



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 01:08 pm BST

PDB ID : 3N8G
Title : Structure of the (SR)Ca²⁺-ATPase Ca²-E1-CaAMPPCP form
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Deposited on : 2010-05-28
Resolution : 2.58 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

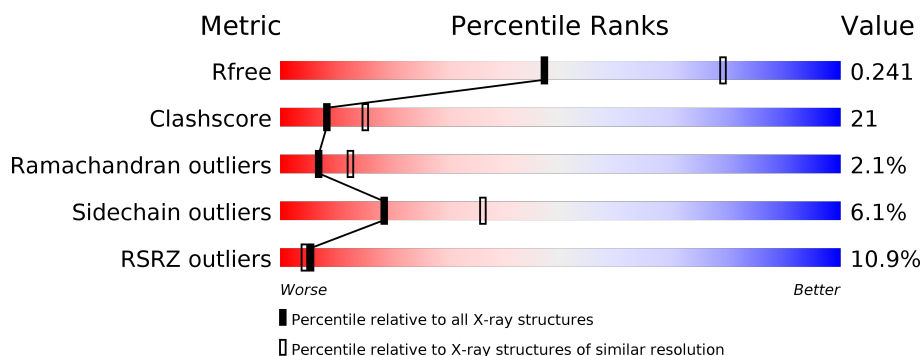
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	994	<div> <div>11%</div> <div>63%</div> <div>33%</div> <div>5%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7798 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 SERCA 1a.

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

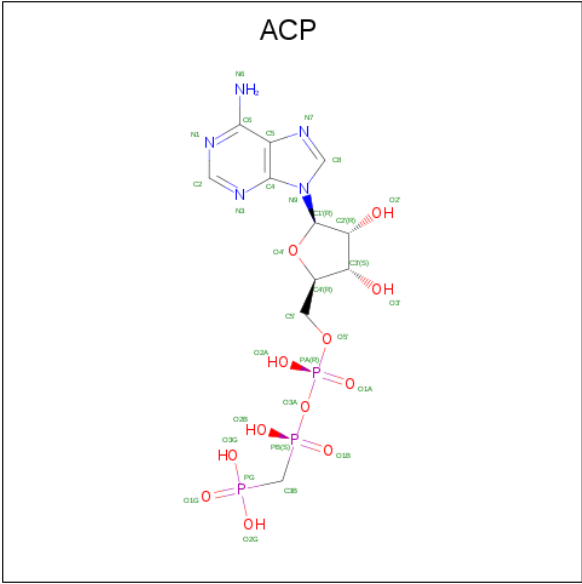
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 4 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

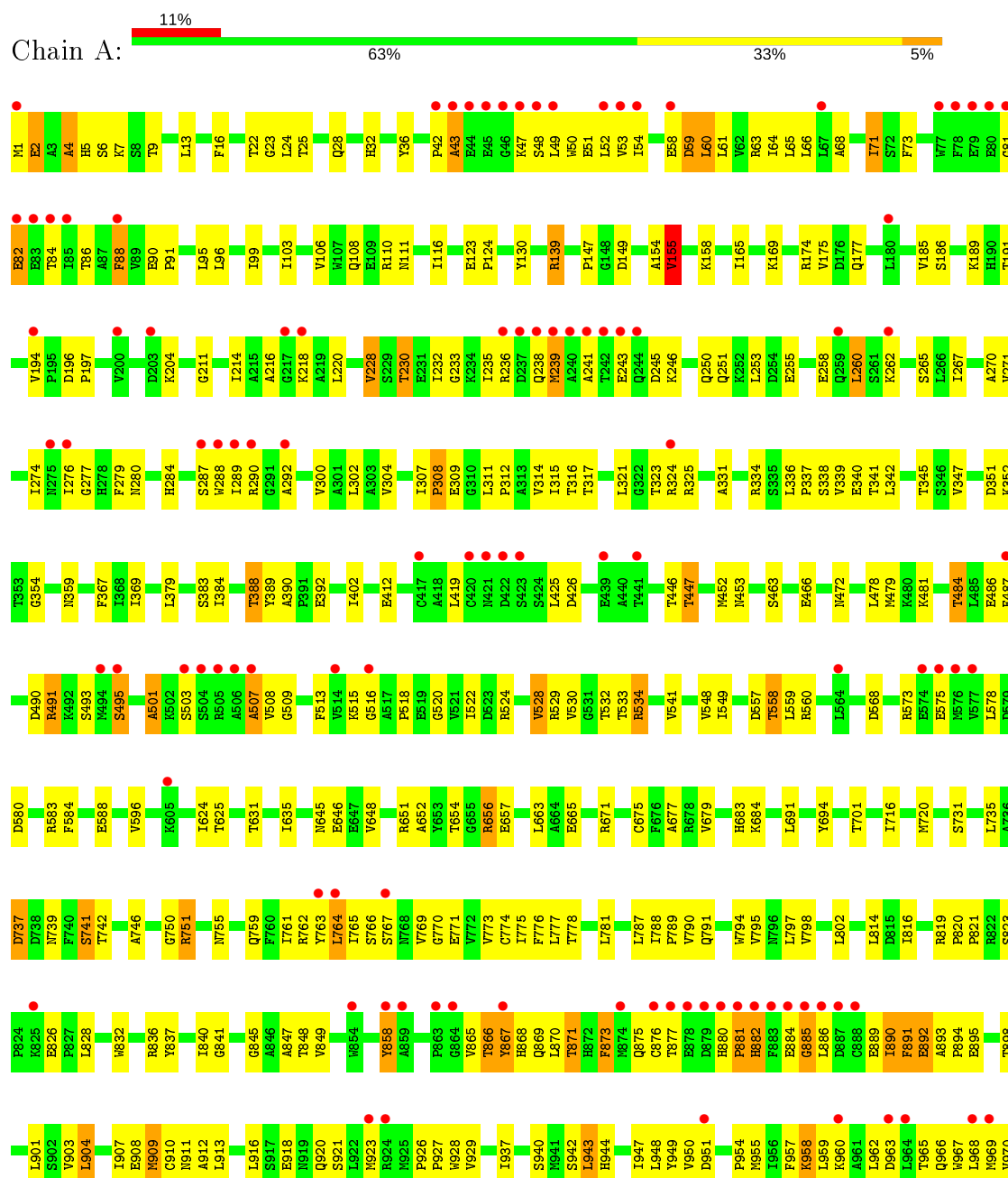
- Molecule 5 is water.

