



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 09:42 PM BST

PDB ID : 1OH8
Title : THE CRYSTAL STRUCTURE OF E. COLI MUTS BINDING TO DNA
WITH AN UNPAIRED THYMIDINE
Authors : Natrajan, G.; Lamers, M.H.; Enzlin, J.H.; Winterwerp, H.H.K.; Perrakis, A.;
Sixma, T.K.
Deposited on : 2003-05-23
Resolution : 2.90 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

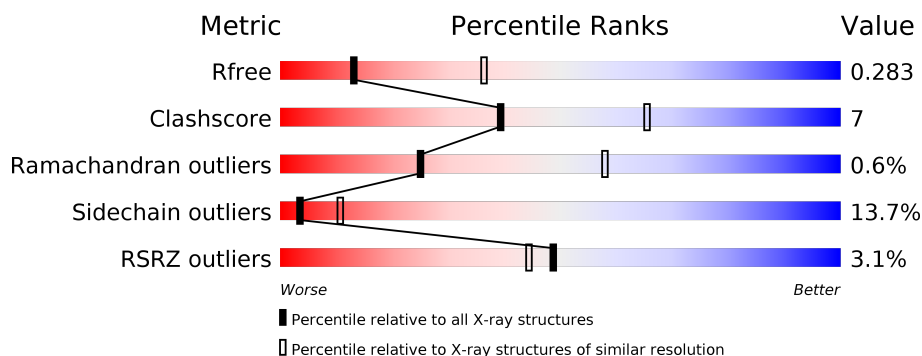
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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>3%</div> <div>71%</div> <div>24%</div> <div>• •</div> </div>
1	B	800	<div> <div>3%</div> <div>70%</div> <div>21%</div> <div>• 6%</div> </div>
2	E	30	<div> <div>7%</div> <div>30%</div> <div>17%</div> <div>53%</div> </div>
3	F	31	<div> <div>3%</div> <div>19%</div> <div>13%</div> <div>13%</div> <div>55%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12905 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			

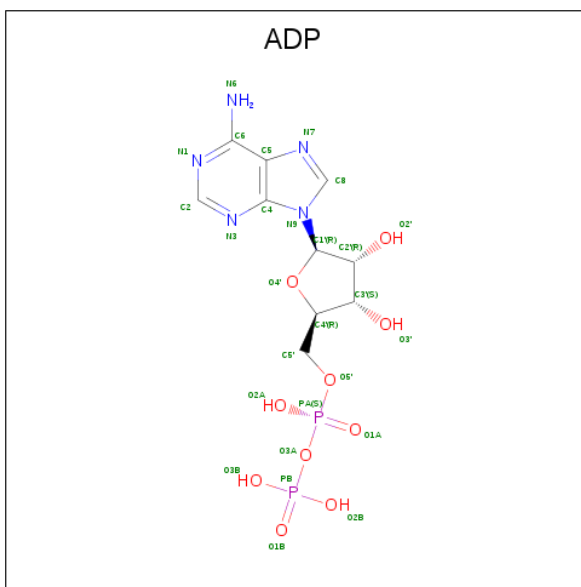
- Molecule 2 is a DNA chain called 5'-D(*AP*GP*CP*TP*GP*CP*CP*AP*GP*GP *CP*A P*CP*CP*AP*GP*TP*GP*TP*CP*AP*GP*CP*GP*TP*CP*CP* TP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	P	0	0	0
			282	134	55	80	13			

- 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*CP*TP*TP*GP*GP*CP* AP*GP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	14	Total	C	N	O	P	0	0	0
			287	136	50	87	14			

- 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	
			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		
			1	1	0	0

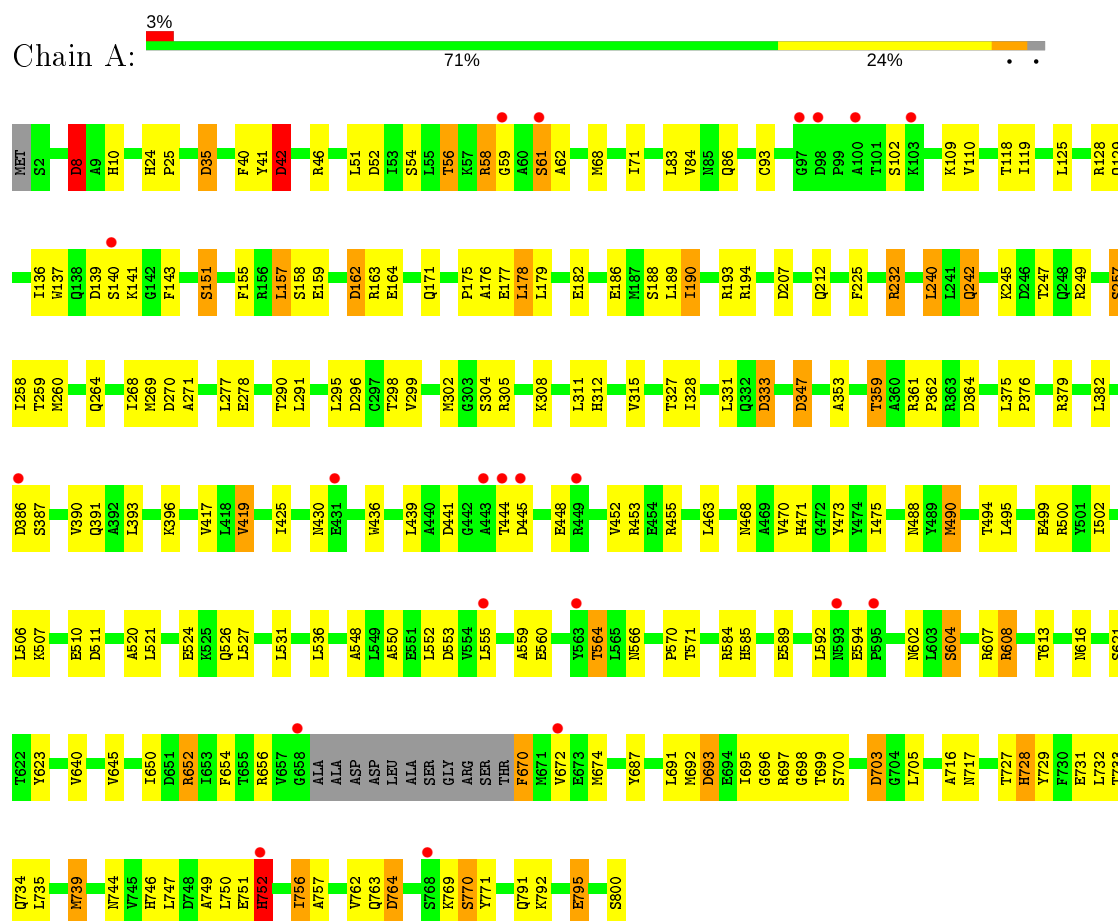
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	80	Total	O		
			80	80	0	0
6	B	56	Total	O		
			56	56	0	0
6	E	1	Total	O		
			1	1	0	0

