Full wwPDB X-ray Structure Validation Report (i)

Nov 6, 2023 – 06:19 AM EST

PDB ID	:	4ORN
Title	:	Blue Fluorescent Protein mKalama1
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Deposited on	:	2014-02-11
Resolution	:	1.71 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 (i)) were used in the production of this report:

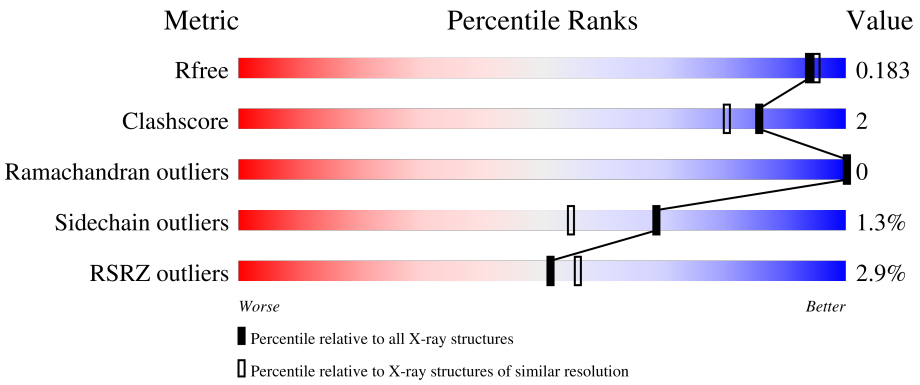
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.71 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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	239	3% 88% 8% ·
1	B	239	3% 92% · ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	B	302	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4288 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 mKalama1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	229	1890	1193	328	362	7	0	9	0
1	B	229	1926	1214	337	368	7	0	13	0

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P42212
A	-1	SER	-	expression tag	UNP P42212
A	0	MET	-	expression tag	UNP P42212
A	1	VAL	-	expression tag	UNP P42212
A	18	MET	LEU	engineered mutation	UNP P42212
A	25	ARG	HIS	engineered mutation	UNP P42212
A	30	ARG	SER	engineered mutation	UNP P42212
A	32	VAL	GLU	engineered mutation	UNP P42212
A	39	HIS	TYR	engineered mutation	UNP P42212
A	50	SER	THR	engineered mutation	UNP P42212
A	64	LEU	PHE	engineered mutation	UNP P42212
A	66	GYS	SER	chromophore	UNP P42212
A	66	GYS	TYR	chromophore	UNP P42212
A	66	GYS	GLY	chromophore	UNP P42212
A	105	SER	ASN	engineered mutation	UNP P42212
A	124	VAL	GLU	engineered mutation	UNP P42212
A	128	THR	ILE	engineered mutation	UNP P42212
A	145	MET	TYR	engineered mutation	UNP P42212
A	147	VAL	SER	engineered mutation	UNP P42212
A	148	GLY	HIS	engineered mutation	UNP P42212
A	153	THR	MET	engineered mutation	UNP P42212
A	163	ALA	VAL	engineered mutation	UNP P42212
A	166	GLU	LYS	engineered mutation	UNP P42212
A	171	VAL	ILE	engineered mutation	UNP P42212
A	175	GLY	SER	engineered mutation	UNP P42212

