



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 11:24 PM BST

PDB ID : 1OH7
Title : THE CRYSTAL STRUCTURE OF E. COLI MUTS BINDING TO DNA
WITH A G:G MISMATCH
Authors : Natrajan, G.; Lamers, M.H.; Enzlin, J.H.; Winterwerp, H.H.K.; Perrakis, A.;
Sixma, T.K.
Deposited on : 2003-05-23
Resolution : 2.50 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 : 2.13.1
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) : 2.13.1

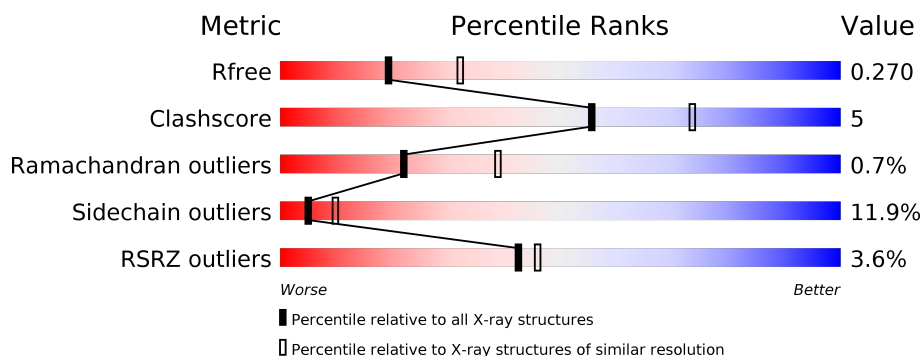
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	800	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>• •</div> </div> </div>
1	B	800	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>18%</div> <div>• 6%</div> </div> </div>
2	E	30	<div> <div>13%</div> <div> <div></div> <div>33%</div> <div>23%</div> <div>• 40%</div> </div> </div>
3	F	30	<div> <div>10%</div> <div> <div></div> <div>17%</div> <div>33%</div> <div>7%</div> <div>43%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13004 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 MUTS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	788	Total	C	N	O	S	0	0	0
			6207	3905	1103	1170	29			
1	B	754	Total	C	N	O	S	0	0	0
			5964	3756	1060	1120	28			

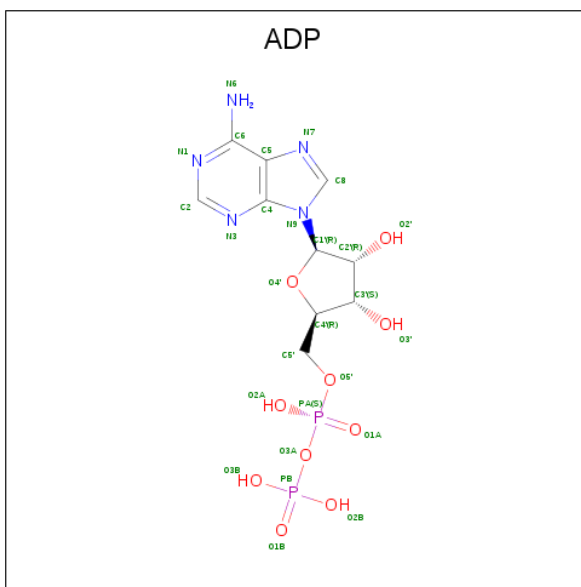
- Molecule 2 is a DNA chain called 5'-D(*AP*GP*CP*TP*GP*CP*CP*AP*GP*GP *CP*A P*CP*CP*AP*GP*TP*GP*TP*CP*AP*GP*CP*GP*TP *CP*CP*TP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	P	0	0	0
			367	174	72	104	17			

- Molecule 3 is a DNA chain called 5'-D(*AP*TP*AP*GP*GP*AP*CP*GP*CP*TP *GP*A P*CP*AP*CP*TP*GP*GP*TP*GP*CP*GP*TP*GP*GP *CP*AP*GP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	17	Total	C	N	O	P	0	0	0
			349	166	65	102	16			

