



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:05 PM GMT

PDB ID : 4BEW  
Title : SERCA bound to phosphate analogue  
Authors : Drachmann, N.D.; Mattle, D.; Laursen, M.; Bublitz, M.; Olesen, C.; Moeller, J.V.; Nissen, P.; Morth, J.P.  
Deposited on : 2013-03-12  
Resolution : 2.50 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

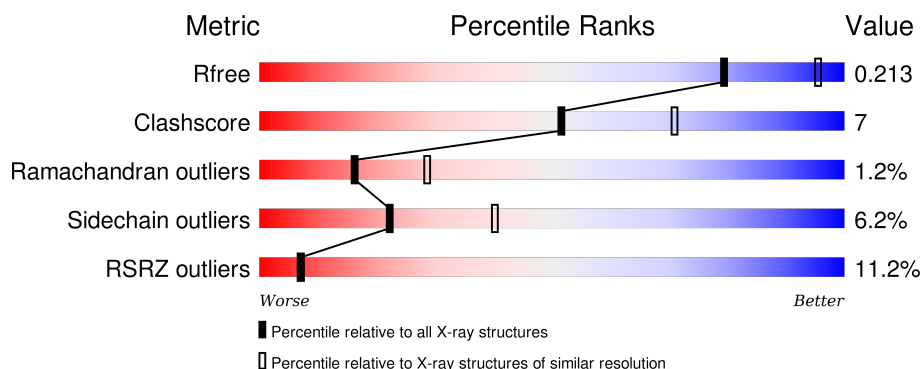
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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>14%</div> <div>77%</div> <div>20%</div> <div>.</div> </div>
1	B	994	<div> <div>8%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	B	1002	-	-	-	X
6	ACP	A	1007	-	-	-	X
6	ACP	B	1007	-	-	-	X
8	ACT	A	3002	-	-	-	X
8	ACT	B	3001	-	-	-	X
8	ACT	B	3002	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15950 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	0	0	0
			7670	4876	1287	1450	57			
1	B	994	Total	C	N	O	S	0	0	0
			7670	4876	1287	1450	57			

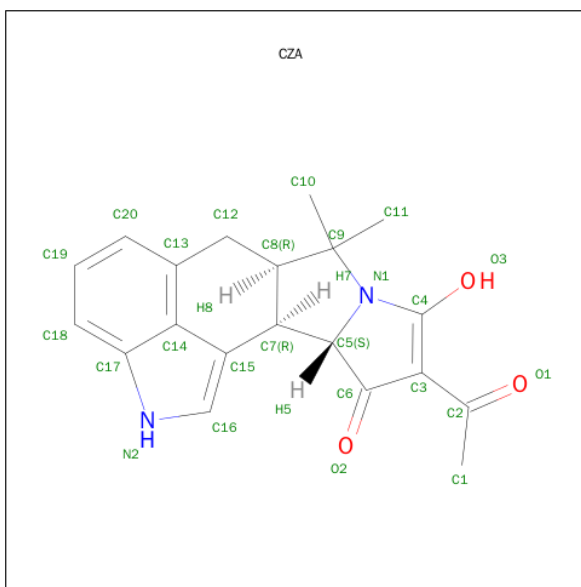
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 4 is (6AR,11AS,11BR)-10-ACETYL-9-HYDROXY-7,7-DIMETHYL-2,6,6A,7,11A,11B-HEXAHYDRO-11H-PYRROLO[1',2':2,3]ISOINDOLO[4,5,6-CD]INDOL-11-ONE (three-letter code: CZA) (formula: C<sub>20</sub>H<sub>20</sub>N<sub>2</sub>O<sub>3</sub>).

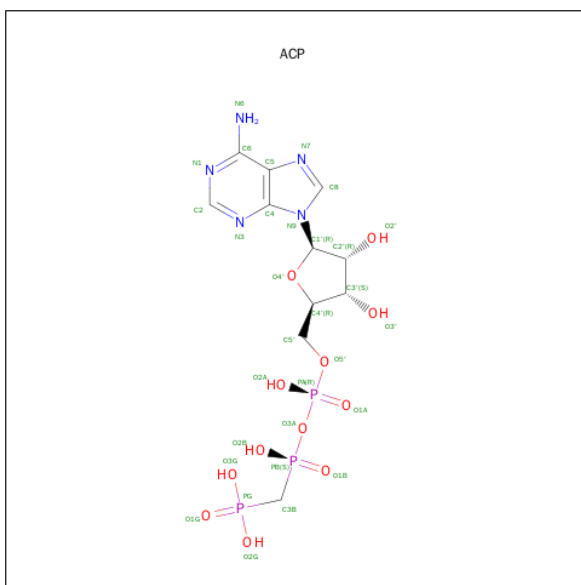


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			25	20	2	3		
4	B	1	Total	C	N	O	0	0
			25	20	2	3		

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

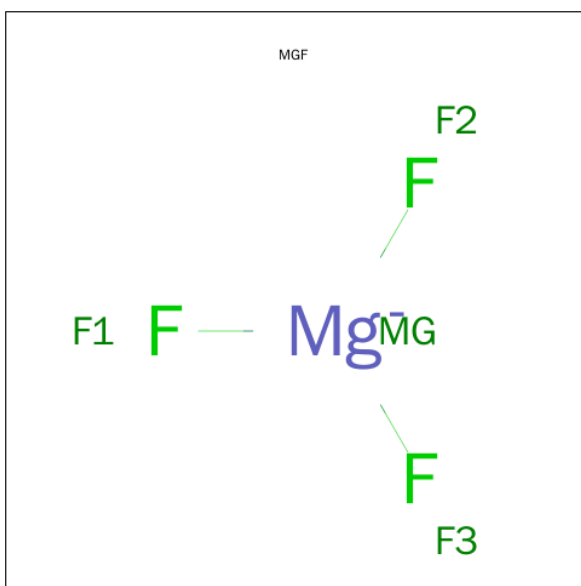
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mn	0	0
			1	1		
5	A	2	Total	Mn	0	0
			2	2		

- Molecule 6 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>).



