Full wwPDB X-ray Structure Validation Report (i)

Aug 25, 2026 – 07:09 am BST

PDB ID	:	5AOR / pdb_00005aor
Title	:	Structure of MLE RNA ADP AlF4 complex
Authors	:	Prabu, J.R.; Conti, E.
Deposited on	:	2015-09-11
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 (i) 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 (i)) were used in the production of this report:

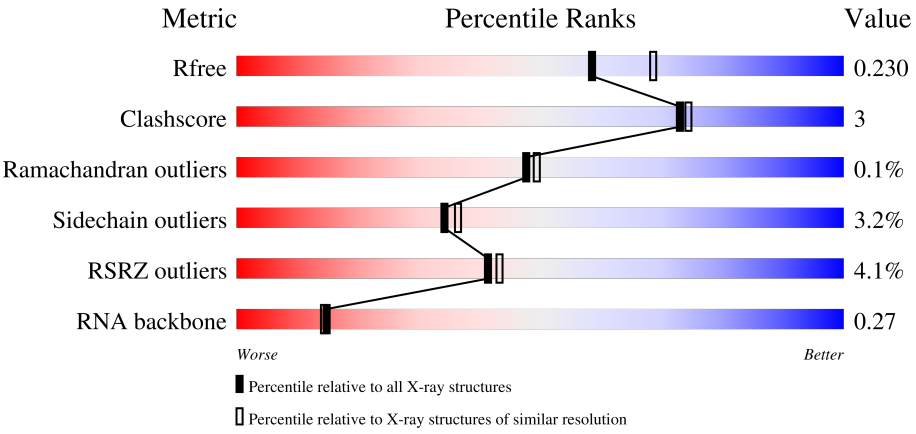
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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}	180053	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)
RNA backbone	3983	1017 (2.40-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1293	3% 71% 6% • 22%
1	B	1293	3% 70% 6% • 23%
2	C	11	9% 73% 27%
2	D	11	9% 45% 36% 9% 9%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16961 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.

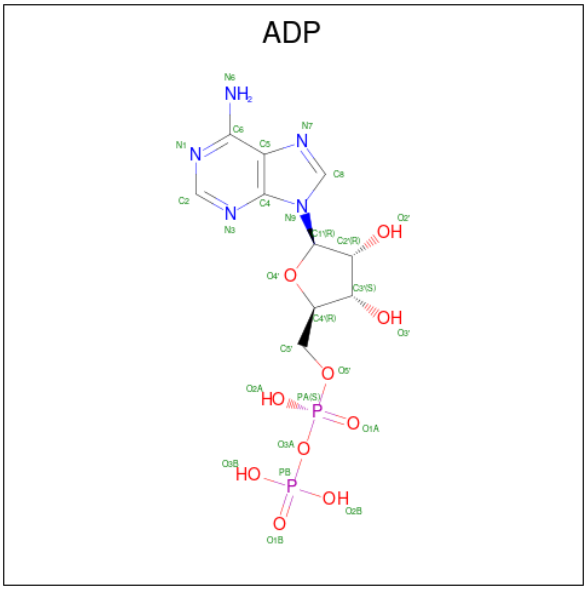
- Molecule 1 is a protein called DOSAGE COMPENSATION REGULATOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1009	Total	C	N	O	S	0	2	0
			8003	5074	1390	1491	48			
1	B	992	Total	C	N	O	S	0	2	0
			7876	4997	1370	1460	49			

- Molecule 2 is a RNA chain called 5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	P	0	0	0
			204	90	20	83	11			
2	D	10	Total	C	N	O	P	0	0	0
			200	90	20	80	10			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

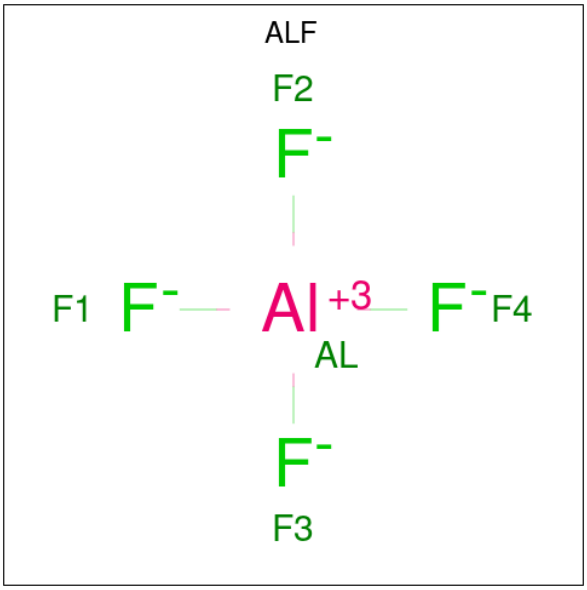


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

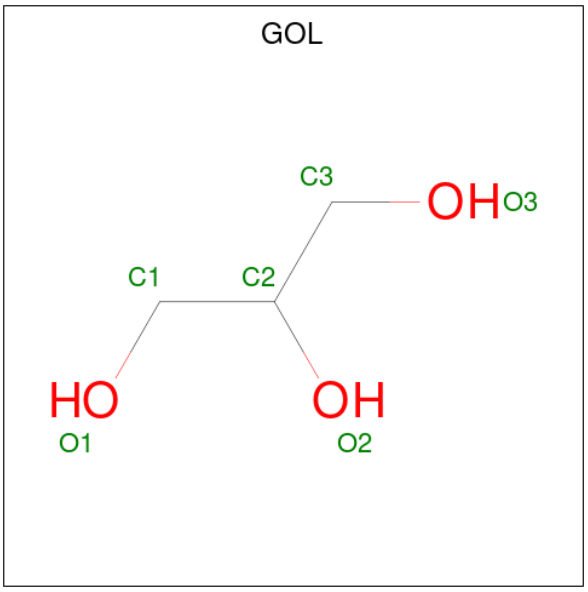
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Al	F	0	0
			5	1	4		
5	B	1	Total	Al	F	0	0
			5	1	4		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	333	Total O 333 333	0	0
7	B	261	Total O 261 261	0	0
7	C	2	Total O 2 2	0	0
7	D	3	Total O 3 3	0	0

