Full wwPDB X-ray Structure Validation Report (i)

Feb 5, 2024 – 10:21 AM EST

PDB ID	:	1T5T
Title	:	Structure of the (SR)Ca2+-ATPase Ca2-E1-ADP:AlF4- form
Authors	:	Sorensen, T.L.-M.; Moller, J.V.; Nissen, P.
Deposited on	:	2004-05-05
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 (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:

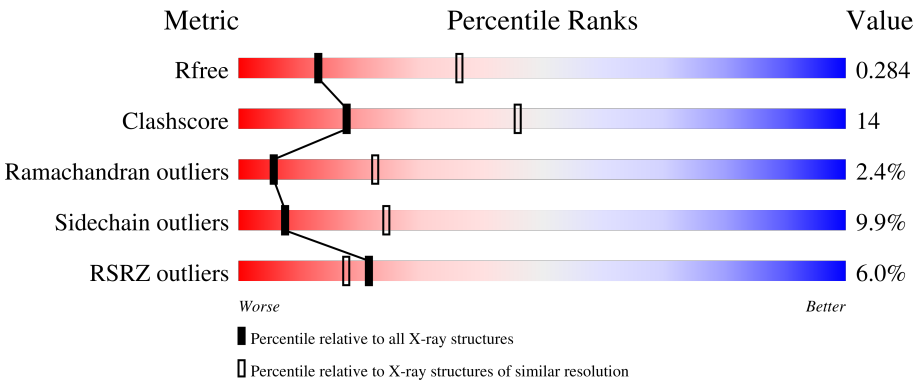
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

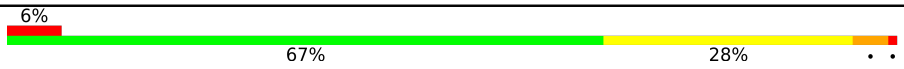
The reported resolution of this entry is 2.90 Å.

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 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	994	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7751 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.

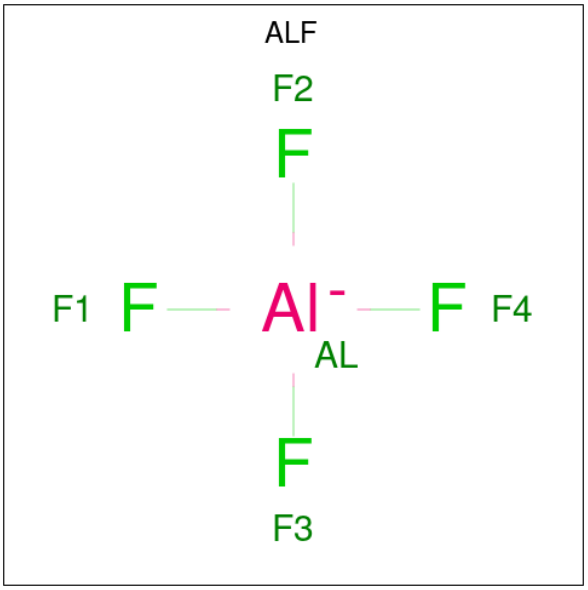
- Molecule 1 is a protein called Sarcoplasmic/endoplasmic reticulum calcium ATPase 1 isoform SERCA1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	994	7671	4876	1287	1451	57	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	994	GLY	-	SEE REMARK 999	UNP P04191

- Molecule 2 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	2	2	2	0	0

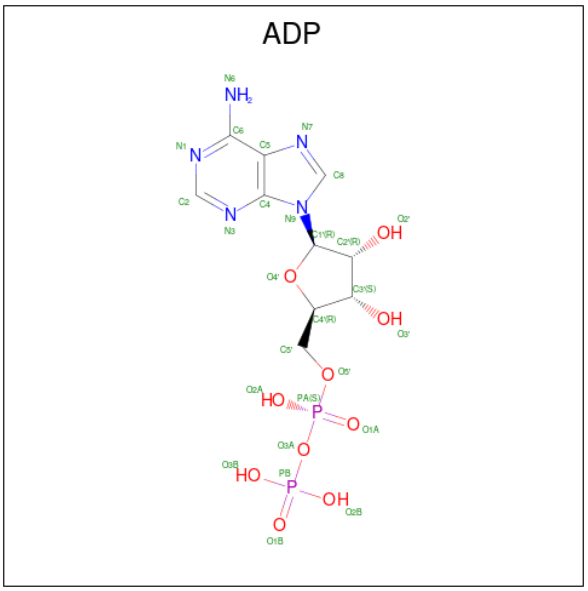
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 7 is water.

