



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:43 AM UTC

PDB ID : 9CPQ / pdb_00009cpq
Title : Crystal structure of SARS-CoV-2 receptor binding domain in complex with antibodies M22-44 and CC12.3
Authors : Feng, Z.; Wilson, I.A.
Deposited on : 2024-07-18
Resolution : 2.88 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
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

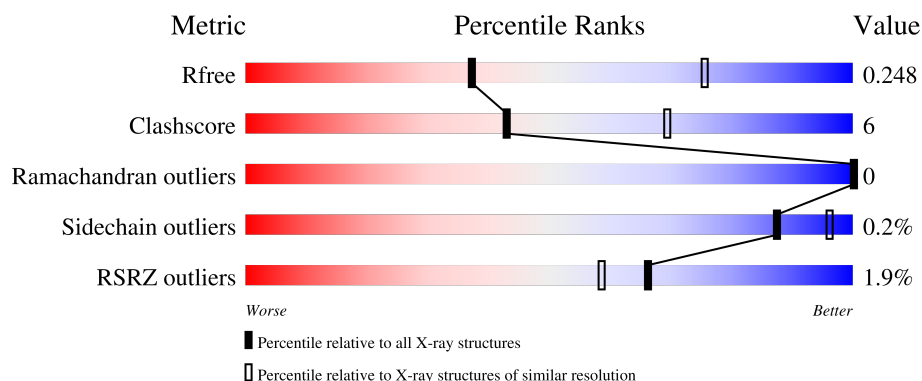
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	205	3% 78% 16% 6%
2	F	220	2% 84% 15% .
3	G	214	4% 86% 13% .
4	H	222	82% 17% .
5	L	220	86% 13% .

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Mol	Chain	Length	Quality of chain
6	B	3	33% 67%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8196 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	0	0
			1527	979	254	286	8			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	531	GLY	-	expression tag	UNP P0DTC2
A	532	HIS	-	expression tag	UNP P0DTC2
A	533	HIS	-	expression tag	UNP P0DTC2
A	534	HIS	-	expression tag	UNP P0DTC2
A	535	HIS	-	expression tag	UNP P0DTC2
A	536	HIS	-	expression tag	UNP P0DTC2
A	537	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called CC12.3 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	218	Total	C	N	O	S	0	0	0
			1632	1034	270	322	6			

- Molecule 3 is a protein called CC12.3 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	212	Total	C	N	O	S	0	0	0
			1626	1016	278	328	4			

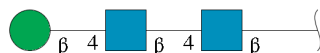
- Molecule 4 is a protein called M22-44 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	220	Total	C	N	O	S	0	0	0
			1636	1039	266	323	8			

- Molecule 5 is a protein called M22-44 Fab light chain.

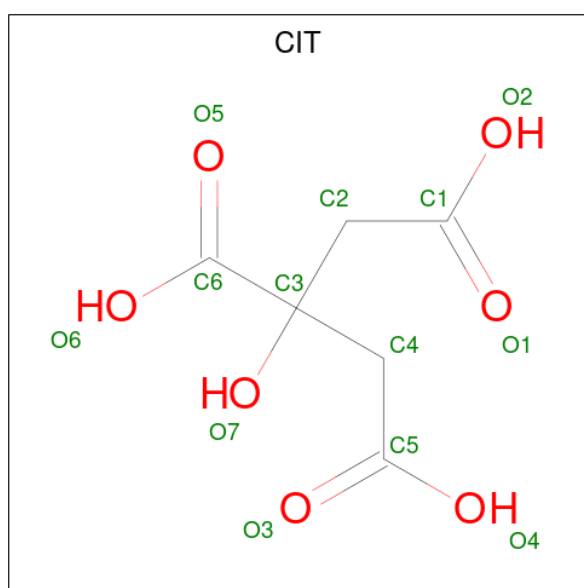
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	217	Total	C	N	O	S	0	0	0
			1690	1063	280	343	4			

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 7 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	6	7		
7	A	1	Total	C	O	0	0
			13	6	7		
7	A	1	Total	C	O	0	0
			13	6	7		

