



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:53 PM GMT

PDB ID : 4MQF  
Title : Crystal structure of the extracellular domain of human GABA(B) receptor  
bound to the antagonist 2-hydroxysaclofen  
Authors : Geng, Y.; Bush, M.; Mosyak, L.; Wang, F.; Fan, Q.R.  
Deposited on : 2013-09-16  
Resolution : 2.22 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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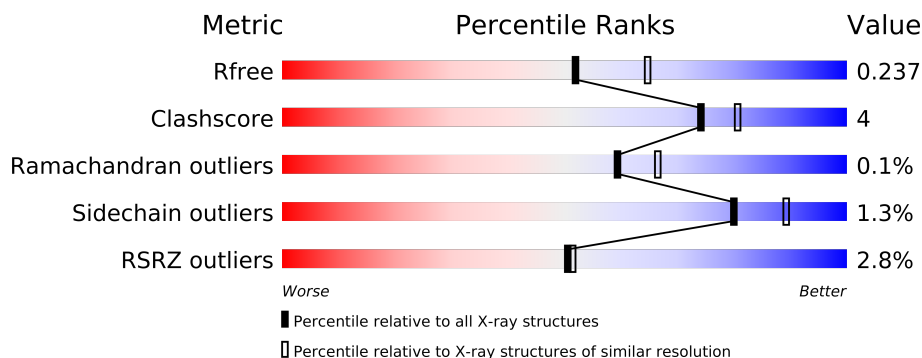
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.22 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))
$R_{free}$	66092	3340 (2.24-2.20)
Clashscore	79885	4208 (2.24-2.20)
Ramachandran outliers	78287	4135 (2.24-2.20)
Sidechain outliers	78261	4136 (2.24-2.20)
RSRZ outliers	66119	3341 (2.24-2.20)

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	420	
2	B	433	

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

Mol	Type	Chain	Res	Geometry	Electron density
5	NAG	A	508	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7070 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 Gamma-aminobutyric acid type B receptor subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	406	3262	2084	549	615	14	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	460	ASP	-	EXPRESSION TAG	UNP Q9UBS5
A	461	TYR	-	EXPRESSION TAG	UNP Q9UBS5
A	462	LYS	-	EXPRESSION TAG	UNP Q9UBS5
A	463	ASP	-	EXPRESSION TAG	UNP Q9UBS5
A	464	ASP	-	EXPRESSION TAG	UNP Q9UBS5
A	465	ASP	-	EXPRESSION TAG	UNP Q9UBS5
A	466	ASP	-	EXPRESSION TAG	UNP Q9UBS5
A	467	LYS	-	EXPRESSION TAG	UNP Q9UBS5

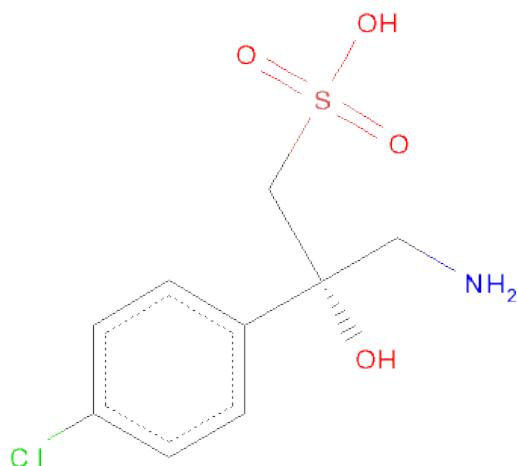
- Molecule 2 is a protein called Gamma-aminobutyric acid type B receptor subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	403	3214	2052	543	604	15	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	467	ASP	-	EXPRESSION TAG	UNP O75899
B	468	TYR	-	EXPRESSION TAG	UNP O75899
B	469	LYS	-	EXPRESSION TAG	UNP O75899
B	470	ASP	-	EXPRESSION TAG	UNP O75899
B	471	ASP	-	EXPRESSION TAG	UNP O75899
B	472	ASP	-	EXPRESSION TAG	UNP O75899
B	473	ASP	-	EXPRESSION TAG	UNP O75899
B	474	LYS	-	EXPRESSION TAG	UNP O75899

- Molecule 3 is 2-HYDROXYSACLOFEN (three-letter code: 2BQ) (formula:  $C_9H_{12}ClNO_4S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			16	9	1	1	4	1		

