Full wwPDB X-ray Structure Validation Report (i)

May 22, 2020 – 05:30 pm BST

PDB ID	:	1XBF
Title	:	X-RAY STRUCTURE NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET CAR10 FROM C. ACETOBUTYLICUM
Authors	:	Kuzin, A.P.; Chen, Y.; Vorobiev, S.; Yong, W.; Acton, T.; Ho, C.-K.; Conover, K.; Cooper, B.; Ciano, M.; Xiao, R.; Montelione, G.; Tong, L.; Hunt, J.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2004-08-30
Resolution	:	2.00 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 following versions of software and data (see references (1)) were used in the production of this report:

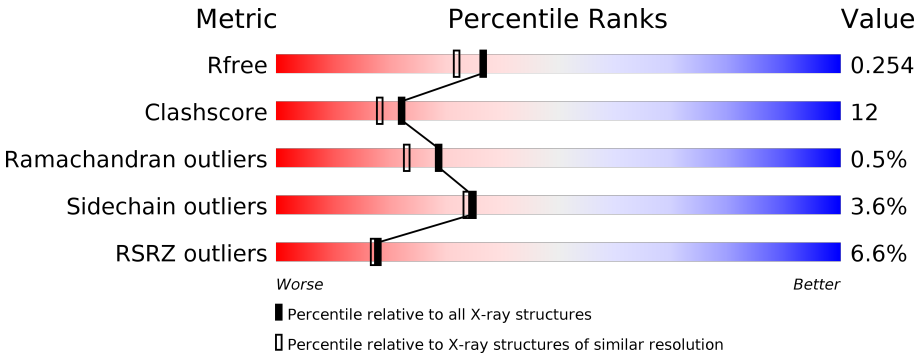
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	140	8% 69% 23% • 6%
1	B	140	3% 76% 15% • 7%
1	C	140	7% 61% 22% • 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3138 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 Clostridium acetobutylicum Q97KL0.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	131	Total	C	N	O	S	Se	0	0	0
			1022	649	171	199	1	2			
1	B	130	Total	C	N	O	S	Se	0	0	0
			1013	644	170	196	1	2			
1	C	121	Total	C	N	O	S	Se	0	0	0
			938	596	157	182	1	2			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MSE	MET	MODIFIED RESIDUE	UNP Q97KL0
A	93	MSE	MET	MODIFIED RESIDUE	UNP Q97KL0
A	133	LEU	-	CLONING ARTIFACT	UNP Q97KL0
A	134	GLU	-	CLONING ARTIFACT	UNP Q97KL0
A	135	HIS	-	EXPRESSION TAG	UNP Q97KL0
A	136	HIS	-	EXPRESSION TAG	UNP Q97KL0
A	137	HIS	-	EXPRESSION TAG	UNP Q97KL0
A	138	HIS	-	EXPRESSION TAG	UNP Q97KL0
A	139	HIS	-	EXPRESSION TAG	UNP Q97KL0
A	140	HIS	-	EXPRESSION TAG	UNP Q97KL0
B	37	MSE	MET	MODIFIED RESIDUE	UNP Q97KL0
B	93	MSE	MET	MODIFIED RESIDUE	UNP Q97KL0
B	133	LEU	-	CLONING ARTIFACT	UNP Q97KL0
B	134	GLU	-	CLONING ARTIFACT	UNP Q97KL0
B	135	HIS	-	EXPRESSION TAG	UNP Q97KL0
B	136	HIS	-	EXPRESSION TAG	UNP Q97KL0
B	137	HIS	-	EXPRESSION TAG	UNP Q97KL0
B	138	HIS	-	EXPRESSION TAG	UNP Q97KL0
B	139	HIS	-	EXPRESSION TAG	UNP Q97KL0
B	140	HIS	-	EXPRESSION TAG	UNP Q97KL0
C	37	MSE	MET	MODIFIED RESIDUE	UNP Q97KL0
C	93	MSE	MET	MODIFIED RESIDUE	UNP Q97KL0
C	133	LEU	-	CLONING ARTIFACT	UNP Q97KL0