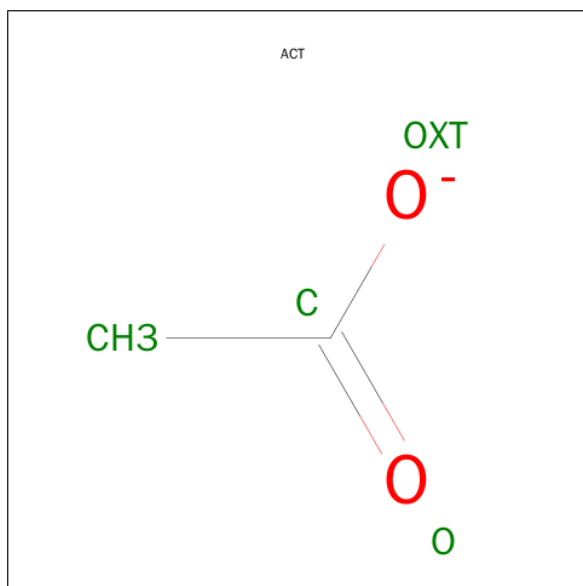
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 31	C 11	N 5	O 12	P 3	0	0
6	B	1	Total 31	C 11	N 5	O 12	P 3	0	0

- Molecule 7 is TRIFLUOROMAGNESATE (three-letter code: MGF) (formula:  $\text{F}_3\text{Mg}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 4	F 3	Mg 1	0	0
7	B	1	Total 4	F 3	Mg 1	0	0

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	268	Total	O	0	0
			268	268		
9	B	199	Total	O	0	0
			199	199		

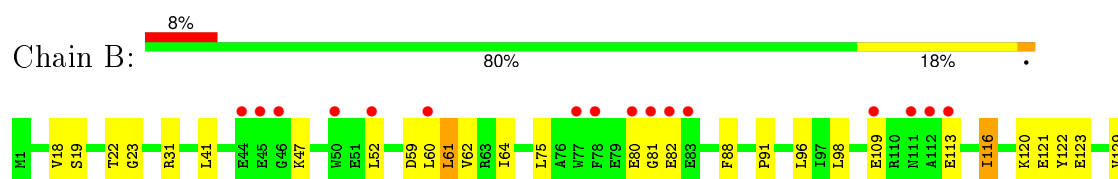
### 3 Residue-property plots

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/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1



- Molecule 1: SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.43Å 108.87Å 274.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.97 – 2.50 45.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (45.97-2.50) 97.6 (45.97-2.50)	Depositor EDS
$R_{merge}$	0.58	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.169 , 0.207 0.177 , 0.213	Depositor DCC
$R_{free}$ test set	3075 reflections (3.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.0	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 60.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 103184 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15950	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, MGF, K, MN, ACP, ACT, CZA