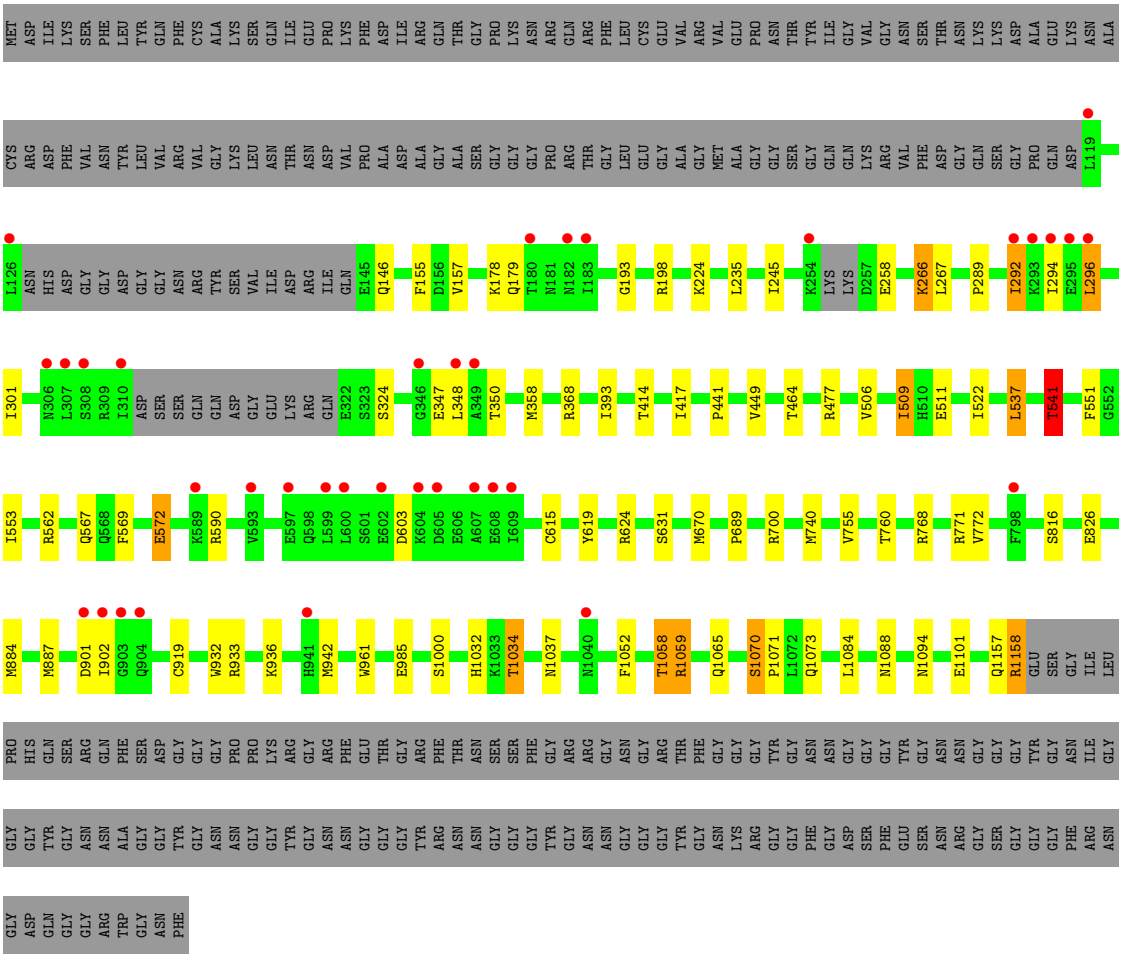
3 Residue-property plots (i)

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: DOSAGE COMPENSATION REGULATOR

Chain A:



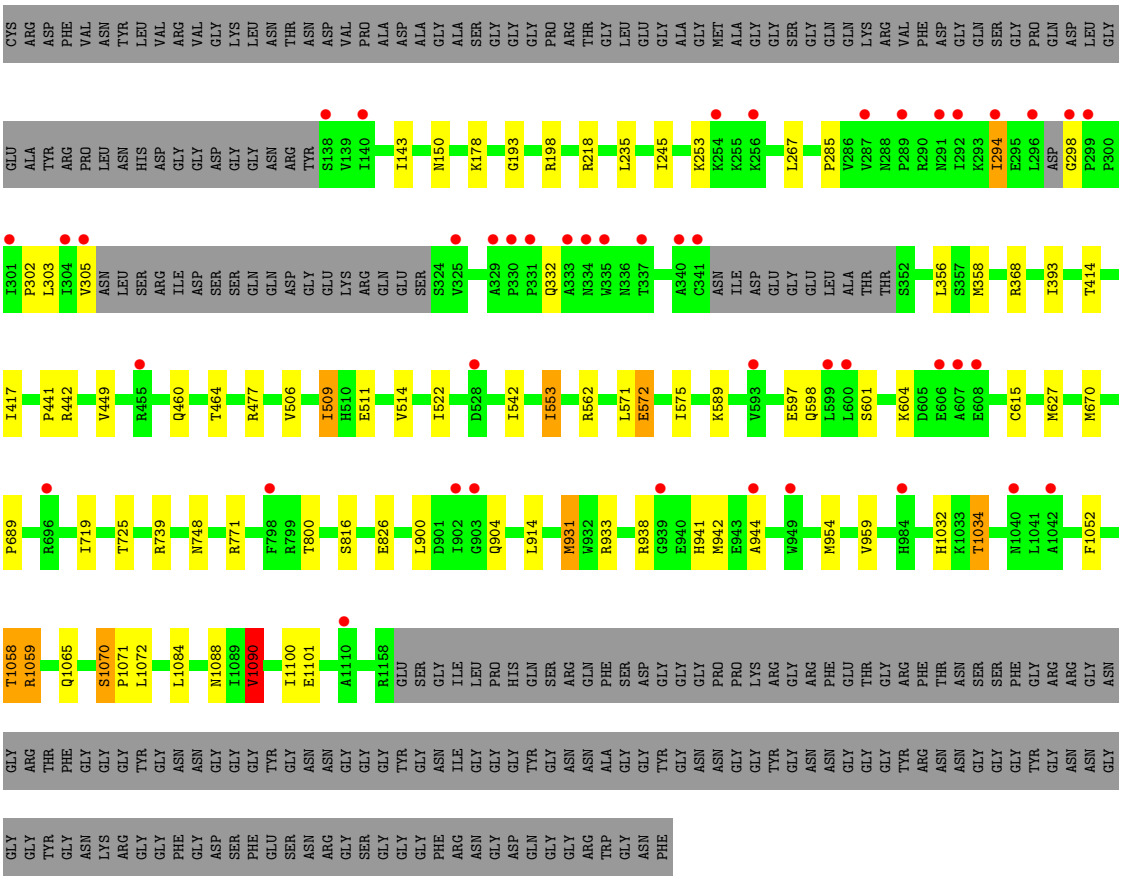


• Molecule 1: DOSAGE COMPENSATION REGULATOR

Chain B:

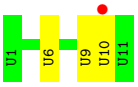






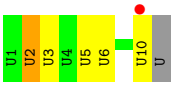
• Molecule 2: 5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP)-3'





• Molecule 2: 5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP)-3'





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	154.37Å 154.37Å 198.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.82 – 2.08 48.82 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.82-2.08) 100.0 (48.82-2.08)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.190 , 0.221 0.198 , 0.230	Depositor DCC
R_{free} test set	7169 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	34.9	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16961	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GOL, ADP, ALF

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	0.81	0/8160	0.93	5/11052 (0.0%)
1	B	0.80	0/8031	0.92	6/10873 (0.1%)
2	C	0.47	0/223	0.85	0/343
2	D	0.65	0/219	1.10	1/336 (0.3%)
All	All	0.80	0/16633	0.93	12/22604 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	258	GLU	N-CA-C	9.06	123.95	111.17
1	A	541	THR	N-CA-CB	-7.92	98.09	111.96
1	A	324	SER	N-CA-C	6.50	118.24	110.19
1	A	572	GLU	CB-CA-C	-6.06	101.37	110.88
1	B	1090	VAL	CB-CA-C	5.83	118.77	110.84
2	D	2	U	C2'-C3'-O3'	5.59	117.89	109.50
1	B	572	GLU	CB-CA-C	-5.46	101.73	110.79
1	B	1070	SER	CB-CA-C	5.33	117.85	109.37
1	B	542	ILE	CB-CA-C	-5.28	101.67	111.18
1	B	460	GLN	N-CA-CB	5.10	118.36	110.46
1	B	931	MET	CG-SD-CE	5.04	111.99	100.90
1	A	1094	ASN	N-CA-C	5.03	119.00	112.86

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	347	GLU	Peptide

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	8003	0	8080	55	0
1	B	7876	0	7963	49	0
2	C	204	0	100	0	0
2	D	200	0	101	1	0
3	A	27	0	12	0	0
3	B	27	0	12	1	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
5	A	5	0	0	1	0
5	B	5	0	0	1	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
7	A	333	0	0	3	0
7	B	261	0	0	1	1
7	C	2	0	0	0	0
7	D	3	0	0	0	0
All	All	16961	0	16284	104	1