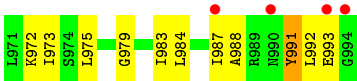
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	92	Total	O	0	0
			92	92		

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 SERCA 1a





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.00 Å 76.00 Å 151.00 Å 90.00° 108.00° 90.00°	Depositor
Resolution (Å)	30.13 – 2.58 38.00 – 2.58	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.13-2.58) 98.4 (38.00-2.58)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.58 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.202 , 0.245 0.197 , 0.241	Depositor DCC
R_{free} test set	1529 reflections (2.83%)	wwPDB-VP
Wilson B-factor (Å ²)	63.8	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 71.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7798	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.37	0/7812	0.56	1/10592 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	VAL	CB-CA-C	-5.18	101.55	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4	ALA	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	325	0
2	A	3	0	0	0	0
3	A	1	0	0	0	0
4	A	31	0	14	6	0
5	A	92	0	0	2	0
All	All	7798	0	7779	325	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 21.

All (325) 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:478:LEU:HD23	1:A:479:MET:HG2	1.49	0.94
1:A:909:MET:HG2	1:A:937:ILE:HG23	1.51	0.90
1:A:880:HIS:HB3	1:A:881:PRO:HD2	1.50	0.90
1:A:341:THR:HB	1:A:716:ILE:HD11	1.54	0.90
1:A:108:GLN:HG3	1:A:317:THR:HG23	1.54	0.89
1:A:155:VAL:HG13	1:A:216:ALA:HA	1.55	0.87
1:A:962:LEU:HB2	1:A:966:GLN:HG2	1.56	0.87
1:A:875:GLN:HA	1:A:880:HIS:HB2	1.61	0.83
1:A:354:GLY:HA2	1:A:359:ASN:HB2	1.59	0.83
1:A:279:PHE:HE2	1:A:288:TRP:HA	1.44	0.82
1:A:388:THR:HG23	1:A:390:ALA:H	1.43	0.82
1:A:388:THR:CG2	1:A:390:ALA:H	1.93	0.81
1:A:528:VAL:HG21	1:A:541:VAL:HG11	1.61	0.81
1:A:495:SER:HB2	1:A:588:GLU:OE2	1.81	0.81
1:A:648:VAL:HG12	1:A:648:VAL:O	1.81	0.80
1:A:59:ASP:OD2	1:A:60:LEU:HG	1.80	0.80
1:A:865:VAL:HG13	1:A:870:LEU:HG	1.62	0.79
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.82	0.79
1:A:238:GLN:O	1:A:239:MET:HB2	1.83	0.78
1:A:481:LYS:HD3	1:A:484:THR:HG22	1.67	0.76
1:A:24:LEU:HD12	1:A:149:ASP:HB3	1.67	0.76
1:A:836:ARG:HG3	1:A:984:LEU:HD23	1.68	0.76
1:A:798:VAL:HG13	1:A:940:SER:HB3	1.69	0.75
1:A:962:LEU:N	1:A:966:GLN:HG3	2.01	0.75
1:A:944:HIS:O	1:A:947:ILE:HG22	1.88	0.74
1:A:308:PRO:HB3	1:A:764:LEU:HD12	1.69	0.73
1:A:347:VAL:HG11	1:A:691:LEU:HD13	1.71	0.72
1:A:425:LEU:HD11	1:A:447:THR:HG22	1.71	0.72
1:A:947:ILE:HD11	1:A:957:PHE:CD1	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:957:PHE:O	1:A:958:LYS:HB2	1.89	0.72
1:A:267:ILE:O	1:A:271:VAL:HG23	1.90	0.72
1:A:271:VAL:HG22	1:A:776:PHE:CE1	2.24	0.72
1:A:869:GLN:C	1:A:871:THR:H	1.92	0.71
1:A:116:ILE:HD11	1:A:323:THR:HG21	1.71	0.71
1:A:560:ARG:HH22	4:A:1001:ACP:PB	2.14	0.70
1:A:948:LEU:HB3	1:A:949:TYR:CD2	2.25	0.70
1:A:889:GLU:O	1:A:891:PHE:N	2.24	0.70
1:A:279:PHE:CE2	1:A:288:TRP:HA	2.24	0.70
1:A:81:GLY:O	1:A:82:GLU:HB2	1.90	0.69
1:A:909:MET:CG	1:A:937:ILE:HG23	2.22	0.69
