



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 30, 2025 – 05:01 pm BST

PDB ID : 8RB1 / pdb_00008rb1
Title : The crystal structure of DNA-bound human MutSbeta (MSH2_K675R/MSH3_K902R) in the canonical mismatch bound conformation with ADP bound in MSH2 and MSH3
Authors : Thomsen, M.; Neudegger, T.; Thieulin-Pardo, G.; Blaesse, M.; Costanzi, E.; Steinbacher, S.; Plotnikov, N.V.; Dominguez, C.; Iyer, R.R.; Wilkinson, H.A.; Monteagudo, E.; Haque, T.S.; Prasad, B.C.; Finley, M.; Boudet, J.; Vogt, T.F.; Felsenfeld, D.P.
Deposited on : 2023-12-01
Resolution : 2.08 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11

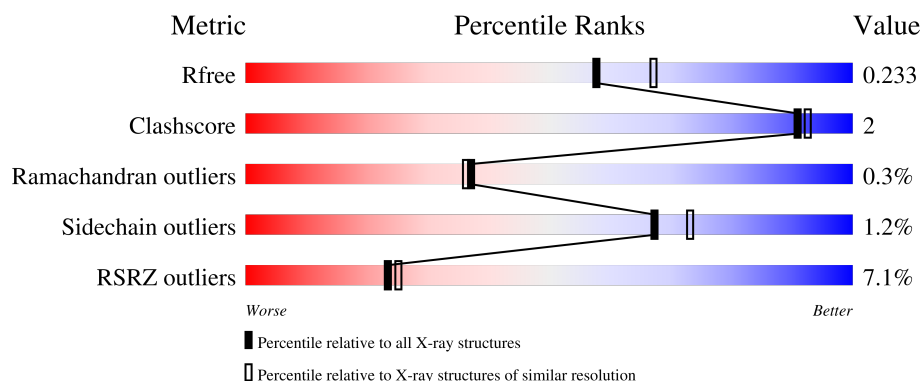
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

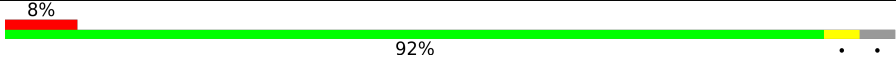

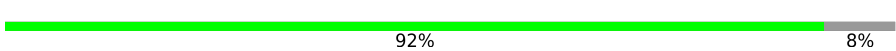
The reported resolution of this entry is 2.08 Å.

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}	164625	7574 (2.10-2.06)
Clashscore	180529	8325 (2.10-2.06)
Ramachandran outliers	177936	8271 (2.10-2.06)
Sidechain outliers	177891	8272 (2.10-2.06)
RSRZ outliers	164620	7574 (2.10-2.06)


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	934	
2	B	918	
3	C	24	

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.44

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Mol	Chain	Length	Quality of chain
4	D	24	 88% 12%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 15637 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 DNA mismatch repair protein Msh2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	895	Total	C	N	O	S	293	1	0
			7083	4495	1202	1348	38			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	675	ARG	LYS	engineered mutation	UNP P43246

- Molecule 2 is a protein called DNA mismatch repair protein Msh3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	853	Total	C	N	O	S	218	6	0
			6876	4384	1178	1282	32			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	217	GLY	-	expression tag	UNP P20585
B	218	PRO	-	expression tag	UNP P20585
B	902	ARG	LYS	engineered mutation	UNP P20585
B	949	ARG	GLN	conflict	UNP P20585

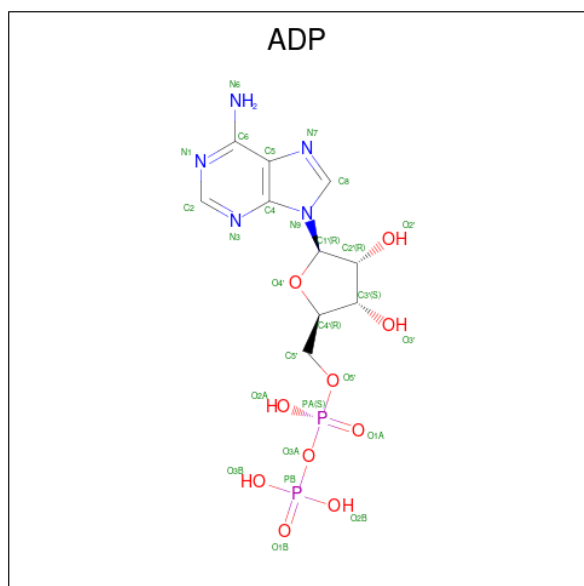
- Molecule 3 is a DNA chain called DNA (5'-D(*TP*CP*TP*AP*TP*CP*TP*GP*AP*AP*GP*CP*CP*GP*AP*TP*CP*GP*AP*TP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	22	Total	C	N	O	P	0	0	0
			449	215	82	131	21			

- Molecule 4 is a DNA chain called DNA (5'-D(*TP*CP*AP*TP*CP*GP*AP*TP*CP*GP*CP*AP*GP*CP*TP*TP*CP*AP*GP*AP*TP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	24	Total	C	N	O	P	0	0	0
			489	234	90	142	23			

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

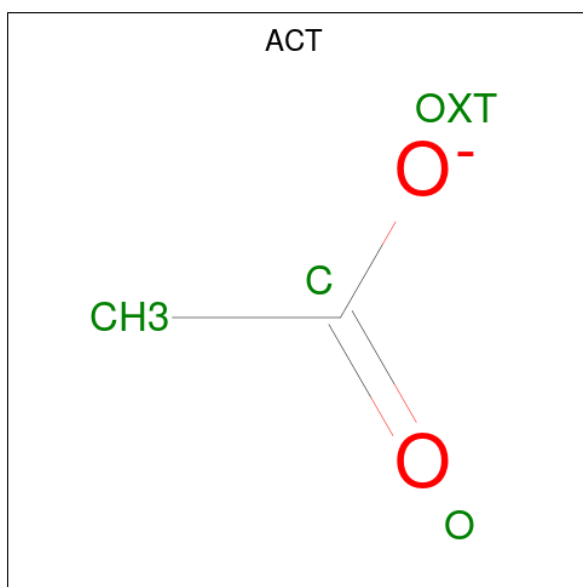
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Cl 1 1	0	0

