



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:22 PM UTC

PDB ID : 2E4Z / pdb_00002e4z
Title : Crystal structure of the ligand-binding region of the group III metabotropic glutamate receptor
Authors : Muto, T.; Tsuchiya, D.; Morikawa, K.; Jingami, H.
Deposited on : 2006-12-17
Resolution : 3.30 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

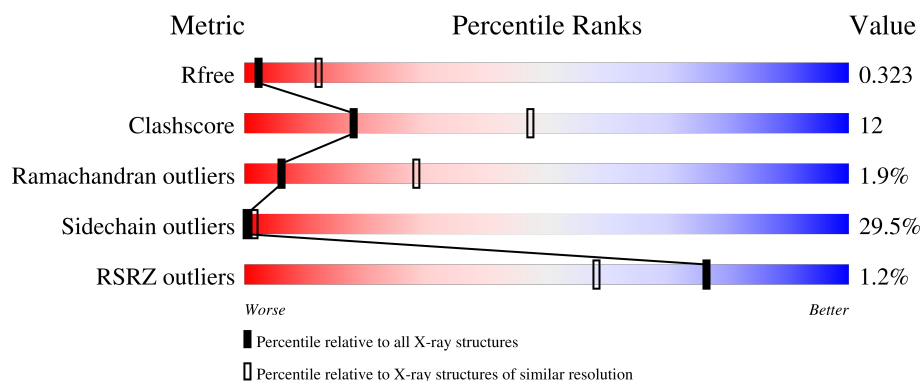
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	501	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3305 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 Metabotropic glutamate receptor 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	434	3293	2082	565	631	15	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	522	LEU	-	cloning artifact	UNP P35400
A	523	VAL	-	cloning artifact	UNP P35400
A	524	PRO	-	cloning artifact	UNP P35400
A	525	ARG	-	cloning artifact	UNP P35400
A	526	GLY	-	cloning artifact	UNP P35400
A	527	SER	-	cloning artifact	UNP P35400
A	528	HIS	-	expression tag	UNP P35400
A	529	HIS	-	expression tag	UNP P35400
A	530	HIS	-	expression tag	UNP P35400
A	531	HIS	-	expression tag	UNP P35400
A	532	HIS	-	expression tag	UNP P35400
A	533	HIS	-	expression tag	UNP P35400

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).

