (0%)	84	92
1	D	484/603 (80%)	478 (99%)	6 (1%)	63	78
All	All	2013/2412 (84%)	1997 (99%)	16 (1%)	73	85

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	559	LEU
1	A	589	GLU
1	A	721	ASP
1	A	991	LYS
1	A	1092	ASP
1	B	589	GLU
1	B	991	LYS
1	B	1185	ASP
1	C	589	GLU
1	C	991	LYS
1	D	559	LEU
1	D	574	LEU
1	D	589	GLU
1	D	705	VAL
1	D	991	LYS
1	D	1088	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	688	HIS
1	A	783	GLN
1	A	862	GLN
1	A	998	HIS
1	A	1130	GLN
1	B	688	HIS
1	B	1130	GLN

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Mol	Chain	Res	Type
1	C	600	GLN
1	C	688	HIS
1	C	1016	ASN
1	C	1068	GLN
1	D	600	GLN
1	D	688	HIS
1	D	783	GLN
1	D	873	GLN
1	D	938	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 65 ligands modelled in this entry, 4 are monoatomic - leaving 61 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	$\# Z > 2$
5	EDO	A	1315	-	3,3,3	0.23	0	2,2,2	0.31	0
5	EDO	C	1303	-	3,3,3	0.25	0	2,2,2	0.48	0
5	EDO	C	1307	-	3,3,3	0.25	0	2,2,2	0.36	0
5	EDO	D	1311	-	3,3,3	0.17	0	2,2,2	0.39	0
5	EDO	C	1313	-	3,3,3	0.13	0	2,2,2	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	1307	-	3,3,3	0.09	0	2,2,2	0.40	0
4	DMS	A	1303	-	3,3,3	0.71	0	3,3,3	0.40	0
4	DMS	B	1316	-	3,3,3	0.68	0	3,3,3	0.31	0
5	EDO	B	1303	-	3,3,3	0.34	0	2,2,2	0.29	0
4	DMS	A	1319	-	3,3,3	0.63	0	3,3,3	0.40	0
5	EDO	A	1306	-	3,3,3	0.27	0	2,2,2	0.26	0
5	EDO	C	1309	-	3,3,3	0.35	0	2,2,2	0.29	0
5	EDO	B	1304	-	3,3,3	0.34	0	2,2,2	0.26	0
5	EDO	B	1313	-	3,3,3	0.22	0	2,2,2	0.44	0
4	DMS	B	1314	-	3,3,3	0.65	0	3,3,3	0.37	0
4	DMS	A	1312	-	3,3,3	0.66	0	3,3,3	0.63	0
5	EDO	A	1320	-	3,3,3	0.13	0	2,2,2	0.41	0
2	ADP	D	1301	3	27,29,29	0.88	1 (3%)	42,45,45	0.67	1 (2%)
4	DMS	D	1314	-	3,3,3	0.67	0	3,3,3	0.36	0
5	EDO	D	1304	-	3,3,3	0.41	0	2,2,2	0.10	0
2	ADP	B	1301	3	27,29,29	1.02	3 (11%)	42,45,45	0.58	1 (2%)
6	A1J1I	C	1310	-	19,20,20	0.90	1 (5%)	22,26,26	0.83	2 (9%)
6	A1J1I	D	1308	-	19,20,20	0.91	2 (10%)	22,26,26	0.80	2 (9%)
4	DMS	D	1305	-	3,3,3	0.68	0	3,3,3	0.31	0
5	EDO	A	1305	-	3,3,3	0.18	0	2,2,2	0.53	0
4	DMS	D	1313	-	3,3,3	0.66	0	3,3,3	0.38	0
6	A1J1I	B	1307	-	19,20,20	0.96	2 (10%)	22,26,26	0.83	2 (9%)
4	DMS	C	1305	-	3,3,3	0.60	0	3,3,3	0.34	0
4	DMS	D	1306	-	3,3,3	0.60	0	3,3,3	0.46	0
4	DMS	A	1304	-	3,3,3	0.69	0	3,3,3	0.45	0
5	EDO	B	1309	-	3,3,3	0.34	0	2,2,2	0.15	0
5	EDO	B	1310	-	3,3,3	0.36	0	2,2,2	0.23	0
5	EDO	D	1310	-	3,3,3	0.24	0	2,2,2	0.10	0
5	EDO	A	1314	-	3,3,3	0.25	0	2,2,2	0.04	0
6	A1J1I	A	1311	-	19,20,20	0.94	1 (5%)	22,26,26	0.84	2 (9%)
5	EDO	D	1303	-	3,3,3	0.13	0	2,2,2	0.51	0
5	EDO	A	1317	-	3,3,3	0.25	0	2,2,2	0.37	0
5	EDO	B	1306	-	3,3,3	0.31	0	2,2,2	0.16	0
4	DMS	B	1305	-	3,3,3	0.59	0	3,3,3	0.23	0
5	EDO	A	1316	-	3,3,3	0.19	0	2,2,2	0.37	0
5	EDO	A	1310	-	3,3,3	0.32	0	2,2,2	0.05	0
5	EDO	A	1318	-	3,3,3	0.26	0	2,2,2	0.27	0
5	EDO	D	1312	-	3,3,3	0.60	0	2,2,2	0.05	0
5	EDO	B	1312	-	3,3,3	0.31	0	2,2,2	0.29	0
5	EDO	C	1314	-	3,3,3	0.28	0	2,2,2	0.33	0
4	DMS	A	1321	-	3,3,3	0.59	0	3,3,3	0.55	0
5	EDO	C	1312	-	3,3,3	0.21	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	C	1308	-	3,3,3	0.43	0	2,2,2	0.06	0
5	EDO	A	1313	-	3,3,3	0.30	0	2,2,2	0.16	0
5	EDO	D	1307	-	3,3,3	0.29	0	2,2,2	0.22	0
5	EDO	C	1304	-	3,3,3	0.14	0	2,2,2	0.33	0
2	ADP	C	1301	3	27,29,29	0.91	1 (3%)	42,45,45	0.66	1 (2%)
5	EDO	D	1309	-	3,3,3	0.25	0	2,2,2	0.22	0
5	EDO	B	1311	-	3,3,3	0.26	0	2,2,2	0.25	0
5	EDO	A	1309	-	3,3,3	0.48	0	2,2,2	0.08	0
5	EDO	C	1311	-	3,3,3	0.41	0	2,2,2	0.11	0
4	DMS	B	1315	-	3,3,3	0.64	0	3,3,3	0.40	0
4	DMS	B	1308	-	3,3,3	0.64	0	3,3,3	0.58	0
5	EDO	C	1306	-	3,3,3	0.19	0	2,2,2	0.36	0
2	ADP	A	1301	3	27,29,29	1.04	3 (11%)	42,45,45	0.63	1 (2%)
5	EDO	A	1308	-	3,3,3	0.11	0	2,2,2	0.35	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
5	EDO	A	1315	-	-	1/1/1/1	-
5	EDO	C	1303	-	-	1/1/1/1	-
5	EDO	D	1311	-	-	0/1/1/1	-
5	EDO	C	1313	-	-	1/1/1/1	-
5	EDO	A	1307	-	-	0/1/1/1	-
5	EDO	B	1303	-	-	1/1/1/1	-
5	EDO	A	1306	-	-	1/1/1/1	-
5	EDO	C	1309	-	-	1/1/1/1	-
5	EDO	B	1304	-	-	1/1/1/1	-
5	EDO	B	1313	-	-	1/1/1/1	-
5	EDO	A	1320	-	-	1/1/1/1	-
5	EDO	D	1304	-	-	1/1/1/1	-
2	ADP	D	1301	3	-	7/16/32/32	0/3/3/3
6	A1J1I	C	1310	-	-	5/11/12/12	0/2/2/2
2	ADP	B	1301	3	-	2/16/32/32	0/3/3/3
6	A1J1I	D	1308	-	-	5/11/12/12	0/2/2/2
5	EDO	A	1305	-	-	0/1/1/1	-
6	A1J1I	B	1307	-	-	5/11/12/12	0/2/2/2
5	EDO	B	1309	-	-	1/1/1/1	-
5	EDO	B	1310	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	D	1310	-	-	1/1/1/1	-
5	EDO	A	1314	-	-	0/1/1/1	-
6	A1J1I	A	1311	-	-	5/11/12/12	0/2/2/2
5	EDO	D	1303	-	-	1/1/1/1	-
5	EDO	A	1317	-	-	1/1/1/1	-
5	EDO	B	1306	-	-	0/1/1/1	-
5	EDO	A	1316	-	-	0/1/1/1	-
5	EDO	A	1310	-	-	0/1/1/1	-
5	EDO	A	1318	-	-	1/1/1/1	-
5	EDO	D	1312	-	-	1/1/1/1	-
5	EDO	B	1312	-	-	1/1/1/1	-
5	EDO	C	1314	-	-	1/1/1/1	-
5	EDO	C	1312	-	-	1/1/1/1	-
5	EDO	C	1308	-	-	0/1/1/1	-
5	EDO	A	1313	-	-	1/1/1/1	-
5	EDO	D	1307	-	-	1/1/1/1	-
5	EDO	C	1304	-	-	0/1/1/1	-
2	ADP	C	1301	3	-	6/16/32/32	0/3/3/3
5	EDO	D	1309	-	-	0/1/1/1	-
5	EDO	B	1311	-	-	0/1/1/1	-
5	EDO	A	1309	-	-	1/1/1/1	-
5	EDO	C	1311	-	-	1/1/1/1	-
5	EDO	C	1307	-	-	0/1/1/1	-
5	EDO	C	1306	-	-	0/1/1/1	-
2	ADP	A	1301	3	-	4/16/32/32	0/3/3/3
5	EDO	A	1308	-	-	0/1/1/1	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	ADP	PB-O1B	-3.54	1.39	1.50
6	A	1311	A1J1I	O-C	-3.43	1.20	1.30
6	B	1307	A1J1I	O-C	-3.40	1.20	1.30
6	D	1308	A1J1I	O-C	-3.34	1.20	1.30
6	C	1310	A1J1I	O-C	-3.30	1.20	1.30
2	B	1301	ADP	PB-O1B	-2.85	1.41	1.50
2	C	1301	ADP	PB-O1B	-2.74	1.41	1.50
2	D	1301	ADP	PB-O1B	-2.59	1.42	1.50
2	B	1301	ADP	PA-O1A	-2.21	1.43	1.50
2	B	1301	ADP	PB-O2B	-2.16	1.46	1.54
6	B	1307	A1J1I	O1-C	2.12	1.29	1.22
6	D	1308	A1J1I	O1-C	2.04	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	ADP	PB-O2B	-2.00	1.47	1.54
2	A	1301	ADP	PA-O1A	-2.00	1.43	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1311	A1J1I	O1-C-C1	-2.93	114.83	121.94
6	C	1310	A1J1I	O1-C-C1	-2.88	114.94	121.94
6	B	1307	A1J1I	O1-C-C1	-2.87	114.96	121.94
2	D	1301	ADP	C4'-O4'-C1'	-2.85	103.17	109.47
6	D	1308	A1J1I	O1-C-C1	-2.71	115.36	121.94
2	C	1301	ADP	C4'-O4'-C1'	-2.48	103.99	109.47
6	A	1311	A1J1I	O-C-C1	2.30	121.94	115.31
6	C	1310	A1J1I	O-C-C1	2.28	121.87	115.31
6	D	1308	A1J1I	O-C-C1	2.27	121.84	115.31
6	B	1307	A1J1I	O-C-C1	2.16	121.54	115.31
2	B	1301	ADP	C4'-O4'-C1'	-2.12	104.79	109.47
2	A	1301	ADP	C4'-O4'-C1'	-2.12	104.79	109.47

