



# wwPDB X-ray Structure Validation Summary Report

Nov 7, 2014 – 04:12 PM EST

PDB ID : 3SAJ  
Title : Crystal Structure of glutamate receptor GluA1 Amino Terminal Domain  
Authors : Jin, R.; Zong, Y.; Yao, G.; Gu, S.  
Deposited on : 2011-06-02  
Resolution : 2.50 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

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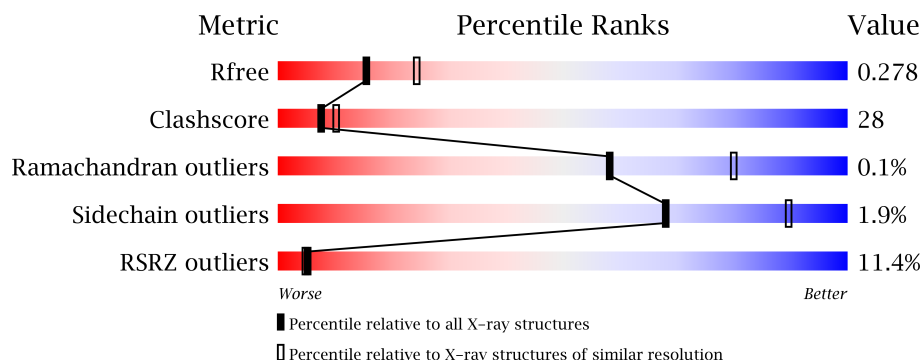
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : trunk24195  
Percentile statistics : 23426  
Refmac : 5.8.0049  
CCP4 : 6.1.3  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk24195

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
$R_{free}$	77520	3163 (2.50-2.50)
Clashscore	88313	3845 (2.50-2.50)
Ramachandran outliers	86584	3762 (2.50-2.50)
C $\alpha$ geometry	86677	3767 (2.50-2.50)
Sidechain outliers	86556	3764 (2.50-2.50)
RSRZ outliers	77580	3164 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	384	
1	B	384	
1	C	384	
1	D	384	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	NAG	D	900	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12534 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Glutamate receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	1	0
			2987	1899	525	550	13			
1	B	366	Total	C	N	O	S	0	0	0
			2959	1882	518	546	13			
1	C	372	Total	C	N	O	S	0	0	0
			3016	1918	530	555	13			
1	D	367	Total	C	N	O	S	0	0	0
			2963	1884	519	547	13			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ILE	-	EXPRESSION TAG	UNP P19490
A	-2	GLU	-	EXPRESSION TAG	UNP P19490
A	-1	GLU	-	EXPRESSION TAG	UNP P19490
A	0	ARG	-	EXPRESSION TAG	UNP P19490
A	1	GLY	-	EXPRESSION TAG	UNP P19490
A	2	ALA	-	EXPRESSION TAG	UNP P19490
A	3	MET	-	EXPRESSION TAG	UNP P19490
A	375	LEU	-	EXPRESSION TAG	UNP P19490
A	376	GLU	-	EXPRESSION TAG	UNP P19490
A	377	VAL	-	EXPRESSION TAG	UNP P19490
A	378	LEU	-	EXPRESSION TAG	UNP P19490
A	379	PHE	-	EXPRESSION TAG	UNP P19490
A	380	GLN	-	EXPRESSION TAG	UNP P19490
B	-3	ILE	-	EXPRESSION TAG	UNP P19490
B	-2	GLU	-	EXPRESSION TAG	UNP P19490
B	-1	GLU	-	EXPRESSION TAG	UNP P19490
B	0	ARG	-	EXPRESSION TAG	UNP P19490
B	1	GLY	-	EXPRESSION TAG	UNP P19490
B	2	ALA	-	EXPRESSION TAG	UNP P19490
B	3	MET	-	EXPRESSION TAG	UNP P19490
B	375	LEU	-	EXPRESSION TAG	UNP P19490

