Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:25 AM GMT

PDB ID	:	3AR2
Title	:	Calcium pump crystal structure with bound AMPPCP and Ca2+
Authors	:	Toyoshima, C.; Yonekura, S.; Tsueda, J.; Iwasawa, S.
Deposited on	:	2010-11-24
Resolution	:	2.50 Å(reported)

The following versions of software and data (see references (i)) 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 (i)

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	Percentile Ranks	Value
Rfree		0.275
Clashscore		19
Ramachandran outliers		1.7%
Sidechain outliers		4.5%
RSRZ outliers		10.7%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
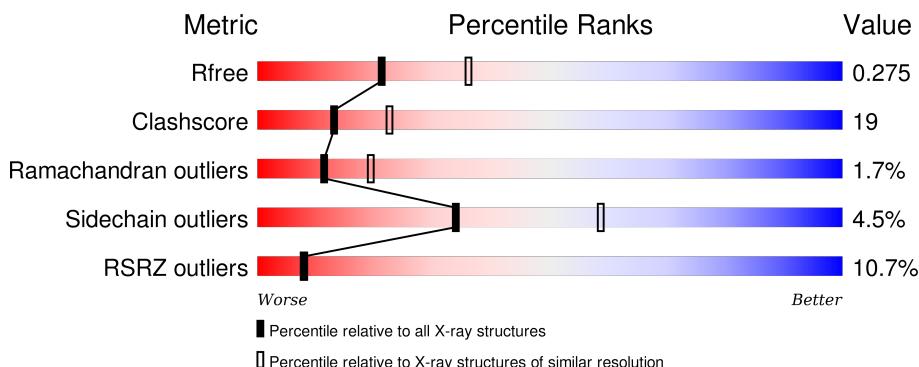
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 >=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 <=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	995	11% / 61% / 35% / ·

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7808 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
			Total	C	N	O	S			
1	A	995	7674	4878	1287	1452	57	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ACE	-	ACETYLATION	UNP P04191
A	994	GLY	ASP	SEE REMARK 999	UNP P04191

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

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

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).

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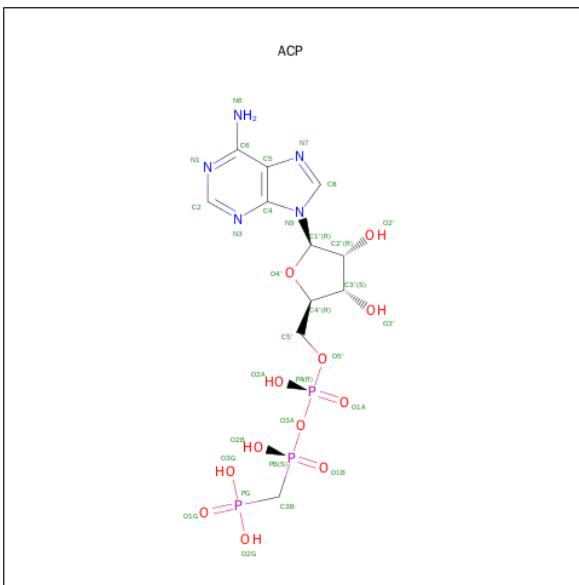
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).

