Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 12:28 PM EDT

PDB ID	:	4Y3U
Title	:	The structure of phospholamban bound to the calcium pump SERCA1a
Authors	:	Hurley, T.D.
Deposited on	:	2015-02-10
Resolution	:	3.51 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

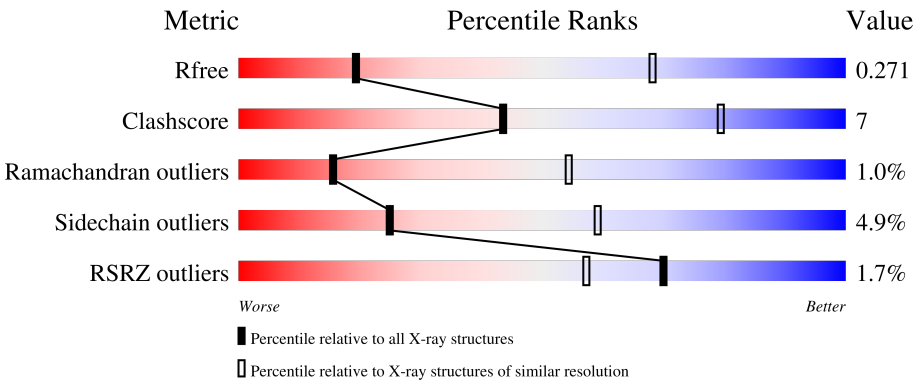
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.51 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 77% 20% • •
2	B	50	44% 14% • 40%
3	C	23	70% 30%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7812 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	970	7489	4767	1255	1410	57	0	0	0

- Molecule 2 is a protein called Cardiac phospholamban.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	30	242	161	40	37	4	0	0	0

- Molecule 3 is a protein called Cardiac phospholamban.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	16	80	48	16	16	0	0	0

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

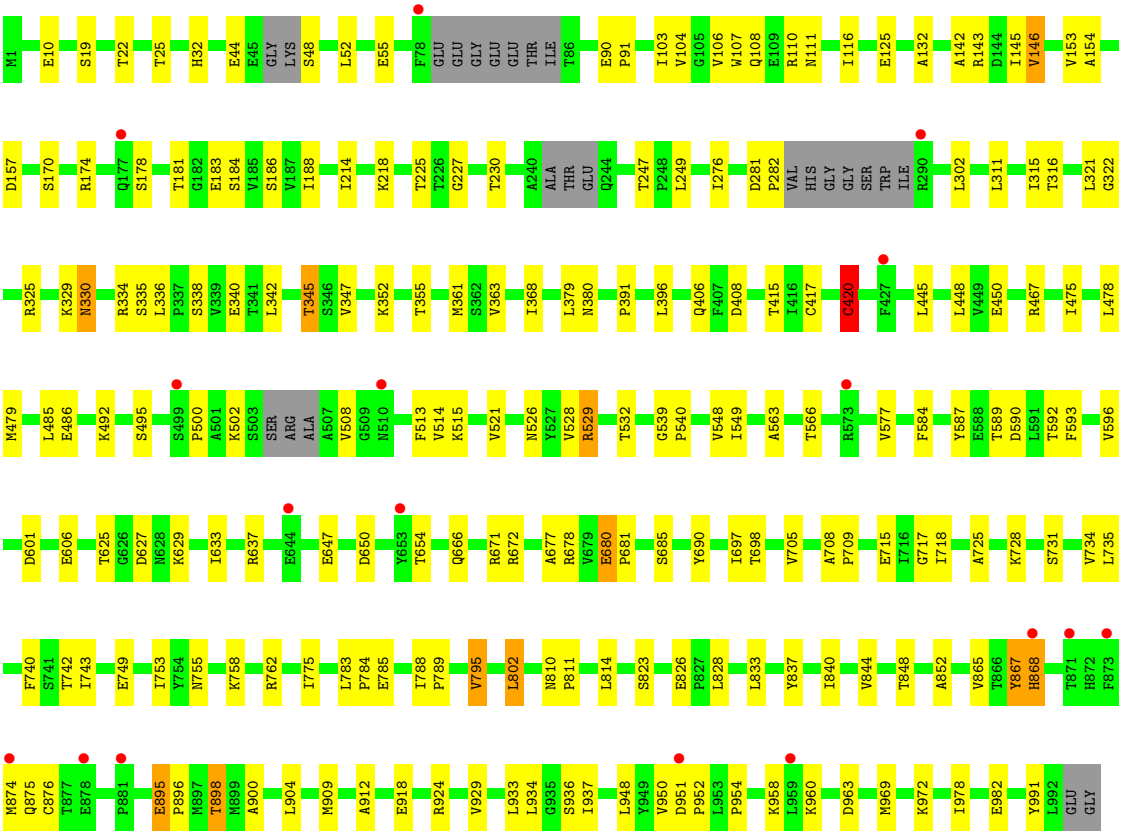
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
4	A	1	1	1	0	0

