



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 11:36 pm BST

PDB ID : 1T5S  
Title : Structure of the (SR)Ca<sup>2+</sup>-ATPase Ca<sup>2</sup>-E1-AMPPCP form  
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Deposited on : 2004-05-05  
Resolution : 2.60 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](mailto: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.

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

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

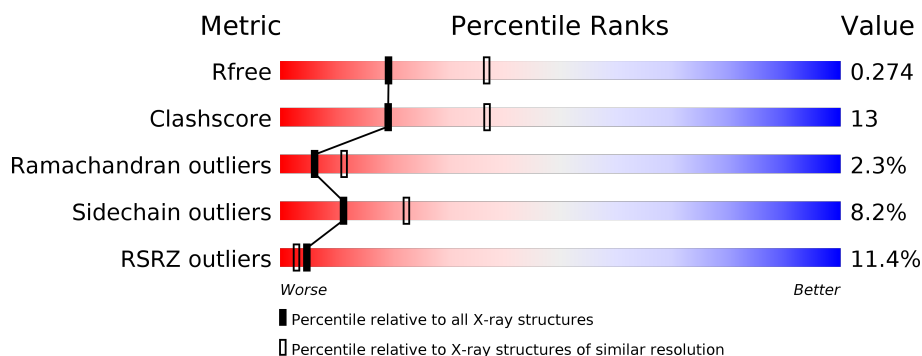
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 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	994	<div> <div>11%</div> <div>71%</div> <div>24%</div> <div>5%</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7746 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
1	A	994	Total	C	N	O	S	0	0	0
			7671	4876	1287	1451	57			

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

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 5 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

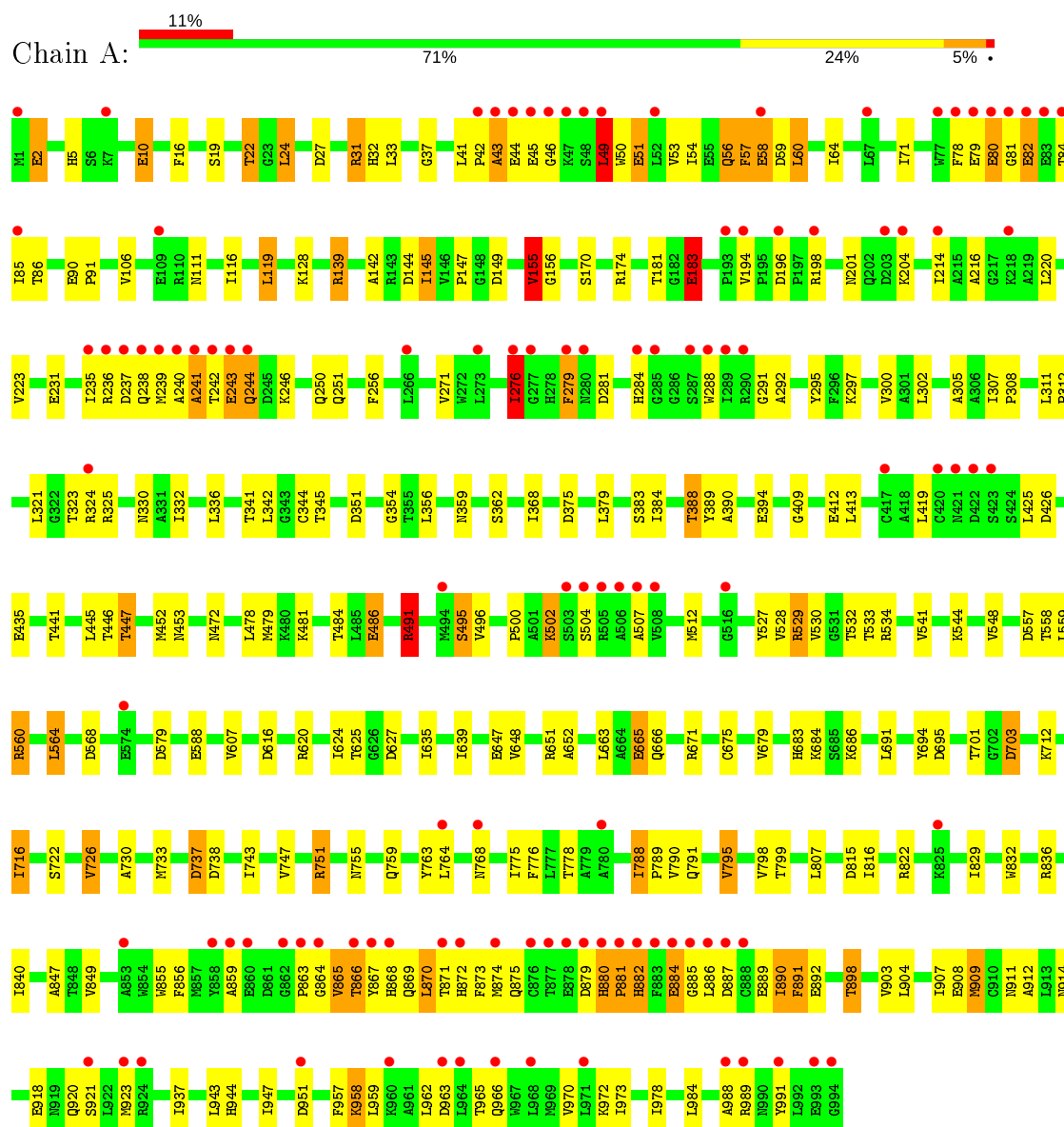
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	40	Total O 40 40	0	0