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	ADP	C5'-O5'-PA-O1A
2	C	1301	ADP	C5'-O5'-PA-O1A
2	D	1301	ADP	PA-O3A-PB-O3B
2	D	1301	ADP	C5'-O5'-PA-O1A
2	B	1301	ADP	O4'-C1'-N9-C4
5	D	1312	EDO	O1-C1-C2-O2
2	C	1301	ADP	O4'-C1'-N9-C4
5	A	1306	EDO	O1-C1-C2-O2
5	A	1309	EDO	O1-C1-C2-O2
5	A	1313	EDO	O1-C1-C2-O2
5	A	1315	EDO	O1-C1-C2-O2
5	B	1304	EDO	O1-C1-C2-O2
5	B	1312	EDO	O1-C1-C2-O2
5	B	1313	EDO	O1-C1-C2-O2
5	C	1309	EDO	O1-C1-C2-O2
5	C	1311	EDO	O1-C1-C2-O2
5	C	1312	EDO	O1-C1-C2-O2
5	D	1307	EDO	O1-C1-C2-O2
6	B	1307	A1J1I	N-C5-S-C6

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Mol	Chain	Res	Type	Atoms
6	C	1310	A1J1I	N-C5-S-C6
6	A	1311	A1J1I	O1-C-C1-C5
6	B	1307	A1J1I	O1-C-C1-C5
6	C	1310	A1J1I	O1-C-C1-C5
6	D	1308	A1J1I	O1-C-C1-C5
5	A	1318	EDO	O1-C1-C2-O2
2	B	1301	ADP	O4'-C1'-N9-C8
2	D	1301	ADP	O4'-C1'-N9-C4
5	A	1317	EDO	O1-C1-C2-O2
5	C	1314	EDO	O1-C1-C2-O2
5	D	1304	EDO	O1-C1-C2-O2
6	D	1308	A1J1I	O-C-C1-C5
2	C	1301	ADP	O4'-C1'-N9-C8
2	D	1301	ADP	O4'-C1'-N9-C8
2	A	1301	ADP	PA-O3A-PB-O2B
2	C	1301	ADP	PA-O3A-PB-O2B
2	D	1301	ADP	PA-O3A-PB-O2B
2	A	1301	ADP	C5'-O5'-PA-O3A
2	C	1301	ADP	C5'-O5'-PA-O3A
2	D	1301	ADP	C5'-O5'-PA-O3A
2	A	1301	ADP	C5'-O5'-PA-O2A
2	C	1301	ADP	C5'-O5'-PA-O2A
2	D	1301	ADP	C5'-O5'-PA-O2A
6	A	1311	A1J1I	N-C5-S-C6
6	D	1308	A1J1I	N-C5-S-C6
6	A	1311	A1J1I	O-C-C1-C5
6	B	1307	A1J1I	O-C-C1-C5
6	C	1310	A1J1I	O-C-C1-C5
5	C	1303	EDO	O1-C1-C2-O2
5	B	1309	EDO	O1-C1-C2-O2
5	B	1303	EDO	O1-C1-C2-O2
5	D	1303	EDO	O1-C1-C2-O2
5	D	1310	EDO	O1-C1-C2-O2
6	C	1310	A1J1I	O-C-C1-C2
6	B	1307	A1J1I	O1-C-C1-C2
6	B	1307	A1J1I	O-C-C1-C2
6	A	1311	A1J1I	O-C-C1-C2
6	D	1308	A1J1I	O-C-C1-C2
6	C	1310	A1J1I	O1-C-C1-C2
6	A	1311	A1J1I	O1-C-C1-C2
6	D	1308	A1J1I	O1-C-C1-C2
5	A	1320	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	C	1313	EDO	O1-C1-C2-O2