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Chain	Residue	Modelled	Actual	Comment	Reference
B	376	GLU	-	EXPRESSION TAG	UNP P19490
B	377	VAL	-	EXPRESSION TAG	UNP P19490
B	378	LEU	-	EXPRESSION TAG	UNP P19490
B	379	PHE	-	EXPRESSION TAG	UNP P19490
B	380	GLN	-	EXPRESSION TAG	UNP P19490
C	-3	ILE	-	EXPRESSION TAG	UNP P19490
C	-2	GLU	-	EXPRESSION TAG	UNP P19490
C	-1	GLU	-	EXPRESSION TAG	UNP P19490
C	0	ARG	-	EXPRESSION TAG	UNP P19490
C	1	GLY	-	EXPRESSION TAG	UNP P19490
C	2	ALA	-	EXPRESSION TAG	UNP P19490
C	3	MET	-	EXPRESSION TAG	UNP P19490
C	375	LEU	-	EXPRESSION TAG	UNP P19490
C	376	GLU	-	EXPRESSION TAG	UNP P19490
C	377	VAL	-	EXPRESSION TAG	UNP P19490
C	378	LEU	-	EXPRESSION TAG	UNP P19490
C	379	PHE	-	EXPRESSION TAG	UNP P19490
C	380	GLN	-	EXPRESSION TAG	UNP P19490
D	-3	ILE	-	EXPRESSION TAG	UNP P19490
D	-2	GLU	-	EXPRESSION TAG	UNP P19490
D	-1	GLU	-	EXPRESSION TAG	UNP P19490
D	0	ARG	-	EXPRESSION TAG	UNP P19490
D	1	GLY	-	EXPRESSION TAG	UNP P19490
D	2	ALA	-	EXPRESSION TAG	UNP P19490
D	3	MET	-	EXPRESSION TAG	UNP P19490
D	375	LEU	-	EXPRESSION TAG	UNP P19490
D	376	GLU	-	EXPRESSION TAG	UNP P19490
D	377	VAL	-	EXPRESSION TAG	UNP P19490
D	378	LEU	-	EXPRESSION TAG	UNP P19490
D	379	PHE	-	EXPRESSION TAG	UNP P19490
D	380	GLN	-	EXPRESSION TAG	UNP P19490

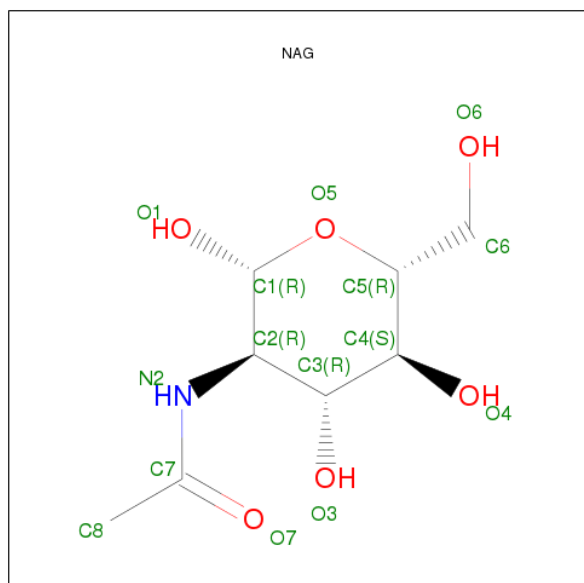
- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			39	22	2	15		
2	B	3	Total	C	N	O	0	0
			39	22	2	15		
2	D	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	49	Total	O	0	0
			49	49		
6	B	29	Total	O	0	0
			29	29		
6	C	41	Total	O	0	0
			41	41		
6	D	24	Total	O	0	0
			24	24		