3 Residue-property plots (i)

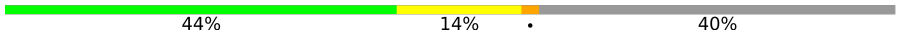
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1

Chain A:



• Molecule 2: Cardiac phospholamban

Chain B: 

• Molecule 3: Cardiac phospholamban

Chain C:
X101
X116
UNK
UNK
UNK
UNK
UNK
UNK
UNK
UNK

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.74Å 91.83Å 316.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.79 – 3.51 48.74 – 3.51	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.79-3.51) 99.0 (48.74-3.51)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.235 , 0.277 0.231 , 0.271	Depositor DCC
R_{free} test set	1195 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	107.0	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 86.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	7812	wwPDB-VP
Average B, all atoms (Å^2)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.30	0/7622	0.52	0/10331
2	B	0.27	0/244	0.44	0/329
All	All	0.30	0/7866	0.51	0/10660

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7489	0	7589	104	0
2	B	242	0	269	7	0
3	C	80	0	18	0	0
4	A	1	0	0	0	0
All	All	7812	0	7876	105	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 (105) 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:549:ILE:HD11	1:A:596:VAL:HG21	1.62	0.81
1:A:895:GLU:H	1:A:896:PRO:HD2	1.49	0.77
1:A:181:THR:OG1	1:A:183:GLU:HG2	1.88	0.73
1:A:788:ILE:HG13	1:A:789:PRO:HD2	1.69	0.73
1:A:898:THR:HG23	1:A:958:LYS:HB2	1.72	0.72
1:A:909:MET:HE2	1:A:937:ILE:HA	1.78	0.66
1:A:762:ARG:HG3	1:A:837:TYR:CE1	2.32	0.65
1:A:103:ILE:HB	2:B:37:LEU:HD21	1.78	0.64
1:A:529:ARG:NH1	1:A:592:THR:HG21	2.12	0.64
1:A:325:ARG:HH11	2:B:23:GLN:HE22	1.44	0.64
1:A:342:LEU:O	1:A:345:THR:HG23	1.99	0.62
1:A:361:MET:HG2	1:A:601:ASP:HB2	1.80	0.61
1:A:329:LYS:O	1:A:330:ASN:HB2	2.00	0.61
1:A:379:LEU:HD12	1:A:548:VAL:HG21	1.82	0.61
1:A:526:ASN:HD22	1:A:590:ASP:HA	1.65	0.61
1:A:227:GLY:O	1:A:230:THR:HG22	2.02	0.60
1:A:25:THR:HA	1:A:132:ALA:HB3	1.85	0.58
1:A:281:ASP:HB3	1:A:282:PRO:HD3	1.86	0.58
1:A:539:GLY:N	1:A:540:PRO:HD2	2.19	0.58
1:A:840:ILE:O	1:A:844:VAL:HG12	2.05	0.57
1:A:762:ARG:NH2	1:A:918:GLU:HA	2.20	0.56
1:A:762:ARG:HH21	1:A:918:GLU:HA	1.71	0.56
1:A:52:LEU:HA	1:A:55:GLU:HG3	1.88	0.55
1:A:513:PHE:HD1	1:A:566:THR:HG22	1.72	0.55
1:A:352:LYS:HE2	1:A:627:ASP:OD2	2.06	0.55
1:A:322:GLY:HA3	1:A:753:ILE:HD11	1.89	0.55
1:A:495:SER:HB3	1:A:514:VAL:HG22	1.88	0.55
1:A:107:TRP:HH2	2:B:30:ASN:HA	1.70	0.55
1:A:391:PRO:HB3	1:A:450:GLU:HB3	1.89	0.55
1:A:802:LEU:HB3	1:A:936:SER:HB2	1.89	0.54
1:A:154:ALA:N	1:A:157:ASP:OD2	2.31	0.53
1:A:950:VAL:O	1:A:954:PRO:HD3	2.08	0.53
1:A:500:PRO:HG3	1:A:508:VAL:O	2.08	0.53
1:A:650:ASP:O	1:A:672:ARG:NH1	2.35	0.53
1:A:19:SER:HB3	1:A:22:THR:HB	1.91	0.52
1:A:32:HIS:HB3	1:A:146:VAL:CG1	2.40	0.51
1:A:749:GLU:O	1:A:753:ILE:HG12	2.11	0.51
1:A:852:ALA:HB2	1:A:900:ALA:HB2	1.93	0.51
1:A:867:TYR:O	1:A:868:HIS:HB2	2.11	0.51
1:A:450:GLU:OE1	1:A:467:ARG:NH1	2.43	0.51
1:A:363:VAL:HG11	1:A:448:LEU:HD22	1.93	0.51
