



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:55 PM EDT

PDB ID : 4MR7 / pdb_00004mr7
Title : Crystal structure of the extracellular domain of human GABA(B) receptor bound to the antagonist CGP54626
Authors : Geng, Y.; Bush, M.; Mosyak, L.; Wang, F.; Fan, Q.R.
Deposited on : 2013-09-17
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

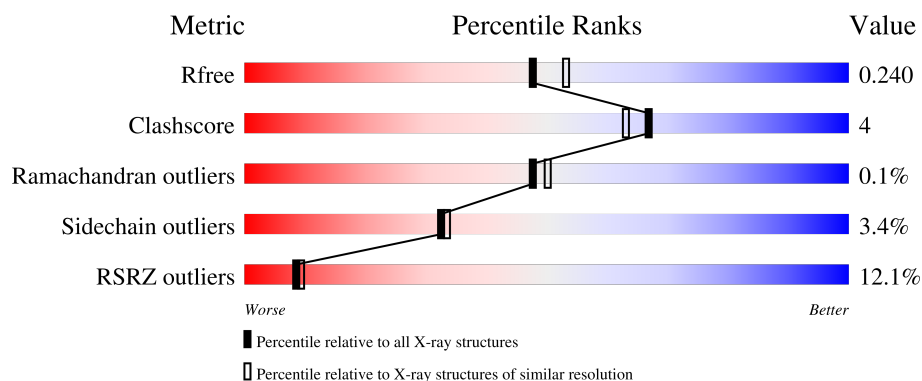
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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 of 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	420	
2	B	433	
3	C	6	
4	D	4	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7148 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	C	N	O	S	0	0	0
			3271	2090	551	616	14			

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

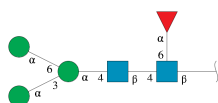
- Molecule 2 is a protein called Gamma-aminobutyric acid type B receptor subunit 2.

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

There are 8 discrepancies between the modelled and reference sequences:

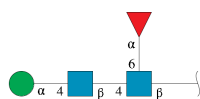
Chain	Residue	Modelled	Actual	Comment	Reference
B	467	ASP	-	expression tag	UNP O75899
B	468	TYR	-	expression tag	UNP O75899
B	469	LYS	-	expression tag	UNP O75899
B	470	ASP	-	expression tag	UNP O75899
B	471	ASP	-	expression tag	UNP O75899
B	472	ASP	-	expression tag	UNP O75899
B	473	ASP	-	expression tag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

- Molecule 3 is an oligosaccharide called α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[α -L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



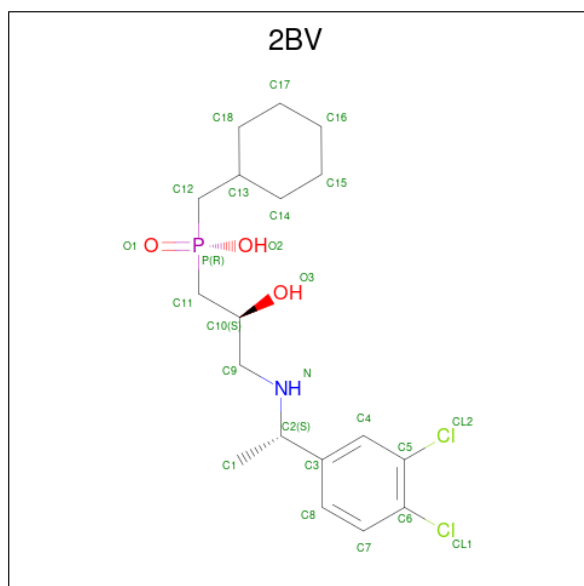
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 4 is an oligosaccharide called α -D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[α -L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



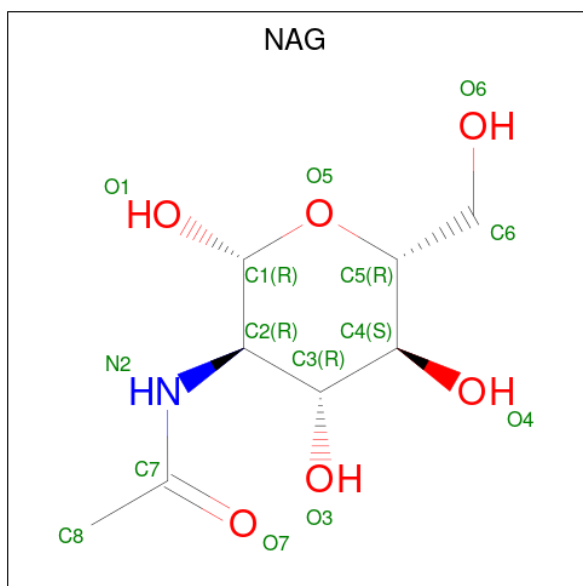
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 5 is (R)-(cyclohexylmethyl)[(2S)-3-{[(1S)-1-(3,4-dichlorophenyl)ethyl]amino}-2-hydroxypropyl]phosphinic acid (CCD ID: 2BV) (formula: $C_{18}H_{28}Cl_2NO_3P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	P	
			25	18	2	1	3	1	
									0
									0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