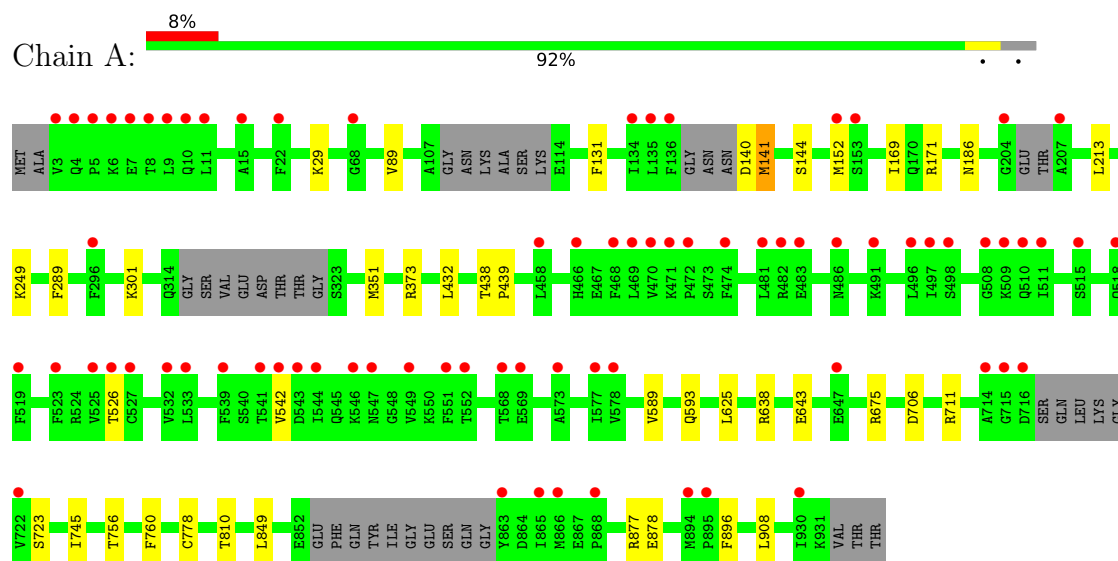
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	305	Total O 305 305	0	0
10	B	289	Total O 289 289	0	0
10	C	15	Total O 15 15	0	0
10	D	18	Total O 18 18	0	0

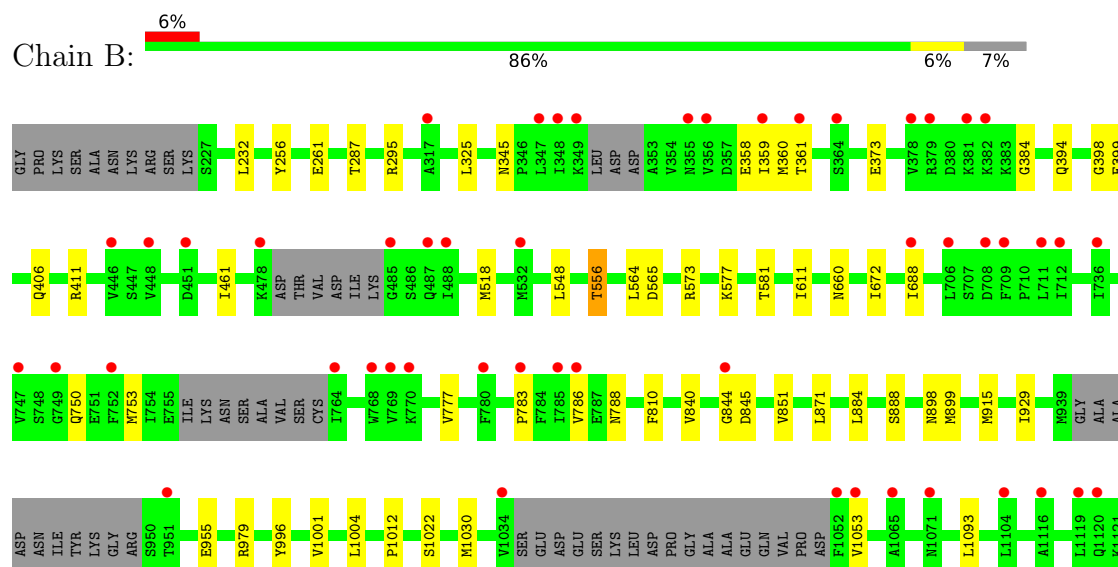
3 Residue-property plots [i](#)

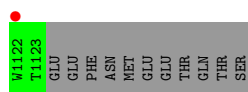
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: DNA mismatch repair protein Msh2



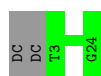
- Molecule 2: DNA mismatch repair protein Msh3






- Molecule 3: DNA (5'-D(*TP*CP*TP*AP*TP*CP*TP*GP*AP*AP*GP*CP*CP*GP*AP*TP*CP*GP*AP*TP*GP*G)-3')

Chain C:  92% 8%



- Molecule 4: DNA (5'-D(*TP*CP*AP*TP*CP*GP*AP*TP*CP*GP*CP*AP*GP*CP*TP*TP*CP*AP*GP*AP*TP*AP*GP*G)-3')

Chain D:  88% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.70Å 91.68Å 94.02Å 67.34° 87.16° 75.86°	Depositor
Resolution (Å)	86.66 – 2.08 86.66 – 2.08	Depositor EDS
% Data completeness (in resolution range)	96.2 (86.66-2.08) 96.2 (86.66-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.198 , 0.235 0.202 , 0.233	Depositor DCC
R_{free} test set	1718 reflections (1.39%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15637	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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: ACT, CL, EDO, ADP, MG