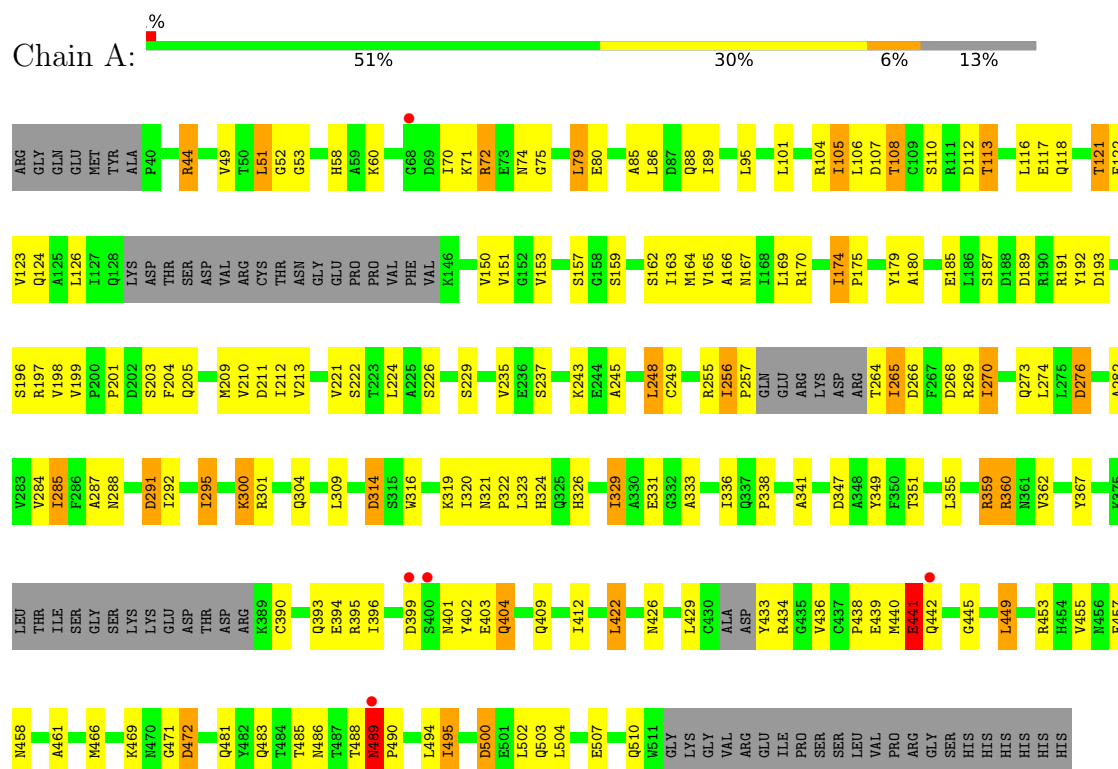


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	12	6	1	4	1	0	0

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: Metabotropic glutamate receptor 7



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.43Å 92.43Å 114.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	12.00 – 3.30 12.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (12.00-3.30) 97.5 (12.00-3.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.270 , 0.324 0.265 , 0.323	Depositor DCC
R_{free} test set	625 reflections (7.05%)	wwPDB-VP
Wilson B-factor (Å ²)	98.0	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 69.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.041 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3305	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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: 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	0.45	0/3364	0.86	0/4579

