



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:48 am BST

PDB ID : 3P42
Title : Structure of GfcC (YmcB), protein encoded by the E. coli group 4 capsule operon
Authors : Saper, M.A.; Sathiyamoorthy, K.
Deposited on : 2010-10-05
Resolution : 1.91 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

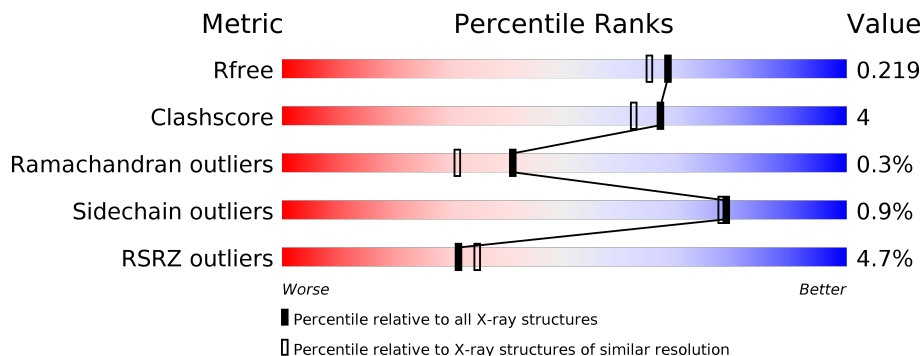
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 $\leq 5\%$. 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	236	
1	B	236	
1	C	236	
1	D	236	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 14977 atoms, of which 7143 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 Predicted protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	Se			
1	A	234	3637	1156	1816	321	341	3	0	0	0
1	B	225	3506	1110	1760	305	328	3	0	1	0
1	C	226	3545	1122	1780	308	332	3	0	4	0
1	D	229	3572	1134	1787	309	339	3	0	2	0

There are 36 discrepancies between the modelled and reference sequences:

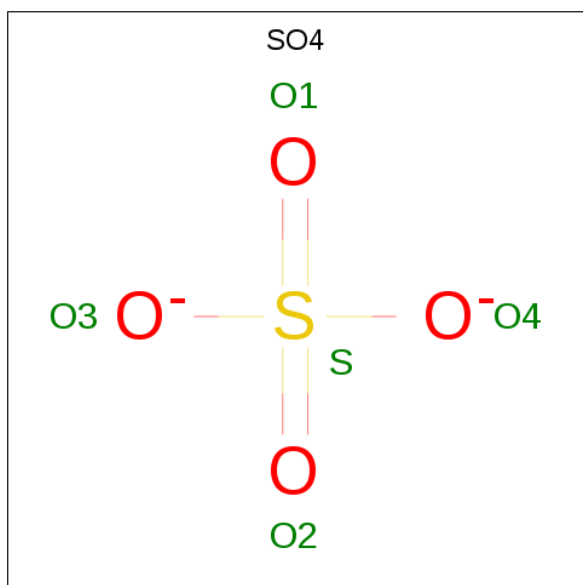
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MSE	-	EXPRESSION TAG	UNP B7UN63
A	249	LEU	-	EXPRESSION TAG	UNP B7UN63
A	250	GLU	-	EXPRESSION TAG	UNP B7UN63
A	251	HIS	-	EXPRESSION TAG	UNP B7UN63
A	252	HIS	-	EXPRESSION TAG	UNP B7UN63
A	253	HIS	-	EXPRESSION TAG	UNP B7UN63
A	254	HIS	-	EXPRESSION TAG	UNP B7UN63
A	255	HIS	-	EXPRESSION TAG	UNP B7UN63
A	256	HIS	-	EXPRESSION TAG	UNP B7UN63
B	21	MSE	-	EXPRESSION TAG	UNP B7UN63
B	249	LEU	-	EXPRESSION TAG	UNP B7UN63
B	250	GLU	-	EXPRESSION TAG	UNP B7UN63
B	251	HIS	-	EXPRESSION TAG	UNP B7UN63
B	252	HIS	-	EXPRESSION TAG	UNP B7UN63
B	253	HIS	-	EXPRESSION TAG	UNP B7UN63
B	254	HIS	-	EXPRESSION TAG	UNP B7UN63
B	255	HIS	-	EXPRESSION TAG	UNP B7UN63
B	256	HIS	-	EXPRESSION TAG	UNP B7UN63
C	21	MSE	-	EXPRESSION TAG	UNP B7UN63
C	249	LEU	-	EXPRESSION TAG	UNP B7UN63
C	250	GLU	-	EXPRESSION TAG	UNP B7UN63