### 3 Residue-property plots

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

- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1 isoform SERCA1a



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.44Å 76.26Å 151.16Å 90.00° 108.70° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60 38.13 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.60) 99.8 (38.13-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, $R_{free}$	0.242 , 0.285 0.236 , 0.274	Depositor DCC
$R_{free}$ test set	1529 reflections (2.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.1	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 76.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7746	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, ACP, CA, K

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	0.50	0/7812	0.88	24/10592 (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	5

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	703	ASP	CB-CG-OD2	11.32	128.49	118.30
1	A	491	ARG	NE-CZ-NH1	9.47	125.04	120.30
1	A	737	ASP	CB-CG-OD2	7.11	124.70	118.30
1	A	155	VAL	CB-CA-C	-6.96	98.17	111.40
1	A	351	ASP	CB-CG-OD2	6.55	124.19	118.30
1	A	144	ASP	CB-CG-OD2	6.43	124.08	118.30
1	A	27	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	560	ARG	NE-CZ-NH2	6.17	123.39	120.30
1	A	627	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	887	ASP	CB-CG-OD2	6.06	123.75	118.30
1	A	491	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	529	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	59	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	695	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	579	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	616	ASP	CB-CG-OD2	5.44	123.20	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	951	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	281	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	879	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	49	LEU	CA-CB-CG	5.18	127.22	115.30
1	A	815	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	57	PHE	N-CA-C	-5.08	97.27	111.00
1	A	237	ASP	CB-CG-OD2	5.06	122.86	118.30
1	A	568	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (5) 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	880	HIS	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	7671	0	7765	199	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	31	0	14	0	0
6	A	40	0	0	0	0
All	All	7746	0	7779	199	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 13.