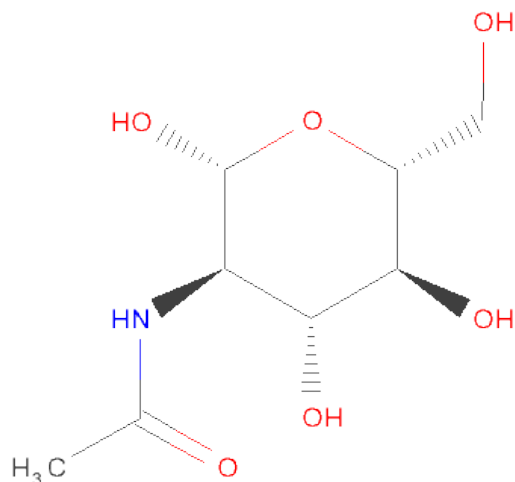
- Molecule 4 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	6	Total	C	N	O	0	0
			71	40	2	29		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	460	ASP	-	EXPRESSION TAG	UNP Q9UBS5
A	461	TYR	-	EXPRESSION TAG	UNP Q9UBS5
A	462	LYS	-	EXPRESSION TAG	UNP Q9UBS5
A	463	ASP	-	EXPRESSION TAG	UNP Q9UBS5
A	464	ASP	-	EXPRESSION TAG	UNP Q9UBS5
A	465	ASP	-	EXPRESSION TAG	UNP Q9UBS5
A	466	ASP	-	EXPRESSION TAG	UNP Q9UBS5
A	467	LYS	-	EXPRESSION TAG	UNP Q9UBS5

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	4	Total	C	N	O	0	0
			49	28	2	19		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	467	ASP	-	EXPRESSION TAG	UNP O75899
B	468	TYR	-	EXPRESSION TAG	UNP O75899
B	469	LYS	-	EXPRESSION TAG	UNP O75899
B	470	ASP	-	EXPRESSION TAG	UNP O75899
B	471	ASP	-	EXPRESSION TAG	UNP O75899
B	472	ASP	-	EXPRESSION TAG	UNP O75899
B	473	ASP	-	EXPRESSION TAG	UNP O75899
B	474	LYS	-	EXPRESSION TAG	UNP O75899

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	201	Total	O	0	0
			201	201		

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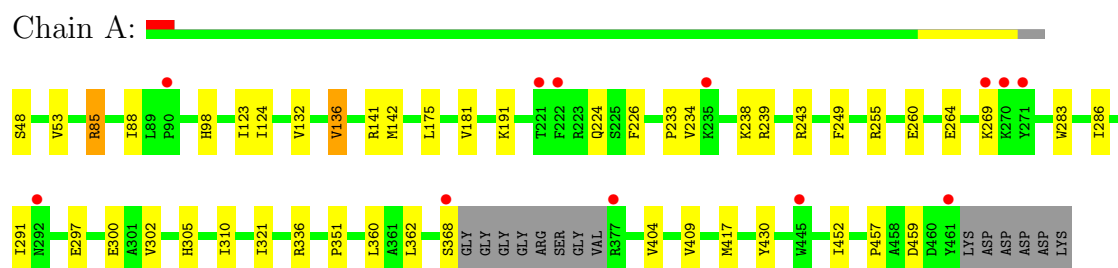
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	243	Total 243	O 243	0	0

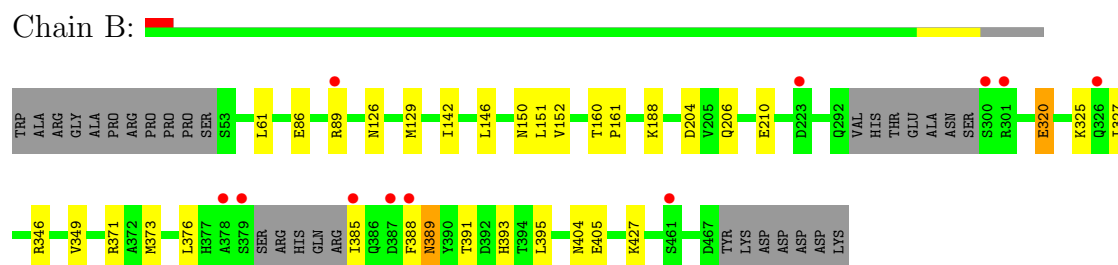
### 3 Residue-property plots

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: Gamma-aminobutyric acid type B receptor subunit 1



