W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:45 am GMT

PDB ID : 4MRM
Title : Crystal structure of the extracellular domain of human GABA(B) receptor bound to the antagonist phaclofen
Authors : Geng, Y.; Bush, M.; Mosyak, L.; Wang, F.; Fan, Q.R.
Deposited on : 2013-09-17
Resolution : 2.86 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

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 2.86 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	Percentile Ranks	Value
Rfree		0.229
Clashscore		9
Ramachandran outliers		0.1%
Sidechain outliers		1.4%
RSRZ outliers		2.4%

Worse — Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
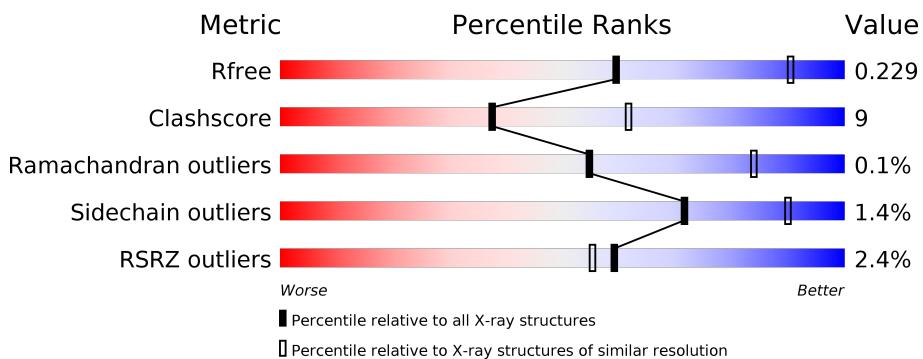
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2469 (2.90-2.82)
Clashscore	112137	2749 (2.90-2.82)
Ramachandran outliers	110173	2687 (2.90-2.82)
Sidechain outliers	110143	2690 (2.90-2.82)
RSRZ outliers	101464	2487 (2.90-2.82)

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. 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 <=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	420	3% / 72% 24% ··
2	B	433	2% / 85% 7% 8%
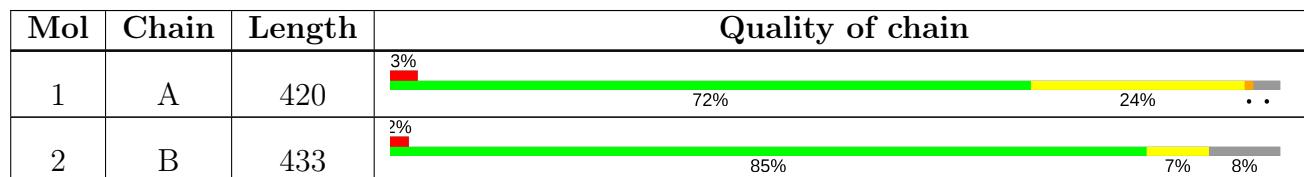
2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 6753 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 Gamma-aminobutyric acid type B receptor subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total 3271	C 2090	N 551	O 616	S 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
2	B	400	Total 3189	C 2037	N 539	O 598	S 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 PHACLOFEN (three-letter code: 2BY) (formula: $C_9H_{13}ClNO_3P$).

2BY
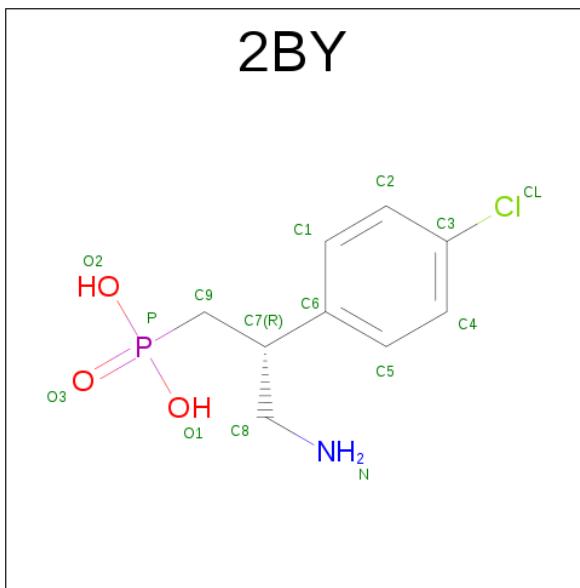
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 15	C 9	Cl 1	N 1	O 3	P 1	0	0