All (199) 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	1.74	0.90
1:A:889:GLU:O	1:A:891:PHE:N	2.06	0.89
1:A:116:ILE:HD11	1:A:323:THR:HG21	1.57	0.87
1:A:679:VAL:HG23	1:A:683:HIS:CB	2.04	0.87
1:A:957:PHE:O	1:A:958:LYS:HG2	1.77	0.84
1:A:679:VAL:HG23	1:A:683:HIS:HB2	1.61	0.82
1:A:495:SER:HB2	1:A:588:GLU:OE2	1.79	0.82
1:A:71:ILE:HD11	1:A:300:VAL:HG11	1.62	0.81
1:A:914:ASN:HD21	1:A:978:ILE:HA	1.48	0.79
1:A:354:GLY:HA2	1:A:359:ASN:HB2	1.65	0.78
1:A:679:VAL:CG2	1:A:683:HIS:HB2	2.14	0.77
1:A:868:HIS:O	1:A:871:THR:N	2.17	0.77
1:A:957:PHE:O	1:A:958:LYS:CG	2.32	0.76
1:A:528:VAL:HG21	1:A:541:VAL:HG11	1.70	0.73
1:A:31:ARG:HH11	1:A:31:ARG:HG3	1.52	0.73
1:A:41:LEU:HD13	1:A:236:ARG:HD2	1.71	0.73
1:A:41:LEU:CD1	1:A:236:ARG:HD2	2.21	0.71
1:A:884:GLU:O	1:A:886:LEU:N	2.23	0.71
1:A:558:THR:HG21	1:A:635:ILE:CG1	2.20	0.70
1:A:880:HIS:HB3	1:A:881:PRO:HD2	1.72	0.69
1:A:41:LEU:HD13	1:A:236:ARG:CD	2.22	0.69
1:A:679:VAL:CG2	1:A:683:HIS:CB	2.71	0.69
1:A:889:GLU:O	1:A:891:PHE:O	2.11	0.69
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.95	0.66
1:A:558:THR:HG21	1:A:635:ILE:HG13	1.79	0.65
1:A:962:LEU:HB2	1:A:966:GLN:HG2	1.79	0.65
1:A:81:GLY:HA2	1:A:297:LYS:NZ	2.12	0.64
1:A:139:ARG:HD3	1:A:435:GLU:OE1	1.97	0.64
1:A:155:VAL:HG13	1:A:216:ALA:HA	1.79	0.64
1:A:875:GLN:O	1:A:880:HIS:CG	2.51	0.63
1:A:486:GLU:O	1:A:491:ARG:NH2	2.32	0.62
1:A:10:GLU:O	1:A:10:GLU:OE1	2.18	0.62
1:A:441:THR:OG1	1:A:560:ARG:NH1	2.32	0.62
1:A:671:ARG:HD2	1:A:694:TYR:CE1	2.34	0.62
1:A:639:ILE:O	1:A:639:ILE:HG22	2.00	0.61
1:A:607:VAL:HG12	1:A:639:ILE:HG23	1.82	0.60
1:A:53:VAL:HG12	1:A:106:VAL:HG22	1.83	0.60
1:A:898:THR:HG21	1:A:958:LYS:O	2.02	0.60
1:A:155:VAL:HA	1:A:214:ILE:HG22	1.84	0.60
1:A:43:ALA:HB3	1:A:236:ARG:HH12	1.67	0.59
1:A:530:VAL:O	1:A:533:THR:HB	2.02	0.59
1:A:86:THR:HG22	1:A:790:VAL:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:THR:HG21	1:A:635:ILE:HG12	1.84	0.59
1:A:558:THR:O	1:A:558:THR:HG22	2.04	0.58
1:A:145:ILE:HD12	1:A:223:VAL:HG21	1.84	0.58
1:A:5:HIS:HD2	1:A:194:VAL:HG23	1.69	0.58
1:A:836:ARG:HG3	1:A:984:LEU:HD23	1.86	0.58
1:A:866:THR:HG22	1:A:867:TYR:H	1.69	0.57
1:A:481:LYS:HD3	1:A:484:THR:HG22	1.86	0.57
1:A:241:ALA:C	1:A:243:GLU:N	2.47	0.57
1:A:116:ILE:HD11	1:A:323:THR:CG2	2.34	0.57
1:A:57:PHE:O	1:A:58:GLU:CB	2.53	0.57
1:A:90:GLU:HG2	1:A:790:VAL:HG22	1.86	0.56
1:A:648:VAL:HG13	1:A:651:ARG:HG3	1.86	0.56
1:A:832:TRP:CH2	1:A:988:ALA:HB2	2.40	0.56
1:A:276:ILE:HD11	1:A:291:GLY:O	2.06	0.56
1:A:170:SER:HB2	1:A:486:GLU:HG2	1.88	0.56
1:A:625:THR:O	1:A:679:VAL:HG12	2.06	0.55
1:A:558:THR:CG2	1:A:635:ILE:HG13	2.36	0.55
1:A:60:LEU:H	1:A:60:LEU:HD23	1.72	0.54
1:A:864:GLY:O	1:A:866:THR:N	2.40	0.54
1:A:24:LEU:HD22	1:A:149:ASP:HB3	1.89	0.54
1:A:856:PHE:O	1:A:863:PRO:O	2.26	0.54
1:A:869:GLN:HG2	1:A:869:GLN:O	2.08	0.54
1:A:884:GLU:HA	1:A:884:GLU:OE1	2.08	0.54
1:A:847:ALA:HB1	1:A:973:ILE:HG22	1.90	0.54
