Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:06 PM GMT

PDB ID	:	3W5D
Title	:	Crystal structure of the calcium pump in the E2+Pi state
Authors	:	Toyoshima, C.; Iwasawa, S.; Ogawa, H.; Hirata, A.; Tsueda, J.; Inesi, G.
Deposited on	:	2013-01-27
Resolution	:	2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

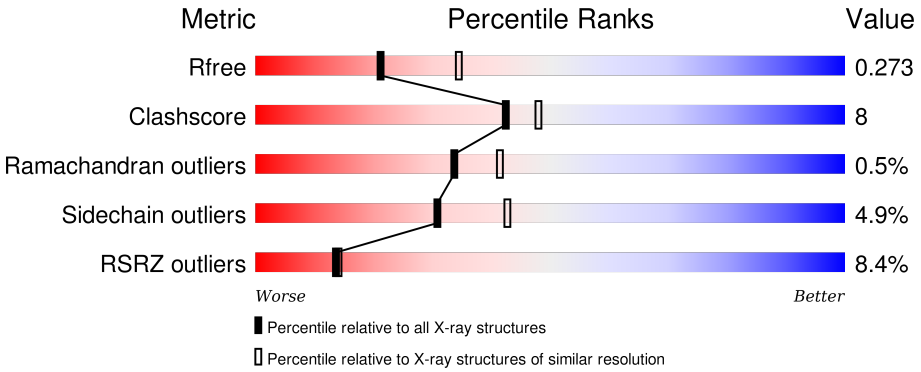
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.45 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	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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	8% 79% 20%

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
3	PTY	A	1002	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PTY	A	1003	-	-	-	X
3	PTY	A	1005	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7811 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 SERCA1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	995	Total	C	N	O	S	0	0	0
			7674	4878	1287	1452	57			

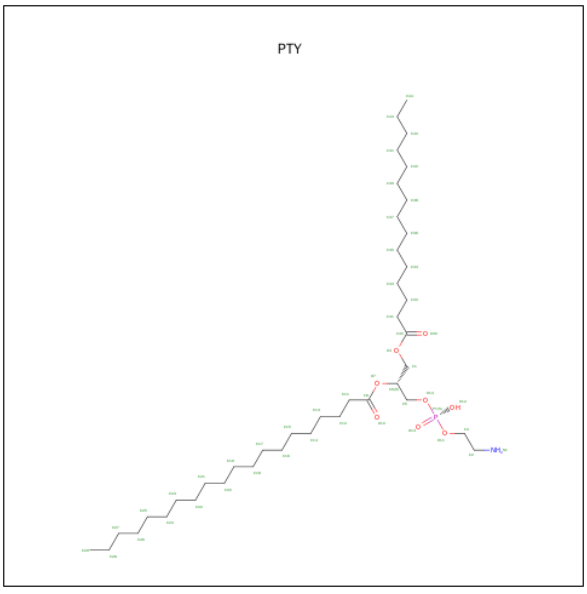
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ACE	-	ACETYLATION	UNP B6CAM1

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

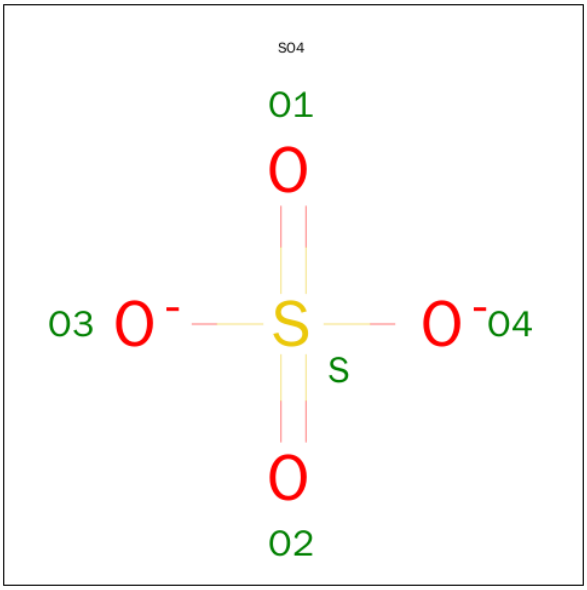
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
3	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
3	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
3	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
3	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