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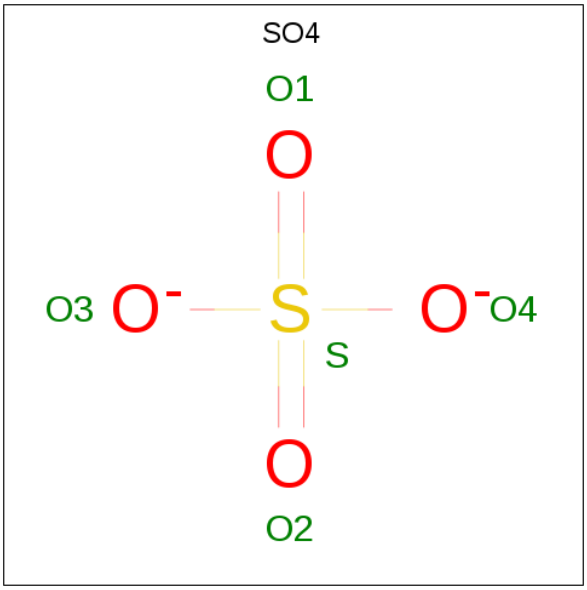
Chain	Residue	Modelled	Actual	Comment	Reference
C	134	GLU	-	CLONING ARTIFACT	UNP Q97KL0
C	135	HIS	-	EXPRESSION TAG	UNP Q97KL0
C	136	HIS	-	EXPRESSION TAG	UNP Q97KL0
C	137	HIS	-	EXPRESSION TAG	UNP Q97KL0
C	138	HIS	-	EXPRESSION TAG	UNP Q97KL0
C	139	HIS	-	EXPRESSION TAG	UNP Q97KL0
C	140	HIS	-	EXPRESSION TAG	UNP Q97KL0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	44	Total O 44 44	0	0

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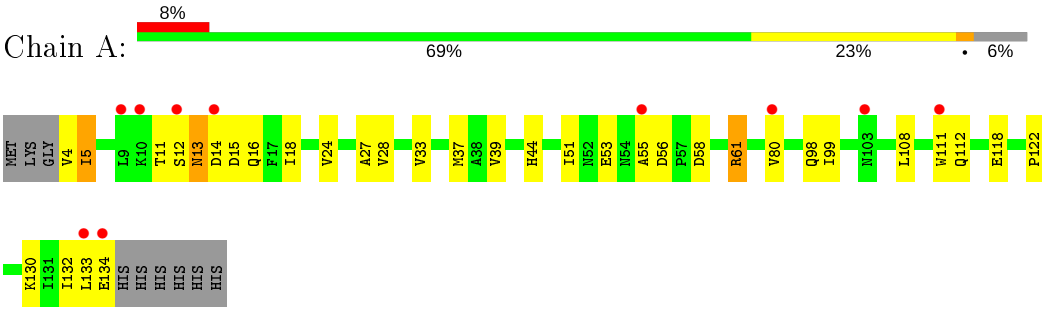
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	57	Total O 57 57	0	0
3	C	39	Total O 39 39	0	0

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 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.

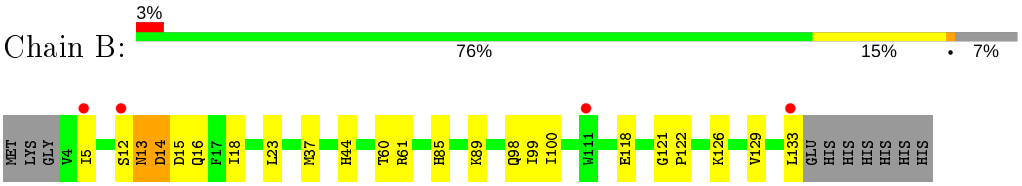
- Molecule 1: Clostridium acetobutylicum Q97KL0

Chain A:



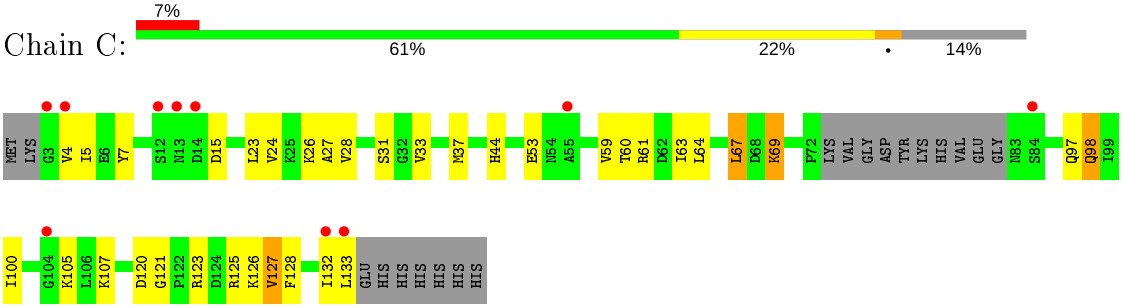
- Molecule 1: Clostridium acetobutylicum Q97KL0

Chain B:



- Molecule 1: Clostridium acetobutylicum Q97KL0

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.43Å 87.46Å 49.14Å 90.00° 116.65° 90.00°	Depositor
Resolution (Å)	19.63 – 2.00 24.58 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.3 (19.63-2.00) 98.2 (24.58-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.17 (at 2.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.203 , 0.248 0.213 , 0.254	Depositor DCC
R_{free} test set	2340 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	23.0	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 57.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3138	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.42% 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

5.1 Standard geometry

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	0.35	0/1038	0.59	0/1401
1	B	0.35	0/1029	0.60	0/1389
1	C	0.37	0/951	0.62	0/1283
All	All	0.36	0/3018	0.60	0/4073

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

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	1022	0	1019	27	0
1	B	1013	0	1013	21	0
1	C	938	0	939	30	0
2	A	15	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	44	0	0	2	0
3	B	57	0	0	1	0
3	C	39	0	0	3	0
All	All	3138	0	2971	70	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 12.