1:A:302:LEU:HD13	1:A:775:ILE:HD12	1.90	0.53
1:A:243:GLU:HA	1:A:244:GLN:HG3	1.91	0.53
1:A:42:PRO:O	1:A:43:ALA:C	2.46	0.53
1:A:276:ILE:HD13	1:A:295:TYR:HB2	1.90	0.53
1:A:865:VAL:HG13	1:A:870:LEU:HG	1.91	0.53
1:A:145:ILE:CD1	1:A:223:VAL:HG21	2.39	0.52
1:A:308:PRO:HB3	1:A:764:LEU:HD12	1.92	0.52
1:A:81:GLY:HA2	1:A:297:LYS:HZ2	1.73	0.52
1:A:383:SER:O	1:A:384:ILE:HD13	2.09	0.52
1:A:246:LYS:HB2	1:A:250:GLN:CD	2.31	0.51
1:A:527:TYR:CD1	1:A:534:ARG:HD3	2.46	0.51
1:A:388:THR:HG22	1:A:390:ALA:H	1.76	0.51
1:A:502:LYS:HD2	1:A:502:LYS:N	2.25	0.51
1:A:648:VAL:O	1:A:648:VAL:HG12	2.10	0.51
1:A:871:THR:O	1:A:872:HIS:CG	2.64	0.51
1:A:271:VAL:HG22	1:A:776:PHE:HE1	1.75	0.51
1:A:139:ARG:HG2	1:A:426:ASP:OD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLU:HB2	1:A:91:PRO:HD3	1.92	0.50
1:A:246:LYS:HG3	1:A:251:GLN:HG3	1.93	0.50
1:A:947:ILE:HD11	1:A:957:PHE:CG	2.46	0.50
1:A:891:PHE:O	1:A:892:GLU:CB	2.60	0.50
1:A:666:GLN:HE22	1:A:686:LYS:NZ	2.10	0.50
1:A:722:SER:OG	1:A:738:ASP:OD2	2.22	0.50
1:A:909:MET:HG2	1:A:937:ILE:HG23	1.93	0.50
1:A:944:HIS:O	1:A:947:ILE:HG22	2.11	0.50
1:A:671:ARG:HD2	1:A:694:TYR:CD1	2.47	0.50
1:A:679:VAL:HG23	1:A:683:HIS:CG	2.47	0.50
1:A:90:GLU:CG	1:A:790:VAL:HG22	2.42	0.50
1:A:276:ILE:HD11	1:A:292:ALA:HA	1.93	0.49
1:A:419:LEU:O	1:A:481:LYS:NZ	2.42	0.49
1:A:43:ALA:CB	1:A:236:ARG:NH1	2.76	0.49
1:A:256:PHE:CE1	1:A:829:ILE:HD11	2.47	0.49
1:A:920:GLN:HA	1:A:989:ARG:HH21	1.78	0.49
1:A:43:ALA:HB3	1:A:236:ARG:NH1	2.28	0.48
1:A:240:ALA:O	1:A:241:ALA:C	2.52	0.48
1:A:279:PHE:CZ	1:A:288:TRP:C	2.86	0.48
1:A:491:ARG:NH1	1:A:588:GLU:OE2	2.46	0.48
1:A:875:GLN:O	1:A:880:HIS:CB	2.61	0.48
1:A:962:LEU:HB2	1:A:966:GLN:CG	2.43	0.48
1:A:639:ILE:CG2	1:A:639:ILE:O	2.62	0.48
1:A:41:LEU:HD13	1:A:236:ARG:HD3	1.95	0.47
1:A:909:MET:HE2	1:A:909:MET:HA	1.96	0.47
1:A:33:LEU:O	1:A:37:GLY:N	2.36	0.47
1:A:875:GLN:O	1:A:880:HIS:HB2	2.14	0.47
1:A:142:ALA:O	1:A:145:ILE:HG23	2.14	0.47
1:A:235:ILE:O	1:A:235:ILE:HG22	2.14	0.47
1:A:19:SER:HB2	1:A:22:THR:HG23	1.96	0.47
1:A:111:ASN:HB3	1:A:324:ARG:CD	2.45	0.47
1:A:453:ASN:O	1:A:453:ASN:OD1	2.33	0.47
1:A:368:ILE:HD12	1:A:409:GLY:HA3	1.97	0.46
1:A:671:ARG:HG3	1:A:694:TYR:CE2	2.51	0.46
1:A:884:GLU:OE1	1:A:884:GLU:CA	2.62	0.46
1:A:889:GLU:O	1:A:890:ILE:C	2.51	0.46
1:A:174:ARG:HB2	1:A:216:ALA:HB3	1.98	0.46
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.97	0.46
1:A:495:SER:CB	1:A:588:GLU:OE2	2.58	0.46
1:A:880:HIS:O	1:A:881:PRO:C	2.53	0.46
1:A:751:ARG:HB3	1:A:816:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:962:LEU:N	1:A:966:GLN:HG3	2.30	0.46
1:A:321:LEU:HD21	1:A:325:ARG:CZ	2.46	0.45
1:A:891:PHE:O	1:A:892:GLU:HB3	2.16	0.45
1:A:2:GLU:HG3	1:A:16:PHE:CE1	2.50	0.45
1:A:276:ILE:HG23	1:A:276:ILE:O	2.16	0.45
1:A:354:GLY:HA3	1:A:703:ASP:OD1	2.16	0.45
1:A:903:VAL:HA	1:A:970:VAL:HG13	1.98	0.45
1:A:31:ARG:HH11	1:A:31:ARG:CG	2.27	0.45
1:A:170:SER:CB	1:A:486:GLU:HG2	2.47	0.45