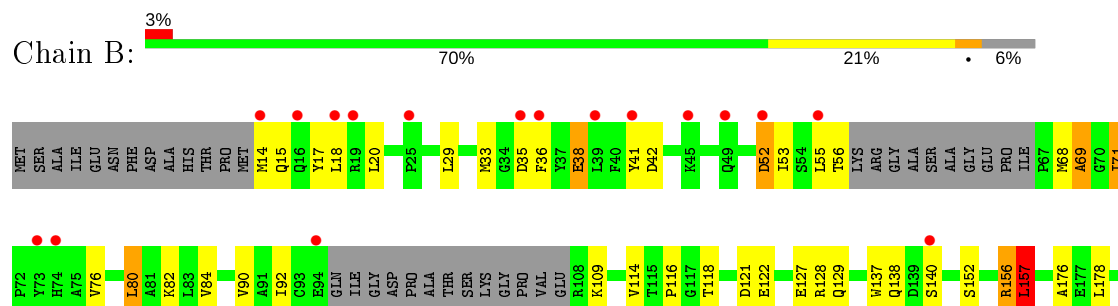
3 Residue-property plots

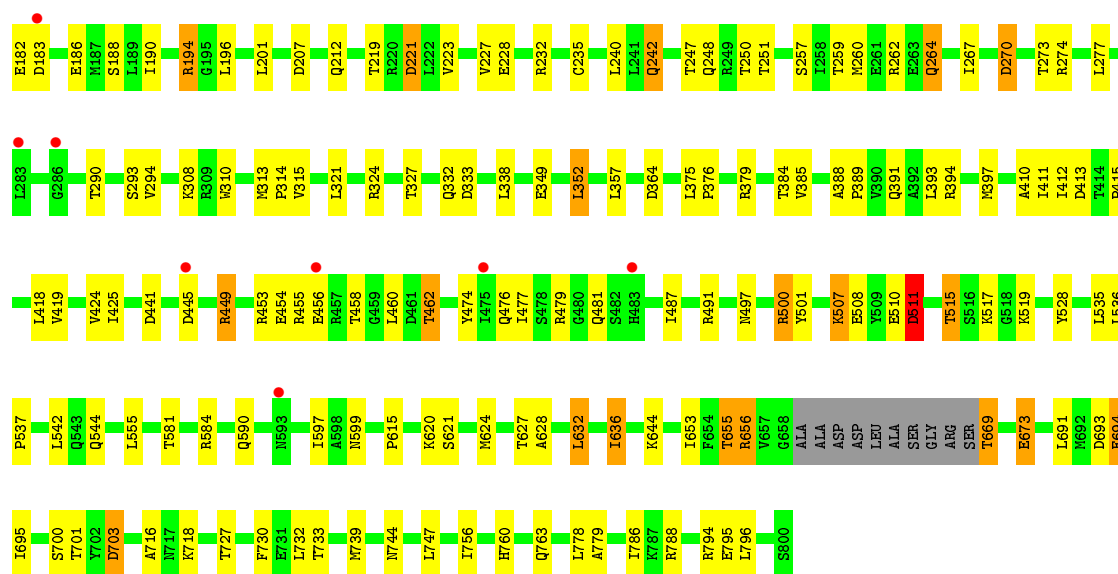
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

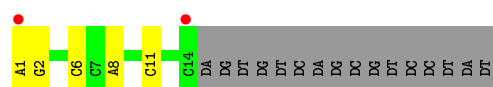
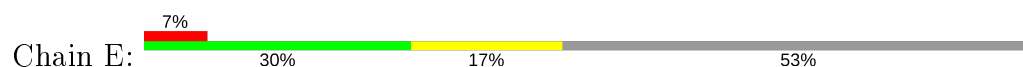


• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

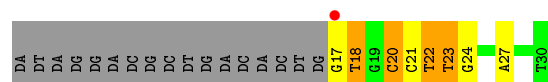
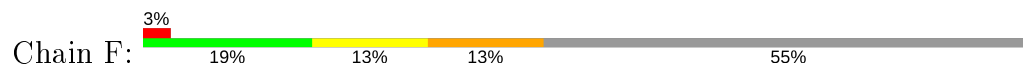




• Molecule 2: 5'-D(*AP*GP*CP*TP*GP*CP*CP*AP*GP*GP *CP*AP*CP*CP*AP*GP*TP*GP*TP*CP*AP*GP*CP*GP*TP*CP*CP* TP*AP*T)-3'



