Full wwPDB X-ray Structure Validation Report (i)

Apr 8, 2024 – 12:21 PM EDT

PDB ID	:	8SBH
Title	:	YeiE effector binding domain from E. coli
Authors	:	Momany, C.; Nune, M.; Brondani, J.C.; Afful, D.; Neidle, E.
Deposited on	:	2023-04-03
Resolution	:	1.93 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:

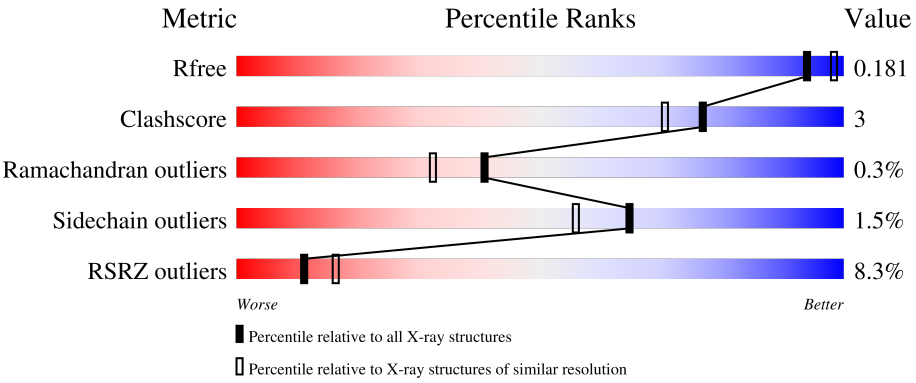
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 1.93 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	209	2% 89% 6% 5%
1	B	209	13% 86% 10% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6986 atoms, of which 3331 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.

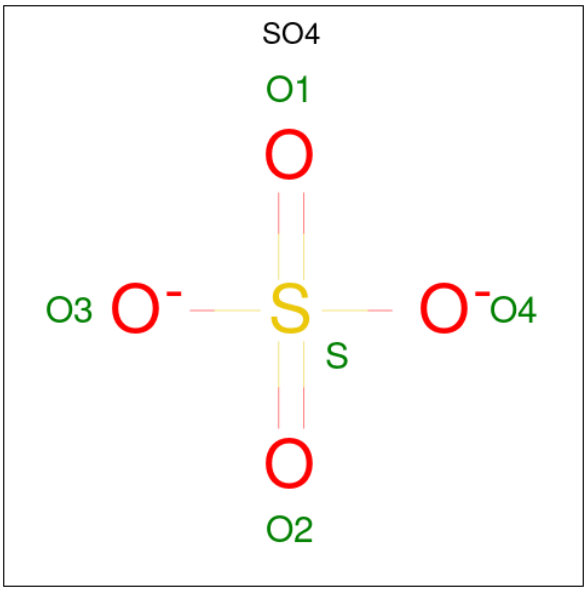
- Molecule 1 is a protein called Transcriptional regulator YeiE, LysR family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	199	Total	C	H	N	O	S	0	5	0
			3249	1027	1633	288	289	12			
1	B	199	Total	C	H	N	O	S	0	2	0
			3210	1017	1612	284	287	10			

There are 12 discrepancies between the modelled and reference sequences:

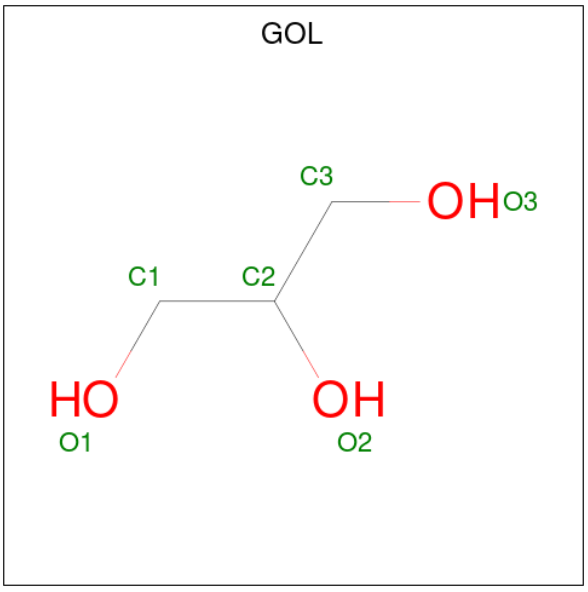
Chain	Residue	Modelled	Actual	Comment	Reference
A	90	MET	-	initiating methionine	UNP P0ACR4
A	294	HIS	-	expression tag	UNP P0ACR4
A	295	HIS	-	expression tag	UNP P0ACR4
A	296	HIS	-	expression tag	UNP P0ACR4
A	297	HIS	-	expression tag	UNP P0ACR4
A	298	HIS	-	expression tag	UNP P0ACR4
B	90	MET	-	initiating methionine	UNP P0ACR4
B	294	HIS	-	expression tag	UNP P0ACR4
B	295	HIS	-	expression tag	UNP P0ACR4
B	296	HIS	-	expression tag	UNP P0ACR4
B	297	HIS	-	expression tag	UNP P0ACR4
B	298	HIS	-	expression tag	UNP P0ACR4