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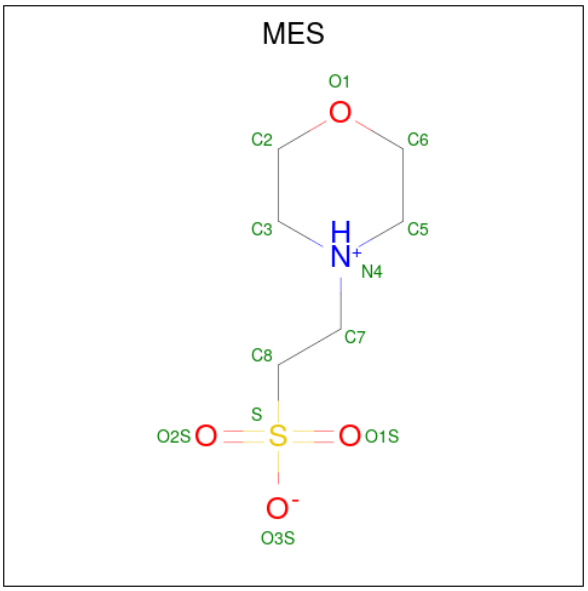
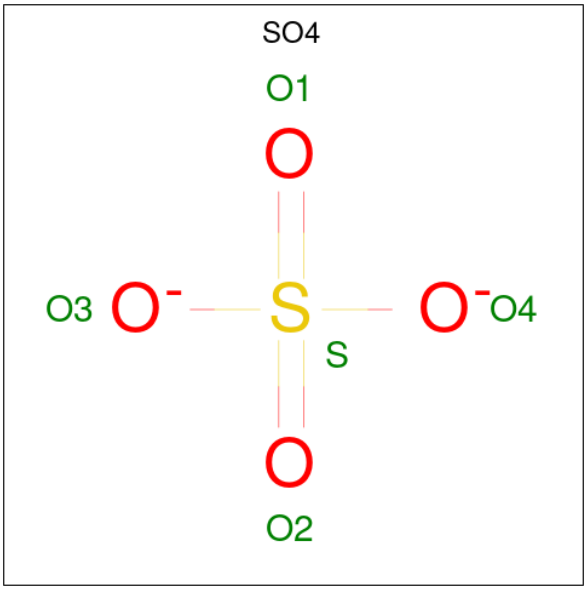
Chain	Residue	Modelled	Actual	Comment	Reference
A	192	SER	PRO	engineered mutation	UNP P42212
A	203	VAL	THR	engineered mutation	UNP P42212
A	205	VAL	SER	engineered mutation	UNP P42212
A	206	LYS	ALA	engineered mutation	UNP P42212
A	224	ARG	VAL	engineered mutation	UNP P42212
A	231	PRO	HIS	engineered mutation	UNP P42212
B	-2	SER	-	expression tag	UNP P42212
B	-1	SER	-	expression tag	UNP P42212
B	0	MET	-	expression tag	UNP P42212
B	1	VAL	-	expression tag	UNP P42212
B	18	MET	LEU	engineered mutation	UNP P42212
B	25	ARG	HIS	engineered mutation	UNP P42212
B	30	ARG	SER	engineered mutation	UNP P42212
B	32	VAL	GLU	engineered mutation	UNP P42212
B	39	HIS	TYR	engineered mutation	UNP P42212
B	50	SER	THR	engineered mutation	UNP P42212
B	64	LEU	PHE	engineered mutation	UNP P42212
B	66	GYS	SER	chromophore	UNP P42212
B	66	GYS	TYR	chromophore	UNP P42212
B	66	GYS	GLY	chromophore	UNP P42212
B	105	SER	ASN	engineered mutation	UNP P42212
B	124	VAL	GLU	engineered mutation	UNP P42212
B	128	THR	ILE	engineered mutation	UNP P42212
B	145	MET	TYR	engineered mutation	UNP P42212
B	147	VAL	SER	engineered mutation	UNP P42212
B	148	GLY	HIS	engineered mutation	UNP P42212
B	153	THR	MET	engineered mutation	UNP P42212
B	163	ALA	VAL	engineered mutation	UNP P42212
B	166	GLU	LYS	engineered mutation	UNP P42212
B	171	VAL	ILE	engineered mutation	UNP P42212
B	175	GLY	SER	engineered mutation	UNP P42212
B	192	SER	PRO	engineered mutation	UNP P42212
B	203	VAL	THR	engineered mutation	UNP P42212
B	205	VAL	SER	engineered mutation	UNP P42212
B	206	LYS	ALA	engineered mutation	UNP P42212
B	224	ARG	VAL	engineered mutation	UNP P42212
B	231	PRO	HIS	engineered mutation	UNP P42212

