



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:50 AM UTC

PDB ID : 5GMQ / pdb_00005gmq
Title : Structure of MERS-CoV RBD in complex with a fully human antibody MCA1
Authors : Chen, C.; Wang, J.M.; Zou, T.T.; Gao, X.P.; Cui, S.; Jin, Q.
Deposited on : 2016-07-15
Resolution : 2.70 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

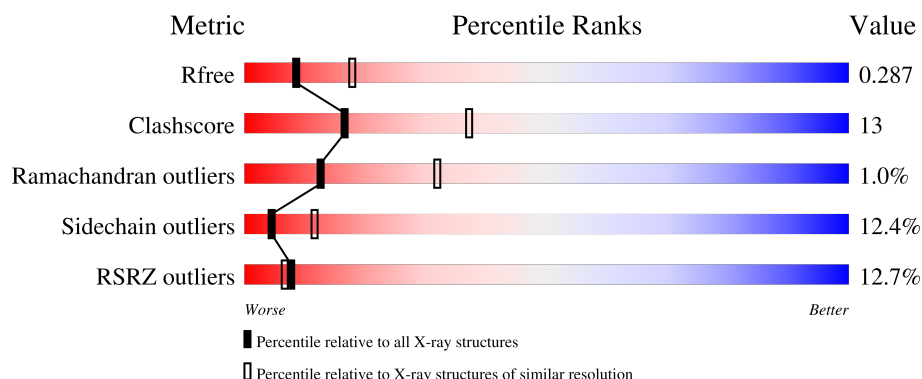
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	229	 4% 67% 20% 10%
2	B	231	 15% 63% 29% 5%
3	C	215	 18% 62% 32% 2%
4	D	3	 67% 33%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4919 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 S protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1585	1012	253	309	11			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	366	MET	-	initiating methionine	UNP V5RDT9
A	589	HIS	-	expression tag	UNP V5RDT9
A	590	HIS	-	expression tag	UNP V5RDT9
A	591	HIS	-	expression tag	UNP V5RDT9
A	592	HIS	-	expression tag	UNP V5RDT9
A	593	HIS	-	expression tag	UNP V5RDT9
A	594	HIS	-	expression tag	UNP V5RDT9

- Molecule 2 is a protein called MCA1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	225	Total	C	N	O	S	0	0	0
			1671	1052	278	334	7			

- Molecule 3 is a protein called MCA1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	209	Total	C	N	O	S	0	0	0
			1607	1003	273	327	4			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			36	20	1	15			

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	2	2		

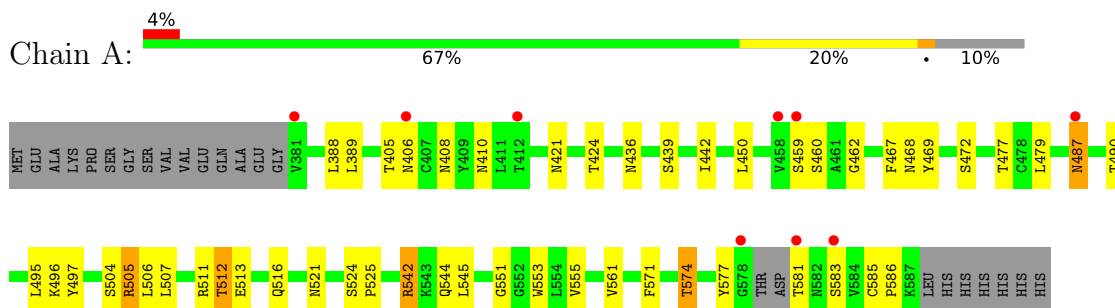
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total	O	0	0
			5	5		
6	B	3	Total	O	0	0
			3	3		
6	C	8	Total	O	0	0
			8	8		