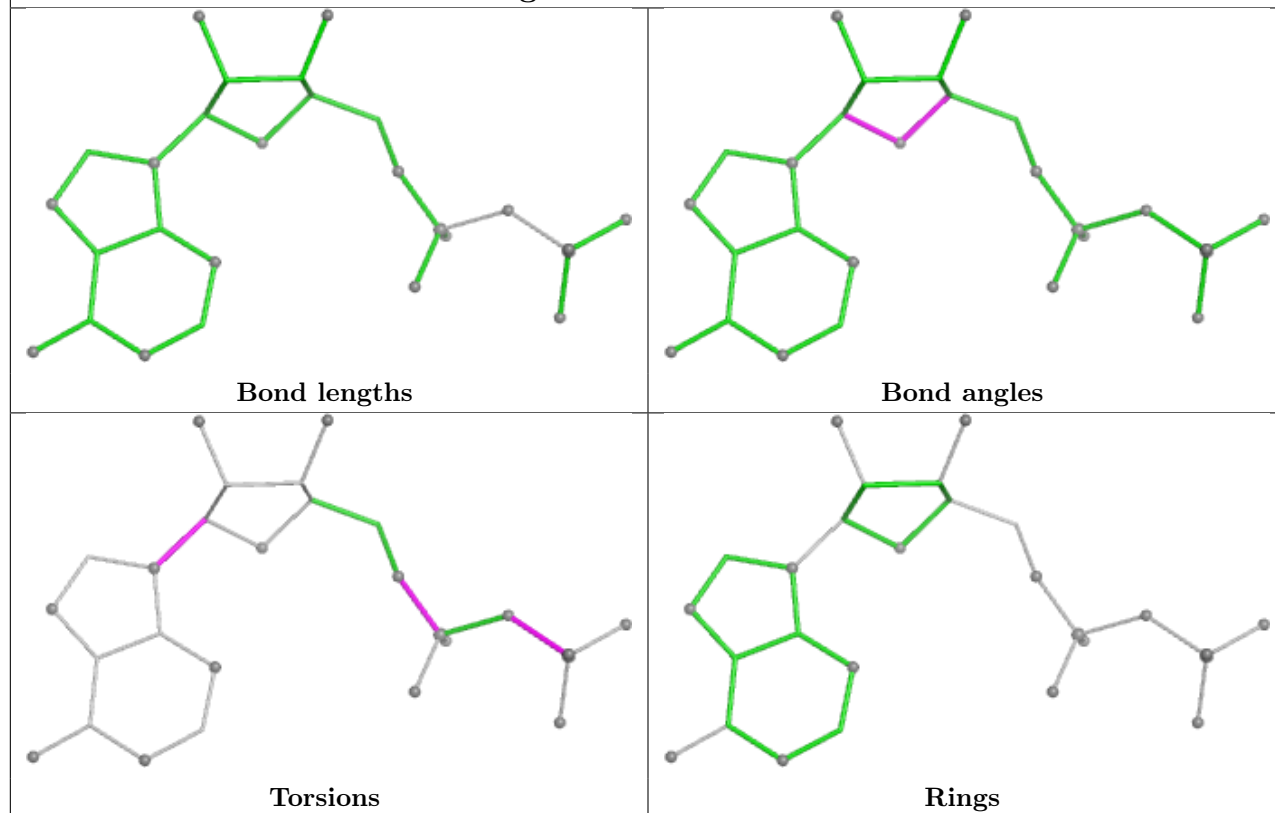
There are no ring outliers.

10 monomers are involved in 11 short contacts:

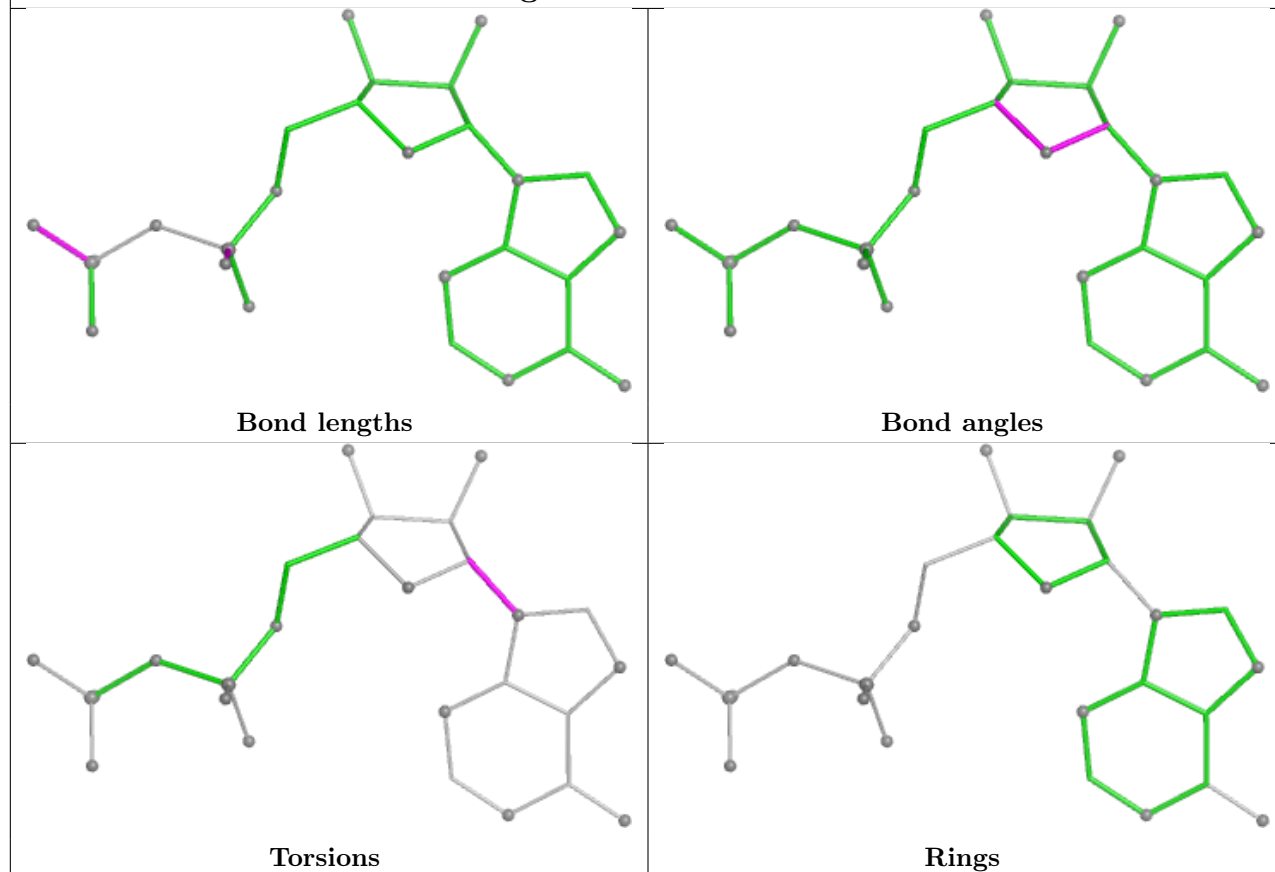
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1311	EDO	1	0
5	A	1307	EDO	1	0
4	B	1316	DMS	2	0
5	A	1320	EDO	1	0
5	D	1304	EDO	1	0
4	D	1305	DMS	1	0
4	D	1313	DMS	2	0
4	C	1305	DMS	1	0
5	C	1304	EDO	1	0
5	A	1308	EDO	1	0

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.