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

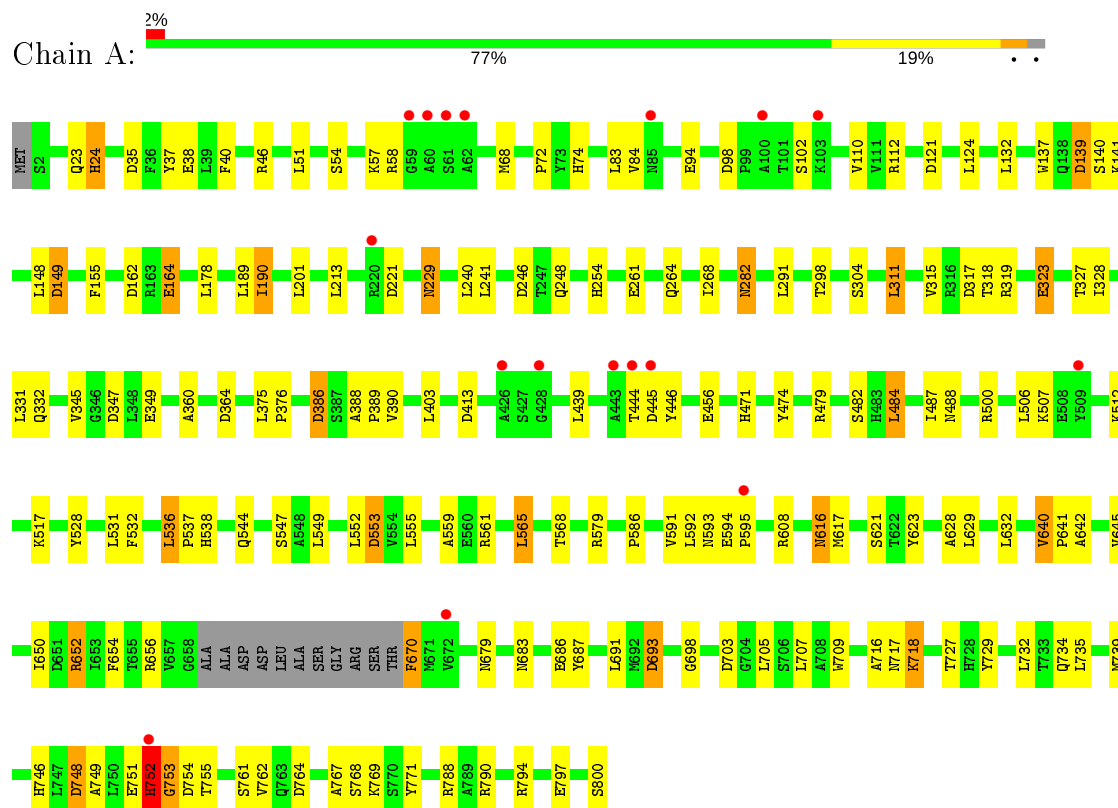
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	46	Total	O	0	0
			46	46		
6	B	41	Total	O	0	0
			41	41		
6	F	2	Total	O	0	0
			2	2		

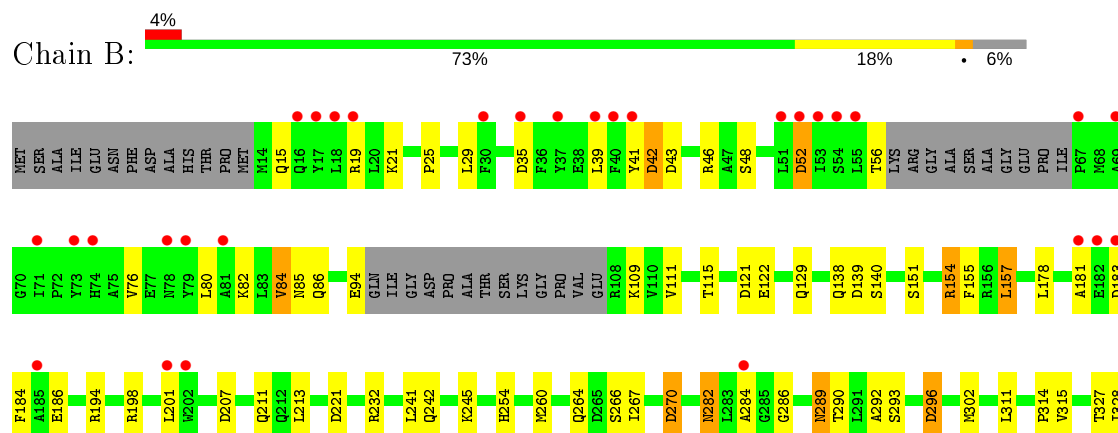
3 Residue-property plots

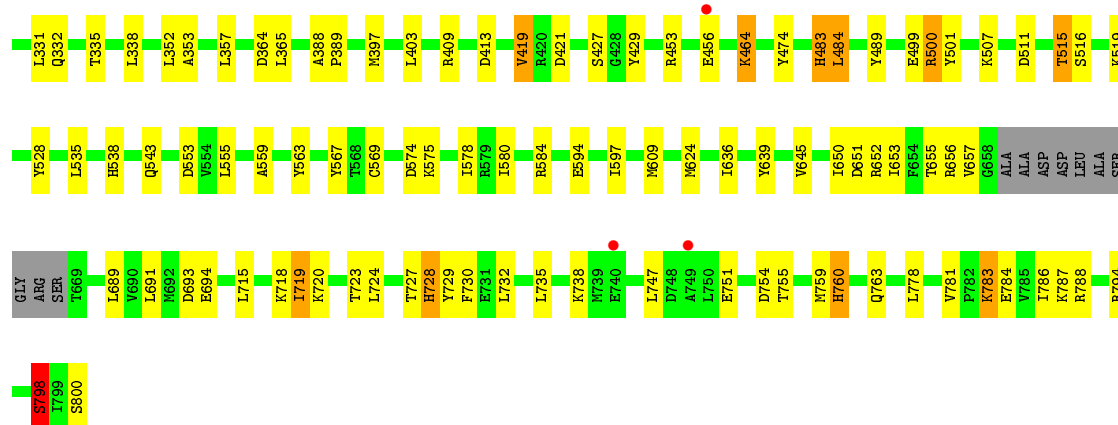
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

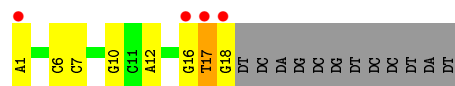
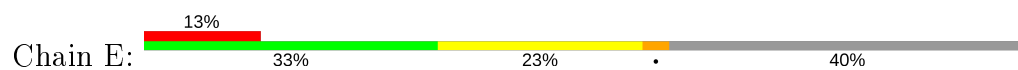


• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS





- Molecule 2: 5'-D(*AP*GP*CP*TP*GP*CP*CP*AP*GP*GP *CP*AP*CP*CP*AP*GP*TP*GP*TP*CP*AP*GP*CP*GP*TP *CP*CP*TP*AP*T)-3'



- Molecule 3: 5'-D(*AP*TP*AP*GP*GP*AP*CP*GP*CP*TP *GP*AP*CP*AP*CP*TP*GP*GP*TP*GP*CP*GP*TP*GP*GP *CP*AP*GP*CP*T)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.41Å 91.81Å 260.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 39.75 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.5 (15.00-2.50) 91.5 (39.75-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.228 , 0.276 0.230 , 0.270	Depositor DCC
R_{free} test set	1335 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13004	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: 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	0.65	1/6313 (0.0%)	0.86	16/8544 (0.2%)
1	B	0.62	0/6062	0.86	16/8199 (0.2%)
2	E	1.04	1/412 (0.2%)	1.70	7/634 (1.1%)
3	F	1.06	1/391 (0.3%)	1.90	15/603 (2.5%)
All	All	0.67	3/13178 (0.0%)	0.96	54/17980 (0.3%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	16	DT	C1'-N1	5.51	1.56	1.49
1	A	315	VAL	CB-CG1	5.36	1.64	1.52
2	E	10	DG	C3'-O3'	-5.04	1.37	1.44

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	22	DG	O4'-C1'-N9	-14.30	97.99	108.00
2	E	17	DT	O4'-C1'-N1	10.70	115.49	108.00
1	A	693	ASP	CB-CG-OD2	9.39	126.75	118.30
2	E	7	DC	O4'-C1'-N1	-8.90	101.77	108.00
3	F	20	DG	O4'-C1'-N9	8.14	113.70	108.00
1	B	754	ASP	CB-CG-OD2	8.03	125.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	553	ASP	CB-CG-OD2	7.78	125.31	118.30
3	F	20	DG	P-O3'-C3'	7.77	129.02	119.70
3	F	27	DA	O4'-C1'-N9	-7.57	102.70	108.00
1	A	553	ASP	CB-CG-OD2	7.30	124.87	118.30
1	A	413	ASP	CB-CG-OD2	6.97	124.57	118.30
1	A	364	ASP	CB-CG-OD2	6.93	124.54	118.30
1	B	270	ASP	CB-CG-OD2	6.86	124.48	118.30
1	A	246	ASP	CB-CG-OD2	6.82	124.44	118.30
1	A	221	ASP	CB-CG-OD2	6.70	124.33	118.30
1	B	221	ASP	CB-CG-OD2	6.38	124.04	118.30
1	B	364	ASP	CB-CG-OD2	6.36	124.03	118.30
3	F	23	DT	C5-C4-O4	-6.27	120.51	124.90
2	E	17	DT	O4'-C4'-C3'	-6.22	102.01	104.50
1	B	157	LEU	CA-CB-CG	6.21	129.57	115.30
1	B	183	ASP	CB-CG-OD2	6.18	123.87	118.30
3	F	30	DT	C1'-O4'-C4'	-5.90	104.20	110.10
1	A	754	ASP	CB-CG-OD2	5.85	123.57	118.30
1	A	748	ASP	CB-CG-OD2	5.81	123.53	118.30
3	F	15	DC	O4'-C1'-N1	5.69	111.98	108.00
1	A	139	ASP	CB-CG-OD2	5.59	123.33	118.30
3	F	18	DG	O4'-C4'-C3'	-5.57	102.27	104.50
1	B	651	ASP	CB-CG-OD2	5.55	123.29	118.30
1	A	162	ASP	CB-CG-OD2	5.54	123.29	118.30
2	E	1	DA	O4'-C1'-N9	5.52	111.86	108.00
1	B	413	ASP	CB-CG-OD2	5.43	123.19	118.30
2	E	12	DA	O4'-C1'-N9	5.43	111.80	108.00
3	F	26	DC	O4'-C1'-N1	5.43	111.80	108.00
1	B	52	ASP	CB-CG-OD2	5.37	123.14	118.30
1	B	569	CYS	CA-CB-SG	-5.37	104.34	114.00
2	E	6	DC	C2-N3-C4	5.37	122.58	119.90
1	B	296	ASP	CB-CG-OD2	5.37	123.13	118.30
3	F	19	DT	C6-C5-C7	-5.32	119.71	122.90
1	A	98	ASP	CB-CG-OD2	5.30	123.07	118.30
3	F	23	DT	N3-C4-O4	5.30	123.08	119.90
3	F	23	DT	OP1-P-OP2	5.30	127.55	119.60
1	A	317	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	121	ASP	CB-CG-OD2	5.29	123.06	118.30
3	F	14	DA	O4'-C1'-N9	5.28	111.69	108.00
1	B	42	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	764	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	386	ASP	CB-CG-OD2	5.26	123.03	118.30
2	E	16	DG	O4'-C1'-N9	5.12	111.58	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	30	DT	O4'-C1'-C2'	-5.10	101.82	105.90
1	A	347	ASP	CB-CG-OD2	5.09	122.89	118.30
1	B	207	ASP	CB-CG-OD2	5.09	122.88	118.30
3	F	28	DG	N3-C4-N9	-5.07	122.96	126.00
1	A	579	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	B	35	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	189	LEU	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	6207	0	6251	71	0
1	B	5964	0	6018	58	0
2	E	367	0	202	1	0
3	F	349	0	193	2	0
4	A	27	0	12	0	0
5	A	1	0	0	0	0
6	A	46	0	0	5	0
6	B	41	0	0	1	0
6	F	2	0	0	0	0
All	All	13004	0	12676	130	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 5.