PC1
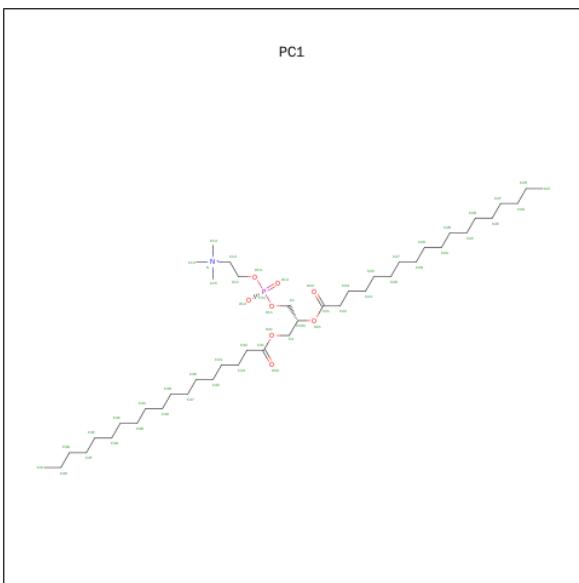
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 20	C 10	N 1	O 8	P 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	79	Total 79	O 79	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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
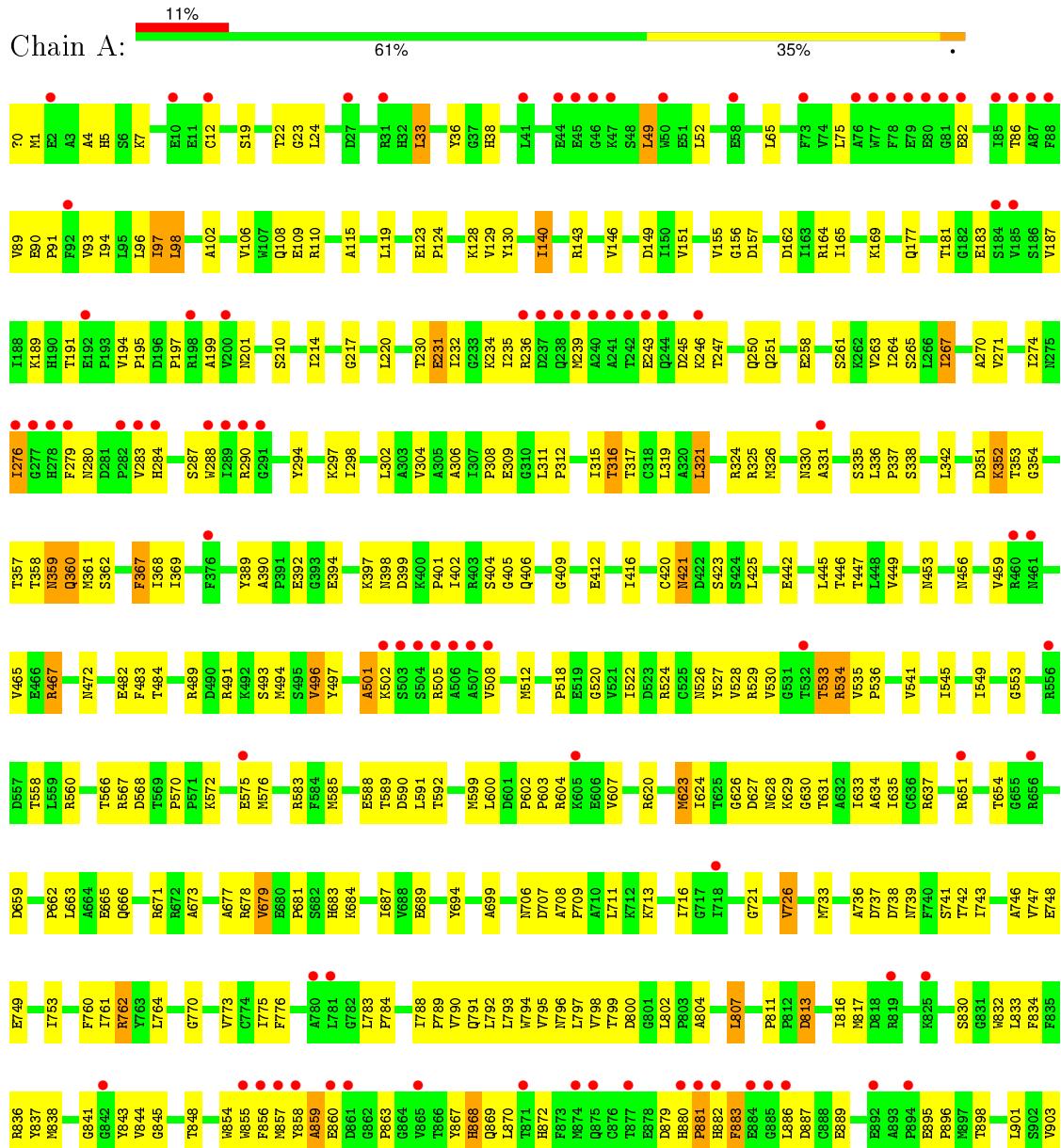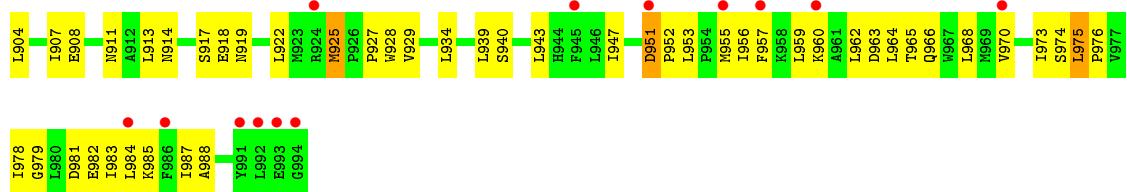
4   Data and refinement statistics   (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	162.00Å 75.31Å 151.54Å 90.00° 108.97° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.50) 99.4 (15.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.247 , 0.272 0.244 , 0.275	Depositor DCC
R_{free} test set	3001 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	63.3	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 78.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	1 of 59360 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7808	wwPDB-VP
Average B, all atoms (Å^2)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ACP, NA, CA, PC1, ACE

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	0.43	0/7813	0.58	1/10594 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	489	ARG	NE-CZ-NH2	-8.16	116.22	120.30

There are no chirality outliers.

There are no planarity outliers.

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	7674	0	7764	295	0
2	A	3	0	0	0	0
3	A	31	0	14	2	0
4	A	1	0	0	0	0
5	A	20	0	18	0	0
6	A	79	0	0	2	0
All	All	7808	0	7796	295	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 19.