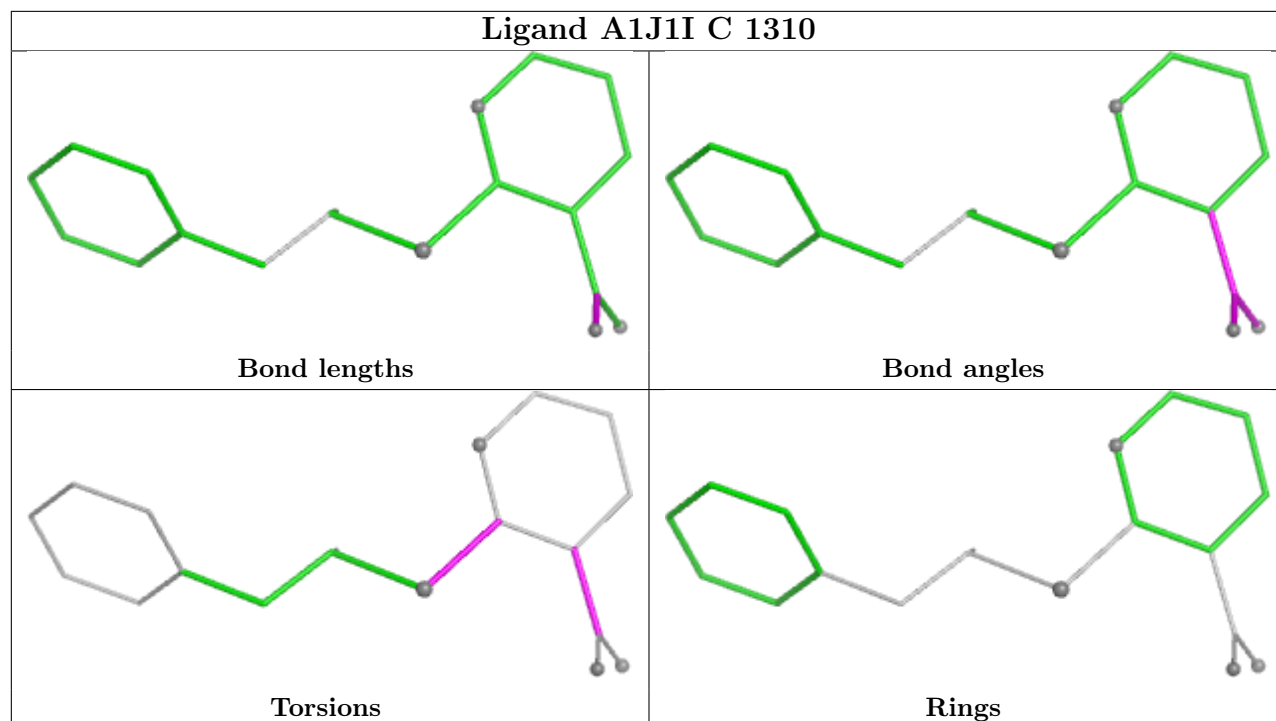
Ligand ADP D 1301



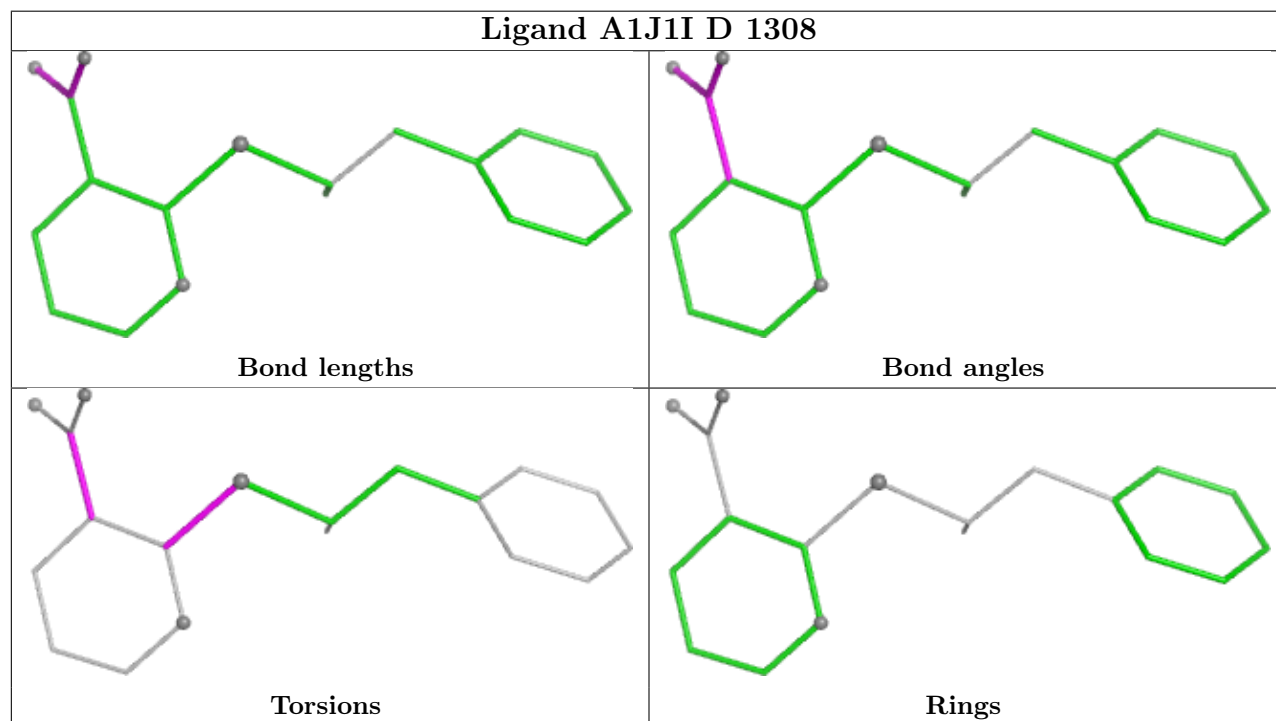
Ligand ADP B 1301



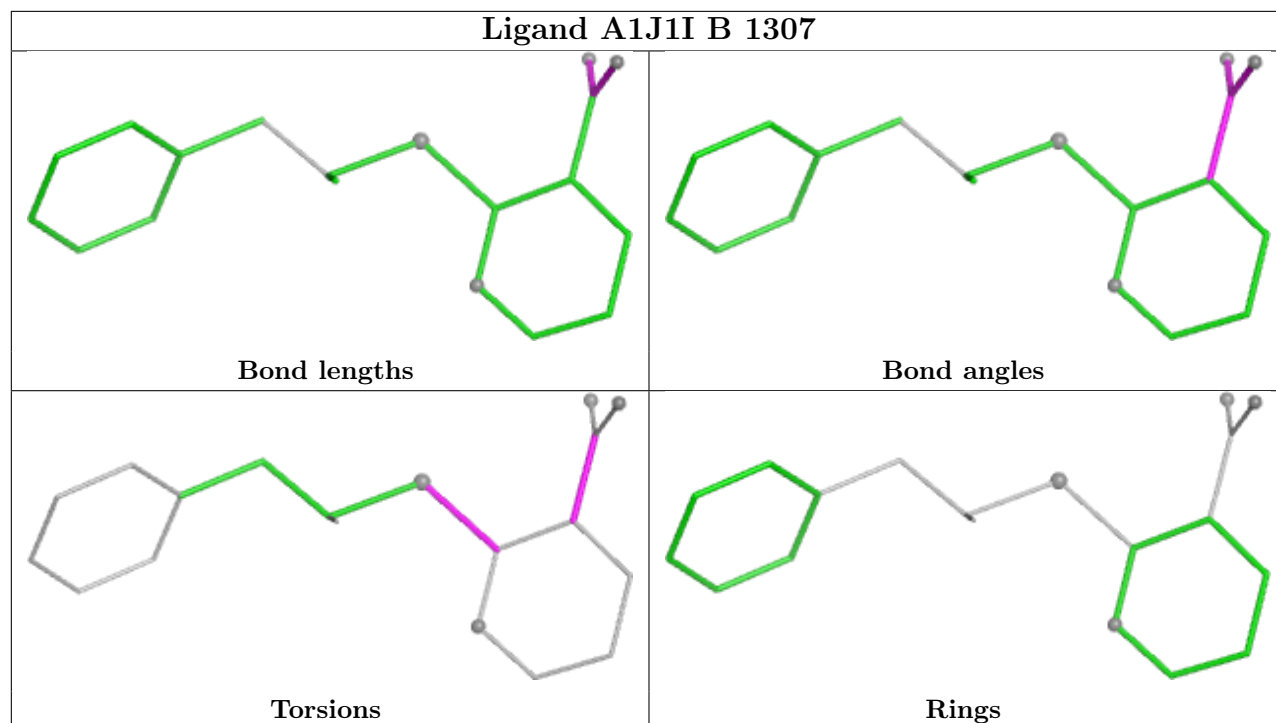