1:A:788:ILE:HG23	1:A:789:PRO:HD2	1.75	0.68
1:A:53:VAL:HG12	1:A:106:VAL:HG22	1.75	0.68
1:A:962:LEU:HG	1:A:966:GLN:HE21	1.59	0.68
1:A:60:LEU:HD12	1:A:61:LEU:HG	1.77	0.66
1:A:32:HIS:HD2	1:A:147:PRO:O	1.78	0.66
1:A:969:MET:O	1:A:973:ILE:HG13	1.95	0.66
1:A:904:LEU:O	1:A:908:GLU:HG3	1.96	0.65
1:A:778:THR:HG23	1:A:849:VAL:HG22	1.77	0.65
1:A:5:HIS:CE1	1:A:204:LYS:HE2	2.31	0.65
1:A:491:ARG:HD2	1:A:588:GLU:OE1	1.95	0.65
1:A:95:LEU:O	1:A:99:ILE:HG12	1.95	0.65
1:A:271:VAL:HG22	1:A:776:PHE:HE1	1.62	0.65
1:A:5:HIS:HD2	1:A:194:VAL:HG23	1.61	0.65
1:A:656:ARG:HG2	1:A:657:GLU:N	2.11	0.65
1:A:341:THR:CB	1:A:716:ILE:HD11	2.25	0.64
1:A:962:LEU:H	1:A:966:GLN:HG3	1.62	0.64
1:A:580:ASP:O	1:A:583:ARG:HG2	1.98	0.63
1:A:947:ILE:HD11	1:A:957:PHE:CG	2.33	0.63
1:A:279:PHE:HZ	1:A:288:TRP:C	2.02	0.63
1:A:950:VAL:O	1:A:954:PRO:HD3	1.98	0.63
1:A:534:ARG:HH21	1:A:568:ASP:HB2	1.63	0.62
1:A:389:TYR:HB3	1:A:425:LEU:HD21	1.81	0.62
1:A:90:GLU:HG2	1:A:790:VAL:HG22	1.80	0.62
1:A:665:GLU:HA	1:A:665:GLU:OE1	2.00	0.61
1:A:302:LEU:HD13	1:A:775:ILE:HD12	1.82	0.61
1:A:158:LYS:HE3	1:A:211:GLY:HA2	1.81	0.61
1:A:979:GLY:O	1:A:983:ILE:HG12	2.01	0.61
1:A:869:GLN:HG2	1:A:869:GLN:O	2.00	0.61
1:A:557:ASP:HB3	1:A:559:LEU:HD21	1.84	0.60
1:A:671:ARG:HD2	1:A:694:TYR:CE1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:VAL:HG11	1:A:106:VAL:HG13	1.83	0.60
1:A:4:ALA:HB3	1:A:7:LYS:HG3	1.84	0.60
1:A:383:SER:O	1:A:384:ILE:HD13	2.02	0.59
1:A:948:LEU:HD22	1:A:960:LYS:HA	1.82	0.59
1:A:230:THR:HG22	1:A:233:GLY:H	1.66	0.59
1:A:847:ALA:HB1	1:A:973:ILE:HG22	1.83	0.59
1:A:99:ILE:O	1:A:103:ILE:HG13	2.02	0.59
1:A:255:GLU:O	1:A:258:GLU:HB3	2.02	0.58
1:A:992:LEU:O	1:A:993:GLU:HG3	2.03	0.58
1:A:965:THR:HA	1:A:968:LEU:HD12	1.85	0.58
1:A:948:LEU:HB3	1:A:949:TYR:CE2	2.39	0.58
1:A:177:GLN:HE22	1:A:189:LYS:NZ	2.02	0.58
1:A:894:PRO:HB3	1:A:958:LYS:HB3	1.84	0.57
1:A:59:ASP:O	1:A:63:ARG:HG3	2.04	0.57
1:A:351:ASP:OD1	4:A:1001:ACP:O3G	2.23	0.57
1:A:890:ILE:HD12	1:A:891:PHE:H	1.69	0.57
1:A:24:LEU:CD1	1:A:149:ASP:HB3	2.34	0.56
1:A:880:HIS:O	1:A:881:PRO:C	2.43	0.56
1:A:271:VAL:HA	1:A:274:ILE:HD12	1.86	0.56
1:A:490:ASP:OD1	1:A:491:ARG:N	2.37	0.56
1:A:530:VAL:O	1:A:533:THR:HB	2.04	0.56
1:A:116:ILE:HD11	1:A:323:THR:CG2	2.33	0.56
1:A:338:SER:HA	1:A:716:ILE:HD12	1.88	0.56
1:A:654:THR:HG21	1:A:656:ARG:NH1	2.20	0.56
1:A:71:ILE:HD11	1:A:300:VAL:HG11	1.88	0.56
1:A:560:ARG:NH2	4:A:1001:ACP:O1B	2.38	0.56
1:A:869:GLN:C	1:A:871:THR:N	2.59	0.56
1:A:90:GLU:HB2	1:A:91:PRO:HD3	1.87	0.56
1:A:880:HIS:HB3	1:A:881:PRO:CD	2.30	0.56
1:A:814:LEU:HD12	1:A:920:GLN:HE21	1.70	0.55
1:A:246:LYS:HG3	1:A:251:GLN:HG3	1.87	0.55
1:A:369:ILE:HG13	1:A:528:VAL:HG13	1.87	0.55
1:A:867:TYR:O	1:A:868:HIS:HB2	2.06	0.55
1:A:174:ARG:HB2	1:A:216:ALA:HB3	1.89	0.55
1:A:5:HIS:CD2	1:A:194:VAL:HG23	2.41	0.55
1:A:869:GLN:OE1	1:A:871:THR:O	2.25	0.55
1:A:367:PHE:CD2	1:A:379:LEU:HD13	2.41	0.54
1:A:891:PHE:O	1:A:892:GLU:HB2	2.07	0.54
1:A:891:PHE:O	1:A:892:GLU:CB	2.55	0.54
1:A:379:LEU:HD12	1:A:548:VAL:HG21	1.90	0.54
1:A:507:ALA:C	1:A:509:GLY:H	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ALA:CB	1:A:7:LYS:HG3	2.38	0.53
