Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:54 PM GMT

PDB ID	:	4UAO
Title	:	Crystal structure of Apical Membrane Antigen 1 from Plasmodium Knowlesi in complex with an invasion inhibitory antibody
Authors	:	Vulliez-Le Normand, B.; Saul, F.A.; Bentley, G.A.
Deposited on	:	2014-08-11
Resolution	:	3.10 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:

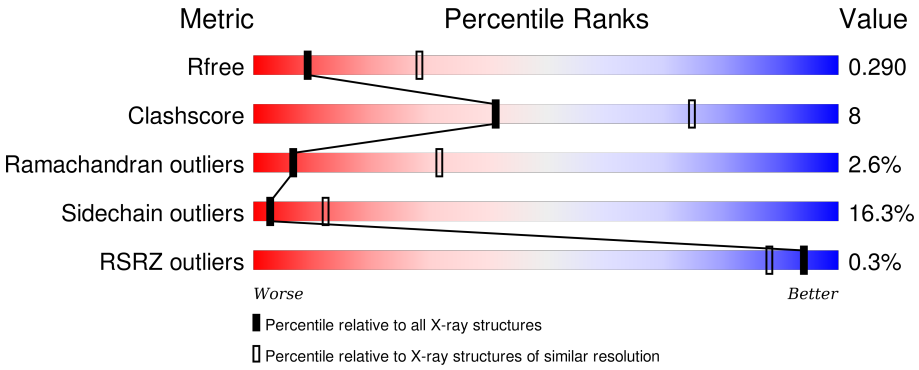
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	370	% 59% 27% • 10%
2	B	214	66% 31% •
3	C	223	67% 29% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6004 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 Apical merozoite antigen 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	2	0
			2672	1676	466	513	17			

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	GLU	-	cloning artifact	UNP B3L5E1
A	42	PHE	-	cloning artifact	UNP B3L5E1
A	107	LYS	ASN	engineered mutation	UNP B3L5E1
A	178	ASN	SER	engineered mutation	UNP B3L5E1
A	189	GLU	ASN	engineered mutation	UNP B3L5E1
A	240	ARG	SER	engineered mutation	UNP B3L5E1
A	388	GLY	-	cloning artifact	UNP B3L5E1
A	389	LEU	-	expression tag	UNP B3L5E1
A	390	GLU	-	expression tag	UNP B3L5E1
A	391	GLN	-	expression tag	UNP B3L5E1
A	392	LYS	-	expression tag	UNP B3L5E1
A	393	LEU	-	expression tag	UNP B3L5E1
A	394	ILE	-	expression tag	UNP B3L5E1
A	395	SER	-	expression tag	UNP B3L5E1
A	396	GLU	-	expression tag	UNP B3L5E1
A	397	GLU	-	expression tag	UNP B3L5E1
A	398	ASP	-	expression tag	UNP B3L5E1
A	399	LEU	-	expression tag	UNP B3L5E1
A	400	ASN	-	expression tag	UNP B3L5E1
A	401	SER	-	expression tag	UNP B3L5E1
A	402	ALA	-	expression tag	UNP B3L5E1
A	403	VAL	-	expression tag	UNP B3L5E1
A	404	ASP	-	expression tag	UNP B3L5E1
A	405	HIS	-	expression tag	UNP B3L5E1
A	406	HIS	-	expression tag	UNP B3L5E1
A	407	HIS	-	expression tag	UNP B3L5E1
A	408	HIS	-	expression tag	UNP B3L5E1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	409	HIS	-	expression tag	UNP B3L5E1
A	410	HIS	-	expression tag	UNP B3L5E1

- Molecule 2 is a protein called immunoglobulin R31C2 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1652	1021	283	337	11			

- Molecule 3 is a protein called immunoglobulin R31C2 VH and CH1 regions.