1:A:875:GLN:HA	1:A:880:HIS:HB2	1.99	0.45
1:A:743:ILE:O	1:A:747:VAL:HG23	2.17	0.45
1:A:788:ILE:HG22	1:A:791:GLN:HG3	1.98	0.44
1:A:903:VAL:O	1:A:907:ILE:HG22	2.17	0.44
1:A:388:THR:CG2	1:A:390:ALA:H	2.30	0.44
1:A:379:LEU:HD12	1:A:548:VAL:HG21	1.98	0.44
1:A:201:ASN:HA	1:A:204:LYS:HG3	1.99	0.44
1:A:81:GLY:HA2	1:A:297:LYS:HZ1	1.80	0.44
1:A:957:PHE:O	1:A:958:LYS:CD	2.65	0.44
1:A:962:LEU:O	1:A:963:ASP:C	2.55	0.44
1:A:201:ASN:HD21	1:A:231:GLU:CG	2.30	0.44
1:A:119:LEU:HD11	1:A:330:ASN:HA	1.99	0.44
1:A:652:ALA:HA	1:A:675:CYS:O	2.16	0.44
1:A:78:PHE:O	1:A:80:GLU:N	2.50	0.44
1:A:855:TRP:O	1:A:859:ALA:HB3	2.18	0.44
1:A:496:VAL:O	1:A:512:MET:HA	2.17	0.44
1:A:156:GLY:HA2	1:A:726:VAL:CG1	2.47	0.44
1:A:43:ALA:O	1:A:45:GLU:N	2.51	0.44
1:A:866:THR:HG22	1:A:867:TYR:N	2.33	0.44
1:A:19:SER:CB	1:A:22:THR:HG23	2.48	0.44
1:A:51:GLU:O	1:A:54:ILE:HB	2.18	0.44
1:A:763:TYR:CE1	1:A:912:ALA:HB2	2.53	0.43
1:A:712:LYS:HG3	1:A:730:ALA:HB1	1.99	0.43
1:A:788:ILE:HG12	1:A:789:PRO:HD2	2.00	0.43
1:A:305:ALA:O	1:A:768:ASN:ND2	2.51	0.43
1:A:875:GLN:N	1:A:875:GLN:HE21	2.16	0.43
1:A:389:TYR:HB3	1:A:425:LEU:HD21	2.01	0.43
1:A:478:LEU:HD23	1:A:479:MET:HG2	2.01	0.43
1:A:528:VAL:HG12	1:A:528:VAL:O	2.18	0.43
1:A:909:MET:HG3	1:A:937:ILE:HG12	2.00	0.42
1:A:624:ILE:CG2	1:A:684:LYS:HG2	2.50	0.42
1:A:679:VAL:CG2	1:A:683:HIS:HB3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:ASP:HB3	1:A:559:LEU:CD2	2.49	0.42
1:A:947:ILE:HD11	1:A:957:PHE:CD1	2.55	0.42
1:A:64:ILE:HG21	1:A:307:ILE:CD1	2.49	0.42
1:A:665:GLU:HA	1:A:665:GLU:OE2	2.19	0.42
1:A:271:VAL:HG22	1:A:776:PHE:CE1	2.53	0.42
1:A:170:SER:HB2	1:A:486:GLU:CG	2.48	0.42
1:A:24:LEU:HD22	1:A:149:ASP:CB	2.50	0.42
1:A:648:VAL:O	1:A:648:VAL:CG1	2.68	0.42
1:A:413:LEU:HD22	1:A:564:LEU:HD13	2.02	0.42
1:A:10:GLU:C	1:A:10:GLU:OE1	2.58	0.42
1:A:341:THR:HB	1:A:716:ILE:HD12	2.02	0.41
1:A:869:GLN:C	1:A:871:THR:H	2.24	0.41
1:A:840:ILE:HG21	1:A:911:ASN:HD22	1.85	0.41
1:A:32:HIS:HD2	1:A:147:PRO:O	2.03	0.41
1:A:865:VAL:O	1:A:866:THR:O	2.37	0.41
1:A:904:LEU:O	1:A:908:GLU:HG3	2.21	0.41
1:A:921:SER:CB	1:A:923:MET:HG2	2.51	0.41
1:A:755:ASN:O	1:A:759:GLN:NE2	2.53	0.41
1:A:156:GLY:HA2	1:A:726:VAL:HG13	2.02	0.41
1:A:119:LEU:HD13	1:A:332:ILE:HG13	2.02	0.41
1:A:446:THR:HG23	1:A:472:ASN:ND2	2.36	0.41
1:A:425:LEU:HD11	1:A:447:THR:HG22	2.02	0.41
1:A:181:THR:OG1	1:A:183:GLU:HB2	2.21	0.41
1:A:311:LEU:N	1:A:312:PRO:CD	2.83	0.41
1:A:778:THR:HG23	1:A:849:VAL:HG22	2.01	0.41
1:A:795:VAL:O	1:A:799:THR:OG1	2.39	0.41
1:A:560:ARG:HD3	1:A:560:ARG:HH11	1.69	0.41
1:A:441:THR:CG2	1:A:560:ARG:NH1	2.84	0.41
1:A:119:LEU:HD11	1:A:330:ASN:C	2.41	0.40
1:A:880:HIS:C	1:A:882:HIS:N	2.75	0.40
1:A:452:MET:O	1:A:453:ASN:C	2.59	0.40
1:A:342:LEU:HA	1:A:345:THR:OG1	2.21	0.40
1:A:491:ARG:HD2	1:A:588:GLU:OE1	2.22	0.40
1:A:49:LEU:O	1:A:50:TRP:C	2.60	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	992/994 (100%)	909 (92%)	60 (6%)	23 (2%)	<b>6</b> <b>11</b>