1:A:90:GLU:CG	1:A:790:VAL:HG22	2.37	0.53
1:A:890:ILE:HD12	1:A:891:PHE:N	2.23	0.53
1:A:769:VAL:O	1:A:773:VAL:HG23	2.09	0.53
1:A:968:LEU:O	1:A:972:LYS:HB2	2.09	0.53
1:A:139:ARG:HG2	1:A:426:ASP:OD2	2.08	0.53
1:A:279:PHE:CZ	1:A:288:TRP:C	2.83	0.53
1:A:916:LEU:HD11	1:A:927:PRO:HA	1.90	0.52
1:A:65:LEU:HG	1:A:304:VAL:HG13	1.91	0.52
1:A:165:ILE:HG22	1:A:191:THR:HG22	1.90	0.52
1:A:1:MET:N	1:A:36:TYR:CE1	2.75	0.52
1:A:765:ILE:HG21	1:A:837:TYR:CD2	2.45	0.52
1:A:533:THR:CG2	1:A:534:ARG:N	2.72	0.52
1:A:962:LEU:HB2	1:A:966:GLN:CG	2.35	0.52
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.90	0.52
1:A:868:HIS:O	1:A:871:THR:N	2.43	0.52
1:A:42:PRO:O	1:A:43:ALA:C	2.48	0.52
1:A:534:ARG:HH21	1:A:568:ASP:CB	2.22	0.52
1:A:654:THR:HA	1:A:677:ALA:O	2.10	0.52
1:A:557:ASP:HB3	1:A:559:LEU:CD2	2.39	0.52
1:A:774:CYS:HB2	1:A:848:THR:HG21	1.91	0.52
1:A:737:ASP:HB3	1:A:739:ASN:H	1.74	0.51
1:A:155:VAL:HG13	1:A:216:ALA:CA	2.36	0.51
1:A:507:ALA:C	1:A:509:GLY:N	2.62	0.51
1:A:648:VAL:CG1	1:A:648:VAL:O	2.53	0.51
1:A:81:GLY:O	1:A:82:GLU:CB	2.58	0.51
1:A:279:PHE:HZ	1:A:289:ILE:N	2.09	0.51
1:A:867:TYR:HD1	1:A:868:HIS:CD2	2.28	0.51
1:A:884:GLU:O	1:A:886:LEU:N	2.44	0.51
1:A:48:SER:HB3	1:A:53:VAL:HG23	1.93	0.51
1:A:773:VAL:CG1	1:A:845:GLY:HA3	2.41	0.51
1:A:23:GLY:HA3	1:A:130:TYR:O	2.11	0.50
1:A:446:THR:HG23	1:A:472:ASN:ND2	2.25	0.50
1:A:761:ILE:O	1:A:765:ILE:HG12	2.10	0.50
1:A:58:GLU:HG3	1:A:63:ARG:HH21	1.77	0.50
1:A:279:PHE:CE1	1:A:292:ALA:N	2.79	0.50
1:A:321:LEU:HD21	1:A:325:ARG:NH2	2.26	0.50
1:A:337:PRO:O	1:A:340:GLU:HG2	2.11	0.50
1:A:388:THR:HG23	1:A:389:TYR:N	2.26	0.50
1:A:49:LEU:HD12	1:A:50:TRP:HE3	1.76	0.50
1:A:755:ASN:O	1:A:759:GLN:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:VAL:O	1:A:907:ILE:HG22	2.12	0.50
1:A:751:ARG:NH1	5:A:1043:HOH:O	2.44	0.49
1:A:49:LEU:HD12	1:A:50:TRP:N	2.27	0.49
1:A:42:PRO:O	1:A:43:ALA:O	2.31	0.49
1:A:762:ARG:HG3	1:A:837:TYR:HE1	1.76	0.49
1:A:270:ALA:O	1:A:274:ILE:HG13	2.11	0.49
1:A:277:GLY:C	1:A:279:PHE:H	2.15	0.49
1:A:763:TYR:CE1	1:A:912:ALA:HB2	2.47	0.49
1:A:388:THR:HG23	1:A:390:ALA:N	2.22	0.49
1:A:86:THR:CG2	1:A:790:VAL:HG21	2.43	0.49
1:A:402:ILE:C	1:A:402:ILE:HD12	2.32	0.49
1:A:486:GLU:CD	1:A:486:GLU:H	2.17	0.48
1:A:766:SER:HB2	1:A:840:ILE:HB	1.95	0.48
1:A:823:SER:HB3	1:A:826:GLU:OE2	2.13	0.48
1:A:893:ALA:HB1	1:A:895:GLU:OE1	2.13	0.48
1:A:880:HIS:CB	1:A:881:PRO:HD2	2.34	0.48
1:A:230:THR:CG2	1:A:232:ILE:HG22	2.43	0.48
1:A:25:THR:OG1	1:A:28:GLN:HG3	2.14	0.48
1:A:652:ALA:HA	1:A:675:CYS:O	2.14	0.48
1:A:154:ALA:HB2	1:A:218:LYS:HG3	1.96	0.48
1:A:991:TYR:CE1	1:A:993:GLU:HB2	2.48	0.48
1:A:86:THR:HG22	1:A:790:VAL:HG21	1.96	0.48
1:A:177:GLN:HE22	1:A:189:LYS:HZ3	1.60	0.48
1:A:336:LEU:N	1:A:337:PRO:HD2	2.28	0.48
1:A:60:LEU:HG	1:A:60:LEU:H	1.54	0.48
1:A:648:VAL:HG13	1:A:651:ARG:HB2	1.96	0.48
1:A:558:THR:HG21	1:A:635:ILE:HG13	1.95	0.47
1:A:873:PHE:O	1:A:873:PHE:CG	2.67	0.47
1:A:529:ARG:HH22	1:A:568:ASP:CG	2.15	0.47
1:A:770:GLY:HA2	1:A:841:GLY:O	2.14	0.47
1:A:836:ARG:CG	1:A:984:LEU:HD23	2.43	0.47