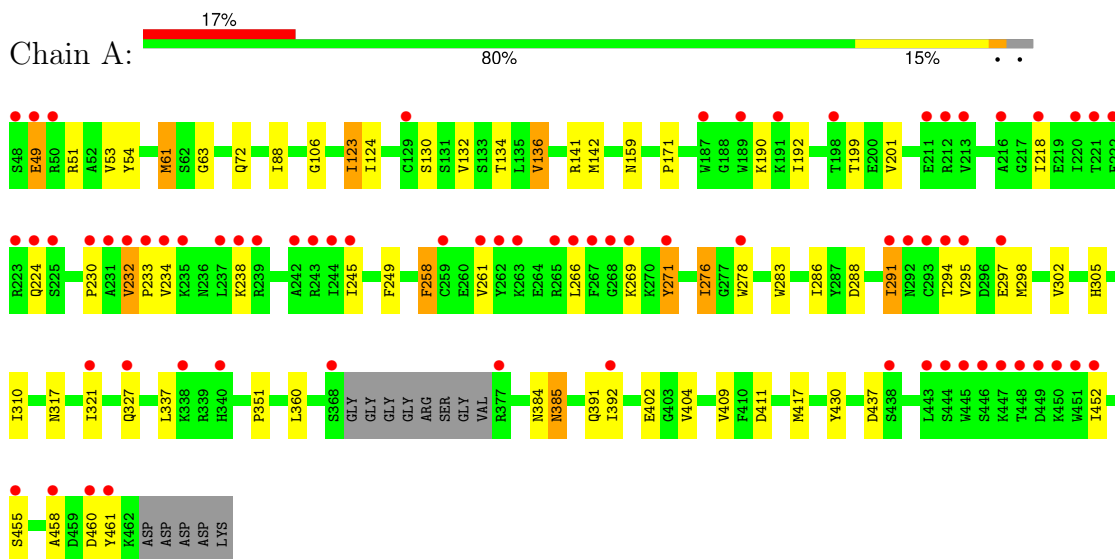
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	218	Total	O		
			218	218	0	0
7	B	286	Total	O		
			286	286	0	0

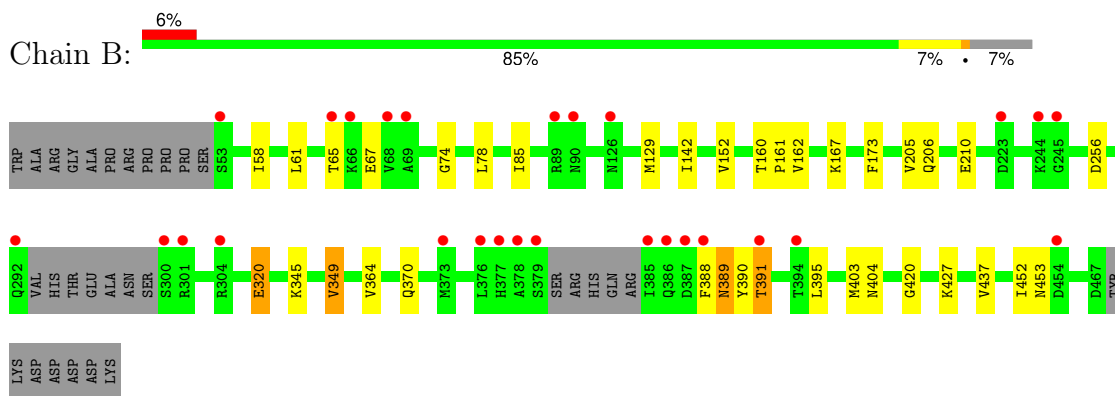
3 Residue-property plots [i](#)

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.

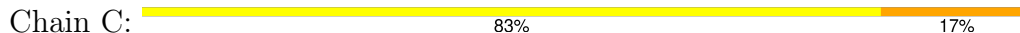
- Molecule 1: Gamma-aminobutyric acid type B receptor subunit 1



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



- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 4: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  25% 25% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.67Å 113.21Å 73.46Å 90.00° 97.11° 90.00°	Depositor
Resolution (Å)	21.67 – 2.15 21.67 – 2.15	Depositor EDS
% Data completeness (in resolution range)	86.0 (21.67-2.15) 86.2 (21.67-2.15)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 2.16Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER	Depositor
R, R_{free}	0.203 , 0.240 0.205 , 0.240	Depositor DCC
R_{free} test set	2709 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7148	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2BV, NAG, MAN, FUC

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	0.86	1/3354 (0.0%)	1.29	29/4547 (0.6%)
2	B	0.88	0/3287	1.25	10/4449 (0.2%)
All	All	0.87	1/6641 (0.0%)	1.27	39/8996 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	MET	SD-CE	-7.24	1.61	1.79

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	VAL	N-CA-CB	8.84	117.34	110.45
2	B	389	ASN	N-CA-C	-7.42	98.46	109.81
1	A	460	ASP	CA-C-N	7.32	130.41	120.38
1	A	460	ASP	C-N-CA	7.32	130.41	120.38
2	B	390	TYR	CA-C-N	7.25	132.98	120.58
2	B	390	TYR	C-N-CA	7.25	132.98	120.58
1	A	49	GLU	CB-CG-CD	7.12	124.70	112.60
1	A	258	PHE	CA-CB-CG	-7.03	106.77	113.80
1	A	238	LYS	CA-C-N	6.37	129.14	120.54
1	A	238	LYS	C-N-CA	6.37	129.14	120.54
1	A	411	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	437	ASP	CA-C-N	5.73	128.24	120.38
1	A	437	ASP	C-N-CA	5.73	128.24	120.38
2	B	452	ILE	CA-C-N	5.59	130.08	121.19
2	B	452	ILE	C-N-CA	5.59	130.08	121.19
1	A	159	ASN	CA-CB-CG	5.51	118.11	112.60
2	B	85	ILE	CA-C-N	5.34	127.76	120.54
2	B	85	ILE	C-N-CA	5.34	127.76	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	ASP	CA-CB-CG	5.33	117.92	112.60
1	A	54	TYR	N-CA-C	5.31	118.06	109.40
1	A	385	ASN	CA-C-N	5.29	130.98	121.66
1	A	385	ASN	C-N-CA	5.29	130.98	121.66
2	B	349	VAL	N-CA-CB	5.26	116.78	110.31
1	A	106	GLY	CA-C-N	5.25	127.32	120.28
1	A	106	GLY	C-N-CA	5.25	127.32	120.28
1	A	271	TYR	N-CA-C	5.23	117.76	109.50
2	B	256	ASP	CA-C-N	5.19	127.49	120.38
2	B	256	ASP	C-N-CA	5.19	127.49	120.38
1	A	234	VAL	CA-C-N	5.19	127.18	120.44
1	A	234	VAL	C-N-CA	5.19	127.18	120.44
1	A	458	ALA	CA-C-N	5.08	127.60	120.28
1	A	458	ALA	C-N-CA	5.08	127.60	120.28
1	A	317	ASN	CA-CB-CG	5.04	117.64	112.60
1	A	63	GLY	CA-C-N	5.04	125.69	119.99
1	A	63	GLY	C-N-CA	5.04	125.69	119.99
1	A	461	TYR	N-CA-C	5.04	117.42	111.33
1	A	245	ILE	N-CA-C	5.03	115.10	107.75
1	A	199	THR	CA-C-N	5.01	127.31	120.54
1	A	199	THR	C-N-CA	5.01	127.31	120.54

