



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:18 AM GMT

PDB ID : 3LMK  
Title : Ligand Binding Domain of Metabotropic glutamate receptor mGluR5 complexed with glutamate  
Authors : Dobrovetsky, E.; Khutoreskaya, G.; Seitova, A.; Cossar, D.; Edwards, A.M.; Arrowsmith, C.H.; Bountra, C.; Weigelt, J.; Bochkarev, A.; Structural Genomics Consortium (SGC)  
Deposited on : 2010-01-30  
Resolution : 2.44 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

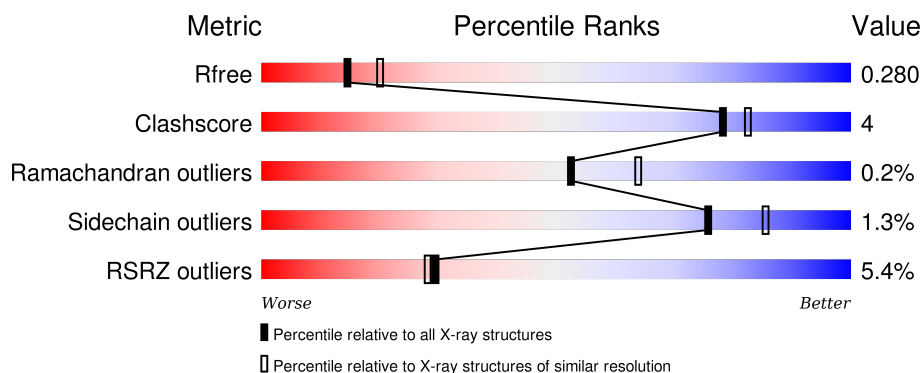
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.44 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))
$R_{free}$	91344	1003 (2.46-2.42)
Clashscore	102246	1071 (2.46-2.42)
Ramachandran outliers	100387	1065 (2.46-2.42)
Sidechain outliers	100360	1065 (2.46-2.42)
RSRZ outliers	91569	1005 (2.46-2.42)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	492	<div> <div>5%</div> <div>80%</div> <div>8%</div> <div>11%</div> </div>
1	B	492	<div> <div>4%</div> <div>81%</div> <div>9%</div> <div>11%</div> </div>

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
2	NAG	B	1	X	-	-	-
4	MG	A	508	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6884 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 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3352	2127	576	621	28			
1	B	439	Total	C	N	O	S	0	0	0
			3392	2152	577	635	28			

There are 10 discrepancies between the modelled and reference sequences:

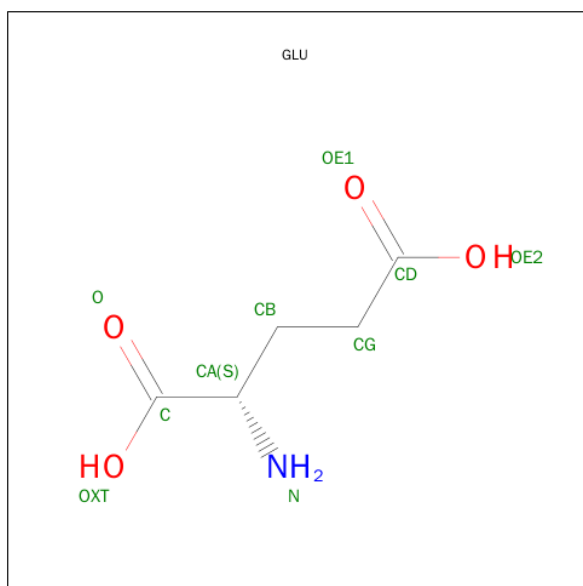
Chain	Residue	Modelled	Actual	Comment	Reference
A	14	GLY	-	EXPRESSION TAG	UNP P41594
A	15	ALA	-	EXPRESSION TAG	UNP P41594
A	16	MET	-	EXPRESSION TAG	UNP P41594
A	17	ASP	-	EXPRESSION TAG	UNP P41594
A	241	SER	CYS	ENGINEERED	UNP P41594
B	14	GLY	-	EXPRESSION TAG	UNP P41594
B	15	ALA	-	EXPRESSION TAG	UNP P41594
B	16	MET	-	EXPRESSION TAG	UNP P41594
B	17	ASP	-	EXPRESSION TAG	UNP P41594
B	241	SER	CYS	ENGINEERED	UNP P41594