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	1.03	0/7192	1.50	0/9689
2	B	1.02	0/7000	1.50	6/9448 (0.1%)
3	C	0.34	0/503	0.83	0/775
4	D	0.35	0/548	0.76	0/844
All	All	0.99	0/15243	1.46	6/20756 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	844	GLY	CA-C-O	-6.05	118.09	122.45
2	B	1012	PRO	N-CA-C	5.81	117.78	110.70
2	B	1030	MET	CA-C-N	5.34	125.18	120.10
2	B	1030	MET	C-N-CA	5.34	125.18	120.10
2	B	871	LEU	CA-C-N	5.24	125.08	120.10
2	B	871	LEU	C-N-CA	5.24	125.08	120.10

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	7083	0	7146	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	6876	0	6979	27	0
3	C	449	0	250	0	0
4	D	489	0	272	2	0
5	A	27	0	12	1	0
5	B	27	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	20	0	30	0	0
7	B	20	0	30	0	0
8	A	12	0	9	0	0
8	B	4	0	3	0	0
9	B	1	0	0	0	0
10	A	305	0	0	3	0
10	B	289	0	0	2	0
10	C	15	0	0	0	0
10	D	18	0	0	0	0
All	All	15637	0	14743	46	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 2.

All (46) 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:849:LEU:O	1:A:877:ARG:NH2	2.30	0.65
2:B:295:ARG:NH1	2:B:345:ASN:OD1	2.33	0.61
1:A:351:MET:HE1	1:A:706:ASP:HA	1.85	0.59
2:B:358:GLU:O	2:B:360:MET:N	2.35	0.56
2:B:548:LEU:HD21	2:B:581:THR:HG22	1.91	0.52
1:A:638:ARG:NE	1:A:643:GLU:OE2	2.39	0.51
2:B:398:GLY:HA2	2:B:518:MET:HE3	1.93	0.51
1:A:723:SER:HA	2:B:899:MET:HG3	1.93	0.50
2:B:788:ASN:ND2	10:B:1305:HOH:O	2.43	0.50
1:A:675:ARG:HD3	5:A:1001:ADP:O1B	2.12	0.50
2:B:955:GLU:OE2	2:B:979:ARG:O	2.30	0.50
1:A:526:THR:HG21	4:D:32:DA:OP1	2.12	0.49
2:B:565:ASP:OD2	2:B:573:ARG:NE	2.45	0.49
2:B:564:LEU:HD21	2:B:915:MET:HE3	1.94	0.49
1:A:810:THR:HA	10:A:1184:HOH:O	2.11	0.49
1:A:171:ARG:HA	1:A:289:PHE:CE2	2.48	0.48
1:A:141:MET:HE1	1:A:169:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:564:LEU:HA	2:B:840:VAL:HG21	1.97	0.47
2:B:232:LEU:HA	2:B:325:LEU:HD21	1.97	0.47
2:B:556[A]:THR:HG21	2:B:573:ARG:HH22	1.80	0.47
2:B:394:GLN:NE2	2:B:399:GLU:OE1	2.48	0.47
1:A:711:ARG:NE	1:A:711:ARG:HA	2.30	0.47
1:A:89:VAL:HG11	1:A:131:PHE:CD2	2.50	0.46
2:B:384:GLY:O	2:B:411:ARG:NH2	2.49	0.45
1:A:438:THR:HB	1:A:439:PRO:HD3	1.98	0.45
1:A:373:ARG:HD2	10:A:1290:HOH:O	2.16	0.45
2:B:851:VAL:HA	2:B:929:ILE:O	2.16	0.45
2:B:256:TYR:CD1	2:B:287:THR:HG22	2.52	0.45
4:D:27:DC:H2"	4:D:28:DA:C8	2.52	0.44
1:A:186:ASN:OD1	1:A:301:LYS:NZ	2.51	0.43
2:B:611:ILE:HD13	2:B:672:ILE:HD13	2.00	0.43
2:B:577:LYS:O	2:B:581:THR:HG23	2.18	0.43
2:B:548:LEU:HD21	2:B:581:THR:CG2	2.49	0.43
2:B:688:ILE:HD11	2:B:810:PHE:HE1	1.84	0.43
2:B:884:LEU:HB3	2:B:1004:LEU:HD22	2.01	0.43
2:B:581:THR:HG21	10:B:1333:HOH:O	2.20	0.42
1:A:625:LEU:HD12	1:A:625:LEU:N	2.35	0.42
1:A:589:VAL:O	1:A:593:GLN:HG3	2.19	0.41
2:B:750:GLN:CB	2:B:753:MET:HE2	2.50	0.41
2:B:996:TYR:CE2	2:B:1001:VAL:CG2	3.03	0.41
1:A:745:ILE:O	1:A:778:CYS:HA	2.20	0.41
1:A:908:LEU:HD23	1:A:908:LEU:HA	1.96	0.41
2:B:899:MET:HA	2:B:899:MET:HE2	2.02	0.41
1:A:760:PHE:CD2	2:B:1093:LEU:HD22	2.56	0.40
2:B:783:PRO:O	2:B:786:VAL:HB	2.21	0.40
1:A:140:ASP:N	10:A:1114:HOH:O	2.54	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	882/934 (94%)	855 (97%)	25 (3%)	2 (0%)	44	44
2	B	847/918 (92%)	827 (98%)	15 (2%)	5 (1%)	22	18
All	All	1729/1852 (93%)	1682 (97%)	40 (2%)	7 (0%)	37	28

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	896	PHE
2	B	359	ILE
2	B	361	THR
1	A	141	MET
2	B	777	VAL
2	B	888[B]	SER
2	B	888[C]	SER