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	33	0
2	B	3214	0	3161	13	0
3	C	71	0	61	1	0
4	D	49	0	43	2	0
5	A	25	0	28	0	0
6	A	14	0	13	1	0
7	A	218	0	0	3	0
7	B	286	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7148	0	6499	48	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:VAL:HG11	7:A:605:HOH:O	1.84	0.77
1:A:141:ARG:HH11	1:A:142:MET:HE3	1.50	0.76
2:B:320:GLU:HG2	2:B:427:LYS:HB2	1.65	0.76
1:A:232:VAL:HG23	1:A:233:PRO:HD3	1.76	0.66
1:A:224:GLN:HB3	1:A:233:PRO:HB3	1.78	0.66
1:A:130:SER:O	1:A:134:THR:HG23	1.99	0.62
1:A:288:ASP:HB3	1:A:291:ILE:HG12	1.83	0.61
1:A:288:ASP:O	1:A:291:ILE:HG13	2.00	0.60
1:A:321:ILE:HG12	1:A:402:GLU:O	2.01	0.60
1:A:302:VAL:O	1:A:305:HIS:HD2	1.86	0.58
1:A:294:THR:OG1	1:A:297:GLU:HG2	2.05	0.57
2:B:65:THR:HG22	2:B:67:GLU:H	1.70	0.57
2:B:404:ASN:HD22	4:D:1:NAG:H83	1.70	0.57
7:A:742:HOH:O	3:C:4:MAN:H5	2.05	0.56
1:A:88:ILE:CD1	6:A:502:NAG:H82	2.37	0.55
1:A:302:VAL:O	1:A:305:HIS:CD2	2.60	0.54
2:B:129:MET:HB2	2:B:152:VAL:O	2.09	0.52
1:A:409:VAL:HG23	1:A:417:MET:HB2	1.90	0.52
2:B:206:GLN:HE21	2:B:210:GLU:HG2	1.75	0.51
1:A:283:TRP:HA	1:A:286:ILE:HD12	1.91	0.50
1:A:61:MET:CE	1:A:72:GLN:HE21	2.24	0.50
1:A:171:PRO:HG2	1:A:310:ILE:HG21	1.94	0.49
2:B:61:LEU:HD13	2:B:142:ILE:HD13	1.96	0.48
1:A:232:VAL:CG2	1:A:233:PRO:HD3	2.41	0.48
1:A:258:PHE:HA	1:A:261:VAL:HB	1.96	0.47
1:A:124:ILE:HD13	1:A:360:LEU:HD13	1.95	0.47
2:B:173:PHE:CD2	2:B:420:GLY:HA2	2.50	0.47
2:B:453:ASN:HA	7:B:755:HOH:O	2.14	0.46
2:B:388:PHE:HB2	2:B:395:LEU:HD23	1.97	0.46
1:A:49:GLU:HG2	1:A:51:ARG:NH1	2.30	0.46
1:A:53:VAL:HG13	1:A:123:ILE:HG12	1.98	0.45
1:A:269:LYS:HE2	1:A:452:ILE:HG22	1.99	0.45
1:A:190:LYS:HA	1:A:218:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:389:ASN:C	2:B:391:THR:H	2.24	0.45
1:A:61:MET:CE	1:A:72:GLN:NE2	2.81	0.43
1:A:276:ILE:HD12	1:A:278:TRP:CZ2	2.54	0.43
2:B:364:VAL:HG12	2:B:403:MET:HE2	2.00	0.43
1:A:295:VAL:HG23	7:A:816:HOH:O	2.18	0.42
2:B:160:THR:HA	2:B:161:PRO:HD3	1.93	0.42
1:A:269:LYS:HG3	1:A:452:ILE:HB	2.00	0.42
1:A:132:VAL:O	1:A:136:VAL:HG13	2.20	0.42
1:A:351:PRO:HB3	1:A:404:VAL:HG23	2.02	0.42
4:D:2:NAG:O3	4:D:3:MAN:H2	2.19	0.42
1:A:305:HIS:HE1	1:A:430:TYR:OH	2.03	0.41
1:A:298:MET:HE2	1:A:298:MET:HB2	1.93	0.41
1:A:327:GLN:H	1:A:327:GLN:CD	2.28	0.41
2:B:74:GLY:O	2:B:78:LEU:HG	2.21	0.41
1:A:291:ILE:HD13	1:A:298:MET:CE	2.51	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%)	391 (97%)	11 (3%)	1 (0%)	43	44
2	B	397/433 (92%)	388 (98%)	9 (2%)	0	100	100
All	All	800/853 (94%)	779 (97%)	20 (2%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	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%)	340 (96%)	14 (4%)	28	27
2	B	349/375 (93%)	339 (97%)	10 (3%)	37	39
All	All	703/737 (95%)	679 (97%)	24 (3%)	32	33

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	ILE
1	A	136	VAL
1	A	192	ILE
1	A	249	PHE
1	A	266	LEU
1	A	271	TYR
1	A	276	ILE
1	A	291	ILE
1	A	337	LEU
1	A	384	ASN
1	A	385	ASN
1	A	391	GLN
1	A	392	ILE
1	A	455	SER
2	B	58	ILE
2	B	162	VAL
2	B	167	LYS
2	B	205	VAL
2	B	320	GLU
2	B	345	LYS
2	B	349	VAL
2	B	370	GLN
2	B	391	THR
2	B	437	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	197	GLN
1	A	224	GLN
1	A	240	GLN
1	A	305	HIS
1	A	384	ASN
1	A	407	HIS
2	B	90	ASN
2	B	110	ASN
2	B	150	ASN
2	B	180	ASN
2	B	206	GLN
2	B	254	GLN
2	B	337	GLN
2	B	459	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 ⓘ

