



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:33 PM GMT

PDB ID : 3B9R  
Title : SERCA Ca<sup>2+</sup>-ATPase E2 aluminium fluoride complex without thapsigargin  
Authors : Olesen, C.; Picard, M.; Winther, A.M.L.; Morth, J.P.; Moller, J.V.; Nissen, P.  
Deposited on : 2007-11-06  
Resolution : 3.00 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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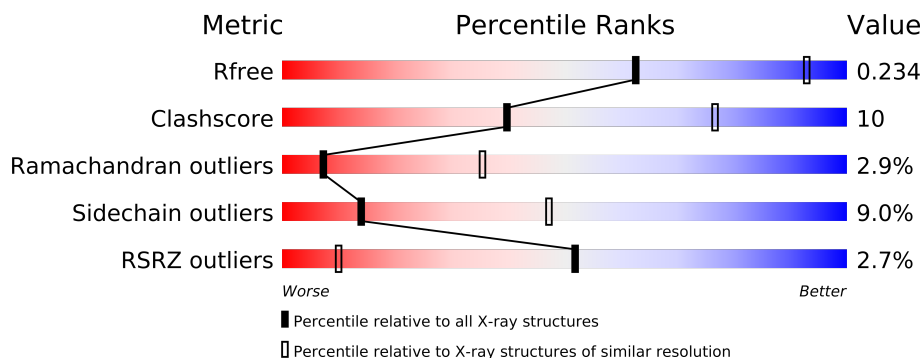
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 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))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	994	
1	B	994	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	A	996	-	X
3	MG	B	996	-	X
5	ACP	A	998	-	X

## 2 Entry composition i

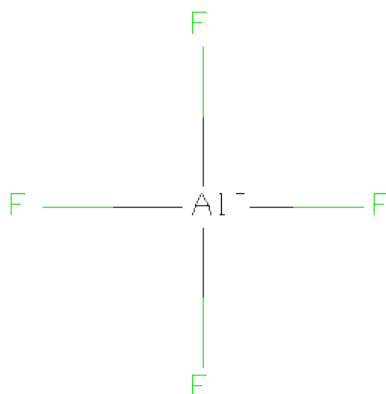
There are 6 unique types of molecules in this entry. The entry contains 15426 atoms, of which 0 are hydrogen and 0 are deuterium.

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/endoplasmicreticulum calcium ATPase 1.

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

- Molecule 2 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula:  $\text{AlF}_4^-$ ).



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

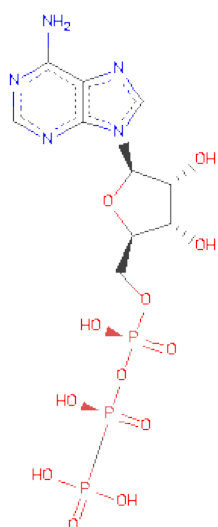
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula:  $\text{Mg}$ ).

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

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

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

- Molecule 5 is PHOSPHOMETHYLPHOSPHONICACID 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 31 11 5 12 3	0	0
5	B	1	Total C N O P 31 11 5 12 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	4	Total O 4 4	0	0

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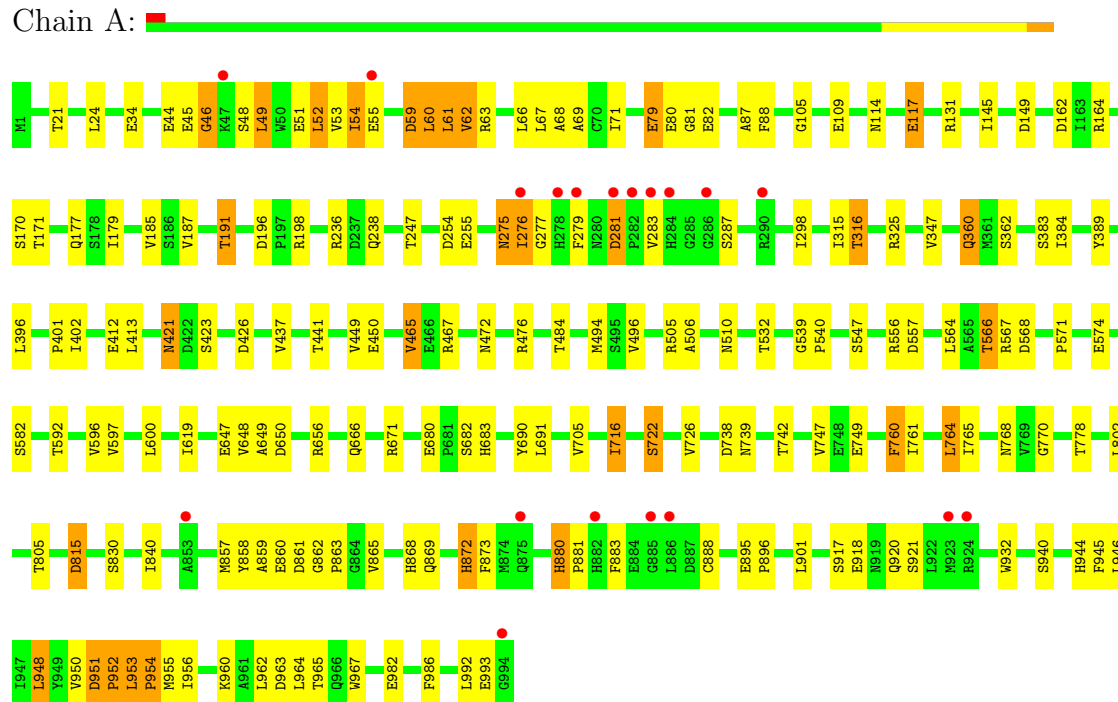
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	4	Total	O	0	0
			4	4		

