



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:35 am BST

PDB ID : 5AOR
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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

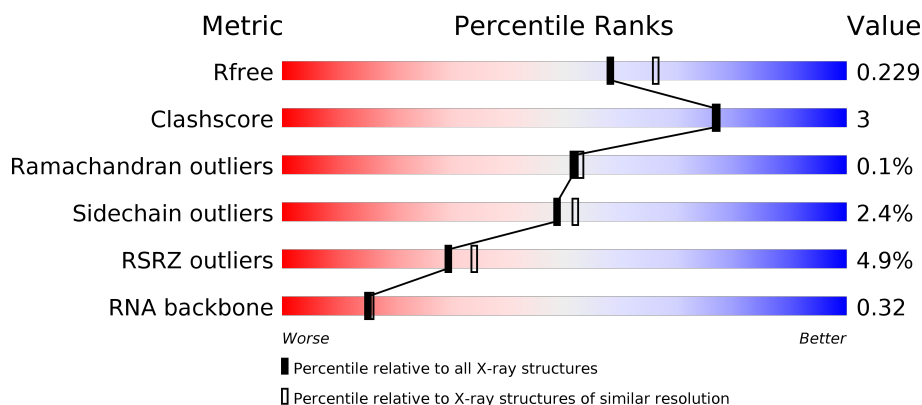
1 Overall quality at a glance

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}	130704	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)
RNA backbone	3102	1004 (2.54-1.62)

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 on 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	1293	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>5%</div> <div>22%</div> </div> </div>
1	B	1293	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>5%</div> <div>23%</div> </div> </div>
2	C	11	<div> <div>73%</div> <div>27%</div> </div>
2	D	11	<div> <div>9%</div> <div> <div></div> <div>45%</div> <div>45%</div> <div>9%</div> </div> </div>

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.

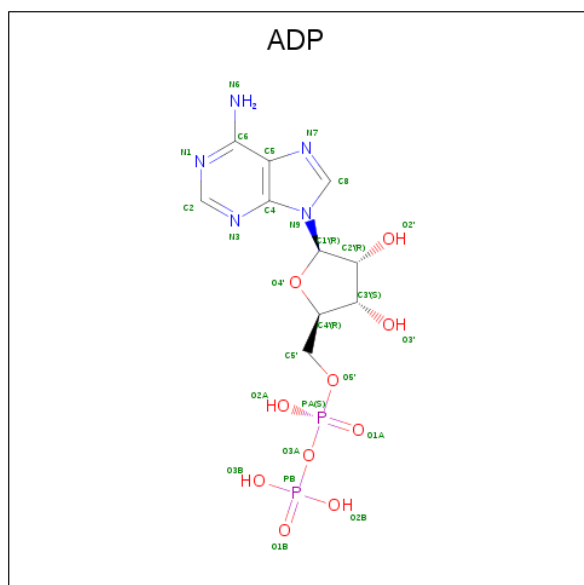
- Molecule 1 is a protein called DOSAGE COMPENSATION REGULATOR.

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)-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 (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

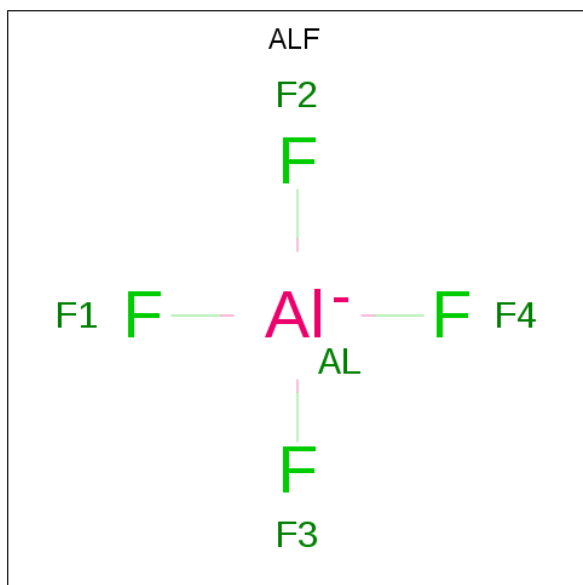


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is TETRAFLUOROALUMINATE ION (three-letter code: 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 (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