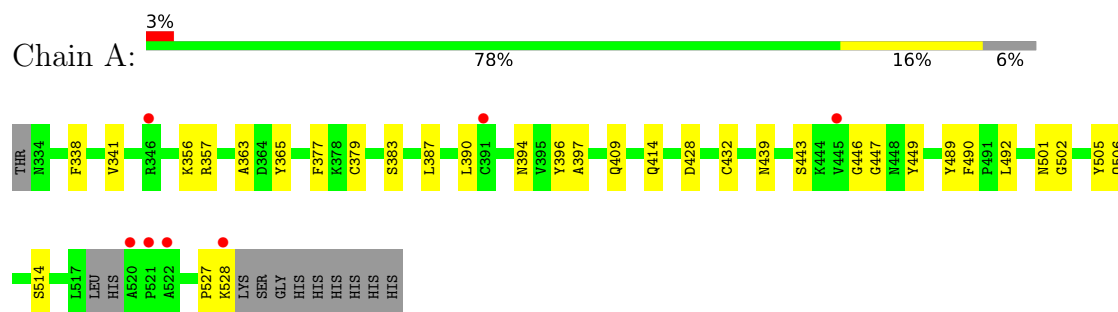
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total 1	O 1	0	0
8	G	2	Total 2	O 2	0	0
8	H	2	Total 2	O 2	0	0
8	L	2	Total 2	O 2	0	0

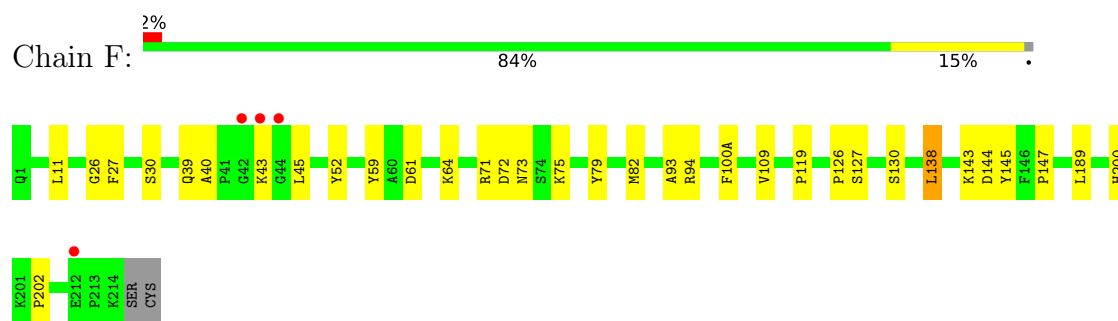
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