All (295) 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:369:ILE:HD11	1:A:545:ILE:HD11	1.45	0.98
1:A:567:ARG:HD3	1:A:570:PRO:HA	1.46	0.96
1:A:624:ILE:HG21	1:A:684:LYS:HG2	1.47	0.96
1:A:342:LEU:HG	1:A:716:ILE:HD13	1.53	0.91
1:A:624:ILE:CG2	1:A:684:LYS:HG2	2.03	0.89
1:A:65:LEU:HD22	1:A:309:GLU:HG2	1.56	0.88
1:A:528:VAL:HG11	1:A:541:VAL:HG11	1.54	0.87
1:A:308:PRO:HB3	1:A:764:LEU:HD23	1.57	0.85
1:A:773:VAL:HG23	1:A:845:GLY:HA3	1.58	0.84
1:A:129:VAL:HG12	1:A:151:VAL:HG22	1.62	0.79
1:A:94:ILE:HD11	1:A:793:LEU:HD22	1.65	0.79
1:A:631:THR:O	1:A:635:ILE:HG12	1.84	0.78
1:A:679:VAL:HG22	1:A:683:HIS:CB	2.14	0.77
1:A:75:LEU:HD22	1:A:297:LYS:HD3	1.64	0.77
1:A:65:LEU:CD2	1:A:309:GLU:HG2	2.17	0.74
1:A:330:ASN:HB2	1:A:737:ASP:HB2	1.70	0.74
1:A:951:ASP:HB3	1:A:952:PRO:HD3	1.70	0.74
1:A:90:GLU:HB2	1:A:91:PRO:HD3	1.68	0.73
1:A:361:MET:HE3	1:A:599:MET:SD	2.29	0.72
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.71	0.71
1:A:762:ARG:HG2	1:A:837:TYR:HE1	1.55	0.71
1:A:90:GLU:HG2	1:A:790:VAL:CG1	2.21	0.71
1:A:369:ILE:CD1	1:A:545:ILE:HD11	2.21	0.70
1:A:770:GLY:HA3	1:A:844:VAL:CG2	2.22	0.70
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.92	0.70
1:A:679:VAL:HG22	1:A:683:HIS:CG	2.27	0.70
1:A:572:LYS:HB2	1:A:575:GLU:HG2	1.72	0.69
1:A:770:GLY:HA3	1:A:844:VAL:HG23	1.75	0.69
1:A:361:MET:HE1	1:A:560:ARG:HD3	1.75	0.69
1:A:96:LEU:HD23	1:A:797:LEU:HD11	1.74	0.69
1:A:928:TRP:HA	1:A:934:LEU:HD11	1.76	0.68
1:A:210:SER:O	1:A:232:ILE:HG12	1.94	0.68
1:A:671:ARG:HD3	1:A:694:TYR:CZ	2.29	0.67
1:A:1:MET:HE3	1:A:12:CYS:HA	1.76	0.66
1:A:518:PRO:O	1:A:522:ILE:HD13	1.96	0.66
1:A:115:ALA:HB2	1:A:324:ARG:HH12	1.59	0.66
1:A:904:LEU:O	1:A:908:GLU:HG3	1.96	0.66
1:A:791:GLN:HG2	1:A:901:LEU:HD22	1.78	0.66
1:A:308:PRO:HB3	1:A:764:LEU:CD2	2.25	0.66
1:A:898:THR:HG22	1:A:962:LEU:HD11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:869:GLN:NE2	1:A:872:HIS:H	1.94	0.65
1:A:679:VAL:HG22	1:A:683:HIS:HB3	1.78	0.65
1:A:922:LEU:HD22	1:A:927:PRO:HG3	1.78	0.65
1:A:748:GLU:HG3	1:A:817:MET:HG2	1.78	0.64
1:A:129:VAL:HG22	1:A:140:ILE:HD12	1.78	0.64
1:A:743:ILE:O	1:A:747:VAL:HG23	1.98	0.64
1:A:880:HIS:N	1:A:881:PRO:HD2	2.12	0.64
1:A:770:GLY:HA2	1:A:773:VAL:HG22	1.79	0.64
1:A:421:ASN:HD21	1:A:423:SER:HB2	1.61	0.64
1:A:94:ILE:HD12	1:A:304:VAL:HG11	1.79	0.63
1:A:108:GLN:HG2	1:A:317:THR:HG23	1.80	0.63
1:A:883:PHE:HB3	1:A:886:LEU:HD12	1.80	0.63
1:A:90:GLU:HG2	1:A:790:VAL:HG13	1.80	0.62
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.81	0.62
1:A:352:LYS:HE2	1:A:353:THR:OG1	1.98	0.62
1:A:181:THR:OG1	1:A:183:GLU:HG2	2.00	0.62
1:A:629:LYS:HA	1:A:677:ALA:CB	2.30	0.62
1:A:798:VAL:HG13	1:A:940:SER:HB3	1.82	0.61
1:A:115:ALA:HB2	1:A:324:ARG:NH1	2.15	0.61
1:A:939:LEU:O	1:A:943:LEU:HB2	2.01	0.61
1:A:983:ILE:O	1:A:987:ILE:HG12	2.01	0.61
1:A:261:SER:O	1:A:265:SER:HB2	2.01	0.60
1:A:389:TYR:HA	1:A:447:THR:HG21	1.84	0.60
1:A:793:LEU:O	1:A:796:ASN:HB3	2.02	0.59
1:A:94:ILE:CD1	1:A:793:LEU:HD22	2.32	0.59
1:A:230:THR:C	1:A:232:ILE:H	2.04	0.59
1:A:947:ILE:HD13	1:A:953:LEU:HD23	1.84	0.59
1:A:762:ARG:HH21	1:A:836:ARG:HH12	1.48	0.59
1:A:94:ILE:HD11	1:A:793:LEU:HD13	1.85	0.59
1:A:762:ARG:HG2	1:A:837:TYR:CE1	2.38	0.59
1:A:762:ARG:NH2	1:A:836:ARG:HH12	2.00	0.58
1:A:311:LEU:HD13	1:A:761:ILE:HD11	1.86	0.58