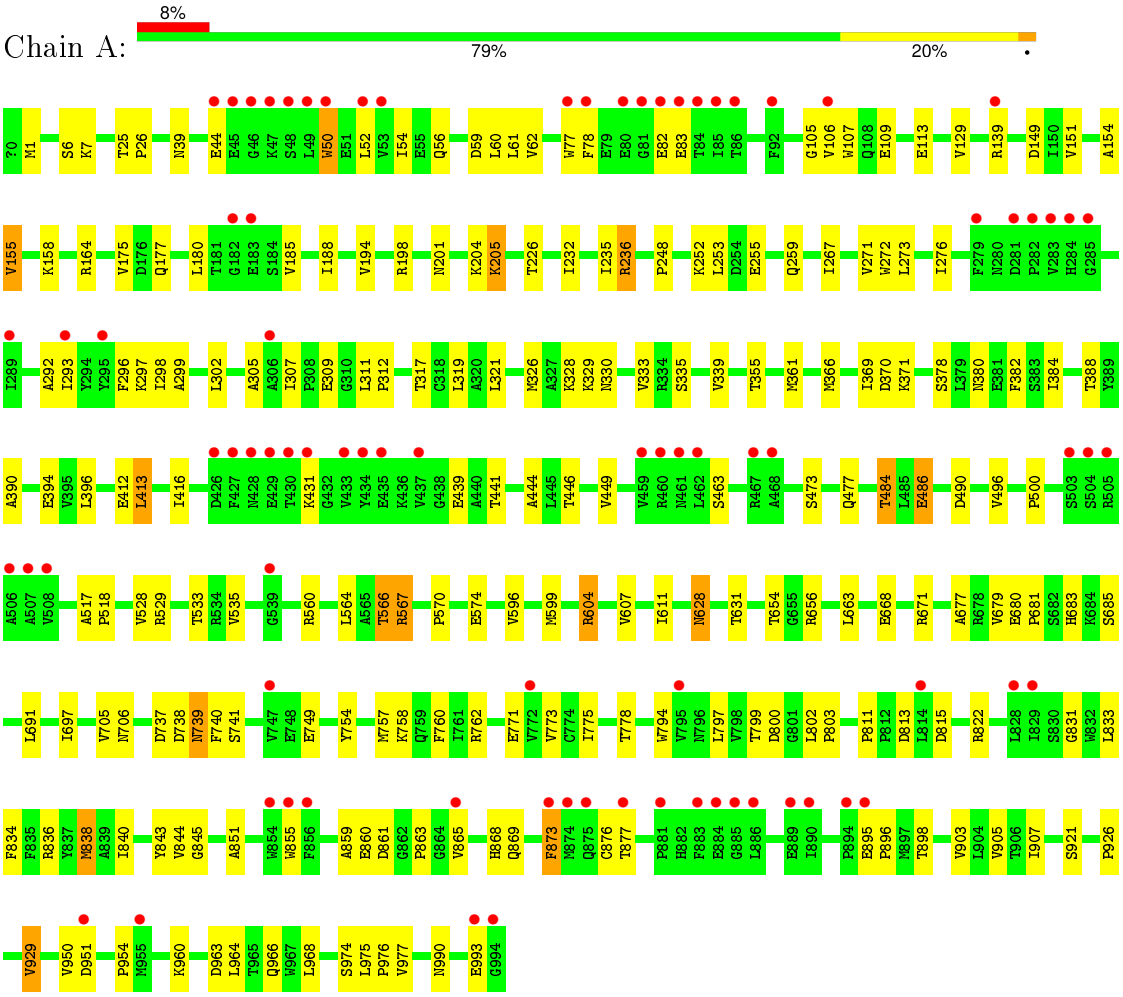
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total	O	0	0
			31	31		