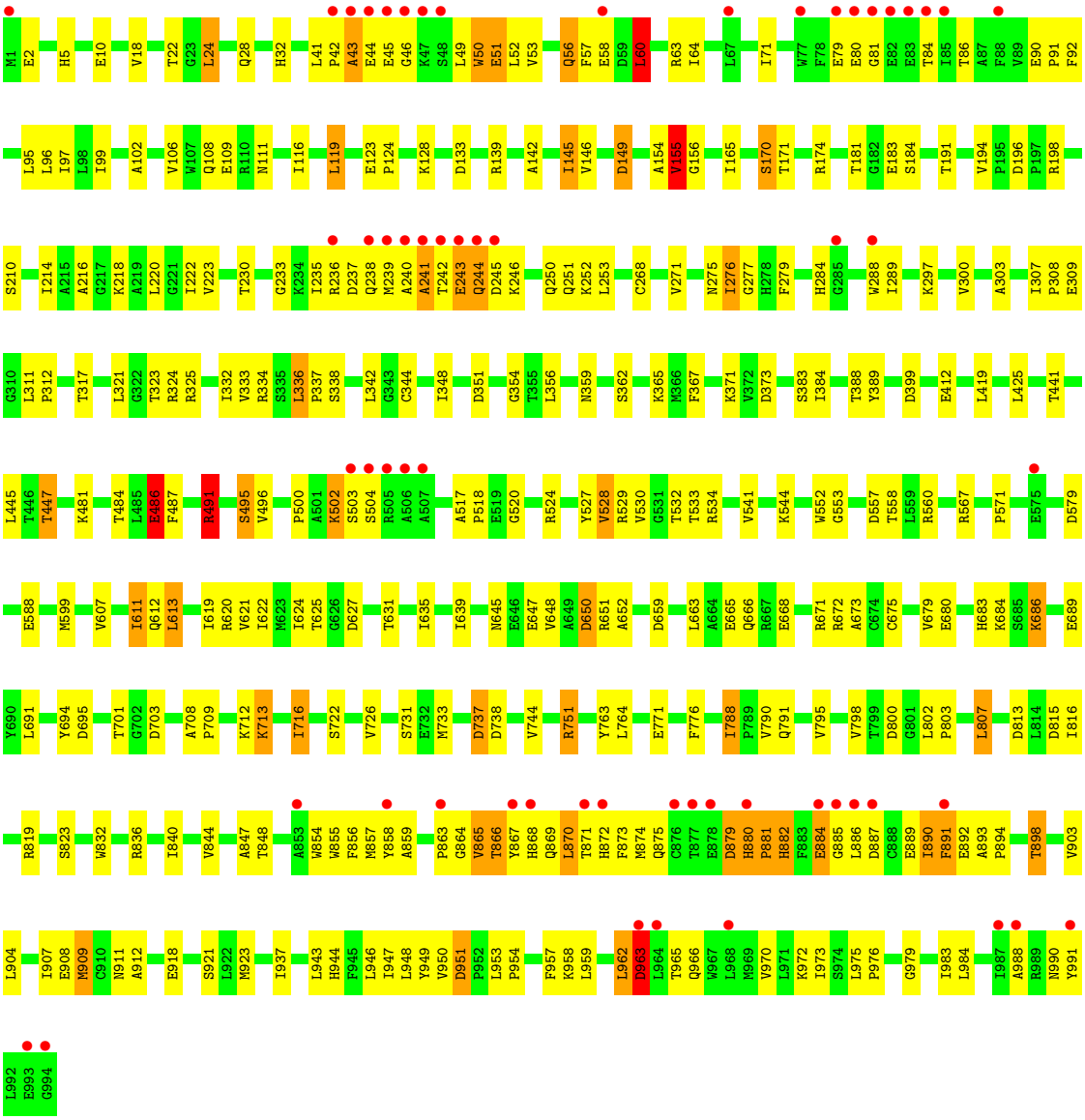
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	43	43	43	0	0

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: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1 isoform SERCA1A

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	162.48Å 75.62Å 151.65Å 90.00° 108.82° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 42.43 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.90) 99.9 (42.43-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.30 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.246 , 0.293 0.233 , 0.284	Depositor DCC
R_{free} test set	1153 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å^2)	74.0	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 81.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7751	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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 (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.49	0/7812	0.88	21/10592 (0.2%)

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	7

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	491	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	650	ASP	CB-CG-OD2	6.84	124.46	118.30
1	A	557	ASP	CB-CG-OD2	6.72	124.34	118.30
1	A	659	ASP	CB-CG-OD2	6.62	124.26	118.30
1	A	951	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	703	ASP	CB-CG-OD2	6.47	124.12	118.30
1	A	887	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	815	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	737	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	155	VAL	CB-CA-C	-5.73	100.51	111.40
1	A	599	MET	CG-SD-CE	-5.51	91.38	100.20
1	A	237	ASP	CB-CG-OD2	5.47	123.23	118.30
1	A	879	ASP	CB-CG-OD2	5.36	123.13	118.30
1	A	351	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	627	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	133	ASP	CB-CG-OD2	5.20	122.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	695	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	373	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	245	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	813	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	149	ASP	N-CA-CB	5.00	119.61	110.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	238	GLN	Peptide
1	A	243	GLU	Peptide
1	A	500	PRO	Peptide
1	A	56	GLN	Peptide
1	A	80	GLU	Peptide
1	A	880	HIS	Peptide
1	A	990	ASN	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	7671	0	7765	210	0
2	A	5	0	0	0	0
3	A	2	0	0	0	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	27	0	12	1	0
7	A	43	0	0	1	0
All	All	7751	0	7777	210	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 14.