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

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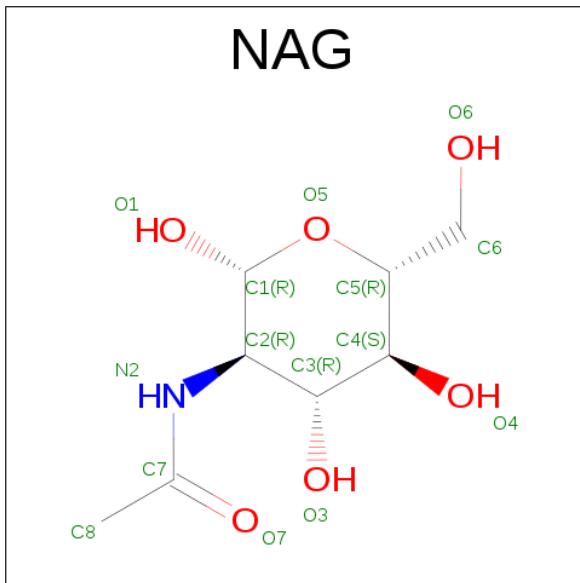
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	4	Total 50	C 28	N 2	O 20	0	0

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 7 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	91	Total 91	O 91	0	0
7	B	95	Total 95	O 95	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 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: Gamma-aminobutyric acid type B receptor subunit 1
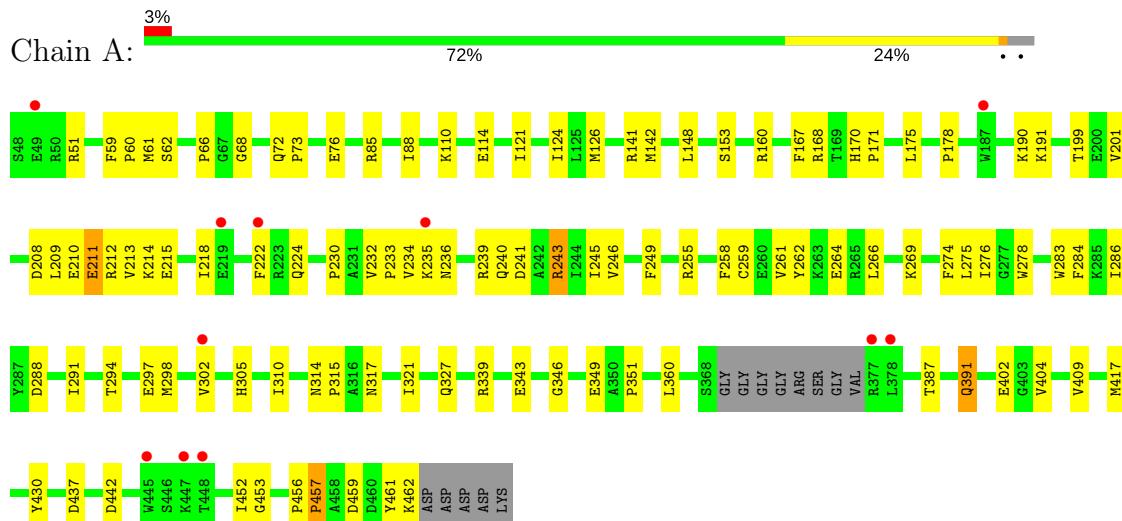
• Molecule 2: Gamma-aminobutyric acid type B receptor subunit 2
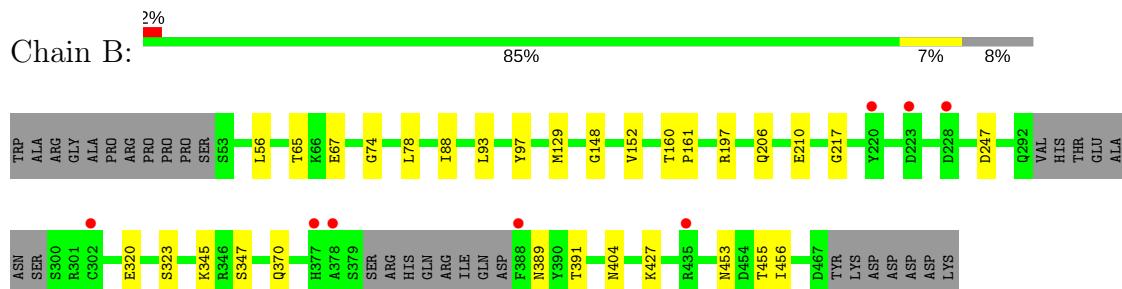
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.07Å 111.94Å 73.47Å 90.00° 97.67° 90.00°	Depositor
Resolution (Å)	47.21 – 2.86 47.20 – 2.86	Depositor EDS
% Data completeness (in resolution range)	94.2 (47.21-2.86) 92.2 (47.20-2.86)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.69 (at 2.86Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.208 , 0.232 0.211 , 0.229	Depositor DCC
R_{free} test set	1207 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	38.4	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 53.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6753	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, 2BY, 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	0.54	0/3354	0.69	0/4547
2	B	0.45	0/3262	0.64	0/4415
All	All	0.50	0/6616	0.67	0/8962