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 (104) 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:572:GLU:N	1:B:627:MET:HE1	1.90	0.87
1:B:571:LEU:HG	1:B:627:MET:HE2	1.60	0.83
1:A:884:MET:HE1	1:A:1000:SER:HB3	1.63	0.79
1:B:267:LEU:HD21	1:B:1072:LEU:HD11	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:TYR:O	1:A:624:ARG:NH1	2.23	0.71
1:B:572:GLU:CA	1:B:627:MET:HE1	2.21	0.70
1:A:541:THR:HG23	1:A:760:THR:HG23	1.75	0.68
1:A:590:ARG:HD2	1:A:631:SER:HB2	1.76	0.68
1:A:933:ARG:HD3	1:A:961:TRP:CH2	2.29	0.68
1:A:1058:THR:HB	7:A:3304:HOH:O	1.95	0.66
1:B:944:ALA:HA	1:B:954:MET:CE	2.27	0.65
1:B:514:VAL:HG11	1:B:800:THR:HG21	1.78	0.65
1:B:1032:HIS:HD2	1:B:1034:THR:HB	1.63	0.64
1:A:1032:HIS:HD2	1:A:1034:THR:HB	1.63	0.64
1:B:670:MET:HE1	1:B:689:PRO:HD3	1.78	0.64
1:A:670:MET:HE1	1:A:689:PRO:HD3	1.78	0.63
1:A:884:MET:HE1	1:A:1000:SER:CB	2.29	0.62
1:A:541:THR:CG2	1:A:760:THR:HG23	2.29	0.61
1:A:1032:HIS:CD2	1:A:1034:THR:HB	2.35	0.61
1:B:442:ARG:HD3	1:B:719:ILE:HA	1.83	0.61
1:B:464:THR:HG22	1:B:477:ARG:CZ	2.31	0.61
1:B:1032:HIS:CD2	1:B:1034:THR:HB	2.35	0.60
1:A:884:MET:N	1:A:884:MET:HE2	2.17	0.59
1:B:393:ILE:HG21	1:B:417:ILE:HD12	1.84	0.58
1:B:572:GLU:HA	1:B:627:MET:HE1	1.85	0.57
1:B:193:GLY:O	1:B:198:ARG:NH1	2.37	0.56
1:A:567:GLN:HG2	1:A:569:PHE:CE2	2.40	0.56
1:A:292:ILE:HG13	1:A:301:ILE:HG21	1.86	0.56
1:A:670:MET:HE1	1:A:689:PRO:CD	2.36	0.56
1:B:670:MET:HE1	1:B:689:PRO:CD	2.36	0.56
1:A:541:THR:HG23	1:A:541:THR:O	2.07	0.55
1:A:464:THR:HG21	7:A:3101:HOH:O	2.06	0.55
1:A:464:THR:HG22	1:A:477:ARG:CZ	2.37	0.55
1:B:572:GLU:HG2	1:B:615:CYS:SG	2.46	0.55
1:A:572:GLU:HG2	1:A:615:CYS:SG	2.46	0.54
1:B:572:GLU:HA	1:B:627:MET:CE	2.37	0.54
1:A:193:GLY:O	1:A:198:ARG:NH1	2.38	0.54
1:B:938:ARG:NH1	1:B:942:MET:SD	2.81	0.53
1:A:740:MET:HE2	1:A:755:VAL:HG11	1.89	0.53
1:A:884:MET:HE1	1:A:887:MET:CE	2.38	0.53
1:A:393:ILE:HG21	1:A:417:ILE:HD12	1.90	0.52
1:B:267:LEU:CD2	1:B:1072:LEU:HD11	2.39	0.52
1:B:771[A]:ARG:NH2	5:B:2161:ALF:F2	2.32	0.52
1:A:901:ASP:OD1	1:A:902:ILE:N	2.43	0.52
1:A:884:MET:CE	1:A:1000:SER:CB	2.89	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:THR:CG2	1:A:541:THR:O	2.59	0.49
1:A:506:VAL:CG1	1:A:509:ILE:HD13	2.43	0.49
1:B:506:VAL:CG1	1:B:509:ILE:HD13	2.43	0.49
1:B:1034:THR:CG2	7:B:3251:HOH:O	2.62	0.48
1:B:1070:SER:HB3	1:B:1071:PRO:HD2	1.96	0.48
1:A:1070[A]:SER:HB3	1:A:1071:PRO:HD2	1.96	0.47
1:A:884:MET:CE	1:A:1000:SER:HB3	2.39	0.47
1:A:932:TRP:CZ2	1:A:936:LYS:HD2	2.50	0.47
1:B:914:LEU:CD2	1:B:931:MET:HE1	2.45	0.47
1:B:1052:PHE:HA	1:B:1065:GLN:O	2.15	0.47
1:A:1070[B]:SER:OG	1:A:1073:GLN:HG3	2.15	0.46
1:A:771[A]:ARG:NH2	5:A:2161:ALF:F2	2.37	0.46
1:B:900:LEU:HD22	1:B:904:GLN:HG3	1.97	0.46
1:B:414:THR:HG22	1:B:449:VAL:HG11	1.98	0.46
1:A:506:VAL:HG12	1:A:509:ILE:HD13	1.96	0.46
1:B:294:ILE:CG2	1:B:298:GLY:HA2	2.46	0.46
1:A:1034:THR:CG2	7:A:3306:HOH:O	2.64	0.46
1:B:506:VAL:HG12	1:B:509:ILE:HD13	1.97	0.46
1:B:944:ALA:HA	1:B:954:MET:HE1	1.97	0.45
1:B:1084:LEU:HD11	1:B:1088:ASN:HA	1.98	0.45
1:B:1090:VAL:HG11	1:B:1100:ILE:CG2	2.46	0.45
1:A:292:ILE:HG21	1:A:1084:LEU:HD23	1.99	0.45
1:A:933:ARG:NH2	1:A:985:GLU:OE2	2.45	0.45
1:A:266:LYS:C	1:A:267:LEU:HD12	2.42	0.45
1:B:914:LEU:HD22	1:B:931:MET:HE1	1.99	0.45
1:B:575:ILE:HD12	1:B:627:MET:CE	2.47	0.44
1:B:302:PRO:C	1:B:303:LEU:HD12	2.43	0.44
1:A:1157:GLN:O	1:A:1158:ARG:CB	2.66	0.44
1:A:414:THR:HG22	1:A:449:VAL:HG11	1.99	0.44
1:A:567:GLN:HG2	1:A:569:PHE:CZ	2.53	0.44
1:A:919:CYS:CA	1:A:1037:ASN:HD21	2.31	0.44
1:A:1157:GLN:O	1:A:1158:ARG:HB2	2.17	0.43
1:A:884:MET:CE	1:A:887:MET:CE	2.96	0.43
1:A:1052:PHE:HA	1:A:1065:GLN:O	2.17	0.43
1:A:1058:THR:HG22	1:A:1059:ARG:N	2.33	0.43
1:A:441:PRO:HG3	1:A:511:GLU:HG3	2.01	0.43
1:A:294:ILE:HG23	1:A:296:LEU:HG	2.00	0.43
1:A:1058:THR:CG2	1:A:1059:ARG:N	2.82	0.43
1:A:1084:LEU:HD11	1:A:1088:ASN:HA	1.99	0.43
1:B:1090:VAL:CG1	1:B:1100:ILE:HG22	2.49	0.43
1:B:941:HIS:HD2	1:B:942:MET:HE3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:GLU:O	1:B:601:SER:N	2.52	0.42
1:B:1058:THR:HG22	1:B:1059:ARG:N	2.34	0.42
1:A:1058:THR:CG2	1:A:1059:ARG:H	2.33	0.42
1:B:285:PRO:HG2	1:B:305:VAL:HG21	2.02	0.42
1:A:537:LEU:HD21	1:A:551:PHE:CE2	2.55	0.42
1:B:739:ARG:NH2	2:D:5:U:OP1	2.53	0.42
1:B:941:HIS:CD2	1:B:942:MET:CE	3.03	0.42
1:B:441:PRO:HG3	1:B:511:GLU:HG3	2.02	0.41
1:B:150:ASN:HD22	1:B:150:ASN:HA	1.73	0.41
1:B:725:THR:HG21	3:B:2159:ADP:C5	2.56	0.41
1:A:155:PHE:CZ	1:A:157:VAL:HG12	2.56	0.41
1:A:289:PRO:HA	1:A:292:ILE:HD13	2.03	0.41
1:A:884:MET:HE3	1:A:1000:SER:OG	2.21	0.41
1:A:224:LYS:NZ	1:A:603:ASP:O	2.50	0.41
1:B:1058:THR:CG2	1:B:1059:ARG:N	2.83	0.41
1:B:1090:VAL:HG11	1:B:1100:ILE:HG23	2.02	0.41
1:B:1058:THR:CG2	1:B:1059:ARG:H	2.34	0.40
1:B:944:ALA:CA	1:B:954:MET:HE1	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:3085:HOH:O	7:B:3085:HOH:O[7_557]	1.81	0.39