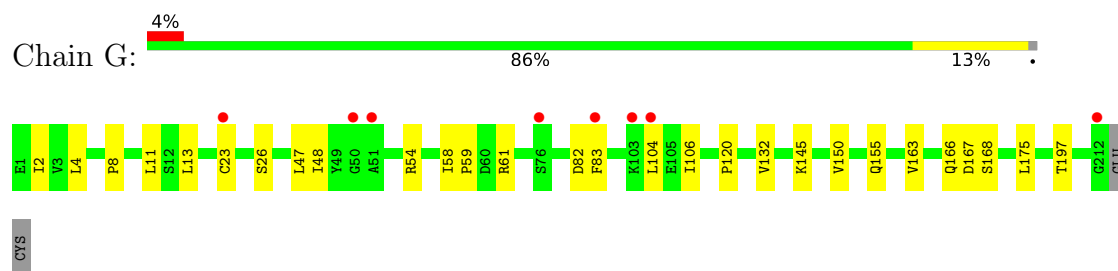
- Molecule 1: Spike protein S1



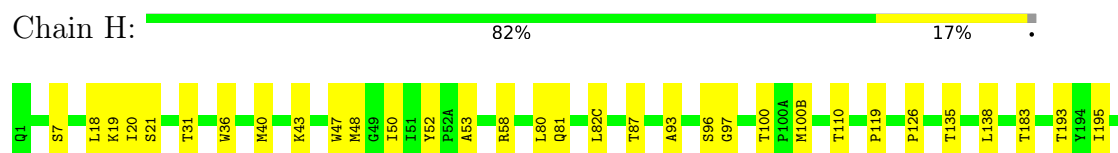
- Molecule 2: CC12.3 Fab heavy chain

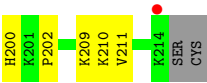


- Molecule 3: CC12.3 Fab light chain

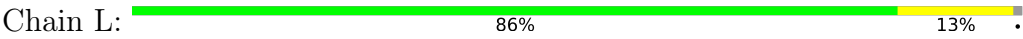


- Molecule 4: M22-44 Fab heavy chain

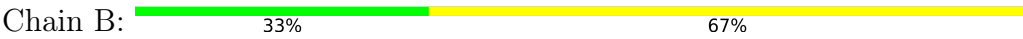




• Molecule 5: M22-44 Fab light chain



• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	109.92Å 109.92Å 225.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.88 49.39 – 2.88	Depositor EDS
% Data completeness (in resolution range)	95.1 (49.39-2.88) 95.2 (49.39-2.88)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.21rc1_5127: ???)	Depositor
R, R_{free}	0.202 , 0.251 0.201 , 0.248	Depositor DCC
R_{free} test set	2000 reflections (6.23%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8196	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, CIT

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	0.12	0/1569	0.27	0/2133
2	F	0.13	0/1672	0.27	0/2276
3	G	0.14	0/1661	0.30	0/2254
4	H	0.12	0/1677	0.29	0/2284
5	L	0.13	0/1728	0.31	0/2350
All	All	0.13	0/8307	0.29	0/11297

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1527	0	1446	22	0
2	F	1632	0	1594	21	0
3	G	1626	0	1586	19	0
4	H	1636	0	1619	24	0
5	L	1690	0	1640	18	0
6	B	39	0	34	0	0
7	A	39	0	15	2	0
8	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	2	0	0	0	0
8	H	2	0	0	0	0
8	L	2	0	0	1	0
All	All	8196	0	7934	100	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 6.