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	3293	0	3095	78	0
2	A	12	0	13	0	0
All	All	3305	0	3108	78	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 (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:A:453:ARG:NH1	1:A:471:GLY:HA3	1.85	0.91
1:A:453:ARG:NH1	1:A:471:GLY:CA	2.38	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LEU:HD21	1:A:105:ILE:HG21	1.58	0.83
1:A:453:ARG:HH12	1:A:471:GLY:HA3	1.43	0.82
1:A:79:LEU:CD2	1:A:105:ILE:HG21	2.19	0.73
1:A:341:ALA:HB3	1:A:461:ALA:HB1	1.74	0.69
1:A:201:PRO:HD3	1:A:472:ASP:HB3	1.77	0.67
1:A:481:GLN:HB3	1:A:495:ILE:HG12	1.75	0.67
1:A:449:LEU:CD2	1:A:453:ARG:HE	2.08	0.67
1:A:453:ARG:HH11	1:A:471:GLY:CA	2.06	0.66
1:A:486:ASN:O	1:A:489:ASN:ND2	2.29	0.65
1:A:489:ASN:C	1:A:489:ASN:HD22	2.02	0.65
1:A:224:LEU:HD23	1:A:285:ILE:HG23	1.78	0.64
1:A:75:GLY:O	1:A:79:LEU:HB2	2.01	0.60
1:A:189:ASP:O	1:A:193:ASP:HB3	2.01	0.60
1:A:287:ALA:HB1	1:A:291:ASP:HB3	1.85	0.59
1:A:165:VAL:C	1:A:167:ASN:H	2.10	0.58
1:A:213:VAL:HG11	1:A:248:LEU:HD13	1.84	0.58
1:A:44:ARG:HG3	1:A:104:ARG:HH11	1.68	0.58
1:A:453:ARG:HH11	1:A:471:GLY:HA2	1.68	0.58
1:A:300:LYS:HB2	1:A:329:ILE:HG12	1.86	0.56
1:A:399:ASP:HB2	1:A:402:TYR:O	2.06	0.56
1:A:108:THR:HG22	1:A:110:SER:H	1.70	0.55
1:A:72:ARG:HB3	1:A:367:TYR:HE1	1.72	0.54
1:A:481:GLN:HG2	1:A:483:GLN:HE21	1.72	0.54
1:A:170:ARG:NH1	1:A:193:ASP:OD2	2.40	0.54
1:A:58:HIS:HD2	1:A:107:ASP:OD1	1.89	0.54
1:A:409:GLN:HE21	1:A:461:ALA:HB3	1.73	0.54
1:A:270:ILE:HG21	1:A:295:ILE:HD11	1.90	0.53
1:A:123:VAL:HG13	1:A:126:LEU:HD12	1.90	0.53
1:A:193:ASP:O	1:A:449:LEU:HD11	2.08	0.53
1:A:157:SER:HB2	1:A:179:TYR:HE1	1.75	0.51
1:A:438:PRO:HA	1:A:441:GLU:HB2	1.93	0.51
1:A:449:LEU:HD22	1:A:453:ARG:HE	1.75	0.51
1:A:80:GLU:HG3	1:A:349:TYR:HE2	1.75	0.50
1:A:273:GLN:O	1:A:276:ASP:HB2	2.12	0.50
1:A:175:PRO:HD3	1:A:445:GLY:HA3	1.93	0.49
1:A:445:GLY:O	1:A:449:LEU:HB2	2.12	0.49
1:A:489:ASN:N	1:A:490:PRO:CD	2.76	0.49
1:A:324:HIS:C	1:A:326:HIS:H	2.22	0.48
1:A:151:VAL:HG11	1:A:422:LEU:HD21	1.96	0.47
1:A:314:ASP:HB2	1:A:338:PRO:HD3	1.95	0.47
1:A:489:ASN:ND2	1:A:489:ASN:C	2.71	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:SER:HB2	1:A:179:TYR:CE1	2.49	0.47
1:A:212:ILE:HG12	1:A:504:LEU:HD13	1.96	0.47
1:A:52:GLY:HA3	1:A:153:VAL:HG22	1.97	0.46
1:A:265:ILE:H	1:A:265:ILE:HG13	1.52	0.46
1:A:209:MET:HE2	1:A:284:VAL:HG13	1.98	0.46
1:A:329:ILE:H	1:A:329:ILE:HG13	1.36	0.46
1:A:321:ASN:N	1:A:322:PRO:HD2	2.30	0.45
1:A:300:LYS:HE2	1:A:301:ARG:HG3	1.99	0.45
1:A:122:PHE:HA	1:A:150:VAL:HG21	1.98	0.44
1:A:44:ARG:CG	1:A:104:ARG:HH11	2.29	0.44
1:A:211:ASP:HB3	1:A:502:LEU:HD22	1.99	0.44
1:A:53:GLY:HA3	1:A:105:ILE:HG13	1.99	0.43
1:A:85:ALA:HB2	1:A:412:ILE:HG12	2.00	0.43
1:A:489:ASN:N	1:A:490:PRO:HD3	2.32	0.43
1:A:108:THR:HG22	1:A:110:SER:N	2.33	0.43
1:A:113:THR:O	1:A:117:GLU:HG3	2.18	0.43
1:A:163:ILE:HG23	1:A:192:TYR:CE2	2.53	0.43
1:A:165:VAL:C	1:A:167:ASN:N	2.74	0.43
1:A:285:ILE:HD13	1:A:316:TRP:HZ3	1.83	0.43
1:A:393:GLN:C	1:A:395:ARG:H	2.27	0.43
1:A:106:LEU:HD22	1:A:118:GLN:HE21	1.84	0.43
1:A:256:ILE:HA	1:A:257:PRO:HD3	1.84	0.43
1:A:157:SER:HA	1:A:180:ALA:HB3	2.00	0.43
1:A:282:ALA:HA	1:A:309:LEU:HB2	2.00	0.42
1:A:359:ARG:O	1:A:360:ARG:C	2.62	0.42
1:A:80:GLU:HG3	1:A:349:TYR:CE2	2.53	0.42
1:A:51:LEU:HD13	1:A:101:LEU:HD13	2.00	0.42
1:A:204:PHE:CD1	1:A:204:PHE:N	2.87	0.41
1:A:169:LEU:HB3	1:A:174:ILE:HB	2.03	0.41
1:A:333:ALA:O	1:A:481:GLN:HA	2.20	0.41
1:A:204:PHE:N	1:A:204:PHE:HD1	2.19	0.41
1:A:440:MET:O	1:A:442:GLN:N	2.53	0.41
1:A:44:ARG:HG3	1:A:104:ARG:HD3	2.03	0.41
1:A:121:THR:C	1:A:123:VAL:H	2.27	0.40
1:A:288:ASN:ND2	1:A:291:ASP:HB2	2.37	0.40

There are no symmetry-related clashes.