All (130) 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:794:ARG:O	1:B:798:SER:HB2	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:760:HIS:ND1	6:B:2036:HOH:O	2.17	0.76
1:A:727:THR:HG22	1:A:729:TYR:H	1.52	0.73
1:A:652:ARG:HD2	1:A:654:PHE:CZ	2.28	0.69
1:B:511:ASP:O	1:B:515:THR:OG1	2.10	0.68
1:B:656:ARG:O	1:B:656:ARG:HG3	1.96	0.66
1:A:718:LYS:HD3	6:A:2039:HOH:O	1.97	0.65
1:B:282:ASN:HD22	1:B:284:ALA:H	1.49	0.59
1:B:327:THR:HG21	1:B:555:LEU:HD13	1.84	0.59
1:A:670:PHE:N	1:A:670:PHE:CD2	2.70	0.58
1:B:254:HIS:HB2	1:B:543:GLN:NE2	2.18	0.58
1:A:37:TYR:OH	1:A:94:GLU:OE2	2.21	0.58
1:A:327:THR:HG23	1:A:390:VAL:HG22	1.87	0.56
1:A:749:ALA:HB3	1:A:771:TYR:CE2	2.40	0.56
1:A:705:LEU:CD1	1:A:732:LEU:HD21	2.36	0.56
1:B:328:ILE:HG23	1:B:559:ALA:HA	1.88	0.56
1:A:727:THR:HG21	1:A:732:LEU:HD12	1.89	0.55
1:B:151:SER:O	1:B:353:ALA:HB2	2.06	0.55
1:A:727:THR:HG22	1:A:729:TYR:N	2.21	0.54
1:B:332:GLN:HE21	1:B:563:TYR:HD1	1.54	0.54
1:A:632:LEU:C	1:A:632:LEU:HD23	2.29	0.54
1:B:567:TYR:HB3	1:B:639:TYR:HB3	1.89	0.54
1:B:419:VAL:HG11	1:B:528:TYR:CD2	2.43	0.54
1:B:82:LYS:O	1:B:86:GLN:HG3	2.08	0.54
1:A:148:LEU:HB3	1:A:240:LEU:HD21	1.90	0.53
1:A:72:PRO:HB2	1:A:74:HIS:CE1	2.44	0.53
1:A:474:TYR:HB2	1:A:500:ARG:HB3	1.91	0.52
1:B:311:LEU:HD23	1:B:636:ILE:HD13	1.89	0.52
1:B:655:THR:O	1:B:655:THR:OG1	2.27	0.52
1:A:38:GLU:OE2	3:F:22:DG:N7	2.43	0.52
1:A:282:ASN:HD22	1:A:282:ASN:C	2.13	0.52
1:A:268:ILE:HB	1:A:652:ARG:HG2	1.91	0.51
1:A:586:PRO:HG3	1:A:641:PRO:HG3	1.92	0.51
1:A:698:GLY:HA3	1:A:703:ASP:HB3	1.92	0.51
1:A:229:ASN:ND2	6:A:2016:HOH:O	2.33	0.51
1:B:728:HIS:HE1	1:B:729:TYR:CE2	2.29	0.51
1:A:375:LEU:N	1:A:376:PRO:CD	2.74	0.50
1:A:213:LEU:HD23	1:A:241:LEU:HD22	1.94	0.50
1:B:403:LEU:HD11	1:B:538:HIS:HD2	1.77	0.50
1:A:291:LEU:HD13	1:A:629:LEU:HD22	1.92	0.50
1:B:267:ILE:HB	1:B:314:PRO:HG2	1.94	0.49
1:A:640:VAL:HG11	1:A:645:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:THR:HG22	1:A:331:LEU:HD12	1.93	0.49
1:A:23:GLN:CB	1:A:24:HIS:CE1	2.95	0.49
1:A:752:HIS:HE1	1:A:755:THR:HG23	1.77	0.49
1:B:80:LEU:O	1:B:84:VAL:HB	2.13	0.49
1:B:282:ASN:ND2	1:B:286:GLY:H	2.11	0.49
1:A:752:HIS:CE1	1:A:755:THR:HG23	2.48	0.48
1:A:132:LEU:HD23	1:A:149:ASP:HB2	1.96	0.48
1:A:40:PHE:CE1	1:A:68:MET:HG3	2.49	0.48
1:A:752:HIS:O	1:A:753:GLY:C	2.52	0.48
1:A:767:ALA:HB3	6:A:2043:HOH:O	2.13	0.48
1:B:715:LEU:HD23	1:B:719:ILE:HD12	1.96	0.48
1:B:691:LEU:CD2	1:B:724:LEU:HD12	2.44	0.47
1:A:446:TYR:C	1:A:446:TYR:CD1	2.87	0.47
1:B:289:ASN:N	1:B:289:ASN:HD22	2.12	0.47
1:A:148:LEU:CB	1:A:240:LEU:HD21	2.45	0.47
1:A:623:TYR:CD1	1:A:762:VAL:HG21	2.50	0.47
1:B:483:HIS:CE1	1:B:484:LEU:HD21	2.50	0.47
1:A:323:GLU:HG3	1:A:389:PRO:HG3	1.97	0.47
1:B:694:GLU:HG2	1:B:727:THR:HA	1.96	0.47
1:B:474:TYR:CE1	1:B:500:ARG:HD2	2.50	0.47
1:A:735:LEU:CD2	1:A:739:MET:HG3	2.44	0.47
1:A:23:GLN:HB3	1:A:24:HIS:CE1	2.50	0.46
1:A:471:HIS:CD2	1:A:471:HIS:N	2.83	0.46
1:A:240:LEU:C	1:A:240:LEU:HD23	2.36	0.46
