wwPDB X-ray Structure Validation Summary Report (i)

Jan 4, 2024 – 07:07 am GMT

PDB ID	:	4UIM
Title	:	crystal structure of quinine-dependent Fab 314.3
Authors	:	Zhu, J.; Zhu, J.; Bougie, D.W.; Aster, R.H.; Springer, T.A.
Deposited on	:	2015-03-30
Resolution	:	2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i)) were used in the production of this report:

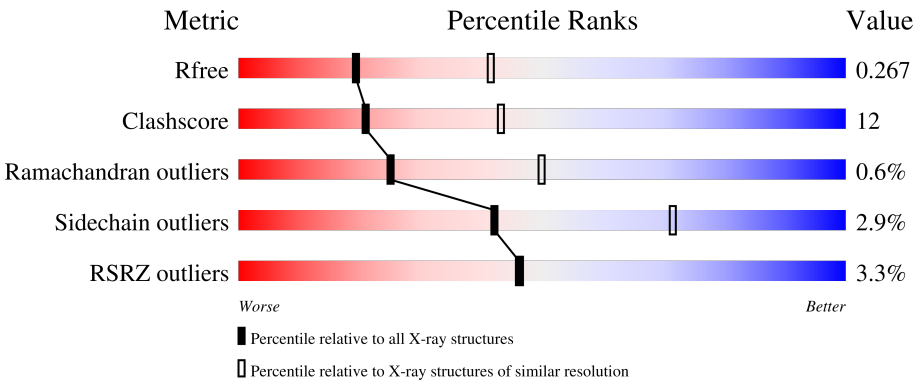
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	225	5% 76% 23% •
1	C	225	3% 79% 18% • •
1	E	225	4% 70% 28%
1	H	225	3% 72% 24% • •
2	B	214	% 79% 21%

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Mol	Chain	Length	Quality of chain
2	D	214	4% 75% 23%
2	F	214	3% 71% 25%
2	L	214	4% 81% 19%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26543 atoms, of which 12917 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.

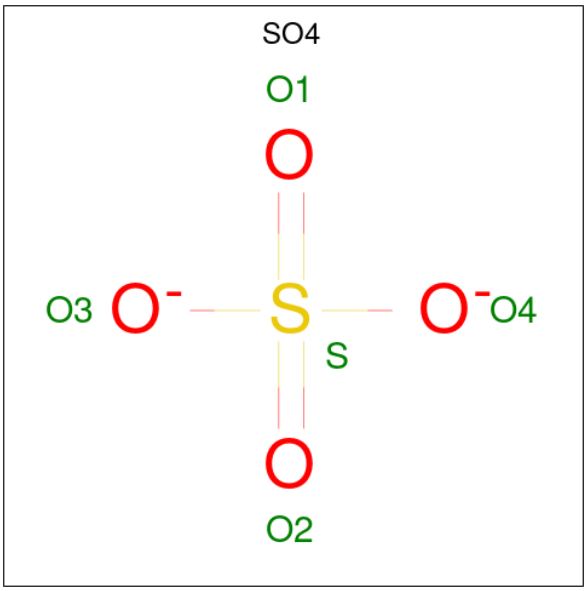
- Molecule 1 is a protein called FAB 314.3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	224	3348	1070	1649	283	337	9	0	0	0
1	C	221	3303	1057	1626	279	332	9	0	0	0
1	E	224	3348	1070	1649	283	337	9	0	0	0
1	H	222	3361	1072	1657	285	338	9	0	4	0

- Molecule 2 is a protein called FAB 314.3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	214	3256	1030	1590	281	348	7	0	3	0
2	D	214	3233	1024	1578	279	345	7	0	0	0
2	F	214	3245	1027	1584	280	347	7	0	2	0
2	L	214	3245	1028	1584	279	347	7	0	1	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