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Chain	Residue	Modelled	Actual	Comment	Reference
C	251	HIS	-	EXPRESSION TAG	UNP B7UN63
C	252	HIS	-	EXPRESSION TAG	UNP B7UN63
C	253	HIS	-	EXPRESSION TAG	UNP B7UN63
C	254	HIS	-	EXPRESSION TAG	UNP B7UN63
C	255	HIS	-	EXPRESSION TAG	UNP B7UN63
C	256	HIS	-	EXPRESSION TAG	UNP B7UN63
D	21	MSE	-	EXPRESSION TAG	UNP B7UN63
D	249	LEU	-	EXPRESSION TAG	UNP B7UN63
D	250	GLU	-	EXPRESSION TAG	UNP B7UN63
D	251	HIS	-	EXPRESSION TAG	UNP B7UN63
D	252	HIS	-	EXPRESSION TAG	UNP B7UN63
D	253	HIS	-	EXPRESSION TAG	UNP B7UN63
D	254	HIS	-	EXPRESSION TAG	UNP B7UN63
D	255	HIS	-	EXPRESSION TAG	UNP B7UN63
D	256	HIS	-	EXPRESSION TAG	UNP B7UN63

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	218	Total 222	O 222	0	4
3	B	157	Total 159	O 159	0	2
3	C	203	Total 206	O 206	0	3
3	D	115	Total 115	O 115	0	0

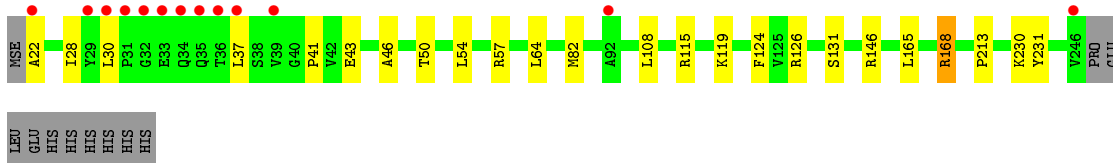
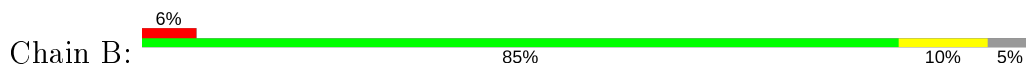
3 Residue-property plots [i](#)

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.

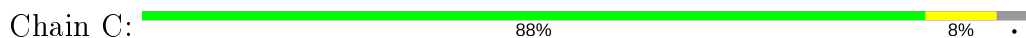
- Molecule 1: Predicted protein



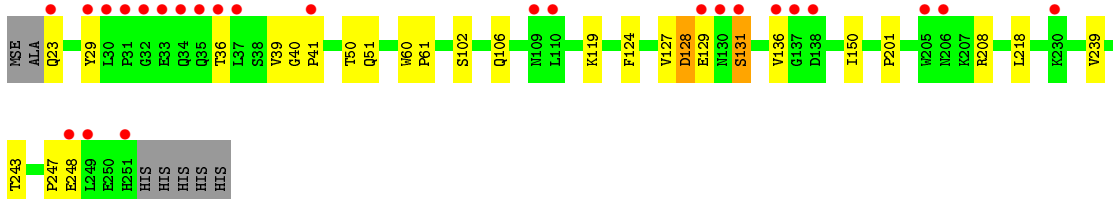
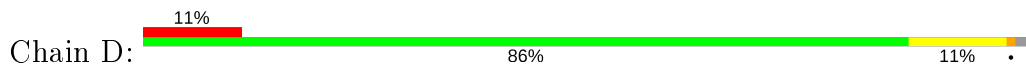
- Molecule 1: Predicted protein



- Molecule 1: Predicted protein



- Molecule 1: Predicted protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.83Å 99.98Å 69.02Å 90.00° 91.74° 90.00°	Depositor
Resolution (Å)	34.49 – 1.91 49.99 – 1.77	Depositor EDS
% Data completeness (in resolution range)	98.5 (34.49-1.91) 86.9 (49.99-1.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 1.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.173 , 0.217 0.176 , 0.219	Depositor DCC
R_{free} test set	3915 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.043 for l,k,-h 0.037 for h,-k,-l 0.026 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14977	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.40	0/1864	0.57	0/2552
1	B	0.37	0/1786	0.54	0/2444
1	C	0.39	0/1817	0.55	0/2487
1	D	0.33	0/1828	0.54	0/2502
All	All	0.38	0/7295	0.55	0/9985

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	1821	1816	1805	11	0
1	B	1746	1760	1756	22	0
1	C	1765	1780	1762	9	0
1	D	1785	1787	1778	19	0
2	B	10	0	0	0	0
2	D	5	0	0	0	0
3	A	222	0	0	1	0
3	B	159	0	0	1	0
3	C	206	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	115	0	0	0	0
All	All	7834	7143	7101	56	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 4.