• 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*CP*TP*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	89.38Å 91.72Å 259.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 19.86 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (15.00-2.90) 98.7 (19.86-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.217 , 0.292 0.215 , 0.283	Depositor DCC
R_{free} test set	2372 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.647	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12905	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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	0.48	0/6313	0.77	15/8544 (0.2%)
1	B	0.46	0/6062	0.76	14/8199 (0.2%)
2	E	0.88	0/316	1.52	3/485 (0.6%)
3	F	0.85	0/320	1.66	6/492 (1.2%)
All	All	0.50	0/13011	0.84	38/17720 (0.2%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	20	DC	O4'-C1'-N1	8.87	114.21	108.00
3	F	27	DA	O4'-C1'-N9	-8.46	102.08	108.00
1	A	8	ASP	CB-CG-OD2	8.14	125.63	118.30
3	F	18	DT	O4'-C1'-N1	8.11	113.68	108.00
1	A	693	ASP	CB-CG-OD2	6.56	124.20	118.30
1	B	42	ASP	CB-CG-OD2	6.36	124.03	118.30
1	A	296	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	52	ASP	CB-CG-OD2	6.05	123.74	118.30
1	B	221	ASP	CB-CG-OD2	6.03	123.72	118.30
1	A	364	ASP	CB-CG-OD2	5.90	123.61	118.30
2	E	6	DC	P-O3'-C3'	5.89	126.77	119.70
1	A	511	ASP	CB-CG-OD2	5.85	123.56	118.30
1	B	121	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	386	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	413	ASP	CB-CG-OD2	5.73	123.46	118.30
1	B	364	ASP	CB-CG-OD2	5.73	123.45	118.30
1	B	157	LEU	CA-CB-CG	5.72	128.45	115.30
1	A	162	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	207	ASP	CB-CG-OD2	5.65	123.38	118.30
1	B	511	ASP	CB-CG-OD2	5.55	123.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	ASP	CB-CG-OD2	5.51	123.25	118.30
1	A	441	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	764	ASP	CB-CG-OD2	5.44	123.20	118.30
1	B	445	ASP	CB-CG-OD2	5.42	123.18	118.30
3	F	20	DC	O4'-C4'-C3'	-5.40	102.34	104.50
1	B	632	LEU	CA-CB-CG	5.33	127.55	115.30
1	B	703	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	42	ASP	CB-CG-OD2	5.29	123.06	118.30
2	E	2	DG	O4'-C1'-N9	-5.25	104.33	108.00
3	F	22	DT	C1'-O4'-C4'	-5.25	104.85	110.10
1	A	333	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	441	ASP	CB-CG-OD2	5.22	122.99	118.30
3	F	23	DT	C5-C4-O4	-5.21	121.25	124.90
2	E	11	DC	O4'-C1'-N1	5.21	111.64	108.00
1	B	52	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	445	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	333	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	347	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6207	0	6251	103	0
1	B	5964	0	6018	86	0
2	E	282	0	157	2	0
3	F	287	0	159	5	0
4	A	27	0	12	1	0
5	A	1	0	0	0	0
6	A	80	0	0	5	0
6	B	56	0	0	3	0
6	E	1	0	0	0	0
All	All	12905	0	12597	188	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 7.