1:A:621:SER:OG	1:A:693:ASP:OD2	2.33	0.46
1:B:732:LEU:O	1:B:735:LEU:HB2	2.15	0.46
1:B:388:ALA:N	1:B:389:PRO:CD	2.78	0.46
1:A:628:ALA:HB2	1:A:691:LEU:HD11	1.95	0.46
1:A:23:GLN:HB2	1:A:24:HIS:CE1	2.50	0.46
1:A:121:ASP:HB2	1:A:124:LEU:HD12	1.96	0.46
1:A:616:ASN:O	1:A:617:MET:HB2	2.16	0.46
1:A:132:LEU:CD2	1:A:149:ASP:HB2	2.45	0.46
1:B:597:ILE:HB	1:B:760:HIS:HB3	1.98	0.46
1:B:728:HIS:CE1	1:B:729:TYR:CZ	3.04	0.45
1:A:594:GLU:HB2	1:A:595:PRO:HD2	1.99	0.45
1:A:751:GLU:C	1:A:752:HIS:O	2.54	0.45
1:B:728:HIS:HE1	1:B:729:TYR:CZ	2.34	0.45
1:B:409:ARG:O	1:B:429:TYR:HB2	2.16	0.45
1:B:578:ILE:HD11	1:B:689:LEU:HD13	1.97	0.45
1:A:164:GLU:HG3	1:A:679:ASN:CG	2.37	0.45
1:A:652:ARG:HG3	1:A:652:ARG:HH11	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:THR:O	1:B:293:SER:OG	2.30	0.45
1:B:267:ILE:HG21	1:B:653:ILE:HD12	1.98	0.45
1:A:608:ARG:NH1	1:A:716:ALA:O	2.50	0.45
1:A:51:LEU:HD21	1:A:83:LEU:HD21	1.98	0.45
1:A:650:ILE:HA	1:A:687:TYR:O	2.16	0.45
1:B:39:LEU:HD23	1:B:43:ASP:HB3	1.99	0.45
1:A:328:ILE:HG23	1:A:559:ALA:HA	2.00	0.44
1:A:623:TYR:CE1	1:A:762:VAL:HG21	2.52	0.44
1:B:292:ALA:O	1:B:296:ASP:CB	2.65	0.44
1:B:489:TYR:HB3	1:B:501:TYR:CD2	2.53	0.44
1:A:561:ARG:HD3	1:A:565:LEU:HD11	2.00	0.43
1:A:327:THR:HG21	1:A:555:LEU:HD13	2.00	0.43
1:A:360:ALA:O	1:A:528:TYR:OH	2.33	0.43
1:B:181:ALA:O	1:B:184:PHE:HB2	2.19	0.43
1:B:787:LYS:HE3	1:B:787:LYS:HB3	1.89	0.43
1:A:345:VAL:HG11	1:A:549:LEU:HD13	2.01	0.43
1:B:290:THR:HG23	1:B:293:SER:H	1.84	0.43
1:A:298:THR:HB	1:A:553:ASP:OD2	2.19	0.43
1:B:474:TYR:CD1	1:B:500:ARG:HD2	2.54	0.43
1:A:532:PHE:O	1:A:536:LEU:HB2	2.19	0.42
1:A:536:LEU:N	1:A:537:PRO:CD	2.83	0.42
1:B:609:MET:HE2	1:B:723:THR:HB	2.02	0.42
1:B:580:ILE:HG12	1:B:645:VAL:HG22	2.01	0.42
1:B:781:VAL:HB	1:B:786:ILE:HD11	2.01	0.42
1:B:655:THR:HG22	1:B:691:LEU:HD12	2.01	0.42
1:B:656:ARG:O	1:B:656:ARG:CG	2.65	0.42
1:A:388:ALA:N	1:A:389:PRO:CD	2.82	0.41
1:B:515:THR:HB	1:B:519:LYS:HZ2	1.86	0.41
1:B:464:LYS:NZ	3:F:19:DT:OP1	2.54	0.41
1:A:482:SER:C	1:A:484:LEU:H	2.23	0.41
1:B:624:MET:HE2	1:B:691:LEU:HB3	2.02	0.41
1:B:657:VAL:HA	1:B:693:ASP:HB2	2.01	0.41
1:A:132:LEU:HG	6:A:2012:HOH:O	2.20	0.41
1:A:291:LEU:HD23	1:A:311:LEU:HG	2.02	0.41
1:B:21:LYS:NZ	1:B:41:TYR:O	2.54	0.41
6:A:2036:HOH:O	1:B:730:PHE:HB3	2.21	0.41
1:A:568:THR:HG23	1:A:642:ALA:O	2.21	0.41
1:B:728:HIS:CE1	1:B:729:TYR:CE2	3.08	0.41
2:E:17:DT:H2''	2:E:18:DG:O5'	2.21	0.41
1:A:403:LEU:HD21	1:A:538:HIS:ND1	2.36	0.40
1:B:138:GLN:HE22	1:B:186:GLU:HG3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:LEU:HD23	1:B:241:LEU:HD22	2.03	0.40
1:B:515:THR:HB	1:B:519:LYS:NZ	2.36	0.40
1:A:24:HIS:CE1	1:A:110:VAL:HG21	2.57	0.40
1:A:679:ASN:OD1	1:A:683:ASN:ND2	2.55	0.40
1:A:709:TRP:CD1	1:A:709:TRP:C	2.95	0.40
1:B:331:LEU:O	1:B:332:GLN:C	2.58	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	784/800 (98%)	737 (94%)	42 (5%)	5 (1%)	25	43
1	B	746/800 (93%)	706 (95%)	35 (5%)	5 (1%)	22	39
All	All	1530/1600 (96%)	1443 (94%)	77 (5%)	10 (1%)	22	39