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	424/501 (85%)	378 (89%)	38 (9%)	8 (2%)	6	28

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	ALA
1	A	441	GLU
1	A	500	ASP
1	A	404	GLN
1	A	485	THR
1	A	245	ALA
1	A	360	ARG
1	A	489	ASN

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	339/425 (80%)	239 (70%)	100 (30%)	0	2

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	49	VAL
1	A	51	LEU

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Mol	Chain	Res	Type
1	A	60	LYS
1	A	70	ILE
1	A	71	LYS
1	A	72	ARG
1	A	74	ASN
1	A	79	LEU
1	A	86	LEU
1	A	88	GLN
1	A	89	ILE
1	A	95	LEU
1	A	105	ILE
1	A	108	THR
1	A	112	ASP
1	A	113	THR
1	A	116	LEU
1	A	121	THR
1	A	124	GLN
1	A	159	SER
1	A	162	SER
1	A	164	MET
1	A	174	ILE
1	A	185	GLU
1	A	187	SER
1	A	191	ARG
1	A	196	SER
1	A	197	ARG
1	A	198	VAL
1	A	199	VAL
1	A	203	SER
1	A	205	GLN
1	A	210	VAL
1	A	221	VAL
1	A	222	SER
1	A	226	SER
1	A	229	SER
1	A	235	VAL
1	A	237	SER
1	A	243	LYS
1	A	248	LEU
1	A	249	CYS
1	A	255	ARG
1	A	256	ILE

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Mol	Chain	Res	Type
1	A	264	THR
1	A	265	ILE
1	A	266	ASP
1	A	268	ASP
1	A	269	ARG
1	A	270	ILE
1	A	274	LEU
1	A	276	ASP
1	A	285	ILE
1	A	291	ASP
1	A	292	ILE
1	A	295	ILE
1	A	300	LYS
1	A	304	GLN
1	A	314	ASP
1	A	319	LYS
1	A	320	ILE
1	A	323	LEU
1	A	329	ILE
1	A	331	GLU
1	A	336	ILE
1	A	347	ASP
1	A	351	THR
1	A	355	LEU
1	A	359	ARG
1	A	362	VAL
1	A	390	CYS
1	A	394	GLU
1	A	396	ILE
1	A	401	ASN
1	A	403	GLU
1	A	404	GLN
1	A	422	LEU
1	A	426	ASN
1	A	429	LEU
1	A	433	TYR
1	A	434	ARG
1	A	436	VAL
1	A	439	GLU
1	A	441	GLU
1	A	449	LEU
1	A	455	VAL

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Mol	Chain	Res	Type
1	A	457	PHE
1	A	458	ASN
1	A	466	MET
1	A	469	LYS
1	A	472	ASP
1	A	488	THR
1	A	489	ASN
1	A	494	LEU
1	A	495	ILE
1	A	500	ASP
1	A	503	GLN
1	A	507	GLU
1	A	510	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	74	ASN
1	A	77	HIS
1	A	88	GLN
1	A	118	GLN
1	A	294	GLN
1	A	321	ASN
1	A	326	HIS
1	A	409	GLN
1	A	426	ASN
1	A	483	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is 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	MES	A	1001	-	12,12,12	1.21	1 (8%)	15,16,16	1.38	2 (13%)

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	1001	-	-	3/6/14/14	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	MES	C8-S	3.64	1.82	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	MES	O2S-S-C8	3.69	112.31	106.73
2	A	1001	MES	O3S-S-C8	2.06	110.04	106.00

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	MES	C7-C8-S-O3S
2	A	1001	MES	C7-C8-S-O1S
2	A	1001	MES	C7-C8-S-O2S

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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 [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	434/501 (86%)	-0.34	5 (1%) 76 58	16, 40, 61, 74	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	442	GLN	3.0
1	A	400	SER	2.7
1	A	489	ASN	2.5
1	A	399	ASP	2.3
1	A	68	GLY	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 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
2	MES	A	1001	12/12	0.79	0.09	56,71,88,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.