All (210) 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:241:ALA:C	1:A:243:GLU:H	1.67	0.97
1:A:889:GLU:O	1:A:891:PHE:N	2.02	0.92
1:A:495:SER:HB2	1:A:588:GLU:OE2	1.74	0.86
1:A:279:PHE:HZ	1:A:288:TRP:C	1.86	0.79
1:A:868:HIS:O	1:A:871:THR:N	2.16	0.78
1:A:884:GLU:O	1:A:886:LEU:N	2.18	0.76
1:A:155:VAL:HG13	1:A:216:ALA:HA	1.71	0.72
1:A:354:GLY:HA2	1:A:359:ASN:HB2	1.71	0.72
1:A:679:VAL:HG22	1:A:683:HIS:HB2	1.72	0.72
1:A:558:THR:HG21	1:A:635:ILE:CG1	2.19	0.71
1:A:880:HIS:HB3	1:A:881:PRO:HD2	1.71	0.71
1:A:145:ILE:CD1	1:A:223:VAL:HG21	2.20	0.71
1:A:671:ARG:HD2	1:A:694:TYR:CE1	2.26	0.71
1:A:791:GLN:NE2	1:A:958:LYS:HG3	2.06	0.70
1:A:856:PHE:O	1:A:863:PRO:O	2.09	0.70
1:A:486:GLU:O	1:A:491:ARG:NH2	2.26	0.68
1:A:832:TRP:CH2	1:A:988:ALA:HB2	2.28	0.68
1:A:558:THR:HG21	1:A:635:ILE:HG13	1.76	0.67
1:A:279:PHE:O	1:A:279:PHE:CG	2.46	0.67
1:A:528:VAL:HG21	1:A:541:VAL:HG11	1.76	0.67
1:A:279:PHE:CZ	1:A:288:TRP:C	2.68	0.67
1:A:41:LEU:HD13	1:A:236:ARG:HD2	1.75	0.67
1:A:679:VAL:CG2	1:A:683:HIS:CB	2.73	0.67
1:A:866:THR:HG22	1:A:867:TYR:H	1.60	0.66
1:A:857:MET:CE	1:A:867:TYR:HA	2.25	0.66
1:A:271:VAL:HG22	1:A:776:PHE:HE1	1.61	0.65
1:A:679:VAL:CG2	1:A:683:HIS:HB2	2.26	0.65
1:A:116:ILE:HD11	1:A:323:THR:HG21	1.78	0.65
1:A:875:GLN:O	1:A:880:HIS:CG	2.50	0.65
1:A:650:ASP:OD1	1:A:672:ARG:NE	2.30	0.64
1:A:145:ILE:HD12	1:A:223:VAL:HG21	1.80	0.64
1:A:49:LEU:O	1:A:52:LEU:N	2.30	0.63
1:A:181:THR:OG1	1:A:183:GLU:HB2	1.97	0.63
1:A:71:ILE:HD11	1:A:300:VAL:HG11	1.81	0.63
1:A:441:THR:OG1	1:A:560:ARG:NH1	2.33	0.62
1:A:155:VAL:HA	1:A:214:ILE:HG22	1.81	0.62
1:A:791:GLN:HE22	1:A:958:LYS:HG3	1.65	0.62
1:A:894:PRO:HB2	1:A:959:LEU:HB2	1.81	0.61
1:A:864:GLY:O	1:A:866:THR:N	2.33	0.61
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.99	0.61
1:A:241:ALA:C	1:A:243:GLU:N	2.42	0.61
1:A:156:GLY:HA2	1:A:726:VAL:HG13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:GLU:HA	1:A:244:GLN:HG3	1.82	0.60
1:A:95:LEU:O	1:A:99:ILE:HG12	2.02	0.60
1:A:722:SER:OG	1:A:738:ASP:OD2	2.13	0.60
1:A:530:VAL:O	1:A:533:THR:HB	2.01	0.59
1:A:142:ALA:O	1:A:145:ILE:HG23	2.02	0.59
1:A:671:ARG:HG3	1:A:694:TYR:CE2	2.37	0.59
1:A:791:GLN:NE2	1:A:958:LYS:CG	2.66	0.58
1:A:751:ARG:HB3	1:A:816:ILE:HD11	1.84	0.58
1:A:894:PRO:HB3	1:A:958:LYS:HB3	1.85	0.58
1:A:558:THR:HG21	1:A:635:ILE:HG12	1.86	0.58
1:A:894:PRO:O	1:A:898:THR:OG1	2.21	0.58
1:A:884:GLU:HA	1:A:884:GLU:OE1	2.04	0.58
1:A:889:GLU:O	1:A:891:PHE:O	2.22	0.58
1:A:962:LEU:HB2	1:A:966:GLN:HG2	1.87	0.57
1:A:145:ILE:HD11	1:A:223:VAL:HG21	1.87	0.57
1:A:771:GLU:OE2	1:A:908:GLU:OE1	2.23	0.56
1:A:28:GLN:O	1:A:32:HIS:ND1	2.39	0.55
1:A:235:ILE:HG22	1:A:235:ILE:O	2.07	0.55
1:A:611:ILE:HD13	1:A:621:VAL:HG11	1.89	0.55
1:A:181:THR:HG1	1:A:183:GLU:HB2	1.70	0.55
1:A:947:ILE:HD11	1:A:957:PHE:CE1	2.42	0.55
1:A:102:ALA:O	1:A:106:VAL:HG23	2.06	0.54
1:A:671:ARG:HD2	1:A:694:TYR:CZ	2.42	0.54
1:A:909:MET:HG2	1:A:937:ILE:HG23	1.89	0.54
1:A:875:GLN:O	1:A:880:HIS:HB2	2.06	0.54
1:A:154:ALA:HB2	1:A:218:LYS:HG3	1.89	0.54
1:A:41:LEU:HD13	1:A:236:ARG:CD	2.36	0.54
1:A:81:GLY:HA2	1:A:297:LYS:NZ	2.23	0.54
