



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:40 AM UTC

PDB ID : 6HYS / pdb_00006hys
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

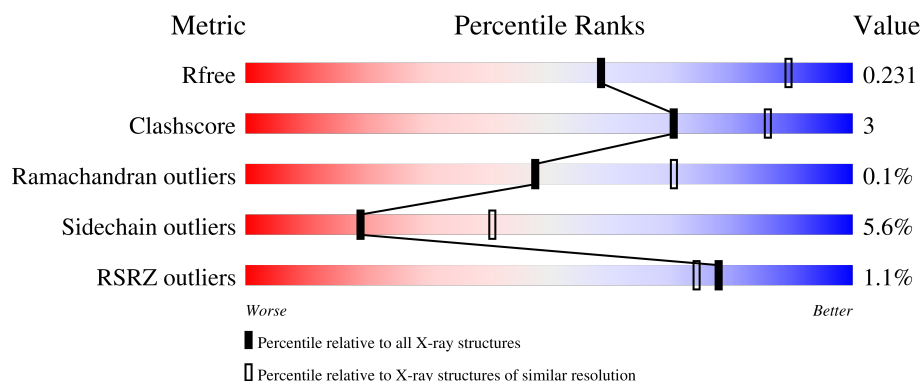
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	673	0% 78% 15% 6%
1	B	673	0% 80% 12% 6%
1	C	673	2% 82% 11% 6%
1	D	673	0% 82% 11% 6%

2 Entry composition [i](#)

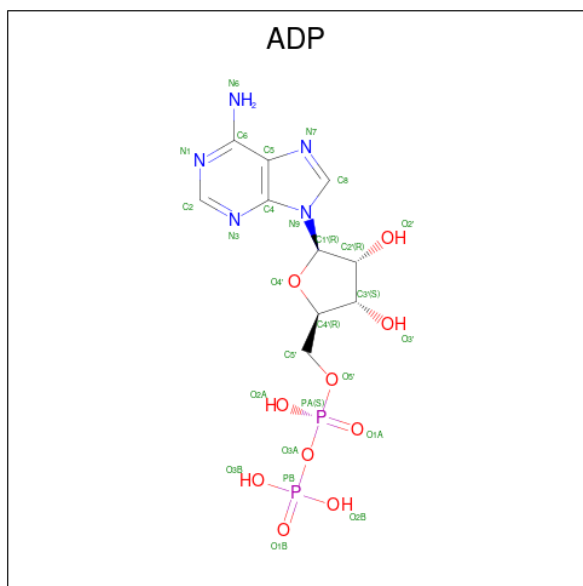
There are 7 unique types of molecules in this entry. The entry contains 19875 atoms, of which 0 are hydrogens and 0 are deuteriums.

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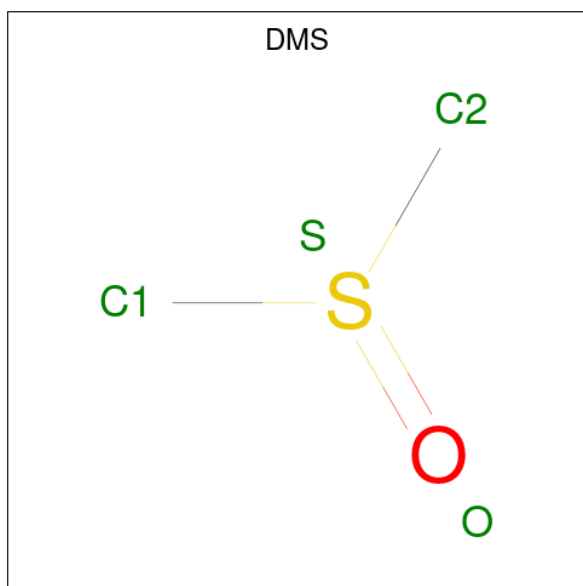
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	1
			46	20	10	14	2		

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

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

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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		

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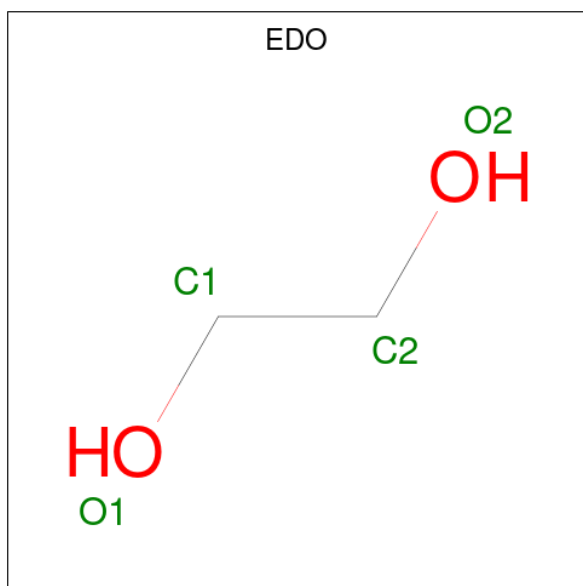
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	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	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	C	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	C	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	C	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	C	1	Total 4	C 2	O 1	S 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 (CCD ID: EDO) (formula: C₂H₆O₂).



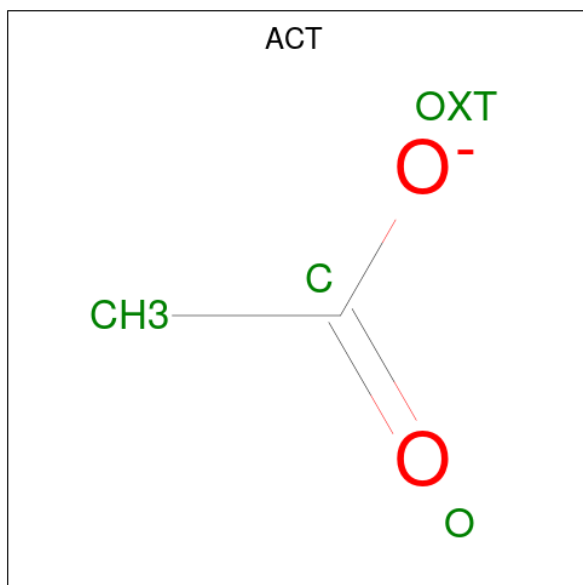
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	2	2		
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 ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 7 is water.

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

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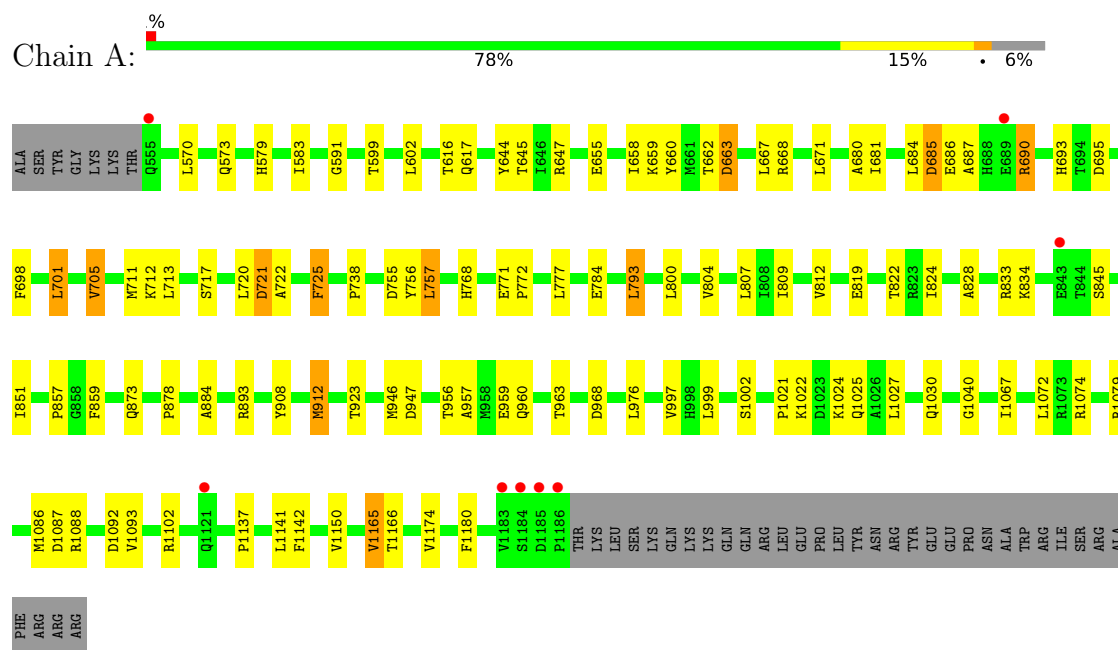
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	101	Total 101	O 101	0	0