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	ALA
1	A	507	ALA
1	A	865	VAL
1	A	881	PRO
1	A	882	HIS
1	A	885	GLY
1	A	890	ILE
1	A	958	LYS
1	A	959	LEU
1	A	46	GLY
1	A	79	GLU
1	A	82	GLU
1	A	155	VAL
1	A	241	ALA
1	A	870	LEU
1	A	874	MET
1	A	44	GLU
1	A	49	LEU
1	A	239	MET
1	A	242	THR
1	A	866	THR
1	A	183	GLU
1	A	276	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	840/840 (100%)	771 (92%)	69 (8%)	11	22

All (69) 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	31	ARG
1	A	51	GLU
1	A	56	GLN
1	A	58	GLU
1	A	60	LEU
1	A	80	GLU
1	A	82	GLU
1	A	84	THR
1	A	85	ILE
1	A	119	LEU
1	A	128	LYS
1	A	139	ARG
1	A	145	ILE
1	A	155	VAL
1	A	183	GLU
1	A	196	ASP
1	A	198	ARG
1	A	220	LEU
1	A	244	GLN
1	A	276	ILE
1	A	279	PHE
1	A	284	HIS
1	A	336	LEU
1	A	344	CYS
1	A	356	LEU
1	A	362	SER

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Mol	Chain	Res	Type
1	A	375	ASP
1	A	388	THR
1	A	394	GLU
1	A	445	LEU
1	A	447	THR
1	A	486	GLU
1	A	491	ARG
1	A	495	SER
1	A	502	LYS
1	A	504	SER
1	A	532	THR
1	A	544	LYS
1	A	564	LEU
1	A	620	ARG
1	A	647	GLU
1	A	663	LEU
1	A	665	GLU
1	A	691	LEU
1	A	701	THR
1	A	716	ILE
1	A	726	VAL
1	A	733	MET
1	A	737	ASP
1	A	751	ARG
1	A	788	ILE
1	A	795	VAL
1	A	798	VAL
1	A	807	LEU
1	A	822	ARG
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	965	THR
1	A	972	LYS
1	A	991	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	111	ASN
1	A	114	ASN
1	A	250	GLN
1	A	259	GLN
1	A	666	GLN
1	A	755	ASN
1	A	868	HIS
1	A	875	GLN
1	A	880	HIS
1	A	882	HIS
1	A	911	ASN
1	A	914	ASN
1	A	920	GLN
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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are 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	$\# Z  > 2$
5	ACP	A	1001	3	27,33,33	1.36	3 (11%)	32,52,52	1.75	8 (25%)

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
5	ACP	A	1001	3	-	0/15/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	ACP	PB-O3A	4.33	1.63	1.58
5	A	1001	ACP	PB-O2B	-3.39	1.48	1.56
5	A	1001	ACP	C5-C4	2.50	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	ACP	C4-C5-N7	-4.22	105.00	109.40
5	A	1001	ACP	N3-C2-N1	-4.07	122.31	128.68
5	A	1001	ACP	O3G-PG-O2G	3.36	117.88	108.08
5	A	1001	ACP	O2B-PB-O1B	3.05	120.26	110.07
5	A	1001	ACP	PA-O3A-PB	-2.86	123.50	132.56
5	A	1001	ACP	C1'-N9-C4	-2.39	122.45	126.64
5	A	1001	ACP	C2-N1-C6	2.30	122.69	118.75
5	A	1001	ACP	O1G-PG-C3B	-2.10	106.73	111.24