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	0.41	0/7811	0.58	1/10592 (0.0%)
1	B	0.40	0/7811	0.57	1/10592 (0.0%)
All	All	0.41	0/15622	0.58	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	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	567	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	476	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	555	GLY	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	7670	0	7762	114	0
1	B	7670	0	7762	97	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	25	0	20	2	0
4	B	25	0	20	2	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
6	A	31	0	14	0	0
6	B	31	0	14	0	0
7	A	4	0	0	0	0
7	B	4	0	0	0	0
8	A	8	0	6	2	0
8	B	8	0	6	2	0
9	A	268	0	0	3	0
9	B	199	0	0	2	0
All	All	15950	0	15604	211	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (211) 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:894:PRO:HB2	1:A:960:LYS:HB2	1.61	0.81
1:A:216:ALA:HB1	8:A:3001:ACT:H2	1.64	0.79
1:B:61:LEU:HD12	4:B:1005:CZA:H8	1.69	0.75
1:B:869:GLN:NE2	1:B:882:HIS:O	2.20	0.71
1:A:249:LEU:HD13	1:A:757:MET:HE2	1.72	0.69
1:B:856:PHE:HA	1:B:863:PRO:HG2	1.75	0.69
1:A:247:THR:HG22	1:A:250:GLN:H	1.57	0.69
1:A:242:THR:HG22	1:A:244:GLN:HG3	1.74	0.68
1:A:85:ILE:HG12	1:A:86:THR:HG23	1.76	0.68
1:A:246:LYS:HB2	1:A:250:GLN:HG3	1.75	0.68
1:B:116:ILE:HD13	1:B:236:ARG:HG2	1.77	0.67
1:B:216:ALA:HB1	8:B:3001:ACT:H2	1.77	0.65
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:756:ASN:HB3	1:B:808:GLY:HA2	1.81	0.62
1:B:963:ASP:H	1:B:966:GLN:HG3	1.65	0.61
1:B:369:ILE:HG13	1:B:528:VAL:HG13	1.81	0.61
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.82	0.60
1:A:756:ASN:HB3	1:A:808:GLY:HA2	1.82	0.60
1:A:450:GLU:OE1	1:A:467:ARG:NH2	2.34	0.59
1:A:416:ILE:HD11	1:A:566:THR:HG22	1.85	0.59
1:B:907:ILE:HG23	1:B:977:VAL:HG11	1.84	0.59
1:A:862:GLY:H	1:A:863:PRO:HD3	1.68	0.58
1:A:60:LEU:HA	1:A:63:ARG:HD2	1.85	0.58
1:A:866:THR:HB	1:A:869:GLN:HB2	1.86	0.58
1:A:113:GLU:OE2	1:A:334:ARG:NH1	2.37	0.57
1:B:122:TYR:HA	1:B:158:LYS:HE3	1.85	0.57
1:B:816:ILE:HG23	1:B:817:MET:HG2	1.86	0.57
1:A:256:PHE:HA	1:A:259:GLN:HB2	1.85	0.57
1:B:844:VAL:HG22	1:B:907:ILE:HG21	1.88	0.55
1:A:923:MET:HE1	1:A:986:PHE:HE1	1.71	0.55
1:A:377:CYS:HB2	1:A:541:VAL:HG22	1.89	0.55
1:A:227:GLY:O	8:A:3002:ACT:H3	2.07	0.55
1:B:247:THR:HG21	1:B:337:PRO:HB2	1.90	0.54
1:A:307:ILE:HG21	4:A:1005:CZA:H102	1.89	0.54
1:B:857:MET:HA	1:B:865:VAL:HA	1.89	0.54
1:B:338:SER:HA	1:B:341:THR:HG23	1.90	0.54
1:A:921:SER:OG	1:A:989:ARG:NH2	2.40	0.54
1:A:381:GLU:O	1:A:397:LYS:HE2	2.07	0.54
1:B:953:LEU:HD23	1:B:956:ILE:HD11	1.90	0.53
1:A:549:ILE:HD11	1:A:596:VAL:HG21	1.90	0.53
1:A:947:ILE:HG12	1:A:953:LEU:HD13	1.91	0.53
1:B:962:LEU:HB3	1:B:966:GLN:HB2	1.91	0.53
1:B:319:LEU:HB3	1:B:336:LEU:HG	1.91	0.53
1:B:981:ASP:HA	1:B:984:LEU:HD12	1.90	0.53
1:B:695:ASP:OD2	1:B:825:LYS:NZ	2.29	0.53
1:A:248:PRO:O	1:A:252:LYS:HG2	2.08	0.53
1:B:271:VAL:HG21	1:B:302:LEU:HD11	1.91	0.52
1:B:691:LEU:HB3	1:B:698:THR:HG21	1.90	0.52
1:A:380:ASN:OD1	1:A:397:LYS:HE3	2.10	0.52
1:A:607:VAL:O	1:A:611:ILE:HG12	2.09	0.52
1:B:311:LEU:HD22	1:B:315:ILE:HG13	1.92	0.51
1:A:670:CYS:HB3	1:A:691:LEU:HD13	1.92	0.51
1:A:840:ILE:O	1:A:844:VAL:HG12	2.11	0.51
1:B:887:ASP:O	1:B:890:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:ARG:HH21	1:B:568:ASP:HB2	1.76	0.51
1:B:22:THR:HG22	1:B:23:GLY:O	2.11	0.50
1:A:482:GLU:HG2	1:A:573:ARG:NH1	2.26	0.50