### 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 errors 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.

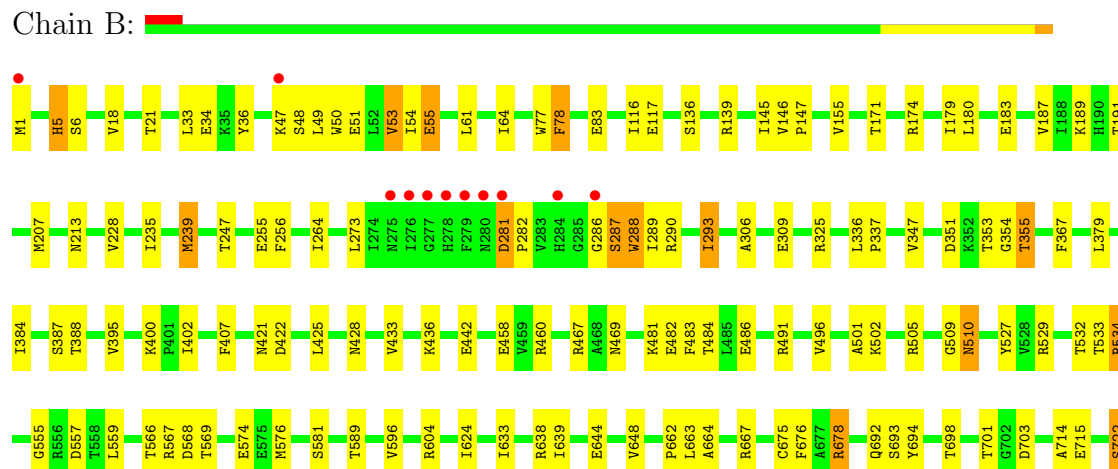
- Molecule 1: Sarcoplasmic/endoplasmicreticulum calcium ATPase 1

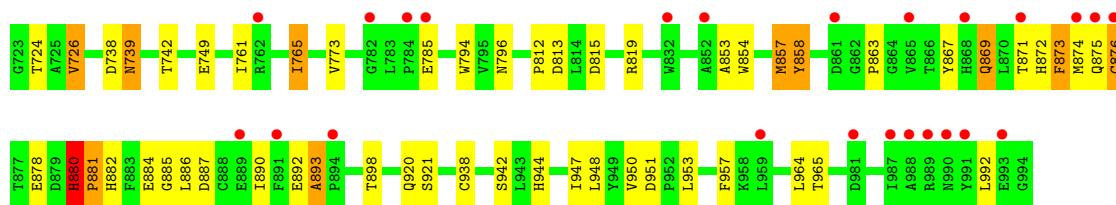
Chain A:



- Molecule 1: Sarcoplasmic/endoplasmicreticulum calcium ATPase 1

Chain B:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.98Å 94.43Å 136.18Å 90.00° 107.79° 90.00°	Depositor
Resolution (Å)	19.99 – 3.00 47.21 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.99-3.00) 99.5 (47.21-3.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 3.01Å)	Xtriage
Refinement program	phenix.refine	Depositor
R, $R_{free}$	0.185 , 0.235 0.187 , 0.234	Depositor DCC
$R_{free}$ test set	1040 reflections (1.63%)	DCC
Wilson B-factor (Å <sup>2</sup> )	77.3	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 82.2	EDS
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 63839 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15426	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ALF, K, ACP, 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	0.60	0/7812	0.80	1/10592 (0.0%)
1	B	0.54	0/7812	0.74	1/10592 (0.0%)
All	All	0.57	0/15624	0.77	2/21184 (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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	VAL	CG1-CB-CG2	-5.13	102.69	110.90
1	A	162	ASP	CB-CG-OD1	5.11	122.90	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	55	GLU	Peptide

### 5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7671	0	0	78	0
1	B	7671	0	0	69	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	31	0	0	0	0
5	B	31	0	0	0	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
All	All	15426	0	0	147	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (147) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:50:TRP:O	1:B:53:VAL:CG1	2.31	0.79
1:A:951:ASP:CB	1:A:952:PRO:CD	2.64	0.75
1:B:876:CYS:SG	1:B:882:HIS:CE1	2.85	0.70
1:A:953:LEU:CB	1:A:954:PRO:CD	2.74	0.65
1:A:963:ASP:OD1	1:A:964:LEU:N	2.30	0.64
1:A:316:THR:O	1:A:316:THR:CG2	2.44	0.64
1:A:953:LEU:O	1:A:955:MET:N	2.29	0.64
1:A:412:GLU:OE2	1:A:566:THR:CG2	2.49	0.60
1:B:722:SER:OG	1:B:738:ASP:OD1	2.20	0.60
1:B:5:HIS:CD2	1:B:6:SER:N	2.69	0.59
1:A:815:ASP:O	1:A:815:ASP:CG	2.39	0.59
1:A:649:ALA:O	1:A:650:ASP:CB	2.50	0.59
1:A:951:ASP:O	1:A:953:LEU:N	2.35	0.59
1:A:450:GLU:OE2	1:A:467:ARG:NH2	2.36	0.59
1:A:60:LEU:O	1:A:62:VAL:N	2.37	0.58
1:A:60:LEU:C	1:A:62:VAL:N	2.58	0.57
1:A:722:SER:OG	1:A:738:ASP:OD1	2.24	0.56
1:B:288:TRP:C	1:B:290:ARG:N	2.59	0.56
1:A:953:LEU:C	1:A:955:MET:N	2.59	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:362:SER:N	1:A:600:LEU:O	2.38	0.56
1:B:880:HIS:N	1:B:881:PRO:CD	2.69	0.56
1:B:678:ARG:CG	1:B:678:ARG:NH1	2.68	0.55
1:A:196:ASP:OD1	1:A:198:ARG:N	2.39	0.55
1:A:946:LEU:O	1:A:950:VAL:CG2	2.55	0.55
1:A:79:GLU:O	1:A:79:GLU:CG	2.56	0.54