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	779/808 (96%)	770 (99%)	9 (1%)	67	73
2	B	769/818 (94%)	757 (98%)	12 (2%)	58	64
All	All	1548/1626 (95%)	1527 (99%)	21 (1%)	67	68

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	144	SER
1	A	152	MET
1	A	213	LEU
1	A	249	LYS
1	A	432	LEU
1	A	542	VAL
1	A	756	THR
1	A	878	GLU

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Mol	Chain	Res	Type
2	B	261	GLU
2	B	373	GLU
2	B	406	GLN
2	B	461	ILE
2	B	556[A]	THR
2	B	556[B]	THR
2	B	660	ASN
2	B	845	ASP
2	B	898[A]	ASN
2	B	898[B]	ASN
2	B	1022	SER
2	B	1053	VAL

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

Mol	Chain	Res	Type
1	A	4	GLN
1	A	263	ASN
1	A	377	GLN
1	A	574	GLN
2	B	524	ASN
2	B	566	HIS
2	B	610	GLN
2	B	690	ASN
2	B	819	HIS
2	B	1027	ASN
2	B	1058	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 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
7	EDO	A	1004	-	3,3,3	0.11	0	2,2,2	0.37	0
5	ADP	A	1001	6	24,29,29	0.65	0	29,45,45	0.76	1 (3%)
7	EDO	B	1205	-	3,3,3	0.08	0	2,2,2	0.29	0
7	EDO	A	1009	-	3,3,3	0.08	0	2,2,2	0.26	0
7	EDO	B	1204	-	3,3,3	0.11	0	2,2,2	0.33	0
7	EDO	B	1209	-	3,3,3	0.10	0	2,2,2	0.32	0
8	ACT	A	1006	-	3,3,3	0.89	0	3,3,3	0.82	0
8	ACT	A	1008	-	3,3,3	0.95	0	3,3,3	0.82	0
8	ACT	B	1203	-	3,3,3	0.95	0	3,3,3	0.83	0
5	ADP	B	1201	6	24,29,29	0.66	0	29,45,45	0.78	1 (3%)
7	EDO	A	1005	-	3,3,3	0.11	0	2,2,2	0.28	0
7	EDO	B	1206	-	3,3,3	0.08	0	2,2,2	0.16	0
8	ACT	A	1007	-	3,3,3	0.96	0	3,3,3	0.75	0
7	EDO	A	1003	-	3,3,3	0.12	0	2,2,2	0.37	0
7	EDO	B	1207	-	3,3,3	0.08	0	2,2,2	0.28	0
7	EDO	A	1010	-	3,3,3	0.14	0	2,2,2	0.34	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
7	EDO	A	1004	-	-	1/1/1/1	-
5	ADP	A	1001	6	-	3/12/32/32	0/3/3/3
7	EDO	B	1205	-	-	1/1/1/1	-
7	EDO	A	1009	-	-	0/1/1/1	-
7	EDO	B	1204	-	-	0/1/1/1	-
7	EDO	B	1209	-	-	1/1/1/1	-
5	ADP	B	1201	6	-	2/12/32/32	0/3/3/3
7	EDO	A	1005	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	B	1206	-	-	1/1/1/1	-
7	EDO	A	1003	-	-	1/1/1/1	-
7	EDO	B	1207	-	-	0/1/1/1	-
7	EDO	A	1010	-	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1201	ADP	C5-C6-N6	2.24	123.75	120.35
5	A	1001	ADP	C5-C6-N6	2.05	123.47	120.35

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	ADP	PA-O3A-PB-O2B
5	B	1201	ADP	PA-O3A-PB-O2B
7	A	1010	EDO	O1-C1-C2-O2
7	A	1003	EDO	O1-C1-C2-O2
7	B	1206	EDO	O1-C1-C2-O2
7	B	1209	EDO	O1-C1-C2-O2
5	B	1201	ADP	PA-O3A-PB-O1B
7	A	1004	EDO	O1-C1-C2-O2
7	B	1205	EDO	O1-C1-C2-O2
5	A	1001	ADP	PA-O3A-PB-O3B
5	A	1001	ADP	PA-O3A-PB-O1B