1:A:331:ALA:HB2	1:A:742:THR:HG21	1.96	0.47
1:A:260:LEU:HA	1:A:260:LEU:HD12	1.71	0.47
1:A:49:LEU:HG	1:A:52:LEU:H	1.79	0.47
1:A:267:ILE:O	1:A:270:ALA:HB3	2.15	0.47
1:A:892:GLU:OE1	1:A:892:GLU:HA	2.15	0.47
1:A:771:GLU:O	1:A:774:CYS:HB3	2.14	0.47
1:A:53:VAL:CG1	1:A:106:VAL:HG13	2.45	0.47
1:A:311:LEU:O	1:A:315:ILE:HG13	2.14	0.47
1:A:463:SER:OG	1:A:466:GLU:HG3	2.15	0.47
1:A:53:VAL:CG1	1:A:106:VAL:HG22	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LEU:HD23	1:A:797:LEU:HD21	1.97	0.46
1:A:832:TRP:CH2	1:A:988:ALA:HB2	2.50	0.46
1:A:238:GLN:O	1:A:239:MET:CB	2.60	0.46
1:A:889:GLU:O	1:A:891:PHE:CD2	2.68	0.46
1:A:59:ASP:CG	1:A:60:LEU:H	2.18	0.46
1:A:528:VAL:HG21	1:A:541:VAL:CG1	2.39	0.46
1:A:777:LEU:O	1:A:781:LEU:HB2	2.16	0.46
1:A:957:PHE:O	1:A:958:LYS:CB	2.62	0.46
1:A:241:ALA:C	1:A:243:GLU:H	2.19	0.46
1:A:515:LYS:O	4:A:1001:ACP:H2	2.15	0.46
1:A:169:LYS:HA	1:A:169:LYS:HD3	1.79	0.46
1:A:890:ILE:O	1:A:893:ALA:N	2.47	0.46
1:A:491:ARG:NH2	1:A:584:PHE:HD1	2.14	0.46
1:A:54:ILE:HD13	1:A:106:VAL:HG21	1.98	0.46
1:A:24:LEU:HD22	1:A:28:GLN:HB3	1.97	0.46
1:A:671:ARG:HG3	1:A:694:TYR:CE2	2.51	0.46
1:A:4:ALA:HB1	1:A:6:SER:H	1.81	0.45
1:A:821:PRO:HB3	5:A:1043:HOH:O	2.16	0.45
1:A:875:GLN:O	1:A:880:HIS:CG	2.70	0.45
1:A:983:ILE:O	1:A:987:ILE:HG13	2.15	0.45
1:A:68:ALA:O	1:A:71:ILE:HG12	2.17	0.45
1:A:991:TYR:C	1:A:991:TYR:CD1	2.87	0.45
1:A:334:ARG:NH1	1:A:731:SER:O	2.49	0.45
1:A:518:PRO:O	1:A:522:ILE:HD12	2.16	0.45
1:A:246:LYS:HB2	1:A:250:GLN:CD	2.37	0.45
1:A:926:PRO:O	1:A:929:VAL:HG22	2.17	0.45
1:A:501:ALA:O	1:A:503:SER:N	2.49	0.45
1:A:66:LEU:HA	1:A:66:LEU:HD12	1.87	0.45
1:A:882:HIS:CD2	1:A:885:GLY:H	2.35	0.45
1:A:679:VAL:HB	1:A:683:HIS:HB2	1.98	0.45
1:A:339:VAL:O	1:A:750:GLY:HA3	2.17	0.45
1:A:123:GLU:HA	1:A:124:PRO:HD3	1.75	0.45
1:A:311:LEU:O	1:A:314:VAL:HG12	2.16	0.45
1:A:481:LYS:HD3	1:A:484:THR:CG2	2.43	0.44
1:A:486:GLU:O	1:A:491:ARG:NH2	2.49	0.44
1:A:351:ASP:HA	1:A:624:ILE:O	2.18	0.44
1:A:175:VAL:HG22	1:A:214:ILE:HD13	1.99	0.44
1:A:61:LEU:HD13	1:A:308:PRO:HD2	2.00	0.44
1:A:64:ILE:HG21	1:A:307:ILE:CD1	2.48	0.44
1:A:43:ALA:HB3	1:A:236:ARG:NH1	2.32	0.44
1:A:926:PRO:HB2	1:A:928:TRP:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:VAL:HG21	1:A:302:LEU:HD23	1.99	0.44
1:A:903:VAL:HA	1:A:970:VAL:HG13	2.00	0.44
1:A:794:TRP:CD2	1:A:947:ILE:HD12	2.53	0.44
1:A:948:LEU:CD2	1:A:960:LYS:HA	2.48	0.44
1:A:279:PHE:HD2	1:A:280:ASN:OD1	2.00	0.44
1:A:873:PHE:C	1:A:873:PHE:CD2	2.88	0.44
1:A:529:ARG:NH2	1:A:568:ASP:OD2	2.51	0.44
1:A:739:ASN:OD1	1:A:741:SER:HB2	2.18	0.44
1:A:196:ASP:HA	1:A:197:PRO:HD3	1.81	0.44
1:A:352:LYS:HD2	1:A:635:ILE:CD1	2.48	0.44
1:A:645:ASN:O	1:A:646:GLU:C	2.56	0.43
1:A:774:CYS:HB2	1:A:848:THR:CG2	2.48	0.43
1:A:354:GLY:CA	1:A:359:ASN:HB2	2.39	0.43
1:A:943:LEU:HD12	1:A:943:LEU:HA	1.86	0.43
1:A:91:PRO:O	1:A:95:LEU:HG	2.18	0.43
1:A:287:SER:HB3	1:A:290:ARG:HB2	1.99	0.43
1:A:342:LEU:HA	1:A:342:LEU:HD12	1.83	0.43
1:A:580:ASP:HB3	1:A:583:ARG:HE	1.84	0.43
1:A:549:ILE:HD11	1:A:596:VAL:HG21	2.00	0.43
1:A:751:ARG:HB3	1:A:816:ILE:HD11	2.01	0.43
1:A:867:TYR:CD1	1:A:868:HIS:CD2	3.07	0.43