3 Residue-property plots (i)

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: SERCA1a

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	71.25Å 71.25Å 587.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.45 47.65 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.00-2.45) 99.9 (47.65-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.51 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.241 , 0.271 0.238 , 0.273	Depositor DCC
R_{free} test set	2900 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	58.9	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Outliers	0 of 57796 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7811	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: NA, SO4, ACE, PTY

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	0.51	5/7813 (0.1%)	0.61	1/10594 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	TRP	CD2-CE2	5.25	1.47	1.41
1	A	77	TRP	CD2-CE2	5.22	1.47	1.41
1	A	794	TRP	CD2-CE2	5.17	1.47	1.41
1	A	50	TRP	CD2-CE2	5.11	1.47	1.41
1	A	272	TRP	CD2-CE2	5.05	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	413	LEU	CA-CB-CG	5.43	127.79	115.30

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	7765	129	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	95	0	55	2	0
4	A	10	0	0	0	0
5	A	31	0	0	0	0
All	All	7811	0	7820	129	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 8.

All (129) 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:990:ASN:HD21	3:A:1003:PTY:HC31	1.32	0.93
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.57	0.85
1:A:873:PHE:CE2	1:A:876:CYS:HA	2.19	0.78
1:A:775:ILE:O	1:A:778:THR:HG22	1.85	0.77
1:A:963:ASP:CB	1:A:966:GLN:HE21	2.00	0.74
1:A:963:ASP:HB2	1:A:966:GLN:HE21	1.53	0.74
1:A:129:VAL:HG12	1:A:151:VAL:HG12	1.68	0.74
1:A:873:PHE:HE2	1:A:876:CYS:HA	1.55	0.71
1:A:567:ARG:HD2	1:A:570:PRO:HA	1.73	0.70
1:A:628:ASN:HD22	1:A:628:ASN:C	1.95	0.70
1:A:271:VAL:HG11	1:A:298:ILE:HD11	1.72	0.70
1:A:412:GLU:OE2	1:A:566:THR:HG21	1.93	0.68
1:A:380:ASN:HB3	1:A:382:PHE:CE1	2.28	0.67
1:A:56:GLN:OE1	1:A:105:GLY:HA3	1.95	0.67
1:A:844:VAL:HG22	1:A:907:ILE:HG21	1.77	0.66
1:A:668:GLU:O	1:A:671:ARG:HG2	1.98	0.64
1:A:484:THR:HB	1:A:496:VAL:HG12	1.78	0.64
1:A:843:TYR:OH	1:A:976:PRO:HG2	1.97	0.64
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.98	0.64
1:A:628:ASN:ND2	1:A:631:THR:H	1.94	0.64
1:A:369:ILE:HG13	1:A:528:VAL:CG1	2.29	0.63