All (70) 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:B:12:SER:H	1:B:16:GLN:HE22	1.08	0.94
1:C:15:ASP:HB3	1:C:64:LEU:HD22	1.64	0.79
1:C:44:HIS:HE1	1:C:126:LYS:H	1.31	0.76
1:A:39:VAL:HG21	1:C:37:MSE:HE3	1.69	0.75
1:A:44:HIS:HE1	1:A:126:LYS:H	1.39	0.70
1:A:5:ILE:HD13	1:A:5:ILE:H	1.54	0.70
1:A:44:HIS:CE1	1:A:126:LYS:H	2.10	0.68
1:B:12:SER:H	1:B:16:GLN:NE2	1.87	0.68
1:B:5:ILE:HG23	1:B:129:VAL:HB	1.75	0.68
1:C:44:HIS:CE1	1:C:126:LYS:H	2.11	0.67
1:B:12:SER:N	1:B:16:GLN:HE22	1.89	0.67
1:A:16:GLN:HE21	1:A:18:ILE:HD11	1.61	0.66
1:B:44:HIS:HE1	1:B:126:LYS:H	1.43	0.64
1:B:44:HIS:CE1	1:B:126:LYS:H	2.17	0.62
1:A:12:SER:O	1:A:122:PRO:HB3	2.03	0.58
1:C:7:TYR:HB2	1:C:127:VAL:HG23	1.86	0.57
1:B:37:MSE:HE1	1:B:100:ILE:HG13	1.87	0.57
1:A:132:ILE:HD11	1:C:37:MSE:HE2	1.86	0.56
1:C:61:ARG:C	1:C:61:ARG:HD3	2.26	0.55
1:A:99:ILE:HD12	1:A:99:ILE:N	2.21	0.55
1:A:5:ILE:N	1:A:5:ILE:HD13	2.23	0.53
1:B:16:GLN:CD	1:B:18:ILE:HD11	2.29	0.53
1:A:61:ARG:HD3	3:A:228:HOH:O	2.09	0.52
1:B:100:ILE:HG21	1:C:4:VAL:HG21	1.91	0.51
1:B:85:HIS:O	1:B:89:LYS:HG3	2.10	0.51
1:C:69:LYS:O	1:C:69:LYS:HD2	2.11	0.51
1:C:120:ASP:O	1:C:123:ARG:HD2	2.11	0.50
1:C:4:VAL:HG11	1:C:128:PHE:HB3	1.91	0.50
1:C:60:THR:HG23	3:C:233:HOH:O	2.09	0.50
1:C:121:GLY:HA2	1:C:123:ARG:HG3	1.93	0.50
1:B:133:LEU:H	1:B:133:LEU:HD23	1.76	0.50
1:B:14:ASP:HA	1:B:121:GLY:O	2.13	0.49
1:B:99:ILE:HD12	1:B:99:ILE:N	2.26	0.49
1:A:15:ASP:HA	1:A:118:GLU:O	2.11	0.49
1:C:53:GLU:HG2	1:C:59:VAL:HG21	1.95	0.48
1:A:13:ASN:HD22	1:A:14:ASP:H	1.61	0.48
1:B:15:ASP:HA	1:B:118:GLU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:VAL:HG11	1:C:100:ILE:HG21	1.96	0.48
1:A:130:LYS:HD2	1:C:100:ILE:HG23	1.95	0.47
1:B:12:SER:O	1:B:122:PRO:HB3	2.14	0.47
1:A:33:VAL:HG22	1:A:133:LEU:HD13	1.96	0.47
1:A:111:TRP:HB2	3:A:236:HOH:O	2.15	0.46
1:A:51:ILE:CG2	1:A:112:GLN:HG2	2.45	0.46
1:A:24:VAL:O	1:A:28:VAL:HG23	2.16	0.46
1:C:24:VAL:O	1:C:28:VAL:HG23	2.16	0.45
1:C:31:SER:OG	1:C:33:VAL:HG22	2.16	0.45
1:A:133:LEU:HD12	1:A:134:GLU:H	1.81	0.45
1:A:108:LEU:HD13	1:A:112:GLN:O	2.17	0.45
1:B:37:MSE:HE3	1:B:99:ILE:C	2.37	0.45
1:C:123:ARG:NH2	3:C:221:HOH:O	2.47	0.45
1:B:13:ASN:HD22	1:B:14:ASP:H	1.65	0.44
1:A:11:THR:HG22	1:A:18:ILE:HD11	1.99	0.44
1:A:37:MSE:HE3	1:A:98:GLN:HB2	1.98	0.44
1:B:37:MSE:HE2	1:B:98:GLN:HG3	2.00	0.44
1:C:97:GLN:HA	1:C:97:GLN:NE2	2.32	0.44
1:B:98:GLN:HE22	1:C:98:GLN:CD	2.22	0.43
1:C:123:ARG:HD3	1:C:125:ARG:CZ	2.47	0.43
1:A:11:THR:HG22	1:A:18:ILE:CD1	2.48	0.43
1:C:132:ILE:HG22	1:C:133:LEU:N	2.34	0.43
1:A:4:VAL:HG21	1:C:107:LYS:HE3	2.01	0.43
1:C:23:LEU:O	1:C:26:LYS:HB3	2.19	0.42
1:A:5:ILE:HD11	1:A:27:ALA:HB1	2.02	0.41
1:B:60:THR:HG23	3:B:258:HOH:O	2.21	0.41
1:B:13:ASN:ND2	1:B:14:ASP:H	2.19	0.41
1:A:130:LYS:HD3	1:C:37:MSE:HE1	2.02	0.41
1:C:5:ILE:HD12	1:C:27:ALA:HB1	2.03	0.41
1:C:97:GLN:HA	1:C:97:GLN:HE21	1.86	0.41
1:C:105:LYS:HD2	3:C:228:HOH:O	2.19	0.40
1:A:56:ASP:OD1	1:A:58:ASP:HB2	2.21	0.40
1:C:63:ILE:O	1:C:67:LEU:HB2	2.21	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	129/140 (92%)	124 (96%)	3 (2%)	2 (2%)	9 4
1	B	128/140 (91%)	121 (94%)	7 (6%)	0	100 100
1	C	117/140 (84%)	113 (97%)	4 (3%)	0	100 100
All	All	374/420 (89%)	358 (96%)	14 (4%)	2 (0%)	29 23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ALA
1	A	80	VAL