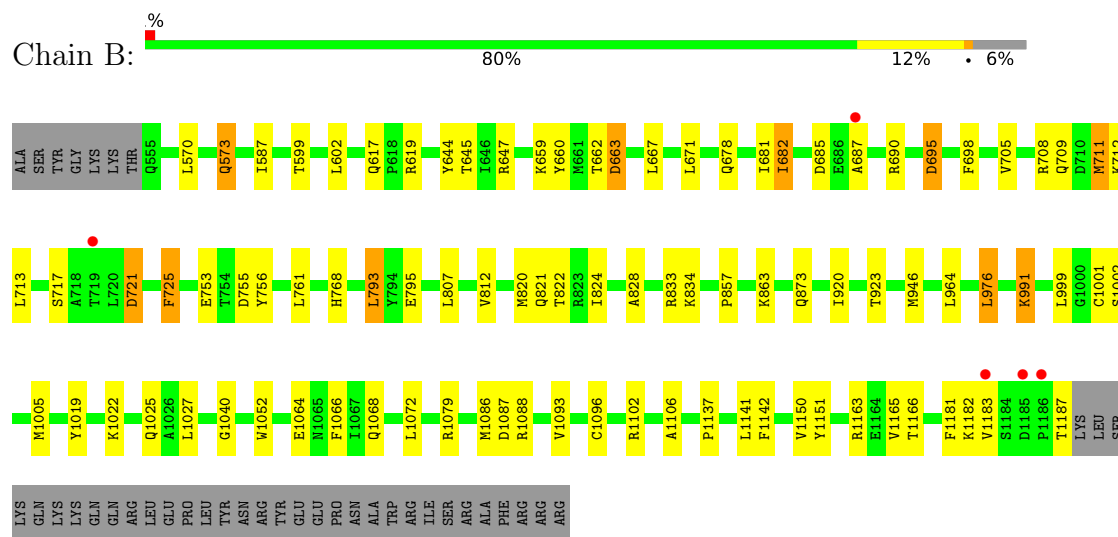
3 Residue-property plots

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.

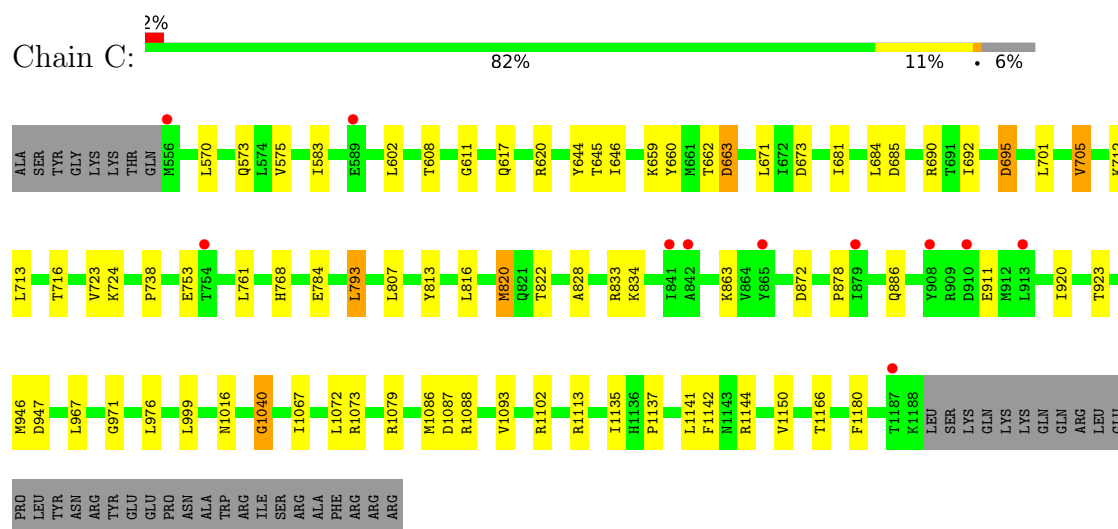
• Molecule 1: ATP-dependent RNA helicase DHX8



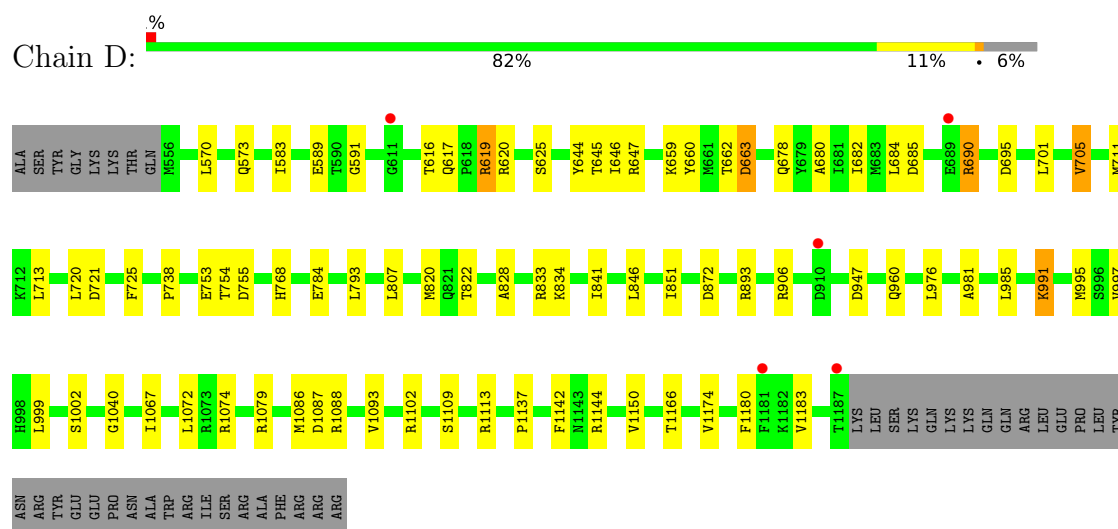
• Molecule 1: ATP-dependent RNA helicase DHX8



• 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	66.96Å 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
$\langle I/\sigma(I) \rangle$ 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 , 92.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

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: DMS, ACT, EDO, MG, 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	0.91	2/4910 (0.0%)	1.36	23/6674 (0.3%)
1	B	0.90	0/4913	1.36	19/6676 (0.3%)
1	C	0.88	1/4825 (0.0%)	1.34	15/6565 (0.2%)
1	D	0.89	1/4842 (0.0%)	1.35	20/6578 (0.3%)
All	All	0.89	4/19490 (0.0%)	1.35	77/26493 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	851	ILE	CG1-CD1	-6.36	1.26	1.51
1	A	912	MET	SD-CE	-5.76	1.65	1.79
1	A	771	GLU	C-N	5.48	1.38	1.33
1	C	1135	ILE	CA-C	5.05	1.58	1.52

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	721	ASP	CA-CB-CG	8.97	121.57	112.60
1	D	1180	PHE	CA-CB-CG	8.78	122.58	113.80
1	B	1182	LYS	CA-C-N	8.41	137.10	121.97
1	B	1182	LYS	C-N-CA	8.41	137.10	121.97
1	B	1181	PHE	CA-C-N	7.63	136.11	121.54
1	B	1181	PHE	C-N-CA	7.63	136.11	121.54
1	C	1180	PHE	CA-CB-CG	7.41	121.20	113.80
1	C	673	ASP	CA-CB-CG	6.99	119.59	112.60
1	B	663	ASP	CA-CB-CG	6.69	119.29	112.60
1	A	685	ASP	CA-CB-CG	6.49	119.09	112.60
1	B	1182	LYS	N-CA-C	-6.42	97.12	110.80
1	D	1040	GLY	N-CA-C	6.36	120.01	110.97
1	A	1040	GLY	N-CA-C	6.32	119.95	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1040	GLY	N-CA-C	6.29	119.90	110.97
1	A	755	ASP	CA-CB-CG	6.29	118.89	112.60
1	B	1040	GLY	N-CA-C	6.18	119.75	110.97
1	C	1016	ASN	CA-CB-CG	6.16	118.76	112.60
1	A	957	ALA	CA-C-N	6.03	128.28	120.44
1	A	957	ALA	C-N-CA	6.03	128.28	120.44
1	B	1079	ARG	CA-C-N	5.83	128.09	120.28
1	B	1079	ARG	C-N-CA	5.83	128.09	120.28
1	D	663	ASP	CA-CB-CG	5.78	118.38	112.60
1	C	663	ASP	CA-CB-CG	5.74	118.34	112.60
1	B	599	THR	CA-C-N	5.72	127.94	120.28
1	B	599	THR	C-N-CA	5.72	127.94	120.28
1	A	725	PHE	CA-CB-CG	5.67	119.47	113.80
1	A	968	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	772	PRO	CA-C-O	-5.60	116.87	120.90
1	B	725	PHE	CA-CB-CG	5.60	119.40	113.80
1	D	906	ARG	CA-C-N	5.59	128.33	120.28
1	D	906	ARG	C-N-CA	5.59	128.33	120.28
1	B	755	ASP	CA-CB-CG	5.54	118.14	112.60
1	C	872	ASP	CA-CB-CG	5.49	118.09	112.60
1	C	1150	VAL	N-CA-CB	5.49	119.53	111.52
1	A	1180	PHE	CA-CB-CG	5.45	119.25	113.80
1	A	997	VAL	N-CA-C	-5.44	105.41	110.53
1	A	1079	ARG	CA-C-N	5.44	127.57	120.28
1	A	1079	ARG	C-N-CA	5.44	127.57	120.28
1	D	1150	VAL	N-CA-CB	5.44	119.46	111.52
1	C	1079	ARG	CA-C-N	5.43	127.56	120.28
1	C	1079	ARG	C-N-CA	5.43	127.56	120.28
1	B	1150	VAL	N-CA-CB	5.41	119.42	111.52
1	A	721	ASP	CA-C-N	5.38	128.49	120.31
1	A	721	ASP	C-N-CA	5.38	128.49	120.31
1	A	1150	VAL	N-CA-CB	5.36	119.34	111.52
1	B	721	ASP	CA-C-N	5.32	128.80	120.82
1	B	721	ASP	C-N-CA	5.32	128.80	120.82
1	A	680	ALA	N-CA-C	-5.29	106.96	113.41
1	D	1079	ARG	CA-C-N	5.28	127.35	120.28
1	D	1079	ARG	C-N-CA	5.28	127.35	120.28
1	B	685	ASP	CA-CB-CG	5.24	117.84	112.60
1	B	619	ARG	CA-C-N	5.21	127.52	120.65
1	B	619	ARG	C-N-CA	5.21	127.52	120.65
1	C	692	ILE	N-CA-CB	5.20	116.28	110.51
1	D	755	ASP	CA-CB-CG	5.18	117.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	784	GLU	CA-C-N	5.16	127.20	120.28
1	C	784	GLU	C-N-CA	5.16	127.20	120.28
1	A	819	GLU	CA-C-N	5.15	128.14	120.31
1	A	819	GLU	C-N-CA	5.15	128.14	120.31
1	D	721	ASP	CA-CB-CG	5.15	117.75	112.60
1	D	720	LEU	CA-C-N	5.13	127.41	120.38
1	D	720	LEU	C-N-CA	5.13	127.41	120.38
1	D	725	PHE	CA-CB-CG	5.13	118.93	113.80
1	A	784	GLU	CA-C-N	5.08	127.08	120.28
1	A	784	GLU	C-N-CA	5.08	127.08	120.28
1	D	784	GLU	CA-C-N	5.07	127.08	120.28
1	D	784	GLU	C-N-CA	5.07	127.08	120.28
1	C	575	VAL	N-CA-CB	5.07	117.43	110.54
1	D	680	ALA	N-CA-C	-5.06	107.24	113.41
1	D	619	ARG	CA-C-N	5.05	127.31	120.65
1	D	619	ARG	C-N-CA	5.05	127.31	120.65
1	C	886	GLN	CA-C-N	5.03	126.98	120.44
1	C	886	GLN	C-N-CA	5.03	126.98	120.44
1	D	872	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	908	TYR	CA-C-N	5.03	126.98	120.44
1	A	908	TYR	C-N-CA	5.03	126.98	120.44
1	D	997	VAL	N-CA-C	-5.02	105.70	110.42