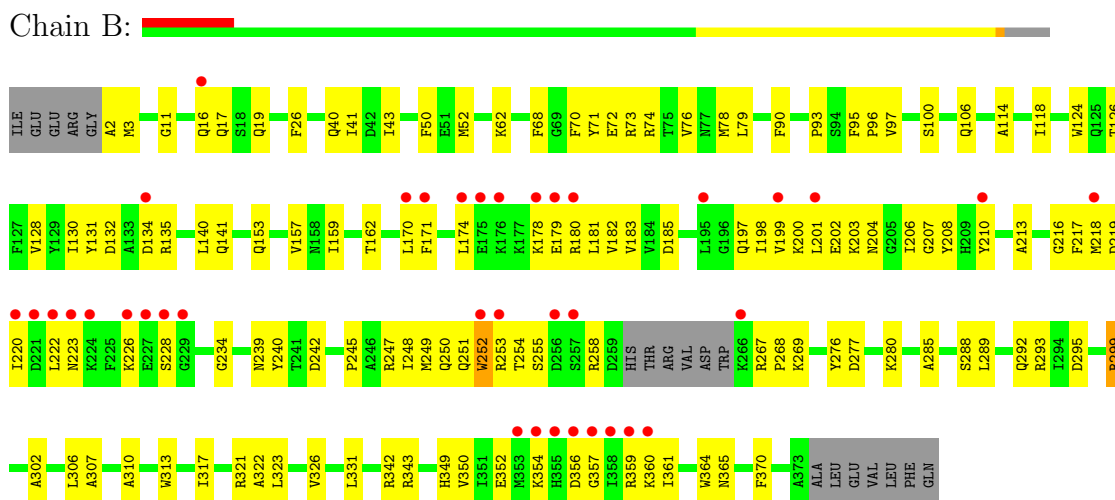
### 3 Residue-property plots

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.