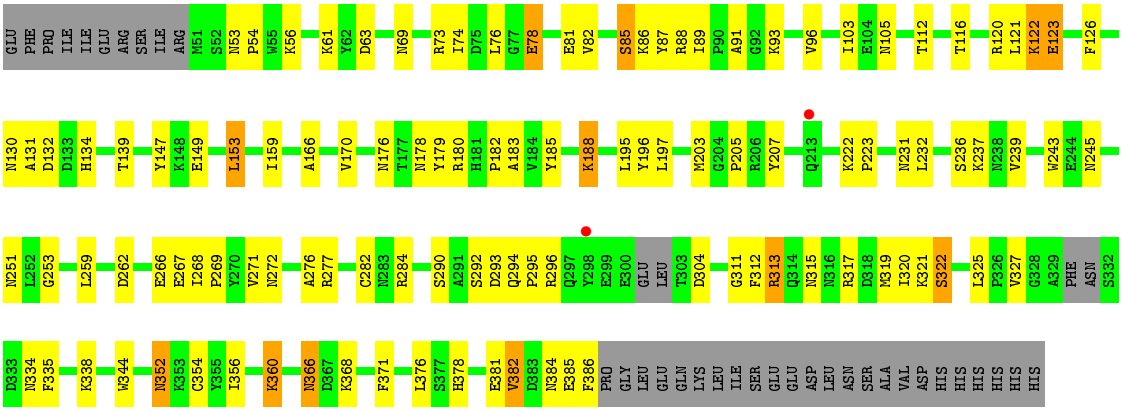
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	223	Total	C	N	O	S	0	0	0
			1680	1058	277	336	9			

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.

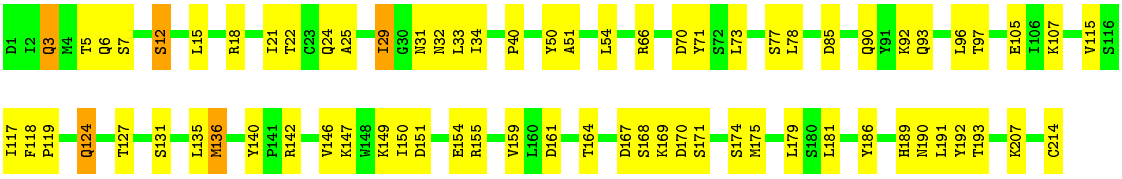
- Molecule 1: Apical merozoite antigen 1

Chain A:



- Molecule 2: immunoglobulin R31C2 light chain

Chain B:



- Molecule 3: immunoglobulin R31C2 VH and CH1 regions

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	165.86Å 71.81Å 90.69Å 90.00° 116.37° 90.00°	Depositor
Resolution (Å)	40.77 – 3.10 40.77 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.6 (40.77-3.10) 97.6 (40.77-3.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.188 , 0.266 0.208 , 0.290	Depositor DCC
R_{free} test set	838 reflections (5.15%)	DCC
Wilson B-factor (Å^2)	65.8	Xtriage
Anisotropy	0.752	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 89.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	1 of 17120 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6004	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% 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

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	0.53	0/2737	0.78	0/3691
2	B	0.52	0/1684	0.82	1/2280 (0.0%)
3	C	0.51	0/1722	0.83	1/2349 (0.0%)
All	All	0.52	0/6143	0.81	2/8320 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	214	GLU	C-N-CA	7.03	139.28	121.70
2	B	29	ILE	N-CA-C	-5.08	97.29	111.00