- 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	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 27 6 15 6	0	1

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 14 3 8 3	0	0
3	A	1	Total C H O 14 3 8 3	0	0
3	A	1	Total C H O 14 3 8 3	0	0
3	A	1	Total C H O 14 3 8 3	0	0
3	A	1	Total C H O 14 3 8 3	0	0
3	A	1	Total C H O 13 3 7 3	0	0
3	A	1	Total C H O 14 3 8 3	0	0
3	A	1	Total C H O 14 3 8 3	0	0
3	B	1	Total C H O 14 3 8 3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0

- Molecule 5 is water.

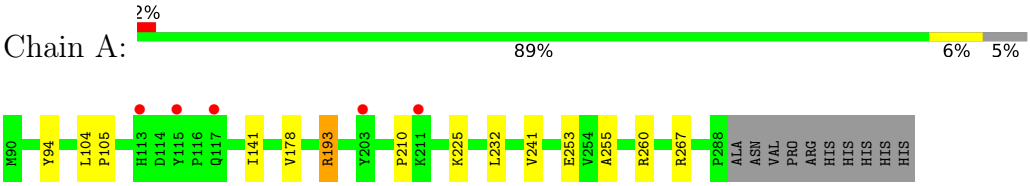
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	177	Total O 184 184	0	7
5	B	172	Total O 175 175	0	3

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.

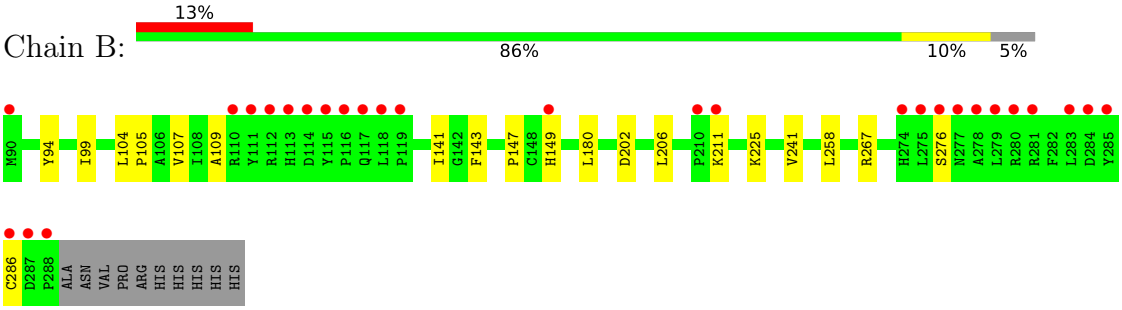
• Molecule 1: Transcriptional regulator YeiE, LysR family

Chain A:



• Molecule 1: Transcriptional regulator YeiE, LysR family

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	71.10Å 71.10Å 196.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.80 – 1.93 31.80 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.5 (31.80-1.93) 94.9 (31.80-1.93)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.166 , 0.181 0.167 , 0.181	Depositor DCC
R_{free} test set	1119 reflections (2.89%)	wwPDB-VP
Wilson B-factor (Å^2)	21.6	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 62.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6986	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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: GOL, CME, SO4, CL

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	0/1647	0.53	0/2236
1	B	0.27	0/1627	0.53	0/2210
All	All	0.27	0/3274	0.53	0/4446

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	1616	1633	1620	10	0
1	B	1598	1612	1611	11	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
3	A	60	78	80	0	0
3	B	6	8	8	0	0
4	B	1	0	0	0	0
5	A	184	0	0	2	0
5	B	175	0	0	0	0
All	All	3655	3331	3319	20	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 3.