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	42	0
1	B	4814	0	4542	36	0
1	C	4726	0	4384	28	0
1	D	4743	0	4423	25	0
2	A	46	0	24	0	0
2	B	46	0	24	0	0
2	C	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	4	0
4	B	32	0	48	2	0
4	C	36	0	54	1	0
4	D	28	0	42	2	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	129	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 (129) 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:B:682:ILE:HD12	1:B:711:MET:HE1	1.45	0.99
1:A:1141:LEU:HD12	1:A:1165:VAL:HG12	1.60	0.82
1:B:690:ARG:HH11	1:B:695:ASP:CG	1.96	0.74
1:D:625:SER:HB3	2:D:1301[B]:ADP:HN62	1.55	0.71
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:A:1030:GLN:HG3	4:A:1312:DMS:H11	1.78	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:985:LEU:O	4:D:1306:DMS:H21	2.07	0.54
1:A:1067:ILE:HG21	1:A:1072:LEU:HD11	1.90	0.54
1:A:800:LEU:HB3	1:A:804:VAL:HG21	1.90	0.53
1:C:690:ARG:HH21	1:C:695:ASP:CG	2.17	0.53
1:A:756:TYR:HB2	1:A:857:PRO:HB3	1.90	0.53
1:B:1163:ARG:HD2	4:B:1308:DMS:H13	1.89	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:964:LEU:HD22	1:B:991:LYS:HG3	1.92	0.51
1:A:668[A]:ARG:HH22	4:A:1307:DMS:H11	1.76	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:HH22	1:C:947:ASP:HB2	1.77	0.48
1:C:878:PRO:HB3	4:C:1307:DMS:H12	1.95	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:724:LYS:HD3	1:C:946:MET:HE3	1.97	0.46
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:878:PRO:HB3	4:A:1310:DMS:H12	1.97	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:C:1086:MET:HE3	1:C:1093:VAL:HG22	1.99	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:D:981:ALA:HA	4:D:1306:DMS:H12	1.99	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:D:682:ILE:HB	1:D:711:MET:HE3	1.98	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:D:1086:MET:HE3	1:D:1093:VAL:HG22	1.98	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:B:1005:MET:HE3	1:B:1106:ALA:HB3	2.00	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:A:884:ALA:HB2	1:A:912:MET:HE1	1.99	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:B:1086:MET:HE3	1:B:1093:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:999:LEU:O	1:C:1102:ARG:HD3	2.18	0.43
1:A:725:PHE:CE1	1:A:946:MET:HE1	2.54	0.43
1:A:720:LEU:C	1:A:722:ALA:H	2.25	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
1:A:1086:MET:HE3	1:A:1093:VAL:HG22	2.01	0.42
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:B:725:PHE:CE1	1:B:946:MET:HE1	2.55	0.42
1:D:999:LEU:O	1:D:1102:ARG:HD3	2.19	0.42
1:A:859:PHE:CZ	4:A:1310:DMS:H22	2.55	0.41
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:B:1163:ARG:CD	4:B:1308:DMS:H13	2.51	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%)	43	66
1	B	633/673 (94%)	607 (96%)	25 (4%)	1 (0%)	43	66
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%)	48	70

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%)	441 (94%)	27 (6%)	18	39
1	B	466/596 (78%)	437 (94%)	29 (6%)	16	36
1	C	435/596 (73%)	415 (95%)	20 (5%)	24	49
1	D	452/596 (76%)	426 (94%)	26 (6%)	18	39
All	All	1821/2384 (76%)	1719 (94%)	102 (6%)	19	40

All (102) 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	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	793	LEU
1	A	807	LEU
1	A	822	THR
1	A	873	GLN
1	A	923	THR
1	A	976	LEU
1	A	1002	SER
1	A	1027	LEU
1	A	1074	ARG
1	A	1088	ARG
1	A	1092	ASP
1	A	1165	VAL
1	A	1166	THR
1	A	1174	VAL
1	B	573	GLN
1	B	647	ARG
1	B	663	ASP
1	B	667	LEU
1	B	671	LEU
1	B	678	GLN
1	B	682	ILE
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

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Mol	Chain	Res	Type
1	B	795[B]	GLU
1	B	807	LEU
1	B	820	MET
1	B	822	THR
1	B	873	GLN
1	B	920	ILE
1	B	976	LEU
1	B	991	LYS
1	B	1002	SER
1	B	1064	GLU
1	B	1088	ARG
1	B	1166	THR
1	B	1187	THR
1	C	573	GLN
1	C	663	ASP
1	C	671	LEU
1	C	695	ASP
1	C	705	VAL
1	C	713	LEU
1	C	723	VAL
1	C	753	GLU
1	C	793	LEU
1	C	807	LEU
1	C	820	MET
1	C	822	THR
1	C	911	GLU
1	C	920	ILE
1	C	976	LEU
1	C	1073	ARG
1	C	1088	ARG
1	C	1113	ARG
1	C	1144	ARG
1	C	1166	THR
1	D	573	GLN
1	D	589	GLU
1	D	619	ARG
1	D	647	ARG
1	D	663	ASP
1	D	678	GLN
1	D	690	ARG
1	D	695	ASP
1	D	705	VAL

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Mol	Chain	Res	Type
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	822	THR
1	D	976	LEU
1	D	991	LYS
1	D	995	MET
1	D	1002	SER
1	D	1074	ARG
1	D	1088	ARG
1	D	1144	ARG
1	D	1166	THR
1	D	1174	VAL
1	D	1183	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	561	GLN
1	A	821	GLN
1	A	873	GLN
1	A	886	GLN
1	A	916	ASN
1	A	924	ASN
1	A	938	ASN
1	A	960	GLN
1	A	998	HIS
1	A	1152	HIS
1	B	573	GLN
1	B	688	HIS
1	B	709	GLN
1	B	886	GLN
1	B	916	ASN
1	B	1025	GLN
1	B	1152	HIS
1	C	821	GLN
1	C	883	GLN
1	C	916	ASN
1	C	924	ASN