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	3271	0	3193	97	0
2	B	3189	0	3138	18	0
3	A	15	0	11	0	0
4	A	14	0	13	0	0
5	A	50	0	43	0	0
6	B	28	0	25	2	0
7	A	91	0	0	1	0
7	B	95	0	0	4	0
All	All	6753	0	6423	114	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 9.

All (114) 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:222:PHE:CZ	1:A:240:GLN:OE1	2.17	0.98
1:A:262:TYR:OH	1:A:297:GLU:OE1	1.82	0.97
1:A:262:TYR:CZ	1:A:297:GLU:OE1	2.22	0.92
1:A:222:PHE:CE1	1:A:240:GLN:OE1	2.24	0.91
2:B:404:ASN:HD22	6:B:501:NAG:H83	1.35	0.89
1:A:269:LYS:O	1:A:457:PRO:HG3	1.77	0.83
1:A:213:VAL:HG13	1:A:218:ILE:HB	1.60	0.83
1:A:85:ARG:HB3	1:A:88:ILE:HD12	1.59	0.83
1:A:305:HIS:CE1	1:A:430:TYR:OH	2.35	0.80
1:A:387:THR:O	1:A:391:GLN:NE2	2.18	0.76
1:A:230:PRO:O	1:A:234:VAL:HG23	1.87	0.74
1:A:269:LYS:O	1:A:457:PRO:CG	2.38	0.71
1:A:305:HIS:HE1	1:A:430:TYR:OH	1.72	0.71
1:A:346:GLY:HA2	1:A:349:GLU:OE1	1.90	0.71
1:A:305:HIS:CE1	1:A:430:TYR:HH	2.10	0.70
1:A:276:ILE:HG21	1:A:278:TRP:NE1	2.06	0.69
1:A:255:ARG:HB3	1:A:291:ILE:HD11	1.72	0.69
1:A:110:LYS:HE2	2:B:148:GLY:O	1.93	0.69
1:A:85:ARG:CB	1:A:88:ILE:HD12	2.24	0.67
1:A:269:LYS:HE2	1:A:453:GLY:HA3	1.77	0.66
1:A:317:ASN:OD1	1:A:327:GLN:OE1	2.14	0.64
2:B:404:ASN:ND2	6:B:501:NAG:H83	2.09	0.64
1:A:141:ARG:NH1	1:A:142:MET:HE2	2.14	0.63
1:A:339:ARG:HB3	1:A:343:GLU:OE2	1.98	0.63
1:A:211:GLU:HG3	1:A:212:ARG:N	2.15	0.62
1:A:321:ILE:HG12	1:A:402:GLU:O	2.00	0.61
1:A:210:GLU:O	1:A:214:LYS:HG3	2.01	0.61
1:A:276:ILE:HG21	1:A:278:TRP:CE2	2.36	0.61
1:A:213:VAL:HG12	1:A:218:ILE:O	2.02	0.60
1:A:266:LEU:O	1:A:266:LEU:HG	2.02	0.60
1:A:302:VAL:O	1:A:305:HIS:HD2	1.86	0.59
1:A:294:THR:OG1	1:A:297:GLU:HG3	2.03	0.58
1:A:141:ARG:HH11	1:A:142:MET:CE	2.15	0.58
1:A:124:ILE:HD13	1:A:360:LEU:HD13	1.86	0.57
1:A:190:LYS:HA	1:A:218:ILE:HG23	1.87	0.57
1:A:199:THR:HG22	1:A:201:VAL:HG22	1.87	0.56
1:A:284:PHE:CG	1:A:302:VAL:HG21	2.40	0.56
1:A:85:ARG:CB	1:A:88:ILE:CD1	2.82	0.56
1:A:160:ARG:HB3	7:A:664:HOH:O	2.03	0.56
1:A:141:ARG:HH11	1:A:142:MET:HE2	1.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:PRO:HG2	1:A:310:ILE:HG21	1.88	0.55
1:A:59:PHE:HB3	1:A:68:GLY:HA3	1.89	0.55
1:A:224:GLN:HB3	1:A:233:PRO:HB3	1.90	0.54
2:B:65:THR:HG22	2:B:67:GLU:H	1.71	0.54
1:A:241:ASP:OD1	1:A:243:ARG:NE	2.41	0.54
1:A:339:ARG:HB3	1:A:343:GLU:CD	2.29	0.53
1:A:232:VAL:O	1:A:235:LYS:HB3	2.08	0.53
1:A:291:ILE:HG21	1:A:298:MET:CE	2.38	0.53
1:A:236:ASN:HA	1:A:239:ARG:HD3	1.91	0.53
1:A:213:VAL:CG1	1:A:218:ILE:HB	2.35	0.53
1:A:291:ILE:HG21	1:A:298:MET:HE1	1.91	0.53
1:A:339:ARG:HD2	1:A:343:GLU:CD	2.29	0.53
1:A:461:TYR:O	1:A:462:LYS:C	2.48	0.52
1:A:283:TRP:HA	1:A:286:ILE:HD12	1.92	0.52
1:A:72:GLN:O	1:A:76:GLU:HG3	2.09	0.52