10 monosaccharides 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	NAG	C	1	1,3	14,14,15	0.36	0	17,19,21	2.52	2 (11%)
3	NAG	C	2	3	14,14,15	0.36	0	17,19,21	2.38	4 (23%)
3	MAN	C	3	3	11,11,12	0.33	0	15,15,17	1.88	5 (33%)
3	MAN	C	4	3	11,11,12	0.34	0	15,15,17	1.03	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	C	5	3	11,11,12	0.49	0	15,15,17	1.14	1 (6%)
3	FUC	C	6	3	10,10,11	0.61	0	14,14,16	1.83	2 (14%)
4	NAG	D	1	4,2	14,14,15	0.33	0	17,19,21	0.97	1 (5%)
4	NAG	D	2	4	14,14,15	0.27	0	17,19,21	0.83	0
4	MAN	D	3	4	11,11,12	0.45	0	15,15,17	1.32	2 (13%)
4	FUC	D	4	4	10,10,11	0.48	0	14,14,16	0.65	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	NAG	C	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
3	MAN	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
3	FUC	C	6	3	-	-	0/1/1/1
4	NAG	D	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	MAN	D	3	4	-	1/2/19/22	0/1/1/1
4	FUC	D	4	4	-	-	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C1-O5-C5	9.34	124.71	112.19
3	C	2	NAG	C1-O5-C5	7.99	122.89	112.19
3	C	6	FUC	C1-O5-C5	5.29	125.44	112.97
3	C	3	MAN	C1-O5-C5	4.40	118.09	112.19
3	C	2	NAG	O5-C1-C2	4.11	117.65	111.29
3	C	5	MAN	C1-O5-C5	3.86	117.36	112.19
3	C	6	FUC	C1-C2-C3	3.67	114.99	109.64
4	D	3	MAN	C1-O5-C5	3.42	116.77	112.19
3	C	3	MAN	C1-C2-C3	3.35	114.52	109.64
3	C	1	NAG	O5-C1-C2	3.02	115.97	111.29
4	D	1	NAG	C1-C2-N2	2.68	114.65	110.43
4	D	3	MAN	C1-C2-C3	2.51	113.29	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	MAN	O3-C3-C4	-2.37	104.80	110.38
3	C	4	MAN	C1-C2-C3	-2.27	106.34	109.64
3	C	2	NAG	C1-C2-N2	-2.24	106.90	110.43
3	C	2	NAG	C3-C4-C5	2.05	113.95	110.23
3	C	3	MAN	O3-C3-C2	-2.04	105.89	110.05
3	C	3	MAN	O6-C6-C5	2.02	118.21	111.33

There are no chirality outliers.

All (11) torsion outliers are listed below:

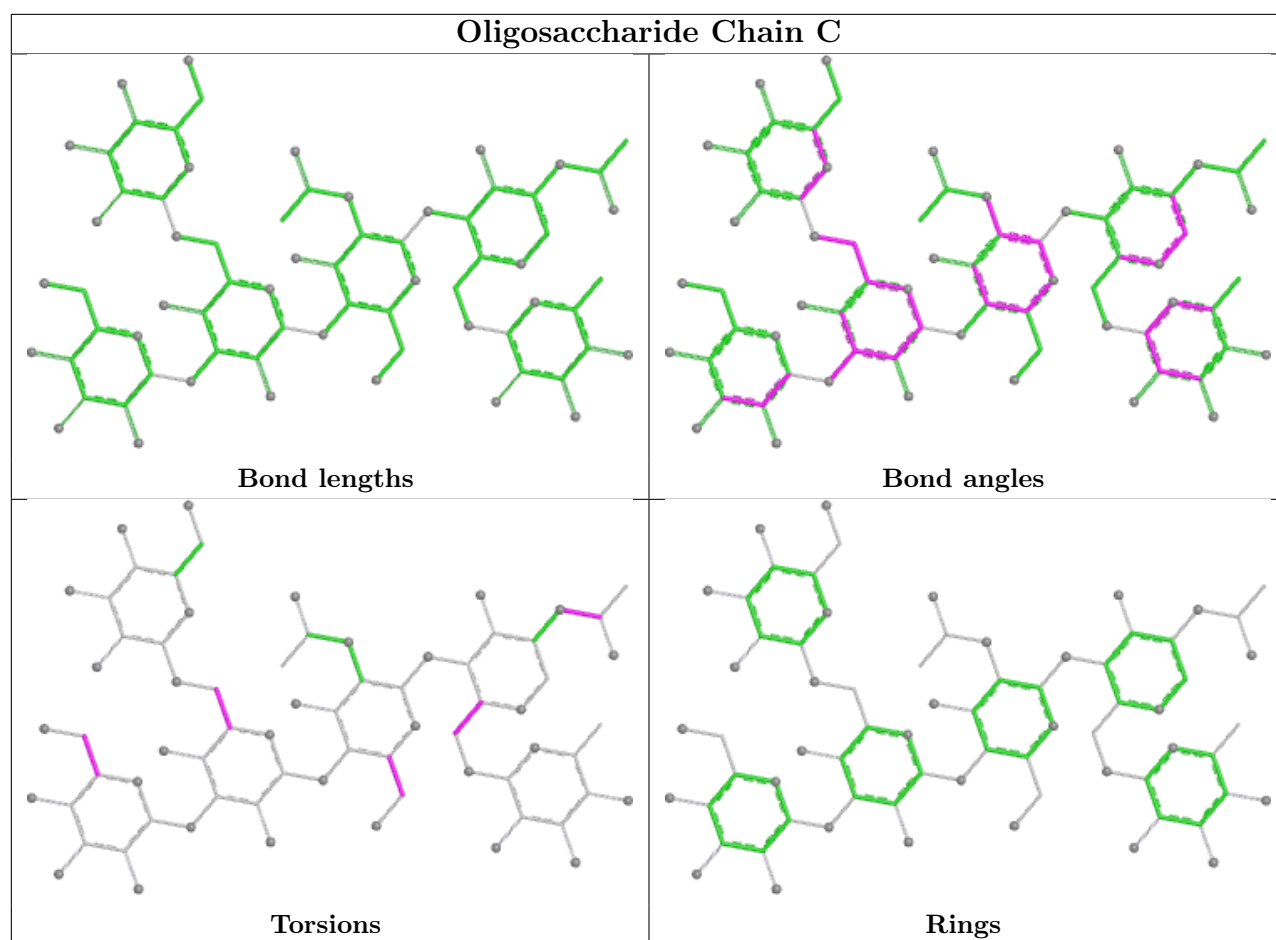
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	3	MAN	O5-C5-C6-O6
3	C	3	MAN	C4-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
3	C	1	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	D	3	MAN	O5-C5-C6-O6
3	C	4	MAN	C4-C5-C6-O6