1:A:875:GLN:O	1:A:880:HIS:CB	2.56	0.53
1:A:909:MET:HA	1:A:909:MET:HE2	1.91	0.53
1:A:170:SER:HB3	1:A:486:GLU:HG2	1.90	0.52
1:A:947:ILE:HD11	1:A:957:PHE:CZ	2.43	0.52
1:A:869:GLN:O	1:A:869:GLN:HG2	2.09	0.52
1:A:607:VAL:HG12	1:A:639:ILE:HG23	1.91	0.52
1:A:389:TYR:HB3	1:A:425:LEU:HD21	1.91	0.52
1:A:639:ILE:HG22	1:A:639:ILE:O	2.09	0.51
1:A:108:GLN:HG3	1:A:317:THR:HG23	1.93	0.51
1:A:553:GLY:CA	1:A:631:THR:HG22	2.41	0.51
1:A:650:ASP:OD1	1:A:650:ASP:O	2.28	0.51
1:A:857:MET:HE3	1:A:867:TYR:HA	1.93	0.51
1:A:43:ALA:HB3	1:A:236:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:VAL:O	1:A:866:THR:O	2.28	0.51
1:A:558:THR:CG2	1:A:635:ILE:HG13	2.41	0.50
1:A:49:LEU:O	1:A:50:TRP:C	2.49	0.50
1:A:651:ARG:HB2	1:A:673:ALA:HA	1.93	0.50
1:A:891:PHE:O	1:A:892:GLU:CB	2.59	0.50
1:A:788:ILE:HG22	1:A:791:GLN:HG3	1.94	0.50
1:A:92:PHE:O	1:A:96:LEU:HB2	2.12	0.50
1:A:419:LEU:O	1:A:481:LYS:NZ	2.44	0.50
1:A:666:GLN:HE22	1:A:686:LYS:NZ	2.09	0.50
1:A:962:LEU:O	1:A:963:ASP:C	2.51	0.50
1:A:240:ALA:O	1:A:241:ALA:C	2.51	0.49
1:A:865:VAL:HG13	1:A:870:LEU:HG	1.95	0.49
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.95	0.49
1:A:679:VAL:HG23	1:A:683:HIS:CG	2.48	0.49
1:A:527:TYR:CD1	1:A:534:ARG:HD3	2.48	0.49
1:A:246:LYS:HB2	1:A:250:GLN:CD	2.33	0.48
1:A:869:GLN:C	1:A:871:THR:H	2.17	0.48
1:A:962:LEU:HB2	1:A:966:GLN:CG	2.43	0.48
1:A:613:LEU:HD23	1:A:744:VAL:HG11	1.96	0.48
1:A:41:LEU:CD1	1:A:236:ARG:HD2	2.41	0.48
1:A:43:ALA:HB3	1:A:236:ARG:HH12	1.78	0.48
1:A:165:ILE:HG22	1:A:191:THR:HG22	1.95	0.48
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.95	0.48
1:A:890:ILE:O	1:A:893:ALA:CB	2.62	0.48
1:A:624:ILE:O	1:A:684:LYS:HE2	2.13	0.48
1:A:889:GLU:O	1:A:890:ILE:C	2.51	0.48
1:A:243:GLU:CA	1:A:244:GLN:HG3	2.44	0.48
1:A:246:LYS:HG3	1:A:251:GLN:HG3	1.95	0.48
1:A:502:LYS:HB2	1:A:504:SER:OG	2.13	0.48
1:A:679:VAL:HG23	1:A:683:HIS:CB	2.43	0.48
1:A:57:PHE:O	1:A:58:GLU:HB3	2.14	0.47
1:A:170:SER:CB	1:A:486:GLU:HG2	2.44	0.47
1:A:174:ARG:HB2	1:A:216:ALA:HB3	1.96	0.47
1:A:308:PRO:HB3	1:A:764:LEU:CD1	2.44	0.47
1:A:86:THR:CG2	1:A:790:VAL:HG21	2.44	0.47
1:A:840:ILE:HG21	1:A:911:ASN:HD22	1.79	0.47
1:A:847:ALA:HB1	1:A:973:ILE:HG22	1.96	0.47
1:A:791:GLN:HE21	1:A:958:LYS:CG	2.28	0.47
1:A:64:ILE:HG21	1:A:307:ILE:CD1	2.45	0.47
1:A:383:SER:O	1:A:384:ILE:HD13	2.13	0.47
1:A:42:PRO:O	1:A:43:ALA:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:VAL:HG12	1:A:106:VAL:HG22	1.96	0.47
1:A:763:TYR:CE1	1:A:912:ALA:HB2	2.50	0.47
1:A:884:GLU:OE1	1:A:884:GLU:CA	2.62	0.47
1:A:689:GLU:OE1	1:A:713:LYS:HD3	2.14	0.47
1:A:947:ILE:HD11	1:A:957:PHE:CD1	2.51	0.46
1:A:947:ILE:HD11	1:A:957:PHE:CE2	2.50	0.46
1:A:708:ALA:O	1:A:709:PRO:C	2.53	0.46
1:A:652:ALA:HA	1:A:675:CYS:O	2.14	0.46
1:A:279:PHE:HZ	1:A:289:ILE:N	2.13	0.46
1:A:553:GLY:HA3	1:A:631:THR:HG22	1.97	0.46
1:A:871:THR:O	1:A:872:HIS:CG	2.69	0.46
1:A:275:ASN:C	1:A:277:GLY:H	2.19	0.46
1:A:791:GLN:HE21	1:A:958:LYS:HG2	1.79	0.46
1:A:954:PRO:O	1:A:958:LYS:N	2.48	0.46
1:A:271:VAL:HG22	1:A:776:PHE:CE1	2.45	0.46
1:A:840:ILE:HG21	1:A:911:ASN:ND2	2.30	0.46
1:A:975:LEU:N	1:A:976:PRO:CD	2.79	0.46
