



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 08:34 PM BST

PDB ID : 6N4X
Title : Metabotropic Glutamate Receptor 5 Apo Form Ligand Binding Domain
Authors : Koehl, A.; Hu, H.; Feng, D.; Sun, B.; Weis, W.I.; Skiniotis, G.S.; Mathiesen, J.M.; Kobilka, B.K.
Deposited on : 2018-11-20
Resolution : 4.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) 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	:	2.13.1
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)	:	2.13.1

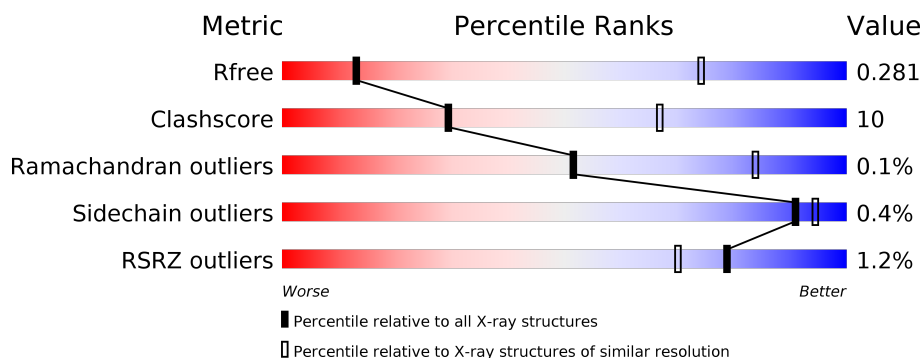
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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 ≥ 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	877	<div> <div>%</div> <div> <div></div> <div>45%</div> <div>13%</div> <div>42%</div> </div> </div>
1	B	877	<div> <div>%</div> <div> <div></div> <div>43%</div> <div>13%</div> <div>44%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7736 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	506	Total	C	N	O	S	0	0	0
			3897	2456	666	739	36			
1	B	487	Total	C	N	O	S	0	0	0
			3754	2362	646	712	34			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP P41594
A	-4	LYS	-	expression tag	UNP P41594
A	-3	THR	-	expression tag	UNP P41594
A	-2	ILE	-	expression tag	UNP P41594
A	-1	ILE	-	expression tag	UNP P41594
A	0	ALA	-	expression tag	UNP P41594
A	1	LEU	-	expression tag	UNP P41594
A	2	SER	-	expression tag	UNP P41594
A	3	TYR	-	expression tag	UNP P41594
A	4	ILE	-	expression tag	UNP P41594
A	5	PHE	-	expression tag	UNP P41594
A	6	CYS	-	expression tag	UNP P41594
A	7	LEU	-	expression tag	UNP P41594
A	8	VAL	-	expression tag	UNP P41594
A	9	PHE	-	expression tag	UNP P41594
A	10	ALA	-	expression tag	UNP P41594
A	11	ASP	-	expression tag	UNP P41594
A	12	TYR	-	expression tag	UNP P41594
A	13	LYS	-	expression tag	UNP P41594
A	14	ASP	-	expression tag	UNP P41594
A	15	ASP	-	expression tag	UNP P41594
A	16	ASP	-	expression tag	UNP P41594
A	17	ASP	-	expression tag	UNP P41594
A	18	ALA	-	expression tag	UNP P41594
A	19	ALA	-	expression tag	UNP P41594

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	866	HIS	-	expression tag	UNP P41594
A	867	HIS	-	expression tag	UNP P41594
A	868	HIS	-	expression tag	UNP P41594
A	869	HIS	-	expression tag	UNP P41594
A	870	HIS	-	expression tag	UNP P41594
A	871	HIS	-	expression tag	UNP P41594
B	-5	MET	-	initiating methionine	UNP P41594
B	-4	LYS	-	expression tag	UNP P41594
B	-3	THR	-	expression tag	UNP P41594
B	-2	ILE	-	expression tag	UNP P41594
B	-1	ILE	-	expression tag	UNP P41594
B	0	ALA	-	expression tag	UNP P41594
B	1	LEU	-	expression tag	UNP P41594
B	2	SER	-	expression tag	UNP P41594
B	3	TYR	-	expression tag	UNP P41594
B	4	ILE	-	expression tag	UNP P41594
B	5	PHE	-	expression tag	UNP P41594
B	6	CYS	-	expression tag	UNP P41594
B	7	LEU	-	expression tag	UNP P41594
B	8	VAL	-	expression tag	UNP P41594
B	9	PHE	-	expression tag	UNP P41594
B	10	ALA	-	expression tag	UNP P41594
B	11	ASP	-	expression tag	UNP P41594
B	12	TYR	-	expression tag	UNP P41594
B	13	LYS	-	expression tag	UNP P41594
B	14	ASP	-	expression tag	UNP P41594
B	15	ASP	-	expression tag	UNP P41594
B	16	ASP	-	expression tag	UNP P41594
B	17	ASP	-	expression tag	UNP P41594
B	18	ALA	-	expression tag	UNP P41594
B	19	ALA	-	expression tag	UNP P41594
B	866	HIS	-	expression tag	UNP P41594
B	867	HIS	-	expression tag	UNP P41594
B	868	HIS	-	expression tag	UNP P41594
B	869	HIS	-	expression tag	UNP P41594
B	870	HIS	-	expression tag	UNP P41594
B	871	HIS	-	expression tag	UNP P41594