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Mol	Chain	Res	Type
1	C	1089	HIS
1	C	1143	ASN
1	C	1152	HIS
1	D	561	GLN
1	D	881	GLN
1	D	924	ASN
1	D	1068	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
4	DMS	B	1312	-	3,3,3	0.32	0	3,3,3	0.29	0
4	DMS	A	1307	-	3,3,3	0.27	0	3,3,3	0.56	0
2	ADP	B	1301[B]	-	28,29,29	0.32	0	43,45,45	0.68	0
4	DMS	A	1303	-	3,3,3	0.29	0	3,3,3	0.14	0
4	DMS	C	1312	-	3,3,3	0.33	0	3,3,3	0.25	0
5	EDO	B	1306	-	3,3,3	0.56	0	2,2,2	0.35	0
4	DMS	B	1308	-	3,3,3	0.27	0	3,3,3	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	C	1309	-	3,3,3	0.34	0	3,3,3	0.44	0
4	DMS	C	1310	-	3,3,3	0.34	0	3,3,3	0.39	0
4	DMS	C	1306	-	3,3,3	0.31	0	3,3,3	0.37	0
5	EDO	D	1303	-	3,3,3	0.63	0	2,2,2	0.34	0
4	DMS	A	1311	-	3,3,3	0.32	0	3,3,3	0.22	0
4	DMS	C	1305	-	3,3,3	0.30	0	3,3,3	0.31	0
4	DMS	B	1310	-	3,3,3	0.26	0	3,3,3	0.28	0
4	DMS	C	1304	-	3,3,3	0.31	0	3,3,3	0.27	0
4	DMS	C	1307	-	3,3,3	0.29	0	3,3,3	0.15	0
4	DMS	B	1307	-	3,3,3	0.25	0	3,3,3	0.43	0
5	EDO	C	1303	-	3,3,3	0.58	0	2,2,2	0.15	0
4	DMS	D	1307	-	3,3,3	0.39	0	3,3,3	0.31	0
4	DMS	C	1311	-	3,3,3	0.33	0	3,3,3	0.35	0
6	ACT	D	1312	-	3,3,3	1.10	0	3,3,3	1.27	0
4	DMS	D	1308	-	3,3,3	0.30	0	3,3,3	0.23	0
5	EDO	A	1305	-	3,3,3	0.55	0	2,2,2	0.31	0
2	ADP	D	1301[A]	-	28,29,29	0.38	0	43,45,45	0.70	2 (4%)
4	DMS	A	1310	-	3,3,3	0.25	0	3,3,3	0.24	0
4	DMS	B	1311	-	3,3,3	0.25	0	3,3,3	0.15	0
4	DMS	A	1309	-	3,3,3	0.29	0	3,3,3	0.36	0
2	ADP	D	1301[B]	-	28,29,29	0.38	0	43,45,45	0.76	2 (4%)
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
4	DMS	D	1309	-	3,3,3	0.33	0	3,3,3	0.24	0
4	DMS	D	1306	-	3,3,3	0.20	0	3,3,3	0.26	0
4	DMS	B	1304	-	3,3,3	0.34	0	3,3,3	0.36	0
4	DMS	B	1303	-	3,3,3	0.29	0	3,3,3	0.25	0
6	ACT	A	1308	-	3,3,3	1.44	0	3,3,3	1.05	0
4	DMS	D	1311	-	3,3,3	0.33	0	3,3,3	0.45	0
2	ADP	A	1301[B]	-	28,29,29	0.34	0	43,45,45	0.73	1 (2%)
2	ADP	A	1301[A]	-	28,29,29	0.33	0	43,45,45	0.58	0
5	EDO	A	1304	-	3,3,3	0.65	0	2,2,2	0.06	0
4	DMS	B	1305	-	3,3,3	0.23	0	3,3,3	0.28	0
4	DMS	D	1310	-	3,3,3	0.33	0	3,3,3	0.06	0
4	DMS	A	1312	-	3,3,3	0.27	0	3,3,3	0.42	0
4	DMS	A	1306	-	3,3,3	0.31	0	3,3,3	0.27	0
6	ACT	B	1309	-	3,3,3	1.26	0	3,3,3	0.97	0
2	ADP	C	1301	3	28,29,29	0.47	0	43,45,45	0.90	3 (6%)
4	DMS	A	1313	-	3,3,3	0.29	0	3,3,3	0.32	0
5	EDO	D	1304	-	3,3,3	0.42	0	2,2,2	0.67	0
2	ADP	B	1301[A]	-	28,29,29	0.35	0	43,45,45	0.64	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	B	1301[B]	-	-	2/16/32/32	0/3/3/3
5	EDO	B	1306	-	-	1/1/1/1	-
5	EDO	C	1303	-	-	0/1/1/1	-
2	ADP	C	1301	3	-	5/16/32/32	0/3/3/3
5	EDO	D	1303	-	-	0/1/1/1	-
5	EDO	A	1305	-	-	0/1/1/1	-
2	ADP	A	1301[B]	-	-	5/16/32/32	0/3/3/3
2	ADP	A	1301[A]	-	-	2/16/32/32	0/3/3/3
5	EDO	A	1304	-	-	0/1/1/1	-
2	ADP	D	1301[A]	-	-	0/16/32/32	0/3/3/3
2	ADP	D	1301[B]	-	-	5/16/32/32	0/3/3/3
5	EDO	D	1304	-	-	0/1/1/1	-
2	ADP	B	1301[A]	-	-	5/16/32/32	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1301	ADP	C4'-O4'-C1'	-2.56	103.80	109.47
2	C	1301	ADP	O3B-PB-O2B	2.55	117.37	107.80
2	C	1301	ADP	O2A-PA-O5'	2.06	116.89	107.57
2	D	1301[A]	ADP	O3B-PB-O2B	2.04	115.44	107.80
2	D	1301[B]	ADP	O3B-PB-O2B	2.04	115.44	107.80
2	D	1301[A]	ADP	O2B-PB-O1B	-2.03	102.93	110.83
2	D	1301[B]	ADP	O2B-PB-O1B	-2.03	102.93	110.83
2	A	1301[B]	ADP	C4'-O4'-C1'	-2.01	105.03	109.47

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301[B]	ADP	C5'-O5'-PA-O1A
2	A	1301[B]	ADP	C5'-O5'-PA-O3A
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

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Mol	Chain	Res	Type	Atoms
2	D	1301[B]	ADP	C5'-O5'-PA-O2A
2	C	1301	ADP	O4'-C1'-N9-C4
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	C	1301	ADP	O4'-C1'-N9-C8
2	A	1301[B]	ADP	C5'-O5'-PA-O2A
2	B	1301[A]	ADP	C5'-O5'-PA-O1A
2	B	1301[A]	ADP	C5'-O5'-PA-O2A
2	B	1301[A]	ADP	C5'-O5'-PA-O3A
2	C	1301	ADP	C5'-O5'-PA-O1A
2	C	1301	ADP	C5'-O5'-PA-O3A
2	D	1301[B]	ADP	C5'-O5'-PA-O1A
2	D	1301[B]	ADP	C5'-O5'-PA-O3A
2	D	1301[B]	ADP	O4'-C1'-N9-C8
5	B	1306	EDO	O1-C1-C2-O2
2	B	1301[A]	ADP	PA-O3A-PB-O1B
2	B	1301[B]	ADP	PA-O3A-PB-O1B
2	D	1301[B]	ADP	O4'-C1'-N9-C4