All (100) 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)
4:H:126:PRO:HG3	4:H:138:LEU:HB3	1.59	0.85
2:F:126:PRO:HG3	2:F:138:LEU:HB3	1.61	0.83
2:F:11:LEU:HB2	2:F:147:PRO:HG3	1.70	0.74
5:L:6:GLN:O	5:L:100:GLN:NE2	2.23	0.70
3:G:106:ILE:H	3:G:166:GLN:HE22	1.38	0.69
4:H:20:ILE:HD11	4:H:80:LEU:HD23	1.78	0.66
2:F:59:TYR:HB2	2:F:64:LYS:HG3	1.77	0.65
1:A:489:TYR:OH	2:F:94:ARG:NH2	2.31	0.64
2:F:30:SER:HB3	2:F:73:ASN:HD22	1.65	0.62
3:G:8:PRO:HG3	3:G:11:LEU:HD12	1.82	0.61
1:A:383:SER:HG	4:H:96:SER:HG	1.47	0.61
3:G:2:ILE:HG13	3:G:26:SER:HB3	1.82	0.61
3:G:150:VAL:HB	3:G:155:GLN:HE21	1.66	0.60
3:G:83:PHE:HA	3:G:104:LEU:HB3	1.84	0.60
3:G:106:ILE:H	3:G:166:GLN:NE2	1.99	0.59
2:F:82:MET:HE1	2:F:109:VAL:HG21	1.85	0.59
2:F:30:SER:HB3	2:F:73:ASN:ND2	2.18	0.59
4:H:87:THR:HG23	4:H:110:THR:HA	1.84	0.59
1:A:409:GLN:HA	1:A:414:GLN:HG2	1.85	0.58
1:A:490:PHE:HD1	1:A:492:LEU:H	1.51	0.58
3:G:120:PRO:HD3	3:G:132:VAL:HG22	1.87	0.56
2:F:93:ALA:HB1	2:F:100(A):PHE:HB3	1.89	0.55
1:A:490:PHE:HE1	1:A:492:LEU:HB2	1.72	0.54
4:H:200:HIS:CD2	4:H:202:PRO:HD2	2.43	0.54
1:A:365:TYR:CD1	1:A:387:LEU:HB3	2.43	0.53
3:G:163:VAL:HG22	3:G:175:LEU:HD12	1.91	0.53
1:A:356:LYS:HB3	1:A:397:ALA:HB3	1.90	0.53
5:L:160:GLN:NE2	8:L:301:HOH:O	2.42	0.52
1:A:338:PHE:HE2	1:A:363:ALA:HB1	1.74	0.52
1:A:490:PHE:CE1	1:A:492:LEU:HB2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:LEU:HD23	1:A:390:LEU:HD12	1.90	0.52
1:A:439:ASN:O	1:A:443:SER:OG	2.25	0.52
5:L:90:GLN:HE21	5:L:93:SER:H	1.58	0.51
2:F:72:ASP:HB2	2:F:79:TYR:HE2	1.75	0.51
2:F:200:HIS:CD2	2:F:202:PRO:HD2	2.45	0.51
4:H:19:LYS:HD2	4:H:81:GLN:HE21	1.75	0.51
3:G:83:PHE:CZ	3:G:106:ILE:HG13	2.45	0.51
4:H:48:MET:HE1	4:H:80:LEU:HD21	1.92	0.51
4:H:47:TRP:HZ2	4:H:50:ILE:HB	1.75	0.50
4:H:36:TRP:HB3	4:H:48:MET:HE2	1.94	0.50
3:G:83:PHE:CE2	3:G:106:ILE:HG13	2.46	0.50
2:F:39:GLN:HB2	2:F:45:LEU:HD23	1.94	0.50
4:H:195:ILE:HG12	4:H:210:LYS:HG3	1.93	0.49
3:G:47:LEU:C	3:G:48:ILE:HD12	2.38	0.49
3:G:59:PRO:HB2	3:G:61:ARG:HG2	1.93	0.49
3:G:61:ARG:HH22	3:G:82:ASP:CG	2.20	0.49
5:L:90:GLN:NE2	5:L:93:SER:H	2.11	0.49
1:A:396:TYR:HB2	1:A:514:SER:HB3	1.94	0.49
2:F:72:ASP:CG	2:F:75:LYS:HG3	2.38	0.48
5:L:186:TYR:O	5:L:192:TYR:OH	2.32	0.48
5:L:145:LYS:HB3	5:L:197:THR:HB	1.96	0.48
2:F:127:SER:H	2:F:130:SER:HB2	1.78	0.48
5:L:90:GLN:HG2	5:L:92:TYR:H	1.79	0.47
1:A:527:PRO:O	1:A:528:LYS:HG3	2.14	0.47
7:A:603:CIT:H42	2:F:26:GLY:HA2	1.96	0.47
4:H:135:THR:HG23	4:H:183:THR:HG23	1.95	0.47
5:L:27(D):TYR:HB3	5:L:28:ILE:HG22	1.97	0.47
3:G:4:LEU:HD22	3:G:23:CYS:SG	2.55	0.46
2:F:119:PRO:HB3	2:F:145:TYR:HB3	1.97	0.46
2:F:40:ALA:HB3	2:F:43:LYS:HB3	1.97	0.46
3:G:83:PHE:CD2	3:G:104:LEU:HD22	2.51	0.46
1:A:447:GLY:HA3	1:A:449:TYR:CE1	2.50	0.45
4:H:40:MET:HE3	4:H:43:LYS:HD2	1.98	0.45
5:L:19:ALA:HB3	5:L:75:ILE:HB	1.99	0.45
3:G:145:LYS:HB3	3:G:197:THR:HB	1.99	0.45
2:F:61:ASP:HA	2:F:64:LYS:HE3	1.99	0.45
5:L:144:ALA:HB2	5:L:198:HIS:HD2	1.83	0.44
4:H:52:TYR:CE2	4:H:53:ALA:HB3	2.52	0.44
4:H:47:TRP:CD1	4:H:100(B):MET:HE1	2.53	0.44
1:A:428:ASP:O	5:L:27(D):TYR:OH	2.36	0.44
3:G:54:ARG:HD3	3:G:58:ILE:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:18:LEU:HB2	4:H:82(C):LEU:HD11	2.00	0.43
1:A:377:PHE:CG	4:H:31:THR:HG22	2.54	0.43
1:A:446:GLY:O	1:A:449:TYR:HE1	2.01	0.43
4:H:193:THR:HB	4:H:210:LYS:HE2	2.00	0.43
4:H:93:ALA:HB1	4:H:100(B):MET:HB3	2.00	0.43
5:L:201:LEU:HD13	5:L:205:VAL:HG13	2.01	0.43
2:F:143:LYS:NZ	2:F:144:ASP:OD2	2.47	0.43
3:G:11:LEU:HD21	3:G:13:LEU:HG	2.00	0.43
3:G:167:ASP:OD1	3:G:168:SER:N	2.52	0.42
2:F:52:TYR:O	2:F:71:ARG:NH2	2.42	0.42
4:H:119:PRO:HD3	4:H:200:HIS:ND1	2.34	0.42
1:A:357:ARG:NH2	1:A:394:ASN:OD1	2.52	0.42
5:L:80:ALA:HA	5:L:106:ILE:HD11	2.01	0.42
5:L:3:GLN:HB2	5:L:26:SER:HB3	2.00	0.42
5:L:33:LEU:HB3	5:L:51:ALA:HB2	2.01	0.42
4:H:138:LEU:HD13	4:H:211:VAL:HG21	2.02	0.42
2:F:119:PRO:HD3	2:F:200:HIS:ND1	2.35	0.42
7:A:601:CIT:O2	7:A:601:CIT:O7	2.34	0.41
4:H:50:ILE:HG22	4:H:58:ARG:HB2	2.02	0.41
5:L:4:LEU:HD11	5:L:90:GLN:HB3	2.01	0.41
1:A:341:VAL:HG11	1:A:397:ALA:HB1	2.01	0.41
4:H:7:SER:HB3	4:H:21:SER:HB3	2.03	0.41
1:A:379:CYS:HA	1:A:432:CYS:HA	2.02	0.41
4:H:97:GLY:O	4:H:100:THR:OG1	2.29	0.41
1:A:502:GLY:O	1:A:506:GLN:HG3	2.21	0.41
1:A:501:ASN:HB3	1:A:505:TYR:HB2	2.02	0.41
4:H:209:LYS:NZ	5:L:123:GLU:OE2	2.54	0.41
5:L:108:ARG:HG3	5:L:109:THR:O	2.21	0.41
2:F:27:PHE:CZ	2:F:94:ARG:HD2	2.56	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	189/205 (92%)	187 (99%)	2 (1%)	0	100	100
2	F	216/220 (98%)	215 (100%)	1 (0%)	0	100	100
3	G	210/214 (98%)	203 (97%)	7 (3%)	0	100	100
4	H	218/222 (98%)	217 (100%)	1 (0%)	0	100	100
5	L	215/220 (98%)	213 (99%)	2 (1%)	0	100	100
All	All	1048/1081 (97%)	1035 (99%)	13 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	166/177 (94%)	166 (100%)	0	100	100
2	F	184/186 (99%)	182 (99%)	2 (1%)	65	86
3	G	183/185 (99%)	183 (100%)	0	100	100
4	H	185/187 (99%)	185 (100%)	0	100	100
5	L	193/195 (99%)	193 (100%)	0	100	100
All	All	911/930 (98%)	909 (100%)	2 (0%)	87	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	138	LEU
2	F	189	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	ASN
1	A	394	ASN
2	F	39	GLN