1:B:354:GLY:O	1:B:604:ARG:NH1	2.40	0.54
1:B:286:GLY:O	1:B:287:SER:C	2.46	0.54
1:A:865:VAL:CB	1:A:868:HIS:CD2	2.91	0.54
1:B:676:PHE:CD1	1:B:676:PHE:N	2.76	0.54
1:B:47:LYS:O	1:B:47:LYS:CG	2.56	0.53
1:A:60:LEU:CD1	1:A:61:LEU:N	2.72	0.53
1:B:325:ARG:NH1	1:B:749:GLU:OE2	2.41	0.53
1:B:878:GLU:CB	1:B:880:HIS:CD2	2.92	0.53
1:A:648:VAL:O	1:A:649:ALA:C	2.46	0.52
1:A:865:VAL:C	1:A:868:HIS:CD2	2.83	0.52
1:A:67:LEU:O	1:A:71:ILE:N	2.43	0.52
1:A:51:GLU:O	1:A:52:LEU:C	2.48	0.52
1:B:235:ILE:O	1:B:239:MET:CG	2.58	0.52
1:A:901:LEU:CD2	1:A:944:HIS:CE1	2.93	0.52
1:A:760:PHE:CD1	1:A:760:PHE:C	2.83	0.52
1:A:51:GLU:O	1:A:53:VAL:N	2.44	0.51
1:B:692:GLN:NE2	1:B:715:GLU:OE1	2.43	0.51
1:A:666:GLN:NE2	1:A:690:TYR:OH	2.44	0.51
1:A:449:VAL:CG2	1:A:472:ASN:ND2	2.72	0.51
1:A:962:LEU:O	1:A:965:THR:OG1	2.29	0.51
1:B:815:ASP:OD1	1:B:819:ARG:NH2	2.44	0.51
1:B:938:CYS:O	1:B:942:SER:N	2.44	0.51
1:A:948:LEU:O	1:A:954:PRO:CG	2.59	0.51
1:B:281:ASP:N	1:B:282:PRO:CD	2.74	0.50
1:A:880:HIS:CG	1:A:881:PRO:CD	2.94	0.50
1:B:171:THR:CG2	1:B:486:GLU:OE1	2.59	0.50
1:B:146:VAL:O	1:B:147:PRO:C	2.49	0.49
1:A:114:ASN:OD1	1:A:117:GLU:CB	2.61	0.49
1:A:325:ARG:NH1	1:A:749:GLU:OE2	2.45	0.49
1:A:51:GLU:O	1:A:54:ILE:N	2.45	0.49
1:B:481:LYS:CG	1:B:496:VAL:CG1	2.91	0.49
1:A:67:LEU:O	1:A:69:ALA:N	2.45	0.49
1:A:680:GLU:N	1:A:683:HIS:ND1	2.61	0.49
1:A:865:VAL:CA	1:A:868:HIS:CD2	2.96	0.48
1:B:884:GLU:O	1:B:886:LEU:N	2.47	0.48
1:A:858:TYR:O	1:A:860:GLU:N	2.46	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:505:ARG:O	1:A:506:ALA:CB	2.62	0.48
1:B:351:ASP:OD2	1:B:355:THR:CG2	2.61	0.48
1:B:529:ARG:NH2	1:B:568:ASP:OD2	2.47	0.47
1:A:59:ASP:OD1	1:A:59:ASP:N	2.46	0.47
1:A:895:GLU:N	1:A:896:PRO:CD	2.77	0.47
1:A:656:ARG:NH1	1:A:656:ARG:CG	2.77	0.47
1:B:77:TRP:CD1	1:B:78:PHE:CE1	3.03	0.47
1:B:869:GLN:CG	1:B:872:HIS:ND1	2.78	0.47
1:A:79:GLU:O	1:A:81:GLY:N	2.48	0.47
1:B:667:ARG:NH2	1:B:693:SER:O	2.48	0.47
1:B:648:VAL:O	1:B:648:VAL:CG1	2.63	0.46
1:A:281:ASP:O	1:A:283:VAL:N	2.48	0.46
1:A:275:ASN:O	1:A:277:GLY:N	2.48	0.46
1:B:509:GLY:O	1:B:510:ASN:C	2.54	0.46
1:B:853:ALA:C	1:B:854:TRP:CD1	2.89	0.46
1:B:667:ARG:NH1	1:B:694:TYR:CE1	2.84	0.45
1:B:892:GLU:O	1:B:893:ALA:C	2.54	0.45
1:A:105:GLY:O	1:A:109:GLU:CG	2.64	0.45
1:A:79:GLU:OE1	1:A:79:GLU:N	2.50	0.45
1:A:716:ILE:CD1	1:A:716:ILE:N	2.80	0.45
1:B:48:SER:O	1:B:49:LEU:C	2.55	0.45
1:B:944:HIS:O	1:B:944:HIS:CD2	2.70	0.45
1:B:555:GLY:C	1:B:557:ASP:N	2.69	0.45
1:A:917:SER:OG	1:A:918:GLU:N	2.50	0.44
1:B:951:ASP:O	1:B:953:LEU:N	2.51	0.44
1:B:483:PHE:CZ	1:B:576:MET:CE	3.00	0.44
1:B:964:LEU:O	1:B:965:THR:CB	2.64	0.44
1:B:256:PHE:CZ	1:B:765:ILE:CD1	3.01	0.44