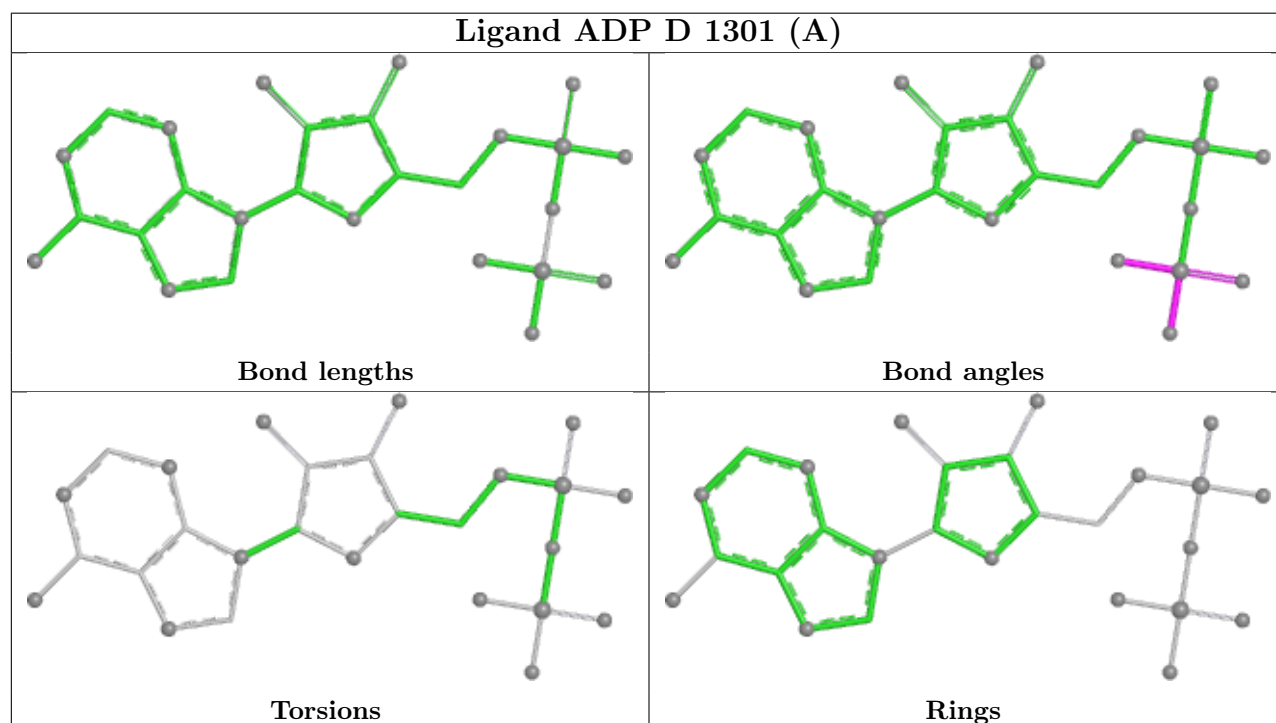
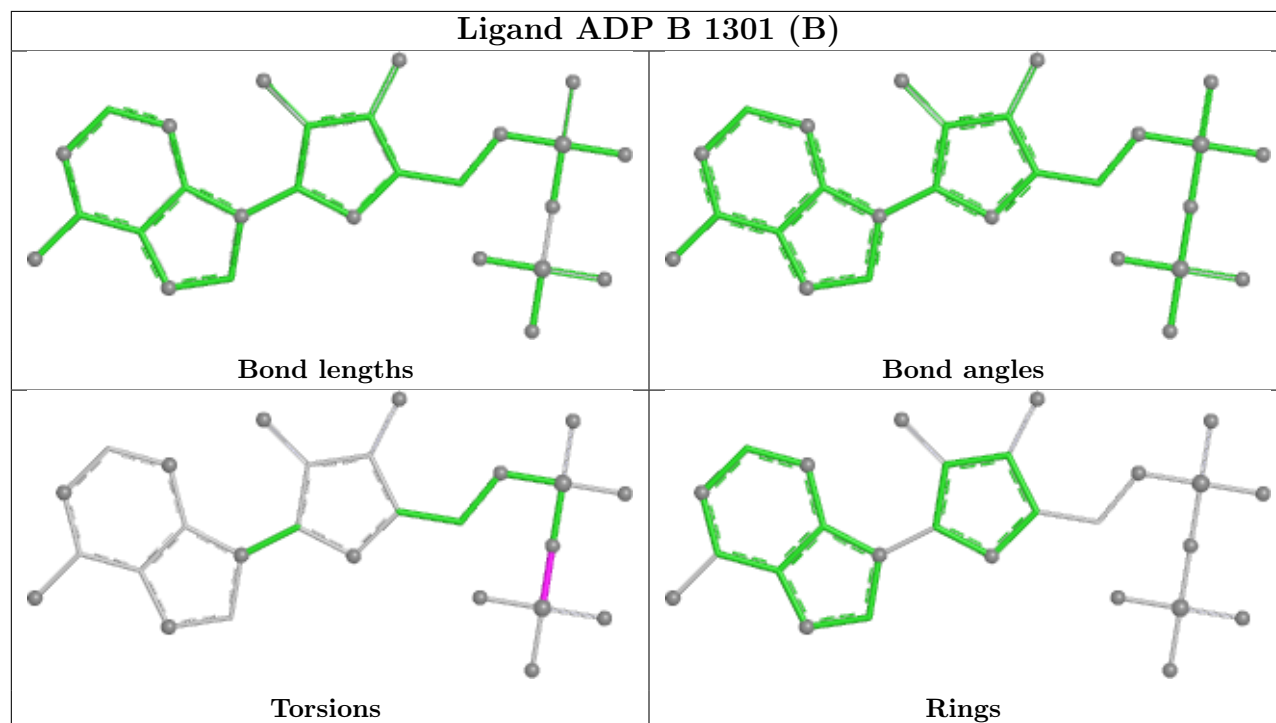
There are no ring outliers.

7 monomers are involved in 10 short contacts:

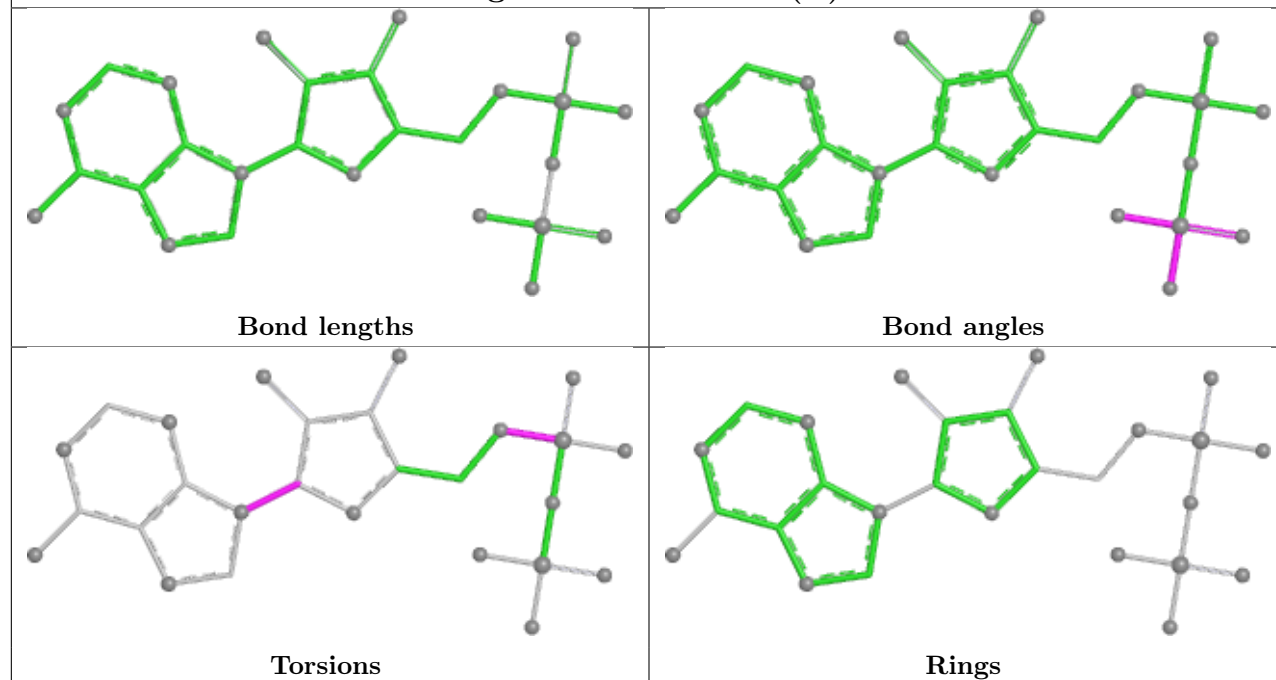
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1307	DMS	1	0
4	B	1308	DMS	2	0
4	C	1307	DMS	1	0
4	A	1310	DMS	2	0
2	D	1301[B]	ADP	1	0
4	D	1306	DMS	2	0
4	A	1312	DMS	1	0

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

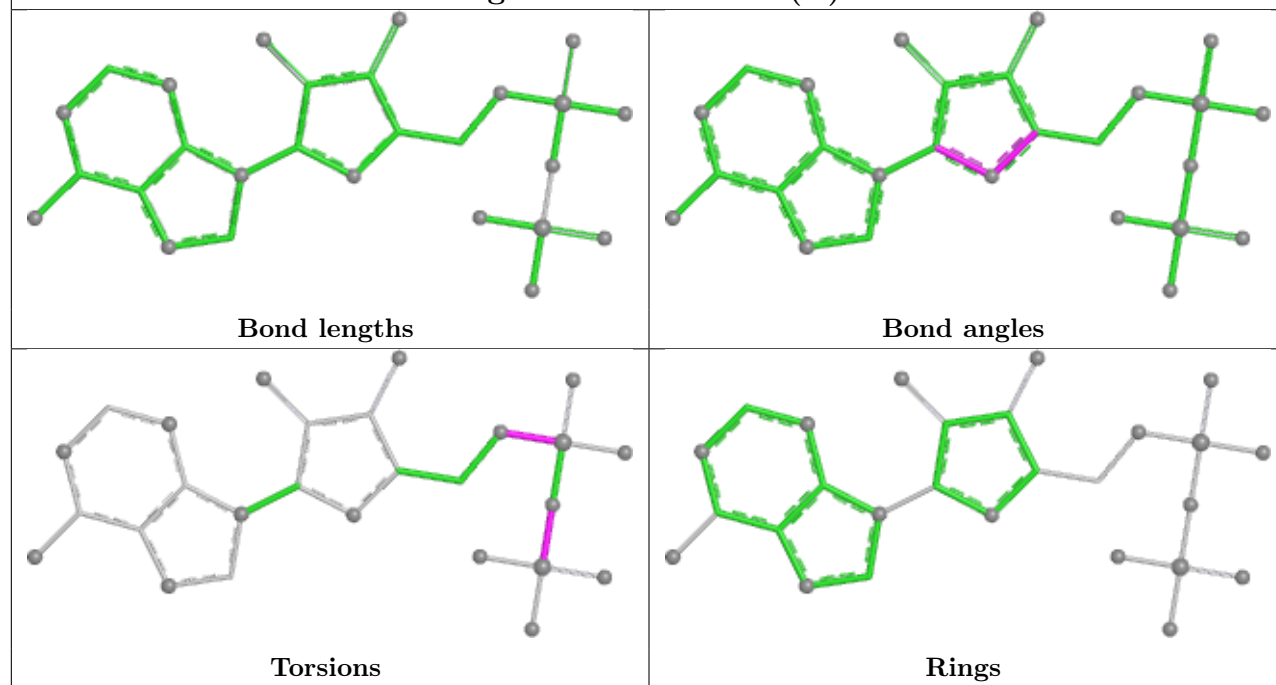
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