Ligand A1J1I C 1310



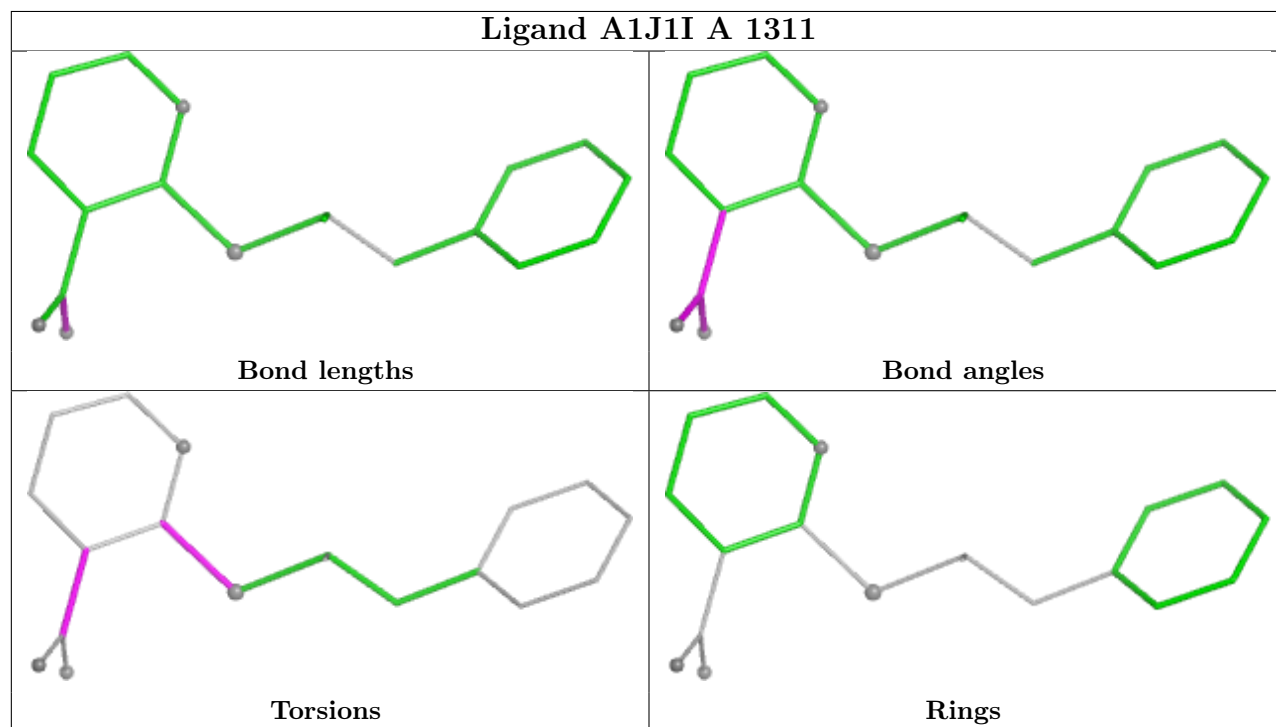
Ligand A1J1I D 1308

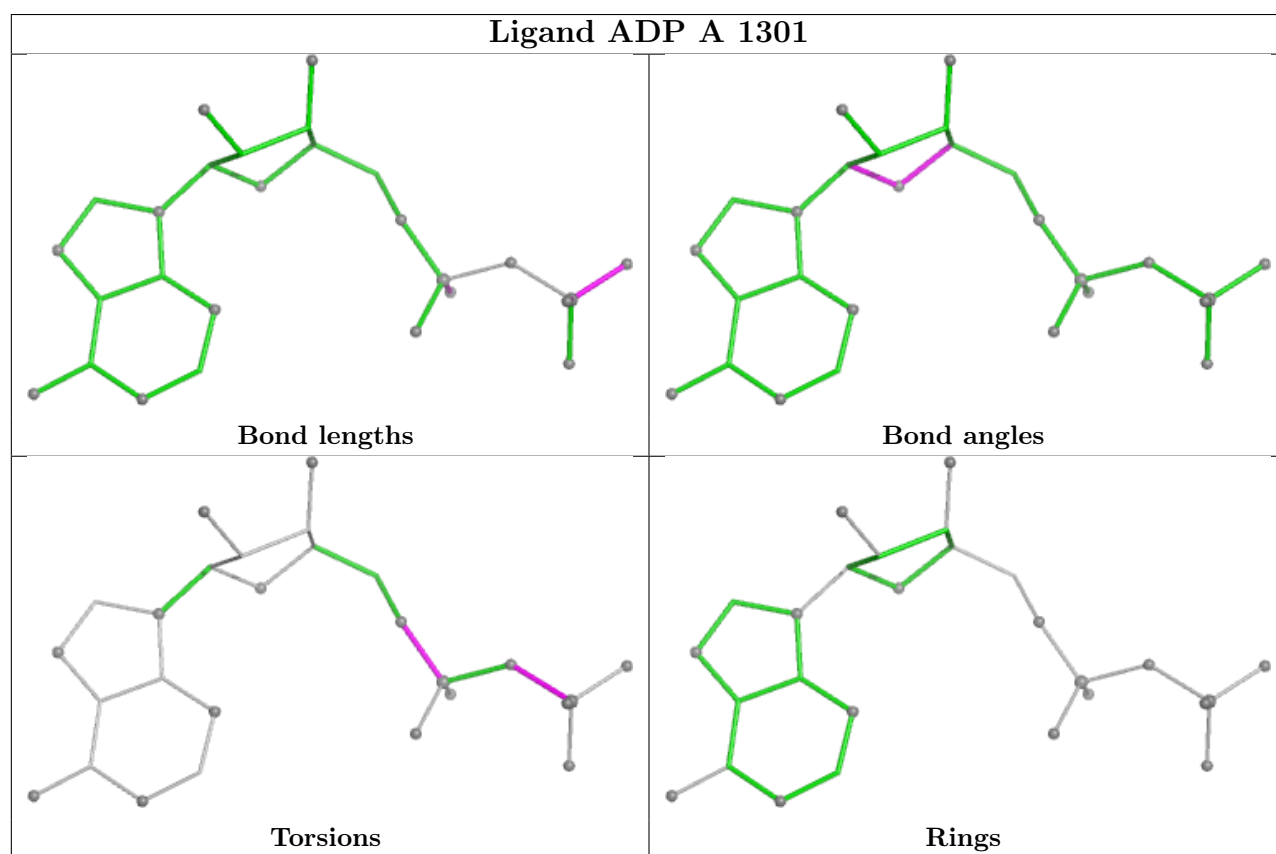
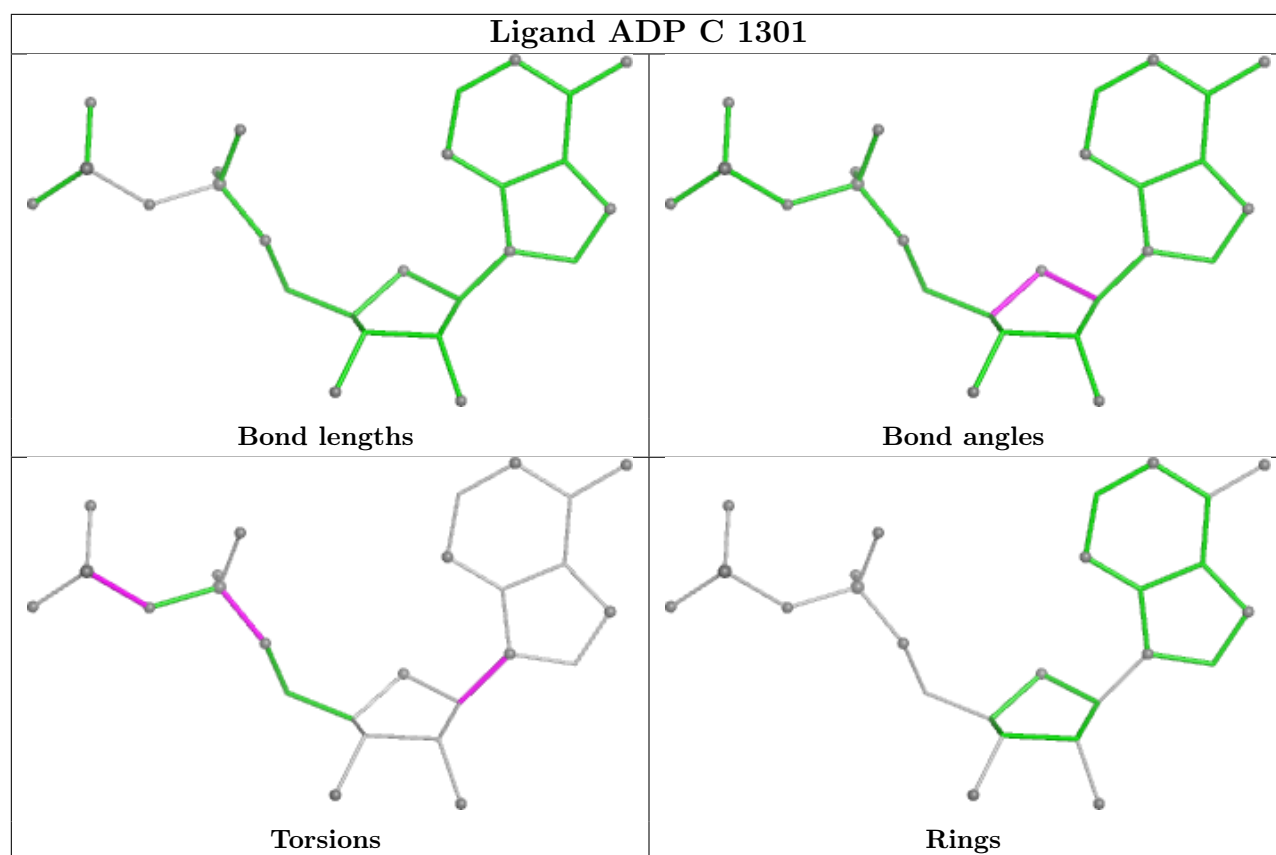