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is GLUTAMIC ACID (three-letter code: GLU) (formula:  $C_5H_9NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	5	1	4		
3	B	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Mg 1	0	0
4	A	2	Total 2	Mg 2	0	0

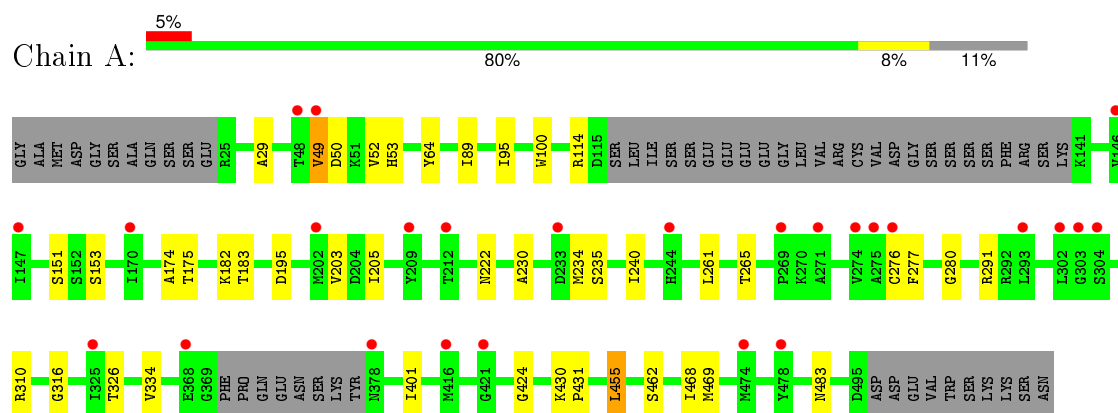
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	35	Total 35	O 35	0	0
5	B	54	Total 54	O 54	0	0

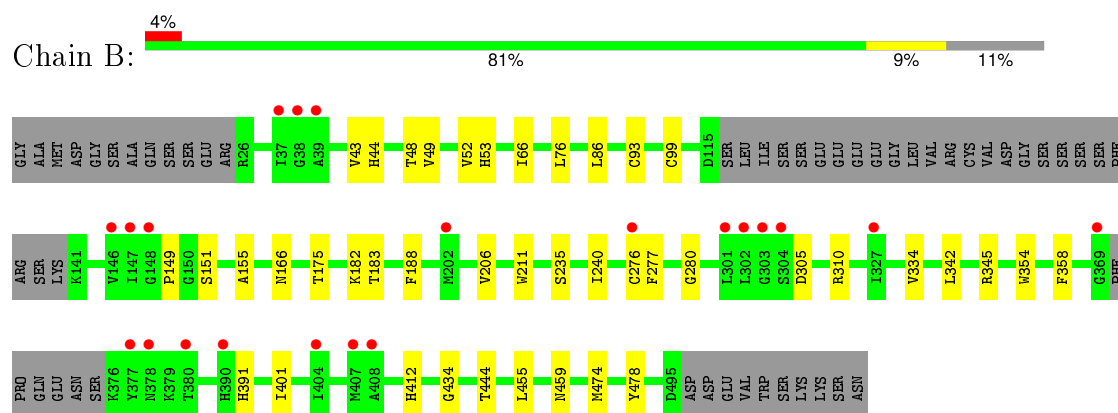
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 5



- Molecule 1: Metabotropic glutamate receptor 5



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.88Å 98.35Å 155.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.08 – 2.44 24.59 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.3 (83.08-2.44) 99.5 (24.59-2.44)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 2.44Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.232 , 0.281 0.229 , 0.280	Depositor DCC
$R_{free}$ test set	2095 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.8	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 45.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 41502 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6884	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, NAG

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	0.43	0/3425	0.55	0/4636
1	B	0.44	0/3467	0.56	0/4692
All	All	0.43	0/6892	0.56	0/9328