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	1003/1293 (78%)	969 (97%)	33 (3%)	1 (0%)	48 49
1	B	986/1293 (76%)	965 (98%)	20 (2%)	1 (0%)	48 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1989/2586 (77%)	1934 (97%)	53 (3%)	2 (0%)	48 49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	553	ILE
1	B	553	ILE

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	890/1091 (82%)	860 (97%)	30 (3%)	32 34
1	B	876/1091 (80%)	847 (97%)	29 (3%)	33 35
All	All	1766/2182 (81%)	1707 (97%)	59 (3%)	34 35

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	178	LYS
1	A	179	GLN
1	A	235	LEU
1	A	245	ILE
1	A	266	LYS
1	A	292	ILE
1	A	296	LEU
1	A	348	LEU
1	A	350	THR
1	A	358	MET
1	A	368	ARG
1	A	509	ILE
1	A	522	ILE
1	A	537	LEU
1	A	541	THR

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Mol	Chain	Res	Type
1	A	562	ARG
1	A	700	ARG
1	A	768	ARG
1	A	772	VAL
1	A	816	SER
1	A	826	GLU
1	A	942	MET
1	A	1034	THR
1	A	1058	THR
1	A	1059	ARG
1	A	1070[A]	SER
1	A	1070[B]	SER
1	A	1101	GLU
1	A	1158	ARG
1	B	143	ILE
1	B	178	LYS
1	B	218	ARG
1	B	235	LEU
1	B	245	ILE
1	B	253	LYS
1	B	294	ILE
1	B	332	GLN
1	B	356	LEU
1	B	358[A]	MET
1	B	358[B]	MET
1	B	368	ARG
1	B	509	ILE
1	B	522	ILE
1	B	553	ILE
1	B	562	ARG
1	B	589	LYS
1	B	598	GLN
1	B	604	LYS
1	B	748	ASN
1	B	816	SER
1	B	826	GLU
1	B	933	ARG
1	B	959	VAL
1	B	1034	THR
1	B	1058	THR
1	B	1059	ARG
1	B	1090	VAL

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Mol	Chain	Res	Type
1	B	1101	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	ASN
1	A	370	ASN
1	A	764	GLN
1	A	972	GLN
1	A	1032	HIS
1	A	1037	ASN
1	A	1157	GLN
1	B	150	ASN
1	B	175	ASN
1	B	179	GLN
1	B	182	ASN
1	B	223	ASN
1	B	270	ASN
1	B	369	GLN
1	B	567	GLN
1	B	646	HIS
1	B	684	GLN
1	B	941	HIS
1	B	1032	HIS
1	B	1125	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	9/11 (81%)	3 (33%)	1 (11%)
2	D	9/11 (81%)	4 (44%)	0
All	All	18/22 (81%)	7 (38%)	1 (5%)

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	6	U
2	C	9	U
2	C	10	U
2	D	2	U

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Mol	Chain	Res	Type
2	D	3	U
2	D	6	U
2	D	10	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	9	U

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 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	ADP	A	2159	4,5	27,29,29	1.44	3 (11%)	42,45,45	1.88	9 (21%)
3	ADP	B	2159	4,5	27,29,29	1.36	5 (18%)	42,45,45	1.88	11 (26%)
6	GOL	B	2162	-	5,5,5	0.37	0	5,5,5	0.15	0
5	ALF	A	2161	7,3	0,4,4	-	-	-		
6	GOL	A	2163	-	5,5,5	0.36	0	5,5,5	0.17	0
5	ALF	B	2161	7,3	0,4,4	-	-	-		

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
6	GOL	B	2162	-	-	3/4/4/4	-
6	GOL	A	2163	-	-	2/4/4/4	-
3	ADP	A	2159	4,5	-	2/16/32/32	0/3/3/3
3	ADP	B	2159	4,5	-	2/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2159	ADP	C5-C4	4.58	1.47	1.39
3	B	2159	ADP	C5-C4	3.97	1.46	1.39
3	A	2159	ADP	C5-C6	3.00	1.49	1.41
3	A	2159	ADP	C8-N7	2.78	1.36	1.31
3	B	2159	ADP	C5-C6	2.59	1.48	1.41
3	B	2159	ADP	C8-N7	2.56	1.36	1.31
3	B	2159	ADP	C4-N9	-2.17	1.32	1.37
3	B	2159	ADP	C5-N7	-2.08	1.35	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2159	ADP	C5-C4-N3	-5.41	119.70	126.75
3	B	2159	ADP	C5-C4-N3	-4.90	120.36	126.75
3	B	2159	ADP	N3-C2-N1	-4.26	121.94	128.60
3	A	2159	ADP	N3-C4-N9	4.10	133.83	127.08
3	B	2159	ADP	N3-C4-N9	4.06	133.76	127.08
3	A	2159	ADP	C2-N3-C4	4.02	121.24	111.75
3	A	2159	ADP	N3-C2-N1	-3.86	122.56	128.60
3	B	2159	ADP	C2-N3-C4	3.83	120.80	111.75
3	B	2159	ADP	C4-N9-C8	3.42	109.43	105.73
3	A	2159	ADP	C4-C5-N7	-3.36	106.53	110.62
3	A	2159	ADP	C6-C5-N7	3.10	137.79	132.02
3	A	2159	ADP	C4-N9-C8	3.03	109.01	105.73
3	B	2159	ADP	C6-C5-N7	2.80	137.24	132.02
3	A	2159	ADP	C5-N7-C8	2.80	107.48	103.51
3	B	2159	ADP	C4-C5-N7	-2.71	107.31	110.62
3	B	2159	ADP	N9-C8-N7	-2.57	110.39	113.91
3	B	2159	ADP	O3B-PB-O2B	2.50	117.19	107.64
3	A	2159	ADP	N9-C8-N7	-2.49	110.51	113.91
3	B	2159	ADP	C5-N7-C8	2.45	106.99	103.51
3	B	2159	ADP	C2-N1-C6	2.36	122.81	118.77