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

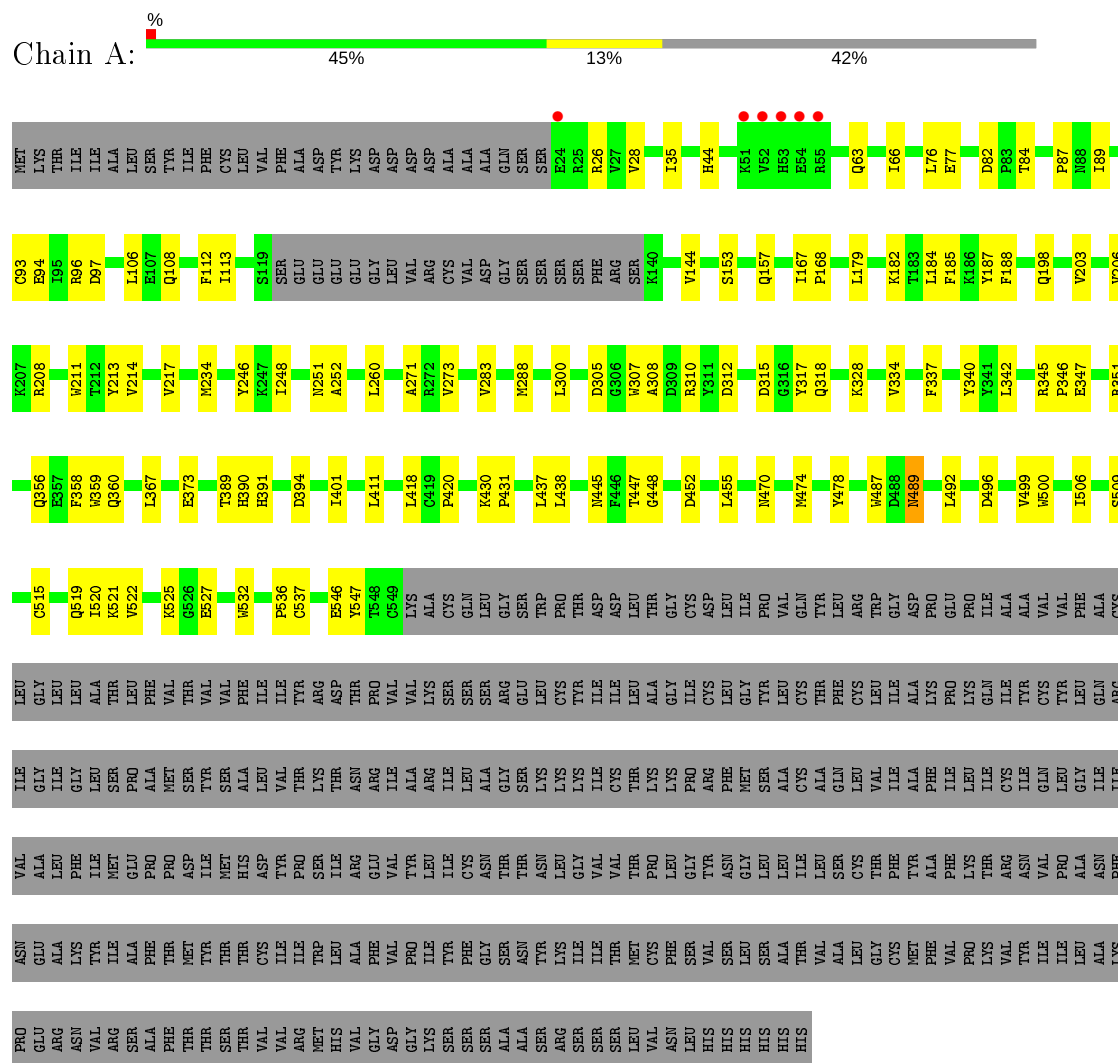
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		