2:B:197:ARG:NH2	2:B:247:ASP:O	2.43	0.52
2:B:217:GLY:HA3	7:B:667:HOH:O	2.09	0.51
1:A:175:LEU:HD23	1:A:310:ILE:HG12	1.92	0.51
1:A:208:ASP:OD2	1:A:212:ARG:NE	2.41	0.51
1:A:222:PHE:CE2	1:A:240:GLN:OE1	2.62	0.51
1:A:61:MET:HE1	1:A:72:GLN:NE2	2.26	0.50
1:A:339:ARG:HD2	1:A:343:GLU:OE1	2.12	0.50
1:A:61:MET:CE	1:A:72:GLN:NE2	2.75	0.49
1:A:409:VAL:HG23	1:A:417:MET:HB2	1.94	0.49
1:A:302:VAL:O	1:A:305:HIS:CD2	2.65	0.49
1:A:85:ARG:HB3	1:A:88:ILE:CD1	2.35	0.49
2:B:323:SER:HA	7:B:688:HOH:O	2.13	0.48
1:A:235:LYS:HA	1:A:264:GLU:OE1	2.13	0.48
1:A:269:LYS:HE2	1:A:452:ILE:O	2.13	0.48
1:A:339:ARG:HB3	1:A:343:GLU:CG	2.42	0.48
1:A:213:VAL:HG13	1:A:218:ILE:CB	2.39	0.48
1:A:258:PHE:HA	1:A:261:VAL:HB	1.95	0.47
1:A:51:ARG:HA	1:A:51:ARG:HD3	1.74	0.46
1:A:209:LEU:O	1:A:213:VAL:HG23	2.16	0.46
1:A:230:PRO:O	1:A:233:PRO:HD2	2.16	0.46
1:A:168:ARG:HD2	1:A:170:HIS:O	2.16	0.46
1:A:60:PRO:O	1:A:66:PRO:HA	2.15	0.46
1:A:456:PRO:HA	1:A:457:PRO:HD3	1.86	0.46
2:B:206:GLN:HE21	2:B:210:GLU:HG2	1.80	0.46
1:A:153:SER:HB3	1:A:170:HIS:CE1	2.50	0.46
1:A:175:LEU:O	1:A:178:PRO:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:LEU:HG	2:B:97:TYR:HB3	1.98	0.45
1:A:351:PRO:HB3	1:A:404:VAL:HG23	1.99	0.45
1:A:191:LYS:HB2	1:A:459:ASP:HB2	1.99	0.45
1:A:230:PRO:C	1:A:233:PRO:HD2	2.37	0.45
2:B:129:MET:HB2	2:B:152:VAL:O	2.17	0.45
1:A:314:ASN:OD1	1:A:315:PRO:HD2	2.18	0.44
1:A:437:ASP:HB3	1:A:442:ASP:HB3	1.98	0.44
1:A:72:GLN:HB3	1:A:73:PRO:HD3	2.00	0.44
2:B:320:GLU:OE1	2:B:427:LYS:HB2	2.17	0.44
1:A:148:LEU:HA	1:A:167:PHE:O	2.18	0.43
2:B:453:ASN:HA	7:B:655:HOH:O	2.17	0.43
1:A:126:MET:HG3	1:A:148:LEU:O	2.18	0.43
1:A:141:ARG:NH1	1:A:142:MET:CE	2.79	0.43
1:A:59:PHE:CE2	1:A:72:GLN:HG3	2.54	0.43
1:A:275:LEU:HD12	1:A:305:HIS:CE1	2.53	0.42
2:B:389:ASN:C	2:B:391:THR:H	2.22	0.42
1:A:259:CYS:O	1:A:262:TYR:HB3	2.20	0.42
1:A:241:ASP:OD2	1:A:243:ARG:NH2	2.52	0.42
1:A:275:LEU:HD12	1:A:305:HIS:ND1	2.34	0.41
2:B:347:SER:HA	7:B:685:HOH:O	2.20	0.41
2:B:88:ILE:HA	2:B:93:LEU:HD12	2.01	0.41
1:A:199:THR:CG2	1:A:201:VAL:HG22	2.50	0.41
1:A:211:GLU:O	1:A:215:GLU:HG3	2.20	0.41
2:B:455:THR:OG1	2:B:456:ILE:N	2.53	0.41
1:A:288:ASP:HB3	1:A:291:ILE:HD12	2.01	0.41
1:A:283:TRP:HA	1:A:286:ILE:CD1	2.50	0.41
1:A:259:CYS:HB2	1:A:291:ILE:HG23	2.03	0.41
1:A:246:VAL:HG22	1:A:274:PHE:HB2	2.02	0.41
1:A:459:ASP:N	1:A:459:ASP:OD1	2.51	0.41
2:B:160:THR:HA	2:B:161:PRO:HD3	1.98	0.41
1:A:262:TYR:CE1	1:A:297:GLU:HB3	2.55	0.40
1:A:284:PHE:CD2	1:A:302:VAL:HG21	2.57	0.40
2:B:74:GLY:O	2:B:78:LEU:HG	2.22	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	403/420 (96%)	392 (97%)	10 (2%)	1 (0%)	51	80
2	B	394/433 (91%)	382 (97%)	12 (3%)	0	100	100
All	All	797/853 (93%)	774 (97%)	22 (3%)	1 (0%)	55	84