1:A:491:ARG:NH1	1:A:588:GLU:OE2	2.49	0.46
1:A:875:GLN:HA	1:A:880:HIS:HB2	1.98	0.46
1:A:844:VAL:O	1:A:848:THR:HG22	2.16	0.46
1:A:854:TRP:NE1	1:A:858:TYR:CD2	2.84	0.46
1:A:276:ILE:HA	1:A:279:PHE:HB2	1.97	0.45
1:A:903:VAL:O	1:A:907:ILE:HG22	2.17	0.45
1:A:24:LEU:HG	1:A:28:GLN:HB3	1.99	0.45
1:A:156:GLY:HA2	1:A:726:VAL:CG1	2.43	0.45
1:A:880:HIS:C	1:A:882:HIS:N	2.70	0.45
1:A:921:SER:HB3	1:A:923:MET:HG2	1.98	0.45
1:A:668:GLU:OE2	1:A:694:TYR:OH	2.35	0.45
1:A:60:LEU:H	1:A:60:LEU:HD23	1.81	0.45
1:A:171:THR:OG1	1:A:486:GLU:OE2	2.29	0.45
1:A:803:PRO:O	1:A:807:LEU:HD22	2.17	0.45
1:A:18:VAL:HG21	1:A:222:ILE:HD12	1.98	0.45
1:A:365:LYS:NZ	7:A:1031:HOH:O	2.47	0.44
1:A:679:VAL:CG2	1:A:683:HIS:HB3	2.48	0.44
1:A:866:THR:HG22	1:A:867:TYR:N	2.28	0.44
1:A:342:LEU:HD13	1:A:716:ILE:HG13	2.00	0.44
1:A:648:VAL:CG1	1:A:648:VAL:O	2.65	0.44
1:A:855:TRP:O	1:A:859:ALA:HB3	2.17	0.44
1:A:890:ILE:O	1:A:893:ALA:HB2	2.18	0.44
1:A:58:GLU:HA	1:A:63:ARG:NE	2.32	0.44
1:A:625:THR:O	1:A:679:VAL:HG12	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ILE:HG13	1:A:146:VAL:N	2.33	0.44
1:A:944:HIS:O	1:A:947:ILE:HG22	2.18	0.44
1:A:49:LEU:O	1:A:51:GLU:N	2.50	0.43
1:A:111:ASN:HB3	1:A:324:ARG:CD	2.48	0.43
1:A:909:MET:CG	1:A:937:ILE:HG23	2.48	0.43
1:A:90:GLU:HB2	1:A:91:PRO:HD3	2.00	0.43
1:A:308:PRO:HB3	1:A:764:LEU:HD12	2.00	0.43
1:A:948:LEU:HB3	1:A:949:TYR:CD2	2.53	0.43
1:A:333:VAL:HG13	1:A:338:SER:OG	2.18	0.43
1:A:620:ARG:NH2	1:A:622:ILE:HD11	2.33	0.43
1:A:875:GLN:HE21	1:A:875:GLN:N	2.16	0.43
1:A:567:ARG:CZ	1:A:571:PRO:HD3	2.48	0.43
1:A:904:LEU:O	1:A:908:GLU:HG3	2.17	0.43
1:A:51:GLU:O	1:A:52:LEU:C	2.57	0.43
1:A:869:GLN:NE2	1:A:872:HIS:C	2.72	0.43
1:A:891:PHE:O	1:A:892:GLU:HB3	2.19	0.43
1:A:119:LEU:HD13	1:A:332:ILE:HG13	2.01	0.43
1:A:367:PHE:HD1	1:A:552:TRP:CH2	2.37	0.43
1:A:97:ILE:HD11	1:A:800:ASP:O	2.19	0.43
1:A:558:THR:HG22	1:A:558:THR:O	2.19	0.42
1:A:321:LEU:HD21	1:A:325:ARG:NH2	2.35	0.42
1:A:979:GLY:O	1:A:983:ILE:HG12	2.19	0.42
1:A:671:ARG:HD2	1:A:694:TYR:CD1	2.54	0.42
1:A:866:THR:HG22	1:A:867:TYR:CD2	2.55	0.42
1:A:425:LEU:HD11	1:A:447:THR:HG22	2.00	0.42
1:A:230:THR:O	1:A:233:GLY:N	2.52	0.42
1:A:348:ILE:HD12	1:A:619:ILE:HG21	2.02	0.42
1:A:336:LEU:N	1:A:337:PRO:HD2	2.35	0.41
1:A:81:GLY:HA2	1:A:297:LYS:HZ1	1.86	0.41
1:A:836:ARG:HG3	1:A:984:LEU:HD23	2.02	0.41
1:A:880:HIS:O	1:A:881:PRO:C	2.58	0.41
1:A:123:GLU:HA	1:A:124:PRO:HD3	1.89	0.41
1:A:334:ARG:NH1	1:A:731:SER:O	2.52	0.41
1:A:5:HIS:HD2	1:A:194:VAL:HG23	1.86	0.41
1:A:43:ALA:C	1:A:45:GLU:H	2.23	0.41
1:A:639:ILE:O	1:A:639:ILE:CG2	2.69	0.41
1:A:957:PHE:O	1:A:958:LYS:HG2	2.21	0.41
1:A:921:SER:CB	1:A:923:MET:HG2	2.51	0.41
1:A:268:CYS:SG	1:A:303:ALA:HB2	2.61	0.41
1:A:487:PHE:CE2	6:A:1001:ADP:C4	3.09	0.41
1:A:903:VAL:HA	1:A:970:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:950:VAL:O	1:A:954:PRO:HD3	2.21	0.41
1:A:648:VAL:O	1:A:648:VAL:HG12	2.21	0.40
1:A:517:ALA:HA	1:A:518:PRO:HD3	1.90	0.40
1:A:520:GLY:O	1:A:524:ARG:HG3	2.21	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	992/994 (100%)	908 (92%)	60 (6%)	24 (2%)	6 22