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2159	ADP	PA-O3A-PB-O3B
3	B	2159	ADP	PA-O3A-PB-O3B
6	A	2163	GOL	C1-C2-C3-O3
6	B	2162	GOL	O1-C1-C2-C3
6	B	2162	GOL	O1-C1-C2-O2
6	A	2163	GOL	O2-C2-C3-O3
3	A	2159	ADP	PA-O3A-PB-O2B
3	B	2159	ADP	PA-O3A-PB-O2B
6	B	2162	GOL	O2-C2-C3-O3

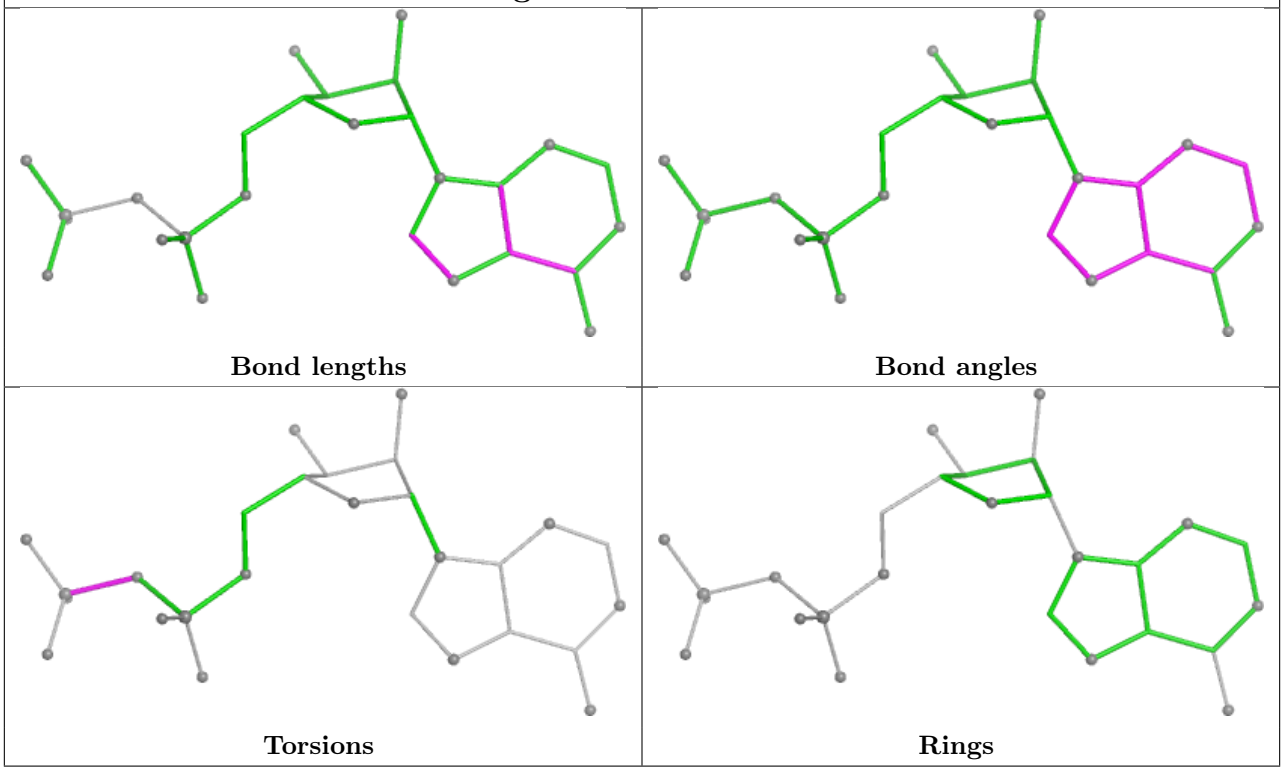
There are no ring outliers.

3 monomers are involved in 3 short contacts:

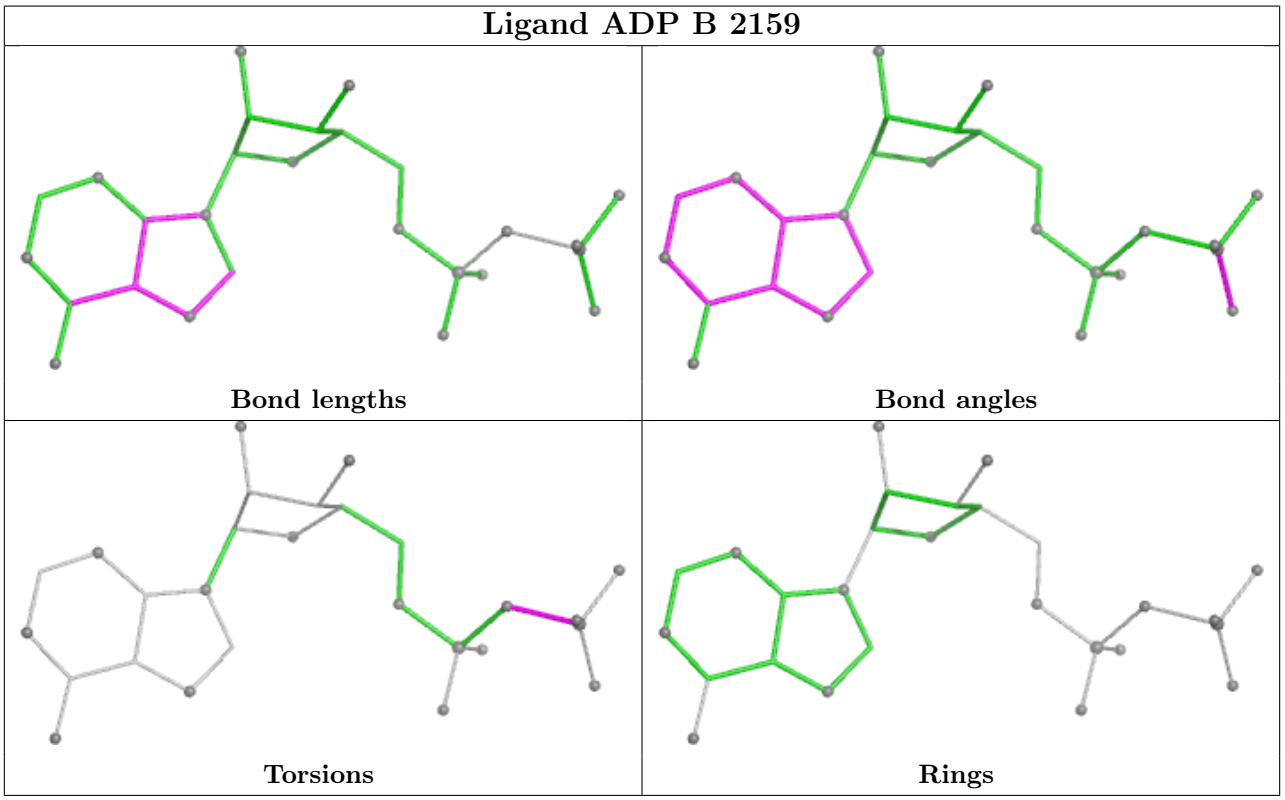
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2159	ADP	1	0
5	A	2161	ALF	1	0
5	B	2161	ALF	1	0

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

Ligand ADP A 2159



Ligand ADP B 2159



5.7 Other polymers

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	1009/1293 (78%)	0.06	36 (3%)	46	48	15, 37, 83, 157	2 (0%)
1	B	992/1293 (76%)	0.24	44 (4%)	39	40	16, 42, 79, 129	2 (0%)
2	C	11/11 (100%)	0.30	1 (9%)	15	15	33, 51, 126, 127	0
2	D	10/11 (90%)	0.09	1 (10%)	12	13	30, 56, 115, 139	0
All	All	2022/2608 (77%)	0.15	82 (4%)	41	43	15, 39, 80, 157	4 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	348	LEU	6.2
1	A	607	ALA	6.0
1	A	310	ILE	5.3
1	A	600	LEU	5.1
1	A	902	ILE	4.9
1	B	325	VAL	4.8
1	B	294	ILE	4.7
1	B	593	VAL	4.6
1	A	294	ILE	4.5
1	A	296	LEU	4.5
1	B	600	LEU	4.3
1	B	296	LEU	4.2
1	A	119	LEU	4.0
1	A	599	LEU	4.0
1	A	593	VAL	3.8
1	A	292	ILE	3.7
1	A	349	ALA	3.7
1	B	903	GLY	3.5
1	B	599	LEU	3.5
1	A	798	PHE	3.5
1	A	307	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	305	VAL	3.5
1	B	340	ALA	3.4
1	B	289	PRO	3.2
1	B	607	ALA	3.1
1	B	902	ILE	3.0
1	A	1040	ASN	3.0
1	B	334	ASN	3.0
1	B	333	ALA	2.9
1	A	602	GLU	2.9
1	B	939	GLY	2.9
2	D	10	U	2.8
1	B	254	LYS	2.8
1	A	346	GLY	2.8
1	A	903	GLY	2.8
1	B	299	PRO	2.8
1	B	335	TRP	2.8
1	B	949	TRP	2.8
1	B	138	SER	2.8
1	B	301	ILE	2.8
1	A	597	GLU	2.7
1	B	331	PRO	2.7
1	A	182	ASN	2.7
1	A	183	ILE	2.7
1	A	901	ASP	2.7
1	A	308	SER	2.6
1	B	798	PHE	2.6
1	B	944	ALA	2.6
1	A	904	GLN	2.5
1	B	608	GLU	2.5
1	A	605	ASP	2.5
1	B	287	VAL	2.4
1	A	254	LYS	2.4
1	B	606	GLU	2.3
1	B	140	ILE	2.3
1	A	608	GLU	2.3
1	A	180	THR	2.3
1	B	330	PRO	2.3
1	B	291	ASN	2.3
1	B	984	HIS	2.2
2	C	10	U	2.2
1	B	304	ILE	2.2
1	B	1042	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	455	ARG	2.2
1	A	609	ILE	2.1
1	B	292	ILE	2.1
1	B	298	GLY	2.1
1	B	329	ALA	2.1
1	A	306	ASN	2.1
1	B	1040	ASN	2.1
1	A	589	LYS	2.1
1	A	604	LYS	2.1
1	A	126	LEU	2.1
1	B	1110	ALA	2.1
1	B	341	CYS	2.0
1	B	528	ASP	2.0
1	A	941	HIS	2.0
1	A	293	LYS	2.0
1	B	256	LYS	2.0
1	A	295	GLU	2.0
1	B	696	ARG	2.0
1	B	337	THR	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	MG	A	2162	1/1	0.81	0.22	55,55,55,55	0
6	GOL	B	2162	6/6	0.84	0.14	63,68,73,75	0
6	GOL	A	2163	6/6	0.86	0.15	64,77,81,81	0
3	ADP	A	2159	27/27	0.98	0.05	26,30,34,36	0

