



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:09 AM UTC

PDB ID : 8A1I / pdb_00008a1i
Title : Crystal structure of murine Armc8 isoform beta
Authors : van gen Hassend, P.M.; Schindelin, H.
Deposited on : 2022-06-01
Resolution : 2.69 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

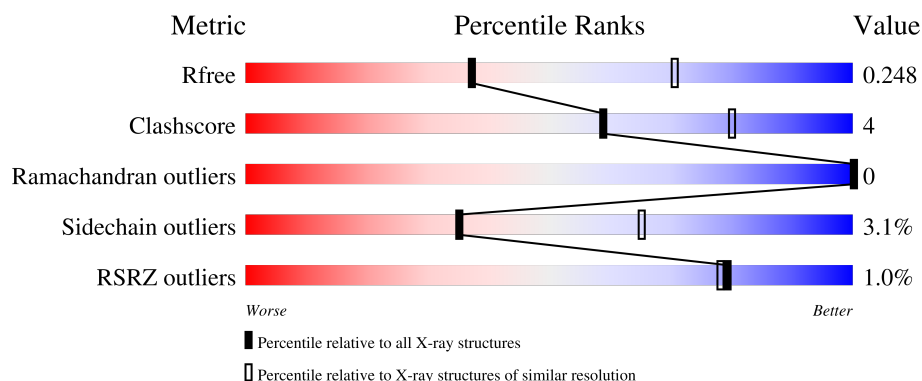
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	401	80% 12% • 8%
1	I	401	79% 11% 10%
1	P	401	79% 12% • 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17596 atoms, of which 8912 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 Isoform 2 of Armadillo repeat-containing protein 8.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	370	Total	C	H	N	O	S	Se	76	0	0
			5896	1844	2995	498	536	13	10			
1	I	360	Total	C	H	N	O	S	Se	75	0	0
			5708	1788	2896	480	521	13	10			
1	P	366	Total	C	H	N	O	S	Se	75	0	0
			5836	1826	2965	491	531	13	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	379	ILE	-	insertion	UNP Q9DBR3-2
A	380	ILE	-	insertion	UNP Q9DBR3-2
I	379	ILE	-	insertion	UNP Q9DBR3-2
I	380	ILE	-	insertion	UNP Q9DBR3-2
P	379	ILE	-	insertion	UNP Q9DBR3-2
P	380	ILE	-	insertion	UNP Q9DBR3-2

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

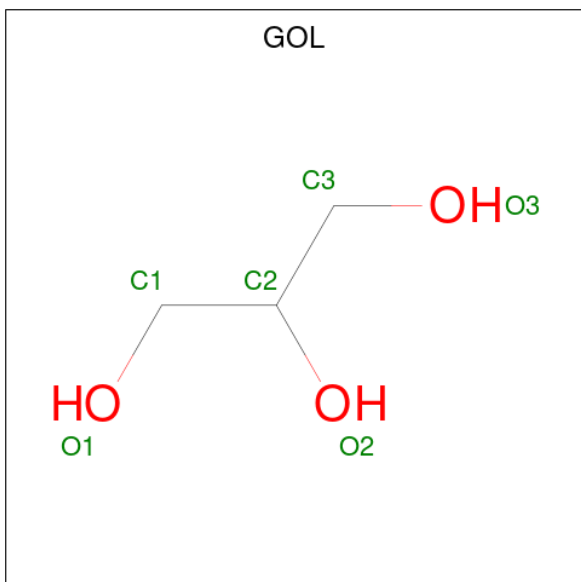


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	I	2	Total	Cl	0	0
			2	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 14 3 8 3	2	0
4	A	1	Total C H O 12 3 6 3	0	0
4	A	1	Total C H O 12 3 6 3	0	0
4	I	1	Total C H O 12 3 6 3	1	0
4	I	1	Total C H O 13 3 7 3	1	0
4	P	1	Total C H O 11 3 5 3	0	0
4	P	1	Total C H O 11 3 5 3	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	10	Total O 10 10	0	0
6	I	12	Total O 12 12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	16	Total	O	0	0
			16	16		