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Mol	Chain	Res	Type
2	F	81	GLN
2	F	82(A)	ASN
2	F	164	HIS
2	F	171	GLN
2	F	199	ASN
3	G	27	GLN
3	G	38	GLN
3	G	166	GLN
4	H	64	GLN
4	H	81	GLN
4	H	164	HIS
5	L	27	GLN
5	L	38	GLN
5	L	137	ASN
5	L	138	ASN
5	L	160	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 ⓘ

3 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	$\# Z > 2$
6	NAG	B	1	1,6	14,14,15	0.75	0	17,19,21	2.54	5 (29%)
6	NAG	B	2	6	14,14,15	0.75	0	17,19,21	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BMA	B	3	6	11,11,12	0.83	0	15,15,17	1.69	1 (6%)

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	B	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	B	2	6	-	1/6/23/26	0/1/1/1
6	BMA	B	3	6	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1	NAG	C2-N2-C7	7.73	133.26	122.90
6	B	3	BMA	C1-O5-C5	4.77	118.58	112.19
6	B	1	NAG	C1-C2-N2	4.60	117.67	110.43
6	B	1	NAG	O7-C7-N2	2.46	126.33	121.98
6	B	1	NAG	O3-C3-C2	-2.11	105.03	109.40
6	B	1	NAG	C4-C3-C2	2.06	114.04	111.02

There are no chirality outliers.