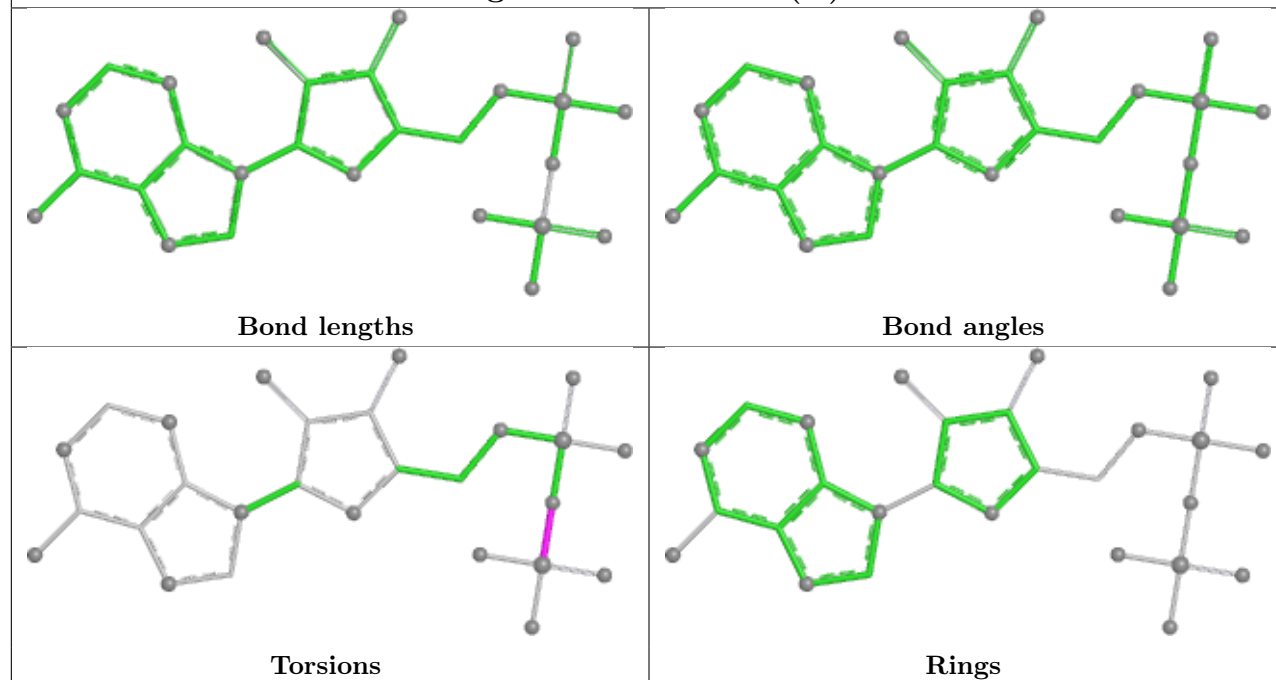
Ligand ADP D 1301 (B)



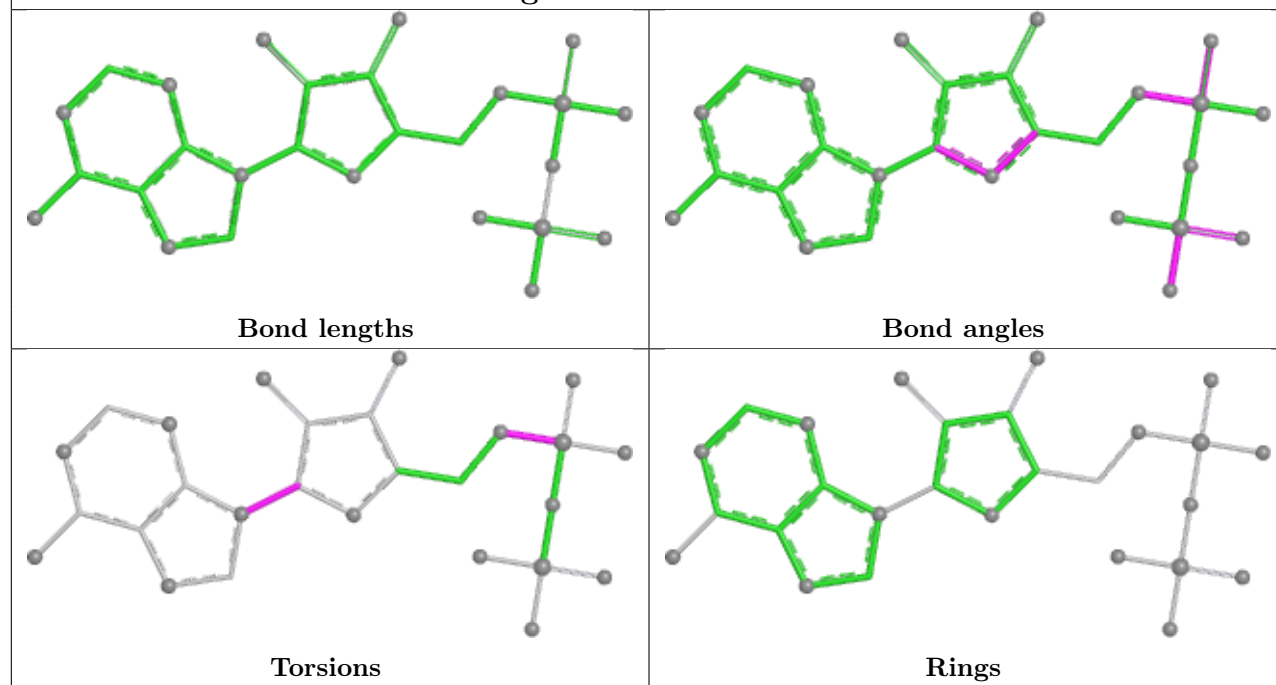
Ligand ADP A 1301 (B)

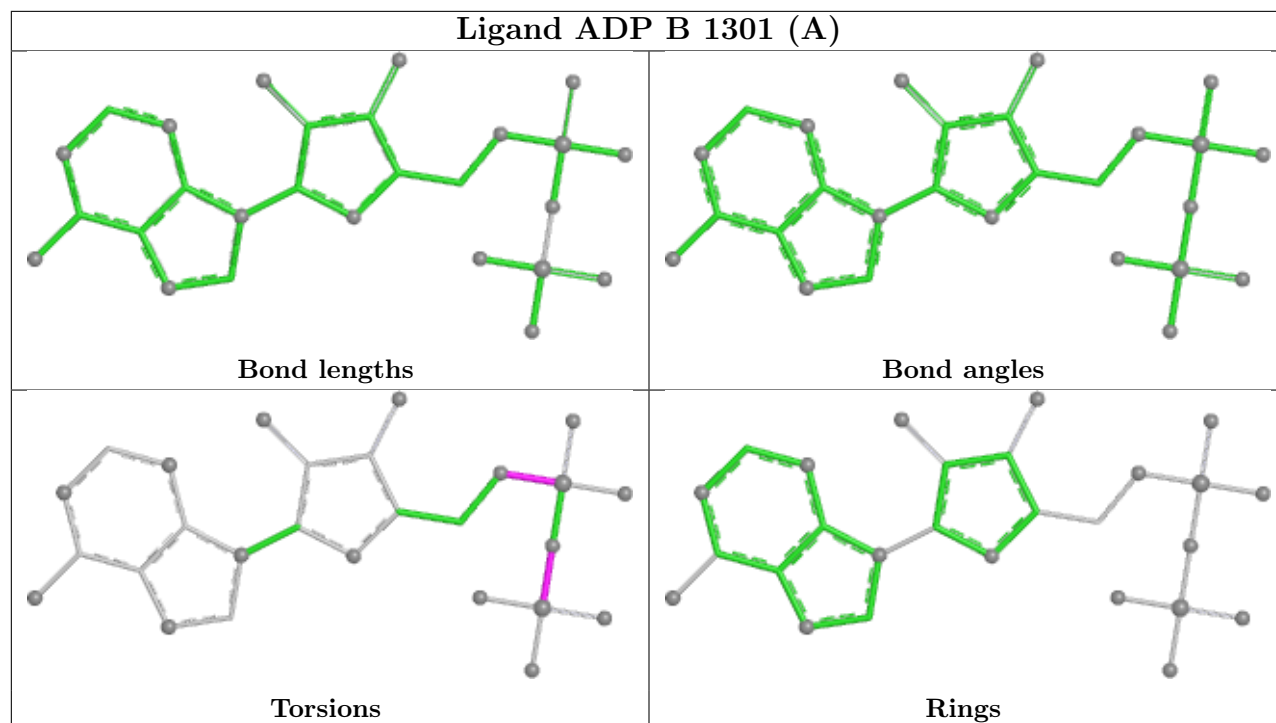


Ligand ADP A 1301 (A)