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	24	12	2	8	2	0	1
			Total	C	N	O	S		
2	A	1	12	6	1	4	1	0	0

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



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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	1	1	1	0	0
			Total	Cl		
4	B	3	3	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	210	210	210	0	0
			Total	O		
5	B	192	192	192	0	0

3 Residue-property plots (i)

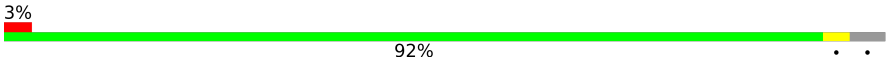
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

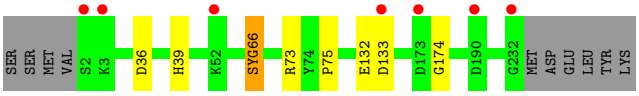
• Molecule 1: mKalama1

Chain A:

• Molecule 1: mKalama1

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.51Å 83.46Å 92.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.66 – 1.71 60.66 – 1.71	Depositor EDS
% Data completeness (in resolution range)	99.8 (60.66-1.71) 99.8 (60.66-1.71)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.37 (at 1.71Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.158 , 0.183 0.158 , 0.183	Depositor DCC
R_{free} test set	3421 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4288	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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: CSD, SO4, MES, GYS, 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	0.58	0/1898	0.72	0/2558
1	B	0.59	0/1934	0.74	0/2608
All	All	0.58	0/3832	0.73	0/5166

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	1890	0	1847	11	0
1	B	1926	0	1877	7	0
2	A	36	0	36	0	0
3	A	15	0	0	0	0
3	B	15	0	0	2	0
4	A	1	0	0	0	0
4	B	3	0	0	0	0
5	A	210	0	0	3	0
5	B	192	0	0	3	0
All	All	4288	0	3760	17	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 2.

All (17) 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:73[B]:ARG:NH1	3:B:302:SO4:O4	1.98	0.96
1:B:73[B]:ARG:NH1	3:B:302:SO4:S	2.53	0.82
1:B:36:ASP:OD1	5:B:538:HOH:O	2.09	0.69
1:B:174[A]:GLY:O	5:B:576:HOH:O	2.11	0.67
1:A:2:SER:HB2	1:A:5:GLU:H	1.64	0.63
1:A:115[A]:GLU:OE1	1:B:75:PRO:HG3	2.03	0.59
1:A:2:SER:N	1:A:5:GLU:OE2	2.45	0.49
1:A:184:GLN:OE1	1:A:186:THR:OG1	2.32	0.45
1:A:168[B]:ARG:NH2	5:A:587:HOH:O	2.26	0.45
1:A:2:SER:O	1:A:5:GLU:HG2	2.17	0.45
1:A:122:ARG:NH2	5:A:502:HOH:O	2.52	0.42
1:A:77:HIS:CD2	1:A:231:PRO:HA	2.55	0.42
1:A:70:CSD:OD2	1:A:84:PHE:HB3	2.20	0.41
1:A:22[A]:VAL:HG23	1:A:27:PHE:HE1	1.85	0.41
1:A:39:HIS:NE2	5:A:452:HOH:O	2.34	0.40
1:B:39:HIS:CE1	5:B:554:HOH:O	2.73	0.40
1:B:66:GYS:N2	1:B:66:GYS:HD1	2.36	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	232/239 (97%)	229 (99%)	3 (1%)	0	100	100
1	B	236/239 (99%)	233 (99%)	3 (1%)	0	100	100
All	All	468/478 (98%)	462 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	205/206 (100%)	202 (98%)	3 (2%)	65	49
1	B	208/206 (101%)	206 (99%)	2 (1%)	76	65
All	All	413/412 (100%)	408 (99%)	5 (1%)	69	58

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

Mol	Chain	Res	Type
1	A	3	LYS
1	A	132	GLU
1	A	157	GLN
1	B	132	GLU
1	B	133	ASP

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)