1:B:51:GLU:O	1:B:54:ILE:CB	2.65	0.44
1:A:917:SER:OG	1:A:920:GLN:CB	2.66	0.44
1:B:407:PHE:CD2	1:B:407:PHE:N	2.85	0.44
1:B:189:LYS:NZ	1:B:207:MET:O	2.50	0.44
1:B:527:TYR:CE2	1:B:534:ARG:NH1	2.86	0.43
1:A:62:VAL:CG1	1:A:63:ARG:N	2.81	0.43
1:B:309:GLU:OE1	1:B:796:ASN:ND2	2.51	0.43
1:A:164:ARG:NH1	1:A:191:THR:O	2.52	0.43
1:A:568:ASP:OD1	1:A:592:THR:OG1	2.35	0.43
1:A:557:ASP:O	1:A:557:ASP:OD1	2.37	0.43
1:A:421:ASN:ND2	1:A:423:SER:OG	2.51	0.43
1:B:293:ILE:CG2	1:B:293:ILE:O	2.67	0.43
1:A:764:LEU:O	1:A:768:ASN:ND2	2.51	0.43
1:B:501:ALA:O	1:B:502:LYS:CG	2.66	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:761:ILE:CG2	1:B:761:ILE:O	2.67	0.43
1:A:45:GLU:O	1:A:46:GLY:C	2.57	0.43
1:A:88:PHE:O	1:A:88:PHE:CD1	2.72	0.43
1:A:53:VAL:O	1:A:55:GLU:N	2.52	0.43
1:A:298:ILE:C	1:A:298:ILE:CD1	2.87	0.43
1:A:131:ARG:NH2	1:A:149:ASP:OD1	2.52	0.43
1:B:662:PRO:O	1:B:664:ALA:N	2.52	0.43
1:B:264:ILE:CD1	1:B:306:ALA:CB	2.97	0.42
1:B:1:MET:CB	1:B:36:TYR:CE1	3.03	0.42
1:B:992:LEU:O	1:B:992:LEU:CG	2.68	0.42
1:B:428:ASN:C	1:B:428:ASN:OD1	2.58	0.42
1:B:567:ARG:NH1	1:B:569:THR:O	2.52	0.42
1:B:5:HIS:CD2	1:B:5:HIS:C	2.93	0.42
1:B:726:VAL:CG2	1:B:726:VAL:O	2.68	0.42
1:A:539:GLY:N	1:A:540:PRO:CD	2.83	0.42
1:A:53:VAL:C	1:A:55:GLU:N	2.73	0.42
1:B:873:PHE:CE1	1:B:876:CYS:CA	3.03	0.42
1:B:965:THR:O	1:B:965:THR:CG2	2.68	0.42
1:A:596:VAL:CG1	1:A:597:VAL:N	2.83	0.42
1:B:422:ASP:N	1:B:442:GLU:OE1	2.53	0.42
1:A:383:SER:O	1:A:396:LEU:N	2.53	0.41
1:B:336:LEU:N	1:B:337:PRO:CD	2.82	0.41
1:B:920:GLN:O	1:B:921:SER:C	2.58	0.41
1:A:872:HIS:O	1:A:873:PHE:CD1	2.74	0.41
1:B:78:PHE:N	1:B:78:PHE:CD1	2.88	0.41
1:A:921:SER:OG	1:A:982:GLU:OE1	2.39	0.41
1:A:276:ILE:O	1:A:279:PHE:CD2	2.74	0.41
1:A:360:GLN:OE1	1:A:389:TYR:N	2.54	0.41
1:B:878:GLU:CB	1:B:880:HIS:NE2	2.83	0.41
1:B:425:LEU:O	1:B:469:ASN:ND2	2.54	0.41
1:B:873:PHE:CZ	1:B:881:PRO:CG	3.04	0.41
1:A:413:LEU:CD1	1:A:564:LEU:CD1	2.99	0.41
1:A:279:PHE:C	1:A:279:PHE:CD1	2.94	0.41
1:A:945:PHE:CZ	1:A:967:TRP:CZ2	3.09	0.41
1:A:49:LEU:CD1	1:A:52:LEU:N	2.84	0.40
1:B:857:MET:O	1:B:858:TYR:CD2	2.74	0.40
1:A:67:LEU:C	1:A:69:ALA:N	2.75	0.40
1:B:77:TRP:CD1	1:B:78:PHE:CD1	3.09	0.40
1:B:83:GLU:OE1	1:B:83:GLU:N	2.54	0.40
1:A:49:LEU:C	1:A:51:GLU:N	2.73	0.40
1:A:861:ASP:CG	1:A:862:GLY:N	2.74	0.40
1:B:183:GLU:OE2	1:B:353:THR:OG1	2.39	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:992:LEU:CG	1:A:993:GLU:N	2.85	0.40
1:B:703:ASP:O	1:B:724:THR:N	2.54	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%)	858 (86%)	106 (11%)	28 (3%)	8	37
1	B	992/994 (100%)	853 (86%)	110 (11%)	29 (3%)	7	35
All	All	1984/1988 (100%)	1711 (86%)	216 (11%)	57 (3%)	7	35