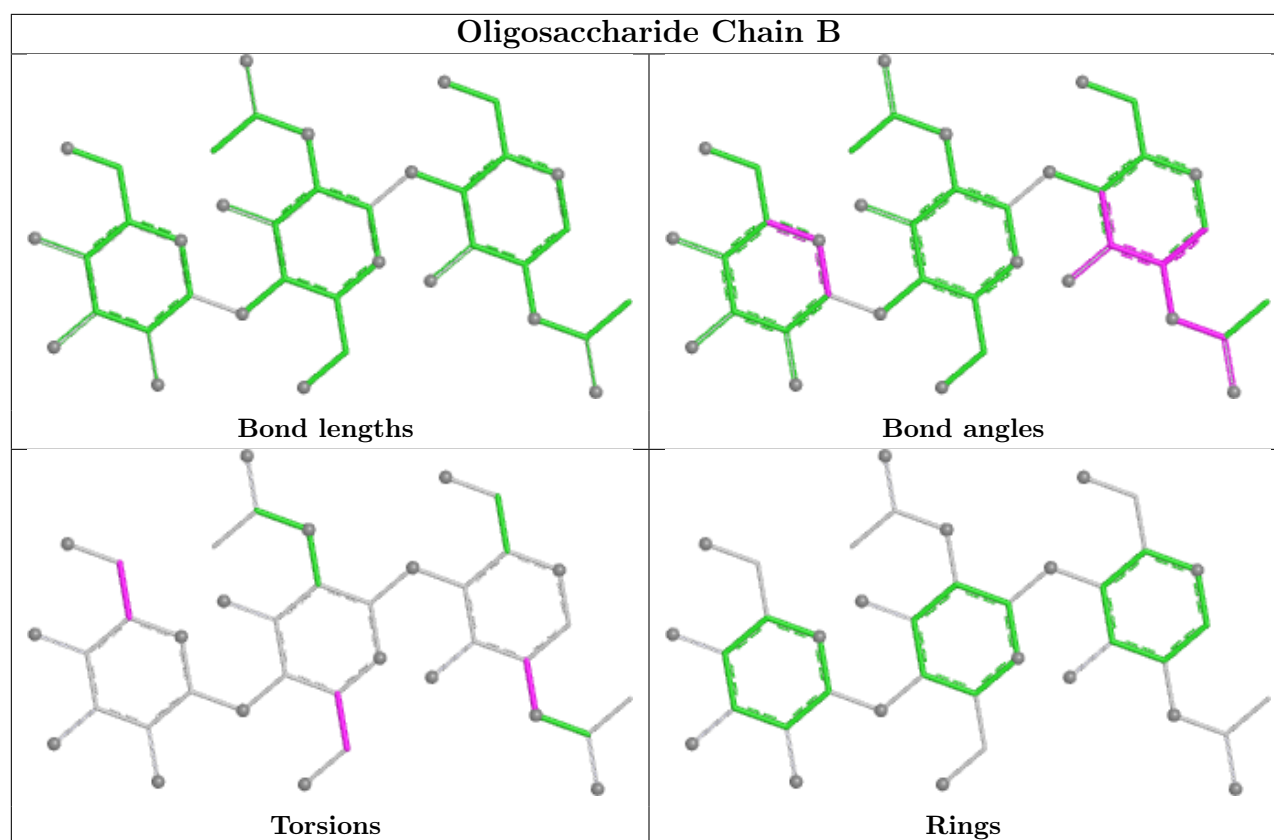
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1	NAG	C1-C2-N2-C7
6	B	2	NAG	O5-C5-C6-O6
6	B	3	BMA	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