1:A:302:LEU:HD13	1:A:775:ILE:HD12	1.85	0.58
1:A:287:SER:HB2	1:A:290:ARG:HB2	1.86	0.58
1:A:280:ASN:HD21	1:A:288:TRP:HA	1.69	0.58
1:A:446:THR:HG23	1:A:472:ASN:ND2	2.19	0.57
1:A:368:ILE:HD12	1:A:409:GLY:HA3	1.86	0.57
1:A:162:ASP:OD2	1:A:230:THR:HA	2.04	0.57
1:A:258:GLU:HA	1:A:261:SER:HB3	1.87	0.57
1:A:491:ARG:NH1	1:A:588:GLU:OE1	2.38	0.57
1:A:917:SER:HB2	1:A:925:MET:HE2	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:VAL:HG22	1:A:217:GLY:N	2.20	0.56
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.88	0.56
1:A:354:GLY:HA2	1:A:359:ASN:HB2	1.87	0.56
1:A:361:MET:CE	1:A:560:ARG:HD3	2.36	0.55
1:A:792:LEU:O	1:A:795:VAL:HG12	2.05	0.55
1:A:963:ASP:HB2	1:A:966:GLN:HG3	1.88	0.55
1:A:683:HIS:O	1:A:687:ILE:HG12	2.07	0.55
1:A:367:PHE:C	1:A:367:PHE:CD2	2.80	0.55
1:A:352:LYS:NZ	1:A:627:ASP:OD2	2.40	0.55
1:A:412:GLU:OE2	1:A:529:ARG:NH1	2.39	0.55
1:A:38:HIS:CD2	1:A:143:ARG:HH21	2.24	0.55
1:A:491:ARG:HD2	1:A:493:SER:OG	2.08	0.54
1:A:856:PHE:HD1	1:A:870:LEU:HD21	1.73	0.54
1:A:416:ILE:HD11	1:A:566:THR:CG2	2.37	0.54
1:A:357:THR:HA	1:A:603:PRO:HA	1.89	0.54
1:A:965:THR:HG23	1:A:968:LEU:HD12	1.88	0.54
1:A:681:PRO:HG3	1:A:706:ASN:HB2	1.90	0.54
1:A:530:VAL:HB	1:A:533:THR:HG22	1.90	0.54
1:A:788:ILE:HB	1:A:789:PRO:HD2	1.90	0.54
1:A:1:MET:HG2	1:A:4:ALA:HB2	1.89	0.53
1:A:102:ALA:O	1:A:106:VAL:HG12	2.09	0.53
1:A:156:GLY:HA2	1:A:726:VAL:CG1	2.38	0.53
1:A:760:PHE:HA	1:A:807:LEU:HD23	1.89	0.53
1:A:267:ILE:HG22	1:A:776:PHE:CE1	2.43	0.53
1:A:165:ILE:HG22	1:A:191:THR:HG22	1.90	0.53
1:A:155:VAL:HG22	1:A:217:GLY:H	1.74	0.53
1:A:5:HIS:HD2	1:A:194:VAL:HG13	1.74	0.53
1:A:421:ASN:ND2	1:A:442:GLU:HB3	2.23	0.53
1:A:201:ASN:ND2	1:A:231:GLU:OE2	2.42	0.53
1:A:312:PRO:O	1:A:315:ILE:HG22	2.09	0.52
1:A:813:ASP:HA	1:A:925:MET:HE1	1.91	0.52
1:A:518:PRO:HB3	1:A:549:ILE:HD13	1.92	0.52
1:A:308:PRO:CB	1:A:764:LEU:HD23	2.32	0.52
1:A:952:PRO:O	1:A:956:ILE:HG13	2.10	0.52
1:A:834:PHE:O	1:A:838:MET:HG2	2.10	0.52
1:A:271:VAL:HA	1:A:274:ILE:HG12	1.91	0.52
1:A:397:LYS:CB	1:A:402:ILE:HD12	2.40	0.51
1:A:210:SER:HB3	1:A:232:ILE:HD13	1.93	0.51
1:A:604:ARG:HB2	1:A:607:VAL:CG2	2.40	0.51
1:A:843:TYR:OH	1:A:976:PRO:HG2	2.10	0.51
1:A:123:GLU:OE1	1:A:124:PRO:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ILE:HD12	1:A:306:ALA:HB1	1.93	0.51
1:A:811:PRO:HG3	1:A:929:VAL:CG1	2.40	0.51
1:A:629:LYS:HD2	1:A:654:THR:CG2	2.41	0.51
1:A:802:LEU:HD12	1:A:939:LEU:HD23	1.93	0.51
1:A:491:ARG:HD2	1:A:588:GLU:OE2	2.11	0.51
1:A:520:GLY:O	1:A:524:ARG:HG3	2.11	0.51
1:A:128:LYS:NZ	1:A:157:ASP:OD2	2.33	0.50
1:A:589:THR:HG22	1:A:590:ASP:N	2.27	0.50
1:A:739:ASN:HD21	1:A:741:SER:HB2	1.77	0.49
1:A:895:GLU:N	1:A:896:PRO:HD2	2.27	0.49
1:A:895:GLU:HG2	1:A:960:LYS:HD3	1.94	0.49
1:A:979:GLY:O	1:A:983:ILE:HG12	2.12	0.49
1:A:748:GLU:HG3	1:A:817:MET:CG	2.43	0.49
1:A:276:ILE:HA	1:A:279:PHE:CE2	2.47	0.49
1:A:342:LEU:HD22	1:A:747:VAL:HG22	1.93	0.49
1:A:335:SER:OG	1:A:337:PRO:HD2	2.12	0.49
1:A:589:THR:HG22	1:A:590:ASP:H	1.77	0.49
1:A:624:ILE:HG22	1:A:684:LYS:HG2	1.91	0.49
1:A:773:VAL:CG2	1:A:845:GLY:HA3	2.37	0.49
1:A:533:THR:HG23	1:A:534:ARG:N	2.28	0.49
1:A:651:ARG:HA	1:A:673:ALA:HA	1.94	0.49
1:A:716:ILE:HD11	1:A:733:MET:HE2	1.94	0.48
1:A:975:LEU:N	1:A:976:PRO:HD2	2.28	0.48
1:A:331:ALA:HB2	1:A:742:THR:HG21	1.95	0.48