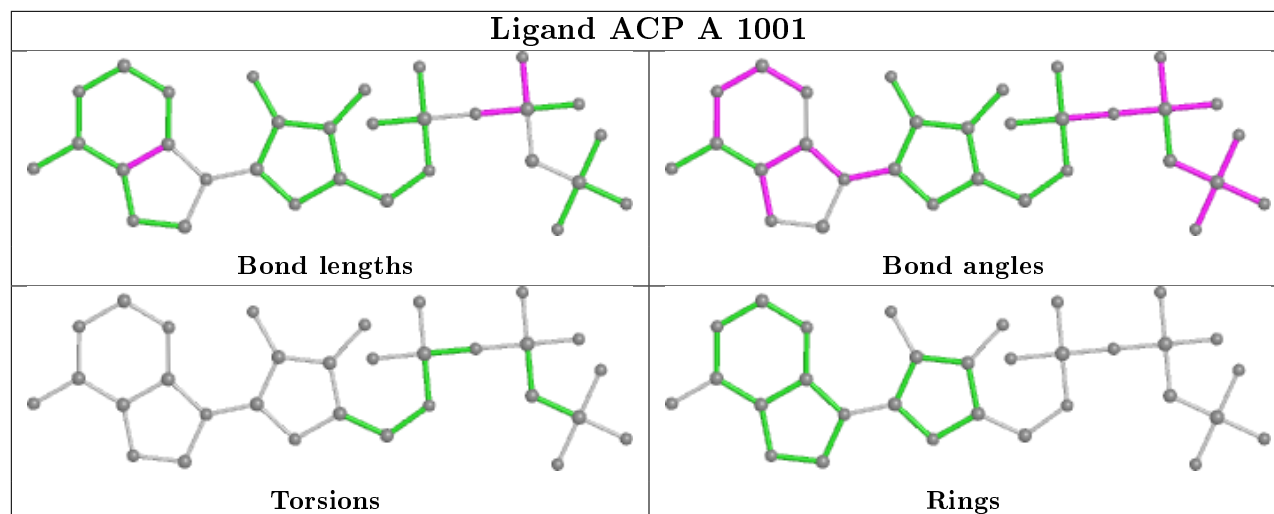
There are no chirality outliers.

There are no torsion outliers.

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	994/994 (100%)	0.75	113 (11%) <b>5</b> <b>3</b>	40, 71, 127, 142	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	506	ALA	11.9
1	A	877	THR	9.8
1	A	240	ALA	8.7
1	A	863	PRO	8.4
1	A	994	GLY	8.2
1	A	83	GLU	7.9
1	A	1	MET	7.7
1	A	47	LYS	7.6
1	A	876	CYS	7.5
1	A	84	THR	6.9
1	A	82	GLU	6.4
1	A	886	LEU	6.3
1	A	505	ARG	6.1
1	A	85	ILE	6.0
1	A	241	ALA	5.9
1	A	507	ALA	5.8
1	A	239	MET	5.8
1	A	81	GLY	5.7
1	A	883	PHE	5.6
1	A	963	ASP	5.1
1	A	242	THR	5.1
1	A	887	ASP	5.1
1	A	288	TRP	5.0
1	A	80	GLU	4.6
1	A	878	GLU	4.6
1	A	79	GLU	4.5
1	A	45	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	993	GLU	4.4
1	A	864	GLY	4.3
1	A	884	GLU	4.3
1	A	504	SER	4.3
1	A	46	GLY	4.2
1	A	881	PRO	4.1
1	A	503	SER	4.1
1	A	885	GLY	4.0
1	A	58	GLU	4.0
1	A	277	GLY	4.0
1	A	964	LEU	3.9
1	A	49	LEU	3.9
1	A	880	HIS	3.9
1	A	243	GLU	3.8
1	A	43	ALA	3.7
1	A	859	ALA	3.7
1	A	991	TYR	3.7
1	A	285	GLY	3.5
1	A	48	SER	3.5
1	A	236	ARG	3.4
1	A	951	ASP	3.4
1	A	879	ASP	3.4
1	A	289	ILE	3.4
1	A	764	LEU	3.4
1	A	825	LYS	3.3
1	A	280	ASN	3.3
1	A	290	ARG	3.3
1	A	780	ALA	3.2
1	A	52	LEU	3.2
1	A	77	TRP	3.2
1	A	923	MET	3.0
1	A	872	HIS	3.0
1	A	858	TYR	3.0
1	A	273	LEU	3.0
1	A	421	ASN	3.0
1	A	423	SER	2.9
1	A	42	PRO	2.9
1	A	78	PHE	2.9
1	A	287	SER	2.9
1	A	874	MET	2.8
1	A	768	ASN	2.8
1	A	238	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	266	LEU	2.8
1	A	868	HIS	2.8
1	A	237	ASP	2.8
1	A	194	VAL	2.7
1	A	853	ALA	2.7
1	A	203	ASP	2.7
1	A	924	ARG	2.7
1	A	244	GLN	2.6
1	A	888	CYS	2.6
1	A	198	ARG	2.6
1	A	882	HIS	2.5
1	A	276	ILE	2.5
1	A	968	LEU	2.5
1	A	44	GLU	2.5
1	A	494	MET	2.5
1	A	516	GLY	2.5
1	A	871	THR	2.4
1	A	960	LYS	2.4
1	A	420	CYS	2.4
1	A	67	LEU	2.4
1	A	204	LYS	2.3
1	A	867	TYR	2.3
1	A	279	PHE	2.3
1	A	862	GLY	2.3
1	A	422	ASP	2.3
1	A	109	GLU	2.2
1	A	860	GLU	2.2
1	A	417	CYS	2.2
1	A	324	ARG	2.2
1	A	574	GLU	2.2
1	A	989	ARG	2.2
1	A	971	LEU	2.2
1	A	866	THR	2.2
1	A	284	HIS	2.1
1	A	218	LYS	2.1
1	A	196	ASP	2.1
1	A	7	LYS	2.1
1	A	214	ILE	2.1
1	A	235	ILE	2.1
1	A	508	VAL	2.1
1	A	988	ALA	2.1
1	A	193	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	921	SER	2.0
1	A	966	GLN	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