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	571	PRO
1	A	859	ALA
1	A	863	PRO
1	A	883	PHE
1	A	952	PRO
1	A	953	LEU
1	A	954	PRO
1	B	288	TRP
1	B	289	ILE
1	B	881	PRO
1	A	46	GLY
1	A	54	ILE
1	A	62	VAL
1	A	68	ALA
1	A	869	GLN
1	B	55	GLU
1	B	287	SER

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Mol	Chain	Res	Type
1	B	785	GLU
1	B	813	ASP
1	B	863	PRO
1	B	867	TYR
1	B	876	CYS
1	B	885	GLY
1	A	61	LEU
1	A	275	ASN
1	A	276	ILE
1	A	770	GLY
1	A	888	CYS
1	B	644	GLU
1	B	663	LEU
1	B	714	ALA
1	B	887	ASP
1	B	948	LEU
1	B	957	PHE
1	A	80	GLU
1	A	287	SER
1	A	465	VAL
1	B	858	TYR
1	B	893	ALA
1	A	44	GLU
1	A	59	ASP
1	A	281	ASP
1	A	316	THR
1	B	510	ASN
1	B	638	ARG
1	B	739	ASN
1	B	880	HIS
1	A	87	ALA
1	B	281	ASP
1	B	293	ILE
1	B	950	VAL
1	A	951	ASP
1	B	812	PRO
1	B	247	THR
1	A	880	HIS
1	B	947	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%)	764 (91%)	76 (9%)	14	47
1	B	840/840 (100%)	764 (91%)	76 (9%)	14	47
All	All	1680/1680 (100%)	1528 (91%)	152 (9%)	14	47

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	24	LEU
1	A	34	GLU
1	A	48	SER
1	A	49	LEU
1	A	60	LEU
1	A	66	LEU
1	A	79	GLU
1	A	82	GLU
1	A	117	GLU
1	A	145	ILE
1	A	170	SER
1	A	171	THR
1	A	177	GLN
1	A	179	ILE
1	A	185	VAL
1	A	187	VAL
1	A	191	THR
1	A	236	ARG
1	A	238	GLN
1	A	247	THR
1	A	254	ASP
1	A	255	GLU
1	A	315	ILE
1	A	347	VAL
1	A	360	GLN
1	A	384	ILE
1	A	401	PRO
1	A	402	ILE

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Mol	Chain	Res	Type
1	A	421	ASN
1	A	426	ASP
1	A	437	VAL
1	A	441	THR
1	A	465	VAL
1	A	476	ARG
1	A	484	THR
1	A	494	MET
1	A	496	VAL
1	A	510	ASN
1	A	532	THR
1	A	547	SER
1	A	556	ARG
1	A	566	THR
1	A	567	ARG
1	A	574	GLU
1	A	582	SER
1	A	619	ILE
1	A	647	GLU
1	A	671	ARG
1	A	682	SER
1	A	691	LEU
1	A	705	VAL
1	A	716	ILE
1	A	722	SER
1	A	726	VAL
1	A	739	ASN
1	A	742	THR
1	A	747	VAL
1	A	760	PHE
1	A	761	ILE
1	A	764	LEU
1	A	765	ILE
1	A	778	THR
1	A	802	LEU
1	A	805	THR
1	A	815	ASP
1	A	830	SER
1	A	840	ILE
1	A	857	MET
1	A	872	HIS
1	A	932	TRP

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Mol	Chain	Res	Type
1	A	940	SER
1	A	948	LEU
1	A	956	ILE
1	A	960	LYS
1	A	986	PHE
1	B	5	HIS
1	B	18	VAL
1	B	21	THR
1	B	33	LEU
1	B	34	GLU
1	B	61	LEU
1	B	64	ILE
1	B	78	PHE
1	B	116	ILE
1	B	117	GLU
1	B	136	SER
1	B	139	ARG
1	B	145	ILE
1	B	155	VAL
1	B	174	ARG
1	B	179	ILE
1	B	180	LEU
1	B	187	VAL
1	B	191	THR
1	B	213	ASN
1	B	228	VAL
1	B	239	MET
1	B	255	GLU
1	B	273	LEU
1	B	347	VAL
1	B	355	THR
1	B	367	PHE
1	B	379	LEU
1	B	384	ILE
1	B	387	SER
1	B	388	THR
1	B	395	VAL
1	B	400	LYS
1	B	402	ILE
1	B	421	ASN
1	B	433	VAL
1	B	436	LYS