1:A:880:HIS:C	1:A:882:HIS:H	2.17	0.48
1:A:351:ASP:OD2	3:A:1002:ACP:O3G	2.30	0.48
1:A:553:GLY:CA	1:A:631:THR:HG22	2.43	0.48
1:A:529:ARG:HH22	1:A:568:ASP:CG	2.17	0.48
1:A:848:THR:HG21	1:A:904:LEU:HD13	1.95	0.48
1:A:352:LYS:HB2	1:A:623:MET:CE	2.44	0.48
1:A:659:ASP:HA	1:A:666:GLN:NE2	2.28	0.48
1:A:75:LEU:CD2	1:A:297:LYS:HD3	2.41	0.48
1:A:572:LYS:HB2	1:A:575:GLU:CG	2.43	0.48
1:A:336:LEU:N	1:A:337:PRO:CD	2.77	0.48
1:A:830:SER:HB3	1:A:833:LEU:HB2	1.95	0.48
1:A:89:VAL:HG21	1:A:956:ILE:HG21	1.95	0.47
1:A:352:LYS:HB2	1:A:623:MET:HE2	1.96	0.47
1:A:97:ILE:HD11	1:A:800:ASP:O	2.13	0.47
1:A:524:ARG:HB2	1:A:591:LEU:HD12	1.96	0.47
1:A:854:TRP:O	1:A:859:ALA:HA	2.14	0.47
1:A:287:SER:HB2	1:A:290:ARG:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LYS:HZ3	1:A:220:LEU:HD12	1.79	0.47
1:A:770:GLY:HA2	1:A:841:GLY:O	2.14	0.47
1:A:246:LYS:HE3	1:A:251:GLN:HE21	1.79	0.47
1:A:558:THR:HG22	1:A:634:ALA:HB1	1.96	0.47
1:A:887:ASP:OD2	1:A:889:GLU:HB2	2.15	0.47
1:A:689:GLU:HG3	1:A:713:LYS:HE3	1.95	0.47
1:A:903:VAL:HG22	1:A:970:VAL:HA	1.96	0.47
1:A:358:THR:HG23	1:A:602:PRO:O	2.15	0.47
1:A:352:LYS:CE	1:A:353:THR:OG1	2.62	0.46
1:A:247:THR:HG23	1:A:250:GLN:HE21	1.80	0.46
1:A:23:GLY:HA3	1:A:130:TYR:O	2.15	0.46
1:A:360:GLN:HA	1:A:360:GLN:HE21	1.79	0.46
1:A:24:LEU:HD22	1:A:149:ASP:HB3	1.96	0.46
1:A:7:LYS:NZ	1:A:7:LYS:HB2	2.31	0.46
1:A:389:TYR:O	1:A:425:LEU:HD21	2.15	0.46
1:A:880:HIS:N	1:A:881:PRO:CD	2.79	0.46
1:A:361:MET:CE	1:A:599:MET:SD	3.01	0.46
1:A:981:ASP:O	1:A:985:LYS:N	2.45	0.46
1:A:140:ILE:H	1:A:140:ILE:HD13	1.79	0.46
1:A:425:LEU:HD22	1:A:447:THR:HG22	1.98	0.46
1:A:527:TYR:O	1:A:592:THR:HA	2.16	0.46
1:A:155:VAL:HA	1:A:214:ILE:HG22	1.98	0.46
1:A:232:ILE:N	1:A:232:ILE:HD12	2.32	0.45
1:A:1:MET:CG	1:A:4:ALA:HB2	2.45	0.45
1:A:624:ILE:O	1:A:684:LYS:HE2	2.15	0.45
1:A:361:MET:HE1	1:A:599:MET:HG3	1.99	0.45
1:A:230:THR:C	1:A:232:ILE:N	2.70	0.45
1:A:530:VAL:O	1:A:533:THR:HB	2.15	0.45
1:A:913:LEU:O	1:A:922:LEU:HD21	2.16	0.45
1:A:629:LYS:HD2	1:A:654:THR:HG23	1.98	0.45
1:A:681:PRO:HG3	1:A:706:ASN:CB	2.47	0.45
1:A:816:ILE:HG23	1:A:817:MET:N	2.32	0.45
1:A:389:TYR:CA	1:A:447:THR:HG21	2.47	0.45
1:A:526:ASN:HD22	1:A:590:ASP:HA	1.82	0.45
1:A:911:ASN:O	1:A:914:ASN:HB2	2.16	0.45
1:A:804:ALA:O	1:A:807:LEU:HB2	2.16	0.45
1:A:119:LEU:HD11	1:A:330:ASN:HA	1.99	0.45
1:A:491:ARG:HG3	1:A:585:MET:HB2	1.98	0.45
1:A:620:ARG:NH2	1:A:671:ARG:HA	2.32	0.45
1:A:491:ARG:HH11	1:A:588:GLU:CD	2.20	0.44
1:A:662:PRO:HG2	1:A:665:GLU:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:957:PHE:O	1:A:959:LEU:HG	2.17	0.44
1:A:737:ASP:O	1:A:738:ASP:HB2	2.17	0.44
1:A:19:SER:HB2	1:A:22:THR:HB	1.98	0.44
1:A:482:GLU:HG3	1:A:497:TYR:HD1	1.81	0.44
1:A:33:LEU:HD12	1:A:146:VAL:CG1	2.47	0.44
1:A:283:VAL:HG13	1:A:284:HIS:H	1.82	0.44
1:A:315:ILE:HG23	1:A:316:THR:N	2.33	0.44
1:A:397:LYS:HB3	1:A:402:ILE:HD12	2.00	0.44
1:A:501:ALA:HB3	1:A:505:ARG:HG2	2.00	0.44
1:A:978:ILE:O	1:A:982:GLU:HB2	2.18	0.44
1:A:624:ILE:HG22	1:A:679:VAL:HG11	2.00	0.44
1:A:361:MET:HE2	1:A:560:ARG:HE	1.83	0.44
1:A:353:THR:HG1	3:A:1002:ACP:PG	2.40	0.44
1:A:267:ILE:O	1:A:271:VAL:HG23	2.18	0.44
1:A:231:GLU:HA	1:A:234:LYS:HG2	1.98	0.44
1:A:49:LEU:HD22	1:A:110:ARG:NE	2.33	0.44
1:A:412:GLU:CD	1:A:529:ARG:HH11	2.22	0.43