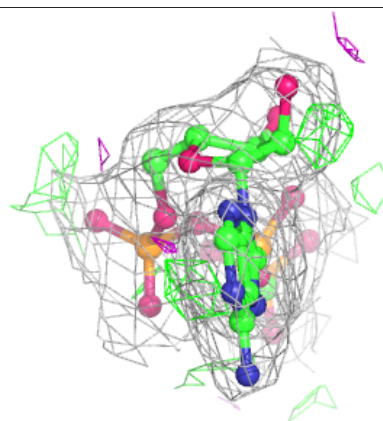
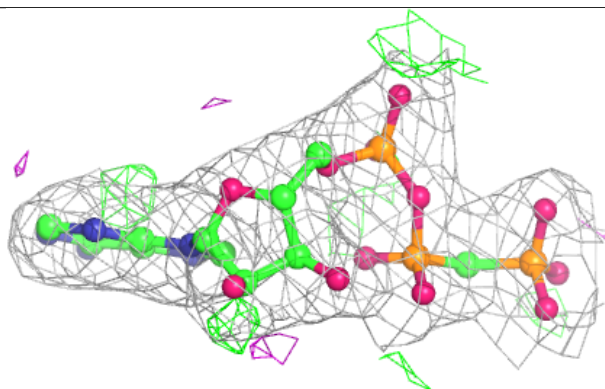
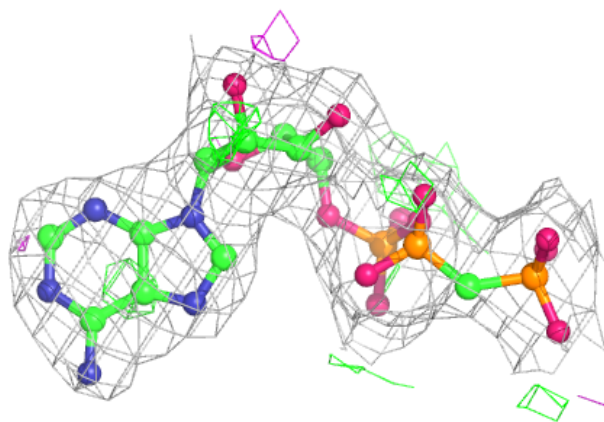
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	1004	1/1	0.78	0.21	83,83,83,83	0
3	MG	A	1005	1/1	0.79	0.29	32,32,32,32	0
2	CA	A	1003	1/1	0.87	0.15	85,85,85,85	0
4	K	A	1006	1/1	0.94	0.10	69,69,69,69	0
5	ACP	A	1001	31/31	0.98	0.27	37,43,45,46	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 ACP 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 ⓘ

There are no such residues in this entry.