ARG
GLN
GLY
VAL
THR
SER
THR

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.64Å 148.18Å 67.14Å 90.00° 90.57° 90.00°	Depositor
Resolution (Å)	19.97 – 2.69 19.97 – 2.69	Depositor EDS
% Data completeness (in resolution range)	73.9 (19.97-2.69) 73.7 (19.97-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.214 , 0.248 0.220 , 0.248	Depositor DCC
R_{free} test set	1310 reflections (3.69%)	wwPDB-VP
Wilson B-factor (Å ²)	75.7	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.002 for l,k,-h 0.046 for h,-k,-l 0.027 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17596	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, GOL, CL, MES

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	0.20	0/2939	0.44	0/3964
1	I	0.19	0/2848	0.41	0/3842
1	P	0.20	0/2906	0.41	0/3918
All	All	0.20	0/8693	0.42	0/11724

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	2901	2995	2994	29	0
1	I	2812	2896	2891	25	0
1	P	2871	2965	2963	25	1
2	A	12	13	13	0	0
3	A	1	0	0	0	0
3	I	2	0	0	0	0
4	A	18	20	24	0	0
4	I	12	13	16	1	0
4	P	12	10	16	0	0
5	I	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	10	0	0	0	0
6	I	12	0	0	0	0
6	P	16	0	0	0	0
All	All	8684	8912	8917	78	1