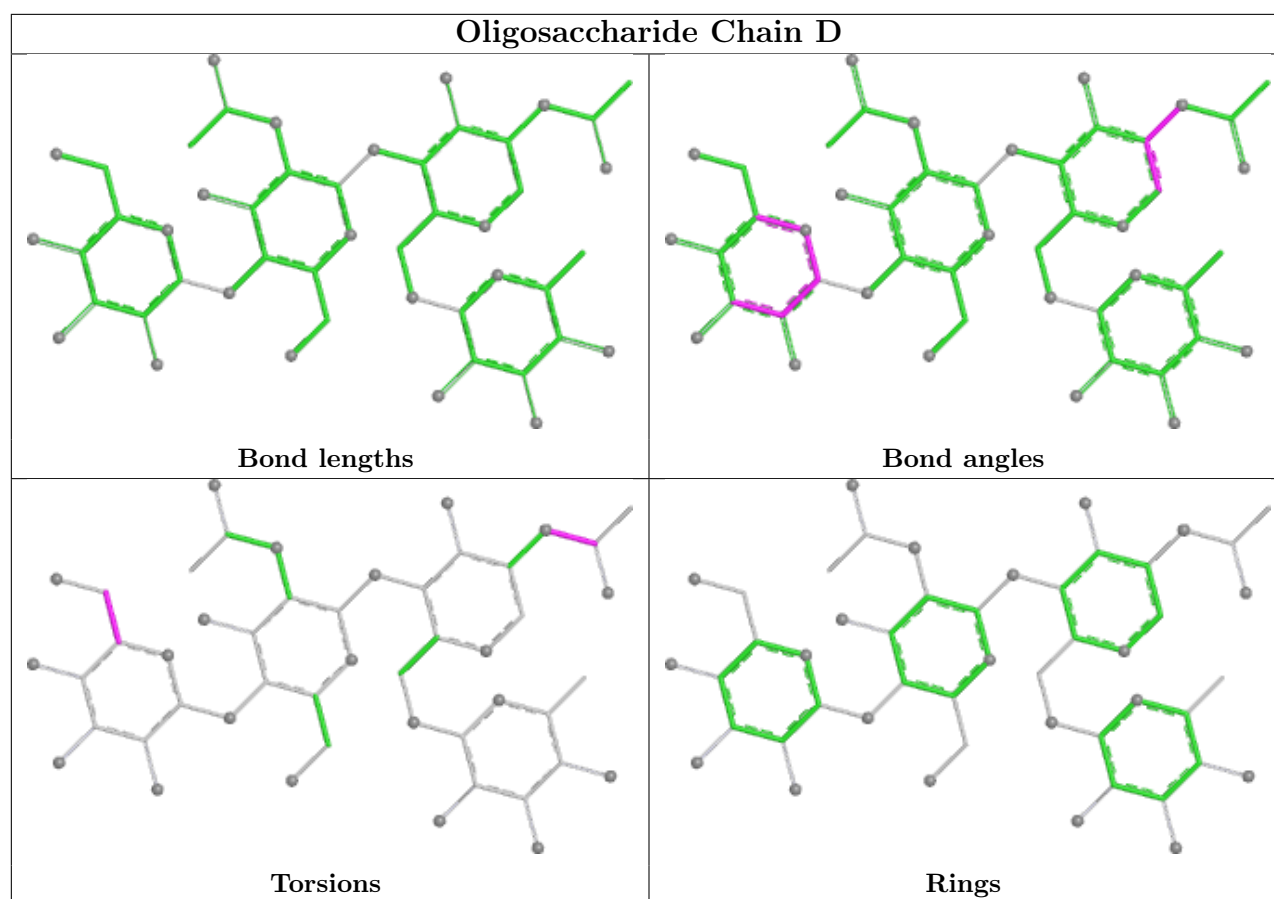
There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2	NAG	1	0
3	C	4	MAN	1	0
4	D	3	MAN	1	0
4	D	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





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	$\# Z > 2$
6	NAG	A	502	1	14,14,15	0.25	0	17,19,21	0.51	0
5	2BV	A	501	-	23,26,26	1.54	4 (17%)	26,36,36	1.51	5 (19%)

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
6	NAG	A	502	1	-	2/6/23/26	0/1/1/1
5	2BV	A	501	-	-	1/19/27/27	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	2BV	C5-C6	4.37	1.49	1.39
5	A	501	2BV	P-C11	3.01	1.82	1.79
5	A	501	2BV	C6-CL1	2.80	1.80	1.73
5	A	501	2BV	P-C12	2.77	1.82	1.79

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	2BV	C1-C2-N	2.83	113.95	108.74
5	A	501	2BV	C17-C18-C13	2.52	117.39	112.08
5	A	501	2BV	C7-C6-CL1	2.51	123.37	118.42
5	A	501	2BV	C8-C3-C4	2.32	121.42	118.74
5	A	501	2BV	C4-C5-CL2	2.08	121.85	118.45

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	2BV	C10-C9-N-C2
6	A	502	NAG	C4-C5-C6-O6
6	A	502	NAG	O5-C5-C6-O6