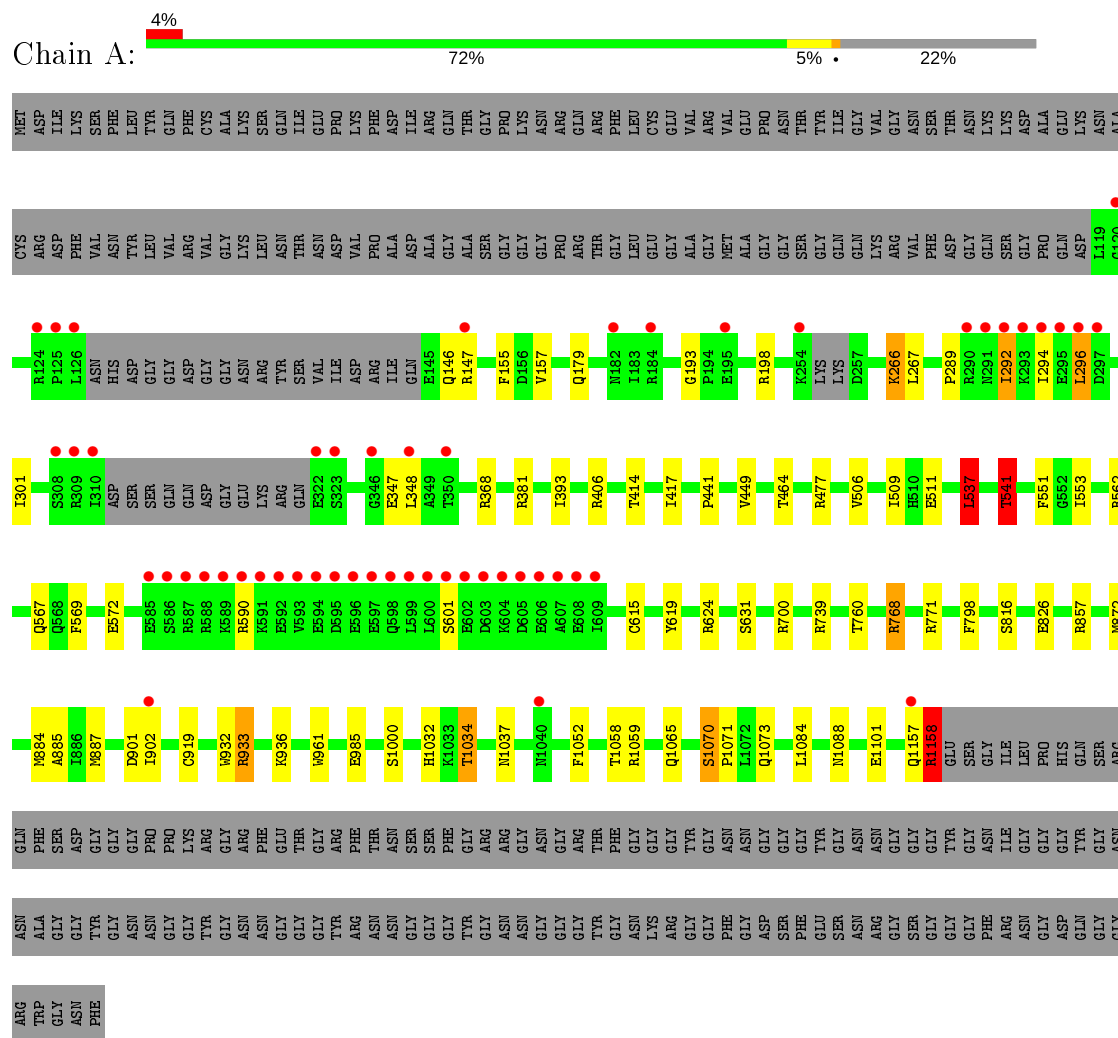
- Molecule 7 is water.