1:B:839:ALA:HB1	1:B:980:LEU:HD11	1.93	0.50
1:A:389:TYR:HB3	1:A:425:LEU:HD11	1.93	0.50
1:A:92:PHE:O	1:A:96:LEU:HB2	2.12	0.50
1:B:767:SER:O	1:B:771:GLU:HG3	2.11	0.50
1:A:651:ARG:NH1	9:A:2247:HOH:O	2.45	0.50
1:B:650:ASP:N	1:B:650:ASP:OD1	2.42	0.50
1:B:151:VAL:HG21	1:B:163:ILE:HD13	1.93	0.49
1:B:764:LEU:O	1:B:768:ASN:ND2	2.44	0.49
1:B:793:LEU:O	1:B:797:LEU:HB2	2.12	0.49
1:B:679:VAL:HB	1:B:683:HIS:HB2	1.94	0.49
1:B:851:ALA:HB1	1:B:899:MET:HB3	1.95	0.49
1:A:773:VAL:HB	1:A:845:GLY:HA3	1.95	0.48
1:A:716:ILE:HD11	1:A:733:MET:HE3	1.95	0.48
1:B:947:ILE:HG12	1:B:953:LEU:HD13	1.96	0.48
1:A:650:ASP:O	1:A:672:ARG:HD2	2.14	0.48
1:A:905:VAL:O	1:A:909:MET:HG2	2.14	0.48
1:B:574:GLU:OE1	1:B:574:GLU:N	2.36	0.48
1:A:815:ASP:OD2	1:A:819:ARG:HD3	2.13	0.48
1:B:325:ARG:NH1	1:B:749:GLU:OE2	2.47	0.47
1:A:271:VAL:HG21	1:A:302:LEU:HD11	1.96	0.47
1:A:835:PHE:HA	1:A:838:MET:HB2	1.96	0.47
1:B:198:ARG:HH22	1:B:660:ASP:HA	1.79	0.47
1:A:774:CYS:O	1:A:778:THR:HG22	2.14	0.47
1:A:814:LEU:H	1:A:814:LEU:HD12	1.79	0.47
1:B:80:GLU:O	1:B:82:GLU:N	2.41	0.47
1:B:855:TRP:CZ3	1:B:863:PRO:HG3	2.48	0.47
1:A:308:PRO:HB3	1:A:768:ASN:ND2	2.29	0.47
1:A:962:LEU:HB3	1:A:966:GLN:HB2	1.96	0.47
1:B:200:VAL:HG22	1:B:680:GLU:CG	2.45	0.47
1:B:910:CYS:HB3	1:B:978:ILE:HG13	1.97	0.47
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.97	0.47
1:B:650:ASP:O	1:B:672:ARG:HD2	2.14	0.47
1:B:963:ASP:HB3	1:B:966:GLN:HG3	1.96	0.47
1:B:922:LEU:O	1:B:927:PRO:HD3	2.16	0.46
1:A:311:LEU:HD21	1:A:761:ILE:HG12	1.98	0.46
1:A:93:VAL:O	1:A:97:ILE:HG12	2.16	0.46
1:A:869:GLN:HB3	1:A:883:PHE:CE1	2.50	0.46
1:B:916:LEU:HD12	1:B:927:PRO:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:771:GLU:O	1:A:775:ILE:HG12	2.15	0.46
1:B:607:VAL:O	1:B:611:ILE:HG12	2.15	0.46
1:A:555:GLY:HA3	1:A:557:ASP:H	1.80	0.46
1:A:852:ALA:HB2	1:A:900:ALA:HB2	1.98	0.46
1:B:413:LEU:HG	1:B:564:LEU:HD12	1.97	0.46
1:A:951:ASP:HB2	1:A:952:PRO:HD3	1.96	0.46
1:A:712:LYS:HB3	1:A:712:LYS:HE2	1.37	0.46
1:A:366:MET:HG2	1:A:384:ILE:HD11	1.98	0.46
1:B:840:ILE:HD11	1:B:981:ASP:HB2	1.98	0.46
1:A:962:LEU:HB2	1:A:967:TRP:NE1	2.31	0.46
1:A:550:LYS:HE2	1:A:551:GLU:N	2.30	0.46
1:A:950:VAL:O	1:A:954:PRO:HD3	2.15	0.46
1:A:983:ILE:O	1:A:987:ILE:HG22	2.16	0.45
1:B:60:LEU:O	1:B:64:ILE:HG12	2.17	0.45
1:B:109:GLU:OE2	1:B:246:LYS:NZ	2.27	0.45
1:B:62:VAL:HG13	4:B:1005:CZA:H13	1.98	0.45
1:A:947:ILE:HG22	1:A:959:LEU:HD12	1.99	0.45
1:B:604:ARG:HB2	1:B:607:VAL:HG23	1.98	0.45
1:A:802:LEU:HG	1:A:939:LEU:HD23	1.98	0.45
1:B:52:LEU:HD23	1:B:52:LEU:HA	1.83	0.45
1:B:201:ASN:HB2	9:B:2059:HOH:O	2.16	0.45
1:A:240:ALA:O	1:A:242:THR:N	2.49	0.45
1:A:200:VAL:HG22	1:A:680:GLU:CG	2.46	0.45
1:A:857:MET:HA	1:A:865:VAL:HA	1.97	0.45
1:B:832:TRP:O	1:B:836:ARG:N	2.47	0.45
1:B:962:LEU:HB2	1:B:967:TRP:CD1	2.53	0.44
1:A:301:ALA:HA	1:A:789:PRO:HG3	1.99	0.44
1:B:757:MET:HG2	1:B:760:PHE:CZ	2.52	0.44
1:B:948:LEU:O	1:B:961:ALA:HB2	2.17	0.44
1:A:336:LEU:HD12	1:A:336:LEU:HA	1.85	0.44
1:B:926:PRO:HA	1:B:927:PRO:HD3	1.82	0.44
1:A:832:TRP:HH2	1:A:987:ILE:HG23	1.82	0.44
1:B:242:THR:O	1:B:244:GLN:N	2.51	0.44
1:A:33:LEU:HD13	1:A:146:VAL:CG1	2.48	0.44
1:A:482:GLU:HG2	1:A:573:ARG:HH12	1.82	0.44
1:B:534:ARG:NH2	1:B:568:ASP:HB2	2.32	0.44
1:B:447:THR:HG22	1:B:451:LYS:HE3	2.00	0.44
1:B:454:VAL:HG22	9:B:2130:HOH:O	2.18	0.44
1:A:887:ASP:HB3	1:A:890:ILE:HG13	2.00	0.44
1:B:88:PHE:C	1:B:91:PRO:HD2	2.38	0.44
1:B:856:PHE:CZ	1:B:891:PHE:HA	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:LEU:HD12	1:B:425:LEU:HA	1.88	0.43