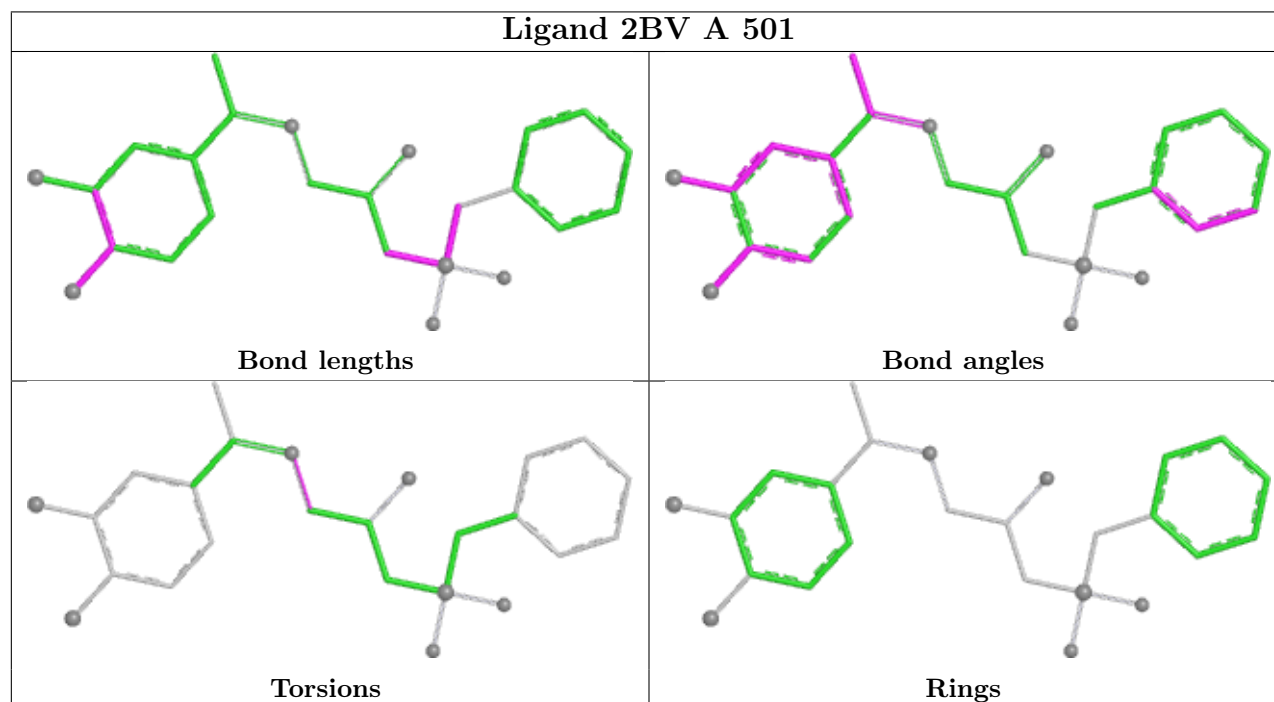
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	502	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	407/420 (96%)	0.67	71 (17%) 4 4	13, 36, 78, 90	0
2	B	403/433 (93%)	0.19	27 (6%) 24 27	11, 29, 64, 103	0
All	All	810/853 (94%)	0.43	98 (12%) 8 9	11, 33, 75, 103	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	379	SER	7.5
2	B	388	PHE	7.3
1	A	368	SER	5.6
2	B	385	ILE	4.8
1	A	222	PHE	4.5
1	A	297	GLU	4.4
2	B	378	ALA	4.4
2	B	300	SER	4.3
1	A	48	SER	4.3
2	B	386	GLN	4.1
1	A	461	TYR	4.1
1	A	291	ILE	4.0
1	A	444	SER	3.9
2	B	377	HIS	3.7
1	A	189	TRP	3.6
1	A	266	LEU	3.6
1	A	267	PHE	3.5
1	A	445	TRP	3.4
2	B	387	ASP	3.4
1	A	212	ARG	3.4
1	A	295	VAL	3.4
1	A	377	ARG	3.4
2	B	244	LYS	3.3
1	A	262	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	49	GLU	3.3
1	A	231	ALA	3.1
2	B	454	ASP	3.1
2	B	304	ARG	3.0
1	A	238	LYS	3.0
2	B	292	GLN	3.0
1	A	198	THR	2.9
1	A	451	TRP	2.9
1	A	218	ILE	2.9
1	A	340	HIS	2.9
1	A	449	ASP	2.9
1	A	458	ALA	2.9
1	A	293	CYS	2.8
1	A	460	ASP	2.8
1	A	271	TYR	2.8
2	B	66	LYS	2.8
1	A	452	ILE	2.8
1	A	220	ILE	2.7
2	B	53	SER	2.7
1	A	216	ALA	2.7
1	A	223	ARG	2.7
1	A	261	VAL	2.7
1	A	450	LYS	2.6
1	A	448	THR	2.6
1	A	455	SER	2.6
1	A	269	LYS	2.6
1	A	294	THR	2.5
1	A	237	LEU	2.5
2	B	301	ARG	2.5
2	B	223	ASP	2.5
1	A	211	GLU	2.5
2	B	373	MET	2.5
1	A	265	ARG	2.5
2	B	89	ARG	2.5
1	A	268	GLY	2.5
1	A	443	LEU	2.4
1	A	234	VAL	2.4
1	A	129	CYS	2.4
1	A	446	SER	2.4
1	A	50	ARG	2.4
1	A	235	LYS	2.4
1	A	292	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	244	ILE	2.4
1	A	321	ILE	2.3
2	B	90	ASN	2.3
1	A	232	VAL	2.3
2	B	68	VAL	2.3
1	A	233	PRO	2.3
1	A	447	LYS	2.3
1	A	187	TRP	2.3
1	A	242	ALA	2.2
2	B	69	ALA	2.2
1	A	221	THR	2.2
1	A	392	ILE	2.2
1	A	213	VAL	2.2
1	A	259	CYS	2.2
2	B	65	THR	2.2
2	B	391	THR	2.2
2	B	394	THR	2.2
2	B	376	LEU	2.1
1	A	338	LYS	2.1
1	A	230	PRO	2.1
1	A	245	ILE	2.1
1	A	243	ARG	2.1
1	A	225	SER	2.1
1	A	438	SER	2.1
1	A	327	GLN	2.1
2	B	126	ASN	2.1
1	A	239	ARG	2.1
2	B	245	GLY	2.1
1	A	224	GLN	2.0
1	A	191	LYS	2.0
1	A	278	TRP	2.0
1	A	263	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