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	354/362 (98%)	346 (98%)	8 (2%)	56	83
2	B	346/375 (92%)	344 (99%)	2 (1%)	89	96
All	All	700/737 (95%)	690 (99%)	10 (1%)	71	90

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	SER
1	A	114	GLU
1	A	121	ILE
1	A	211	GLU
1	A	243	ARG

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Mol	Chain	Res	Type
1	A	245	ILE
1	A	249	PHE
1	A	391	GLN
2	B	345	LYS
2	B	370	GLN

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	72	GLN
1	A	196	GLN
1	A	305	HIS
1	A	391	GLN
1	A	407	HIS
2	B	150	ASN
2	B	206	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 ⓘ

6 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	#$|Z| > 2$
5	NAG	A	503	1,5	14,14,15	0.63	0	15,19,21	3.55	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths				Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	NAG	A	504	5	14,14,15	0.79	0	15,19,21	1.72	3 (20%)
5	MAN	A	505	5	11,11,12	0.98	0	13,15,17	2.39	5 (38%)
5	BMA	A	506	5	11,11,12	0.94	0	13,15,17	2.67	6 (46%)
6	NAG	B	501	2,6	14,14,15	1.66	2 (14%)	15,19,21	2.33	6 (40%)
6	NAG	B	502	6	14,14,15	0.63	0	15,19,21	1.50	3 (20%)