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	2672	0	2545	44	0
2	B	1652	0	1595	31	0
3	C	1680	0	1619	29	0
All	All	6004	0	5759	100	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 (100) 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)
3:C:87:THR:HG23	3:C:110:THR:HA	1.75	0.67
1:A:78:GLU:HB2	1:A:91:ALA:HB2	1.77	0.66
1:A:74:ILE:HG21	1:A:294:GLN:HB3	1.80	0.64
1:A:166:ALA:HB2	1:A:183:ALA:HB2	1.78	0.63
3:C:94:ARG:HD2	3:C:101:ASP:OD1	1.98	0.62
2:B:150:ILE:HD11	2:B:179:LEU:HD21	1.80	0.62
2:B:164:THR:HG22	2:B:174:SER:H	1.66	0.61
1:A:276:ALA:HB2	1:A:354:CYS:HB2	1.83	0.60
1:A:120:ARG:HH11	1:A:122:LYS:HD2	1.68	0.59
1:A:259:LEU:HD13	1:A:269:PRO:HD3	1.88	0.56
2:B:149:LYS:HB2	2:B:193:THR:HG23	1.87	0.56
3:C:100:TYR:HB3	3:C:100(B):GLU:HG2	1.87	0.55
3:C:119:PRO:HB3	3:C:145:TYR:HB3	1.88	0.55
3:C:28:THR:O	3:C:31:ASN:HB2	2.06	0.55
2:B:6:GLN:HE21	2:B:21:ILE:HG21	1.72	0.55
1:A:322:SER:HA	1:A:325:LEU:HD12	1.89	0.54
2:B:149:LYS:HB2	2:B:193:THR:CG2	2.38	0.54
3:C:97:TYR:O	3:C:100:TYR:HB2	2.08	0.54
1:A:96:VAL:HG22	1:A:376:LEU:HD23	1.88	0.54
1:A:120:ARG:HA	1:A:313[A]:ARG:HH22	1.73	0.53
1:A:312[B]:PHE:HA	1:A:320:ILE:HD11	1.89	0.53
1:A:312[A]:PHE:HA	1:A:320:ILE:HD11	1.89	0.53
1:A:74:ILE:HG21	1:A:294:GLN:CB	2.39	0.53
3:C:133:ASN:CG	3:C:134:SER:H	2.11	0.52
2:B:167:ASP:O	2:B:171:SER:HA	2.09	0.52
2:B:151:ASP:HA	2:B:191:LEU:HB3	1.93	0.51
3:C:143:LYS:HA	3:C:176:THR:HG23	1.92	0.51
2:B:66:ARG:HG3	2:B:71:TYR:CE2	2.46	0.50
2:B:147:LYS:NZ	2:B:155:ARG:H	2.09	0.50
1:A:182:PRO:HB2	1:A:195:LEU:HD12	1.94	0.50
2:B:186:TYR:HA	2:B:192:TYR:OH	2.13	0.49
1:A:243:TRP:C	1:A:245:ASN:H	2.16	0.49
2:B:29:ILE:HA	2:B:92:LYS:HG2	1.94	0.49
3:C:204:THR:HG23	3:C:206:VAL:HG23	1.95	0.49
1:A:378:HIS:HB3	1:A:381:GLU:HB2	1.94	0.49
1:A:311:GLY:HA3	1:A:319:MET:HG2	1.95	0.48
1:A:73:ARG:HG2	1:A:223:PRO:HG2	1.95	0.48
3:C:15:GLY:O	3:C:82(B):SER:HA	2.12	0.48
2:B:107:LYS:HA	2:B:140:TYR:OH	2.14	0.47
1:A:276:ALA:O	1:A:352:ASN:HB3	2.15	0.47
2:B:136:MET:CE	2:B:146:VAL:HB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:27:PHE:HD2	3:C:32:TYR:CE1	2.32	0.47
1:A:153:LEU:C	1:A:153:LEU:HD12	2.35	0.47
2:B:25:ALA:HB2	2:B:29:ILE:HD11	1.97	0.47
2:B:3:GLN:O	2:B:25:ALA:HA	2.15	0.47
3:C:70:SER:OG	3:C:79:TYR:HB2	2.16	0.46
1:A:120:ARG:NH1	1:A:122:LYS:HD2	2.30	0.46
3:C:34:MET:SD	3:C:94:ARG:HA	2.56	0.46
3:C:127:GLY:O	3:C:130:LEU:HG	2.16	0.46
2:B:124:GLN:HG3	3:C:122:TYR:CD2	2.50	0.45