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	444	THR
1	A	753	GLY
1	B	798	SER
1	A	229	ASN
1	A	752	HIS
1	B	154	ARG
1	B	718	LYS
1	B	783	LYS
1	B	25	PRO
1	A	190	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	656/664 (99%)	583 (89%)	73 (11%)	6	11
1	B	631/664 (95%)	551 (87%)	80 (13%)	4	8
All	All	1287/1328 (97%)	1134 (88%)	153 (12%)	5	10

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	35	ASP
1	A	46	ARG
1	A	54	SER
1	A	57	LYS
1	A	58	ARG
1	A	84	VAL
1	A	102	SER
1	A	112	ARG
1	A	137	TRP
1	A	139	ASP
1	A	140	SER
1	A	141	LYS
1	A	149	ASP
1	A	155	PHE
1	A	164	GLU
1	A	178	LEU
1	A	190	ILE
1	A	201	LEU
1	A	248	GLN
1	A	254	HIS
1	A	261	GLU
1	A	264	GLN
1	A	282	ASN
1	A	304	SER
1	A	311	LEU
1	A	318	THR

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Mol	Chain	Res	Type
1	A	319	ARG
1	A	323	GLU
1	A	332	GLN
1	A	349	GLU
1	A	386	ASP
1	A	439	LEU
1	A	445	ASP
1	A	456	GLU
1	A	479	ARG
1	A	484	LEU
1	A	487	ILE
1	A	488	ASN
1	A	506	LEU
1	A	507	LYS
1	A	512	LYS
1	A	517	LYS
1	A	531	LEU
1	A	536	LEU
1	A	544	GLN
1	A	547	SER
1	A	552	LEU
1	A	565	LEU
1	A	591	VAL
1	A	592	LEU
1	A	593	ASN
1	A	616	ASN
1	A	640	VAL
1	A	652	ARG
1	A	656	ARG
1	A	670	PHE
1	A	686	GLU
1	A	707	LEU
1	A	717	ASN
1	A	718	LYS
1	A	734	GLN
1	A	746	HIS
1	A	748	ASP
1	A	752	HIS
1	A	761	SER
1	A	768	SER
1	A	769	LYS
1	A	788	ARG

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Mol	Chain	Res	Type
1	A	790	ARG
1	A	794	ARG
1	A	797	GLU
1	A	800	SER
1	B	15	GLN
1	B	19	ARG
1	B	29	LEU
1	B	42	ASP
1	B	46	ARG
1	B	48	SER
1	B	52	ASP
1	B	56	THR
1	B	76	VAL
1	B	84	VAL
1	B	85	ASN
1	B	94	GLU
1	B	109	LYS
1	B	111	VAL
1	B	115	THR
1	B	122	GLU
1	B	129	GLN
1	B	139	ASP
1	B	140	SER
1	B	154	ARG
1	B	155	PHE
1	B	157	LEU
1	B	178	LEU
1	B	194	ARG
1	B	198	ARG
1	B	201	LEU
1	B	211	GLN
1	B	232	ARG
1	B	242	GLN
1	B	245	LYS
1	B	260	MET
1	B	264	GLN
1	B	266	SER
1	B	270	ASP
1	B	282	ASN
1	B	289	ASN
1	B	302	MET
1	B	315	VAL