1:A:363:VAL:HG11	1:A:448:LEU:HD22	2.00	0.43
1:A:412:GLU:OE2	1:A:566:THR:HG21	2.19	0.43
1:B:832:TRP:NE1	1:B:836:ARG:HD3	2.33	0.43
1:B:120:LYS:HG2	1:B:123:GLU:OE2	2.19	0.43
1:B:880:HIS:HD2	1:B:888:CYS:SG	2.41	0.43
1:A:832:TRP:CH2	1:A:987:ILE:HG23	2.53	0.43
1:A:476:ARG:NH2	9:A:2162:HOH:O	2.50	0.43
1:A:695:ASP:O	1:A:824:PRO:HG2	2.19	0.43
1:A:826:GLU:HA	1:A:827:PRO:HD3	1.84	0.43
1:B:712:LYS:HE2	1:B:712:LYS:HB3	1.67	0.43
1:B:129:VAL:HG12	1:B:151:VAL:HG12	1.99	0.43
1:A:79:GLU:HB3	1:A:84:THR:HG22	2.00	0.43
1:B:135:LYS:HA	1:B:135:LYS:HD2	1.74	0.43
1:A:202:GLN:OE1	1:A:202:GLN:N	2.50	0.42
1:A:667:ARG:HG2	1:A:694:TYR:CE2	2.53	0.42
1:A:305:ALA:HB1	1:A:771:GLU:HB3	2.00	0.42
1:A:559:LEU:HD23	1:A:600:LEU:HB3	2.01	0.42
1:B:620:ARG:NH2	1:B:671:ARG:HA	2.34	0.42
1:B:855:TRP:HA	1:B:859:ALA:HB3	2.01	0.42
1:B:459:VAL:HA	1:B:462:LEU:HG	2.00	0.42
1:A:883:PHE:HD1	1:A:886:LEU:HD11	1.85	0.42
1:A:151:VAL:HG21	1:A:163:ILE:CD1	2.50	0.42
1:B:248:PRO:HA	1:B:251:GLN:HB3	2.02	0.42
1:A:504:SER:C	1:A:506:ALA:H	2.21	0.42
1:A:352:LYS:HA	1:A:356:LEU:HB2	2.01	0.42
1:A:65:LEU:HB2	1:A:307:ILE:HD13	2.00	0.42
1:A:419:LEU:HD11	1:A:479:MET:HB2	2.01	0.42
1:A:64:ILE:HG21	1:A:264:ILE:HD13	2.01	0.42
1:B:151:VAL:HG21	1:B:163:ILE:CD1	2.49	0.42
1:A:981:ASP:HA	1:A:984:LEU:HB2	2.02	0.42
1:A:908:GLU:HA	1:A:911:ASN:HB2	2.02	0.42
1:A:45:GLU:HB2	1:A:46:GLY:H	1.56	0.41
1:A:118:ALA:O	1:A:121:GLU:HB2	2.19	0.41
1:A:495:SER:HB3	1:A:514:VAL:HG22	2.02	0.41
1:A:883:PHE:CD1	1:A:886:LEU:HD11	2.55	0.41
1:A:151:VAL:HG21	1:A:163:ILE:HD13	2.01	0.41
1:B:252:LYS:HA	1:B:252:LYS:HD3	1.92	0.41
1:A:606:GLU:HG3	1:A:739:ASN:OD1	2.19	0.41
1:A:61:LEU:HD12	4:A:1005:CZA:H8	2.02	0.41
1:B:113:GLU:OE2	1:B:334:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:PRO:HB3	1:B:450:GLU:CB	2.50	0.41
1:A:274:ILE:HG21	1:A:780:ALA:HB1	2.02	0.41
1:B:921:SER:OG	1:B:989:ARG:NH2	2.53	0.41
1:B:926:PRO:O	1:B:929:VAL:HG23	2.20	0.41
1:B:757:MET:HA	1:B:760:PHE:CE2	2.55	0.41
1:A:154:ALA:N	1:A:157:ASP:OD2	2.45	0.41
1:B:41:LEU:HD21	8:B:3002:ACT:H1	2.02	0.41
1:A:853:ALA:HA	1:A:856:PHE:HD1	1.86	0.41
1:B:556:ARG:HD2	1:B:644:GLU:HB3	2.02	0.41
1:B:511:LYS:HA	1:B:511:LYS:HD3	1.88	0.41
1:B:950:VAL:HG12	1:B:952:PRO:HD2	2.02	0.41
1:A:272:TRP:O	1:A:276:ILE:N	2.53	0.41
1:A:346:SER:HA	1:A:821:PRO:HG2	2.03	0.41
1:B:652:ALA:HA	1:B:675:CYS:O	2.21	0.41
1:A:694:TYR:HB2	1:A:696:GLU:HG3	2.02	0.41
1:B:654:THR:HA	1:B:677:ALA:O	2.21	0.41
1:A:201:ASN:HB2	9:A:2072:HOH:O	2.21	0.41
1:A:247:THR:HB	1:A:250:GLN:HB3	2.03	0.40
1:A:75:LEU:HD21	1:A:296:PHE:HB2	2.02	0.40
1:A:57:PHE:HE1	1:A:98:LEU:HB3	1.85	0.40
1:B:863:PRO:CD	1:B:864:GLY:HA2	2.51	0.40
1:B:122:TYR:O	1:B:211:GLY:HA2	2.22	0.40
1:A:573:ARG:HB2	1:A:574:GLU:OE2	2.21	0.40
1:A:555:GLY:CA	1:A:557:ASP:H	2.34	0.40
1:B:450:GLU:OE1	1:B:467:ARG:NH2	2.53	0.40
1:B:269:VAL:O	1:B:273:LEU:HG	2.20	0.40
1:A:800:ASP:C	1:A:803:PRO:HD2	2.42	0.40
1:B:308:PRO:O	1:B:311:LEU:HB2	2.22	0.40
1:A:35:LYS:HD3	1:A:36:TYR:CZ	2.56	0.40
1:B:916:LEU:HD23	1:B:916:LEU:HA	1.89	0.40
1:A:77:TRP:C	1:A:79:GLU:H	2.25	0.40
1:B:174:ARG:HB3	1:B:186:SER:HB3	2.04	0.40
1:A:287:SER:OG	1:A:289:ILE:HG22	2.21	0.40
1:A:353:THR:HA	1:A:357:THR:OG1	2.22	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%)	925 (93%)	52 (5%)	15 (2%)	13	22
1	B	992/994 (100%)	930 (94%)	53 (5%)	9 (1%)	21	37
All	All	1984/1988 (100%)	1855 (94%)	105 (5%)	24 (1%)	16	29