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

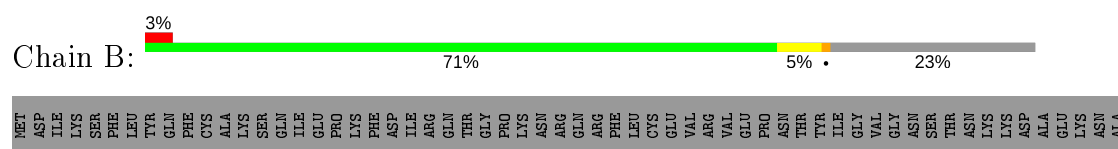
3 Residue-property plots

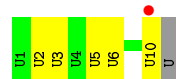
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



• Molecule 1: DOSAGE COMPENSATION REGULATOR





4 Data and refinement statistics

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) 99.9 (48.82-2.08)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.190 , 0.221 0.198 , 0.229	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 , 41.8	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	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.*

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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ALF, GOL, 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	0.59	0/8160	0.81	12/11052 (0.1%)
1	B	0.58	0/8031	0.79	9/10873 (0.1%)
2	C	0.48	0/223	0.76	0/343
2	D	0.73	0/219	0.95	0/336
All	All	0.59	0/16633	0.80	21/22604 (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 (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	768	ARG	NE-CZ-NH1	12.08	126.34	120.30
1	A	768	ARG	NE-CZ-NH2	-10.96	114.82	120.30
1	A	1158	ARG	NE-CZ-NH1	10.03	125.31	120.30
1	A	1158	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	B	375	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	B	931	MET	CG-SD-CE	7.37	111.99	100.20
1	A	739	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	541	THR	N-CA-CB	-6.43	98.09	110.30
1	A	933	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	A	147	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	B	696	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	B	933	ARG	NE-CZ-NH1	5.91	123.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	739	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	B	933	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	562	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	857	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	368	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	739	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	381	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	562	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	537	LEU	CA-CB-CG	5.00	126.81	115.30

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

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	50	0
1	B	7876	0	7963	47	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	97	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 (97) 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:884:MET:HE1	1:A:1000:SER:HB3	1.52	0.91
1:B:572:GLU:N	1:B:627:MET:HE1	1.91	0.86
1:A:884:MET:HE1	1:A:1000:SER:CB	2.07	0.84
1:B:267:LEU:HD21	1:B:1072:LEU:HD11	1.67	0.76
1:A:619:TYR:O	1:A:624:ARG:NH1	2.23	0.71
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:571:LEU:HG	1:B:627:MET:HE2	1.78	0.65
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:572:GLU:HA	1:B:627:MET:HE3	1.80	0.64
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:575:ILE:HD12	1:B:627:MET:HE2	1.82	0.61
1:B:1032:HIS:CD2	1:B:1034:THR:HB	2.35	0.60
1:B:393:ILE:HG21	1:B:417:ILE:HD12	1.84	0.58
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:541:THR:O	1:A:541:THR:HG23	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:THR:O	1:A:541:THR:CG2	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:HE1	1:A:1000:SER:CA	2.44	0.47
1:B:944:ALA:HA	1:B:954:MET:HE3	1.95	0.47
1:A:932:TRP:CZ2	1:A:936:LYS:HD2	2.50	0.47
1:B:355:ASP:HA	1:B:358[A]:MET:HE2	1.96	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:884:MET:CE	1:A:1000:SER:CB	2.89	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: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:1157:GLN:O	1:A:1158:ARG:CB	2.66	0.44
1:B:572:GLU:CA	1:B:627:MET:HE1	2.48	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: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:884:MET:CE	1:A:887:MET:CE	2.96	0.43
1:A:441:PRO:HG3	1:A:511:GLU:HG3	2.01	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:A:294:ILE:HG23	1:A:296:LEU:HG	2.00	0.43
1:B:1090:VAL:CG1	1:B:1100:ILE:HG22	2.49	0.43
1:A:884:MET:HE2	1:A:887:MET:CE	2.49	0.43
1:B:1058:THR:HG22	1:B:1059:ARG:N	2.34	0.42
1:B:597:GLU:O	1:B:601:SER:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:572:GLU:CA	1:B:627:MET:CE	2.98	0.41
1:B:571:LEU:C	1:B:627:MET:HE1	2.38	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:872:MET:HE1	1:A:885:ALA:HB2	2.03	0.41
1:A:289:PRO:HA	1:A:292:ILE:HD13	2.03	0.41
1:B:575:ILE:HD12	1:B:627:MET:CE	2.47	0.41
1:B:941:HIS:CD2	1:B:942:MET:HE2	2.55	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:A:266:LYS:C	1:A:267:LEU:HD12	2.42	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%)	51 53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	986/1293 (76%)	965 (98%)	20 (2%)	1 (0%)	51	53
All	All	1989/2586 (77%)	1934 (97%)	53 (3%)	2 (0%)	51	53