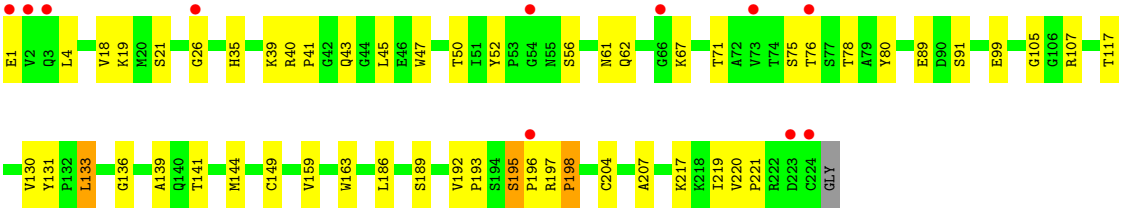
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	24	Total O 24 24	0	0
4	B	23	Total O 23 23	0	0
4	C	33	Total O 33 33	0	0
4	D	19	Total O 19 19	0	0
4	E	31	Total O 31 31	0	0
4	F	16	Total O 16 16	0	0
4	H	33	Total O 33 33	0	0
4	L	15	Total O 15 15	0	0

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.

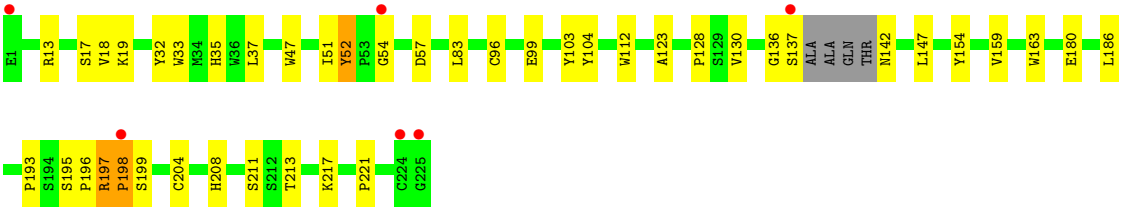
• Molecule 1: FAB 314.3

Chain A:



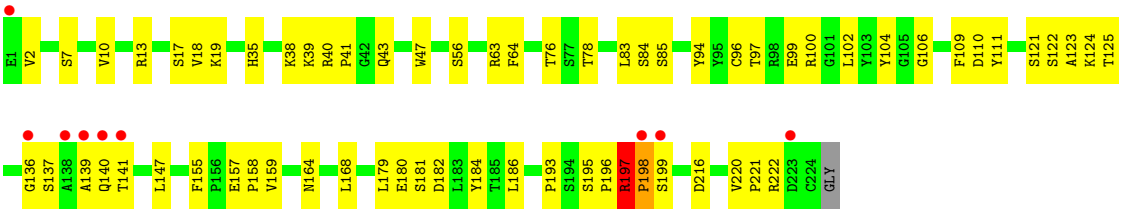
• Molecule 1: FAB 314.3

Chain C:



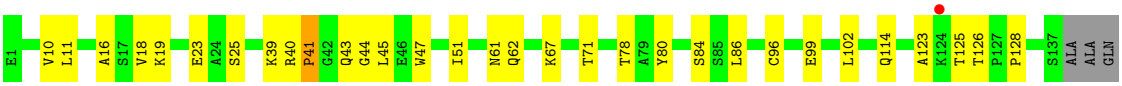
• Molecule 1: FAB 314.3

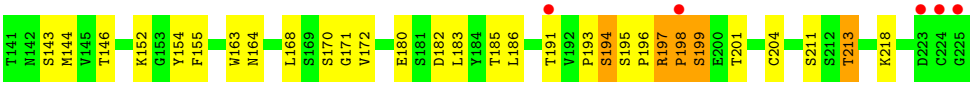
Chain E:



• Molecule 1: FAB 314.3

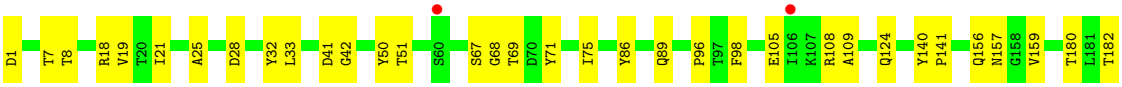
Chain H:

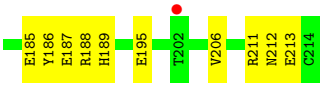




• Molecule 2: FAB 314.3

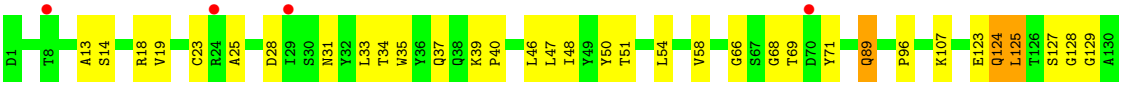
Chain B:

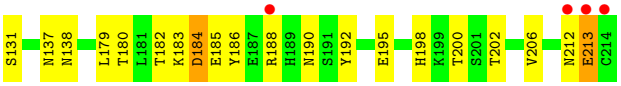




• Molecule 2: FAB 314.3

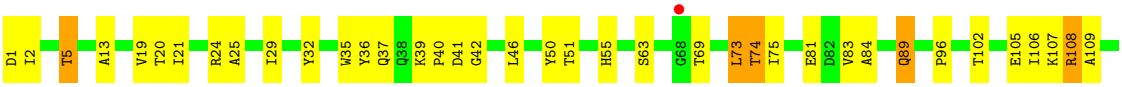
Chain D:





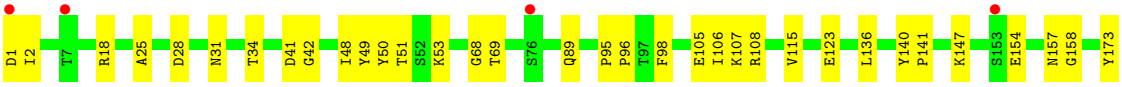
• Molecule 2: FAB 314.3

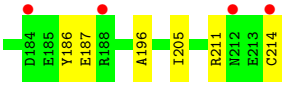
Chain F:



• Molecule 2: FAB 314.3

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.32Å 145.24Å 101.49Å 90.00° 90.88° 90.00°	Depositor
Resolution (Å)	49.37 – 2.70 49.37 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.37-2.70) 99.9 (49.37-2.70)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.222 , 0.260 0.229 , 0.267	Depositor DCC
R_{free} test set	1035 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å^2)	37.4	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	26543	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: SO4

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	0.27	0/1744	0.52	0/2381
1	C	0.27	0/1721	0.52	0/2347
1	E	0.31	0/1744	0.66	1/2381 (0.0%)
1	H	0.29	0/1755	0.52	0/2393
2	B	0.28	0/1709	0.46	0/2320
2	D	0.28	0/1689	0.48	0/2293
2	F	0.31	0/1701	0.62	0/2309
2	L	0.28	0/1698	0.47	0/2305
All	All	0.28	0/13761	0.54	1/18729 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	E	0	1
1	H	0	1
All	All	0	4

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	E	197	ARG	NE-CZ-NH1	6.66	123.63	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	197	ARG	Peptide
1	C	198	PRO	Peptide
1	E	197	ARG	Peptide
1	H	197	ARG	Peptide

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	1699	1649	1652	46	1
1	C	1677	1626	1629	34	2
1	E	1699	1649	1652	58	1
1	H	1704	1657	1656	57	1
2	B	1666	1590	1587	32	0
2	D	1655	1578	1581	43	0
2	F	1661	1584	1582	43	1
2	L	1661	1584	1587	29	1
3	B	5	0	0	1	0
3	H	5	0	0	0	0
4	A	24	0	0	4	0
4	B	23	0	0	2	1
4	C	33	0	0	3	0
4	D	19	0	0	4	0
4	E	31	0	0	3	0
4	F	16	0	0	2	0
4	H	33	0	0	8	0
4	L	15	0	0	4	0
All	All	13626	12917	12926	321	4

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 12.