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	$\# Z > 2$
7	CIT	A	603	-	12,12,12	1.40	1 (8%)	17,17,17	1.49	3 (17%)
7	CIT	A	602	-	12,12,12	1.53	1 (8%)	17,17,17	1.49	3 (17%)
7	CIT	A	601	-	12,12,12	1.47	1 (8%)	17,17,17	1.53	3 (17%)

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
7	CIT	A	603	-	-	10/16/16/16	-
7	CIT	A	602	-	-	3/16/16/16	-
7	CIT	A	601	-	-	9/16/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	602	CIT	C3-C6	3.70	1.57	1.53
7	A	601	CIT	C3-C6	3.43	1.57	1.53
7	A	603	CIT	C3-C6	3.02	1.56	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	601	CIT	O5-C6-C3	-3.44	115.42	122.09
7	A	603	CIT	O5-C6-C3	-3.11	116.06	122.09
7	A	601	CIT	O6-C6-C3	3.10	119.08	113.14
7	A	602	CIT	O5-C6-C3	-2.96	116.37	122.09
7	A	602	CIT	O6-C6-C3	2.87	118.65	113.14
7	A	602	CIT	O7-C3-C6	2.82	112.95	108.96
7	A	603	CIT	O6-C6-C3	2.50	117.94	113.14
7	A	603	CIT	O1-C1-C2	-2.19	116.75	122.95
7	A	601	CIT	O7-C3-C6	2.18	112.04	108.96

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	601	CIT	O7-C3-C6-O5
7	A	601	CIT	O7-C3-C6-O6
7	A	601	CIT	C4-C3-C6-O5
7	A	601	CIT	C4-C3-C6-O6
7	A	602	CIT	C1-C2-C3-C4
7	A	602	CIT	C1-C2-C3-C6
7	A	601	CIT	O1-C1-C2-C3
7	A	603	CIT	C6-C3-C4-C5
7	A	601	CIT	O2-C1-C2-C3
7	A	603	CIT	C2-C3-C6-O6
7	A	603	CIT	C4-C3-C6-O6
7	A	602	CIT	C1-C2-C3-O7
7	A	601	CIT	O7-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
7	A	603	CIT	C2-C3-C4-C5
7	A	603	CIT	O7-C3-C4-C5
7	A	601	CIT	C2-C3-C4-C5
7	A	603	CIT	C2-C3-C6-O5
7	A	603	CIT	C1-C2-C3-O7
7	A	603	CIT	O7-C3-C6-O6
7	A	603	CIT	C4-C3-C6-O5
7	A	603	CIT	O1-C1-C2-C3
7	A	601	CIT	C1-C2-C3-O7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	603	CIT	1	0
7	A	601	CIT	1	0

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	193/205 (94%)	0.06	7 (3%) 46 38	28, 47, 86, 102	0
2	F	218/220 (99%)	0.01	4 (1%) 67 60	33, 49, 83, 94	0
3	G	212/214 (99%)	0.33	8 (3%) 44 36	36, 59, 84, 111	0
4	H	220/222 (99%)	-0.09	1 (0%) 87 83	32, 47, 68, 85	0
5	L	217/220 (98%)	-0.08	0 100 100	33, 51, 72, 85	0
All	All	1060/1081 (98%)	0.04	20 (1%) 66 58	28, 51, 80, 111	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	520	ALA	3.4
3	G	50	GLY	2.8
3	G	83	PHE	2.8
3	G	76	SER	2.8
1	A	521	PRO	2.7
2	F	43	LYS	2.6
2	F	42	GLY	2.6
1	A	346	ARG	2.5
1	A	391	CYS	2.4
1	A	445	VAL	2.4
3	G	51	ALA	2.3
3	G	23	CYS	2.3
2	F	212	GLU	2.3
1	A	528	LYS	2.2
3	G	103	LYS	2.1
3	G	212	GLY	2.1
1	A	522	ALA	2.1
3	G	104	LEU	2.1
2	F	44	GLY	2.1
4	H	214	LYS	2.0