Ligand A1J1I B 1307



Ligand A1J1I A 1311





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%)	0.03	14 (2%) 62 59	21, 47, 74, 91	6 (0%)
1	B	638/680 (93%)	0.05	7 (1%) 78 76	18, 50, 69, 85	10 (1%)
1	C	633/680 (93%)	0.08	9 (1%) 73 71	23, 51, 73, 86	6 (0%)
1	D	632/680 (92%)	0.23	24 (3%) 44 41	21, 54, 81, 93	4 (0%)
All	All	2539/2720 (93%)	0.10	54 (2%) 63 60	18, 51, 74, 93	26 (1%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	844	THR	5.8
1	D	910	ASP	5.6
1	A	1183	VAL	4.4
1	D	916	ASN	4.2
1	D	842	ALA	4.2
1	D	913	LEU	4.0
1	C	1181	PHE	4.0
1	A	741	THR	3.8
1	A	1181	PHE	3.7
1	A	1193	LYS	3.7
1	A	1195	GLN	3.5
1	A	1091	LEU	3.1
1	B	717[A]	SER	3.1
1	D	871	ILE	2.9
1	D	843	GLU	2.9
1	C	846	LEU	2.8
1	D	720	LEU	2.8
1	D	874	LEU	2.8
1	A	844	THR	2.8
1	B	719[A]	THR	2.7
1	D	803	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1196	GLN	2.6
1	D	841	ILE	2.6
1	A	1197	ARG	2.6
1	D	718	ALA	2.5
1	C	870	GLY	2.5
1	D	740	ARG	2.4
1	B	720[A]	LEU	2.4
1	B	1198	LEU	2.4
1	C	1063	TYR	2.3
1	C	1186	PRO	2.3
1	A	1182	LYS	2.3
1	B	1091	LEU	2.3
1	A	1089	HIS	2.3
1	D	847	THR	2.2
1	D	869	THR	2.2
1	D	757	LEU	2.2
1	D	846	LEU	2.2
1	A	1180	PHE	2.2
1	B	721[A]	ASP	2.2
1	D	906	ARG	2.2
1	B	718[A]	ALA	2.2
1	D	908	TYR	2.2
1	C	1089	HIS	2.2
1	D	815	ALA	2.2
1	C	910	ASP	2.1
1	D	862	GLN	2.1
1	D	915	THR	2.1
1	C	845	SER	2.1
1	A	1198	LEU	2.1
1	D	1128	ILE	2.1
1	A	1063	TYR	2.1
1	C	1185	ASP	2.0
1	D	816	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 ⓘ

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	B	1312	4/4	0.67	0.20	74,74,74,74	0
5	EDO	B	1309	4/4	0.72	0.23	82,82,82,82	0
4	DMS	D	1305	4/4	0.73	0.20	102,102,102,103	0
5	EDO	B	1313	4/4	0.73	0.23	73,73,73,73	0
4	DMS	B	1314	4/4	0.74	0.21	113,113,113,113	0
5	EDO	A	1313	4/4	0.77	0.23	80,81,81,81	0
4	DMS	A	1319	4/4	0.77	0.22	89,89,89,89	4
5	EDO	A	1306	4/4	0.78	0.23	64,64,64,64	0
4	DMS	D	1306	4/4	0.78	0.22	91,91,92,92	4
5	EDO	A	1318	4/4	0.78	0.21	75,75,75,75	0
5	EDO	C	1314	4/4	0.78	0.22	68,68,68,68	0
4	DMS	B	1316	4/4	0.79	0.26	90,90,91,91	0
5	EDO	C	1308	4/4	0.79	0.16	65,65,65,65	0
4	DMS	A	1303	4/4	0.79	0.24	81,81,81,81	4
5	EDO	C	1307	4/4	0.80	0.15	70,71,71,71	0
5	EDO	D	1304	4/4	0.80	0.23	70,70,70,70	0
5	EDO	A	1314	4/4	0.81	0.20	67,68,68,68	0
5	EDO	B	1306	4/4	0.82	0.15	66,66,67,67	0
5	EDO	A	1309	4/4	0.82	0.17	50,50,50,50	4
5	EDO	D	1310	4/4	0.82	0.17	54,54,54,54	0
5	EDO	C	1309	4/4	0.83	0.13	55,56,58,58	0
5	EDO	D	1307	4/4	0.83	0.21	94,94,94,94	0
5	EDO	B	1303	4/4	0.83	0.18	67,68,68,68	0
4	DMS	A	1312	4/4	0.84	0.23	90,90,90,90	0
5	EDO	A	1308	4/4	0.84	0.22	77,77,77,78	0
5	EDO	C	1303	4/4	0.85	0.18	70,70,71,71	0
5	EDO	A	1317	4/4	0.85	0.17	77,77,78,78	0
5	EDO	D	1311	4/4	0.85	0.16	67,67,67,67	0
5	EDO	C	1312	4/4	0.86	0.15	64,64,64,65	0
3	MG	D	1302	1/1	0.86	0.09	53,53,53,53	0
4	DMS	A	1304	4/4	0.86	0.22	77,77,77,77	4
5	EDO	A	1316	4/4	0.87	0.18	67,67,67,67	0
5	EDO	B	1304	4/4	0.87	0.17	64,64,64,65	0
4	DMS	D	1314	4/4	0.87	0.20	97,97,97,97	4
4	DMS	B	1315	4/4	0.87	0.32	56,56,56,56	4
5	EDO	A	1315	4/4	0.88	0.15	67,67,67,67	0
5	EDO	D	1309	4/4	0.88	0.16	56,57,57,57	4