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 (78) 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:I:298:VAL:HG23	1:I:360:ALA:HB2	1.60	0.83
1:A:248:LYS:HD2	1:A:252:MSE:HE3	1.68	0.75
1:I:308:ILE:HD11	1:I:315:GLN:HA	1.72	0.71
1:P:17:VAL:HG21	1:P:60:LEU:HD11	1.75	0.69
1:I:154:MSE:HE1	1:I:192:ASN:HB2	1.76	0.68
1:P:298:VAL:HG23	1:P:360:ALA:HB2	1.77	0.66
1:I:250:ILE:CG2	1:I:287:MSE:HE1	2.26	0.66
1:P:250:ILE:CG2	1:P:287:MSE:HE1	2.26	0.64
1:P:54:LYS:O	1:P:58:ILE:HG23	2.00	0.62
1:I:237:PRO:HG3	1:I:263:MSE:HE1	1.81	0.61
1:A:176:LYS:HB3	1:A:180:HIS:CE1	2.37	0.60
1:A:250:ILE:CG2	1:A:287:MSE:HE1	2.32	0.60
1:P:282:PRO:O	1:P:285:VAL:HG22	2.02	0.59
1:P:250:ILE:HG23	1:P:287:MSE:HE1	1.84	0.59
1:A:101:LEU:HB3	1:A:106:ILE:HD13	1.86	0.58
1:A:250:ILE:HG23	1:A:287:MSE:HE1	1.87	0.57
1:I:116:SER:O	1:I:122:ILE:HD11	2.05	0.56
1:I:277:VAL:HG23	1:I:278:LEU:HG	1.88	0.56
1:P:28:LEU:HD21	1:P:43:MSE:HE1	1.87	0.56
1:A:116:SER:O	1:A:122:ILE:HD11	2.06	0.55
1:P:197:LEU:HD12	1:P:236:LEU:HD11	1.88	0.54
1:P:27:ARG:NH2	1:P:42:ASP:OD2	2.41	0.54
1:A:282:PRO:O	1:A:285:VAL:HG22	2.09	0.53
1:A:257:ALA:O	1:A:261:THR:HG23	2.08	0.53
1:P:116:SER:O	1:P:122:ILE:HD11	2.08	0.53
1:A:239:ILE:HG22	1:A:243:MSE:HE2	1.89	0.53
1:A:180:HIS:HB3	1:A:183:ILE:HD12	1.91	0.52
1:P:285:VAL:HG21	1:P:321:THR:HG22	1.93	0.51
1:P:277:VAL:HG23	1:P:278:LEU:HG	1.92	0.51
1:P:28:LEU:CD2	1:P:43:MSE:HE1	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:254:LEU:HB2	1:I:287:MSE:HE2	1.93	0.49
1:I:334:TYR:HB2	1:I:335:PRO:HD3	1.94	0.49
1:A:197:LEU:HD12	1:A:236:LEU:HD11	1.95	0.49
1:A:101:LEU:O	1:A:106:ILE:HG23	2.12	0.49
1:I:239:ILE:HG22	1:I:243:MSE:HE2	1.93	0.49
1:I:250:ILE:HG22	1:I:287:MSE:HE1	1.95	0.49
1:P:143:LEU:O	1:P:143:LEU:HD23	2.13	0.49
1:I:209:LEU:HD13	1:I:243:MSE:HE1	1.93	0.48
1:A:144:TYR:CE2	1:A:180:HIS:HB2	2.48	0.48
1:I:154:MSE:HE1	1:I:192:ASN:CB	2.43	0.48
1:P:328:LEU:HD21	1:P:364:LEU:HD23	1.95	0.48
1:I:282:PRO:O	1:I:285:VAL:HG22	2.13	0.48
1:A:140:GLU:OE1	1:A:176:LYS:HB2	2.14	0.48
1:I:43:MSE:HE1	1:I:66:LEU:HD21	1.96	0.48
1:A:227:VAL:HG21	1:A:268:ALA:HB1	1.95	0.48
1:I:308:ILE:CD1	1:I:315:GLN:HA	2.43	0.47
1:I:257:ALA:O	1:I:261:THR:HG23	2.15	0.47
1:A:254:LEU:HB2	1:A:287:MSE:HE2	1.95	0.47
1:A:240:PHE:HD1	1:A:243:MSE:CE	2.28	0.47
1:I:107:ILE:HD12	1:I:142:LEU:HD13	1.98	0.46
1:A:227:VAL:CG2	1:A:268:ALA:HB1	2.46	0.46
1:P:107:ILE:HB	1:P:108:PRO:HD3	1.98	0.46
1:A:365:TYR:HE2	1:A:383:LEU:HD21	1.81	0.45
1:I:308:ILE:HG23	1:I:367:SER:HB3	1.99	0.45
1:A:37:LEU:O	1:A:40:VAL:HG12	2.17	0.45
1:A:119:LEU:HD23	1:P:35:LYS:HE2	1.99	0.44
1:P:56:ASN:O	1:P:60:LEU:HD13	2.18	0.44
1:I:214:VAL:HG22	4:I:504:GOL:H12	2.00	0.44
1:A:17:VAL:HG22	1:A:56:ASN:OD1	2.17	0.43
1:A:70:LEU:HD23	1:A:70:LEU:O	2.18	0.43
1:A:281:LEU:C	1:A:281:LEU:HD23	2.44	0.43
1:P:70:LEU:HD23	1:P:70:LEU:O	2.19	0.42
1:P:253:GLN:OE1	1:P:286:ARG:NH1	2.51	0.42
1:A:81:THR:O	1:A:85:VAL:HG23	2.19	0.42
1:P:220:PRO:O	1:P:224:MSE:HG2	2.18	0.42
1:I:225:THR:O	1:I:229:VAL:HG23	2.19	0.42
1:I:281:LEU:HB3	1:I:282:PRO:HD3	2.01	0.42
1:A:277:VAL:HG23	1:A:278:LEU:HG	2.02	0.42
1:P:182:THR:HG22	1:P:186:ASN:OD1	2.20	0.41
1:A:150:ILE:HB	1:A:151:PRO:HD3	2.02	0.41
1:I:273:ASP:OD1	1:I:274:SER:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:55:ALA:O	1:P:59:VAL:HG13	2.20	0.41
1:A:203:LYS:HE3	1:A:203:LYS:H	1.86	0.41
1:A:143:LEU:O	1:A:143:LEU:HD23	2.21	0.41
1:I:28:LEU:HD11	1:I:43:MSE:HE2	2.03	0.41
1:I:133:PHE:CD1	1:I:174:CYS:SG	3.14	0.41
1:P:241:VAL:HG13	1:P:279:LYS:HG2	2.02	0.40
1:P:34:GLN:CD	1:P:34:GLN:C	2.89	0.40

All (1) 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:P:16:GLU:OE1	1:P:378:LYS:NZ[1_556]	2.13	0.07

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	366/401 (91%)	364 (100%)	2 (0%)	0	100	100
1	I	356/401 (89%)	352 (99%)	4 (1%)	0	100	100
1	P	362/401 (90%)	359 (99%)	3 (1%)	0	100	100
All	All	1084/1203 (90%)	1075 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	329/344 (96%)	317 (96%)	12 (4%)	31	60
1	I	318/344 (92%)	311 (98%)	7 (2%)	45	74
1	P	325/344 (94%)	314 (97%)	11 (3%)	32	62
All	All	972/1032 (94%)	942 (97%)	30 (3%)	35	65