4 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	GYS	A	66	1	22,22,23	3.70	5 (22%)	27,30,32	2.73	7 (25%)
1	CSD	A	70	1	3,7,8	0.83	0	1,8,10	0.67	0
1	GYS	B	66	1	22,22,23	3.61	5 (22%)	27,30,32	3.07	9 (33%)
1	CSD	B	70	1	3,7,8	1.02	0	1,8,10	0.11	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	GYS	A	66	1	-	0/9/29/30	0/2/2/2
1	CSD	A	70	1	-	0/2/6/8	-
1	GYS	B	66	1	-	0/9/29/30	0/2/2/2
1	CSD	B	70	1	-	0/2/6/8	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	GYS	CB2-CA2	15.02	1.47	1.35
1	B	66	GYS	CB2-CA2	14.50	1.47	1.35
1	B	66	GYS	CA2-C2	-6.19	1.42	1.48
1	A	66	GYS	CA2-C2	-5.18	1.43	1.48
1	A	66	GYS	C1-N2	4.83	1.39	1.32
1	B	66	GYS	C1-N2	3.98	1.38	1.32
1	A	66	GYS	O2-C2	3.32	1.30	1.23
1	A	66	GYS	C2-N3	-3.26	1.32	1.39
1	B	66	GYS	C2-N3	-2.91	1.33	1.39
1	B	66	GYS	O2-C2	2.61	1.28	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	66	GYS	CA2-C2-N3	10.23	108.21	103.37
1	A	66	GYS	CA2-C2-N3	9.50	107.86	103.37
1	B	66	GYS	O2-C2-CA2	-9.02	125.89	130.96
1	A	66	GYS	O2-C2-CA2	-7.71	126.63	130.96
1	B	66	GYS	CG2-CB2-CA2	-3.21	126.01	129.94
1	A	66	GYS	CD2-CG2-CD1	3.20	122.37	117.64
1	B	66	GYS	O3-C3-CA3	-2.86	117.77	126.39
1	B	66	GYS	CD2-CG2-CD1	2.68	121.61	117.64
1	A	66	GYS	O3-C3-CA3	-2.62	118.49	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	66	GYS	CA1-C1-N3	-2.57	121.50	124.85
1	B	66	GYS	CE1-CD1-CG2	-2.48	118.01	121.25
1	A	66	GYS	CG2-CB2-CA2	-2.41	126.99	129.94
1	B	66	GYS	CD2-CG2-CB2	-2.29	113.43	121.22
1	A	66	GYS	CE1-CD1-CG2	-2.11	118.50	121.25
1	B	66	GYS	C2-N3-C1	-2.07	106.92	107.97
1	A	66	GYS	CD2-CG2-CB2	-2.05	114.24	121.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	70	CSD	1	0
1	B	66	GYS	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	SO4	A	303	-	4,4,4	0.24	0	6,6,6	0.18	0
2	MES	A	301[B]	-	12,12,12	2.91	2 (16%)	14,16,16	2.45	3 (21%)
2	MES	A	301[A]	-	12,12,12	2.83	2 (16%)	14,16,16	2.78	7 (50%)
3	SO4	A	304	-	4,4,4	0.18	0	6,6,6	0.35	0
3	SO4	B	303	-	4,4,4	0.17	0	6,6,6	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	B	302	-	4,4,4	0.20	0	6,6,6	0.15	0
3	SO4	A	305	-	4,4,4	0.15	0	6,6,6	0.26	0
2	MES	A	302	-	12,12,12	2.80	2 (16%)	14,16,16	2.61	5 (35%)
3	SO4	B	301	-	4,4,4	0.31	0	6,6,6	0.67	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
2	MES	A	301[B]	-	-	2/6/14/14	0/1/1/1
2	MES	A	302	-	-	2/6/14/14	0/1/1/1
2	MES	A	301[A]	-	-	2/6/14/14	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301[B]	MES	C8-S	-7.69	1.66	1.77
2	A	302	MES	C8-S	-7.54	1.66	1.77
2	A	301[A]	MES	C8-S	-7.26	1.67	1.77
2	A	301[A]	MES	O2S-S	6.33	1.63	1.45
2	A	301[B]	MES	O2S-S	6.32	1.63	1.45
2	A	302	MES	O2S-S	5.90	1.62	1.45