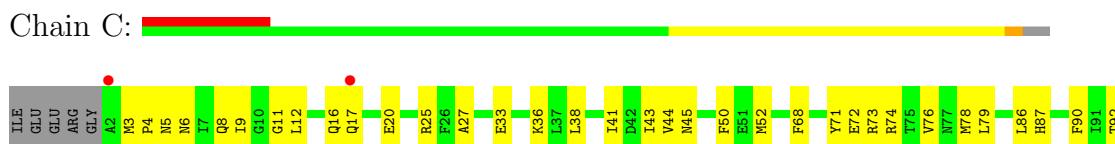
#### • Molecule 1: Glutamate receptor 1

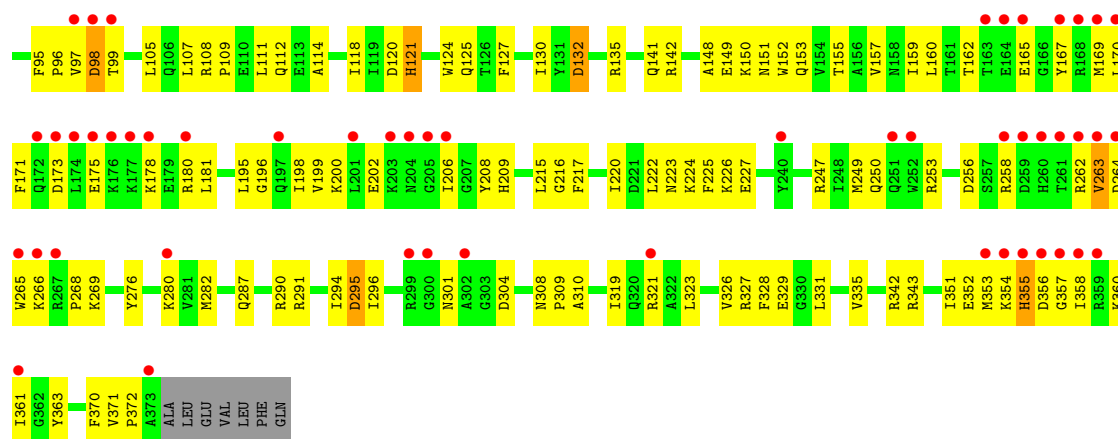


#### • Molecule 1: Glutamate receptor 1



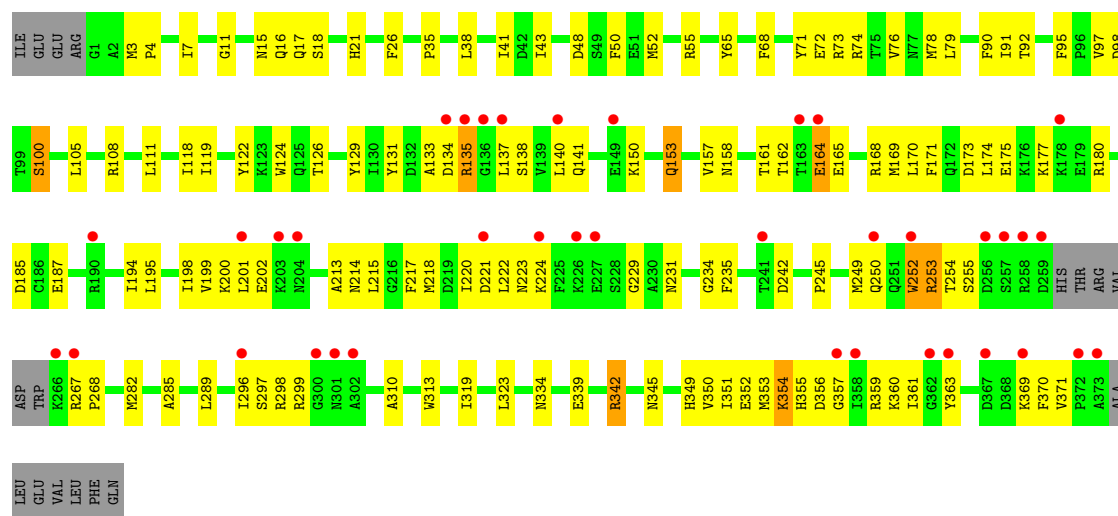
#### • Molecule 1: Glutamate receptor 1





• Molecule 1: Glutamate receptor 1

Chain D:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.59Å 94.42Å 186.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.18 – 2.50 41.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (93.18-2.50) 99.3 (41.46-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.66 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.218 , 0.286 0.235 , 0.278	Depositor DCC
$R_{free}$ test set	2886 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.1	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.2	EDS
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 57162 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12534	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% 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: BMA, NAG, MAN

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	0.56	0/3049	0.66	1/4122 (0.0%)
1	B	0.50	0/3021	0.66	1/4085 (0.0%)
1	C	0.51	1/3082 (0.0%)	0.65	1/4171 (0.0%)
1	D	0.48	0/3025	0.65	2/4090 (0.0%)
All	All	0.52	1/12177 (0.0%)	0.65	5/16468 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	268	PRO	N-CD	5.01	1.54	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	294	ILE	N-CA-C	-5.44	96.32	111.00
1	D	342	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	158	ASN	N-CA-C	-5.34	96.58	111.00
1	D	100	SER	N-CA-C	-5.34	96.59	111.00
1	B	343	ARG	NE-CZ-NH2	-5.33	117.64	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	299	ARG	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2987	0	2956	162	0
1	B	2959	0	2920	173	0
1	C	3016	0	2973	193	0
1	D	2963	0	2925	160	0
2	A	39	0	34	2	0
2	B	39	0	34	2	0
2	D	39	0	34	2	0
3	A	56	0	50	1	0
3	B	56	0	50	1	0
3	C	56	0	50	3	0
3	D	56	0	50	4	0
4	A	14	0	13	1	0
4	B	14	0	13	1	0
4	D	14	0	13	4	0
5	C	83	0	70	1	0
6	A	49	0	0	3	0
6	B	29	0	0	3	0
6	C	41	0	0	4	0
6	D	24	0	0	1	0
All	All	12534	0	12185	675	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