1:A:262:LYS:O	1:A:265:SER:HB2	2.19	0.43
1:A:814:LEU:HD23	1:A:814:LEU:HA	1.88	0.43
1:A:889:GLU:O	1:A:890:ILE:C	2.57	0.43
1:A:921:SER:HB3	1:A:923:MET:H	1.83	0.43
1:A:501:ALA:C	1:A:503:SER:H	2.22	0.43
1:A:49:LEU:HG	1:A:51:GLU:H	1.84	0.43
1:A:720:MET:CE	1:A:735:LEU:HD12	2.49	0.43
1:A:958:LYS:N	1:A:958:LYS:CD	2.82	0.43
1:A:988:ALA:C	1:A:991:TYR:O	2.57	0.43
1:A:342:LEU:HD23	1:A:746:ALA:CB	2.49	0.42
1:A:42:PRO:HD3	1:A:228:VAL:HG22	2.00	0.42
1:A:875:GLN:N	1:A:875:GLN:HE21	2.17	0.42
1:A:516:GLY:HA2	4:A:1001:ACP:N3	2.33	0.42
1:A:491:ARG:HG3	1:A:493:SER:OG	2.19	0.42
1:A:419:LEU:HD12	1:A:513:PHE:CE2	2.54	0.42
1:A:625:THR:O	1:A:679:VAL:HG22	2.19	0.42
1:A:867:TYR:O	1:A:868:HIS:CB	2.67	0.42
1:A:795:VAL:HG13	1:A:901:LEU:HD12	2.01	0.42
1:A:910:CYS:O	1:A:913:LEU:HB2	2.19	0.42
1:A:279:PHE:CD1	1:A:292:ALA:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LYS:HB3	1:A:48:SER:H	1.70	0.42
1:A:49:LEU:HD12	1:A:50:TRP:H	1.83	0.42
1:A:575:GLU:O	1:A:575:GLU:HG2	2.19	0.42
1:A:963:ASP:HA	1:A:967:TRP:HD1	1.85	0.42
1:A:42:PRO:HG2	1:A:43:ALA:H	1.83	0.42
1:A:788:ILE:CG2	1:A:789:PRO:HD2	2.46	0.42
1:A:921:SER:C	1:A:923:MET:N	2.71	0.42
1:A:253:LEU:HD23	1:A:828:LEU:HD21	2.02	0.42
1:A:96:LEU:HB3	1:A:797:LEU:HD13	2.00	0.42
1:A:870:LEU:O	1:A:871:THR:CB	2.67	0.42
1:A:9:THR:O	1:A:13:LEU:HG	2.20	0.42
1:A:96:LEU:HD23	1:A:797:LEU:HD11	2.02	0.42
1:A:487:PHE:CE2	4:A:1001:ACP:C4	3.03	0.42
1:A:185:VAL:HG12	1:A:186:SER:N	2.35	0.42
1:A:2:GLU:HG3	1:A:16:PHE:CE1	2.55	0.42
1:A:342:LEU:HA	1:A:345:THR:OG1	2.19	0.42
1:A:679:VAL:HB	1:A:683:HIS:CB	2.50	0.42
1:A:73:PHE:HE1	1:A:88:PHE:CE1	2.38	0.42
1:A:390:ALA:C	1:A:392:GLU:H	2.23	0.42
1:A:671:ARG:HD2	1:A:694:TYR:CD1	2.54	0.42
1:A:235:ILE:O	1:A:235:ILE:HG22	2.20	0.42
1:A:58:GLU:HG3	1:A:63:ARG:NH2	2.35	0.42
1:A:767:SER:HB3	1:A:908:GLU:OE2	2.19	0.41
1:A:866:THR:HG23	1:A:867:TYR:CD2	2.55	0.41
1:A:338:SER:HA	1:A:716:ILE:CD1	2.49	0.41
1:A:452:MET:O	1:A:453:ASN:C	2.59	0.41
1:A:478:LEU:CD2	1:A:479:MET:HG2	2.35	0.41
1:A:388:THR:HG22	1:A:390:ALA:H	1.77	0.41
1:A:533:THR:HG22	1:A:534:ARG:N	2.35	0.41
1:A:311:LEU:N	1:A:312:PRO:CD	2.83	0.41
1:A:338:SER:O	1:A:342:LEU:HB2	2.20	0.41
1:A:654:THR:HG21	1:A:656:ARG:HH12	1.85	0.41
1:A:762:ARG:CZ	1:A:836:ARG:NH2	2.83	0.41
1:A:819:ARG:HB3	1:A:820:PRO:HD2	2.01	0.41
1:A:958:LYS:HD2	1:A:958:LYS:N	2.35	0.41
1:A:646:GLU:OE1	1:A:651:ARG:NH1	2.53	0.41
1:A:520:GLY:O	1:A:524:ARG:HG3	2.19	0.41
1:A:795:VAL:HG13	1:A:901:LEU:CD1	2.51	0.41
1:A:478:LEU:C	1:A:501:ALA:HB2	2.42	0.41
1:A:865:VAL:O	1:A:866:THR:O	2.37	0.41
1:A:624:ILE:HG22	1:A:684:LYS:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:ARG:HE	1:A:573:ARG:HB3	1.72	0.40
1:A:787:LEU:HA	1:A:791:GLN:OE1	2.21	0.40
1:A:969:MET:SD	1:A:972:LYS:HD3	2.62	0.40
1:A:111:ASN:HB3	1:A:324:ARG:CD	2.51	0.40
1:A:279:PHE:C	1:A:279:PHE:CD2	2.94	0.40
1:A:271:VAL:HG21	1:A:302:LEU:CD2	2.52	0.40
1:A:59:ASP:CG	1:A:312:PRO:HB3	2.42	0.40
1:A:869:GLN:O	1:A:870:LEU:HB2	2.20	0.40
1:A:276:ILE:HA	1:A:276:ILE:HD12	1.76	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%)	911 (92%)	60 (6%)	21 (2%)	7 12