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	3352	0	3183	27	0
1	B	3392	0	3233	23	0
2	A	14	0	13	1	0
2	B	14	0	13	0	0
3	A	10	0	5	2	0
3	B	10	0	5	2	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
5	A	35	0	0	0	0
5	B	54	0	0	0	0
All	All	6884	0	6452	48	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 (48) 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:175:THR:HG1	3:B:507:GLU:N	1.92	0.66
1:A:455:LEU:HD11	2:A:1:NAG:H82	1.83	0.59
1:A:29:ALA:HB3	1:A:95:ILE:HB	1.88	0.56
1:A:175:THR:HG1	3:A:506:GLU:N	2.05	0.55
1:A:205:ILE:HD11	1:A:468:ILE:HG12	1.88	0.54
1:A:153:SER:HB3	1:A:222:ASN:H	1.72	0.54
1:A:203:VAL:HG21	1:A:234:MET:HB3	1.90	0.54
1:A:89:ILE:HG13	1:A:424:GLY:HA2	1.91	0.53
1:A:280:GLY:HA3	1:A:310:ARG:NH1	2.24	0.52
1:B:334:VAL:HG11	1:B:401:ILE:HD12	1.92	0.52
1:B:474:MET:HB2	1:B:478:TYR:CD2	2.46	0.51
1:A:53:HIS:NE2	1:B:183:THR:HA	2.26	0.51
1:A:230:ALA:O	1:A:234:MET:HB2	2.11	0.50
1:B:444:THR:O	1:B:455:LEU:HA	2.12	0.48
1:A:183:THR:HA	1:B:53:HIS:NE2	2.29	0.48
1:B:235:SER:HB2	1:B:240:ILE:HB	1.95	0.48
1:B:182:LYS:HE3	1:B:188:PHE:O	2.14	0.48
1:B:166:ASN:O	1:B:434:GLY:HA3	2.13	0.48
1:B:43:VAL:HG11	1:B:354:TRP:CG	2.50	0.47
1:B:206:VAL:HG13	1:B:211:TRP:HB2	1.96	0.47
1:A:326:THR:OG1	1:A:469:MET:HB2	2.16	0.46
1:B:182:LYS:HE2	1:B:459:ASN:O	2.14	0.46
1:B:149:PRO:HD2	1:B:155:ALA:HA	1.96	0.46
1:A:334:VAL:HG21	1:A:401:ILE:HD12	1.97	0.45
1:B:76:LEU:HD11	1:B:93:CYS:HB3	1.99	0.45
1:A:291:ARG:NH2	1:A:316:GLY:O	2.46	0.45
1:A:430:LYS:HA	1:A:431:PRO:HA	1.80	0.45
1:A:114:ARG:O	1:A:114:ARG:HG3	2.18	0.44
1:B:334:VAL:HG11	1:B:401:ILE:CD1	2.48	0.44
1:B:305:ASP:OD2	3:B:507:GLU:HG3	2.17	0.44
1:A:174:ALA:HA	3:A:506:GLU:O	2.18	0.43
1:B:86:LEU:HG	1:B:412:HIS:HB2	1.99	0.43
1:A:100:TRP:CE2	1:A:151:SER:HB2	2.53	0.43
1:A:182:LYS:HA	1:A:182:LYS:HE2	2.01	0.43
1:A:469:MET:HE2	1:A:483:ASN:HA	2.01	0.43
1:A:100:TRP:CZ2	1:A:151:SER:HB2	2.54	0.42
1:A:175:THR:O	1:A:195:ASP:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:LEU:HD21	1:B:391:HIS:CG	2.55	0.42
1:A:49:VAL:HA	1:A:50:ASP:HA	1.64	0.42
1:A:64:TYR:HE1	1:A:310:ARG:HD3	1.85	0.42
1:A:261:LEU:O	1:A:265:THR:HG23	2.19	0.42
1:B:182:LYS:HD3	1:B:182:LYS:HA	1.73	0.41
1:A:235:SER:HB2	1:A:240:ILE:HB	2.02	0.41
1:B:66:ILE:HG13	1:B:358:PHE:CG	2.55	0.41
1:B:44:HIS:O	1:B:99:CYS:HA	2.21	0.41
1:B:280:GLY:HA3	1:B:310:ARG:NH1	2.36	0.41
1:A:100:TRP:CD1	1:A:100:TRP:O	2.74	0.40
1:B:48:THR:O	1:B:52:VAL:HG23	2.21	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	432/492 (88%)	411 (95%)	20 (5%)	1 (0%)	52	64
1	B	433/492 (88%)	414 (96%)	18 (4%)	1 (0%)	52	64
All	All	865/984 (88%)	825 (95%)	38 (4%)	2 (0%)	52	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	VAL
1	B	49	VAL