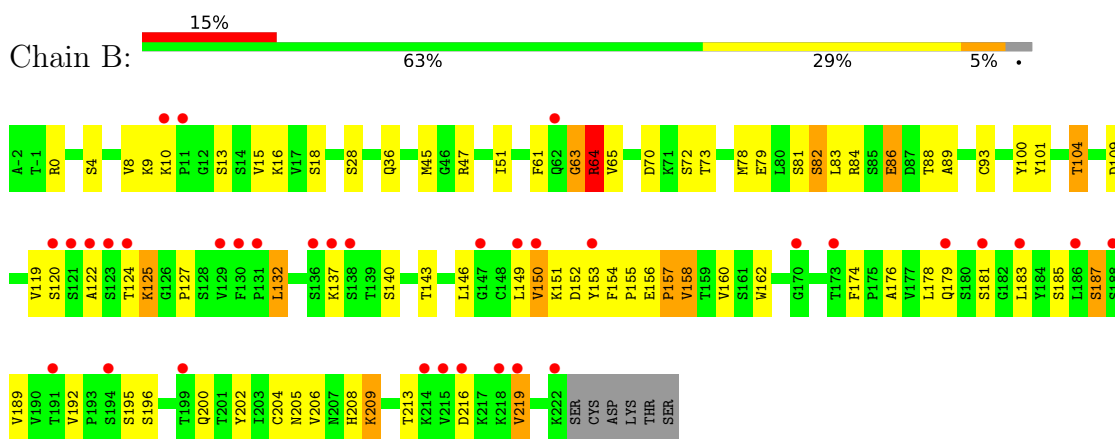
3 Residue-property plots [i](#)

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.

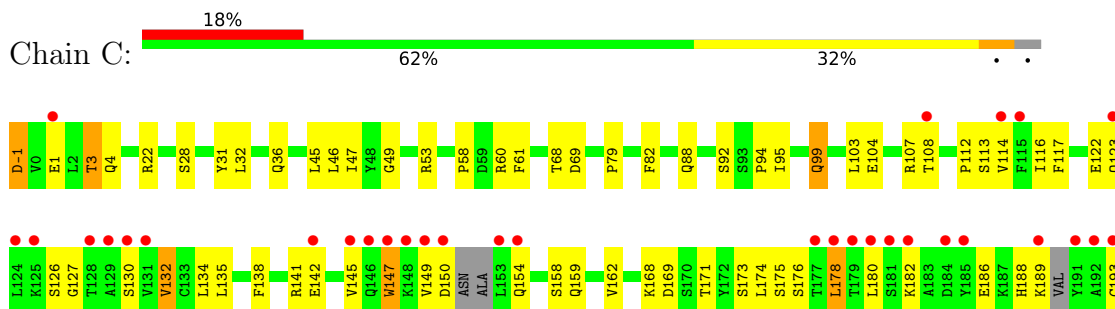
- Molecule 1: S protein

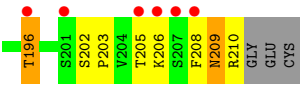


- Molecule 2: MCA1 heavy chain



- Molecule 3: MCA1 light chain





- Molecule 4: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.46Å 153.46Å 97.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.33 – 2.70 40.33 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.33-2.70) 99.3 (40.33-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.239 , 0.285 0.245 , 0.287	Depositor DCC
R_{free} test set	1733 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	59.3	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4919	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: EDO, MAN, NAG

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	0.53	0/1623	0.55	0/2214
2	B	0.47	1/1709 (0.1%)	0.66	3/2325 (0.1%)
3	C	0.46	0/1640	0.65	0/2223
All	All	0.49	1/4972 (0.0%)	0.62	3/6762 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	93	CYS	CB-SG	-5.08	1.64	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	63	GLY	N-CA-C	-7.08	96.40	113.18
2	B	63	GLY	CA-C-N	6.43	133.27	121.70
2	B	63	GLY	C-N-CA	6.43	133.27	121.70

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	1585	0	1551	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1671	0	1644	57	0
3	C	1607	0	1557	53	0
4	D	36	0	31	1	0
5	C	4	0	6	2	0
6	A	5	0	0	1	0
6	B	3	0	0	0	0
6	C	8	0	0	0	0
All	All	4919	0	4789	125	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 13.