3:C:213:ARG:HB3	3:C:213:ARG:HH11	1.81	0.45
2:B:31:ASN:HB2	2:B:50:TYR:CZ	2.51	0.45
2:B:136:MET:HE1	2:B:146:VAL:HB	1.98	0.45
3:C:214:GLU:HA	3:C:215:CYS:HB2	1.98	0.45
1:A:88:ARG:NH2	1:A:293:ASP:HB3	2.31	0.45
2:B:214:CYS:HB3	3:C:213:ARG:HH12	1.81	0.45
1:A:85:SER:HB2	1:A:87:TYR:CE1	2.51	0.45
1:A:295:PRO:HD3	1:A:335:PHE:HD2	1.83	0.44
3:C:13:GLN:O	3:C:16:ARG:HB2	2.17	0.44
2:B:32:ASN:HB2	2:B:92:LYS:HB2	2.00	0.44
2:B:124:GLN:HG3	3:C:122:TYR:CG	2.52	0.44
1:A:147:TYR:HB2	1:A:153:LEU:HD11	2.00	0.44
2:B:124:GLN:HE22	2:B:131:SER:H	1.64	0.43
3:C:11:LEU:HD22	3:C:147:PRO:HG3	2.00	0.43
1:A:159:ILE:HG13	1:A:185:TYR:CD2	2.53	0.43
3:C:40:ALA:HB3	3:C:43:LYS:HB2	1.99	0.43
1:A:82:VAL:HG13	1:A:321:LYS:HE2	1.99	0.43
3:C:95:ARG:HG3	3:C:96:GLY:N	2.34	0.43
1:A:166:ALA:CB	1:A:183:ALA:HB2	2.48	0.43
1:A:81:GLU:HA	1:A:86:LYS:HA	1.99	0.43
1:A:88:ARG:HH22	1:A:293:ASP:HB3	1.83	0.43
1:A:147:TYR:HB3	1:A:153:LEU:HD21	2.00	0.42
1:A:317:ARG:O	1:A:321:LYS:HB2	2.19	0.42
1:A:120:ARG:O	1:A:123:GLU:HB2	2.19	0.42
1:A:268:ILE:HG13	1:A:268:ILE:H	1.56	0.42
2:B:115:VAL:HB	2:B:207:LYS:HD3	2.02	0.42
2:B:118:PHE:HA	2:B:119:PRO:HD3	1.95	0.42
1:A:253:GLY:HA2	1:A:371:PHE:HD1	1.84	0.42
3:C:119:PRO:CB	3:C:145:TYR:HB3	2.50	0.42
1:A:236:SER:H	1:A:239:VAL:HG23	1.84	0.42
2:B:90:GLN:HE21	2:B:97:THR:H	1.67	0.42
1:A:272:ASN:HB2	1:A:356:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:156:SER:H	3:C:196:ASN:HD21	1.67	0.42
1:A:53:ASN:HA	1:A:54:PRO:HD3	1.97	0.41
2:B:31:ASN:OD1	2:B:66:ARG:HD2	2.20	0.41
3:C:29:PHE:HD2	3:C:73:ASN:HA	1.85	0.41
3:C:181:VAL:O	3:C:181:VAL:HG13	2.20	0.41
2:B:96:LEU:HD13	3:C:100(D):PHE:HZ	1.85	0.41
2:B:164:THR:HG22	2:B:174:SER:N	2.33	0.41
1:A:76:LEU:HD12	1:A:294:GLN:HB2	2.03	0.41
2:B:25:ALA:CB	2:B:29:ILE:HD11	2.51	0.41
3:C:20:LEU:HD21	3:C:82:MET:HE1	2.03	0.41
2:B:151:ASP:OD1	2:B:189:HIS:HB3	2.21	0.41
1:A:126:PHE:CD2	1:A:197:LEU:HB2	2.55	0.40
1:A:188:LYS:HB2	1:A:231:ASN:HD22	1.86	0.40
1:A:179:TYR:C	1:A:179:TYR:CD2	2.94	0.40
2:B:12:SER:HB3	2:B:107:LYS:NZ	2.36	0.40
1:A:251:ASN:O	1:A:382:VAL:HA	2.21	0.40
1:A:63:ASP:HB2	1:A:360:LYS:HD3	2.03	0.40
1:A:180:ARG:HB2	1:A:237:LYS:HB3	2.03	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	328/370 (89%)	281 (86%)	37 (11%)	10 (3%)	5 28
2	B	212/214 (99%)	182 (86%)	26 (12%)	4 (2%)	10 40
3	C	221/223 (99%)	194 (88%)	21 (10%)	6 (3%)	6 31
All	All	761/807 (94%)	657 (86%)	84 (11%)	20 (3%)	7 32