All (188) 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:739:MET:CE	1:A:739:MET:SD	2.03	1.47
1:B:458:THR:HB	1:B:460:LEU:HD12	1.50	0.92
1:A:359:THR:HG21	6:A:2010:HOH:O	1.77	0.84
1:A:698:GLY:HA3	1:A:703:ASP:HB3	1.61	0.80
1:B:310:TRP:C	1:B:636:ILE:HD11	2.02	0.80
1:B:310:TRP:HB3	1:B:636:ILE:HD11	1.66	0.75
1:B:511:ASP:O	1:B:515:THR:OG1	2.04	0.75
1:A:652:ARG:HD2	1:A:654:PHE:CZ	2.23	0.74
1:A:245:LYS:NZ	6:A:2031:HOH:O	2.22	0.73
1:B:310:TRP:HB3	1:B:636:ILE:CD1	2.18	0.72
1:B:264:GLN:NE2	1:B:264:GLN:H	1.91	0.68
1:A:157:LEU:C	1:A:157:LEU:HD23	2.14	0.68
3:F:17:DG:N2	3:F:18:DT:N3	2.41	0.67
1:B:655:THR:HG22	1:B:691:LEU:HD12	1.76	0.67
1:B:248:GLN:HB3	1:B:250:THR:HG22	1.76	0.66
1:A:616:ASN:HD21	1:B:669:THR:HG22	1.59	0.66
1:A:302:MET:HG3	1:A:550:ALA:HB2	1.78	0.65
1:A:602:ASN:O	1:A:607:ARG:HD3	1.96	0.65
1:B:264:GLN:HE21	1:B:264:GLN:H	1.43	0.65
1:A:128:ARG:O	1:A:308:LYS:NZ	2.28	0.65
1:B:476:GLN:C	1:B:477:ILE:HD13	2.18	0.65
1:A:750:LEU:O	1:A:756:ILE:O	2.15	0.65
1:A:327:THR:HG21	1:A:555:LEU:HD13	1.79	0.64
1:B:327:THR:HG21	1:B:555:LEU:HD13	1.80	0.64
1:A:10:HIS:ND1	1:A:61:SER:OG	2.26	0.62
1:B:84:VAL:HG13	1:B:116:PRO:HA	1.80	0.62
1:B:128:ARG:O	1:B:308:LYS:NZ	2.32	0.62
1:A:463:LEU:HD21	1:A:475:ILE:HG23	1.82	0.62
1:B:507:LYS:NZ	1:B:510:GLU:OE1	2.33	0.62
1:B:655:THR:CG2	1:B:691:LEU:HD12	2.29	0.62
1:A:746:HIS:CE1	1:A:763:GLN:HB2	2.35	0.61
1:B:138:GLN:HE22	1:B:186:GLU:HG3	1.65	0.61
1:B:730:PHE:HB3	6:B:2048:HOH:O	2.01	0.61
1:B:118:THR:HG21	1:B:247:THR:HG21	1.83	0.60
1:B:477:ILE:HD13	1:B:477:ILE:N	2.17	0.60
1:B:310:TRP:O	1:B:636:ILE:HD11	2.02	0.59
1:B:419:VAL:HG11	1:B:528:TYR:CD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1801:ADP:O1A	6:A:2079:HOH:O	2.17	0.58
1:A:186:GLU:HG2	6:A:2016:HOH:O	2.02	0.58
1:B:267:ILE:HG21	1:B:653:ILE:HD12	1.84	0.58
3:F:23:DT:H2"	3:F:24:DG:C8	2.38	0.57
1:A:58:ARG:CZ	1:A:68:MET:HE1	2.34	0.57
3:F:20:DC:H4'	3:F:21:DC:OP1	2.05	0.57
1:B:656:ARG:O	1:B:656:ARG:HG3	2.04	0.57
1:B:727:THR:HG21	1:B:732:LEU:HD12	1.86	0.57
1:A:608:ARG:NH1	1:A:716:ALA:O	2.38	0.57
1:A:171:GLN:HE22	1:A:271:ALA:HA	1.69	0.57
1:A:171:GLN:NE2	1:A:271:ALA:HA	2.20	0.56
1:B:375:LEU:HD22	1:B:397:MET:HG2	1.88	0.56
1:A:157:LEU:CD2	1:A:260:MET:HG3	2.36	0.56
1:A:728:HIS:CE1	1:A:729:TYR:CZ	2.94	0.55
1:A:490:MET:HG3	1:A:502:ILE:O	2.07	0.54
1:A:792:LYS:O	1:A:795:GLU:HB2	2.07	0.54
1:A:328:ILE:HG23	1:A:559:ALA:HA	1.88	0.54
1:A:650:ILE:HA	1:A:687:TYR:O	2.06	0.54
1:B:716:ALA:HB3	1:B:739:MET:CE	2.38	0.54
1:A:24:HIS:N	1:A:25:PRO:HD3	2.23	0.54
1:A:419:VAL:HG23	6:A:2043:HOH:O	2.08	0.54
1:A:692:MET:HE2	1:A:695:ILE:HD13	1.89	0.54
1:A:699:THR:HB	1:B:615:PRO:HA	1.89	0.53
1:A:570:PRO:HB3	1:A:645:VAL:HB	1.90	0.53
1:B:693:ASP:O	1:B:694:GLU:C	2.47	0.53
1:A:176:ALA:HA	1:A:194:ARG:CZ	2.39	0.53
1:A:396:LYS:HD3	1:A:548:ALA:HB2	1.90	0.53
1:A:268:ILE:HB	1:A:652:ARG:HG2	1.90	0.53
1:B:375:LEU:HB2	1:B:376:PRO:HD3	1.91	0.53
1:A:10:HIS:HD1	1:A:61:SER:HG	1.55	0.52
1:A:616:ASN:ND2	1:B:669:THR:HG22	2.24	0.52
1:A:452:VAL:HG22	1:A:455:ARG:NH2	2.24	0.52
1:B:460:LEU:HD22	1:B:481:GLN:HB3	1.91	0.52
1:A:93:CYS:HA	1:A:110:VAL:HA	1.91	0.52
1:B:620:LYS:HG3	1:B:747:LEU:HD12	1.92	0.52
1:A:749:ALA:HB3	1:A:771:TYR:CZ	2.43	0.52
1:A:291:LEU:HG	1:A:295:LEU:HD12	1.92	0.52
1:A:305:ARG:NH2	1:A:347:ASP:OD2	2.43	0.51
1:B:157:LEU:O	1:B:260:MET:HA	2.11	0.51
1:B:375:LEU:O	1:B:379:ARG:HG3	2.10	0.51
1:A:382:LEU:O	1:A:391:GLN:NE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:GLN:OE1	1:B:242:GLN:HG2	2.11	0.50
1:B:92:ILE:N	1:B:92:ILE:HD13	2.26	0.50
1:A:560:GLU:OE2	1:A:564:THR:OG1	2.24	0.50
1:A:225:PHE:CE1	1:A:257:SER:HB2	2.47	0.50
1:A:430:ASN:HD22	1:A:527:LEU:HD21	1.76	0.50
1:B:599:ASN:ND2	6:B:2038:HOH:O	2.37	0.50
1:B:310:TRP:CB	1:B:636:ILE:HD11	2.39	0.50
1:A:278:GLU:O	1:A:290:THR:HB	2.12	0.49
1:A:727:THR:HG22	1:A:729:TYR:N	2.26	0.49
1:B:515:THR:HB	1:B:519:LYS:HE3	1.95	0.49
1:B:277:LEU:HD21	1:B:655:THR:HG21	1.94	0.49
1:B:17:TYR:CE2	1:B:29:LEU:HD23	2.47	0.49
1:B:474:TYR:CD1	1:B:500:ARG:HD2	2.48	0.49
1:A:178:LEU:HD13	1:A:190:ILE:HG13	1.94	0.49
1:A:470:VAL:HB	1:A:471:HIS:HD2	1.77	0.49
1:A:692:MET:CE	1:A:695:ILE:HD13	2.42	0.49
1:B:157:LEU:HD23	1:B:157:LEU:C	2.34	0.49