All (125) 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)
3:C:53:ARG:NH1	3:C:61:PHE:O	1.94	1.01
2:B:137:LYS:HB3	3:C:206:LYS:HZ3	1.29	0.98
3:C:116:ILE:H	3:C:206:LYS:HZ2	0.97	0.97
2:B:125:LYS:NZ	2:B:152:ASP:O	1.99	0.94
3:C:116:ILE:N	3:C:206:LYS:HZ2	1.66	0.94
3:C:116:ILE:H	3:C:206:LYS:NZ	1.67	0.91
2:B:63:GLY:HA3	2:B:64:ARG:HB2	1.54	0.86
2:B:45:MET:HE1	2:B:78:MET:HE3	1.60	0.83
2:B:137:LYS:HB3	3:C:206:LYS:NZ	1.96	0.81
3:C:188:HIS:O	3:C:210:ARG:NH2	2.15	0.78
1:A:389:LEU:O	1:A:490:THR:OG1	2.05	0.73
2:B:88:THR:HB	2:B:119:VAL:HG22	1.71	0.72
2:B:178:LEU:O	3:C:159:GLN:NE2	2.24	0.70
3:C:107:ARG:HD3	3:C:108:THR:O	1.92	0.69
1:A:477:THR:HG22	1:A:574:THR:HB	1.75	0.69
2:B:10:LYS:O	2:B:13:SER:OG	2.09	0.68
2:B:84:ARG:HD2	2:B:86:GLU:HG2	1.78	0.66
1:A:497:TYR:HB2	1:A:561:VAL:HB	1.77	0.66
2:B:45:MET:HE1	2:B:78:MET:CE	2.25	0.66
1:A:487:ASN:OD1	1:A:487:ASN:N	2.23	0.65
3:C:4:GLN:O	3:C:99:GLN:NE2	2.33	0.62
2:B:196:SER:HB2	2:B:200:GLN:HB3	1.83	0.60
3:C:209:ASN:N	3:C:209:ASN:OD1	2.32	0.60
2:B:154:PHE:HB2	2:B:183:LEU:HD22	1.86	0.58
2:B:65:VAL:HA	2:B:79:GLU:O	2.04	0.57
1:A:467:PHE:O	1:A:524:SER:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:PRO:HB2	2:B:150:VAL:HG23	1.86	0.56
2:B:84:ARG:O	2:B:119:VAL:HG21	2.05	0.56
2:B:162:TRP:CH2	2:B:204:CYS:HB3	2.40	0.56
3:C:116:ILE:HG22	3:C:206:LYS:NZ	2.20	0.56
2:B:82:SER:O	2:B:82:SER:OG	2.22	0.56
2:B:149:LEU:HD23	2:B:151:LYS:HB2	1.88	0.55
3:C:107:ARG:NH1	3:C:169:ASP:O	2.39	0.55
2:B:158:VAL:HG13	2:B:208:HIS:CD2	2.41	0.55
3:C:123:GLN:O	3:C:126:SER:OG	2.25	0.55
1:A:542:ARG:HG3	1:A:553:TRP:CE3	2.42	0.54
2:B:63:GLY:CA	2:B:64:ARG:HB2	2.30	0.54
3:C:182:LYS:O	3:C:186:GLU:HG3	2.07	0.54
1:A:505:ARG:HE	1:A:545:LEU:HD12	1.73	0.54
3:C:189:LYS:HG2	3:C:210:ARG:HB3	1.90	0.54
2:B:127:PRO:HD2	2:B:213:THR:HG21	1.91	0.53
3:C:107:ARG:NH1	3:C:171:THR:HG22	2.23	0.52
2:B:101:TYR:O	2:B:104:THR:HB	2.08	0.52
2:B:70:ASP:OD1	2:B:72:SER:OG	2.27	0.52
3:C:188:HIS:HD2	3:C:189:LYS:H	1.58	0.52
2:B:151:LYS:HG2	2:B:152:ASP:CG	2.35	0.52
1:A:436:ASN:ND2	1:A:577:TYR:OH	2.39	0.52
2:B:9:LYS:O	2:B:119:VAL:HA	2.10	0.52
3:C:127:GLY:HA2	3:C:182:LYS:HB2	1.93	0.51
3:C:1:GLU:OE2	3:C:3:THR:OG1	2.24	0.51
1:A:505:ARG:NH2	1:A:551:GLY:O	2.32	0.51
3:C:36:GLN:HB2	3:C:46:LEU:HD11	1.93	0.51
2:B:78:MET:SD	2:B:78:MET:C	2.94	0.51
1:A:542:ARG:HD2	2:B:100:TYR:CD2	2.46	0.50
3:C:147:TRP:HD1	3:C:193:CYS:HA	1.76	0.50
3:C:196:THR:HG23	3:C:203:PRO:HG3	1.93	0.50
3:C:112:PRO:HB3	3:C:138:PHE:HB3	1.93	0.50
3:C:46:LEU:O	3:C:47:ILE:HD13	2.12	0.50
3:C:188:HIS:H	3:C:210:ARG:NH2	2.09	0.50
2:B:160:VAL:HG22	2:B:206:VAL:HG22	1.94	0.49
2:B:132:LEU:CD1	2:B:149:LEU:HB2	2.42	0.49
1:A:460:SER:C	1:A:462:GLY:H	2.20	0.49
3:C:45:LEU:O	5:C:301:EDO:O2	2.30	0.49
1:A:410:ASN:ND2	6:A:701:HOH:O	2.45	0.49
2:B:109:ASP:HB2	5:C:301:EDO:H22	1.94	0.48
2:B:4:SER:HB3	2:B:18:SER:OG	2.14	0.48
2:B:36:GLN:C	2:B:89:ALA:HB1	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:132:VAL:HA	3:C:176:SER:O	2.13	0.48
2:B:61:PHE:O	2:B:65:VAL:HG12	2.13	0.48