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	82	GLU
1	A	504	SER
1	B	243	GLU
1	B	283	VAL
1	B	865	VAL
1	A	831	GLY
1	A	865	VAL
1	A	46	GLY
1	A	47	LYS
1	A	241	ALA
1	A	827	PRO
1	A	864	GLY
1	B	47	LYS
1	B	867	TYR
1	A	857	MET
1	A	889	GLU
1	B	81	GLY
1	B	826	GLU
1	A	245	ASP
1	A	283	VAL
1	A	951	ASP
1	B	951	ASP
1	B	973	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	840/841 (100%)	786 (94%)	54 (6%)	22	39
1	B	840/841 (100%)	789 (94%)	51 (6%)	23	42
All	All	1680/1682 (100%)	1575 (94%)	105 (6%)	22	40

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	45	GLU
1	A	51	GLU
1	A	109	GLU
1	A	184	SER
1	A	200	VAL
1	A	236	ARG
1	A	245	ASP
1	A	247	THR
1	A	249	LEU
1	A	254	ASP
1	A	278	HIS
1	A	311	LEU
1	A	319	LEU
1	A	334	ARG
1	A	336	LEU
1	A	340	GLU
1	A	341	THR
1	A	342	LEU
1	A	356	LEU
1	A	397	LYS
1	A	465	VAL
1	A	478	LEU
1	A	482	GLU
1	A	533	THR
1	A	534	ARG
1	A	535	VAL