- Molecule 2: Gamma-aminobutyric acid type B receptor subunit 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.28Å 112.63Å 73.22Å 90.00° 97.79° 90.00°	Depositor
Resolution (Å)	32.50 – 2.22 44.48 – 2.22	Depositor EDS
% Data completeness (in resolution range)	90.5 (32.50-2.22) 88.7 (44.48-2.22)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.04 (at 2.22Å)	Xtriage
Refinement program	BUSTER	Depositor
R, $R_{free}$	0.207 , 0.234 0.206 , 0.237	Depositor DCC
$R_{free}$ test set	2536 reflections (5.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 34.4	EDS
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 49428 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7070	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 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: FUC, NAG, 2BQ, 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	0.48	0/3345	0.67	0/4536
2	B	0.49	0/3287	0.66	1/4449 (0.0%)
All	All	0.49	0/6632	0.67	1/8985 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	389	ASN	N-CA-C	-5.30	96.68	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 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	3262	0	3180	31	0
2	B	3214	0	3161	21	0
3	A	16	0	11	0	0
4	A	71	0	61	0	0
5	A	14	0	13	0	0
6	B	49	0	43	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	201	0	0	3	0
7	B	243	0	0	1	0
All	All	7070	0	6469	53	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 4.

All (53) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:234:VAL:HG21	1:A:260:GLU:HB3	1.65	0.78
2:B:86:GLU:HA	2:B:89:ARG:HH21	1.57	0.69
2:B:373:MET:HG2	2:B:385:ILE:HD11	1.75	0.68
2:B:388:PHE:HB2	2:B:395:LEU:HD23	1.80	0.64
2:B:404:ASN:HD22	6:B:501:NAG:H83	1.63	0.63
1:A:238:LYS:HD2	1:A:264:GLU:HB3	1.82	0.62
1:A:53:VAL:HG13	1:A:123:ILE:HG12	1.82	0.61
2:B:320:GLU:HG2	2:B:427:LYS:HB2	1.83	0.61
2:B:126:ASN:HD21	2:B:388:PHE:HD2	1.49	0.59
1:A:269:LYS:HE2	1:A:452:ILE:HG21	1.85	0.58
1:A:283:TRP:HA	1:A:286:ILE:HD12	1.87	0.56
2:B:206:GLN:HE21	2:B:210:GLU:HG2	1.71	0.56
2:B:373:MET:HG2	2:B:385:ILE:CD1	2.35	0.56
1:A:191:LYS:HB2	1:A:459:ASP:HB2	1.87	0.56
1:A:302:VAL:O	1:A:305:HIS:HD2	1.90	0.55
2:B:89:ARG:HG3	7:B:650:HOH:O	2.06	0.55
2:B:346:ARG:O	2:B:349:VAL:HG22	2.07	0.54
2:B:129:MET:HB2	2:B:152:VAL:O	2.07	0.53
2:B:86:GLU:CA	2:B:89:ARG:HH21	2.21	0.52
1:A:269:LYS:HE2	1:A:452:ILE:CG2	2.39	0.52
6:B:502:NAG:O3	6:B:503:MAN:H2	2.08	0.52
1:A:305:HIS:CE1	1:A:430:TYR:OH	2.62	0.51
2:B:376:LEU:HD12	2:B:385:ILE:HG12	1.91	0.51
1:A:238:LYS:HE3	1:A:264:GLU:O	2.13	0.49
1:A:48:SER:HB2	7:A:725:HOH:O	2.13	0.48
1:A:305:HIS:HE1	1:A:430:TYR:OH	1.95	0.48
2:B:150:ASN:ND2	2:B:393:HIS:HA	2.29	0.48
1:A:85:ARG:HB3	1:A:88:ILE:HD12	1.94	0.48
1:A:243:ARG:HB2	1:A:459:ASP:HA	1.95	0.47
1:A:255:ARG:HB3	1:A:291:ILE:HD13	1.95	0.47
1:A:409:VAL:HG23	1:A:417:MET:HB2	1.95	0.47
1:A:351:PRO:HB3	1:A:404:VAL:HG23	1.97	0.47
1:A:224:GLN:HB3	1:A:233:PRO:HB3	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:98:HIS:HD2	7:A:729:HOH:O	1.99	0.46
1:A:302:VAL:O	1:A:305:HIS:CD2	2.67	0.46
1:A:132:VAL:O	1:A:136:VAL:HG13	2.16	0.45
1:A:269:LYS:HG2	1:A:452:ILE:HB	1.99	0.44
2:B:86:GLU:HG3	2:B:89:ARG:NH2	2.33	0.44
2:B:61:LEU:HD13	2:B:142:ILE:HD13	2.00	0.44
1:A:85:ARG:CB	1:A:88:ILE:HD12	2.48	0.43
1:A:226:PHE:HB3	1:A:233:PRO:HG2	2.00	0.43
1:A:297:GLU:O	1:A:300:GLU:HB3	2.19	0.43
1:A:175:LEU:HD23	1:A:310:ILE:HG12	2.00	0.43
2:B:160:THR:HA	2:B:161:PRO:HD3	1.94	0.43
2:B:371:ARG:HD2	2:B:405:GLU:OE1	2.19	0.43
2:B:389:ASN:C	2:B:391:THR:H	2.23	0.42
2:B:146:LEU:HB3	2:B:151:LEU:O	2.19	0.42
1:A:181:VAL:HG21	7:A:723:HOH:O	2.19	0.42
1:A:321:ILE:HD13	1:A:362:LEU:HD11	2.02	0.41
1:A:124:ILE:CD1	1:A:360:LEU:HD13	2.50	0.41
1:A:141:ARG:HH11	1:A:142:MET:HE3	1.85	0.41
2:B:325:LYS:HB3	2:B:327:ILE:HD12	2.03	0.41
1:A:255:ARG:HB3	1:A:291:ILE:CD1	2.51	0.41