### 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	343/424 (81%)	338 (98%)	5 (2%)	72	83
1	B	354/424 (84%)	350 (99%)	4 (1%)	80	87
All	All	697/848 (82%)	688 (99%)	9 (1%)	76	85

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	276	CYS
1	A	277	PHE
1	A	455	LEU
1	A	462	SER
1	B	151	SER
1	B	276	CYS
1	B	277	PHE
1	B	345	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	160	ASN
1	A	218	HIS
1	B	88	ASN
1	B	157	GLN
1	B	166	ASN
1	B	244	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	$\# Z  > 2$
2	NAG	A	1	1	14,14,15	0.51	0	15,19,21	1.20	1 (6%)
3	GLU	A	506	-	3,9,9	0.14	0	2,11,11	0.19	0
2	NAG	B	1	1	14,14,15	0.64	0	15,19,21	2.18	2 (13%)
3	GLU	B	507	-	3,9,9	0.48	0	2,11,11	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
2	NAG	A	1	1	-	0/6/23/26	0/1/1/1
3	GLU	A	506	-	-	0/3/9/9	0/0/0/0
2	NAG	B	1	1	1/1/5/7	0/6/23/26	0/1/1/1
3	GLU	B	507	-	-	0/3/9/9	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C3-C2-N2	3.30	118.45	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAG	C1-O5-C5	3.59	116.81	112.25
2	B	1	NAG	C2-N2-C7	6.86	131.86	123.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	NAG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NAG	1	0
3	A	506	GLU	2	0
3	B	507	GLU	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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	438/492 (89%)	0.28	26 (5%) 26 23	23, 33, 44, 50	1 (0%)
1	B	439/492 (89%)	0.11	21 (4%) 34 33	22, 30, 44, 50	1 (0%)
All	All	877/984 (89%)	0.19	47 (5%) 29 28	22, 32, 44, 50	2 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	276	CYS	12.0
1	B	276	CYS	10.8
1	A	302	LEU	5.1
1	A	275	ALA	4.5
1	B	147	ILE	4.3
1	A	303	GLY	3.9
1	A	474	MET	3.9
1	B	302	LEU	3.7
1	A	271	ALA	3.2
1	B	146	VAL	3.2
1	B	39	ALA	3.1
1	B	38	GLY	3.0
1	A	48	THR	3.0
1	A	304	SER	3.0
1	A	233	ASP	2.9
1	B	202	MET	2.9
1	A	244	HIS	2.9
1	B	390	HIS	2.8
1	B	377	TYR	2.8
1	B	378	ASN	2.8
1	A	368	GLU	2.7
1	A	212	THR	2.7
1	A	293	LEU	2.7
1	A	49	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	327	ILE	2.6
1	B	303	GLY	2.6
1	B	37	ILE	2.6
1	A	325	ILE	2.5
1	A	478	TYR	2.4
1	B	408	ALA	2.4
1	A	146	VAL	2.4
1	B	304	SER	2.4
1	B	148	GLY	2.4
1	A	378	ASN	2.3
1	B	301	LEU	2.3
1	A	147	ILE	2.2
1	B	380	THR	2.2
1	B	407	MET	2.2
1	B	369	GLY	2.1
1	A	416	MET	2.1
1	A	274	VAL	2.1
1	A	209	TYR	2.1
1	A	421	GLY	2.1
1	B	404	ILE	2.1
1	A	269	PRO	2.0
1	A	202	MET	2.0
1	A	170	ILE	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	A	508	1/1	0.97	0.18	2.28	46,46,46,46	0
4	MG	B	506	1/1	0.92	0.17	0.67	64,64,64,64	0
3	GLU	A	506	10/10	0.95	0.12	-0.24	35,35,37,37	0
4	MG	A	507	1/1	0.69	0.09	-1.66	74,74,74,74	0
3	GLU	B	507	10/10	0.98	0.09	-1.80	31,32,34,36	0
2	NAG	B	1	14/15	0.79	0.32	-	67,73,74,74	0
2	NAG	A	1	14/15	0.87	0.30	-	65,70,71,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.