All (20) 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:180:LEU:HD21	1:B:258:LEU:HD21	1.73	0.70
1:B:141:ILE:HD11	1:B:267:ARG:HD2	1.81	0.63
1:A:178:VAL:HG22	1:A:255:ALA:O	2.05	0.56
1:A:225:LYS:HD3	1:A:241:VAL:HG12	1.86	0.56
1:B:147:PRO:O	1:B:149:HIS:CD2	2.63	0.51
1:B:202[A]:ASP:OD1	1:B:206:LEU:HD12	2.10	0.51
1:A:193:ARG:HE	1:A:193:ARG:H	1.58	0.51
1:A:253:GLU:OE2	5:A:401[A]:HOH:O	2.20	0.47
1:B:141:ILE:HD11	1:B:267:ARG:CD	2.44	0.46
1:B:107:VAL:HG11	1:B:286:CYS:SG	2.55	0.46
1:B:141:ILE:HD11	1:B:267:ARG:CG	2.45	0.46
1:A:193:ARG:H	1:A:193:ARG:NE	2.15	0.44
1:B:99:ILE:HD13	1:B:143:PHE:HB3	1.99	0.44
1:A:232:LEU:HD21	1:B:109:ALA:HA	2.01	0.43
1:A:260[A]:ARG:NH2	5:A:408:HOH:O	2.43	0.43
1:B:225:LYS:HD2	1:B:241:VAL:HG12	2.01	0.42
1:B:104:LEU:N	1:B:105:PRO:CD	2.81	0.42
1:A:141:ILE:HD11	1:A:267:ARG:CG	2.49	0.42
1:A:141:ILE:HD11	1:A:267:ARG:HG2	2.02	0.42
1:A:104:LEU:N	1:A:105:PRO:CD	2.84	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	199/209 (95%)	193 (97%)	5 (2%)	1 (0%)	29 17
1	B	198/209 (95%)	194 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	397/418 (95%)	387 (98%)	9 (2%)	1 (0%)	41 32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	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	175/180 (97%)	173 (99%)	2 (1%)	73 67
1	B	173/180 (96%)	170 (98%)	3 (2%)	60 49
All	All	348/360 (97%)	343 (99%)	5 (1%)	65 58

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	TYR
1	A	193	ARG
1	B	94	TYR
1	B	211	LYS
1	B	276	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

3 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CME	A	148[B]	-	8,9,10	1.19	0	5,9,11	0.82	0
1	CME	A	148[A]	-	8,9,10	1.08	0	5,9,11	0.80	0
1	CME	B	148	1	8,9,10	0.95	0	5,9,11	0.53	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	A	148[B]	-	-	3/5/8/10	-
1	CME	A	148[A]	-	-	1/5/8/10	-
1	CME	B	148	1	-	2/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	148[A]	CME	SD-CE-CZ-OH
1	A	148[B]	CME	SD-CE-CZ-OH
1	B	148	CME	N-CA-CB-SG
1	A	148[B]	CME	CE-SD-SG-CB
1	A	148[B]	CME	CA-CB-SG-SD
1	B	148	CME	CE-SD-SG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 for Mogul analysis.