All (2) Ramachandran outliers are listed below:

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

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	890/1091 (82%)	868 (98%)	22 (2%)	47	50
1	B	876/1091 (80%)	853 (97%)	23 (3%)	46	49
All	All	1766/2182 (81%)	1721 (98%)	45 (2%)	49	50

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	179	GLN
1	A	266	LYS
1	A	292	ILE
1	A	296	LEU
1	A	348	LEU
1	A	368	ARG
1	A	406	ARG
1	A	537	LEU
1	A	541	THR
1	A	562	ARG
1	A	601	SER
1	A	700	ARG
1	A	768	ARG

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Mol	Chain	Res	Type
1	A	798	PHE
1	A	816	SER
1	A	826	GLU
1	A	1034	THR
1	A	1070[A]	SER
1	A	1070[B]	SER
1	A	1101	GLU
1	A	1158	ARG
1	B	178	LYS
1	B	218	ARG
1	B	253	LYS
1	B	294	ILE
1	B	332	GLN
1	B	358[A]	MET
1	B	358[B]	MET
1	B	368	ARG
1	B	377	PHE
1	B	406	ARG
1	B	553	ILE
1	B	562	ARG
1	B	589	LYS
1	B	598	GLN
1	B	604	LYS
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	GLN
1	A	370	ASN
1	A	693	GLN
1	A	764	GLN
1	A	972	GLN
1	A	1032	HIS
1	A	1037	ASN

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Mol	Chain	Res	Type
1	A	1157	GLN
1	B	646	HIS
1	B	693	GLN
1	B	941	HIS
1	B	1032	HIS

5.3.3 RNA ⓘ

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
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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
6	GOL	A	2163	-	5,5,5	0.36	0	5,5,5	0.17	0
3	ADP	A	2159	5,4	24,29,29	1.09	1 (4%)	29,45,45	1.30	3 (10%)
6	GOL	B	2162	-	5,5,5	0.37	0	5,5,5	0.15	0
5	ALF	B	2161	3,4,7	0,4,4	0.00	-	-	-	-
3	ADP	B	2159	5,4	24,29,29	1.03	1 (4%)	29,45,45	1.38	5 (17%)
5	ALF	A	2161	3,7	0,4,4	0.00	-	-	-	-

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	A	2163	-	-	2/4/4/4	-
3	ADP	A	2159	5,4	-	2/12/32/32	0/3/3/3
3	ADP	B	2159	5,4	-	2/12/32/32	0/3/3/3
6	GOL	B	2162	-	-	3/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2159	ADP	C5-C4	2.51	1.47	1.40
3	B	2159	ADP	C5-C4	2.08	1.46	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2159	ADP	N3-C2-N1	-4.31	121.94	128.68
3	A	2159	ADP	N3-C2-N1	-3.91	122.56	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2159	ADP	C4-C5-N7	-2.75	106.53	109.40
3	B	2159	ADP	C1'-N9-C4	-2.70	121.90	126.64
3	B	2159	ADP	O3B-PB-O2B	2.50	117.19	107.64
3	B	2159	ADP	C2-N1-C6	2.37	122.81	118.75
3	A	2159	ADP	C1'-N9-C4	-2.09	122.97	126.64
3	B	2159	ADP	C4-C5-N7	-2.00	107.31	109.40

There are no chirality outliers.