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	ALA
1	A	239	MET
1	A	871	THR
1	A	881	PRO
1	A	882	HIS
1	A	890	ILE
1	A	59	ASP
1	A	82	GLU
1	A	507	ALA
1	A	866	THR
1	A	876	CYS
1	A	885	GLY

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Mol	Chain	Res	Type
1	A	892	GLU
1	A	958	LYS
1	A	959	LEU
1	A	84	THR
1	A	867	TYR
1	A	501	ALA
1	A	858	TYR
1	A	877	THR
1	A	155	VAL

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%)	789 (94%)	51 (6%)	18	36

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	22	THR
1	A	60	LEU
1	A	71	ILE
1	A	88	PHE
1	A	110	ARG
1	A	139	ARG
1	A	155	VAL
1	A	220	LEU
1	A	228	VAL
1	A	230	THR
1	A	245	ASP
1	A	260	LEU
1	A	284	HIS
1	A	308	PRO
1	A	309	GLU
1	A	316	THR

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Mol	Chain	Res	Type
1	A	388	THR
1	A	447	THR
1	A	484	THR
1	A	491	ARG
1	A	495	SER
1	A	508	VAL
1	A	528	VAL
1	A	532	THR
1	A	534	ARG
1	A	558	THR
1	A	578	LEU
1	A	631	THR
1	A	656	ARG
1	A	663	LEU
1	A	701	THR
1	A	737	ASP
1	A	741	SER
1	A	751	ARG
1	A	764	LEU
1	A	802	LEU
1	A	858	TYR
1	A	873	PHE
1	A	891	PHE
1	A	898	THR
1	A	904	LEU
1	A	909	MET
1	A	911	ASN
1	A	918	GLU
1	A	942	SER
1	A	943	LEU
1	A	951	ASP
1	A	955	MET
1	A	975	LEU
1	A	991	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	38	HIS
1	A	114	ASN
1	A	177	GLN

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Mol	Chain	Res	Type
1	A	755	ASN
1	A	868	HIS
1	A	875	GLN
1	A	882	HIS
1	A	911	ASN
1	A	920	GLN
1	A	966	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
4	ACP	A	1001	2	27,33,33	1.82	7 (25%)	32,52,52	1.80	7 (21%)

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	ACP	A	1001	2	-	1/15/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	ACP	PG-O1G	3.97	1.58	1.50
4	A	1001	ACP	PB-O2B	-3.61	1.47	1.56
4	A	1001	ACP	PG-O3G	-3.52	1.46	1.54
4	A	1001	ACP	PB-O1B	2.88	1.58	1.51
4	A	1001	ACP	C2'-C1'	2.65	1.57	1.53
4	A	1001	ACP	C2-N3	2.27	1.35	1.32
4	A	1001	ACP	PG-O2G	2.04	1.59	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	ACP	PA-O3A-PB	4.51	146.86	132.56
4	A	1001	ACP	O3G-PG-C3B	3.83	115.69	106.40
4	A	1001	ACP	O2G-PG-O1G	-3.14	104.08	112.39
4	A	1001	ACP	C1'-N9-C4	-2.99	121.40	126.64
4	A	1001	ACP	O1B-PB-C3B	2.68	116.16	109.07
4	A	1001	ACP	O2A-PA-O5'	2.52	119.46	107.75
4	A	1001	ACP	O2'-C2'-C1'	-2.06	103.24	110.85