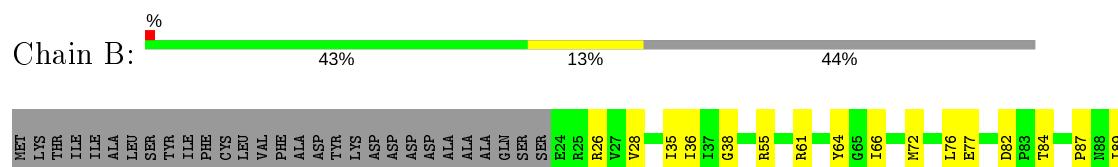
3 Residue-property plots

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 5



• Molecule 1: Metabotropic glutamate receptor 5



GLY	THR	VAL	LEU	TRP	W499	Q360	D195	C93
CYS	PHE	ILE	ILE	GLY	W500	L367		E94
MET	ALA	ALA	ALA	ASP	S501		Q198	I95
PHE	ALA	PHE	LYS	PRO	K502	F370		R96
PRO	LYS	LEU	LYS	PRO	K503	F371	V203	L106
LYS	THR	ILE	GLN	ILE	I506	Q372	D204	E107
VAL	ARG	CYS	CYS	ALA		E373	I205	Q108
THR	ASN	ILE	TYR	VAL	S509	R374	V206	S109
ILE	VAL	GLN	CYS	VAL			R207	I110
ILE	PRO	LEU	TYR	VAL	O515	T389	R208	E111
ALA	ALA	GLY	LEU	PHE		H390		F112
ALA	ASN	ILE	GLN	ALA	Q519	H391	W211	E113
PHE	PHE	ILE	ARG	CYS	Q520	V392	T212	R114
PRO	ASN	VAL	ILE	LEU	Q393	Q393	Y213	D115
GLU	GLU	ALA	GLY	GLY	K521	D394		
ARG	ALA	LEU	ILE	LEU			Q224	S116
ASN	LYS	PHE	GLY	LEU	K525	W397	N222	L117
VAL	TYR	ILE	LEU	ALA				I118
ARG	ILE	MET	SER	THR	T533	I401	M234	SER
ALA	ALA	GLU	PRO	LEU				SER
SER	PHE	PRO	ALA	PHE	P536	I404	H244	GLU
PHE	THR	PRO	MET	VAL	CYS		S245	GLU
THR	MET	ASP	SER	THR	LYS	L411	Y246	GLU
THR	TYR	ILE	TYR	VAL	GLU			GLY
THR	THR	MET	SER	VAL	ASN	L418	A271	LEU
VAL	CYS	ASP	ALA	PHE	GLU	C419	G280	VAL
VAL	ILE	TYR	VAL	ILE	TYR	P420		ARG
ARG	ILE	PRO	THR	TTR	PHE	G421	V283	CYS
MET	TRP	SER	LYS	ARG	ASP	Y422		VAL
HIS	LEU	ILE	THR	ASP	GLU	A428	M288	ASP
VAL	ALA	ARG	ASN	PRO	TYR	K429		GLY
GLY	PHE	GLU	ARG	PRO	THR	K430	D305	SER
ASP	VAL	VAL	ILE	VAL	CYS	P431	G306	SER
GLY	PRO	TRP	ALA	VAL	LYS		W307	SER
LYS	ILE	LEU	ARG	LYS	ALA	L437	R310	ARG
SER	TYR	ILE	ILE	SER	GLN	L438	Y311	PHE
SER	PHE	CYS	LEU	SER	GLN			ARG
SER	GLY	ASN	ALA	SER	LEU	G448		SER
ALA	SER	THR	GLY	ARG	GLY		Y317	K140
ALA	ASN	THR	SER	GLU	SER	D452		K141
SER	TRP	ASN	LYS	LEU	TRP		V334	P142
ARG	LYS	LEU	LYS	CYS	PRO	R465	I143	
SER	ILE	GLY	LYS	TYR	THR		F337	V144
SER	ILE	VAL	ILE	ILE	ASP	N470		G145
SER	THR	VAL	CYS	ILE	ASP		Y340	
LEU	MET	THR	THR	LEU	LEU	K474	Y341	Q157
VAL	CYS	PRO	LYS	ALA	GLY		L342	
ASN	PHE	LEU	LYS	GLY	THR			P168
LEU	SER	GLY	PRO	ILE	LYS	ASP	R345	
HIS	VAL	TYR	ARG	CYS	ASP	THR	P346	L179
HIS	SER	ASN	PHE	LEU	LEU	PHE	E347	
HIS	LEU	GLY	MET	GLY	ILE	D480		K182
SER	SER	LEU	SER	TYR	PRO		R351	T183
HIS	ALA	LEU	ALA	ILE	VAL	W497		L184
THR	VAL	ILE	LYS	CYS	VAL	D488	Q356	F185
THR	THR	ALA	CYS	THR	GLN	D489	E357	K186
ALA	VAL	SER	GLN	PHE	LEU		F358	F187
THR	THR	CYS	LEU	CYS	ARG	D406	F359	F189