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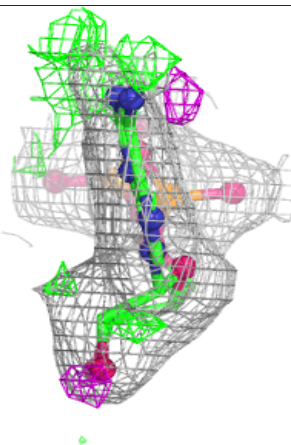
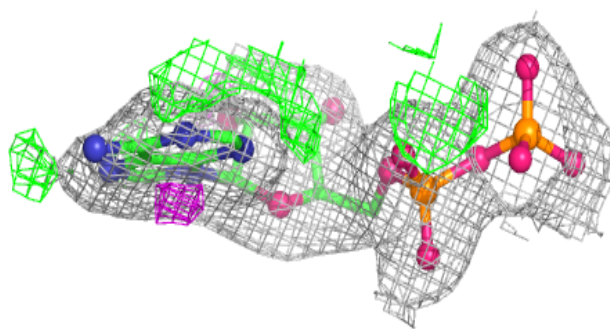
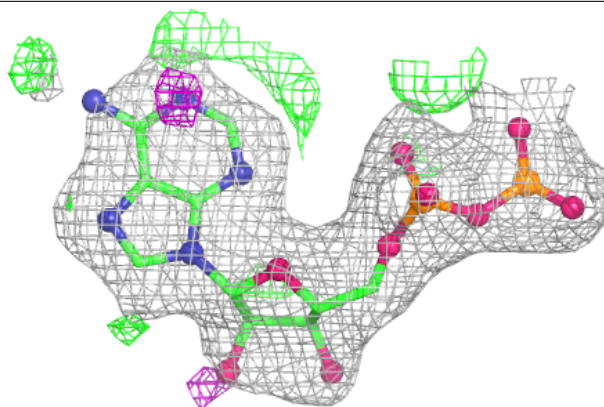
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	C	1311	4/4	0.89	0.13	57,57,58,58	0
4	DMS	A	1321	4/4	0.89	0.23	117,117,117,117	0
4	DMS	D	1313	4/4	0.89	0.21	113,113,113,113	0
5	EDO	B	1311	4/4	0.89	0.12	86,86,86,86	0
5	EDO	D	1312	4/4	0.89	0.13	52,53,53,53	0
4	DMS	B	1305	4/4	0.90	0.20	102,102,103,103	0
4	DMS	B	1308	4/4	0.90	0.18	85,85,85,85	4
3	MG	C	1302	1/1	0.91	0.10	47,47,47,47	0
5	EDO	B	1310	4/4	0.91	0.11	63,64,64,64	0
5	EDO	A	1305	4/4	0.91	0.11	57,58,58,58	0
5	EDO	C	1304	4/4	0.92	0.14	67,67,68,69	0
5	EDO	D	1303	4/4	0.92	0.12	63,63,63,64	0
5	EDO	C	1313	4/4	0.93	0.12	60,60,61,62	0
5	EDO	C	1306	4/4	0.93	0.13	67,67,67,67	0
5	EDO	A	1307	4/4	0.93	0.13	58,58,58,59	0
2	ADP	D	1301	27/27	0.94	0.10	40,51,52,53	27
4	DMS	C	1305	4/4	0.94	0.14	108,108,109,109	0
2	ADP	B	1301	27/27	0.94	0.10	44,53,55,55	0
2	ADP	A	1301	27/27	0.95	0.09	36,47,48,49	0
5	EDO	A	1310	4/4	0.95	0.07	54,54,55,55	0
2	ADP	C	1301	27/27	0.95	0.09	38,48,49,50	27
5	EDO	A	1320	4/4	0.96	0.12	65,66,66,66	0
3	MG	A	1302	1/1	0.96	0.08	42,42,42,42	0
6	A1J1I	A	1311	19/19	0.96	0.07	34,36,40,40	0
6	A1J1I	B	1307	19/19	0.97	0.06	35,37,40,40	0
6	A1J1I	C	1310	19/19	0.97	0.06	38,40,42,42	0
6	A1J1I	D	1308	19/19	0.98	0.05	38,39,40,40	0
3	MG	B	1302	1/1	0.99	0.04	42,42,42,42	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.

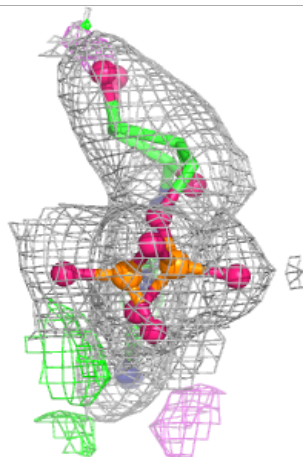
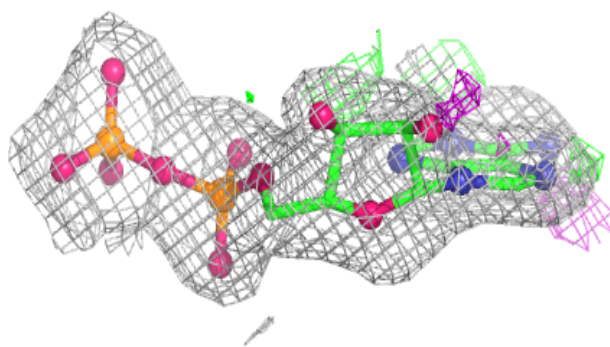
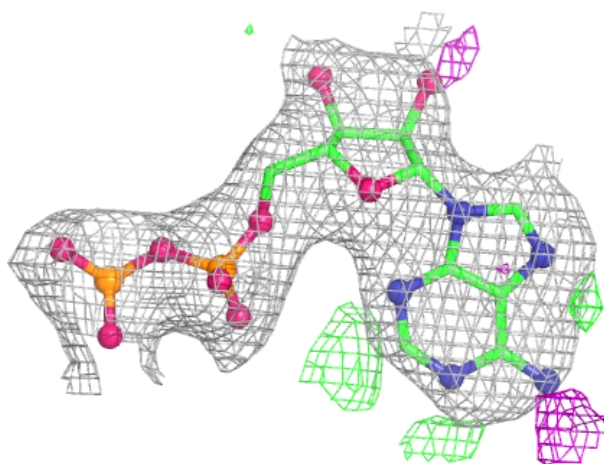
Electron density around ADP D 1301:

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



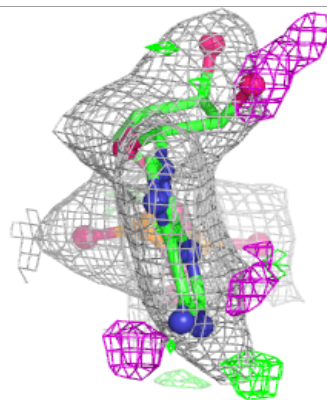
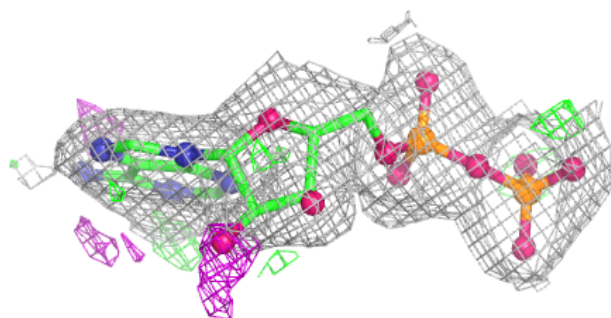
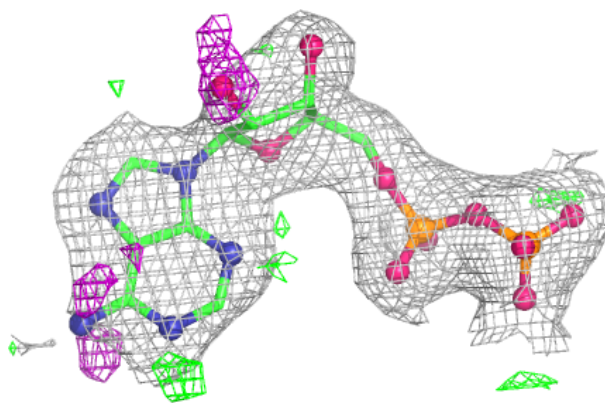
Electron density around ADP B 1301:

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



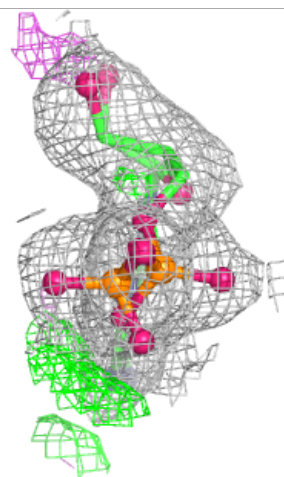
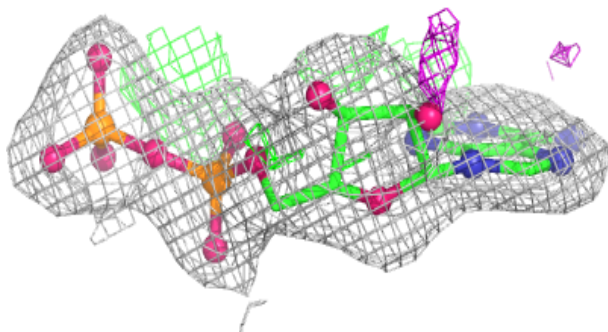
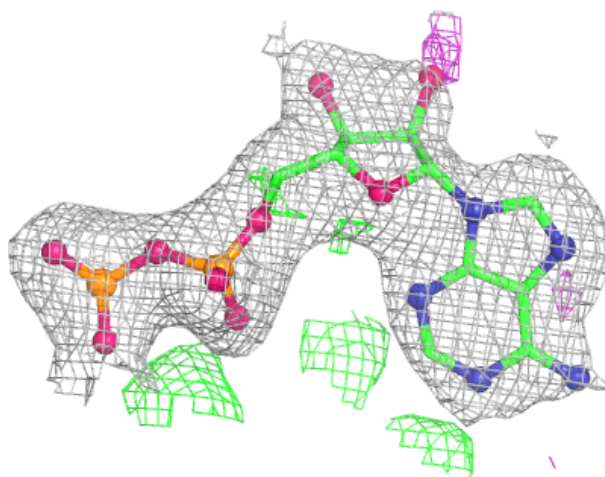
Electron density around ADP A 1301:

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



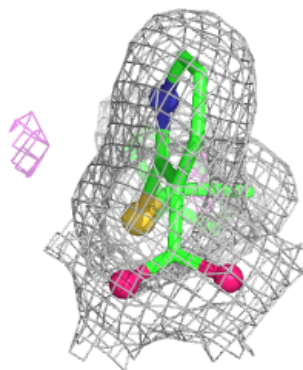
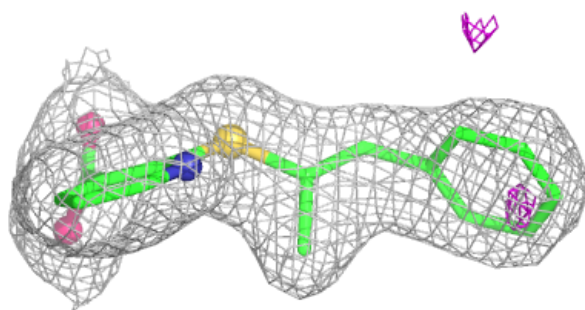
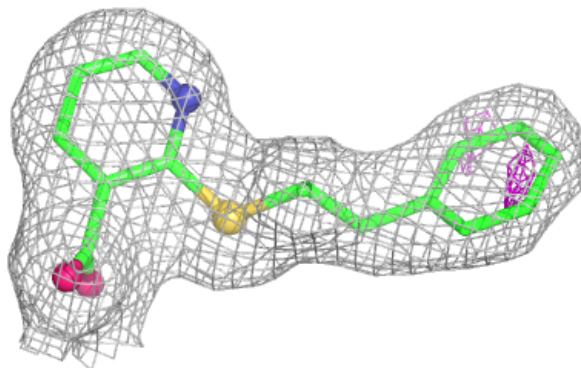
Electron density around ADP C 1301:

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

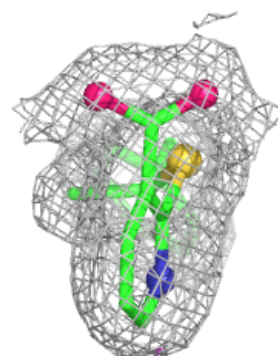
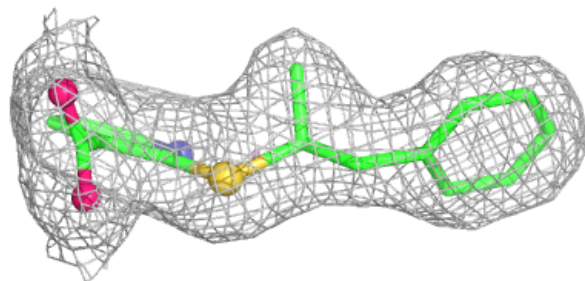
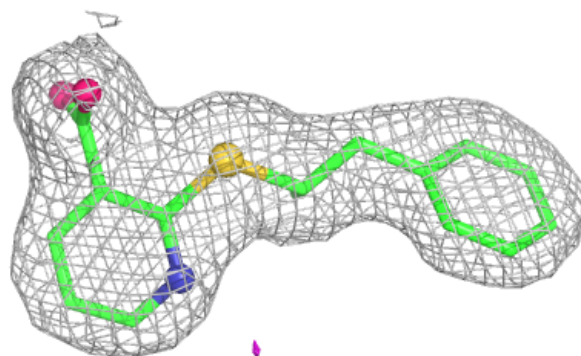


Electron density around A1J1I A 1311:

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

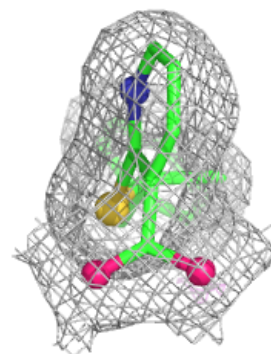
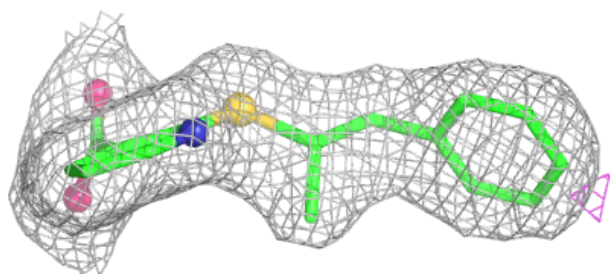
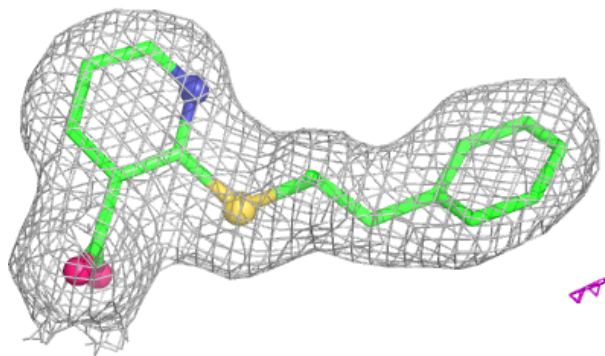
**Electron density around A1J1I B 1307:**

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

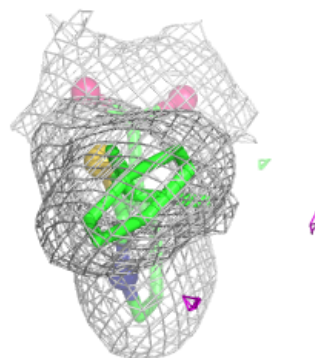
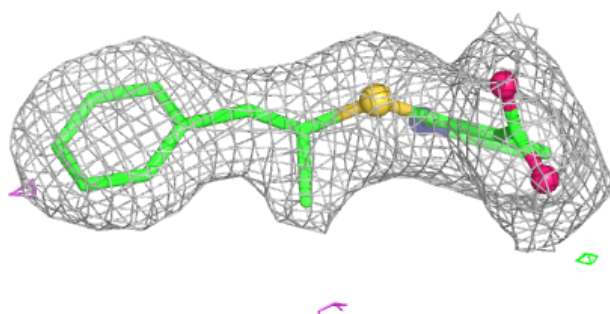
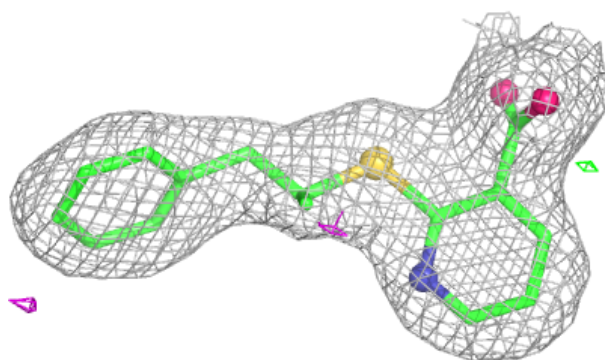


Electron density around A1J1I C 1310:

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

**Electron density around A1J1I D 1308:**

$2mF_o-DF_c$ (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.