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Mol	Chain	Res	Type
1	A	543	GLU
1	A	544	LYS
1	A	550	LYS
1	A	566	THR
1	A	572	LYS
1	A	656	ARG
1	A	679	VAL
1	A	686	LYS
1	A	691	LEU
1	A	698	THR
1	A	712	LYS
1	A	716	ILE
1	A	759	GLN
1	A	760	PHE
1	A	767	SER
1	A	809	PHE
1	A	814	LEU
1	A	816	ILE
1	A	819	ARG
1	A	844	VAL
1	A	865	VAL
1	A	886	LEU
1	A	911	ASN
1	A	936	SER
1	A	956	ILE
1	A	964	LEU
1	A	986	PHE
1	B	18	VAL
1	B	19	SER
1	B	31	ARG
1	B	59	ASP
1	B	61	LEU
1	B	75	LEU
1	B	96	LEU
1	B	98	LEU
1	B	116	ILE
1	B	121	GLU
1	B	200	VAL
1	B	236	ARG
1	B	242	THR
1	B	278	HIS
1	B	309	GLU

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Mol	Chain	Res	Type
1	B	311	LEU
1	B	319	LEU
1	B	336	LEU
1	B	356	LEU
1	B	360	GLN
1	B	406	GLN
1	B	426	ASP
1	B	465	VAL
1	B	478	LEU
1	B	505	ARG
1	B	534	ARG
1	B	543	GLU
1	B	566	THR
1	B	572	LYS
1	B	577	VAL
1	B	605	LYS
1	B	656	ARG
1	B	691	LEU
1	B	701	THR
1	B	712	LYS
1	B	759	GLN
1	B	767	SER
1	B	778	THR
1	B	781	LEU
1	B	799	THR
1	B	813	ASP
1	B	819	ARG
1	B	838	MET
1	B	860	GLU
1	B	866	THR
1	B	877	THR
1	B	889	GLU
1	B	941	MET
1	B	956	ILE
1	B	980	LEU
1	B	992	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	868	HIS

### 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 17 ligands modelled in this entry, 7 are monoatomic - leaving 10 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	CZA	A	1005	5	25,29,29	1.59	6 (24%)	22,48,48	1.41	3 (13%)
6	ACP	A	1007	5	25,33,33	1.58	5 (20%)	31,52,52	2.29	8 (25%)
7	MGF	A	1950	9,1	0,3,3	0.00	-	0,3,3	0.00	-
8	ACT	A	3001	-	1,3,3	0.59	0	0,3,3	0.00	-
8	ACT	A	3002	-	1,3,3	0.45	0	0,3,3	0.00	-
4	CZA	B	1005	5	25,29,29	1.63	8 (32%)	22,48,48	1.54	4 (18%)
6	ACP	B	1007	-	25,33,33	1.63	5 (20%)	31,52,52	2.26	9 (29%)
7	MGF	B	1950	9,1	0,3,3	0.00	-	0,3,3	0.00	-
8	ACT	B	3001	-	1,3,3	1.21	0	0,3,3	0.00	-
8	ACT	B	3002	-	1,3,3	0.23	0	0,3,3	0.00	-

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	CZA	A	1005	5	-	0/4/52/52	0/5/5/5
6	ACP	A	1007	5	-	0/15/38/38	0/3/3/3
7	MGF	A	1950	9,1	-	0/0/0/0	0/0/0/0
8	ACT	A	3001	-	-	0/0/0/0	0/0/0/0
8	ACT	A	3002	-	-	0/0/0/0	0/0/0/0
4	CZA	B	1005	5	-	0/4/52/52	0/5/5/5
6	ACP	B	1007	-	-	0/15/38/38	0/3/3/3
7	MGF	B	1950	9,1	-	0/0/0/0	0/0/0/0
8	ACT	B	3001	-	-	0/0/0/0	0/0/0/0
8	ACT	B	3002	-	-	0/0/0/0	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1007	ACP	PB-O2B	-3.53	1.47	1.56
4	B	1005	CZA	C4-N1	-3.49	1.34	1.39
6	A	1007	ACP	PB-O2B	-3.26	1.48	1.56
6	B	1007	ACP	PG-O2G	-2.71	1.48	1.54
6	A	1007	ACP	PG-O2G	-2.64	1.48	1.54
4	A	1005	CZA	C4-N1	-2.60	1.35	1.39
4	B	1005	CZA	C3-C4	-2.54	1.35	1.40
4	A	1005	CZA	C3-C4	-2.17	1.36	1.40
4	B	1005	CZA	C13-C14	-2.12	1.39	1.44
4	B	1005	CZA	C16-C15	-2.00	1.35	1.38
4	A	1005	CZA	C20-C13	2.00	1.41	1.37
6	A	1007	ACP	C2-N3	2.01	1.35	1.32
4	B	1005	CZA	C20-C13	2.07	1.41	1.37
6	B	1007	ACP	PG-O3G	2.07	1.60	1.54
4	B	1005	CZA	C19-C18	2.22	1.41	1.36
4	A	1005	CZA	C19-C18	2.27	1.41	1.36
4	B	1005	CZA	O3-C4	2.32	1.37	1.31
6	B	1007	ACP	PB-O1B	2.46	1.58	1.51
4	A	1005	CZA	O3-C4	2.46	1.37	1.31
6	A	1007	ACP	PB-O1B	2.57	1.58	1.51
4	B	1005	CZA	C12-C8	3.32	1.57	1.52
6	A	1007	ACP	PG-O1G	3.54	1.58	1.50
6	B	1007	ACP	PG-O1G	3.57	1.58	1.50
4	A	1005	CZA	C12-C8	3.84	1.58	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1007	ACP	O3G-PG-O1G	-5.60	98.08	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1007	ACP	O3G-PG-O1G	-4.91	99.85	112.40
6	A	1007	ACP	C1'-N9-C4	-4.18	120.64	126.94
6	B	1007	ACP	C1'-N9-C4	-3.64	121.45	126.94
4	B	1005	CZA	C12-C13-C14	-2.34	117.45	119.49
6	A	1007	ACP	O2A-PA-O5'	-2.33	96.70	108.46
6	B	1007	ACP	O2A-PA-O5'	-2.29	96.89	108.46
4	A	1005	CZA	C12-C13-C14	-2.11	117.65	119.49
6	A	1007	ACP	C2'-C1'-N9	-2.07	111.12	114.29
6	B	1007	ACP	C4'-O4'-C1'	2.12	112.05	109.72
6	B	1007	ACP	O3G-PG-C3B	2.13	111.57	106.40
4	B	1005	CZA	O1-C2-C3	2.18	124.52	120.31
4	A	1005	CZA	C18-C17-N2	2.28	137.21	130.75
4	B	1005	CZA	C18-C17-N2	2.32	137.32	130.75
6	B	1007	ACP	N3-C2-N1	2.42	130.75	128.89
6	B	1007	ACP	O5'-PA-O1A	2.57	119.58	109.62
6	A	1007	ACP	O2B-PB-C3B	2.59	118.17	106.88
6	A	1007	ACP	O2G-PG-C3B	2.66	112.86	106.40
6	B	1007	ACP	O2G-PG-C3B	2.84	113.29	106.40
6	A	1007	ACP	O5'-PA-O1A	3.18	121.97	109.62
4	A	1005	CZA	C13-C14-C15	4.50	127.78	123.50
4	B	1005	CZA	C13-C14-C15	4.87	128.13	123.50
6	A	1007	ACP	PA-O3A-PB	7.49	153.76	132.73
6	B	1007	ACP	PA-O3A-PB	8.19	155.72	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1005	CZA	2	0
8	A	3001	ACT	1	0
8	A	3002	ACT	1	0
4	B	1005	CZA	2	0
8	B	3001	ACT	1	0
8	B	3002	ACT	1	0