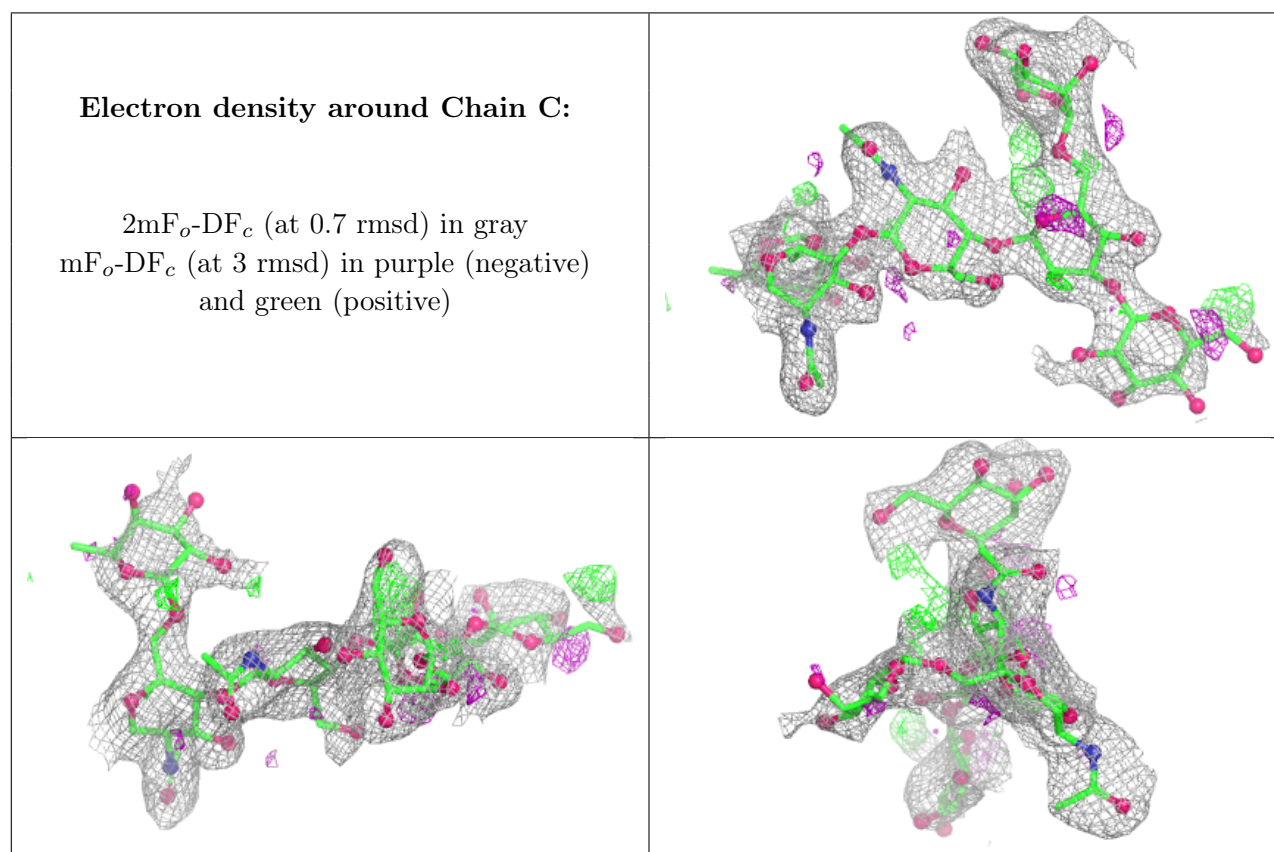
6.3 Carbohydrates [i](#)

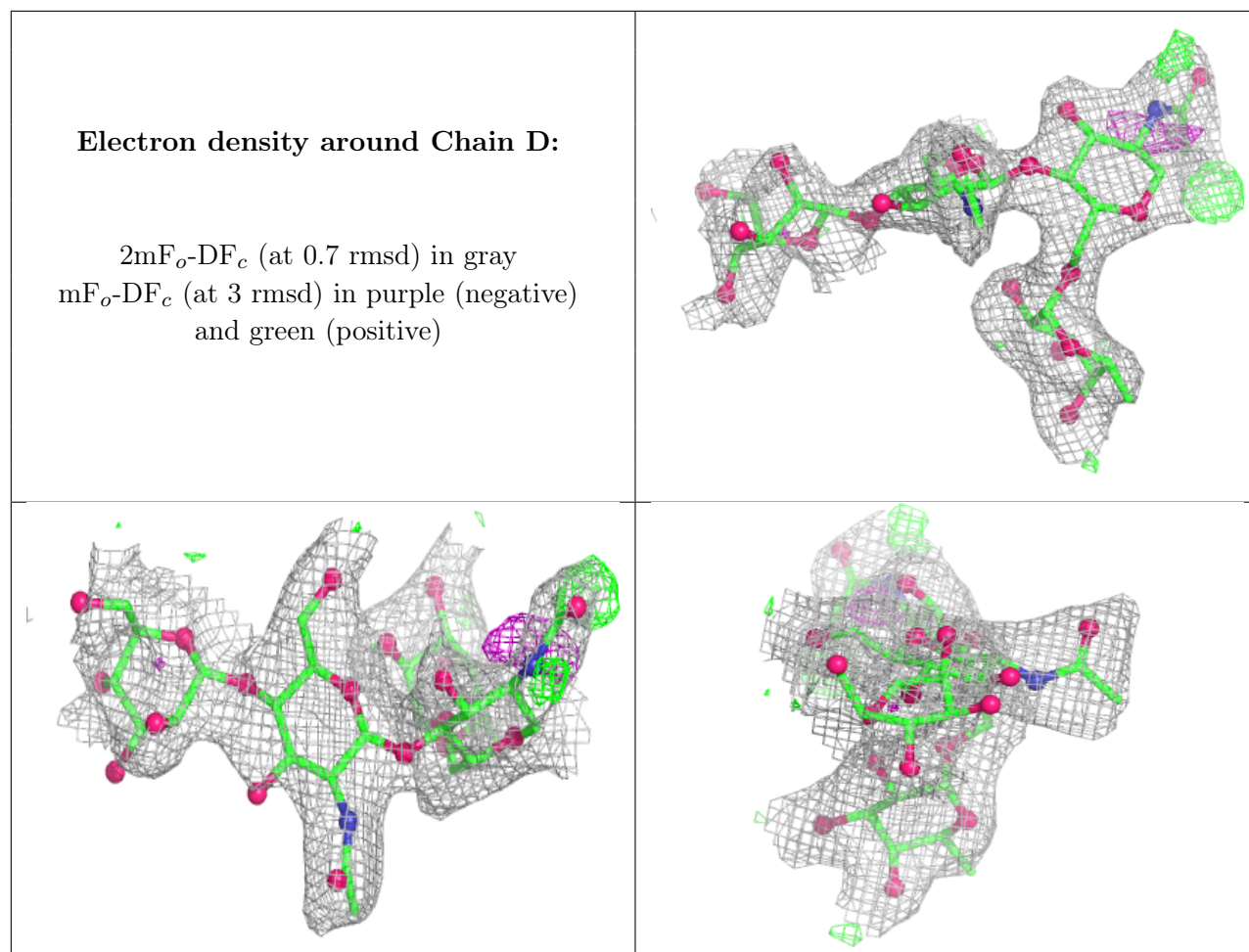
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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(Å ²)	Q<0.9
4	MAN	D	3	11/12	0.34	0.14	86,87,89,90	0
3	MAN	C	4	11/12	0.49	0.22	81,83,83,84	0
3	FUC	C	6	10/11	0.53	0.22	79,83,85,87	0
3	MAN	C	3	11/12	0.58	0.22	71,75,78,81	0
4	NAG	D	2	14/15	0.75	0.12	64,72,77,82	0
4	NAG	D	1	14/15	0.75	0.14	49,54,61,63	0
3	MAN	C	5	11/12	0.76	0.15	66,71,73,73	0
3	NAG	C	2	14/15	0.86	0.13	55,58,61,68	0
3	NAG	C	1	14/15	0.86	0.12	46,48,64,72	0
4	FUC	D	4	10/11	0.90	0.11	51,55,56,56	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