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	402/420 (96%)	390 (97%)	11 (3%)	1 (0%)	56	62
2	B	397/433 (92%)	384 (97%)	13 (3%)	0	100	100
All	All	799/853 (94%)	774 (97%)	24 (3%)	1 (0%)	59	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	457	PRO

### 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	353/362 (98%)	347 (98%)	6 (2%)	73	84
2	B	349/375 (93%)	346 (99%)	3 (1%)	87	94
All	All	702/737 (95%)	693 (99%)	9 (1%)	80	89

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

Mol	Chain	Res	Type
1	A	85	ARG
1	A	136	VAL
1	A	239	ARG
1	A	249	PHE
1	A	336	ARG
1	A	368	SER
2	B	188	LYS
2	B	204	ASP
2	B	320	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	98	HIS
1	A	144	ASN
1	A	196	GLN
1	A	305	HIS
2	B	126	ASN
2	B	150	ASN
2	B	206	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 ⓘ

10 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	$\# Z  > 2$
4	NAG	A	502	1,4	12,14,15	0.22	0	15,19,21	1.18	2 (13%)
4	NAG	A	503	4	12,14,15	0.30	0	15,19,21	1.43	2 (13%)
4	MAN	A	504	4	10,11,12	0.42	0	11,15,17	1.61	3 (27%)
4	MAN	A	505	4	10,11,12	0.45	0	11,15,17	1.03	1 (9%)
4	MAN	A	506	4	10,11,12	0.36	0	11,15,17	0.69	0
4	FUC	A	507	4	9,10,11	0.40	0	10,14,16	0.60	0
6	NAG	B	501	2,6	12,14,15	0.31	0	15,19,21	0.53	0
6	NAG	B	502	6	12,14,15	0.31	0	15,19,21	1.64	4 (26%)
6	MAN	B	503	6	10,11,12	0.45	0	11,15,17	1.31	2 (18%)
6	FUC	B	504	6	9,10,11	0.36	0	10,14,16	0.55	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	NAG	A	502	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	503	4	-	0/6/23/26	0/1/1/1
4	MAN	A	504	4	-	0/2/19/22	0/1/1/1
4	MAN	A	505	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	A	506	4	-	0/2/19/22	0/1/1/1
4	FUC	A	507	4	-	0/0/17/20	0/1/1/1
6	NAG	B	501	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	502	6	-	0/6/23/26	0/1/1/1
6	MAN	B	503	6	-	0/2/19/22	0/1/1/1
6	FUC	B	504	6	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	NAG	O5-C5-C4	4.00	115.73	110.65
6	B	502	NAG	O5-C5-C4	3.77	115.44	110.65
6	B	503	MAN	C4-C3-C2	3.17	114.75	110.50
4	A	505	MAN	C3-C4-C5	2.99	115.53	110.20
4	A	504	MAN	O5-C5-C6	2.75	109.87	106.98
4	A	503	NAG	O5-C5-C6	-2.65	104.20	106.98
6	B	502	NAG	C3-C4-C5	2.61	114.86	110.20
4	A	502	NAG	O5-C5-C6	-2.61	104.25	106.98
4	A	502	NAG	O5-C5-C4	2.60	113.96	110.65
6	B	502	NAG	O4-C4-C3	-2.46	104.83	110.35
6	B	502	NAG	O5-C5-C6	-2.35	104.52	106.98
4	A	504	MAN	O5-C5-C4	2.32	113.60	110.65
4	A	504	MAN	O3-C3-C4	-2.04	105.77	110.35
6	B	503	MAN	C3-C4-C5	2.00	113.78	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