1:B:294:VAL:HG13	1:B:590:GLN:HG3	1.93	0.49
1:A:705:LEU:HD23	1:B:796:LEU:HD13	1.94	0.48
1:B:80:LEU:HD21	1:B:90:VAL:HG11	1.95	0.48
1:B:221:ASP:OD1	1:B:223:VAL:HB	2.12	0.48
1:A:393:LEU:HD13	1:A:552:LEU:CD1	2.44	0.48
1:A:640:VAL:HG11	1:A:645:VAL:HG21	1.95	0.48
1:A:40:PHE:HE1	1:A:68:MET:HE3	1.78	0.48
1:B:273:THR:HG23	1:B:655:THR:OG1	2.13	0.48
1:B:290:THR:HG23	1:B:293:SER:H	1.77	0.48
1:B:412:ILE:HD11	1:B:415:PRO:HA	1.95	0.48
1:A:51:LEU:HD21	1:A:83:LEU:HD21	1.95	0.48
1:A:739:MET:CE	1:A:739:MET:CG	2.90	0.47
1:B:68:MET:O	1:B:69:ALA:HB2	2.14	0.47
1:B:36:PHE:HA	1:B:71:ILE:O	2.13	0.47
1:A:327:THR:HG22	1:A:331:LEU:HD12	1.95	0.47
1:A:212:GLN:HG3	1:A:242:GLN:NE2	2.30	0.47
1:A:8:ASP:N	1:A:8:ASP:OD2	2.46	0.47
1:A:621:SER:OG	1:A:693:ASP:OD2	2.33	0.47
1:B:716:ALA:HB3	1:B:739:MET:HE1	1.96	0.47
1:B:152:SER:HB3	1:B:349:GLU:OE2	2.15	0.46
1:A:751:GLU:O	1:A:752:HIS:C	2.53	0.46
1:B:156:ARG:NH1	1:B:259:THR:HB	2.30	0.46
1:A:430:ASN:ND2	1:A:527:LEU:HD21	2.30	0.46
1:A:155:PHE:O	1:A:258:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:GLY:O	1:A:729:TYR:OH	2.33	0.46
1:A:756:ILE:O	1:A:757:ALA:HB3	2.16	0.46
1:A:362:PRO:HD2	1:A:417:VAL:O	2.15	0.46
1:A:155:PHE:CE1	1:A:258:ILE:HD12	2.51	0.45
3:F:20:DC:H2''	3:F:21:DC:O5'	2.16	0.45
1:B:267:ILE:HB	1:B:314:PRO:HG2	1.98	0.45
1:B:491:ARG:HG3	1:B:501:TYR:CE2	2.52	0.45
1:A:157:LEU:HD23	1:A:158:SER:N	2.31	0.45
1:A:159:GLU:HB3	1:A:232:ARG:HD2	1.98	0.45
1:A:327:THR:HG23	1:A:390:VAL:HG22	1.99	0.45
1:A:56:THR:HG21	3:F:22:DT:H5'	1.99	0.45
1:B:33:MET:HG3	1:B:38:GLU:HG3	1.99	0.45
1:A:473:TYR:HD1	1:A:510:GLU:HG3	1.82	0.44
1:A:61:SER:OG	1:A:62:ALA:N	2.50	0.44
1:B:393:LEU:O	1:B:397:MET:HB2	2.17	0.44
1:B:462:THR:OG1	1:B:481:GLN:OE1	2.35	0.44
2:E:1:DA:H2'	2:E:1:DA:N3	2.31	0.44
1:A:175:PRO:HB2	1:A:177:GLU:O	2.16	0.44
1:B:388:ALA:N	1:B:389:PRO:HD2	2.33	0.44
1:B:732:LEU:HA	1:B:732:LEU:HD23	1.83	0.44
1:B:194:ARG:HD3	6:B:2011:HOH:O	2.18	0.44
1:B:321:LEU:O	1:B:324:ARG:N	2.51	0.44
1:A:151:SER:O	1:A:353:ALA:HB2	2.18	0.44
1:A:733:THR:O	1:A:744:ASN:ND2	2.50	0.44
1:A:51:LEU:HD21	1:A:83:LEU:CG	2.47	0.44
1:A:623:TYR:CE1	1:A:762:VAL:HG21	2.54	0.43
1:A:35:ASP:OD2	2:E:8:DA:H2''	2.18	0.43
1:A:299:VAL:HG22	1:A:553:ASP:OD1	2.18	0.43
1:A:494:THR:OG1	1:A:499:GLU:OE2	2.19	0.43
1:B:385:VAL:O	1:B:391:GLN:NE2	2.46	0.43
1:B:454:GLU:O	1:B:458:THR:OG1	2.25	0.42
1:A:136:ILE:HD13	1:A:190:ILE:HD13	2.01	0.42
1:A:143:PHE:C	1:A:232:ARG:HD3	2.40	0.42
1:A:436:TRP:HB3	1:A:520:ALA:HB2	2.01	0.42
1:A:652:ARG:HD2	1:A:654:PHE:CE1	2.54	0.42
1:B:733:THR:HB	1:B:744:ASN:HD21	1.84	0.42
1:A:163:ARG:HG2	1:A:189:LEU:HD21	2.01	0.42
1:B:536:LEU:N	1:B:537:PRO:CD	2.81	0.42
1:A:119:ILE:HD12	1:A:125:LEU:HD23	2.01	0.42
1:A:375:LEU:O	1:A:379:ARG:HG3	2.19	0.42
1:B:756:ILE:HG22	1:B:778:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:VAL:HB	1:A:471:HIS:CD2	2.54	0.42
1:B:700:SER:O	1:B:701:THR:C	2.58	0.42
1:A:118:THR:HG21	1:A:247:THR:HG21	2.02	0.42
1:A:674:MET:HB3	1:B:779:ALA:CB	2.50	0.42
1:B:410:ALA:O	1:B:425:ILE:HA	2.20	0.41
1:A:270:ASP:O	1:A:271:ALA:C	2.57	0.41
1:A:361:ARG:HB3	1:A:362:PRO:CD	2.50	0.41
1:A:425:ILE:HG12	1:A:524:GLU:HG3	2.02	0.41
1:B:190:ILE:O	1:B:196:LEU:HD11	2.19	0.41
1:A:585:HIS:O	1:A:589:GLU:HG2	2.21	0.41
1:B:624:MET:O	1:B:627:THR:HB	2.20	0.41
1:B:656:ARG:HD3	1:B:673:GLU:HG3	2.01	0.41
1:A:731:GLU:OE2	1:B:701:THR:OG1	2.33	0.41
1:B:310:TRP:CE2	1:B:324:ARG:NH2	2.89	0.41
1:B:449:ARG:HB2	1:B:449:ARG:HE	1.80	0.41
1:B:80:LEU:CD2	1:B:90:VAL:HG11	2.50	0.41
1:A:670:PHE:N	1:A:670:PHE:CD2	2.88	0.41
1:B:240:LEU:HD23	1:B:240:LEU:C	2.41	0.41
1:B:628:ALA:HB2	1:B:691:LEU:HD11	2.03	0.41
1:A:604:SER:O	1:A:608:ARG:HB3	2.21	0.40
1:B:227:VAL:HG12	1:B:260:MET:HB2	2.02	0.40
1:B:352:LEU:HD21	1:B:542:LEU:HB3	2.02	0.40
1:A:240:LEU:CD1	1:A:240:LEU:C	2.90	0.40
1:A:375:LEU:N	1:A:376:PRO:CD	2.84	0.40
1:B:176:ALA:HA	1:B:194:ARG:NH2	2.36	0.40
1:A:157:LEU:CD2	1:A:157:LEU:C	2.85	0.40
1:A:770:SER:HB2	1:B:703:ASP:OD2	2.21	0.40
1:A:495:LEU:HD11	1:A:500:ARG:HD2	2.03	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	784/800 (98%)	733 (94%)	45 (6%)	6 (1%)	19	51
1	B	746/800 (93%)	682 (91%)	61 (8%)	3 (0%)	34	66
All	All	1530/1600 (96%)	1415 (92%)	106 (7%)	9 (1%)	25	58