1:A:353:THR:HA	1:A:357:THR:OG1	2.18	0.43
1:A:246:LYS:HE3	1:A:251:GLN:NE2	2.33	0.43
1:A:0:ACE:H3	1:A:36:TYR:CE1	2.52	0.43
1:A:762:ARG:HH11	1:A:762:ARG:HB3	1.84	0.43
1:A:397:LYS:HB2	1:A:402:ILE:HD12	2.00	0.43
1:A:797:LEU:HD23	1:A:798:VAL:HG23	2.00	0.43
1:A:342:LEU:HG	1:A:716:ILE:CD1	2.35	0.43
1:A:94:ILE:HD11	1:A:793:LEU:CD2	2.42	0.43
1:A:553:GLY:HA2	1:A:631:THR:HG22	2.01	0.43
1:A:96:LEU:HB3	1:A:797:LEU:CD1	2.49	0.43
1:A:880:HIS:O	1:A:882:HIS:N	2.52	0.43
1:A:530:VAL:HB	1:A:533:THR:CG2	2.48	0.43
1:A:879:ASP:HB3	1:A:882:HIS:CE1	2.54	0.43
1:A:86:THR:O	1:A:86:THR:HG22	2.19	0.43
1:A:567:ARG:HD3	1:A:570:PRO:CA	2.33	0.43
1:A:508:VAL:HG12	1:A:508:VAL:O	2.19	0.43
1:A:633:ILE:O	1:A:637:ARG:HG3	2.19	0.43
1:A:783:LEU:HB3	1:A:784:PRO:HD2	1.99	0.42
1:A:836:ARG:HD3	1:A:984:LEU:HD13	2.00	0.42
1:A:529:ARG:NH2	1:A:568:ASP:OD1	2.52	0.42
1:A:795:VAL:O	1:A:799:THR:OG1	2.37	0.42
1:A:707:ASP:O	1:A:711:LEU:HD12	2.19	0.42
1:A:52:LEU:HB3	1:A:106:VAL:HG23	2.01	0.42
1:A:195:PRO:O	1:A:197:PRO:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ILE:HA	1:A:270:ALA:HB3	2.02	0.42
1:A:628:ASN:OD1	1:A:630:GLY:N	2.51	0.42
1:A:459:VAL:HB	1:A:467:ARG:CD	2.49	0.42
1:A:367:PHE:CD2	1:A:367:PHE:O	2.73	0.42
1:A:404:SER:C	1:A:406:GLN:H	2.21	0.42
1:A:394:GLU:OE1	1:A:401:PRO:HB3	2.19	0.42
1:A:964:LEU:HD12	1:A:964:LEU:H	1.84	0.42
1:A:535:VAL:HB	1:A:536:PRO:HD2	2.00	0.42
1:A:483:PHE:HZ	1:A:576:MET:HE1	1.84	0.42
1:A:326:MET:CE	1:A:746:ALA:HB2	2.50	0.41
1:A:553:GLY:O	1:A:558:THR:HA	2.20	0.41
1:A:749:GLU:O	1:A:753:ILE:HG12	2.21	0.41
1:A:699:ALA:HA	1:A:716:ILE:O	2.20	0.41
1:A:529:ARG:NH2	1:A:592:THR:HG21	2.35	0.41
1:A:119:LEU:CD1	1:A:330:ASN:HA	2.51	0.41
1:A:181:THR:HG1	1:A:183:GLU:HG2	1.83	0.41
1:A:533:THR:CG2	1:A:534:ARG:N	2.83	0.41
1:A:904:LEU:O	1:A:907:ILE:HG22	2.21	0.41
1:A:811:PRO:HG3	1:A:929:VAL:HG13	2.03	0.41
1:A:420:CYS:SG	1:A:494:MET:HG2	2.61	0.41
1:A:38:HIS:CG	1:A:143:ARG:HH21	2.38	0.41
1:A:903:VAL:HA	1:A:970:VAL:HG13	2.03	0.41
1:A:97:ILE:CG2	1:A:98:LEU:N	2.83	0.41
1:A:321:LEU:HD22	1:A:325:ARG:CZ	2.51	0.41
1:A:626:GLY:O	1:A:678:ARG:HA	2.21	0.41
1:A:1:MET:CE	1:A:12:CYS:HA	2.49	0.41
1:A:788:ILE:HB	1:A:789:PRO:CD	2.51	0.41
1:A:263:VAL:O	1:A:267:ILE:HG13	2.20	0.41
1:A:855:TRP:HH2	1:A:863:PRO:HD2	1.85	0.41
1:A:624:ILE:CG2	1:A:679:VAL:HG11	2.51	0.41
1:A:974:SER:C	1:A:976:PRO:HD2	2.41	0.41
1:A:721:GLY:HA3	1:A:736:ALA:HA	2.03	0.41
1:A:89:VAL:O	1:A:93:VAL:HG23	2.21	0.40
1:A:858:TYR:O	1:A:860:GLU:N	2.54	0.40
1:A:832:TRP:CE2	1:A:988:ALA:HB2	2.56	0.40
1:A:867:TYR:CE2	1:A:868:HIS:ND1	2.89	0.40
1:A:918:GLU:HG2	1:A:919:ASN:ND2	2.36	0.40
1:A:898:THR:HG21	1:A:960:LYS:O	2.21	0.40
1:A:794:TRP:CZ2	1:A:947:ILE:HG13	2.57	0.40
1:A:189:LYS:HD3	1:A:189:LYS:HA	1.87	0.40
1:A:235:ILE:O	1:A:239:MET:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:HD11	1:A:109:GLU:HG2	2.04	0.40
1:A:800:ASP:OD2	6:A:3401:HOH:O	2.22	0.40
1:A:496:VAL:O	1:A:512:MET:HA	2.21	0.40
1:A:362:SER:HA	6:A:4506:HOH:O	2.20	0.40
1:A:177:GLN:NE2	1:A:187:VAL:HG21	2.35	0.40
1:A:398:ASN:O	1:A:399:ASP:HB2	2.20	0.40
1:A:528:VAL:HG11	1:A:541:VAL:CG1	2.39	0.40
1:A:294:TYR:CZ	1:A:298:ILE:HD11	2.56	0.40
1:A:390:ALA:C	1:A:392:GLU:H	2.25	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	993/995 (100%)	878 (88%)	98 (10%)	17 (2%)	11 19