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301[B]	MES	C5-N4-C3	7.47	125.64	108.83
2	A	302	MES	C5-N4-C3	6.55	123.56	108.83
2	A	301[A]	MES	O1S-S-C8	5.71	113.80	106.92
2	A	301[A]	MES	C5-N4-C3	5.39	120.96	108.83
2	A	302	MES	O1S-S-C8	4.59	112.44	106.92
2	A	301[A]	MES	C7-N4-C3	3.55	120.30	111.23
2	A	302	MES	C7-N4-C3	3.30	119.68	111.23
2	A	301[B]	MES	O1S-S-C8	3.26	110.84	106.92
2	A	301[A]	MES	C7-N4-C5	2.93	118.72	111.23
2	A	301[A]	MES	C2-C3-N4	-2.86	105.77	110.10
2	A	301[A]	MES	O2S-S-C8	-2.78	103.56	106.92
2	A	301[B]	MES	C7-N4-C3	2.74	118.25	111.23
2	A	302	MES	O3S-S-C8	2.31	109.50	105.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301[A]	MES	C6-C5-N4	-2.19	106.78	110.10
2	A	302	MES	C7-N4-C5	2.06	116.51	111.23

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301[A]	MES	C8-C7-N4-C3
2	A	301[B]	MES	C8-C7-N4-C3
2	A	302	MES	C8-C7-N4-C3
2	A	301[A]	MES	C8-C7-N4-C5
2	A	302	MES	C8-C7-N4-C5
2	A	301[B]	MES	C7-C8-S-O3S

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	SO4	2	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	227/239 (94%)	-0.04	6 (2%)	56	60	16, 23, 43, 64	0
1	B	227/239 (94%)	-0.19	7 (3%)	49	53	15, 22, 41, 75	0
All	All	454/478 (94%)	-0.11	13 (2%)	51	56	15, 22, 43, 75	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	232	GLY	4.9
1	B	2	SER	4.3
1	A	231	PRO	3.7
1	A	232	GLY	3.6
1	B	3	LYS	3.4
1	B	173[A]	ASP	3.0
1	A	173	ASP	2.8
1	A	230	THR	2.8
1	B	133	ASP	2.8
1	B	52	LYS	2.6
1	A	133	ASP	2.4
1	B	190	ASP	2.3
1	A	2	SER	2.3

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, 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
1	GYS	A	66	21/22	0.97	0.09	15,17,21,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSD	A	70	8/9	0.98	0.10	15,17,26,30	0
1	GYS	B	66	21/22	0.98	0.07	14,16,20,25	0
1	CSD	B	70	8/9	0.98	0.07	17,19,27,30	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, 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
4	CL	B	306	1/1	0.88	0.07	60,60,60,60	0
2	MES	A	301[B]	12/12	0.89	0.20	24,34,42,43	12
2	MES	A	301[A]	12/12	0.89	0.20	26,34,39,39	12
4	CL	B	304	1/1	0.91	0.09	59,59,59,59	0
3	SO4	B	302	5/5	0.91	0.12	28,31,33,33	5
2	MES	A	302	12/12	0.93	0.16	16,24,29,32	12
3	SO4	B	303	5/5	0.93	0.12	31,32,33,43	0
4	CL	B	305	1/1	0.95	0.08	51,51,51,51	0
3	SO4	B	301	5/5	0.95	0.11	28,28,32,38	5
4	CL	A	306	1/1	0.96	0.04	58,58,58,58	0
3	SO4	A	304	5/5	0.99	0.08	25,29,30,35	5
3	SO4	A	305	5/5	0.99	0.06	23,23,25,26	5
3	SO4	A	303	5/5	0.99	0.09	24,26,31,32	0

6.5 Other polymers (i)

There are no such residues in this entry.