The worst 5 of 321 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:40:ARG:NH1	4:A:2005:HOH:O	2.10	0.84
1:H:44:GLY:O	4:H:2010:HOH:O	1.97	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:170:SER:O	1:H:172:VAL:N	2.13	0.80
1:A:89:GLU:N	1:A:89:GLU:OE1	2.15	0.80
1:E:193:PRO:O	1:E:196:PRO:HD2	1.84	0.78

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:GLY:O	4:B:2021:HOH:O[1_656]	1.99	0.21
1:C:104:TYR:OH	1:H:99:GLU:OE1[1_656]	2.01	0.19
1:A:99:GLU:OE1	1:E:104:TYR:OH[2_656]	2.07	0.13
2:F:127:SER:O	2:L:18:ARG:NH2[2_545]	2.19	0.01

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	222/225 (99%)	213 (96%)	7 (3%)	2 (1%)	17	40
1	C	217/225 (96%)	211 (97%)	6 (3%)	0	100	100
1	E	222/225 (99%)	211 (95%)	9 (4%)	2 (1%)	17	40
1	H	222/225 (99%)	211 (95%)	8 (4%)	3 (1%)	11	28
2	B	215/214 (100%)	210 (98%)	5 (2%)	0	100	100
2	D	212/214 (99%)	206 (97%)	5 (2%)	1 (0%)	29	54
2	F	214/214 (100%)	206 (96%)	6 (3%)	2 (1%)	17	40
2	L	213/214 (100%)	206 (97%)	6 (3%)	1 (0%)	29	54
All	All	1737/1756 (99%)	1674 (96%)	52 (3%)	11 (1%)	25	50

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	198	PRO
1	H	171	GLY
1	A	107	ARG
2	D	213	GLU
2	F	188	ARG

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	192/192 (100%)	184 (96%)	8 (4%)	30	58
1	C	190/192 (99%)	185 (97%)	5 (3%)	46	75
1	E	192/192 (100%)	188 (98%)	4 (2%)	53	80
1	H	194/192 (101%)	187 (96%)	7 (4%)	35	64
2	B	195/192 (102%)	191 (98%)	4 (2%)	53	80
2	D	192/192 (100%)	186 (97%)	6 (3%)	40	69
2	F	194/192 (101%)	186 (96%)	8 (4%)	30	59
2	L	193/192 (100%)	191 (99%)	2 (1%)	76	91
All	All	1542/1536 (100%)	1498 (97%)	44 (3%)	42	71

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	5	THR
1	H	45	LEU
2	F	73	LEU
2	F	108	ARG
1	H	96	CYS

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

Mol	Chain	Res	Type
1	A	173	HIS

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Mol	Chain	Res	Type
2	D	189	HIS
2	F	189	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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	SO4	H	1226	-	4,4,4	0.15	0	6,6,6	0.07	0
3	SO4	B	1215	-	4,4,4	0.14	0	6,6,6	0.14	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1215	SO4	1	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	224/225 (99%)	0.53	11 (4%)	29	28	39, 71, 115, 156	0
1	C	221/225 (98%)	0.45	6 (2%)	54	55	41, 63, 106, 146	0
1	E	224/225 (99%)	0.46	9 (4%)	38	37	38, 60, 107, 158	0
1	H	222/225 (98%)	0.49	6 (2%)	54	55	42, 63, 104, 187	0
2	B	214/214 (100%)	0.44	3 (1%)	75	77	39, 64, 88, 110	0
2	D	214/214 (100%)	0.50	8 (3%)	41	41	46, 72, 102, 160	0
2	F	214/214 (100%)	0.53	6 (2%)	53	54	44, 67, 96, 138	0
2	L	214/214 (100%)	0.60	8 (3%)	41	41	48, 76, 115, 149	0
All	All	1747/1756 (99%)	0.50	57 (3%)	46	46	38, 67, 108, 187	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	225	GLY	7.2
1	H	225	GLY	6.7
1	H	224	CYS	5.1
1	H	223	ASP	4.3
1	A	224	CYS	4.2

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
3	SO4	B	1215	5/5	0.92	0.25	72,73,74,74	0
3	SO4	H	1226	5/5	0.92	0.18	83,86,86,86	0

6.5 Other polymers (i)

There are no such residues in this entry.