3:C:188:HIS:CD2	3:C:189:LYS:H	2.32	0.48
2:B:0:ARG:HB3	2:B:0:ARG:CZ	2.43	0.48
3:C:130:SER:HA	3:C:178:LEU:O	2.14	0.48
2:B:8:VAL:HG21	2:B:155:PRO:HG3	1.96	0.47
3:C:-1:ASP:HB3	3:C:94:PRO:HD2	1.95	0.47
2:B:156:GLU:OE2	2:B:176:ALA:HB3	2.14	0.47
2:B:127:PRO:HB3	2:B:153:TYR:HB3	1.95	0.47
3:C:174:LEU:HD23	3:C:175:SER:N	2.30	0.47
3:C:113:SER:O	3:C:135:LEU:HA	2.15	0.47
2:B:189:VAL:HG21	3:C:134:LEU:HD11	1.97	0.47
3:C:116:ILE:HG22	3:C:206:LYS:HZ2	1.80	0.47
1:A:388:LEU:HD11	1:A:571:PHE:CE1	2.50	0.46
2:B:152:ASP:OD1	2:B:179:GLN:NE2	2.43	0.46
3:C:186:GLU:HA	3:C:210:ARG:NH2	2.31	0.46
3:C:58:PRO:HB3	3:C:60:ARG:NH1	2.31	0.45
2:B:84:ARG:HD2	2:B:86:GLU:CG	2.45	0.45
2:B:137:LYS:HD2	3:C:206:LYS:HE2	1.99	0.45
2:B:64:ARG:NH2	2:B:81:SER:O	2.47	0.45
2:B:205:ASN:ND2	2:B:216:ASP:OD1	2.50	0.45
1:A:507:LEU:HD12	1:A:512:THR:OG1	2.18	0.44
3:C:28:SER:HB3	3:C:31:TYR:CD2	2.52	0.44
3:C:158:SER:O	3:C:159:GLN:HG3	2.18	0.44
2:B:45:MET:HE3	2:B:45:MET:HB3	1.83	0.44
2:B:209:LYS:H	2:B:209:LYS:HG2	1.44	0.44
2:B:146:LEU:HD13	2:B:219:VAL:HG21	1.98	0.44
3:C:127:GLY:O	3:C:182:LYS:N	2.38	0.44
3:C:147:TRP:CD1	3:C:193:CYS:HA	2.52	0.44
1:A:504:SER:HB3	1:A:513:GLU:HG2	1.99	0.44
1:A:421:ASN:HA	4:D:3:MAN:H4	2.00	0.43
2:B:174:PHE:HD2	2:B:187:SER:O	2.01	0.43
3:C:28:SER:HB3	3:C:31:TYR:HD2	1.82	0.43
1:A:505:ARG:NE	1:A:545:LEU:HD12	2.33	0.43
1:A:544:GLN:HB2	1:A:553:TRP:CZ3	2.53	0.43
2:B:15:VAL:O	2:B:79:GLU:HA	2.18	0.43
1:A:405:THR:HG22	1:A:439:SER:O	2.19	0.43
3:C:159:GLN:O	3:C:176:SER:HA	2.19	0.43
3:C:188:HIS:H	3:C:210:ARG:HH22	1.67	0.43
2:B:158:VAL:HG13	2:B:208:HIS:HD2	1.83	0.42
2:B:174:PHE:HE1	3:C:173:SER:O	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:GLN:HB3	1:A:525:PRO:HG2	2.02	0.42
2:B:36:GLN:O	2:B:89:ALA:HB1	2.20	0.42
1:A:406:ASN:HA	1:A:583:SER:HB3	2.02	0.42
1:A:472:SER:HB2	1:A:521:ASN:HD21	1.85	0.42
2:B:153:TYR:HD2	2:B:208:HIS:HE2	1.68	0.42
2:B:0:ARG:CB	2:B:0:ARG:NH1	2.84	0.41
2:B:156:GLU:OE1	2:B:157:PRO:HA	2.21	0.41
3:C:88:GLN:HE21	3:C:95:ILE:HG21	1.85	0.41
2:B:192:VAL:HG11	2:B:202:TYR:CE1	2.56	0.41
2:B:122:ALA:HB1	2:B:183:LEU:HD21	2.02	0.41
3:C:147:TRP:HE1	3:C:193:CYS:HB2	1.86	0.41
3:C:107:ARG:HH12	3:C:171:THR:CG2	2.34	0.41
1:A:408:ASN:HA	1:A:585:CYS:O	2.21	0.40
3:C:47:ILE:CD1	3:C:53:ARG:HG3	2.51	0.40
2:B:132:LEU:HD23	3:C:117:PHE:CD2	2.57	0.40
3:C:186:GLU:HA	3:C:210:ARG:CZ	2.51	0.40
3:C:79:PRO:O	3:C:82:PHE:HD2	2.04	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	201/229 (88%)	188 (94%)	11 (6%)	2 (1%)	12	32
2	B	223/231 (96%)	201 (90%)	20 (9%)	2 (1%)	14	35
3	C	203/215 (94%)	189 (93%)	12 (6%)	2 (1%)	12	32
All	All	627/675 (93%)	578 (92%)	43 (7%)	6 (1%)	12	32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	469	TYR
2	B	64	ARG
3	C	154	GLN
1	A	586	PRO
3	C	49	GLY
2	B	157	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	187/207 (90%)	170 (91%)	17 (9%)	9	22
2	B	186/193 (96%)	162 (87%)	24 (13%)	4	10
3	C	182/186 (98%)	154 (85%)	28 (15%)	2	7
All	All	555/586 (95%)	486 (88%)	69 (12%)	4	11