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	GOL	A	302[B]	-	5,5,5	0.87	0	5,5,5	1.02	0
3	GOL	A	306	-	5,5,5	0.84	0	5,5,5	1.02	0
3	GOL	B	303	-	5,5,5	0.87	0	5,5,5	1.04	0
3	GOL	A	310	-	5,5,5	0.88	0	5,5,5	0.99	0
2	SO4	A	301	-	4,4,4	0.16	0	6,6,6	0.06	0
2	SO4	B	301	-	4,4,4	0.17	0	6,6,6	0.07	0
3	GOL	A	307	-	5,5,5	0.85	0	5,5,5	1.00	0
3	GOL	A	303	-	5,5,5	0.84	0	5,5,5	0.91	0
3	GOL	A	304	-	5,5,5	0.85	0	5,5,5	1.02	0
3	GOL	A	309	-	5,5,5	0.84	0	5,5,5	0.93	0
3	GOL	A	305	-	5,5,5	0.92	0	5,5,5	1.03	0
2	SO4	B	302	-	4,4,4	0.14	0	6,6,6	0.05	0
3	GOL	A	302[A]	-	5,5,5	0.82	0	5,5,5	1.03	0
3	GOL	A	308	-	5,5,5	0.79	0	5,5,5	1.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	302[B]	-	-	2/4/4/4	-
3	GOL	A	306	-	-	0/4/4/4	-
3	GOL	B	303	-	-	3/4/4/4	-
3	GOL	A	310	-	-	2/4/4/4	-
3	GOL	A	307	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	309	-	-	0/4/4/4	-
3	GOL	A	303	-	-	2/4/4/4	-
3	GOL	A	304	-	-	2/4/4/4	-
3	GOL	A	305	-	-	2/4/4/4	-
3	GOL	A	302[A]	-	-	2/4/4/4	-
3	GOL	A	308	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302[A]	GOL	O1-C1-C2-C3
3	A	302[B]	GOL	O1-C1-C2-C3
3	A	303	GOL	O1-C1-C2-C3
3	A	304	GOL	O1-C1-C2-C3
3	A	305	GOL	C1-C2-C3-O3
3	A	308	GOL	C1-C2-C3-O3
3	A	310	GOL	C1-C2-C3-O3
3	A	310	GOL	O2-C2-C3-O3
3	A	302[A]	GOL	O1-C1-C2-O2
3	A	302[B]	GOL	O1-C1-C2-O2
3	A	304	GOL	O1-C1-C2-O2
3	A	308	GOL	O2-C2-C3-O3
3	A	303	GOL	O1-C1-C2-O2
3	A	305	GOL	O2-C2-C3-O3
3	B	303	GOL	O1-C1-C2-O2
3	A	307	GOL	C1-C2-C3-O3
3	B	303	GOL	O1-C1-C2-C3
3	A	307	GOL	O2-C2-C3-O3
3	B	303	GOL	C1-C2-C3-O3

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, 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	198/209 (94%)	-0.01	5 (2%) 57 64	14, 26, 54, 72	0
1	B	198/209 (94%)	0.50	28 (14%) 2 4	14, 26, 87, 109	0
All	All	396/418 (94%)	0.25	33 (8%) 11 16	14, 26, 75, 109	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	118	LEU	7.1
1	B	117	GLN	6.1
1	B	275	LEU	5.1
1	B	210	PRO	5.1
1	B	285	TYR	4.8
1	B	286	CYS	4.6
1	B	115	TYR	4.5
1	B	113	HIS	4.4
1	B	280	ARG	4.4
1	B	281	ARG	4.4
1	B	288	PRO	3.9
1	B	287	ASP	3.9
1	B	274	HIS	3.5
1	B	277	ASN	3.5
1	A	113	HIS	3.0
1	B	211	LYS	3.0
1	B	278	ALA	2.9
1	A	203	TYR	2.8
1	B	284	ASP	2.8
1	B	110	ARG	2.8
1	B	149	HIS	2.8
1	B	114	ASP	2.6
1	B	279	LEU	2.6
1	B	111	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	115	TYR	2.5
1	B	283	LEU	2.5
1	A	211	LYS	2.4
1	A	117	GLN	2.4
1	B	116	PRO	2.3
1	B	119	PRO	2.3
1	B	90	MET	2.3
1	B	112	ARG	2.1
1	B	276	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CME	A	148[A]	10/11	0.84	0.20	35,45,58,58	15
1	CME	A	148[B]	10/11	0.84	0.20	35,45,58,58	15
1	CME	B	148	10/11	0.85	0.21	37,57,87,95	0

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, 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
3	GOL	B	303	6/6	0.80	0.25	47,63,76,76	0
3	GOL	A	307	6/6	0.81	0.47	51,68,81,81	0
3	GOL	A	309	6/6	0.82	0.25	40,48,56,68	0
3	GOL	A	304	6/6	0.84	0.28	41,49,66,66	0
3	GOL	A	308	6/6	0.85	0.19	30,37,56,56	0
3	GOL	A	310	6/6	0.87	0.27	28,60,72,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	302[A]	6/6	0.88	0.24	23,28,35,35	13
3	GOL	A	302[B]	6/6	0.88	0.24	24,31,36,38	14
3	GOL	A	305	6/6	0.92	0.15	40,49,59,63	0
3	GOL	A	303	6/6	0.95	0.15	32,41,52,62	0
3	GOL	A	306	6/6	0.96	0.11	29,39,45,52	0
2	SO4	B	302	5/5	0.99	0.10	20,24,31,32	0
2	SO4	A	301	5/5	0.99	0.09	19,20,21,24	0
2	SO4	B	301	5/5	0.99	0.08	26,29,31,34	0
4	CL	B	304	1/1	0.99	0.08	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.