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Mol	Chain	Res	Type
1	B	458	GLU
1	B	460	ARG
1	B	467	ARG
1	B	482	GLU
1	B	484	THR
1	B	491	ARG
1	B	505	ARG
1	B	532	THR
1	B	533	THR
1	B	534	ARG
1	B	559	LEU
1	B	566	THR
1	B	574	GLU
1	B	581	SER
1	B	589	THR
1	B	596	VAL
1	B	624	ILE
1	B	633	ILE
1	B	639	ILE
1	B	675	CYS
1	B	678	ARG
1	B	698	THR
1	B	701	THR
1	B	722	SER
1	B	726	VAL
1	B	739	ASN
1	B	742	THR
1	B	765	ILE
1	B	773	VAL
1	B	794	TRP
1	B	857	MET
1	B	869	GLN
1	B	871	THR
1	B	873	PHE
1	B	874	MET
1	B	875	GLN
1	B	880	HIS
1	B	890	ILE
1	B	898	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	995	-	4,4,4	1.83	0	0,6,6	0.00	-
5	ACP	A	998	-	33,33,33	3.29	12 (36%)	52,52,52	2.61	20 (38%)
2	ALF	B	995	-	4,4,4	1.74	0	0,6,6	0.00	-
5	ACP	B	998	-	33,33,33	3.45	12 (36%)	52,52,52	2.38	15 (28%)