1:A:48:SER:HB2	1:A:110:ARG:HH11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:952:PRO:HB3	2:B:49:VAL:HG21	1.94	0.50
1:A:978:ILE:O	1:A:982:GLU:HG2	2.11	0.49
1:A:170:SER:HB2	1:A:218:LYS:H	1.77	0.49
1:A:485:LEU:HD22	1:A:584:PHE:CE1	2.47	0.49
1:A:735:LEU:HD22	1:A:742:THR:HB	1.95	0.49
1:A:814:LEU:HD21	1:A:924:ARG:NH1	2.28	0.49
1:A:311:LEU:HD11	1:A:315:ILE:HG21	1.95	0.48
1:A:848:THR:HG21	1:A:904:LEU:HD13	1.95	0.48
1:A:322:GLY:CA	1:A:753:ILE:HD11	2.44	0.48
1:A:680:GLU:HG3	1:A:681:PRO:HD2	1.96	0.47
1:A:865:VAL:HG12	1:A:867:TYR:H	1.78	0.47
1:A:302:LEU:HD13	1:A:775:ILE:HD12	1.95	0.47
1:A:654:THR:HA	1:A:677:ALA:O	2.14	0.47
1:A:529:ARG:HH12	1:A:592:THR:HG21	1.77	0.47
1:A:104:VAL:HG23	2:B:37:LEU:HD23	1.96	0.46
1:A:417:CYS:SG	1:A:445:LEU:HD22	2.55	0.46
1:A:577:VAL:HG12	1:A:587:TYR:OH	2.16	0.45
1:A:708:ALA:N	1:A:709:PRO:HD2	2.31	0.45
1:A:181:THR:HG1	1:A:183:GLU:HG2	1.80	0.45
1:A:811:PRO:HD2	1:A:929:VAL:HG12	1.98	0.45
1:A:355:THR:HG22	1:A:740:PHE:HB2	1.99	0.45
1:A:697:ILE:HG23	1:A:715:GLU:HG2	1.98	0.45
1:A:934:LEU:HA	1:A:937:ILE:HD12	1.99	0.44
1:A:948:LEU:HD22	1:A:960:LYS:HA	1.98	0.44
1:A:420:CYS:HB3	1:A:515:LYS:HD3	1.99	0.44
1:A:874:MET:HG3	1:A:875:GLN:HG3	1.99	0.44
1:A:116:ILE:HG21	1:A:336:LEU:HD11	1.98	0.44
1:A:492:LYS:HE2	1:A:678:ARG:HD3	2.00	0.44
1:A:32:HIS:CB	1:A:146:VAL:HG11	2.48	0.44
1:A:666:GLN:HB3	1:A:690:TYR:CE2	2.52	0.44
1:A:90:GLU:N	1:A:91:PRO:HD2	2.33	0.44
1:A:338:SER:O	1:A:342:LEU:HB2	2.17	0.44
1:A:633:ILE:O	1:A:637:ARG:HG3	2.18	0.44
1:A:969:MET:HA	1:A:972:LYS:HG2	1.99	0.44
1:A:415:THR:HA	1:A:475:ILE:HD13	1.99	0.43
1:A:142:ALA:HA	1:A:145:ILE:HD12	2.00	0.43
1:A:895:GLU:N	1:A:896:PRO:HD2	2.26	0.43
1:A:32:HIS:HB3	1:A:146:VAL:HG11	2.00	0.43
1:A:521:VAL:CG2	1:A:563:ALA:HB3	2.48	0.43
1:A:810:ASN:HA	1:A:811:PRO:HD3	1.86	0.43
1:A:32:HIS:HB3	1:A:146:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ARG:NH1	1:A:186:SER:OG	2.52	0.43
1:A:347:VAL:HB	1:A:698:THR:HG22	2.01	0.43
1:A:758:LYS:NZ	1:A:828:LEU:O	2.48	0.42
1:A:795:VAL:HG21	1:A:904:LEU:HD23	2.02	0.42
1:A:334:ARG:HD2	1:A:734:VAL:HG23	2.01	0.42
1:A:717:GLY:O	1:A:731:SER:HB2	2.20	0.42
1:A:718:ILE:HD13	1:A:743:ILE:HG12	2.01	0.42
1:A:321:LEU:HD22	2:B:23:GLN:HE21	1.84	0.42
1:A:528:VAL:HG12	1:A:593:PHE:HB3	2.02	0.41
1:A:912:ALA:HB1	1:A:933:LEU:HD11	2.01	0.41
1:A:823:SER:HB3	1:A:826:GLU:HG3	2.01	0.41
1:A:867:TYR:HB3	1:A:868:HIS:H	1.70	0.41
1:A:368:ILE:HG13	1:A:380:ASN:HB2	2.01	0.41
1:A:725:ALA:HA	1:A:728:LYS:HD2	2.02	0.41
1:A:475:ILE:HA	1:A:478:LEU:HD12	2.02	0.41
1:A:629:LYS:HD2	1:A:654:THR:HG23	2.03	0.41
2:B:28:LEU:O	2:B:32:PHE:HB2	2.20	0.41
1:A:153:VAL:HB	1:A:214:ILE:HG13	2.03	0.41
1:A:785:GLU:O	1:A:785:GLU:HG2	2.21	0.40
1:A:833:LEU:O	1:A:837:TYR:CD1	2.75	0.40
1:A:895:GLU:H	1:A:896:PRO:CD	2.27	0.40
1:A:783:LEU:HB3	1:A:784:PRO:HD2	2.04	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	958/994 (96%)	891 (93%)	57 (6%)	10 (1%)	15 54
2	B	28/50 (56%)	25 (89%)	3 (11%)	0	100 100
All	All	986/1044 (94%)	916 (93%)	60 (6%)	10 (1%)	15 54