1:A:369:ILE:HG13	1:A:528:VAL:HG13	1.81	0.63
1:A:963:ASP:HB3	1:A:966:GLN:HG3	1.78	0.62
1:A:52:LEU:HD11	1:A:109:GLU:HG3	1.79	0.62
1:A:413:LEU:HD22	1:A:564:LEU:HD12	1.82	0.62
1:A:628:ASN:HD21	1:A:631:THR:H	1.47	0.62
1:A:860:GLU:H	1:A:860:GLU:CD	2.03	0.61
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.82	0.61
1:A:860:GLU:CD	1:A:860:GLU:N	2.54	0.61
1:A:865:VAL:HB	1:A:868:HIS:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LEU:HD21	1:A:232:ILE:HG22	1.83	0.59
1:A:235:ILE:HD13	1:A:705:VAL:HG12	1.85	0.59
1:A:328:LYS:HA	1:A:328:LYS:HE2	1.85	0.59
1:A:205:LYS:HB3	1:A:205:LYS:NZ	2.18	0.59
1:A:975:LEU:N	1:A:976:PRO:HD2	2.19	0.58
1:A:271:VAL:HG11	1:A:298:ILE:CD1	2.33	0.58
1:A:739:ASN:HD22	1:A:740:PHE:N	2.02	0.57
1:A:39:ASN:OD1	1:A:226:THR:HB	2.04	0.57
1:A:394:GLU:HG3	1:A:396:LEU:HD21	1.86	0.56
1:A:865:VAL:HB	1:A:868:HIS:CB	2.35	0.55
1:A:441:THR:HG23	1:A:599:MET:SD	2.46	0.55
1:A:311:LEU:N	1:A:312:PRO:HD2	2.22	0.55
1:A:863:PRO:HB2	1:A:865:VAL:HG22	1.89	0.55
1:A:326:MET:HG2	1:A:749:GLU:HG2	1.89	0.55
1:A:831:GLY:HA3	3:A:1005:PTY:O13	2.08	0.54
1:A:329:LYS:O	1:A:330:ASN:HB2	2.08	0.54
1:A:326:MET:CE	1:A:333:VAL:HG21	2.40	0.52
1:A:370:ASP:HB3	1:A:378:SER:OG	2.10	0.52
1:A:326:MET:HE1	1:A:339:VAL:HG22	1.92	0.52
1:A:201:ASN:HA	1:A:204:LYS:HD2	1.92	0.52
1:A:309:GLU:HB3	1:A:797:LEU:HD11	1.91	0.51
1:A:293:ILE:O	1:A:297:LYS:HB2	2.10	0.51
1:A:380:ASN:HB3	1:A:382:PHE:CZ	2.45	0.51
1:A:758:LYS:O	1:A:762:ARG:HG3	2.10	0.51
1:A:654:THR:HA	1:A:677:ALA:O	2.11	0.51
1:A:1:MET:HE1	1:A:7:LYS:HG3	1.93	0.50
1:A:679:VAL:HG13	1:A:683:HIS:CB	2.38	0.50
1:A:129:VAL:HG12	1:A:151:VAL:CG1	2.39	0.50
1:A:267:ILE:HG22	1:A:302:LEU:HD11	1.93	0.50
1:A:834:PHE:O	1:A:838:MET:HB2	2.12	0.50
1:A:52:LEU:HG	1:A:106:VAL:HG22	1.94	0.49
1:A:361:MET:HB3	1:A:444:ALA:HB2	1.94	0.49
1:A:963:ASP:HB3	1:A:966:GLN:HE21	1.77	0.49
1:A:851:ALA:HB2	1:A:903:VAL:HG21	1.93	0.49
1:A:628:ASN:C	1:A:628:ASN:ND2	2.65	0.49
1:A:326:MET:HE1	1:A:333:VAL:HG21	1.95	0.49
1:A:305:ALA:HB1	1:A:771:GLU:HB3	1.95	0.49
1:A:754:TYR:CE2	1:A:822:ARG:HD2	2.48	0.49
1:A:567:ARG:CD	1:A:570:PRO:HA	2.42	0.48
1:A:50:TRP:O	1:A:54:ILE:HG12	2.13	0.48
1:A:663:LEU:HD12	1:A:663:LEU:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:CE	1:A:7:LYS:HG3	2.43	0.47
1:A:737:ASP:O	1:A:738:ASP:HB2	2.14	0.47
1:A:61:LEU:HD22	1:A:307:ILE:HD12	1.95	0.47
1:A:188:ILE:HD13	1:A:486:GLU:HG2	1.96	0.47
1:A:836:ARG:O	1:A:840:ILE:HG12	2.15	0.47