2 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
3	2BQ	A	501	-	16,16,16	1.76	3 (18%)	24,24,24	1.49	4 (16%)
5	NAG	A	508	1	12,14,15	0.34	0	15,19,21	0.57	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
3	2BQ	A	501	-	-	0/14/15/15	0/1/1/1
5	NAG	A	508	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	2BQ	O3-S	4.79	1.61	1.45
3	A	501	2BQ	C9-S	-3.59	1.68	1.77
3	A	501	2BQ	C7-C6	-2.14	1.50	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	2BQ	O1-S-C9	5.42	112.62	105.64
3	A	501	2BQ	O1-S-O2	-2.24	106.95	111.78
3	A	501	2BQ	O2-S-C9	2.22	111.08	106.96
3	A	501	2BQ	C7-C8-N	-2.04	110.44	116.19

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	406/420 (96%)	0.23	12 (2%) 48 49	14, 35, 72, 87	0
2	B	403/433 (93%)	0.12	11 (2%) 52 53	14, 31, 64, 96	0
All	All	809/853 (94%)	0.17	23 (2%) 50 51	14, 33, 70, 96	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	461	TYR	7.4
2	B	378	ALA	5.1
1	A	377	ARG	4.8
2	B	387	ASP	4.3
2	B	301	ARG	4.2
1	A	269	LYS	4.2
2	B	388	PHE	3.9
1	A	222	PHE	3.8
2	B	300	SER	3.3
1	A	270	LYS	3.3
2	B	89	ARG	3.0
1	A	368	SER	2.8
2	B	385	ILE	2.7
1	A	90	PRO	2.7
2	B	379	SER	2.5
1	A	271	TYR	2.4
2	B	223	ASP	2.3
1	A	235	LYS	2.3
2	B	461	SER	2.3
1	A	292	ASN	2.3
1	A	445	TRP	2.3
1	A	221	THR	2.1
2	B	326	GLN	2.0



## 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(Å <sup>2</sup> )	Q<0.9
4	NAG	A	502	14/15	0.17	22.60	55,59,70,77	0
4	MAN	A	505	11/12	0.35	10.31	90,91,95,96	0
4	FUC	A	507	10/11	0.36	6.99	84,89,90,91	0
4	MAN	A	506	11/12	0.31	3.30	83,85,88,89	0
6	NAG	B	501	14/15	0.18	1.51	54,61,69,70	0
4	MAN	A	504	11/12	0.27	0.49	80,83,84,88	0
6	FUC	B	504	10/11	0.14	0.09	67,67,69,69	0
4	NAG	A	503	14/15	0.23	-0.35	65,69,72,76	0
6	NAG	B	502	14/15	0.16	-	75,79,82,88	0
6	MAN	B	503	11/12	0.39	-	94,98,99,100	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(Å <sup>2</sup> )	Q<0.9
5	NAG	A	508	14/15	0.20	2.42	72,77,79,80	0
3	2BQ	A	501	16/16	0.12	-0.57	13,19,23,30	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.