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

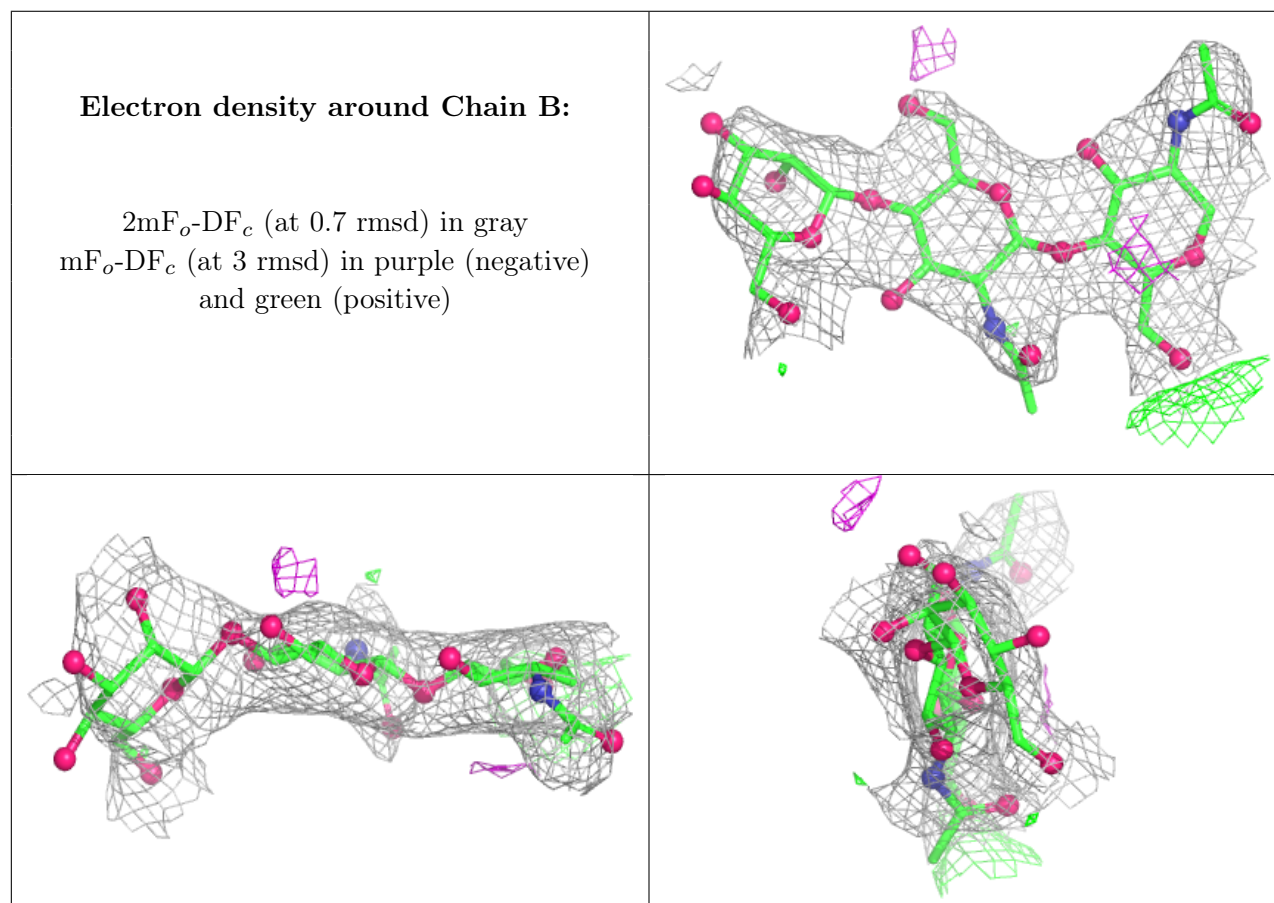
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
6	NAG	B	1	14/15	-	-	52,61,73,80	0
6	NAG	B	2	14/15	-	-	71,86,97,100	0
6	BMA	B	3	11/12	-	-	72,104,115,130	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(Å ²)	Q<0.9
7	CIT	A	601	13/13	0.76	0.15	56,79,99,100	0
7	CIT	A	603	13/13	0.79	0.13	65,75,89,90	0
7	CIT	A	602	13/13	0.86	0.13	64,71,81,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.