1:A:974:SER:O	1:A:977:VAL:HG12	2.15	0.46
1:A:950:VAL:O	1:A:954:PRO:HD2	2.14	0.46
1:A:799:THR:HG21	1:A:905:VAL:HG22	1.97	0.46
1:A:607:VAL:O	1:A:611:ILE:HG12	2.14	0.46
1:A:255:GLU:O	1:A:259:GLN:HG2	2.15	0.46
1:A:6:SER:HA	1:A:194:VAL:O	2.14	0.46
1:A:473:SER:O	1:A:477:GLN:HG2	2.15	0.46
1:A:59:ASP:HB3	1:A:62:VAL:HG22	1.98	0.46
1:A:811:PRO:HG3	1:A:929:VAL:HG13	1.98	0.46
1:A:855:TRP:HA	1:A:859:ALA:HB3	1.97	0.46
1:A:317:THR:O	1:A:321:LEU:HG	2.15	0.45
1:A:813:ASP:HB3	1:A:815:ASP:OD1	2.15	0.45
1:A:185:VAL:HG21	1:A:439:GLU:HG3	1.99	0.45
1:A:898:THR:HG21	1:A:960:LYS:O	2.17	0.45
1:A:298:ILE:O	1:A:302:LEU:HB2	2.16	0.45
1:A:248:PRO:O	1:A:252:LYS:HE3	2.16	0.45
1:A:895:GLU:N	1:A:896:PRO:HD2	2.32	0.45
1:A:757:MET:HA	1:A:760:PHE:CE2	2.52	0.45
1:A:25:THR:HB	1:A:26:PRO:HD2	1.99	0.45
1:A:974:SER:C	1:A:976:PRO:HD2	2.38	0.44
1:A:773:VAL:CG1	1:A:845:GLY:HA3	2.47	0.44
1:A:416:ILE:HD11	1:A:566:THR:HG22	1.99	0.44
1:A:446:THR:O	1:A:449:VAL:HG22	2.18	0.44
1:A:366:MET:HA	1:A:596:VAL:O	2.19	0.43
1:A:309:GLU:CB	1:A:797:LEU:HD11	2.49	0.43
1:A:205:LYS:HB3	1:A:205:LYS:HZ2	1.82	0.43
1:A:388:THR:HG23	1:A:390:ALA:HB3	2.00	0.43
1:A:697:ILE:N	1:A:697:ILE:HD12	2.33	0.43
1:A:380:ASN:HD22	1:A:382:PHE:HZ	1.65	0.43
1:A:273:LEU:HA	1:A:276:ILE:HG13	2.00	0.43
1:A:964:LEU:O	1:A:968:LEU:HB2	2.19	0.42
1:A:441:THR:HG21	1:A:560:ARG:HH12	1.84	0.42
1:A:154:ALA:O	1:A:155:VAL:C	2.57	0.42
1:A:355:THR:HA	1:A:738:ASP:O	2.19	0.42
1:A:604:ARG:CG	1:A:604:ARG:HH11	2.32	0.42
1:A:273:LEU:HD23	1:A:276:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ALA:O	1:A:296:PHE:HD1	2.02	0.42
1:A:697:ILE:N	1:A:697:ILE:CD1	2.83	0.41
1:A:739:ASN:C	1:A:739:ASN:HD22	2.24	0.41
1:A:963:ASP:H	1:A:966:GLN:NE2	2.17	0.41
1:A:205:LYS:H	1:A:205:LYS:HG2	1.64	0.41
1:A:384:ILE:HA	1:A:394:GLU:O	2.20	0.41
1:A:388:THR:CG2	1:A:390:ALA:HB3	2.50	0.41
1:A:802:LEU:HB2	1:A:803:PRO:HD3	2.02	0.41
1:A:604:ARG:HH11	1:A:604:ARG:HG3	1.84	0.41
1:A:680:GLU:HB2	1:A:683:HIS:CD2	2.55	0.41
1:A:298:ILE:HG13	1:A:299:ALA:N	2.35	0.41
1:A:175:VAL:HG12	1:A:177:GLN:HG3	2.02	0.41
1:A:800:ASP:C	1:A:803:PRO:HD2	2.41	0.41
1:A:236:ARG:HD3	1:A:236:ARG:C	2.41	0.41
1:A:739:ASN:ND2	1:A:741:SER:H	2.18	0.40
1:A:517:ALA:HA	1:A:518:PRO:HD3	1.83	0.40
1:A:926:PRO:O	1:A:929:VAL:HB	2.22	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%)	931 (94%)	57 (6%)	5 (0%)	34 41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	VAL
1	A	463	SER
1	A	869	GLN
1	A	993	GLU