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Mol	Chain	Res	Type
1	B	335	THR
1	B	338	LEU
1	B	352	LEU
1	B	357	LEU
1	B	365	LEU
1	B	397	MET
1	B	419	VAL
1	B	421	ASP
1	B	427	SER
1	B	453	ARG
1	B	456	GLU
1	B	464	LYS
1	B	483	HIS
1	B	484	LEU
1	B	499	GLU
1	B	500	ARG
1	B	507	LYS
1	B	515	THR
1	B	516	SER
1	B	535	LEU
1	B	574	ASP
1	B	575	LYS
1	B	584	ARG
1	B	594	GLU
1	B	650	ILE
1	B	652	ARG
1	B	719	ILE
1	B	720	LYS
1	B	728	HIS
1	B	738	LYS
1	B	747	LEU
1	B	751	GLU
1	B	755	THR
1	B	759	MET
1	B	760	HIS
1	B	763	GLN
1	B	778	LEU
1	B	783	LYS
1	B	784	GLU
1	B	788	ARG
1	B	798	SER
1	B	800	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	24	HIS
1	A	49	GLN
1	A	174	ASN
1	A	282	ASN
1	A	312	HIS
1	A	332	GLN
1	A	471	HIS
1	A	488	ASN
1	A	543	GLN
1	A	746	HIS
1	A	752	HIS
1	A	791	GLN
1	B	74	HIS
1	B	126	GLN
1	B	129	GLN
1	B	242	GLN
1	B	282	ASN
1	B	289	ASN
1	B	538	HIS
1	B	714	ASN
1	B	791	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	ADP	A	1801	5	24,29,29	1.19	2 (8%)	29,45,45	1.57	4 (13%)

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
4	ADP	A	1801	5	-	3/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1801	ADP	C2-N3	4.04	1.38	1.32
4	A	1801	ADP	C2-N1	2.44	1.38	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1801	ADP	N3-C2-N1	-5.96	119.36	128.68
4	A	1801	ADP	C3'-C2'-C1'	3.32	105.98	100.98
4	A	1801	ADP	PA-O3A-PB	-3.31	121.48	132.83
4	A	1801	ADP	O3B-PB-O3A	2.15	111.85	104.64

There are no chirality outliers.

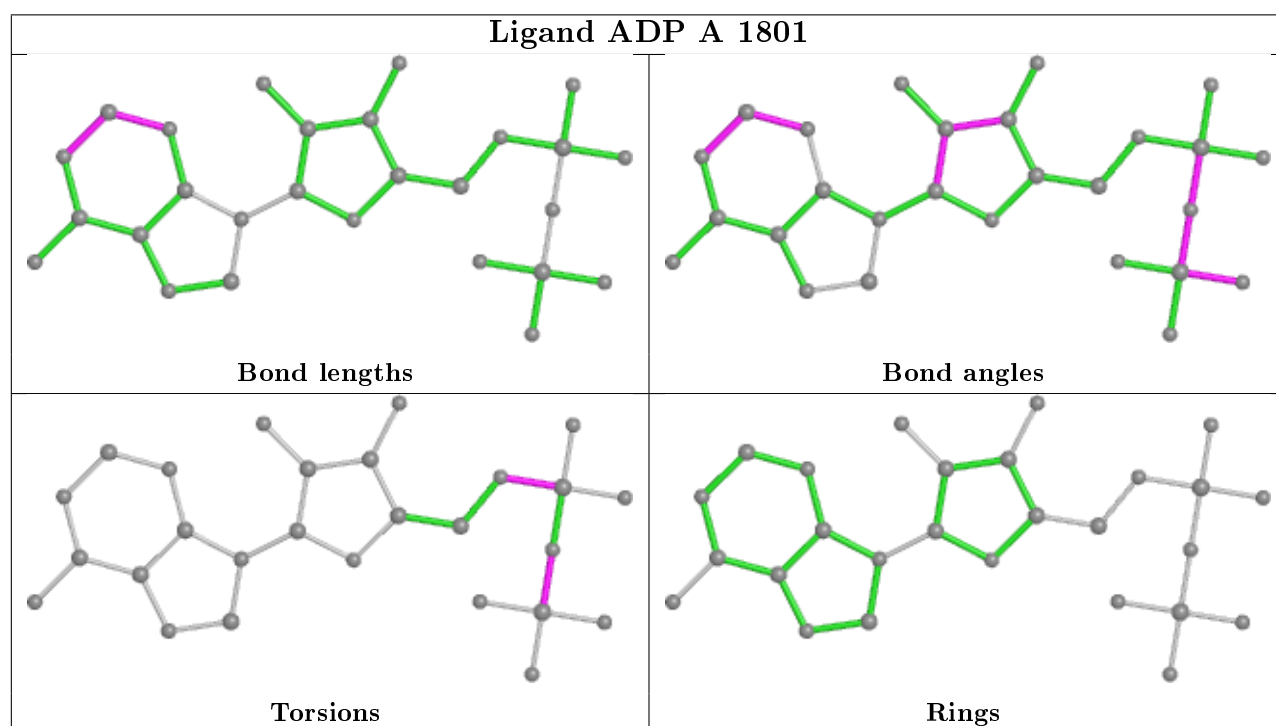
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1801	ADP	PA-O3A-PB-O2B
4	A	1801	ADP	PA-O3A-PB-O1B
4	A	1801	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