The worst 5 of 675 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:73:ARG:HB2	1:D:134:ASP:O	1.25	1.29
1:C:352:GLU:HB2	1:C:361:ILE:CD1	1.65	1.25
1:D:26:PHE:CZ	1:D:252:TRP:HB3	1.72	1.23
1:C:11:GLY:HA3	1:C:41:ILE:HG22	1.23	1.17

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:126:THR:HG22	1:A:153:GLN:HB2	1.22	1.17

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	366/384 (95%)	354 (97%)	12 (3%)	0	100	100
1	B	362/384 (94%)	341 (94%)	20 (6%)	1 (0%)	49	71
1	C	370/384 (96%)	350 (95%)	19 (5%)	1 (0%)	49	71
1	D	363/384 (94%)	342 (94%)	21 (6%)	0	100	100
All	All	1461/1536 (95%)	1387 (95%)	72 (5%)	2 (0%)	58	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	218	MET
1	C	263	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	322/336 (96%)	316 (98%)	6 (2%)	68	89
1	B	320/336 (95%)	318 (99%)	2 (1%)	92	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	326/336 (97%)	318 (98%)	8 (2%)	58 84
1	D	320/336 (95%)	311 (97%)	9 (3%)	54 81
All	All	1288/1344 (96%)	1263 (98%)	25 (2%)	68 89

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	132	ASP
1	C	326	VAL
1	D	253	ARG
1	C	295	ASP
1	C	329	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	349	HIS
1	B	355	HIS
1	C	355	HIS
1	B	204	ASN
1	C	17	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

32 carbohydrates 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	$\# Z  > 2$
2	NAG	A	600	1,2	14,14,15	0.79	0	19,19,21	1.80	5 (26%)
2	NAG	A	601	2	14,14,15	0.47	0	19,19,21	2.28	2 (10%)
2	BMA	A	602	2	11,11,12	0.51	0	15,15,17	1.70	5 (33%)
3	NAG	A	700	1,3	14,14,15	0.60	0	19,19,21	0.72	0
3	NAG	A	701	3	14,14,15	0.59	0	19,19,21	2.09	7 (36%)
3	NAG	A	800	1,3	14,14,15	0.71	0	19,19,21	1.20	1 (5%)
3	NAG	A	801	3	14,14,15	0.59	0	19,19,21	1.26	2 (10%)
2	NAG	B	600	1,2	14,14,15	0.47	0	19,19,21	1.47	3 (15%)
2	NAG	B	601	2	14,14,15	0.48	0	19,19,21	1.39	3 (15%)
2	BMA	B	602	2	11,11,12	0.56	0	15,15,17	1.33	2 (13%)
3	NAG	B	700	1,3	14,14,15	0.61	0	19,19,21	2.36	7 (36%)
3	NAG	B	701	3	14,14,15	0.54	0	19,19,21	1.04	2 (10%)
3	NAG	B	800	1,3	14,14,15	0.65	0	19,19,21	1.44	3 (15%)
3	NAG	B	801	3	14,14,15	0.39	0	19,19,21	1.89	3 (15%)
3	NAG	C	600	1,3	14,14,15	0.67	0	19,19,21	1.74	5 (26%)
3	NAG	C	601	3	14,14,15	0.54	0	19,19,21	1.51	3 (15%)
3	NAG	C	700	1,3	14,14,15	0.59	0	19,19,21	1.08	1 (5%)
3	NAG	C	701	3	14,14,15	0.54	0	19,19,21	1.37	1 (5%)
5	NAG	C	800	1,5	14,14,15	0.62	0	19,19,21	1.40	4 (21%)
5	NAG	C	801	5	14,14,15	0.66	0	19,19,21	1.10	1 (5%)
5	BMA	C	802	5	11,11,12	0.49	0	15,15,17	1.08	1 (6%)
5	MAN	C	803	5	11,11,12	0.70	0	15,15,17	2.08	5 (33%)
5	MAN	C	804	5	11,11,12	0.77	0	15,15,17	1.61	4 (26%)
5	MAN	C	805	5	11,11,12	0.59	0	15,15,17	1.06	1 (6%)
5	MAN	C	806	5	11,11,12	0.59	0	15,15,17	1.28	3 (20%)
2	NAG	D	600	1,2	14,14,15	0.64	0	19,19,21	2.29	5 (26%)
2	NAG	D	601	2	14,14,15	0.66	0	19,19,21	1.74	5 (26%)
2	BMA	D	602	2	11,11,12	0.57	0	15,15,17	1.75	3 (20%)
3	NAG	D	700	1,3	14,14,15	1.45	1 (7%)	19,19,21	1.60	1 (5%)
3	NAG	D	701	3	14,14,15	0.75	0	19,19,21	2.05	5 (26%)
3	NAG	D	800	1,3	14,14,15	1.43	1 (7%)	19,19,21	1.44	2 (10%)
3	NAG	D	801	3	14,14,15	0.58	0	19,19,21	1.14	1 (5%)