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Mol	Chain	Res	Type
1	A	951	ASP

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%)	799 (95%)	41 (5%)	31 43

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLU
1	A	60	LEU
1	A	78	PHE
1	A	82	GLU
1	A	83	GLU
1	A	113	GLU
1	A	139	ARG
1	A	149	ASP
1	A	158	LYS
1	A	164	ARG
1	A	198	ARG
1	A	205	LYS
1	A	236	ARG
1	A	253	LEU
1	A	319	LEU
1	A	335	SER
1	A	371	LYS
1	A	431	LYS
1	A	484	THR
1	A	486	GLU
1	A	490	ASP
1	A	500	PRO
1	A	533	THR
1	A	535	VAL
1	A	566	THR

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Mol	Chain	Res	Type
1	A	567	ARG
1	A	574	GLU
1	A	604	ARG
1	A	628	ASN
1	A	656	ARG
1	A	685	SER
1	A	691	LEU
1	A	706	ASN
1	A	739	ASN
1	A	833	LEU
1	A	838	MET
1	A	861	ASP
1	A	873	PHE
1	A	877	THR
1	A	921	SER
1	A	929	VAL

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

Mol	Chain	Res	Type
1	A	202	GLN
1	A	250	GLN
1	A	275	ASN
1	A	359	ASN
1	A	461	ASN
1	A	510	ASN
1	A	628	ASN
1	A	739	ASN
1	A	919	ASN
1	A	966	GLN
1	A	990	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	PTY	A	1002	-	17,18,49	1.50	2 (11%)	18,23,54	1.57	1 (5%)
3	PTY	A	1003	-	17,18,49	1.61	2 (11%)	18,23,54	1.62	3 (16%)
3	PTY	A	1004	-	17,18,49	1.56	2 (11%)	18,23,54	1.71	1 (5%)
3	PTY	A	1005	-	17,18,49	1.47	2 (11%)	18,23,54	1.67	3 (16%)
3	PTY	A	1006	-	17,18,49	1.56	2 (11%)	18,23,54	1.48	1 (5%)
4	SO4	A	1007	-	4,4,4	0.46	0	6,6,6	0.16	0
4	SO4	A	1008	-	4,4,4	0.54	0	6,6,6	0.14	0