## 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%)	0.56	144 (14%) <b>3</b> <b>3</b>	28, 62, 191, 294	0
1	B	994/994 (100%)	0.29	78 (7%) <b>16</b> <b>17</b>	32, 67, 156, 220	0
All	All	1988/1988 (100%)	0.43	222 (11%) <b>7</b> <b>7</b>	28, 65, 177, 294	0

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	VAL	15.9
1	B	288	TRP	10.6
1	A	284	HIS	10.5
1	A	285	GLY	10.3
1	A	281	ASP	10.0
1	A	282	PRO	9.7
1	A	280	ASN	9.3
1	A	78	PHE	9.3
1	A	948	LEU	8.8
1	A	890	ILE	8.3
1	A	891	PHE	8.3
1	A	874	MET	8.0
1	B	283	VAL	7.6
1	A	875	GLN	7.5
1	B	275	ASN	7.4
1	A	863	PRO	7.3
1	A	81	GLY	7.3
1	B	112	ALA	7.3
1	B	284	HIS	7.3
1	A	77	TRP	7.2
1	B	245	ASP	7.2
1	B	285	GLY	7.1
1	B	287	SER	6.8
1	A	288	TRP	6.8

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Mol	Chain	Res	Type	RSRZ
1	B	992	LEU	6.8
1	A	82	GLU	6.6
1	B	243	GLU	6.6
1	A	994	ASP	6.5
1	A	287	SER	6.5
1	B	280	ASN	6.5
1	B	271	VAL	6.4
1	B	282	PRO	6.4
1	A	970	VAL	6.4
1	B	927	PRO	6.4
1	B	81	GLY	6.1
1	A	286	GLY	6.1
1	A	60	LEU	6.1
1	A	853	ALA	6.1
1	B	276	ILE	6.0
1	B	289	ILE	6.0
1	B	77	TRP	6.0
1	A	856	PHE	6.0
1	A	50	TRP	6.0
1	A	111	ASN	6.0
1	A	868	HIS	5.7
1	A	949	TYR	5.6
1	A	46	GLY	5.6
1	B	279	PHE	5.6
1	A	873	PHE	5.6
1	A	991	TYR	5.5
1	A	80	GLU	5.5
1	A	279	PHE	5.4
1	B	286	GLY	5.4
1	A	292	ALA	5.3
1	B	991	TYR	5.2
1	A	865	VAL	5.0
1	B	986	PHE	4.9
1	A	961	ALA	4.9
1	A	782	GLY	4.9
1	B	295	TYR	4.8
1	A	289	ILE	4.8
1	A	962	LEU	4.8
1	A	74	VAL	4.7
1	B	111	ASN	4.6
1	A	860	GLU	4.6
1	A	857	MET	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	52	LEU	4.6
1	A	858	TYR	4.5
1	B	78	PHE	4.5
1	B	281	ASP	4.5
1	A	266	LEU	4.4
1	B	60	LEU	4.4
1	A	883	PHE	4.4
1	B	928	TRP	4.3
1	A	974	SER	4.3
1	A	967	TRP	4.3
1	A	291	GLY	4.3
1	B	292	ALA	4.2
1	A	85	ILE	4.2
1	A	781	LEU	4.2
1	B	964	LEU	4.2
1	A	881	PRO	4.1
1	A	850	GLY	4.0
1	B	274	ILE	4.0
1	B	924	ARG	4.0
1	B	293	ILE	4.0
1	B	244	GLN	4.0
1	B	278	HIS	3.9
1	A	278	HIS	3.9
1	A	888	CYS	3.9
1	A	925	MET	3.9
1	B	50	TRP	3.9
1	A	945	PHE	3.9
1	A	57	PHE	3.8
1	B	272	TRP	3.7
1	A	837	TYR	3.7
1	A	84	THR	3.7
1	B	994	ASP	3.7
1	A	886	LEU	3.7
1	B	925	MET	3.6
1	A	876	CYS	3.6
1	A	951	ASP	3.6
1	A	899	MET	3.6
1	B	273	LEU	3.6
1	A	892	GLU	3.6
1	B	291	GLY	3.6
1	A	973	ILE	3.6
1	A	64	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	872	HIS	3.5
1	A	49	LEU	3.5
1	A	916	LEU	3.5
1	A	53	VAL	3.4
1	A	968	LEU	3.4
1	B	242	THR	3.4
1	A	106	VAL	3.4
1	A	870	LEU	3.4
1	B	290	ARG	3.4
1	A	993	GLU	3.4
1	A	48	SER	3.4
1	B	262	LYS	3.2
1	B	269	VAL	3.2
1	B	45	GLU	3.2
1	A	778	THR	3.2
1	B	113	GLU	3.1
1	A	867	TYR	3.1
1	B	814	LEU	3.1
1	B	241	ALA	3.1
1	A	990	ASN	3.1
1	A	45	GLU	3.1
1	B	993	GLU	3.1
1	A	965	THR	3.1
1	B	44	GLU	3.0
1	A	829	ILE	3.0
1	A	947	ILE	3.0
1	A	972	LYS	3.0
1	B	829	ILE	3.0
1	A	882	HIS	3.0
1	A	273	LEU	3.0
1	A	107	TRP	3.0
1	A	854	TRP	3.0
1	B	46	GLY	3.0
1	A	894	PRO	3.0
1	A	864	GLY	2.9
1	A	79	GLU	2.9
1	A	844	VAL	2.9
1	B	923	MET	2.9
1	A	971	LEU	2.9
1	A	835	PHE	2.9
1	A	966	GLN	2.8
1	B	264	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	887	ASP	2.8
1	B	951	ASP	2.8
1	B	989	ARG	2.8
1	A	975	LEU	2.8
1	A	923	MET	2.8
1	A	959	LEU	2.7
1	B	52	LEU	2.7
1	A	507	ALA	2.7
1	A	871	THR	2.7
1	A	992	LEU	2.7
1	A	73	PHE	2.7
1	A	63	ARG	2.7
1	B	82	GLU	2.7
1	A	244	GLN	2.7
1	A	963	ASP	2.6
1	A	784	PRO	2.6
1	B	861	ASP	2.6
1	A	889	GLU	2.6
1	B	266	LEU	2.6
1	A	258	GLU	2.6
1	A	848	THR	2.6
1	A	869	GLN	2.6
1	A	293	ILE	2.5
1	A	960	LYS	2.5
1	B	297	LYS	2.5
1	A	989	ARG	2.5
1	B	80	GLU	2.5
1	A	54	ILE	2.5
1	A	846	ALA	2.5
1	A	277	GLY	2.5
1	B	932	TRP	2.5
1	B	832	TRP	2.5
1	B	83	GLU	2.5
1	A	839	ALA	2.5
1	A	55	GLU	2.4
1	A	270	ALA	2.4
1	B	865	VAL	2.4
1	A	243	GLU	2.4
1	A	901	LEU	2.4
1	B	968	LEU	2.4
1	A	964	LEU	2.4
1	A	895	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	890	ILE	2.4
1	A	787	LEU	2.3
1	B	971	LEU	2.3
1	B	251	GLN	2.3
1	A	98	LEU	2.3
1	A	833	LEU	2.3
1	B	922	LEU	2.3
1	B	109	GLU	2.3
1	A	67	LEU	2.3
1	A	855	TRP	2.3
1	A	983	ILE	2.2
1	B	461	ASN	2.2
1	A	110	ARG	2.2
1	A	878	GLU	2.2
1	A	957	PHE	2.2
1	A	926	PRO	2.2
1	A	506	ALA	2.2
1	B	983	ILE	2.2
1	A	920	GLN	2.2
1	A	914	ASN	2.1
1	B	926	PRO	2.1
1	B	256	PHE	2.1
1	B	920	GLN	2.1
1	A	58	GLU	2.1
1	A	814	LEU	2.1
1	A	862	GLY	2.1
1	A	981	ASP	2.1
1	A	780	ALA	2.0
1	A	51	GLU	2.0
1	A	956	ILE	2.0

## 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 [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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
8	ACT	B	3001	4/4	0.91	0.24	7.25	54,70,71,78	0
6	ACP	B	1007	31/31	0.82	0.24	4.53	31,73,150,371	31
8	ACT	A	3002	4/4	0.95	0.21	3.82	39,52,53,58	0
8	ACT	B	3002	4/4	0.88	0.21	3.12	55,60,63,63	0
2	MG	B	1002	1/1	0.99	0.24	2.45	37,37,37,37	0
6	ACP	A	1007	31/31	0.87	0.21	2.20	38,60,388,388	31
8	ACT	A	3001	4/4	0.95	0.18	1.96	55,67,68,74	0
7	MGF	A	1950	4/4	0.99	0.21	1.40	40,40,41,45	0
2	MG	A	1002	1/1	0.99	0.20	0.51	34,34,34,34	0
7	MGF	B	1950	4/4	0.99	0.18	0.12	34,35,35,42	0
4	CZA	A	1005	25/25	0.95	0.15	-0.53	112,124,128,180	0
4	CZA	B	1005	25/25	0.96	0.15	-0.65	75,88,101,104	0
3	K	A	1004	1/1	0.92	0.13	-0.90	78,78,78,78	0
3	K	B	1004	1/1	0.93	0.10	-1.71	84,84,84,84	0
5	MN	A	1006	1/1	0.97	0.06	-	107,107,107,107	0
5	MN	B	1006	1/1	0.95	0.12	-	102,102,102,102	0
5	MN	A	1008	1/1	0.88	0.41	-	174,174,174,174	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.