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	44	LYS
1	A	92	MSE
1	A	130	ARG
1	A	180	HIS
1	A	203	LYS
1	A	209	LEU
1	A	222	VAL
1	A	246	ARG
1	A	252	MSE
1	A	292	ARG
1	A	344	ILE
1	I	51	ASN
1	I	130	ARG
1	I	222	VAL
1	I	230	LEU
1	I	292	ARG
1	I	333	LYS
1	I	358	ARG
1	P	17	VAL
1	P	34	GLN
1	P	60	LEU
1	P	73	GLU
1	P	130	ARG
1	P	159	ARG
1	P	219	ASN
1	P	222	VAL
1	P	292	ARG
1	P	346	ARG
1	P	347	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	GLN
1	A	192	ASN
1	A	195	HIS
1	A	207	GLN
1	A	238	GLN
1	A	355	HIS
1	I	355	HIS
1	P	51	ASN
1	P	187	HIS
1	P	195	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 3 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	$\# Z > 2$
4	GOL	I	504	-	5,5,5	0.94	0	5,5,5	1.02	0
4	GOL	P	501	-	5,5,5	0.89	0	5,5,5	1.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	P	502	-	5,5,5	0.90	0	5,5,5	1.06	0
4	GOL	A	503	-	5,5,5	1.01	0	5,5,5	1.00	0
4	GOL	A	504	-	5,5,5	1.02	0	5,5,5	0.98	0
2	MES	A	501	-	12,12,12	2.18	1 (8%)	15,16,16	1.44	2 (13%)
4	GOL	A	505	-	5,5,5	0.97	0	5,5,5	0.90	0
5	SO4	I	503	-	4,4,4	0.24	0	6,6,6	0.11	0
4	GOL	I	505	-	5,5,5	1.04	0	5,5,5	1.03	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
4	GOL	I	504	-	-	1/4/4/4	-
4	GOL	P	501	-	-	0/4/4/4	-
4	GOL	P	502	-	-	0/4/4/4	-
4	GOL	A	503	-	-	0/4/4/4	-
4	GOL	A	504	-	-	2/4/4/4	-
2	MES	A	501	-	-	1/6/14/14	0/1/1/1
4	GOL	A	505	-	-	2/4/4/4	-
4	GOL	I	505	-	-	1/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	MES	C8-S	-7.24	1.67	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	MES	C5-N4-C3	2.54	114.31	108.84
2	A	501	MES	O1S-S-C8	2.47	110.47	106.73

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	505	GOL	O1-C1-C2-C3
4	A	505	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	I	504	GOL	O1-C1-C2-O2
4	I	505	GOL	O2-C2-C3-O3
4	A	504	GOL	O1-C1-C2-C3
2	A	501	MES	N4-C7-C8-S
4	A	504	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	504	GOL	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	360/401 (89%)	-0.02	3 (0%) 82 81	49, 86, 141, 190	0
1	I	350/401 (87%)	-0.07	5 (1%) 73 72	51, 90, 144, 227	0
1	P	356/401 (88%)	-0.04	3 (0%) 82 81	54, 86, 134, 185	0
All	All	1066/1203 (88%)	-0.04	11 (1%) 79 78	49, 87, 142, 227	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	14	LEU	3.0
1	I	47	VAL	2.6
1	I	71	GLN	2.4
1	I	334	TYR	2.3
1	A	215	LEU	2.3
1	I	70	LEU	2.3
1	P	334	TYR	2.3
1	A	178	PRO	2.2
1	I	72	GLN	2.2
1	A	175	CYS	2.1
1	P	35	LYS	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 oligosaccharides 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	GOL	A	503	6/6	0.72	0.14	93,112,117,117	2
2	MES	A	501	12/12	0.73	0.12	120,130,152,156	0
4	GOL	I	505	6/6	0.81	0.12	89,93,112,112	1
4	GOL	I	504	6/6	0.82	0.12	95,98,118,118	1
4	GOL	A	504	6/6	0.82	0.08	97,100,121,121	0
4	GOL	P	501	6/6	0.82	0.11	106,108,130,130	0
4	GOL	P	502	6/6	0.83	0.11	84,85,102,103	0
5	SO4	I	503	5/5	0.83	0.07	120,121,122,122	0
3	CL	A	502	1/1	0.86	0.09	89,89,89,89	0
4	GOL	A	505	6/6	0.88	0.16	74,75,90,90	0
3	CL	I	501	1/1	0.91	0.07	89,89,89,89	0
3	CL	I	502	1/1	0.96	0.10	84,84,84,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.