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	PTY	A	1002	-	-	0/20/20/53	0/0/0/0
3	PTY	A	1003	-	-	0/20/20/53	0/0/0/0
3	PTY	A	1004	-	-	0/20/20/53	0/0/0/0
3	PTY	A	1005	-	-	0/20/20/53	0/0/0/0
3	PTY	A	1006	-	-	0/20/20/53	0/0/0/0
4	SO4	A	1007	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1008	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1005	PTY	O4-C30	2.40	1.46	1.33
3	A	1002	PTY	O4-C30	2.52	1.46	1.33
3	A	1006	PTY	O4-C30	2.56	1.46	1.33
3	A	1004	PTY	O4-C30	2.59	1.47	1.33
3	A	1003	PTY	O4-C30	2.69	1.47	1.33
3	A	1005	PTY	O7-C8	4.94	1.46	1.35
3	A	1002	PTY	O7-C8	4.96	1.46	1.35
3	A	1006	PTY	O7-C8	5.14	1.47	1.35
3	A	1004	PTY	O7-C8	5.19	1.47	1.35
3	A	1003	PTY	O7-C8	5.32	1.47	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1005	PTY	O7-C8-O10	-2.01	118.91	122.92
3	A	1003	PTY	O4-C1-C6	2.03	114.15	108.69
3	A	1005	PTY	O4-C30-C31	2.12	122.04	112.42
3	A	1003	PTY	C1-O4-C30	2.48	123.41	117.14
3	A	1003	PTY	O7-C8-C11	4.56	119.69	111.10
3	A	1006	PTY	O7-C8-C11	4.66	119.89	111.10
3	A	1002	PTY	O7-C8-C11	4.97	120.48	111.10
3	A	1005	PTY	O7-C8-C11	5.32	121.13	111.10
3	A	1004	PTY	O7-C8-C11	5.66	121.79	111.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	PTY	1	0
3	A	1005	PTY	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^{th} 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	83 (8%) 14 14	36, 67, 126, 200	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	504	SER	14.5
1	A	885	GLY	12.3
1	A	886	LEU	11.8
1	A	883	PHE	11.8
1	A	505	ARG	11.2
1	A	506	ALA	10.3
1	A	82	GLU	10.0
1	A	81	GLY	9.0
1	A	80	GLU	8.6
1	A	46	GLY	8.4
1	A	503	SER	7.3
1	A	85	ILE	7.1
1	A	84	THR	7.0
1	A	507	ALA	7.0
1	A	994	GLY	6.7
1	A	508	VAL	6.3
1	A	855	TRP	5.7
1	A	884	GLU	5.5
1	A	462	LEU	5.3
1	A	279	PHE	5.3
1	A	86	THR	5.2
1	A	459	VAL	5.1
1	A	427	PHE	5.1
1	A	894	PRO	4.7
1	A	993	GLU	4.7
1	A	52	LEU	4.6
1	A	461	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	53	VAL	4.4
1	A	289	ILE	4.2
1	A	78	PHE	4.1
1	A	45	GLU	3.9
1	A	877	THR	3.9
1	A	889	GLU	3.8
1	A	44	GLU	3.7
1	A	49	LEU	3.6
1	A	281	ASP	3.5
1	A	426	ASP	3.4
1	A	92	PHE	3.4
1	A	285	GLY	3.4
1	A	434	TYR	3.3
1	A	874	MET	3.3
1	A	460	ARG	3.3
1	A	828	LEU	3.2
1	A	955	MET	3.1
1	A	468	ALA	3.1
1	A	814	LEU	3.1
1	A	50	TRP	3.0
1	A	284	HIS	3.0
1	A	282	PRO	2.8
1	A	873	PHE	2.8
1	A	183	GLU	2.8
1	A	430	THR	2.8
1	A	795	VAL	2.8
1	A	106	VAL	2.7
1	A	139	ARG	2.7
1	A	856	PHE	2.7
1	A	47	LYS	2.6
1	A	865	VAL	2.6
1	A	77	TRP	2.6
1	A	854	TRP	2.6
1	A	429	GLU	2.5
1	A	182	GLY	2.5
1	A	890	ILE	2.4
1	A	428	ASN	2.4
1	A	433	VAL	2.3
1	A	875	GLN	2.3
1	A	951	ASP	2.3
1	A	48	SER	2.3
1	A	295	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	435	GLU	2.3
1	A	431	LYS	2.2
1	A	437	VAL	2.2
1	A	467	ARG	2.2
1	A	283	VAL	2.2
1	A	306	ALA	2.2
1	A	293	ILE	2.1
1	A	829	ILE	2.1
1	A	895	GLU	2.1
1	A	747	VAL	2.0
1	A	772	VAL	2.0
1	A	539	GLY	2.0
1	A	83	GLU	2.0
1	A	881	PRO	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, 95^{th} 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
3	PTY	A	1002	19/50	0.69	0.35	6.71	107,120,142,142	0
3	PTY	A	1003	19/50	0.90	0.23	4.27	103,108,121,123	0
3	PTY	A	1005	19/50	0.85	0.27	3.01	104,119,136,138	0
3	PTY	A	1006	19/50	0.76	0.26	1.90	105,128,152,156	0
3	PTY	A	1004	19/50	0.86	0.24	1.90	85,117,122,126	0
4	SO4	A	1008	5/5	0.89	0.15	-1.21	85,100,103,108	0
2	NA	A	1001	1/1	0.98	0.04	-4.17	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	A	1007	5/5	0.97	0.12	-	96,99,102,103	0

6.5 Other polymers (i)

There are no such residues in this entry.