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	ALA
1	A	276	ILE
1	A	865	VAL
1	A	881	PRO
1	A	882	HIS
1	A	885	GLY
1	A	890	ILE
1	A	46	GLY
1	A	50	TRP
1	A	79	GLU
1	A	155	VAL
1	A	241	ALA
1	A	399	ASP
1	A	866	THR
1	A	870	LEU
1	A	874	MET
1	A	962	LEU

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Mol	Chain	Res	Type
1	A	963	ASP
1	A	242	THR
1	A	60	LEU
1	A	486	GLU
1	A	879	ASP
1	A	44	GLU
1	A	239	MET

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	840/840 (100%)	757 (90%)	83 (10%)	8 24

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	10	GLU
1	A	22	THR
1	A	24	LEU
1	A	51	GLU
1	A	56	GLN
1	A	60	LEU
1	A	84	THR
1	A	109	GLU
1	A	119	LEU
1	A	128	LYS
1	A	139	ARG
1	A	145	ILE
1	A	149	ASP
1	A	155	VAL
1	A	170	SER
1	A	184	SER
1	A	196	ASP
1	A	198	ARG

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Mol	Chain	Res	Type
1	A	210	SER
1	A	220	LEU
1	A	244	GLN
1	A	252	LYS
1	A	253	LEU
1	A	284	HIS
1	A	309	GLU
1	A	336	LEU
1	A	344	CYS
1	A	356	LEU
1	A	362	SER
1	A	371	LYS
1	A	388	THR
1	A	445	LEU
1	A	447	THR
1	A	484	THR
1	A	486	GLU
1	A	491	ARG
1	A	495	SER
1	A	496	VAL
1	A	502	LYS
1	A	503	SER
1	A	528	VAL
1	A	532	THR
1	A	544	LYS
1	A	579	ASP
1	A	611	ILE
1	A	612	GLN
1	A	613	LEU
1	A	645	ASN
1	A	647	GLU
1	A	663	LEU
1	A	665	GLU
1	A	680	GLU
1	A	686	LYS
1	A	691	LEU
1	A	701	THR
1	A	712	LYS
1	A	713	LYS
1	A	716	ILE
1	A	733	MET
1	A	737	ASP