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	41	TYR
1	A	59	GLY
1	A	752	HIS
1	B	69	ALA
1	B	270	ASP
1	B	694	GLU
1	A	298	THR
1	A	444	THR

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%)	567 (86%)	89 (14%)	3	11
1	B	631/664 (95%)	544 (86%)	87 (14%)	3	10
All	All	1287/1328 (97%)	1111 (86%)	176 (14%)	3	11

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	35	ASP
1	A	42	ASP
1	A	46	ARG
1	A	54	SER
1	A	56	THR
1	A	58	ARG

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Mol	Chain	Res	Type
1	A	61	SER
1	A	71	ILE
1	A	84	VAL
1	A	86	GLN
1	A	102	SER
1	A	109	LYS
1	A	129	GLN
1	A	137	TRP
1	A	139	ASP
1	A	140	SER
1	A	141	LYS
1	A	151	SER
1	A	157	LEU
1	A	162	ASP
1	A	164	GLU
1	A	178	LEU
1	A	179	LEU
1	A	182	GLU
1	A	188	SER
1	A	190	ILE
1	A	193	ARG
1	A	232	ARG
1	A	240	LEU
1	A	242	GLN
1	A	249	ARG
1	A	257	SER
1	A	259	THR
1	A	264	GLN
1	A	269	MET
1	A	277	LEU
1	A	304	SER
1	A	311	LEU
1	A	312	HIS
1	A	315	VAL
1	A	333	ASP
1	A	359	THR
1	A	387	SER
1	A	419	VAL
1	A	439	LEU
1	A	448	GLU
1	A	453	ARG
1	A	468	ASN

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Mol	Chain	Res	Type
1	A	488	ASN
1	A	490	MET
1	A	506	LEU
1	A	507	LYS
1	A	521	LEU
1	A	526	GLN
1	A	531	LEU
1	A	536	LEU
1	A	564	THR
1	A	566	ASN
1	A	571	THR
1	A	584	ARG
1	A	592	LEU
1	A	594	GLU
1	A	604	SER
1	A	608	ARG
1	A	613	THR
1	A	652	ARG
1	A	656	ARG
1	A	670	PHE
1	A	672	VAL
1	A	691	LEU
1	A	697	ARG
1	A	700	SER
1	A	703	ASP
1	A	717	ASN
1	A	728	HIS
1	A	732	LEU
1	A	734	GLN
1	A	735	LEU
1	A	739	MET
1	A	747	LEU
1	A	752	HIS
1	A	756	ILE
1	A	764	ASP
1	A	769	LYS
1	A	770	SER
1	A	791	GLN
1	A	795	GLU
1	A	800	SER
1	B	14	MET
1	B	15	GLN

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Mol	Chain	Res	Type
1	B	18	LEU
1	B	20	LEU
1	B	35	ASP
1	B	38	GLU
1	B	41	TYR
1	B	52	ASP
1	B	53	ILE
1	B	55	LEU
1	B	56	THR
1	B	71	ILE
1	B	76	VAL
1	B	80	LEU
1	B	82	LYS
1	B	109	LYS
1	B	114	VAL
1	B	122	GLU
1	B	127	GLU
1	B	129	GLN
1	B	137	TRP
1	B	140	SER
1	B	156	ARG
1	B	157	LEU
1	B	178	LEU
1	B	182	GLU
1	B	183	ASP
1	B	188	SER
1	B	194	ARG
1	B	201	LEU
1	B	219	THR
1	B	228	GLU
1	B	232	ARG
1	B	235	CYS
1	B	242	GLN
1	B	251	THR
1	B	257	SER
1	B	262	ARG
1	B	264	GLN
1	B	270	ASP
1	B	274	ARG
1	B	313	MET
1	B	315	VAL
1	B	332	GLN