All (9) torsion outliers are listed below:

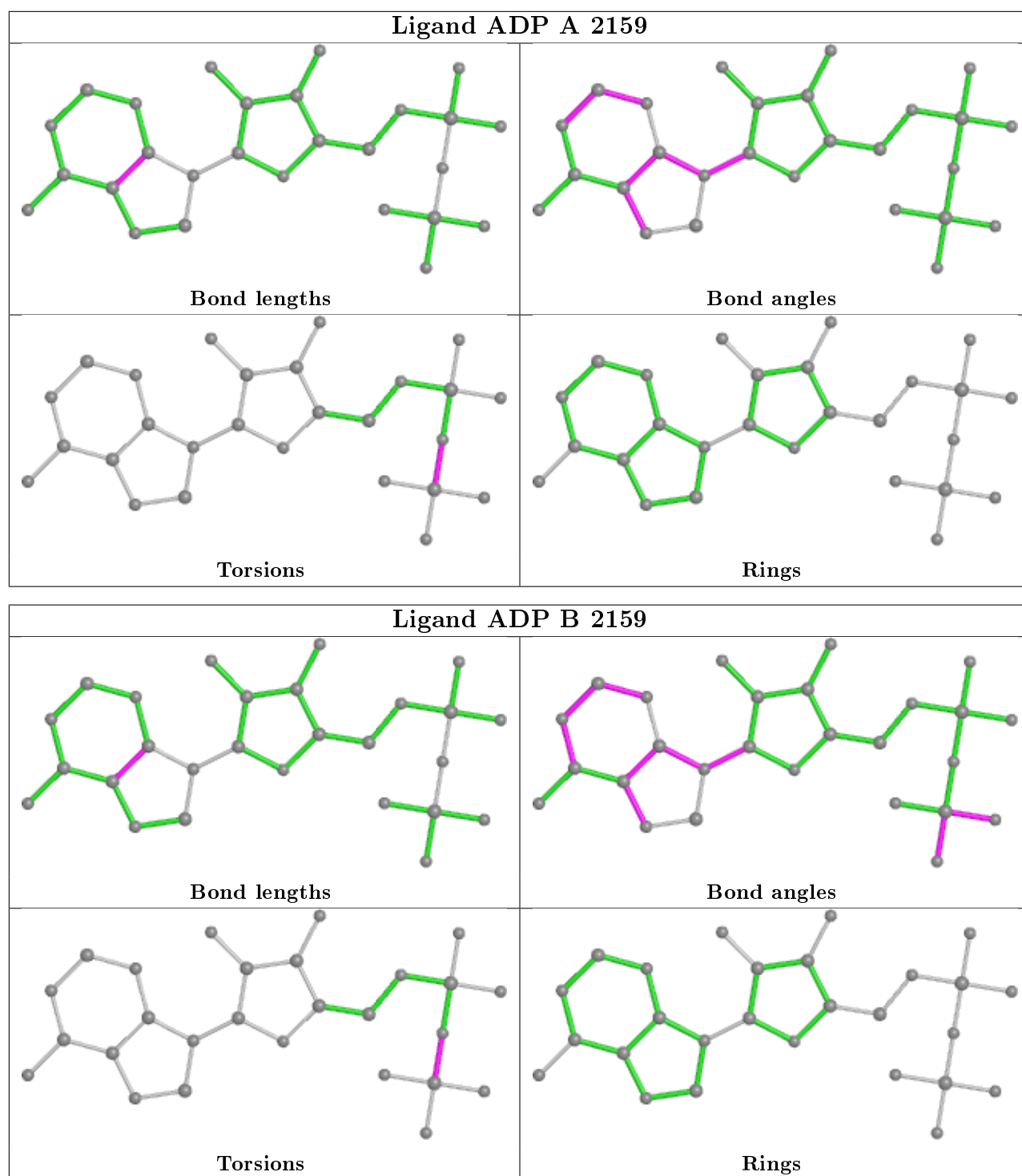
Mol	Chain	Res	Type	Atoms
6	A	2163	GOL	C1-C2-C3-O3
3	A	2159	ADP	PA-O3A-PB-O3B
6	B	2162	GOL	O1-C1-C2-C3
3	B	2159	ADP	PA-O3A-PB-O3B
6	B	2162	GOL	O1-C1-C2-O2
6	A	2163	GOL	O2-C2-C3-O3
3	A	2159	ADP	PA-O3A-PB-O2B
3	B	2159	ADP	PA-O3A-PB-O2B
6	B	2162	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.05	53 (5%) 26 31	22, 37, 83, 157	0
1	B	992/1293 (76%)	0.09	45 (4%) 33 37	22, 42, 79, 129	0
2	C	11/11 (100%)	0.18	0 100 100	33, 51, 126, 127	0
2	D	10/11 (90%)	0.26	1 (10%) 7 9	30, 56, 115, 139	0
All	All	2022/2608 (77%)	0.07	99 (4%) 29 34	22, 39, 80, 157	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	600	LEU	16.5
1	A	607	ALA	15.6
1	A	599	LEU	13.1
1	A	606	GLU	12.6
1	B	294	ILE	11.9
1	A	605	ASP	10.6
1	A	601	SER	10.5
1	A	595	ASP	9.7
1	A	603	ASP	9.6
1	A	598	GLN	9.2
1	A	593	VAL	8.1
1	A	597	GLU	7.3
1	A	322	GLU	6.6
1	A	589	LYS	6.4
1	A	591	LYS	6.4
1	A	602	GLU	6.3
1	B	254	LYS	6.3
1	A	348	LEU	5.9
1	A	292	ILE	5.7
1	B	296	LEU	5.6
1	A	902	ILE	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	590	ARG	5.3
1	A	350	THR	5.2
1	A	594	GLU	5.1
1	B	257	ASP	5.0
1	A	310	ILE	5.0
1	A	596	GLU	4.9
1	A	297	ASP	4.8
1	A	182	ASN	4.7
1	B	593	VAL	4.7
1	A	294	ILE	4.7
1	B	1040	ASN	4.6
1	A	254	LYS	4.4
1	A	308	SER	4.4
1	B	1042	ALA	4.3
1	B	256	LYS	4.3
1	A	588	ARG	4.2
1	B	325	VAL	4.1
1	B	289	PRO	4.1
1	A	295	GLU	4.0
1	A	592	GLU	4.0
1	B	292	ILE	3.9
1	B	290	ARG	3.9
1	B	334	ASN	3.8
1	B	255	LYS	3.8
1	A	323	SER	3.7
1	B	291	ASN	3.7
1	A	585	GLU	3.6
1	A	604	LYS	3.6
1	A	309	ARG	3.6
1	B	335	TRP	3.6
1	B	299	PRO	3.6
1	B	903	GLY	3.5
1	B	1041	LEU	3.5
1	B	298	GLY	3.4
1	B	295	GLU	3.4
1	B	848	ALA	3.4
1	A	296	LEU	3.4
1	A	126	LEU	3.3
1	A	608	GLU	3.3
1	A	184	ARG	3.2
1	A	291	ASN	3.2
1	B	249	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	290	ARG	3.1
1	A	124	ARG	3.1
1	B	598	GLN	3.1
1	B	599	LEU	3.0
1	B	902	ILE	3.0
1	A	346	GLY	2.9
1	B	288	ASN	2.8
1	B	293	LYS	2.8
1	A	587	ARG	2.8
2	D	10	U	2.8
1	B	329	ALA	2.7
1	B	600	LEU	2.7
1	A	1157	GLN	2.7
1	A	293	LYS	2.6
1	B	210	ALA	2.5
1	A	125	PRO	2.5
1	A	586	SER	2.5
1	B	258	GLU	2.4
1	A	195	GLU	2.4
1	B	694	ILE	2.4
1	A	609	ILE	2.4
1	B	597	GLU	2.4
1	B	139	VAL	2.3
1	B	905	ARG	2.3
1	B	906	ARG	2.3
1	B	283	ASP	2.3
1	A	1040	ASN	2.3
1	B	301	ILE	2.3
1	B	606	GLU	2.2
1	B	607	ALA	2.2
1	A	120	GLY	2.2
1	B	209	PRO	2.1
1	A	147	ARG	2.1
1	B	138	SER	2.1
1	B	300	PRO	2.1
1	B	269	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