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	LYS
1	A	205	PRO
2	B	154	GLU
3	C	76	SER
1	A	130	ASN
1	A	352	ASN
1	A	207	TYR
1	A	266	GLU
2	B	51	ALA
3	C	61	ASP
3	C	82(B)	SER
3	C	144	GLY
1	A	366	ASN
2	B	169	LYS
3	C	116	THR
1	A	131	ALA
1	A	132	ASP
1	A	315	ASN
2	B	40	PRO
3	C	149	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	289/325 (89%)	240 (83%)	49 (17%)	2	11
2	B	190/191 (100%)	159 (84%)	31 (16%)	3	12
3	C	187/188 (100%)	158 (84%)	29 (16%)	3	14
All	All	666/704 (95%)	557 (84%)	109 (16%)	3	12

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LYS
1	A	69	ASN
1	A	78	GLU

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Mol	Chain	Res	Type
1	A	85	SER
1	A	89	ILE
1	A	93	LYS
1	A	103	ILE
1	A	105	ASN
1	A	112	THR
1	A	116	THR
1	A	121	LEU
1	A	122	LYS
1	A	123	GLU
1	A	134	HIS
1	A	139	THR
1	A	149	GLU
1	A	153	LEU
1	A	170	VAL
1	A	176	ASN
1	A	178	ASN
1	A	188	LYS
1	A	196	TYR
1	A	203	MET
1	A	222	LYS
1	A	232	LEU
1	A	262	ASP
1	A	267	GLU
1	A	271	VAL
1	A	277	ARG
1	A	282	CYS
1	A	284	ARG
1	A	290	SER
1	A	292	SER
1	A	296	ARG
1	A	304	ASP
1	A	313[A]	ARG
1	A	313[B]	ARG
1	A	322	SER
1	A	327	VAL
1	A	334	ASN
1	A	338	LYS
1	A	344	TRP
1	A	360	LYS
1	A	366	ASN
1	A	368	LYS

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Mol	Chain	Res	Type
1	A	382	VAL
1	A	384	ASN
1	A	385	GLU
1	A	386	PHE
2	B	3	GLN
2	B	5	THR
2	B	7	SER
2	B	12	SER
2	B	15	LEU
2	B	18	ARG
2	B	22	THR
2	B	24	GLN
2	B	33	LEU
2	B	34	ILE
2	B	54	LEU
2	B	70	ASP
2	B	73	LEU
2	B	77	SER
2	B	78	LEU
2	B	85	ASP
2	B	93	GLN
2	B	105	GLU
2	B	117	ILE
2	B	124	GLN
2	B	127	THR
2	B	135	LEU
2	B	136	MET
2	B	142	ARG
2	B	159	VAL
2	B	161	ASP
2	B	168	SER
2	B	170	ASP
2	B	175	MET
2	B	181	LEU
2	B	190	ASN
3	C	1	GLU
3	C	3	GLN
3	C	13	GLN
3	C	20	LEU
3	C	21	SER
3	C	25	SER
3	C	61	ASP

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Mol	Chain	Res	Type
3	C	63	VAL
3	C	64	LYS
3	C	68	THR
3	C	107	VAL
3	C	110	THR
3	C	115	GLU
3	C	140	CYS
3	C	148	GLU
3	C	156	SER
3	C	159	LEU
3	C	161	SER
3	C	163	VAL
3	C	177	LEU
3	C	180	SER
3	C	183	VAL
3	C	185	SER
3	C	187	THR
3	C	189	SER
3	C	194	THR
3	C	196	ASN
3	C	208	LYS
3	C	213	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	27	GLN
2	B	138	ASN
3	C	164	HIS

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	332/370 (89%)	-0.20	2 (0%) 90 80	38, 69, 109, 140	0
2	B	214/214 (100%)	-0.34	0 100 100	43, 67, 89, 121	0
3	C	223/223 (100%)	-0.31	0 100 100	39, 67, 87, 115	0
All	All	769/807 (95%)	-0.28	2 (0%) 94 88	38, 68, 102, 140	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	298	TYR	2.1
1	A	213	GLN	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.