All (56) 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:C:208:ARG:CZ	1:D:127:VAL:HG11	2.24	0.67
1:B:119:LYS:HE2	1:B:124:PHE:CD1	2.30	0.66
1:B:230:LYS:HD2	1:B:231:TYR:CZ	2.36	0.60
1:D:39:VAL:HG11	1:D:51:GLN:HG3	1.82	0.60
1:A:118:VAL:HG12	1:A:133:PRO:HG2	1.83	0.59
1:A:189:MSE:HE1	1:A:199:VAL:HG22	1.84	0.59
1:A:164:TRP:CH2	1:A:166:ALA:HA	2.38	0.57
1:B:64:LEU:HA	3:B:640[B]:HOH:O	2.05	0.55
1:C:189:MSE:HE1	1:C:199:VAL:HG22	1.89	0.55
1:D:127:VAL:O	1:D:131:SER:HB2	2.07	0.54
1:B:22:ALA:HA	1:B:43:GLU:CG	2.36	0.54
1:D:201:PRO:HG2	1:D:208:ARG:HG3	1.89	0.54
1:B:22:ALA:HA	1:B:43:GLU:HG3	1.91	0.53
1:D:127:VAL:O	1:D:128:ASP:HB2	2.10	0.52
1:A:125:VAL:HG22	1:B:213:PRO:HD3	1.91	0.52
1:D:39:VAL:CG1	1:D:51:GLN:HG3	2.40	0.51
1:B:28:ILE:HD11	1:B:54:LEU:HD11	1.93	0.51
1:C:101:LYS:HE2	1:C:105:GLN:NE2	2.26	0.51
1:C:208:ARG:NH2	1:D:127:VAL:HG11	2.27	0.50
1:D:40:GLY:HA2	1:D:41:PRO:C	2.32	0.50
1:C:40:GLY:HA2	1:C:41:PRO:C	2.33	0.49
1:D:247:PRO:C	1:D:248:GLU:HG2	2.33	0.48
1:B:22:ALA:CA	1:B:43:GLU:HG3	2.44	0.48
1:B:28:ILE:CD1	1:B:54:LEU:HD11	2.43	0.48
1:D:29:TYR:CE1	1:D:36:THR:HG21	2.49	0.48
1:B:22:ALA:HB1	1:B:41:PRO:HB2	1.96	0.47
1:C:45:VAL:HG21	1:C:118:VAL:HG21	1.96	0.46
1:A:64:LEU:HD23	1:A:64:LEU:C	2.36	0.46
1:D:23:GLN:HG3	1:D:136:VAL:O	2.16	0.46
1:B:126:ARG:HB3	1:B:131:SER:HB2	1.98	0.45
1:B:22:ALA:N	1:B:43:GLU:CG	2.80	0.45
1:C:168:ARG:HG2	1:C:172:ASP:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:SER:O	1:D:106:GLN:HG3	2.17	0.45
1:B:30:LEU:HD13	1:B:57:ARG:NH2	2.31	0.45
1:D:50:THR:O	1:D:50:THR:HG22	2.18	0.44
1:D:119:LYS:HE2	1:D:124:PHE:CE1	2.52	0.44
1:B:46:ALA:O	1:B:50:THR:HG22	2.17	0.44
1:C:76:LYS:HE3	1:C:76:LYS:HB3	1.87	0.44
1:B:64:LEU:HD11	1:B:115:ARG:HB2	2.00	0.43
1:B:22:ALA:N	1:B:43:GLU:HG2	2.32	0.43
1:A:252:HIS:HB3	1:A:255:HIS:CE1	2.53	0.43
1:B:22:ALA:CA	1:B:43:GLU:CG	2.97	0.43
1:B:82:MSE:HE2	1:B:108:LEU:HA	2.00	0.43
1:D:29:TYR:CD1	1:D:36:THR:HG21	2.53	0.43
1:C:64:LEU:HG	1:C:115:ARG:HG3	2.01	0.42
1:A:55:ARG:CZ	1:B:146:ARG:HD2	2.50	0.42
1:D:60:TRP:N	1:D:61:PRO:CD	2.82	0.42
1:A:166:ALA:HB2	1:B:50:THR:HG21	2.00	0.42
1:D:247:PRO:O	1:D:248:GLU:HG2	2.20	0.42
1:B:165:LEU:HB2	1:B:168:ARG:HD3	2.02	0.41
1:A:40:GLY:HA2	1:A:41:PRO:C	2.41	0.41
1:B:37:LEU:CD1	1:B:37:LEU:N	2.84	0.41
1:D:239:VAL:O	1:D:243:THR:HG23	2.20	0.41
1:D:150:ILE:HD12	1:D:218:LEU:HD22	2.03	0.41
1:A:71:LYS:HE2	3:A:618:HOH:O	2.20	0.41
1:A:82:MSE:HE2	1:A:108:LEU:HD23	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	232/236 (98%)	228 (98%)	3 (1%)	1 (0%)	34 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	224/236 (95%)	218 (97%)	6 (3%)	0	100	100
1	C	228/236 (97%)	226 (99%)	1 (0%)	1 (0%)	34	24
1	D	229/236 (97%)	223 (97%)	5 (2%)	1 (0%)	34	24
All	All	913/944 (97%)	895 (98%)	15 (2%)	3 (0%)	41	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	128	ASP
1	A	250	GLU
1	C	55	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	198/196 (101%)	197 (100%)	1 (0%)	88	89
1	B	190/196 (97%)	189 (100%)	1 (0%)	88	89
1	C	194/196 (99%)	191 (98%)	3 (2%)	65	61
1	D	195/196 (100%)	193 (99%)	2 (1%)	76	75
All	All	777/784 (99%)	770 (99%)	7 (1%)	78	78