Ligand ADP C 1301





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	632/673 (93%)	-0.15	8 (1%) 75 71	28, 62, 89, 127	1 (0%)
1	B	633/673 (94%)	-0.13	5 (0%) 82 80	34, 63, 89, 113	2 (0%)
1	C	633/673 (94%)	0.05	11 (1%) 69 64	37, 70, 101, 123	1 (0%)
1	D	632/673 (93%)	-0.12	5 (0%) 82 80	30, 66, 91, 128	2 (0%)
All	All	2530/2692 (93%)	-0.09	29 (1%) 78 74	28, 65, 93, 128	6 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	589[A]	GLU	5.3
1	A	1184	SER	3.7
1	A	1183	VAL	3.5
1	D	1187	THR	3.2
1	C	842	ALA	3.1
1	A	555	GLN	3.1
1	A	1186	PRO	3.1
1	D	611	GLY	2.9
1	C	1187	THR	2.9
1	B	687	ALA	2.8
1	A	689	GLU	2.7
1	A	1185	ASP	2.7
1	C	841	ILE	2.7
1	C	879	ILE	2.6
1	B	719	THR	2.5
1	B	1185	ASP	2.5
1	C	913	LEU	2.4
1	B	1186	PRO	2.4
1	D	1181	PHE	2.4
1	D	689	GLU	2.4
1	A	843	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	556	MET	2.3
1	D	910	ASP	2.3
1	C	908	TYR	2.1
1	C	910	ASP	2.1
1	C	754	THR	2.1
1	A	1121	GLN	2.1
1	B	1183	VAL	2.1
1	C	865	TYR	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
4	DMS	D	1310	4/4	0.73	0.32	110,111,111,112	0
4	DMS	D	1309	4/4	0.77	0.23	118,118,118,119	0
4	DMS	B	1303	4/4	0.77	0.20	95,97,98,98	0
4	DMS	C	1310	4/4	0.78	0.25	121,122,122,123	0
4	DMS	B	1311	4/4	0.79	0.23	131,131,132,132	0
4	DMS	B	1310	4/4	0.79	0.20	126,126,126,126	0
5	EDO	D	1304	4/4	0.79	0.21	77,78,79,81	0
4	DMS	B	1312	4/4	0.80	0.19	145,145,146,146	0
4	DMS	C	1312	4/4	0.82	0.22	105,106,107,108	0
4	DMS	A	1311	4/4	0.82	0.25	125,125,126,126	0
6	ACT	A	1308	4/4	0.83	0.17	71,74,75,76	0
6	ACT	D	1312	4/4	0.83	0.19	81,82,82,82	0
4	DMS	D	1311	4/4	0.84	0.19	122,123,123,124	0
4	DMS	B	1304	4/4	0.84	0.20	108,108,109,109	0
4	DMS	B	1307	4/4	0.84	0.23	111,112,113,113	0

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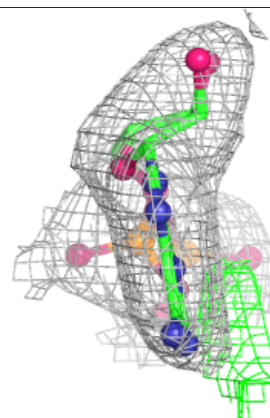
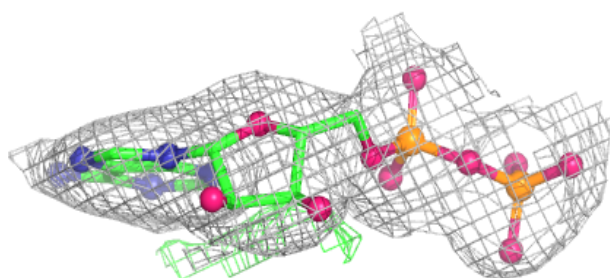
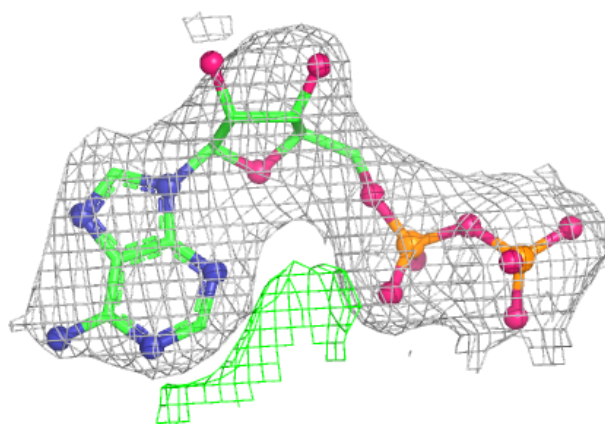
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ACT	B	1309	4/4	0.84	0.16	79,81,82,82	0
4	DMS	A	1307	4/4	0.84	0.22	125,125,125,126	0
4	DMS	D	1306	4/4	0.85	0.20	104,104,104,105	0
4	DMS	A	1306	4/4	0.85	0.16	115,115,115,116	0
4	DMS	A	1313	4/4	0.85	0.20	115,115,115,115	0
4	DMS	D	1305	4/4	0.85	0.16	94,95,96,96	0
5	EDO	D	1303	4/4	0.86	0.17	82,83,84,84	0
4	DMS	D	1307	4/4	0.86	0.17	108,109,110,110	0
4	DMS	C	1306	4/4	0.86	0.22	121,122,122,122	0
5	EDO	A	1305	4/4	0.86	0.22	60,61,63,64	0
5	EDO	B	1306	4/4	0.86	0.24	74,75,75,78	0
4	DMS	C	1311	4/4	0.87	0.18	110,110,111,111	0
4	DMS	C	1309	4/4	0.88	0.20	114,115,116,116	0
4	DMS	C	1305	4/4	0.89	0.19	127,128,128,128	0
4	DMS	B	1308	4/4	0.89	0.19	133,134,134,134	0
5	EDO	C	1303	4/4	0.89	0.17	69,71,71,73	0
4	DMS	A	1309	4/4	0.89	0.16	105,105,106,108	0
4	DMS	A	1312	4/4	0.90	0.17	128,129,129,129	0
4	DMS	C	1304	4/4	0.90	0.14	108,109,109,109	0
4	DMS	D	1308	4/4	0.92	0.17	129,129,129,130	0
4	DMS	C	1307	4/4	0.92	0.17	127,128,128,128	0
4	DMS	C	1308	4/4	0.92	0.16	105,105,105,106	0
4	DMS	A	1310	4/4	0.92	0.21	114,114,114,114	0
4	DMS	B	1305	4/4	0.93	0.18	109,109,110,110	0
5	EDO	A	1304	4/4	0.93	0.11	62,65,66,67	0
2	ADP	C	1301	27/27	0.94	0.09	60,79,84,90	0
4	DMS	A	1303	4/4	0.94	0.11	121,121,121,122	0
2	ADP	B	1301[A]	27/27	0.96	0.09	47,69,75,78	19
2	ADP	D	1301[A]	27/27	0.96	0.08	48,58,64,67	19
2	ADP	D	1301[B]	27/27	0.96	0.08	50,63,69,73	19
2	ADP	B	1301[B]	27/27	0.96	0.09	47,57,59,63	19
2	ADP	A	1301[A]	27/27	0.97	0.07	42,48,59,65	19
2	ADP	A	1301[B]	27/27	0.97	0.07	48,64,67,70	19
3	MG	B	1302	1/1	0.99	0.03	47,47,47,47	0
3	MG	C	1302	1/1	0.99	0.04	65,65,65,65	0
3	MG	D	1302	1/1	0.99	0.04	64,64,64,64	0
3	MG	A	1302	1/1	0.99	0.04	76,76,76,76	0

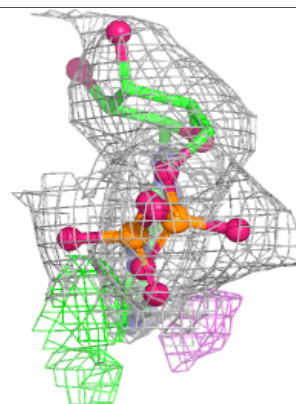
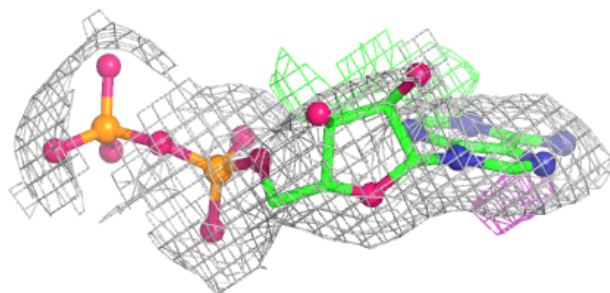
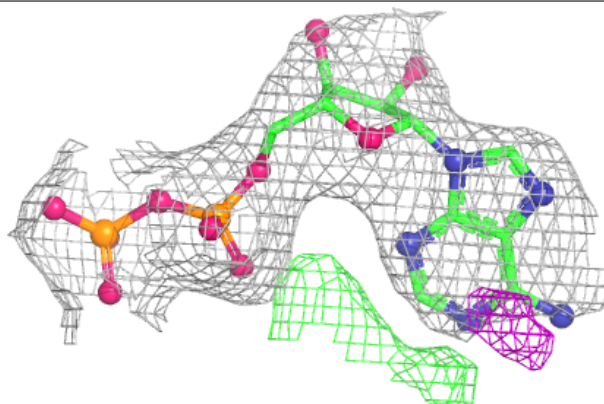
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