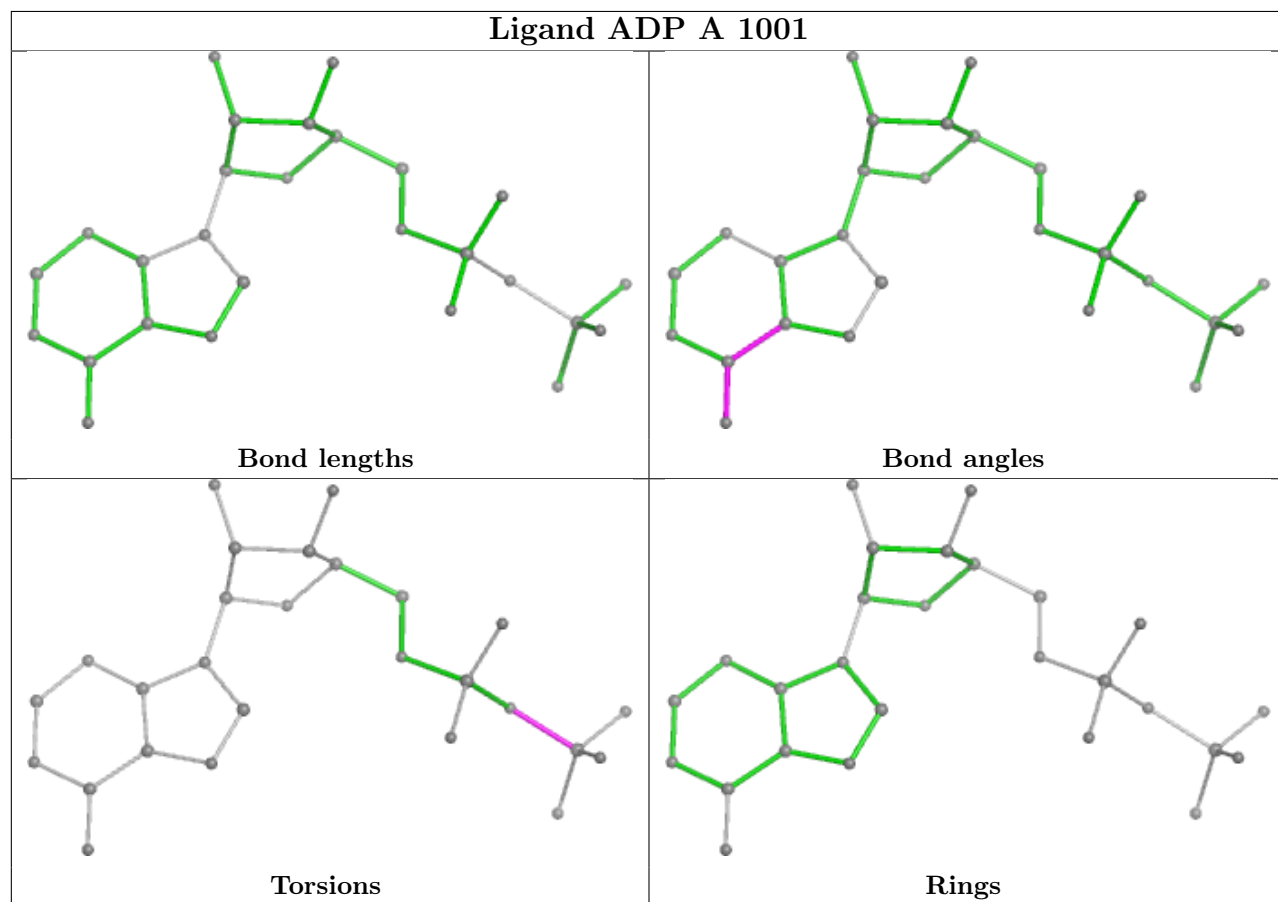
There are no ring outliers.

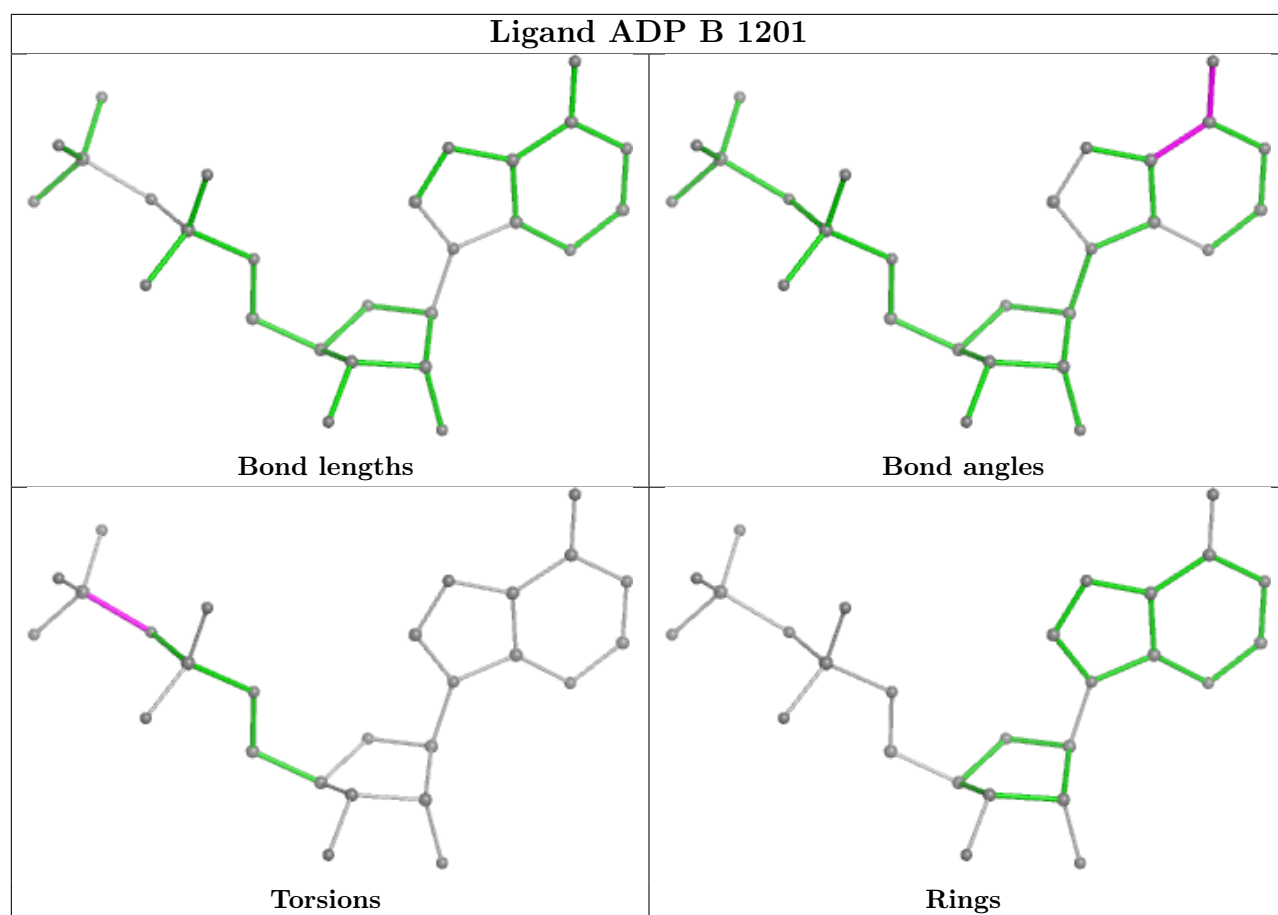
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1001	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	895/934 (95%)	0.56	76 (8%)	18	19	22, 54, 103, 148	92 (10%)
2	B	853/918 (92%)	0.43	51 (5%)	29	31	21, 52, 85, 125	85 (9%)
3	C	22/24 (91%)	0.23	0	100	100	51, 102, 143, 159	0
4	D	24/24 (100%)	0.11	0	100	100	44, 90, 188, 224	0
All	All	1794/1900 (94%)	0.49	127 (7%)	23	25	21, 53, 99, 224	177 (9%)