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	ACP	PG-C3B-PB-O1B

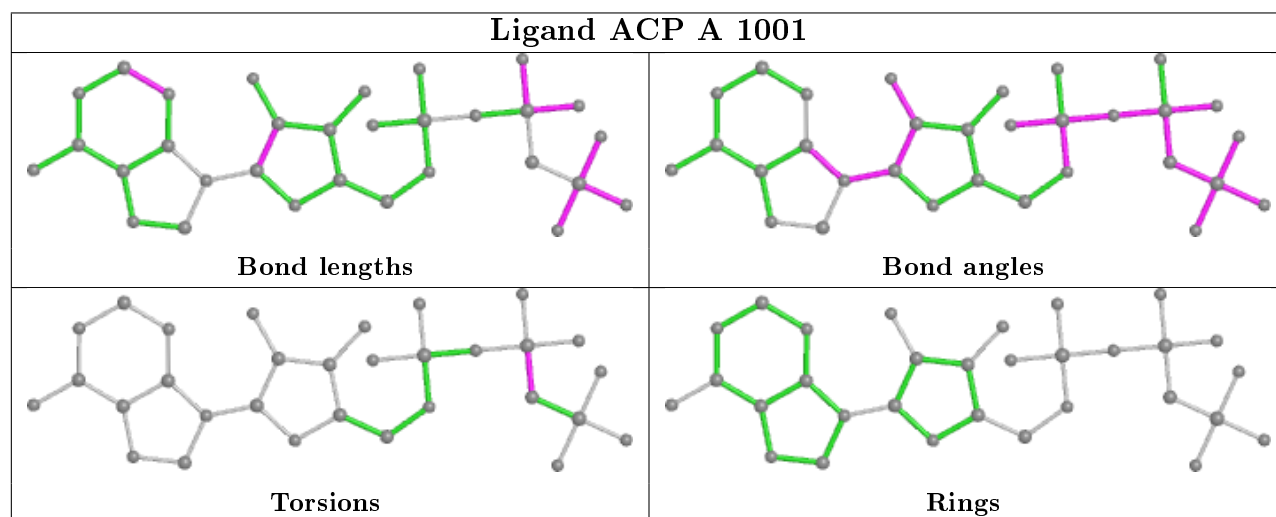
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	ACP	6	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	994/994 (100%)	0.73	108 (10%) 5 4	38, 89, 178, 245	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	506	ALA	14.8
1	A	877	THR	11.6
1	A	83	GLU	11.2
1	A	876	CYS	11.1
1	A	240	ALA	10.7
1	A	81	GLY	9.0
1	A	863	PRO	8.9
1	A	241	ALA	8.3
1	A	864	GLY	7.7
1	A	507	ALA	7.7
1	A	82	GLU	7.7
1	A	505	ARG	7.7
1	A	85	ILE	7.7
1	A	84	THR	7.5
1	A	45	GLU	7.1
1	A	963	ASP	7.0
1	A	239	MET	6.8
1	A	1	MET	6.5
1	A	504	SER	6.4
1	A	242	THR	6.3
1	A	883	PHE	5.7
1	A	47	LYS	5.5
1	A	964	LEU	5.5
1	A	886	LEU	5.3
1	A	80	GLU	5.2
1	A	49	LEU	5.0
1	A	43	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	77	TRP	4.9
1	A	994	GLY	4.8
1	A	44	GLU	4.8
1	A	881	PRO	4.2
1	A	288	TRP	4.2
1	A	243	GLU	4.2
1	A	884	GLU	4.0
1	A	880	HIS	3.9
1	A	289	ILE	3.8
1	A	287	SER	3.7
1	A	46	GLY	3.7
1	A	878	GLU	3.6
1	A	423	SER	3.4
1	A	993	GLU	3.3
1	A	58	GLU	3.3
1	A	987	ILE	3.3
1	A	968	LEU	3.3
1	A	422	ASP	3.1
1	A	882	HIS	3.1
1	A	825	LYS	3.1
1	A	575	GLU	3.0
1	A	859	ALA	3.0
1	A	262	LYS	3.0
1	A	874	MET	3.0
1	A	290	ARG	3.0
1	A	885	GLY	2.9
1	A	990	ASN	2.9
1	A	48	SER	2.9
1	A	879	ASP	2.9
1	A	79	GLU	2.9
1	A	78	PHE	2.9
1	A	923	MET	2.8
1	A	244	GLN	2.8
1	A	420	CYS	2.8
1	A	236	ARG	2.8
1	A	858	TYR	2.8
1	A	217	GLY	2.7
1	A	259	GLN	2.7
1	A	887	ASP	2.7
1	A	194	VAL	2.7
1	A	275	ASN	2.7
1	A	237	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	574	GLU	2.6
1	A	960	LYS	2.6
1	A	88	PHE	2.6
1	A	203	ASP	2.6
1	A	238	GLN	2.6
1	A	417	CYS	2.6
1	A	503	SER	2.6
1	A	421	ASN	2.5
1	A	494	MET	2.5
1	A	200	VAL	2.4
1	A	951	ASP	2.4
1	A	52	LEU	2.4
1	A	924	ARG	2.4
1	A	577	VAL	2.3
1	A	764	LEU	2.3
1	A	867	TYR	2.3
1	A	767	SER	2.3
1	A	854	TRP	2.3
1	A	218	LYS	2.3
1	A	292	ALA	2.3
1	A	67	LEU	2.2
1	A	605	LYS	2.2
1	A	495	SER	2.2
1	A	487	PHE	2.2
1	A	53	VAL	2.1
1	A	516	GLY	2.1
1	A	514	VAL	2.1
1	A	439	GLU	2.1
1	A	576	MET	2.1
1	A	763	TYR	2.1
1	A	276	ILE	2.1
1	A	42	PRO	2.1
1	A	441	THR	2.1
1	A	54	ILE	2.1
1	A	564	LEU	2.1
1	A	969	MET	2.0
1	A	180	LEU	2.0
1	A	324	ARG	2.0
1	A	888	CYS	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](#)

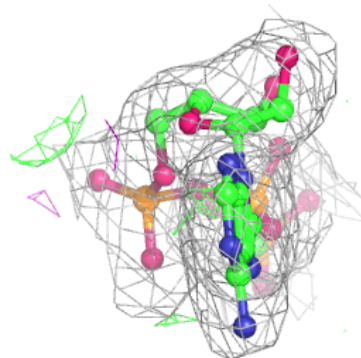
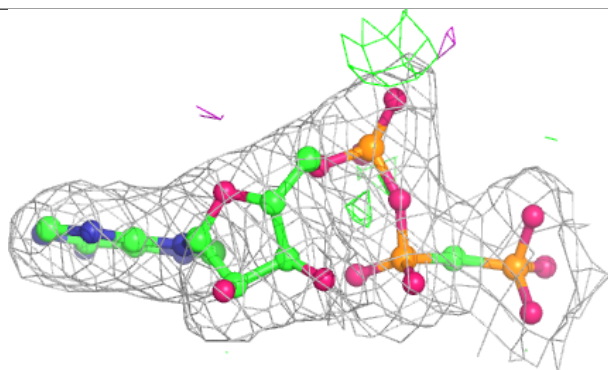
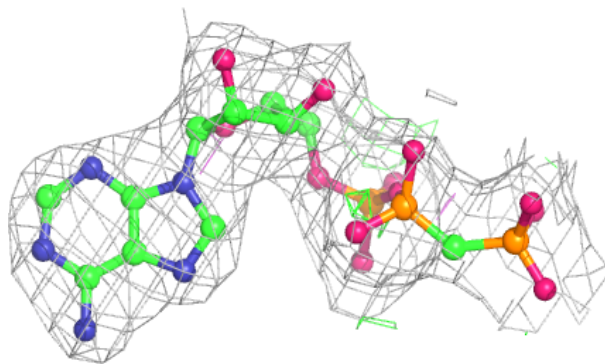
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	K	A	1006	1/1	0.93	0.23	91,91,91,91	0
2	CA	A	1004	1/1	0.94	0.40	107,107,107,107	0
2	CA	A	1003	1/1	0.96	0.28	111,111,111,111	0
2	CA	A	1002	1/1	0.97	0.27	52,52,52,52	0
4	ACP	A	1001	31/31	0.98	0.26	35,46,56,68	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 [i](#)

There are no such residues in this entry.