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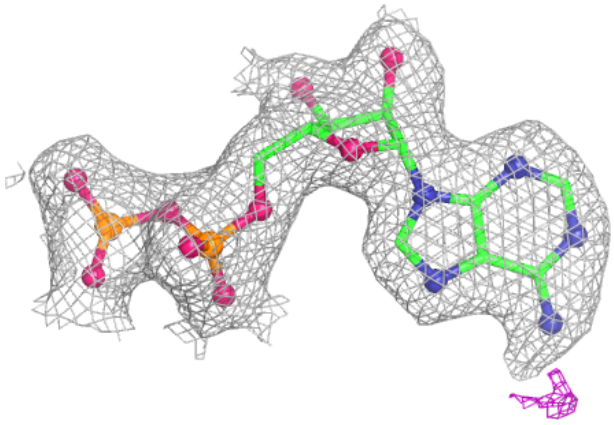
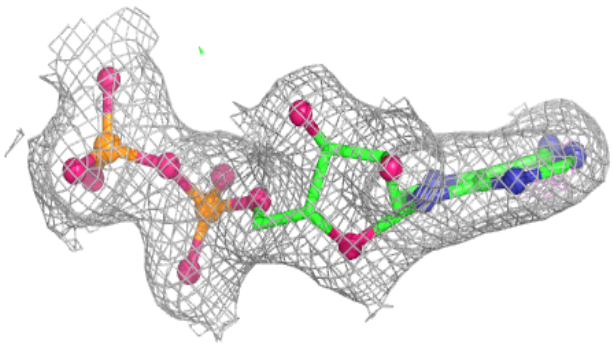
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ALF	A	2161	5/5	0.99	0.02	24,26,28,29	0
5	ALF	B	2161	5/5	0.99	0.04	22,24,26,27	0
3	ADP	B	2159	27/27	0.99	0.04	18,25,33,35	0
4	MG	B	2160	1/1	0.99	0.02	25,25,25,25	0
4	MG	A	2160	1/1	1.00	0.02	27,27,27,27	0

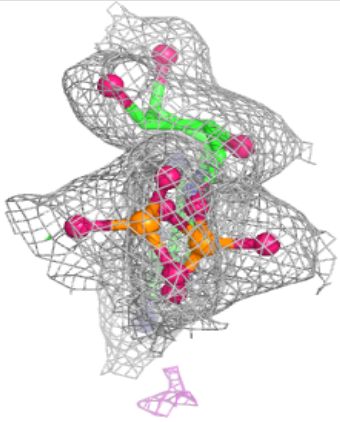
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 2159:

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

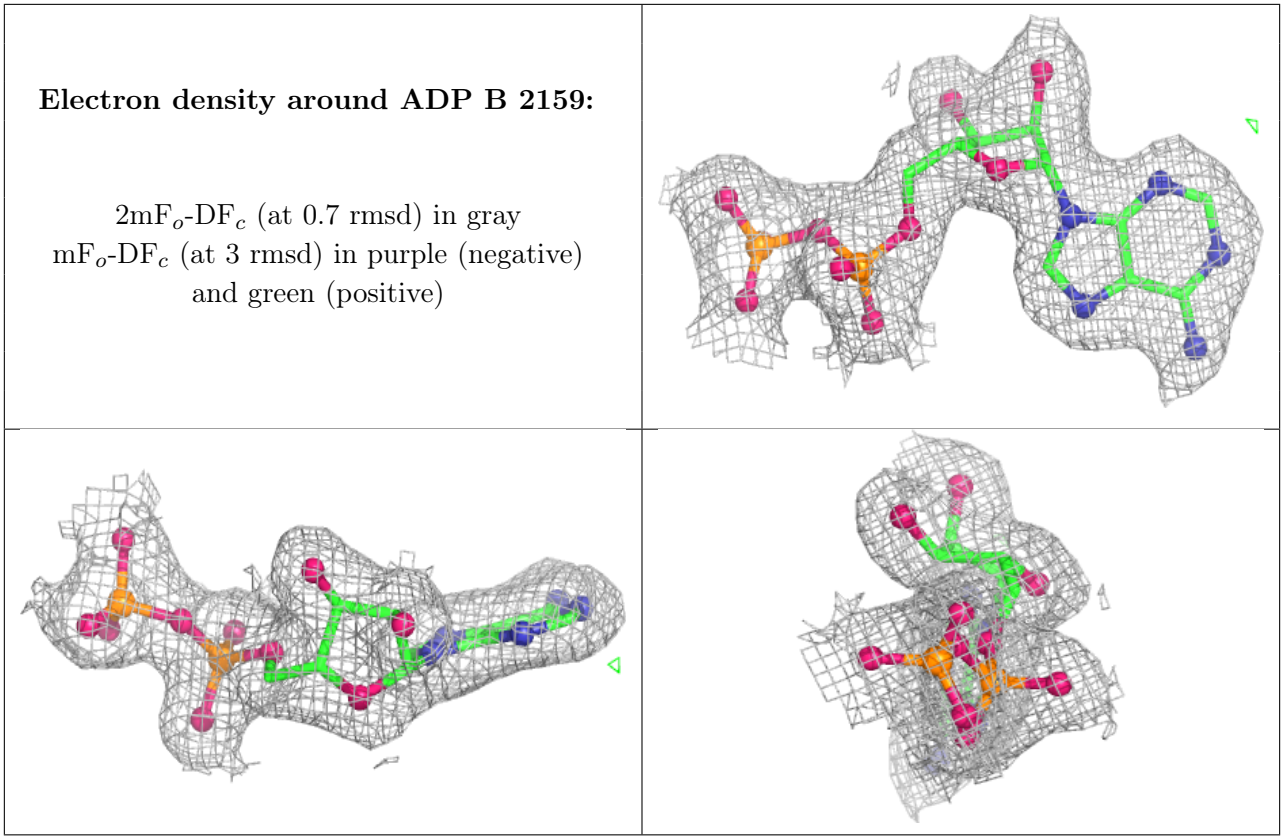






Electron density around ADP B 2159:

$2mF_o$-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.