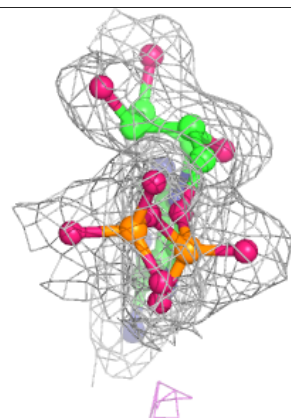
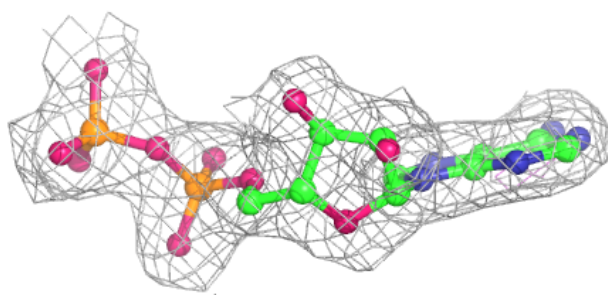
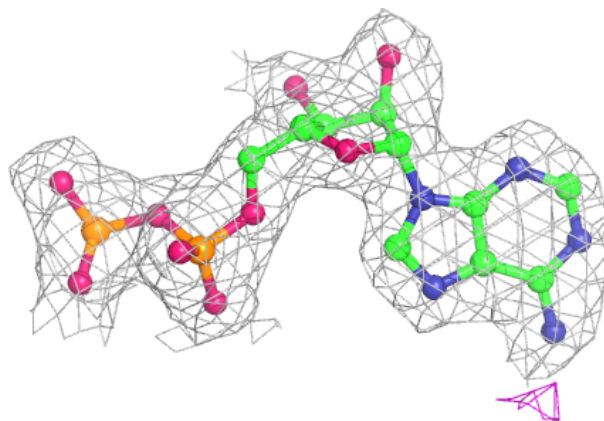
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	B	2162	6/6	0.79	0.27	63,68,73,75	0
6	GOL	A	2163	6/6	0.81	0.40	64,77,81,81	0
4	MG	A	2162	1/1	0.83	0.10	55,55,55,55	0
4	MG	B	2160	1/1	0.98	0.05	25,25,25,25	0
5	ALF	B	2161	5/5	0.98	0.09	22,24,26,27	0
3	ADP	A	2159	27/27	0.98	0.08	26,30,34,36	0
3	ADP	B	2159	27/27	0.99	0.08	18,25,33,35	0
5	ALF	A	2161	5/5	0.99	0.09	24,26,28,29	0
4	MG	A	2160	1/1	1.00	0.07	27,27,27,27	0