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	857	MET
1	A	951	ASP
1	A	245	ASP
1	A	859	ALA
1	A	243	GLU
1	A	338	SER
1	A	501	ALA
1	A	502	LYS
1	A	868	HIS
1	A	231	GLU
1	A	236	ARG
1	A	82	GLU

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Mol	Chain	Res	Type
1	A	453	ASN
1	A	456	ASN
1	A	199	ALA
1	A	405	GLY
1	A	881	PRO

5.3.2　Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	840/840 (100%)	802 (96%)	38 (4%)	34	59

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	49	LEU
1	A	97	ILE
1	A	98	LEU
1	A	140	ILE
1	A	164	ARG
1	A	267	ILE
1	A	276	ILE
1	A	316	THR
1	A	319	LEU
1	A	321	LEU
1	A	352	LYS
1	A	359	ASN
1	A	360	GLN
1	A	367	PHE
1	A	421	ASN
1	A	445	LEU
1	A	449	VAL
1	A	465	VAL
1	A	467	ARG
1	A	484	THR

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Mol	Chain	Res	Type
1	A	496	VAL
1	A	533	THR
1	A	534	ARG
1	A	583	ARG
1	A	600	LEU
1	A	623	MET
1	A	663	LEU
1	A	679	VAL
1	A	726	VAL
1	A	762	ARG
1	A	807	LEU
1	A	813	ASP
1	A	883	PHE
1	A	925	MET
1	A	955	MET
1	A	973	ILE
1	A	975	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	111	ASN
1	A	114	ASN
1	A	201	ASN
1	A	202	GLN
1	A	250	GLN
1	A	251	GLN
1	A	280	ASN
1	A	359	ASN
1	A	360	GLN
1	A	380	ASN
1	A	421	ASN
1	A	472	ASN
1	A	755	ASN
1	A	869	GLN
1	A	872	HIS
1	A	875	GLN
1	A	914	ASN
1	A	919	ASN
1	A	920	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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	ACP	A	1002	2	25,33,33	2.04	6 (24%)	31,52,52	2.33	6 (19%)
5	PC1	A	1011	-	19,19,53	2.03	3 (15%)	20,25,61	1.35	3 (15%)