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Mol	Chain	Res	Type
1	B	338	LEU
1	B	352	LEU
1	B	357	LEU
1	B	384	THR
1	B	394	ARG
1	B	411	ILE
1	B	418	LEU
1	B	424	VAL
1	B	449	ARG
1	B	453	ARG
1	B	455	ARG
1	B	456	GLU
1	B	462	THR
1	B	479	ARG
1	B	487	ILE
1	B	497	ASN
1	B	500	ARG
1	B	507	LYS
1	B	508	GLU
1	B	511	ASP
1	B	515	THR
1	B	517	LYS
1	B	535	LEU
1	B	544	GLN
1	B	581	THR
1	B	584	ARG
1	B	597	ILE
1	B	621	SER
1	B	632	LEU
1	B	636	ILE
1	B	644	LYS
1	B	655	THR
1	B	656	ARG
1	B	669	THR
1	B	673	GLU
1	B	695	ILE
1	B	718	LYS
1	B	760	HIS
1	B	763	GLN
1	B	786	ILE
1	B	788	ARG
1	B	794	ARG

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Mol	Chain	Res	Type
1	B	795	GLU

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

Mol	Chain	Res	Type
1	A	49	GLN
1	A	171	GLN
1	A	242	GLN
1	A	248	GLN
1	A	312	HIS
1	A	339	GLN
1	A	471	HIS
1	A	566	ASN
1	A	602	ASN
1	A	616	ASN
1	A	746	HIS
1	B	85	ASN
1	B	214	ASN
1	B	264	GLN
1	B	276	ASN
1	B	332	GLN
1	B	566	ASN
1	B	590	GLN
1	B	717	ASN
1	B	791	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	1.15	2 (8%)	29,45,45	1.66	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	-	0/12/32/32	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	3.85	1.38	1.32
4	A	1801	ADP	C2-N1	2.15	1.37	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	-6.11	119.12	128.68
4	A	1801	ADP	PA-O3A-PB	-4.61	117.01	132.83
4	A	1801	ADP	O3B-PB-O3A	2.88	114.30	104.64
4	A	1801	ADP	C1'-N9-C4	-2.12	122.92	126.64

There are no chirality outliers.

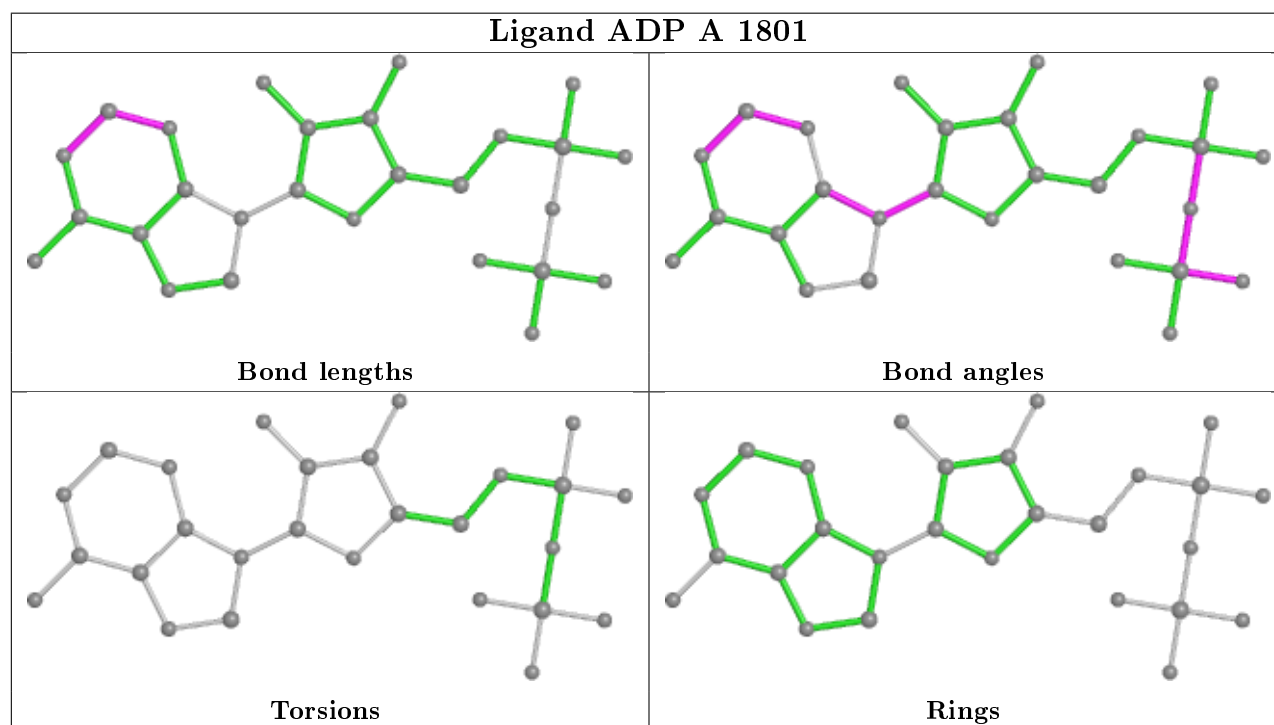
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1801	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 ⓘ