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	788/800 (98%)	0.08	17 (2%) 62 65	8, 21, 28, 42	0
1	B	754/800 (94%)	0.29	33 (4%) 34 37	8, 21, 28, 34	0
2	E	18/30 (60%)	0.76	4 (22%) 0 0	13, 22, 36, 43	0
3	F	17/30 (56%)	0.51	3 (17%) 1 1	11, 24, 35, 38	0
All	All	1577/1660 (95%)	0.20	57 (3%) 42 46	8, 21, 29, 43	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	THR	7.0
2	E	18	DG	6.3
1	A	443	ALA	5.6
1	A	103	LYS	5.5
1	B	54	SER	5.1
1	B	74	HIS	5.0
3	F	14	DA	4.7
1	B	78	ASN	4.7
1	B	53	ILE	4.6
1	B	52	ASP	4.5
3	F	15	DC	4.3
1	B	41	TYR	4.3
1	B	79	TYR	4.3
1	B	185	ALA	4.2
1	A	61	SER	4.1
2	E	17	DT	4.0
2	E	1	DA	3.9
1	B	81	ALA	3.8
1	A	59	GLY	3.8
1	B	17	TYR	3.8
1	B	73	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	51	LEU	3.5
1	B	69	ALA	3.4
1	B	456	GLU	3.4
2	E	16	DG	3.3
1	B	183	ASP	3.3
1	A	509	TYR	3.2
1	B	202	TRP	3.2
1	B	16	GLN	3.0
1	B	37	TYR	3.0
1	B	35	ASP	3.0
1	B	19	ARG	2.9
1	B	71	ILE	2.9
1	B	67	PRO	2.9
1	B	40	PHE	2.7
1	B	55	LEU	2.7
3	F	16	DT	2.7
1	A	672	VAL	2.6
1	A	220	ARG	2.5
1	B	181	ALA	2.5
1	B	201	LEU	2.5
1	B	284	ALA	2.4
1	A	60	ALA	2.4
1	A	426	ALA	2.4
1	A	428	GLY	2.3
1	B	30	PHE	2.3
1	A	100	ALA	2.2
1	A	595	PRO	2.2
1	A	62	ALA	2.2
1	A	85	ASN	2.2
1	B	749	ALA	2.2
1	B	182	GLU	2.2
1	A	445	ASP	2.2
1	B	18	LEU	2.2
1	B	39	LEU	2.2
1	B	740	GLU	2.2
1	A	752	HIS	2.1

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](#)

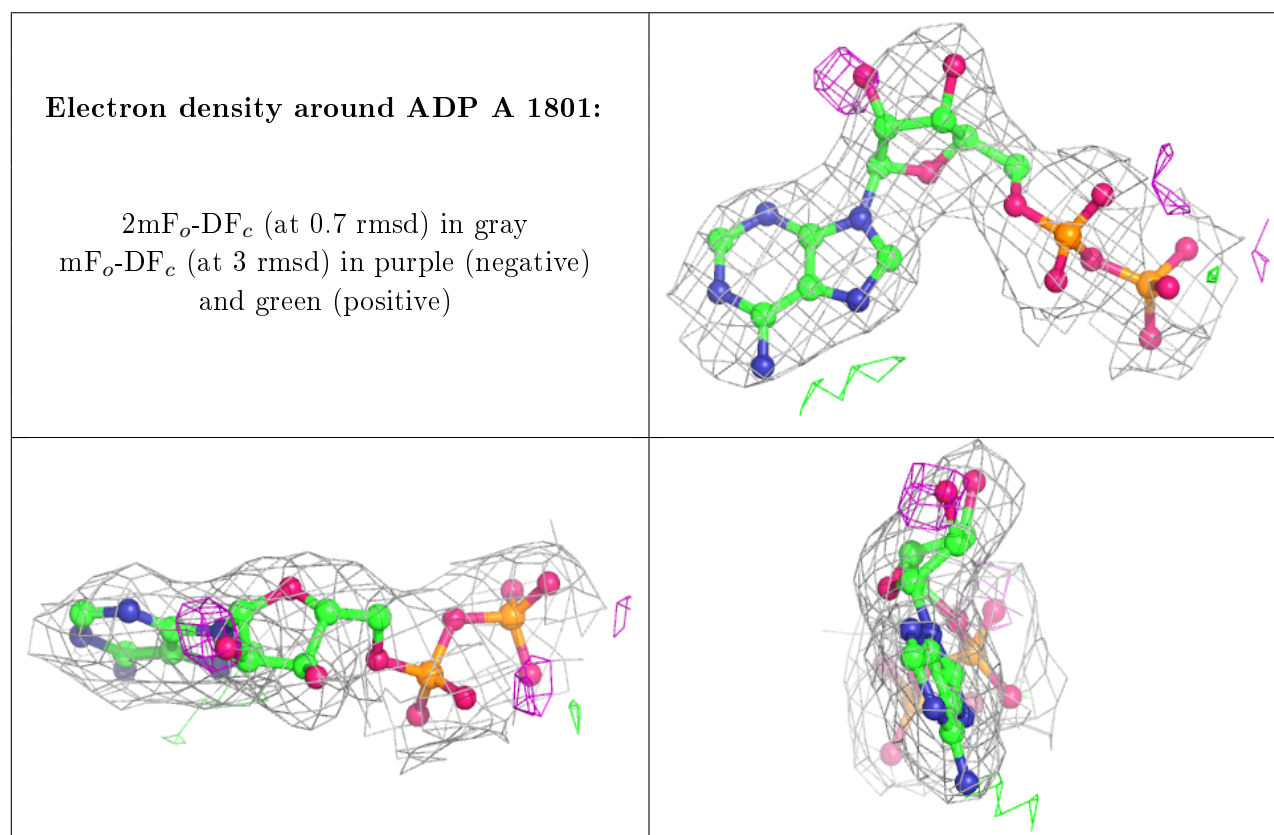
There are no monosaccharides in this entry.

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
5	MG	A	1802	1/1	0.86	0.15	15,15,15,15	0
4	ADP	A	1801	27/27	0.96	0.12	15,17,20,20	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.