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
3	ACP	A	1002	2	-	0/15/38/38	0/3/3/3
5	PC1	A	1011	-	-	0/21/21/57	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1011	PC1	O21-C2	-2.27	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	ACP	PB-O2B	-2.24	1.50	1.56
3	A	1002	ACP	C2-N3	2.20	1.36	1.32
3	A	1002	ACP	O4'-C1'	2.25	1.44	1.41
3	A	1002	ACP	C5-C4	2.74	1.46	1.40
5	A	1011	PC1	O31-C31	5.07	1.47	1.32
3	A	1002	ACP	PB-O3A	5.74	1.64	1.58
3	A	1002	ACP	PG-O1G	6.06	1.64	1.50
5	A	1011	PC1	O21-C21	6.35	1.47	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	ACP	N3-C2-N1	-8.86	122.11	128.89
5	A	1011	PC1	O21-C21-O22	-3.77	120.49	125.50
5	A	1011	PC1	C3-C2-C1	-3.38	104.16	112.07
3	A	1002	ACP	PA-O3A-PB	-3.17	123.82	132.73
3	A	1002	ACP	C4-C5-N7	-2.76	106.94	109.48
3	A	1002	ACP	O2G-PG-O1G	-2.45	106.12	112.40
3	A	1002	ACP	O2A-PA-O1A	2.14	124.14	112.53
5	A	1011	PC1	O31-C3-C2	2.34	114.99	108.69
3	A	1002	ACP	O1B-PB-C3B	5.09	121.82	109.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	ACP	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	994/995 (99%)	0.51	106 (10%)	8	8	48, 111, 207, 257	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	46	GLY	8.4
1	A	503	SER	7.9
1	A	45	GLU	7.7
1	A	241	ALA	7.6
1	A	951	ASP	7.2
1	A	77	TRP	6.7
1	A	992	LEU	6.6
1	A	85	ILE	6.6
1	A	50	TRP	6.4
1	A	508	VAL	6.4
1	A	288	TRP	6.2
1	A	80	GLU	6.2
1	A	505	ARG	6.0
1	A	991	TYR	5.9
1	A	81	GLY	5.9
1	A	506	ALA	5.9
1	A	825	LYS	5.7
1	A	47	LYS	5.6
1	A	243	GLU	5.6
1	A	242	THR	5.3
1	A	881	PRO	5.3
1	A	240	ALA	5.0
1	A	781	LEU	4.8
1	A	875	GLN	4.8
1	A	283	VAL	4.8
1	A	861	ASP	4.7
1	A	236	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	986	PHE	4.7
1	A	276	ILE	4.6
1	A	289	ILE	4.6
1	A	502	LYS	4.3
1	A	279	PHE	4.2
1	A	507	ALA	4.0
1	A	78	PHE	4.0
1	A	87	ALA	4.0
1	A	856	PHE	3.9
1	A	238	GLN	3.8
1	A	504	SER	3.8
1	A	575	GLU	3.7
1	A	244	GLN	3.7
1	A	237	ASP	3.6
1	A	76	ALA	3.6
1	A	885	GLY	3.6
1	A	855	TRP	3.5
1	A	994	GLY	3.4
1	A	290	ARG	3.4
1	A	857	MET	3.4
1	A	886	LEU	3.3
1	A	884	GLU	3.3
1	A	955	MET	3.3
1	A	858	TYR	3.2
1	A	185	VAL	3.2
1	A	874	MET	3.2
1	A	894	PRO	3.2
1	A	92	PHE	3.2
1	A	82	GLU	3.1
1	A	44	GLU	3.1
1	A	291	GLY	3.0
1	A	79	GLU	2.9
1	A	284	HIS	2.9
1	A	88	PHE	2.8
1	A	957	PHE	2.8
1	A	198	ARG	2.8
1	A	993	GLU	2.8
1	A	924	ARG	2.7
1	A	882	HIS	2.7
1	A	871	THR	2.6
1	A	246	LYS	2.6
1	A	780	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	460	ARG	2.6
1	A	73	PHE	2.6
1	A	282	PRO	2.5
1	A	960	LYS	2.5
1	A	27	ASP	2.5
1	A	860	GLU	2.5
1	A	2	GLU	2.5
1	A	984	LEU	2.5
1	A	58	GLU	2.5
1	A	718	ILE	2.4
1	A	31	ARG	2.4
1	A	278	HIS	2.4
1	A	880	HIS	2.4
1	A	556	ARG	2.4
1	A	41	LEU	2.3
1	A	945	PHE	2.3
1	A	877	THR	2.3
1	A	10	GLU	2.3
1	A	331	ALA	2.3
1	A	277	GLY	2.3
1	A	192	GLU	2.3
1	A	461	ASN	2.2
1	A	892	GLU	2.2
1	A	651	ARG	2.2
1	A	200	VAL	2.2
1	A	605	LYS	2.2
1	A	239	MET	2.2
1	A	86	THR	2.2
1	A	532	THR	2.2
1	A	184	SER	2.1
1	A	12	CYS	2.1
1	A	819	ARG	2.1
1	A	970	VAL	2.1
1	A	376	PHE	2.1
1	A	656	ARG	2.1
1	A	865	VAL	2.0
1	A	842	GLY	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. 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, 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	LLDF	B-factors($Å^2$)	Q<0.9
5	PC1	A	1011	20/54	0.79	0.21	0.05	116,118,124,124	0
4	NA	A	1000	1/1	0.91	0.14	-0.77	74,74,74,74	0
3	ACP	A	1002	31/31	0.97	0.11	-0.90	44,55,60,65	0
2	CA	A	1001	1/1	0.98	0.08	-1.85	67,67,67,67	0
2	CA	A	995	1/1	0.98	0.05	-4.05	87,87,87,87	0
2	CA	A	996	1/1	0.96	0.07	-4.35	85,85,85,85	0

6.5 Other polymers (i)

There are no such residues in this entry.