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	600	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	601	2	-	0/6/23/26	0/1/1/1
2	BMA	A	602	2	-	0/2/19/22	0/1/1/1
3	NAG	A	700	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	701	3	-	0/6/23/26	0/1/1/1
3	NAG	A	800	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	801	3	-	0/6/23/26	0/1/1/1
2	NAG	B	600	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	601	2	-	0/6/23/26	0/1/1/1
2	BMA	B	602	2	-	0/2/19/22	0/1/1/1
3	NAG	B	700	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	701	3	-	0/6/23/26	0/1/1/1
3	NAG	B	800	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	801	3	-	0/6/23/26	0/1/1/1
3	NAG	C	600	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	601	3	-	0/6/23/26	0/1/1/1
3	NAG	C	700	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	701	3	-	0/6/23/26	0/1/1/1
5	NAG	C	800	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	801	5	-	0/6/23/26	0/1/1/1
5	BMA	C	802	5	-	0/2/19/22	0/1/1/1
5	MAN	C	803	5	-	0/2/19/22	0/1/1/1
5	MAN	C	804	5	-	0/2/19/22	0/1/1/1
5	MAN	C	805	5	-	0/2/19/22	0/1/1/1
5	MAN	C	806	5	-	0/2/19/22	0/1/1/1
2	NAG	D	600	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	601	2	-	0/6/23/26	0/1/1/1
2	BMA	D	602	2	-	0/2/19/22	0/1/1/1
3	NAG	D	700	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	701	3	-	0/6/23/26	0/1/1/1
3	NAG	D	800	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	801	3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	700	NAG	O5-C1	-5.19	1.35	1.43
3	D	800	NAG	O5-C1	-5.09	1.35	1.43

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	NAG	C1-O5-C5	8.70	123.31	112.13
3	B	801	NAG	C1-O5-C5	6.71	120.75	112.13
2	D	600	NAG	O5-C1-C2	-6.69	104.94	111.68
3	B	700	NAG	C1-O5-C5	6.11	119.98	112.13
3	D	700	NAG	O5-C1-C2	-5.62	106.02	111.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

3 ligands 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	$\# Z  > 2$
4	NAG	A	900	1	14,14,15	0.68	0	19,19,21	2.33	7 (36%)
4	NAG	B	900	1	14,14,15	0.44	0	19,19,21	1.32	3 (15%)
4	NAG	D	900	1	14,14,15	1.15	1 (7%)	19,19,21	3.92	12 (63%)

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	NAG	A	900	1	-	0/6/23/26	0/1/1/1
4	NAG	B	900	1	-	0/6/23/26	0/1/1/1
4	NAG	D	900	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	900	NAG	O5-C5	4.06	1.52	1.43