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	468	PHE	7.0
1	A	469	LEU	4.5
1	A	207	ALA	4.4
2	B	356	VAL	4.4
1	A	542	VAL	4.4
1	A	519	PHE	4.3
1	A	496	LEU	4.2
2	B	448	VAL	4.1
2	B	736	ILE	4.1
1	A	4	GLN	4.1
1	A	11	LEU	4.1
1	A	68	GLY	4.0
1	A	865	ILE	3.9
2	B	747	VAL	3.9
2	B	783	PRO	3.8
2	B	764	ILE	3.8
1	A	471	LYS	3.8
1	A	497	ILE	3.8
1	A	3	VAL	3.7
1	A	526	THR	3.7
1	A	498	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	470	VAL	3.6
1	A	9	LEU	3.5
2	B	1034	VAL	3.5
2	B	770	LYS	3.5
1	A	895	PRO	3.4
1	A	510	GLN	3.4
1	A	544	ILE	3.4
1	A	525	VAL	3.3
1	A	5	PRO	3.3
1	A	22	PHE	3.3
1	A	8	THR	3.2
2	B	381	LYS	3.2
2	B	382	LYS	3.2
2	B	752	PHE	3.1
2	B	532	MET	3.1
1	A	714	ALA	3.0
2	B	446	VAL	3.0
1	A	466	HIS	3.0
1	A	518	GLN	3.0
2	B	711	LEU	3.0
2	B	844	GLY	3.0
1	A	6	LYS	3.0
1	A	511	ILE	2.9
1	A	508	GLY	2.9
1	A	868	PRO	2.8
1	A	573	ALA	2.8
1	A	541	THR	2.8
1	A	527	CYS	2.8
1	A	482	ARG	2.8
1	A	546	LYS	2.7
2	B	1053	VAL	2.7
2	B	348	ILE	2.7
1	A	472	PRO	2.7
2	B	1071	ASN	2.7
2	B	359	ILE	2.7
1	A	549	VAL	2.7
2	B	485	GLY	2.7
2	B	785	ILE	2.7
1	A	894	MET	2.6
2	B	749	GLY	2.6
1	A	486	ASN	2.6
1	A	523	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	930	ILE	2.5
2	B	688	ILE	2.5
1	A	481	LEU	2.5
2	B	378	VAL	2.5
1	A	15	ALA	2.5
2	B	786	VAL	2.5
2	B	487	GLN	2.5
2	B	1120	GLN	2.5
1	A	715	GLY	2.5
1	A	135	LEU	2.5
1	A	577	ILE	2.4
2	B	768	TRP	2.4
1	A	7	GLU	2.4
1	A	532	VAL	2.4
1	A	136	PHE	2.4
1	A	539	PHE	2.4
2	B	1052	PHE	2.4
1	A	474	PHE	2.4
1	A	551	PHE	2.4
1	A	863	TYR	2.4
2	B	488	ILE	2.4
2	B	349	LYS	2.3
2	B	364	SER	2.3
1	A	10	GLN	2.3
1	A	552	THR	2.3
2	B	951	THR	2.3
2	B	780	PHE	2.3
1	A	547	ASN	2.3
1	A	866	MET	2.3
2	B	317	ALA	2.3
1	A	296	PHE	2.3
1	A	458	LEU	2.3
2	B	1104	LEU	2.3
1	A	543	ASP	2.2
2	B	708	ASP	2.2
1	A	722	VAL	2.2
2	B	347	LEU	2.2
1	A	569	GLU	2.2
1	A	716	ASP	2.2
1	A	204	GLY	2.2
2	B	355	ASN	2.2
2	B	379	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	1122	TRP	2.2
1	A	515	SER	2.2
1	A	134	ILE	2.2
1	A	483	GLU	2.2
2	B	706	LEU	2.2
2	B	1065	ALA	2.2
1	A	578	VAL	2.2
2	B	1119	LEU	2.1
1	A	491	LYS	2.1
1	A	509	LYS	2.1
2	B	1116	ALA	2.1
2	B	769	VAL	2.1
1	A	533	LEU	2.1
2	B	709	PHE	2.1
1	A	153	SER	2.1
1	A	568	THR	2.1
2	B	451	ASP	2.1
2	B	712	ILE	2.1
2	B	478	LYS	2.1
1	A	152	MET	2.0
2	B	361	THR	2.0
1	A	647	GLU	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(\AA^2)	Q<0.9
8	ACT	A	1008	4/4	0.76	0.18	94,97,98,98	0