6.4 Ligands [i](#)

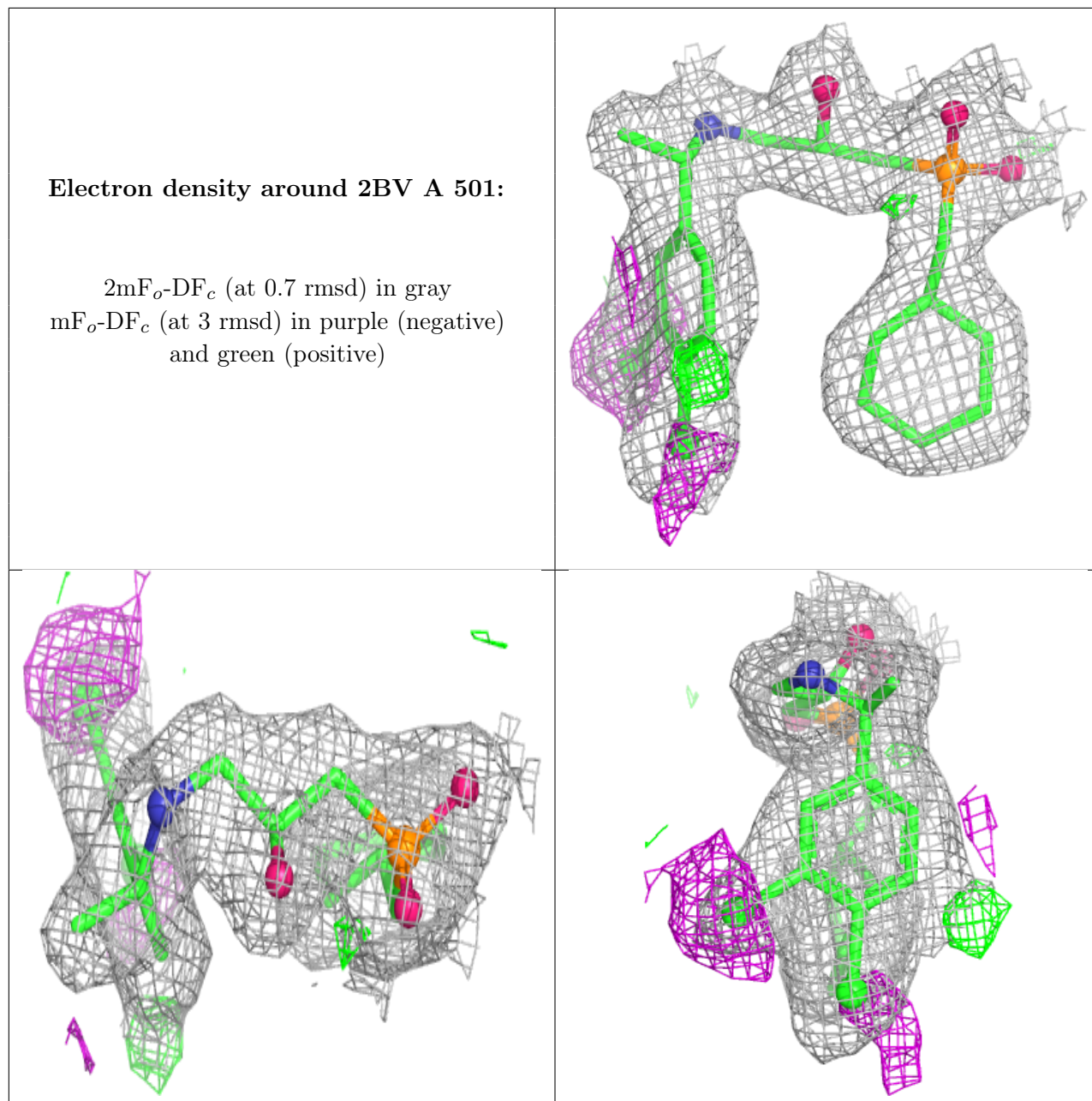
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	A	502	14/15	0.78	0.13	54,61,68,71	0
5	2BV	A	501	25/25	0.94	0.08	14,24,38,50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 2BV A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.