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	900	NAG	O5-C1-C2	-10.18	101.42	111.68
4	D	900	NAG	C2-N2-C7	7.81	133.43	123.42
4	A	900	NAG	O5-C1-C2	-6.06	105.57	111.68
4	D	900	NAG	O5-C5-C4	-5.48	99.74	110.75
4	D	900	NAG	O5-C5-C6	-5.34	97.76	106.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 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	369/384 (96%)	0.60	40 (10%) 6 6	28, 54, 130, 203	0
1	B	366/384 (95%)	0.63	37 (10%) 7 6	29, 68, 114, 159	0
1	C	372/384 (96%)	0.82	53 (14%) 3 3	29, 63, 133, 199	0
1	D	367/384 (95%)	0.58	38 (10%) 6 6	30, 67, 103, 124	0
All	All	1474/1536 (95%)	0.66	168 (11%) 5 5	28, 62, 119, 203	0

The worst 5 of 168 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	263	VAL	15.3
1	A	172	GLN	12.3
1	C	265	TRP	10.0
1	B	220	ILE	8.5
1	C	177	LYS	8.2

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	D	701	14/15	0.39	68.60	160,173,175,176	0
5	MAN	C	804	11/12	0.81	6.45	220,222,223,223	0
5	MAN	C	805	11/12	0.75	4.67	224,224,225,225	0
5	NAG	C	800	14/15	0.30	3.01	127,133,139,143	0
2	NAG	D	601	14/15	0.24	2.90	123,126,132,132	0
3	NAG	C	600	14/15	0.33	2.81	122,135,144,146	0
3	NAG	D	700	14/15	0.32	1.60	150,160,163,167	0
2	NAG	B	601	14/15	0.22	1.52	163,167,174,179	0
2	NAG	B	600	14/15	0.27	1.43	130,140,144,154	0
3	NAG	C	700	14/15	0.29	1.39	144,150,157,159	0
5	NAG	C	801	14/15	0.25	1.21	148,152,156,166	0
2	NAG	D	600	14/15	0.28	1.21	109,119,125,127	0
3	NAG	B	800	14/15	0.21	1.12	139,150,154,161	0
2	NAG	A	600	14/15	0.22	0.98	125,139,144,151	0
3	NAG	A	700	14/15	0.24	0.77	129,137,145,150	0
3	NAG	A	800	14/15	0.23	0.28	129,137,145,153	0
5	MAN	C	806	11/12	0.24	0.22	185,186,187,187	0
3	NAG	C	701	14/15	0.33	0.10	162,164,165,166	0
3	NAG	A	701	14/15	0.30	-0.11	155,158,160,160	0
2	NAG	A	601	14/15	0.31	-0.19	161,166,171,177	0
3	NAG	C	601	14/15	0.23	-0.34	152,156,160,161	0
3	NAG	B	700	14/15	0.31	-0.42	129,143,158,168	0
3	NAG	A	801	14/15	0.26	-0.43	162,166,168,169	0
5	MAN	C	803	11/12	0.30	-0.79	206,210,211,216	0
3	NAG	D	800	14/15	0.14	-0.88	146,155,160,168	0
5	BMA	C	802	11/12	0.21	-1.60	175,181,192,200	0
2	BMA	D	602	11/12	0.15	-8.88	136,138,140,142	0
3	NAG	B	801	14/15	0.21	-	168,172,174,174	0
3	NAG	B	701	14/15	0.47	-	102,175,193,194	0
3	NAG	D	801	14/15	0.23	-	175,180,184,184	0
2	BMA	B	602	11/12	0.31	-	184,186,187,188	0
2	BMA	A	602	11/12	0.50	-	180,183,184,184	0

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	D	900	14/15	0.42	2.77	159,166,173,173	0
4	NAG	A	900	14/15	0.24	1.98	152,159,164,164	0
4	NAG	B	900	14/15	0.26	-0.08	156,165,172,172	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.