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Mol	Chain	Res	Type
1	A	751	ARG
1	A	788	ILE
1	A	795	VAL
1	A	798	VAL
1	A	802	LEU
1	A	807	LEU
1	A	819	ARG
1	A	823	SER
1	A	873	PHE
1	A	884	GLU
1	A	891	PHE
1	A	898	THR
1	A	909	MET
1	A	918	GLU
1	A	943	LEU
1	A	946	LEU
1	A	951	ASP
1	A	953	LEU
1	A	963	ASP
1	A	965	THR
1	A	972	LYS
1	A	991	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	250	GLN
1	A	259	GLN
1	A	280	ASN
1	A	330	ASN
1	A	666	GLN
1	A	755	ASN
1	A	791	GLN
1	A	868	HIS
1	A	869	GLN
1	A	875	GLN
1	A	880	HIS
1	A	882	HIS
1	A	911	ASN
1	A	990	ASN

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 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
2	ALF	A	1002	4,7,6,1	0,4,4	-	-	-		
6	ADP	A	1001	4,2	24,29,29	1.06	2 (8%)	29,45,45	1.28	3 (10%)

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	ADP	A	1001	4,2	-	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)
6	A	1001	ADP	O4'-C1'	2.59	1.44	1.41
6	A	1001	ADP	C2-N3	2.41	1.36	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1001	ADP	C4-C5-N7	-3.98	105.25	109.40
6	A	1001	ADP	PA-O3A-PB	-2.47	124.36	132.83
6	A	1001	ADP	N3-C2-N1	-2.16	125.30	128.68

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1001	ADP	PA-O3A-PB-O3B
6	A	1001	ADP	PA-O3A-PB-O2B
6	A	1001	ADP	C5'-O5'-PA-O1A

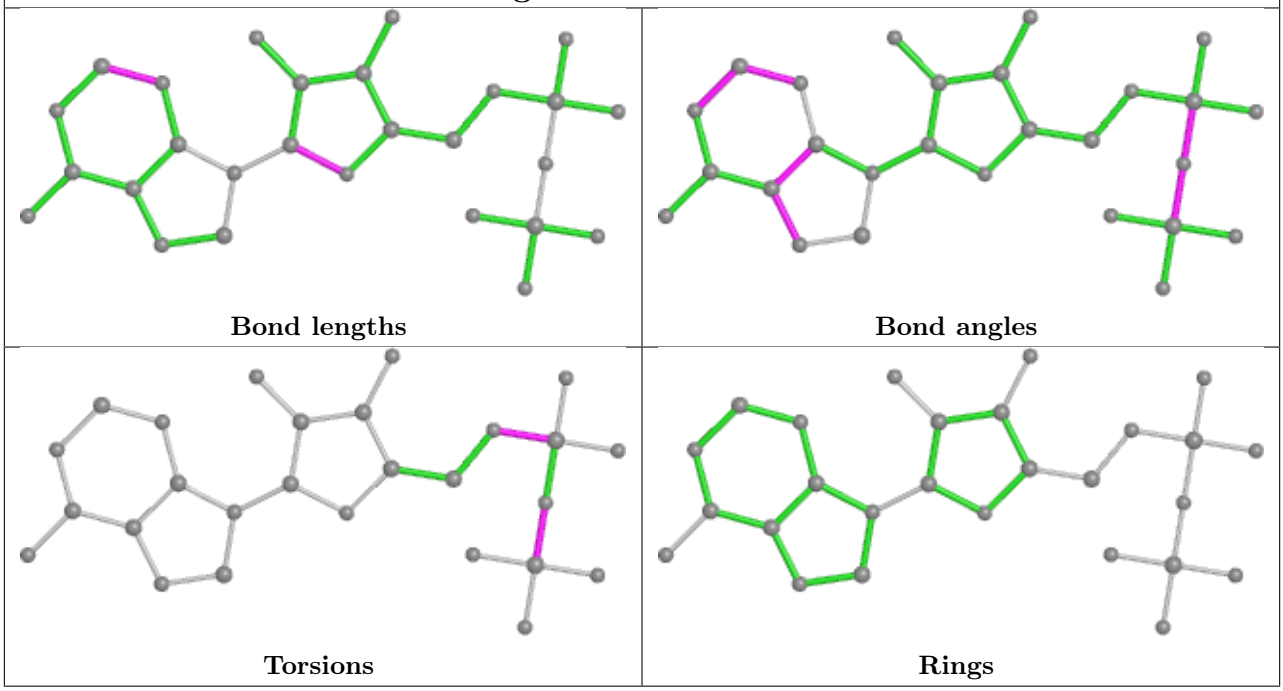
There are no ring outliers.