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	115/121 (95%)	111 (96%)	4 (4%)	36 35
1	B	114/121 (94%)	110 (96%)	4 (4%)	36 35
1	C	106/121 (88%)	102 (96%)	4 (4%)	33 31
All	All	335/363 (92%)	323 (96%)	12 (4%)	35 34

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE

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Mol	Chain	Res	Type
1	A	13	ASN
1	A	53	GLU
1	A	61	ARG
1	B	13	ASN
1	B	14	ASP
1	B	23	LEU
1	B	61	ARG
1	C	67	LEU
1	C	69	LYS
1	C	98	GLN
1	C	127	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	16	GLN
1	A	44	HIS
1	A	54	ASN
1	A	97	GLN
1	B	13	ASN
1	B	16	GLN
1	B	44	HIS
1	B	79	HIS
1	B	87	HIS
1	B	97	GLN
1	B	98	GLN
1	B	103	ASN
1	C	22	ASN
1	C	44	HIS
1	C	83	ASN
1	C	97	GLN
1	C	98	GLN
1	C	103	ASN

5.3.3 RNA

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)

5 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	$\#\|Z\| > 2$
2	SO4	A	201	-	4,4,4	0.22	0	6,6,6	0.07	0
2	SO4	B	202	-	4,4,4	0.25	0	6,6,6	0.11	0
2	SO4	A	205	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	C	203	-	4,4,4	0.31	0	6,6,6	0.12	0
2	SO4	A	204	-	4,4,4	0.28	0	6,6,6	0.06	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.

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

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	129/140 (92%)	0.55	11 (8%)	10	10	14, 31, 48, 65	0
1	B	128/140 (91%)	0.20	4 (3%)	49	48	12, 27, 43, 50	0
1	C	119/140 (85%)	0.37	10 (8%)	11	10	12, 29, 51, 57	0
All	All	376/420 (89%)	0.38	25 (6%)	18	17	12, 29, 49, 65	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	VAL	6.4
1	A	133	LEU	5.3
1	C	133	LEU	4.9
1	A	12	SER	4.8
1	B	133	LEU	4.7
1	C	3	GLY	4.3
1	A	14	ASP	3.5
1	A	111	TRP	3.2
1	C	14	ASP	3.0
1	C	13	ASN	3.0
1	A	103	ASN	2.9
1	A	134	GLU	2.8
1	A	10	LYS	2.7
1	A	124	ASP	2.5
1	B	111	TRP	2.5
1	C	104	GLY	2.4
1	C	132	ILE	2.4
1	B	12	SER	2.3
1	C	12	SER	2.3
1	A	55	ALA	2.2
1	A	9	LEU	2.2
1	C	4	VAL	2.1
1	C	84	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	5	ILE	2.1
1	C	55	ALA	2.1

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. 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	B-factors(Å^2)	Q<0.9
2	SO4	A	205	5/5	0.94	0.18	62,62,62,63	0
2	SO4	A	204	5/5	0.94	0.20	63,63,64,65	0
2	SO4	A	201	5/5	0.99	0.07	30,30,31,33	0
2	SO4	C	203	5/5	0.99	0.07	25,25,28,29	0
2	SO4	B	202	5/5	0.99	0.09	25,27,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.