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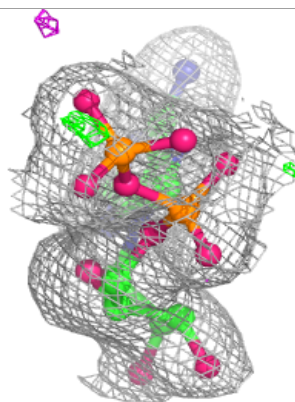
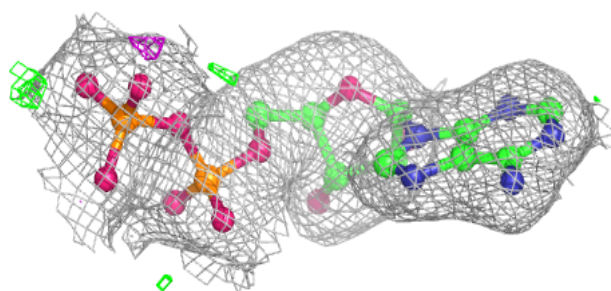
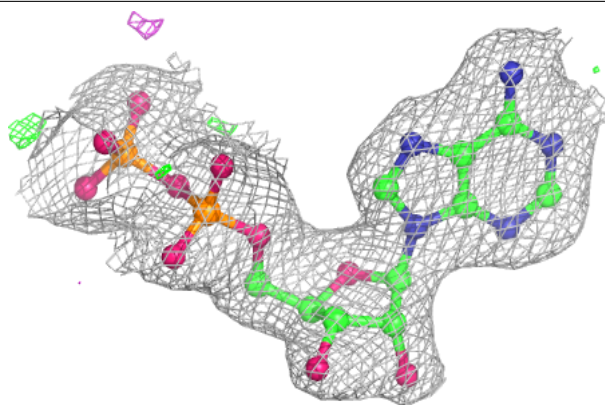
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	EDO	B	1207	4/4	0.81	0.17	79,80,82,87	0
7	EDO	A	1010	4/4	0.82	0.17	80,80,82,82	0
8	ACT	A	1006	4/4	0.84	0.20	63,64,65,67	0
8	ACT	B	1203	4/4	0.85	0.10	67,67,68,68	0
7	EDO	A	1009	4/4	0.86	0.16	81,82,83,83	0
7	EDO	A	1004	4/4	0.86	0.16	64,67,67,68	0
7	EDO	B	1204	4/4	0.87	0.13	62,62,62,63	0
8	ACT	A	1007	4/4	0.88	0.13	62,64,65,70	0
7	EDO	B	1205	4/4	0.89	0.14	68,70,72,73	0
7	EDO	A	1003	4/4	0.89	0.18	64,65,65,65	0
7	EDO	A	1005	4/4	0.90	0.15	72,74,76,76	0
7	EDO	B	1206	4/4	0.92	0.14	79,79,79,79	0
7	EDO	B	1209	4/4	0.92	0.12	77,78,79,80	0
9	CL	B	1208	1/1	0.96	0.07	94,94,94,94	0
5	ADP	B	1201	27/27	0.97	0.06	37,43,48,52	0
5	ADP	A	1001	27/27	0.97	0.05	41,47,48,52	0
6	MG	B	1202	1/1	0.99	0.04	41,41,41,41	0
6	MG	A	1002	1/1	0.99	0.03	39,39,39,39	0

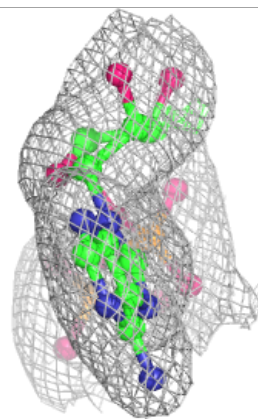
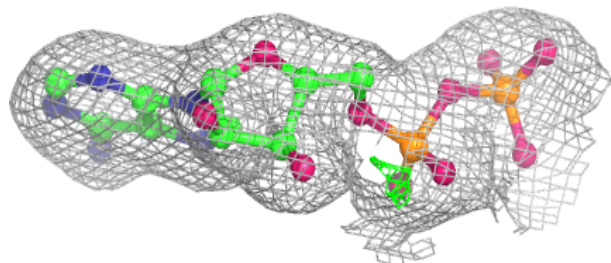
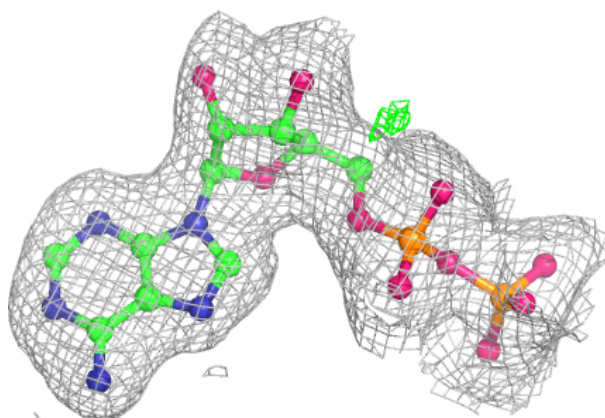
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP B 1201:

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

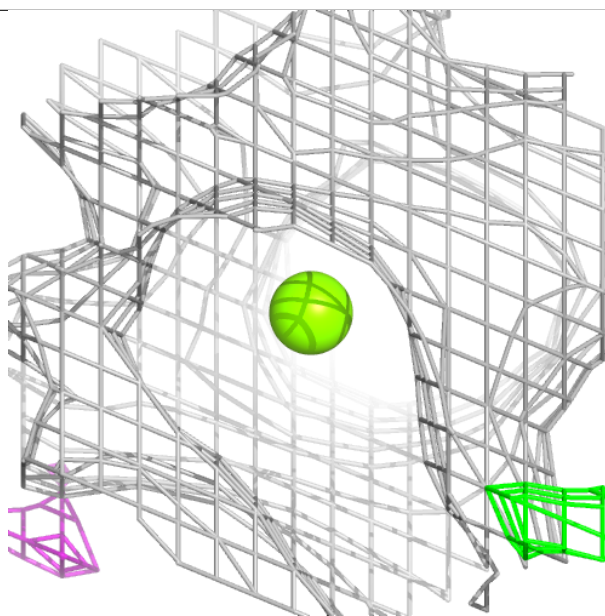
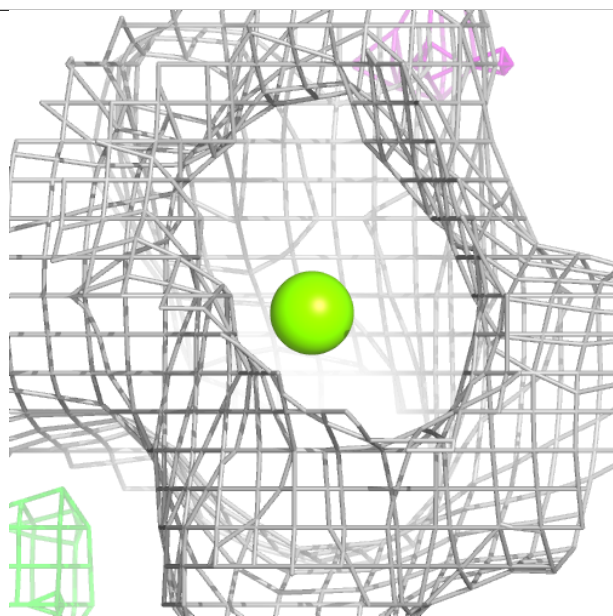
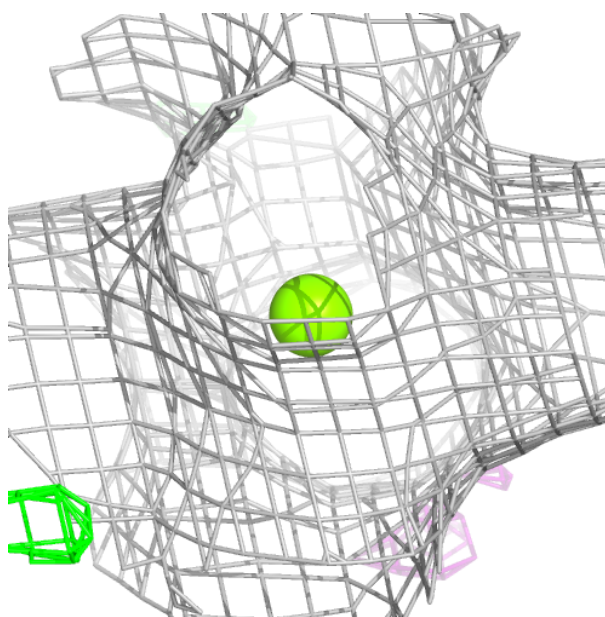
**Electron density around ADP A 1001:**

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



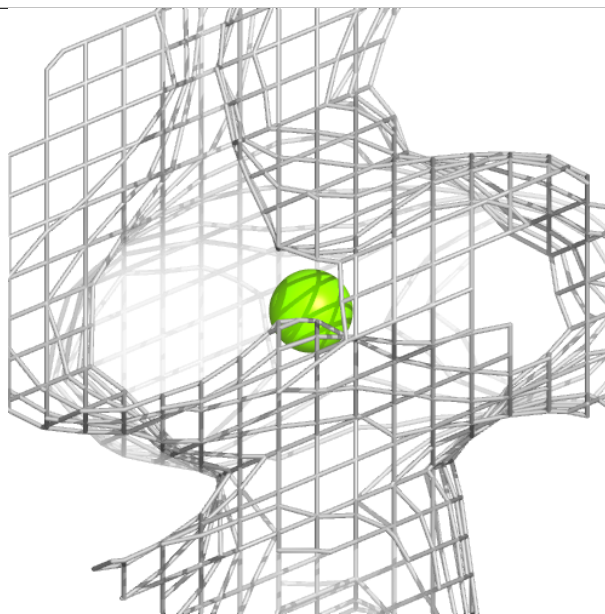
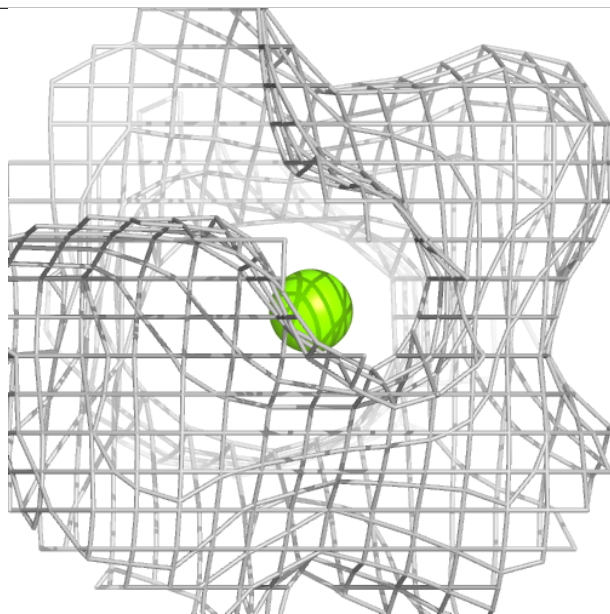
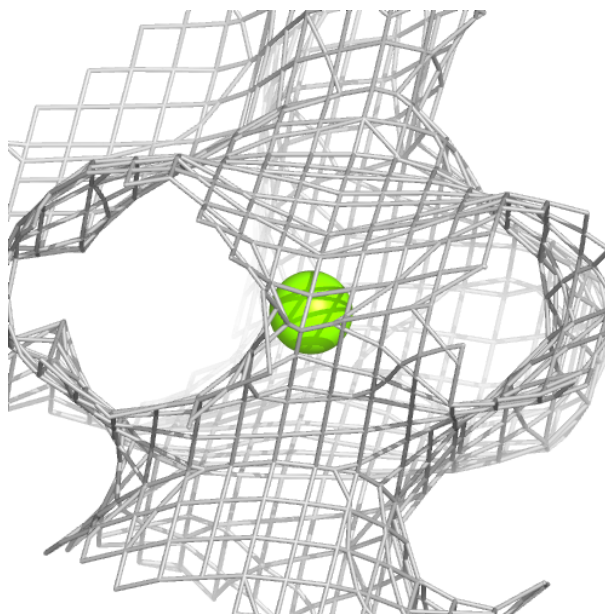
Electron density around MG B 1202:

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



Electron density around MG A 1002:

$2mF_o-DF_c$ (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.