1 monomer is involved in 1 short contact:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 1001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	994/994 (100%)	0.29	60 (6%) 21 18	42, 66, 125, 142	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	994	GLY	11.3
1	A	877	THR	10.1
1	A	240	ALA	8.8
1	A	82	GLU	8.5
1	A	876	CYS	7.8
1	A	1	MET	7.1
1	A	47	LYS	7.0
1	A	993	GLU	6.8
1	A	242	THR	6.5
1	A	239	MET	6.3
1	A	241	ALA	6.0
1	A	83	GLU	5.2
1	A	506	ALA	5.0
1	A	863	PRO	4.9
1	A	45	GLU	4.9
1	A	886	LEU	4.8
1	A	991	TYR	4.5
1	A	505	ARG	4.2
1	A	84	THR	4.2
1	A	964	LEU	4.0
1	A	288	TRP	3.8
1	A	243	GLU	3.7
1	A	868	HIS	3.7
1	A	81	GLY	3.6
1	A	58	GLU	3.6
1	A	46	GLY	3.5
1	A	963	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	968	LEU	3.3
1	A	507	ALA	3.3
1	A	44	GLU	3.3
1	A	236	ARG	3.2
1	A	79	GLU	3.2
1	A	77	TRP	3.2
1	A	878	GLU	3.1
1	A	285	GLY	2.9
1	A	238	GLN	2.9
1	A	80	GLU	2.9
1	A	43	ALA	2.9
1	A	575	GLU	2.9
1	A	67	LEU	2.8
1	A	867	TYR	2.8
1	A	85	ILE	2.8
1	A	987	ILE	2.8
1	A	858	TYR	2.7
1	A	504	SER	2.6
1	A	988	ALA	2.6
1	A	503	SER	2.5
1	A	48	SER	2.5
1	A	42	PRO	2.5
1	A	872	HIS	2.5
1	A	88	PHE	2.4
1	A	885	GLY	2.4
1	A	887	ASP	2.3
1	A	880	HIS	2.3
1	A	871	THR	2.3
1	A	891	PHE	2.2
1	A	244	GLN	2.2
1	A	245	ASP	2.1
1	A	884	GLU	2.1
1	A	853	ALA	2.1

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)

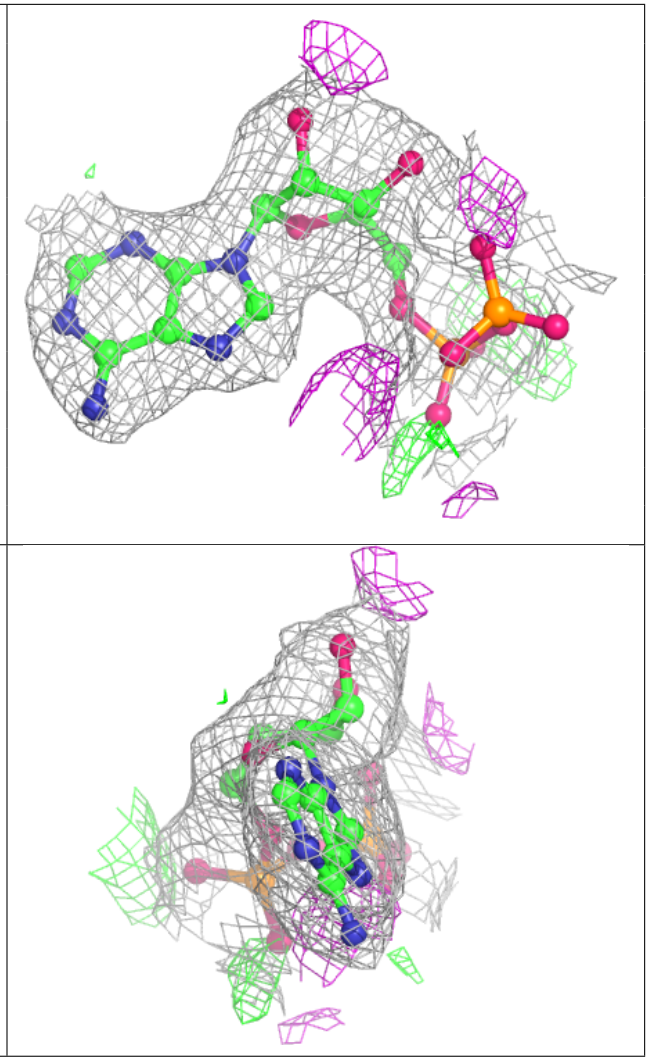
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	A	1007	1/1	0.60	0.20	66,66,66,66	0
3	CA	A	1004	1/1	0.82	0.19	98,98,98,98	0
4	MG	A	1005	1/1	0.83	0.18	39,39,39,39	0
5	K	A	1006	1/1	0.83	0.14	67,67,67,67	0
3	CA	A	1003	1/1	0.98	0.11	92,92,92,92	0
6	ADP	A	1001	27/27	0.98	0.22	32,42,47,47	0
2	ALF	A	1002	5/5	0.99	0.17	39,39,41,44	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 1001:

$2mF_o$-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.