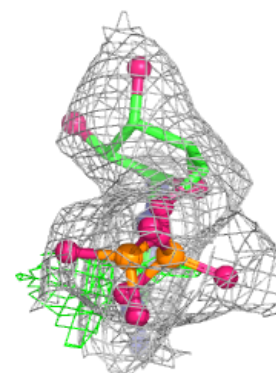
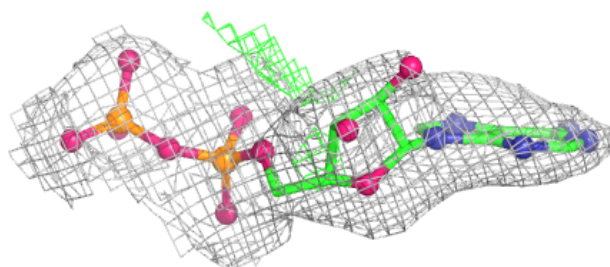
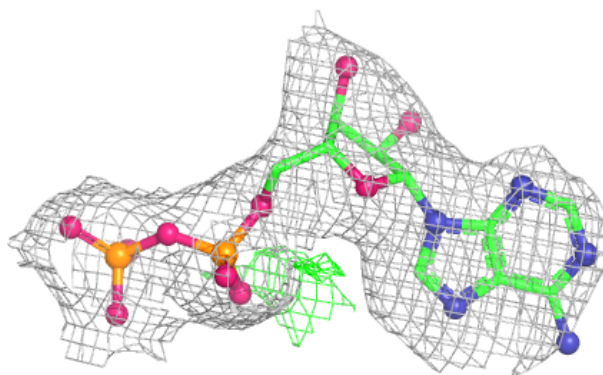
**Electron density around ADP B 1301 (A):**

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

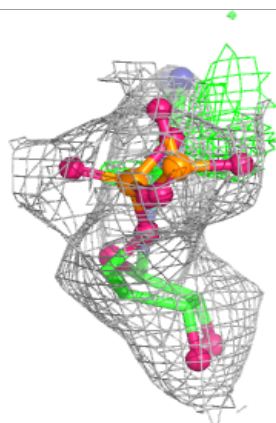
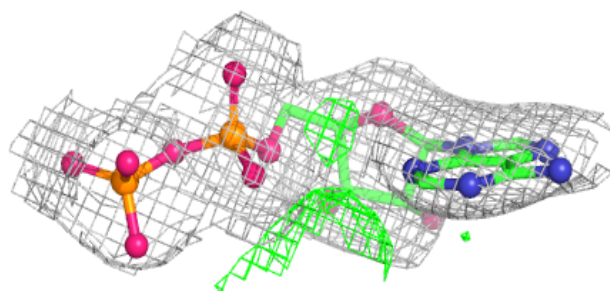
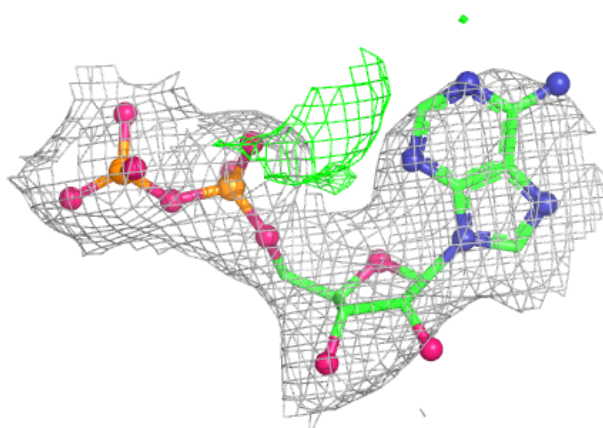


Electron density around ADP D 1301 (A):

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

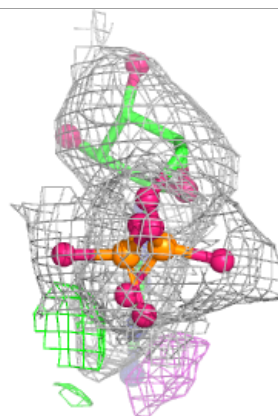
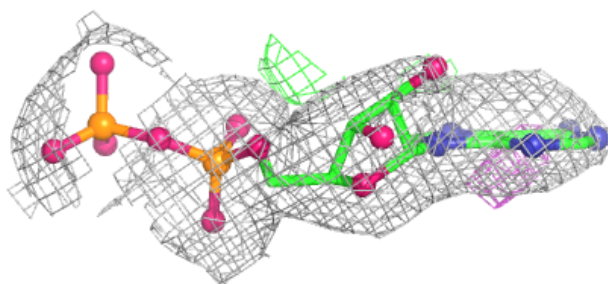
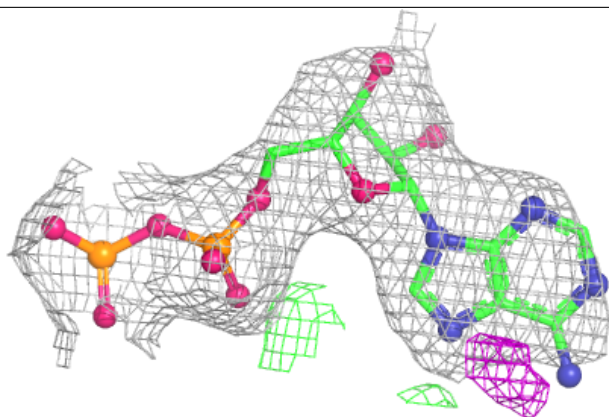
**Electron density around ADP D 1301 (B):**

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

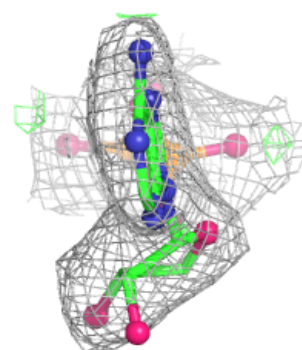
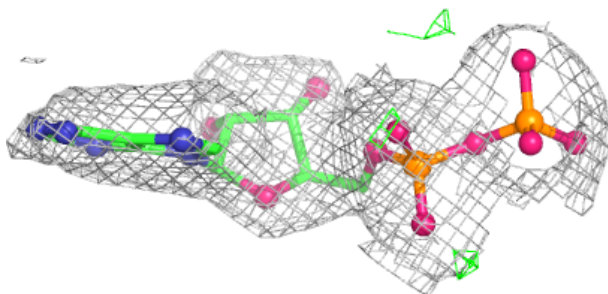
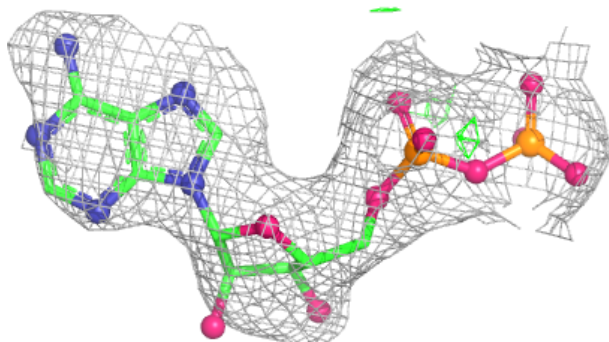


Electron density around ADP B 1301 (B):

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and green (positive)

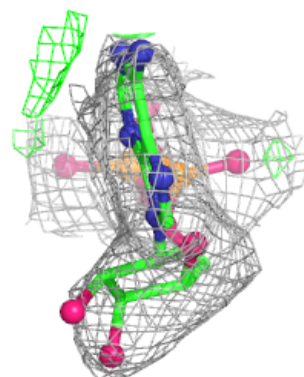
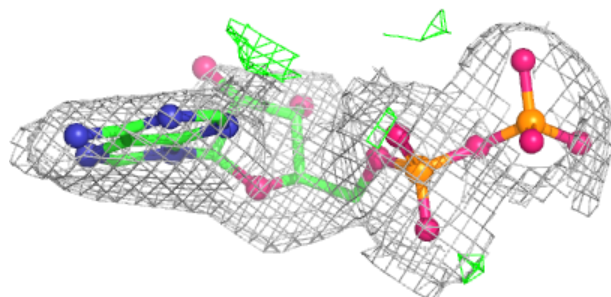
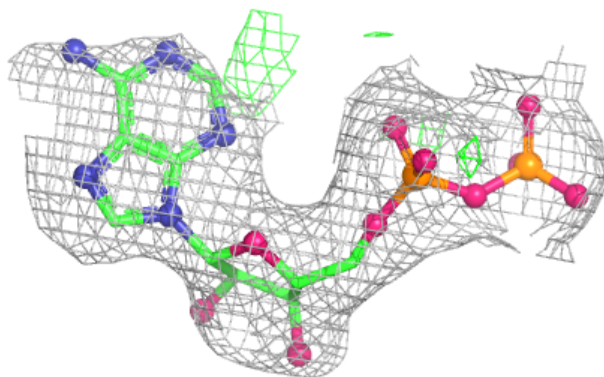
**Electron density around ADP A 1301 (A):**

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 $mF_o - DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.