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	868	HIS
1	A	276	ILE
1	A	802	LEU
1	A	963	ASP
1	A	178	SER
1	A	420	CYS
1	A	867	TYR
1	A	895	GLU
1	A	330	ASN
1	A	502	LYS

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	822/840 (98%)	783 (95%)	39 (5%)	26 60
2	B	29/47 (62%)	26 (90%)	3 (10%)	7 32
All	All	851/887 (96%)	809 (95%)	42 (5%)	25 59

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	44	GLU
1	A	106	VAL
1	A	108	GLN
1	A	111	ASN
1	A	125	GLU
1	A	143	ARG
1	A	146	VAL
1	A	184	SER
1	A	188	ILE
1	A	225	THR
1	A	247	THR
1	A	249	LEU

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Mol	Chain	Res	Type
1	A	316	THR
1	A	335	SER
1	A	340	GLU
1	A	345	THR
1	A	396	LEU
1	A	406	GLN
1	A	408	ASP
1	A	420	CYS
1	A	479	MET
1	A	486	GLU
1	A	529	ARG
1	A	532	THR
1	A	589	THR
1	A	606	GLU
1	A	625	THR
1	A	647	GLU
1	A	671	ARG
1	A	680	GLU
1	A	685	SER
1	A	705	VAL
1	A	755	ASN
1	A	795	VAL
1	A	876	CYS
1	A	898	THR
1	A	951	ASP
1	A	991	TYR
2	B	22	GLN
2	B	32	PHE
2	B	50	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	177	GLN
1	A	251	GLN
1	A	380	ASN
1	A	406	GLN
1	A	526	ASN
1	A	768	ASN
1	A	914	ASN
1	A	944	HIS

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Mol	Chain	Res	Type
2	B	22	GLN
2	B	23	GLN
2	B	27	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	970/994 (97%)	-0.00	17 (1%) 68 55	77, 119, 210, 262	0
2	B	30/50 (60%)	0.18	0 100 100	174, 206, 231, 242	0
3	C	0/23	-	-	-	-
All	All	1000/1067 (93%)	0.00	17 (1%) 70 57	77, 121, 215, 262	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	874	MET	4.8
1	A	959	LEU	3.1
1	A	871	THR	3.1
1	A	881	PRO	2.9
1	A	868	HIS	2.9
1	A	510	ASN	2.7
1	A	878	GLU	2.5
1	A	951	ASP	2.5
1	A	177	GLN	2.4
1	A	573	ARG	2.4
1	A	290	ARG	2.3
1	A	499	SER	2.2
1	A	644	GLU	2.2
1	A	873	PHE	2.1
1	A	78	PHE	2.0
1	A	427	PHE	2.0
1	A	653	TYR	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	K	A	1001	1/1	0.89	0.35	107,107,107,107	0

6.5 Other polymers (i)

There are no such residues in this entry.