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%)	-0.14	21 (2%) 54 50	7, 22, 28, 33	0
1	B	754/800 (94%)	-0.02	25 (3%) 46 41	8, 22, 28, 34	0
2	E	14/30 (46%)	0.37	2 (14%) 2 2	11, 19, 33, 34	0
3	F	14/31 (45%)	0.26	1 (7%) 16 12	8, 12, 36, 39	0
All	All	1570/1661 (94%)	-0.08	49 (3%) 49 44	7, 22, 28, 39	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	74	HIS	5.6
1	A	444	THR	5.3
1	A	445	ASP	5.2
1	A	593	ASN	4.5
1	A	103	LYS	3.9
1	B	25	PRO	3.4
1	A	443	ALA	3.3
2	E	14	DC	3.3
1	A	595	PRO	3.3
1	A	386	ASP	3.1
2	E	1	DA	3.1
1	B	41	TYR	3.1
1	B	35	ASP	3.1
1	B	39	LEU	2.9
1	A	563	TYR	2.9
1	A	140	SER	2.9
1	B	18	LEU	2.9
1	A	752	HIS	2.8
1	B	286	GLY	2.8
1	A	61	SER	2.8
1	A	449	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	672	VAL	2.5
1	B	52	ASP	2.5
1	A	658	GLY	2.5
1	B	14	MET	2.5
1	A	97	GLY	2.5
1	A	98	ASP	2.4
1	B	49	GLN	2.4
1	B	36	PHE	2.4
1	A	768	SER	2.4
1	B	94	GLU	2.4
1	B	73	TYR	2.4
3	F	17	DG	2.4
1	B	183	ASP	2.3
1	A	431	GLU	2.3
1	B	456	GLU	2.3
1	A	100	ALA	2.2
1	B	483	HIS	2.2
1	B	55	LEU	2.2
1	A	59	GLY	2.1
1	A	555	LEU	2.1
1	B	283	LEU	2.1
1	B	19	ARG	2.1
1	B	593	ASN	2.1
1	B	475	ILE	2.1
1	B	45	LYS	2.1
1	B	140	SER	2.0
1	B	16	GLN	2.0
1	B	445	ASP	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 monosaccharides in this entry.

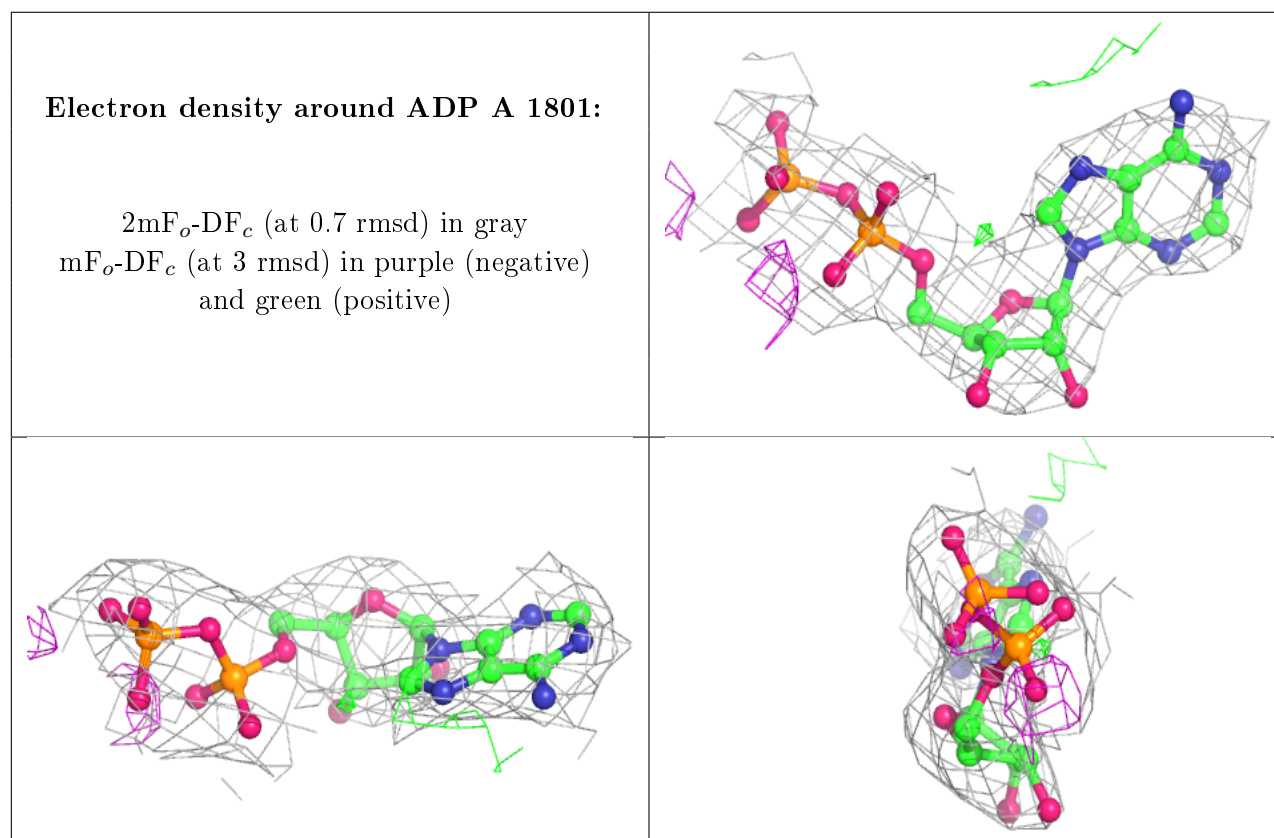
6.4 Ligands [i](#)

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	0.73	0.07	13,13,13,13	0
4	ADP	A	1801	27/27	0.95	0.14	12,16,18,20	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.