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
5	NAG	A	503	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	504	5	-	0/6/23/26	0/1/1/1
5	MAN	A	505	5	-	0/2/19/22	1/1/1/1
5	BMA	A	506	5	-	0/2/19/22	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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	501	NAG	O5-C1	-3.64	1.37	1.43
6	B	501	NAG	C1-C2	4.34	1.58	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	503	NAG	C1-C2-N2	-8.64	95.73	110.49
5	A	505	MAN	O6-C6-C5	-5.41	93.14	111.34
6	B	501	NAG	C1-O5-C5	-4.79	105.56	112.17
5	A	505	MAN	O3-C3-C2	-4.45	101.93	110.02
6	B	501	NAG	C4-C3-C2	-4.16	104.93	111.02
5	A	504	NAG	O4-C4-C3	-3.97	101.73	110.36
6	B	501	NAG	O5-C1-C2	-3.52	106.58	111.47
5	A	504	NAG	O3-C3-C4	-3.35	103.06	110.36
6	B	501	NAG	O6-C6-C5	-2.99	101.28	111.34
5	A	503	NAG	O4-C4-C3	-2.84	104.19	110.36
6	B	502	NAG	C8-C7-N2	-2.72	111.20	116.11
6	B	501	NAG	C3-C4-C5	-2.64	105.56	110.22
5	A	506	BMA	O3-C3-C4	-2.58	104.74	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	502	NAG	O4-C4-C3	-2.38	105.18	110.36
5	A	506	BMA	C6-C5-C4	-2.27	107.69	113.00
5	A	504	NAG	C2-N2-C7	-2.20	119.74	122.94
6	B	502	NAG	C6-C5-C4	-2.17	107.93	113.00
5	A	505	MAN	O2-C2-C1	-2.05	105.01	109.18
5	A	505	MAN	C2-C3-C4	-2.02	107.35	110.88
6	B	501	NAG	C1-C2-N2	2.02	113.93	110.49
5	A	505	MAN	C1-C2-C3	3.20	113.71	109.65
5	A	506	BMA	C2-C3-C4	3.58	117.11	110.88
5	A	506	BMA	C1-C2-C3	3.65	114.28	109.65
5	A	503	NAG	C3-C4-C5	3.71	116.75	110.22
5	A	506	BMA	O5-C1-C2	4.75	118.23	110.79
5	A	503	NAG	O5-C1-C2	4.99	118.42	111.47
5	A	506	BMA	C1-O5-C5	5.07	119.16	112.17
5	A	503	NAG	C1-O5-C5	7.37	122.32	112.17

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	505	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	501	NAG	2	0

5.6 Ligand geometry (i)

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	2BY	A	501	-	15,15,15	1.96	5 (33%)	16,21,21	0.97	0
4	NAG	A	502	1	14,14,15	1.47	2 (14%)	15,19,21	3.34	4 (26%)

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	2BY	A	501	-	-	0/11/11/11	0/1/1/1
4	NAG	A	502	1	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	NAG	C1-C2	-4.32	1.46	1.52
3	A	501	2BY	C6-C7	-2.27	1.47	1.52
3	A	501	2BY	P-O1	-2.24	1.49	1.54
3	A	501	2BY	C3-CL	2.46	1.79	1.74
3	A	501	2BY	P-O2	2.69	1.61	1.54
4	A	502	NAG	O5-C1	2.70	1.48	1.43
3	A	501	2BY	P-O3	5.20	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	NAG	C1-C2-N2	-7.65	97.42	110.49
4	A	502	NAG	C2-N2-C7	-3.22	118.25	122.94
4	A	502	NAG	O5-C1-C2	5.87	119.64	111.47
4	A	502	NAG	C1-O5-C5	7.58	122.61	112.17

There are no chirality outliers.

There are no torsion outliers.

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 (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, 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(Å²)	Q<0.9
1	A	407/420 (96%)	0.16	11 (2%)	55	50	18, 41, 82, 94	0
2	B	400/433 (92%)	-0.04	8 (2%)	65	62	16, 34, 63, 106	0
All	All	807/853 (94%)	0.06	19 (2%)	59	55	16, 37, 77, 106	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	PHE	3.2
2	B	223	ASP	3.2
1	A	447	LYS	3.0
2	B	378	ALA	2.7
1	A	445	TRP	2.5
1	A	187	TRP	2.5
1	A	302	VAL	2.5
2	B	220	TYR	2.5
1	A	49	GLU	2.4
2	B	377	HIS	2.3
1	A	448	THR	2.3
2	B	302	CYS	2.3
2	B	388	PHE	2.2
1	A	219	GLU	2.2
1	A	377	ARG	2.2
1	A	235	LYS	2.2
2	B	228	ASP	2.1
2	B	435	ARG	2.1
1	A	378	LEU	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 (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, 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	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	A	503	14/15	0.87	0.16	-	66,71,74,74	0
5	BMA	A	506	11/12	0.68	0.38	-	99,102,105,106	0
6	NAG	B	502	14/15	0.83	0.18	-	80,84,91,94	0
6	NAG	B	501	14/15	0.82	0.23	-	70,73,77,80	0
5	MAN	A	505	11/12	0.66	0.29	-	89,93,95,95	0
5	NAG	A	504	14/15	0.89	0.21	-	77,81,84,85	0

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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	2BY	A	501	15/15	0.97	0.19	0.44	21,24,28,40	0
4	NAG	A	502	14/15	0.89	0.17	-3.34	74,77,81,82	0

6.5 Other polymers (i)

There are no such residues in this entry.