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	119.08Å 174.10Å 180.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 4.00 49.57 – 4.00	Depositor EDS
% Data completeness (in resolution range)	93.2 (49.57-4.00) 83.5 (49.57-4.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.14 _3211	Depositor
R, R_{free}	0.270 , 0.282 0.268 , 0.281	Depositor DCC
R_{free} test set	1540 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	172.6	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 160.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.064 for -h,l,k	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	7736	wwPDB-VP
Average B, all atoms (Å ²)	184.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: 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	0.25	0/3985	0.45	0/5407
1	B	0.24	0/3836	0.45	0/5200
All	All	0.25	0/7821	0.45	0/10607

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	3897	0	3649	73	0
1	B	3754	0	3546	71	0
2	A	56	0	52	0	0
2	B	28	0	26	0	0
3	B	1	0	0	0	0
All	All	7736	0	7273	143	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 10.

The worst 5 of 143 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:520:ILE:HD13	1:A:546:GLU:C	1.90	0.90
1:A:77:GLU:OE2	1:A:351:ARG:NH1	2.18	0.76
1:B:77:GLU:OE2	1:B:351:ARG:NH1	2.19	0.74
1:B:360:GLN:HE22	1:B:373:GLU:HA	1.52	0.74
1:A:360:GLN:HE22	1:A:373:GLU:HA	1.53	0.73

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	502/877 (57%)	471 (94%)	31 (6%)	0	100	100
1	B	481/877 (55%)	453 (94%)	27 (6%)	1 (0%)	47	79
All	All	983/1754 (56%)	924 (94%)	58 (6%)	1 (0%)	51	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	521	LYS

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	412/763 (54%)	411 (100%)	1 (0%)	93	96

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	399/763 (52%)	397 (100%)	2 (0%)	88	93
All	All	811/1526 (53%)	808 (100%)	3 (0%)	91	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	489	ASN
1	B	465	ARG
1	B	489	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	45	HIS
1	B	74	HIS
1	B	218	HIS
1	A	364	GLN
1	B	198	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	B	902	1	14,14,15	0.36	0	17,19,21	0.63	1 (5%)
2	NAG	A	902	1	14,14,15	0.28	0	17,19,21	0.59	0
2	NAG	A	901	1	14,14,15	0.35	0	17,19,21	0.46	0
2	NAG	A	904	1	14,14,15	0.45	0	17,19,21	0.67	1 (5%)
2	NAG	B	903	1	14,14,15	0.44	0	17,19,21	0.56	0
2	NAG	A	903	1	14,14,15	0.35	0	17,19,21	0.48	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	B	902	1	-	0/6/23/26	0/1/1/1
2	NAG	A	902	1	-	0/6/23/26	0/1/1/1
2	NAG	A	901	1	-	2/6/23/26	0/1/1/1
2	NAG	A	904	1	-	2/6/23/26	0/1/1/1
2	NAG	B	903	1	-	0/6/23/26	0/1/1/1
2	NAG	A	903	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	NAG	C1-O5-C5	2.22	115.20	112.19
2	A	904	NAG	C1-O5-C5	2.19	115.15	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	NAG	O5-C5-C6-O6
2	A	901	NAG	C4-C5-C6-O6
2	A	904	NAG	O5-C5-C6-O6
2	A	904	NAG	C4-C5-C6-O6

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	506/877 (57%)	-0.19	6 (1%) 79 70	127, 180, 254, 270	0
1	B	487/877 (55%)	-0.20	6 (1%) 79 70	114, 183, 252, 292	0
All	All	993/1754 (56%)	-0.19	12 (1%) 79 70	114, 181, 254, 292	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	54	GLU	4.6
1	B	222	ASN	3.8
1	A	51	LYS	3.5
1	B	372	GLN	3.3
1	A	52	VAL	3.2

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 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(\AA^2)	Q<0.9
2	NAG	A	903	14/15	0.59	0.26	214,233,238,244	0
2	NAG	A	901	14/15	0.62	0.28	200,209,217,221	0
2	NAG	B	902	14/15	0.64	0.27	184,210,226,226	0
2	NAG	A	902	14/15	0.72	0.24	200,219,226,230	0
2	NAG	B	903	14/15	0.84	0.24	222,240,245,248	0
2	NAG	A	904	14/15	0.84	0.16	193,206,212,217	0
3	MG	B	901	1/1	0.92	0.10	165,165,165,165	0

6.5 Other polymers [i](#)

There are no such residues in this entry.