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	HIS
1	B	168	ARG
1	C	128	ASP
1	C	194	GLU
1	C	245	ARG
1	D	129	GLU
1	D	131	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	161	GLN

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](#)

3 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	B	1	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	D	2	-	4,4,4	0.17	0	6,6,6	0.20	0
2	SO4	B	3	-	4,4,4	0.15	0	6,6,6	0.28	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 [i](#)

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, 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	231/236 (97%)	-0.05	3 (1%) 77 79	16, 27, 54, 91	0
1	B	222/236 (94%)	0.18	13 (5%) 22 25	20, 31, 66, 171	0
1	C	223/236 (94%)	-0.04	1 (0%) 92 93	16, 26, 57, 86	0
1	D	226/236 (95%)	0.55	25 (11%) 5 6	20, 41, 89, 174	0
All	All	902/944 (95%)	0.16	42 (4%) 31 34	16, 30, 71, 174	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	34	GLN	8.0
1	B	34	GLN	7.4
1	B	246	VAL	7.0
1	D	249	LEU	6.6
1	D	30	LEU	5.7
1	D	32	GLY	5.7
1	D	35	GLN	5.0
1	B	30	LEU	5.0
1	D	37	LEU	5.0
1	B	22	ALA	4.7
1	D	36	THR	4.4
1	A	251	HIS	4.3
1	A	41	PRO	4.1
1	D	31	PRO	4.0
1	B	37	LEU	3.9
1	D	251	HIS	3.8
1	D	136	VAL	3.7
1	D	109	ASN	3.6
1	B	31	PRO	3.4
1	B	29	TYR	3.4
1	B	35	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	29	TYR	3.3
1	D	205	TRP	3.3
1	D	23	GLN	3.3
1	D	137	GLY	3.2
1	B	36	THR	3.1
1	A	256	HIS	2.9
1	D	206	ASN	2.8
1	B	92	ALA	2.7
1	B	33	GLU	2.7
1	D	129	GLU	2.5
1	D	131	SER	2.5
1	B	32	GLY	2.5
1	D	33	GLU	2.4
1	D	110	LEU	2.4
1	D	248	GLU	2.3
1	D	230	LYS	2.3
1	C	248	GLU	2.2
1	D	41	PRO	2.1
1	D	130	ASN	2.1
1	B	39	VAL	2.0
1	D	138	ASP	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. 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
2	SO4	B	3	5/5	0.87	0.18	49,64,67,67	0
2	SO4	D	2	5/5	0.94	0.12	52,53,68,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	B	1	5/5	0.98	0.10	42,57,60,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.