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
2	ALF	A	995	-	-	0/0/0/0	0/0/0/0
5	ACP	A	998	-	-	0/20/38/38	0/1/3/3
2	ALF	B	995	-	-	0/0/0/0	0/0/0/0
5	ACP	B	998	-	-	0/20/38/38	0/1/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	998	ACP	PB-C3B	-12.99	1.68	1.79
5	A	998	ACP	PB-C3B	-12.42	1.69	1.79
5	B	998	ACP	PG-C3B	-9.58	1.71	1.79
5	A	998	ACP	PG-C3B	-8.55	1.72	1.79
5	A	998	ACP	PG-O3G	-4.79	1.45	1.54
5	B	998	ACP	PG-O3G	-4.62	1.45	1.54
5	B	998	ACP	PG-O1G	4.44	1.60	1.50
5	A	998	ACP	PG-O1G	4.44	1.60	1.50
5	A	998	ACP	C8-N9	4.22	1.42	1.36
5	B	998	ACP	C8-N9	4.13	1.42	1.36
5	A	998	ACP	C2'-C1'	3.30	1.58	1.53
5	B	998	ACP	PA-O3A	3.24	1.65	1.59
5	B	998	ACP	C2'-C1'	3.18	1.58	1.53
5	B	998	ACP	C4-N9	3.03	1.42	1.37
5	A	998	ACP	C5-C4	2.92	1.47	1.40
5	A	998	ACP	O4'-C1'	2.90	1.45	1.41
5	A	998	ACP	C4-N9	2.66	1.41	1.37
5	B	998	ACP	PG-O2G	2.66	1.59	1.54
5	B	998	ACP	C5-C4	2.48	1.46	1.40
5	A	998	ACP	PG-O2G	2.48	1.59	1.54
5	B	998	ACP	PB-O3A	2.39	1.65	1.59
5	A	998	ACP	PB-O2B	2.18	1.61	1.56
5	B	998	ACP	PB-O1B	-2.05	1.46	1.51
5	A	998	ACP	PB-O1B	-2.03	1.46	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	998	ACP	O4'-C1'-C2'	-9.09	92.84	106.77
5	A	998	ACP	O4'-C1'-C2'	-8.10	94.36	106.77
5	B	998	ACP	O4'-C4'-C3'	-5.68	93.66	105.17
5	A	998	ACP	O3A-PB-C3B	5.47	123.84	106.62
5	B	998	ACP	O3'-C3'-C4'	5.31	126.71	111.08
5	A	998	ACP	O4'-C1'-N9	-5.11	103.69	108.44
5	A	998	ACP	O4'-C4'-C3'	-5.08	94.87	105.17
5	A	998	ACP	O3'-C3'-C4'	5.01	125.83	111.08
5	A	998	ACP	O2G-PG-O1G	-4.89	99.52	112.56
5	B	998	ACP	PA-O3A-PB	4.82	146.22	131.74
5	B	998	ACP	O3A-PB-C3B	4.39	120.45	106.62
5	A	998	ACP	PB-C3B-PG	4.23	123.71	117.62
5	A	998	ACP	O2B-PB-O3A	-4.21	96.78	107.18
5	B	998	ACP	O3A-PA-O5'	3.84	120.60	103.41
5	A	998	ACP	O3A-PB-O1B	-3.66	103.75	111.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	998	ACP	O2G-PG-O1G	-3.53	103.14	112.56
5	A	998	ACP	C4'-O4'-C1'	-3.35	106.11	109.75
5	B	998	ACP	N3-C4-N9	3.28	131.35	125.43
5	A	998	ACP	O3A-PA-O5'	3.27	118.03	103.41
5	A	998	ACP	C2'-C1'-N9	3.18	121.42	113.27
5	A	998	ACP	C8-N9-C4	-2.96	104.64	106.90
5	A	998	ACP	N3-C4-N9	2.94	130.74	125.43
5	B	998	ACP	C3'-C2'-C1'	2.89	105.43	100.91
5	A	998	ACP	O3G-PG-C3B	2.87	113.37	106.40
5	A	998	ACP	O4'-C4'-C5'	-2.62	100.02	109.36
5	B	998	ACP	O3G-PG-O2G	2.48	116.23	108.35
5	B	998	ACP	O3G-PG-C3B	2.46	112.36	106.40
5	A	998	ACP	O3G-PG-O2G	2.45	116.12	108.35
5	B	998	ACP	O2B-PB-O3A	-2.42	101.19	107.18
5	B	998	ACP	O3A-PB-O1B	-2.17	106.91	111.51
5	B	998	ACP	O4'-C4'-C5'	-2.15	101.68	109.36
5	B	998	ACP	O3G-PG-O1G	-2.15	106.83	112.56
5	A	998	ACP	PA-O3A-PB	2.06	137.92	131.74
5	A	998	ACP	O3G-PG-O1G	-2.01	107.19	112.56
5	A	998	ACP	C2'-C3'-C4'	2.00	106.65	102.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.09	19 (1%) 64 13	36, 86, 210, 329	0
1	B	994/994 (100%)	0.02	35 (3%) 42 8	47, 108, 222, 298	0
All	All	1988/1988 (100%)	-0.03	54 (2%) 52 10	36, 97, 216, 329	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	991	TYR	6.4
1	B	861	ASP	5.4
1	B	280	ASN	4.6
1	B	47	LYS	4.4
1	B	785	GLU	3.8
1	A	281	ASP	3.8
1	B	987	ILE	3.4
1	A	885	GLY	3.3
1	B	276	ILE	3.3
1	A	55	GLU	3.3
1	B	284	HIS	3.3
1	B	993	GLU	3.2
1	B	277	GLY	3.2
1	B	990	ASN	3.2
1	B	852	ALA	3.1
1	B	275	ASN	3.0
1	B	279	PHE	3.0
1	B	281	ASP	3.0
1	B	959	LEU	3.0
1	A	286	GLY	3.0
1	B	782	GLY	2.9
1	A	284	HIS	2.9
1	B	784	PRO	2.9
1	B	832	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	874	MET	2.8
1	A	278	HIS	2.8
1	A	882	HIS	2.8
1	B	278	HIS	2.8
1	A	276	ILE	2.7
1	A	279	PHE	2.7
1	B	894	PRO	2.7
1	B	889	GLU	2.7
1	A	47	LYS	2.7
1	B	988	ALA	2.6
1	A	853	ALA	2.5
1	A	875	GLN	2.5
1	B	868	HIS	2.5
1	B	875	GLN	2.5
1	A	924	ARG	2.5
1	A	923	MET	2.4
1	B	876	CYS	2.5
1	B	981	ASP	2.4
1	B	891	PHE	2.4
1	A	283	VAL	2.3
1	A	886	LEU	2.2
1	B	1	MET	2.2
1	A	994	GLY	2.2
1	B	871	THR	2.2
1	B	286	GLY	2.2
1	B	865	VAL	2.1
1	A	290	ARG	2.1
1	B	989	ARG	2.1
1	A	282	PRO	2.1
1	B	762	ARG	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	A	996	1/1	0.25	4.10	23,23,23,23	0
5	ACP	A	998	31/31	0.24	2.27	63,113,171,279	0
3	MG	B	996	1/1	0.21	2.24	43,43,43,43	0
2	ALF	B	995	5/5	0.22	1.27	42,50,61,69	0
2	ALF	A	995	5/5	0.23	1.25	18,47,49,50	0
5	ACP	B	998	31/31	0.21	0.87	55,101,210,335	0
4	K	A	997	1/1	0.19	0.22	78,78,78,78	0
4	K	B	997	1/1	0.12	-1.18	99,99,99,99	0

## 6.5 Other polymers

There are no such residues in this entry.