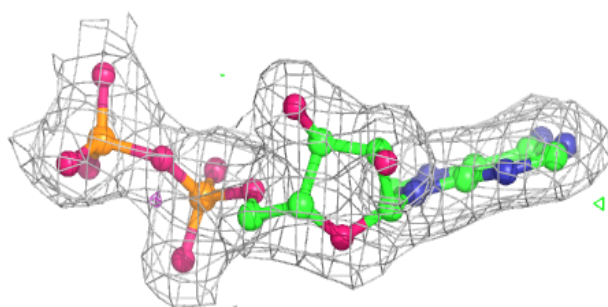
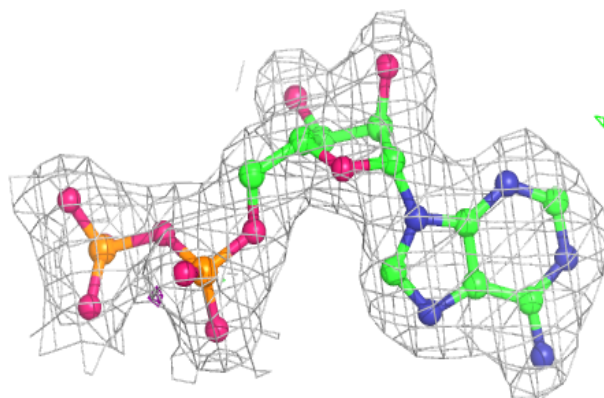
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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