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	424	THR
1	A	442	ILE
1	A	450	LEU
1	A	459	SER
1	A	468	ASN
1	A	479	LEU
1	A	487	ASN
1	A	495	LEU
1	A	496	LYS
1	A	505	ARG
1	A	506	LEU
1	A	511	ARG
1	A	512	THR
1	A	542	ARG
1	A	555	VAL
1	A	574	THR
1	A	581	THR

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Mol	Chain	Res	Type
2	B	16	LYS
2	B	28	SER
2	B	47	ARG
2	B	51	ILE
2	B	64	ARG
2	B	73	THR
2	B	82	SER
2	B	83	LEU
2	B	86	GLU
2	B	104	THR
2	B	120	SER
2	B	124	THR
2	B	125	LYS
2	B	132	LEU
2	B	140	SER
2	B	143	THR
2	B	150	VAL
2	B	158	VAL
2	B	181	SER
2	B	185	SER
2	B	187	SER
2	B	195	SER
2	B	209	LYS
2	B	219	VAL
3	C	-1	ASP
3	C	3	THR
3	C	22	ARG
3	C	32	LEU
3	C	68	THR
3	C	69	ASP
3	C	92	SER
3	C	99	GLN
3	C	103	LEU
3	C	104	GLU
3	C	114	VAL
3	C	122	GLU
3	C	132	VAL
3	C	141	ARG
3	C	142	GLU
3	C	145	VAL
3	C	147	TRP
3	C	149	VAL

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Mol	Chain	Res	Type
3	C	150	ASP
3	C	162	VAL
3	C	168	LYS
3	C	178	LEU
3	C	180	LEU
3	C	196	THR
3	C	202	SER
3	C	205	THR
3	C	208	PHE
3	C	209	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	436	ASN
1	A	475	ASN
1	A	501	ASN
1	A	566	GLN
3	C	25	GLN
3	C	99	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
4	NAG	D	1	4	14,14,15	0.26	0	17,19,21	0.87	2 (11%)
4	MAN	D	2	4	11,11,12	1.02	0	15,15,17	1.43	2 (13%)
4	MAN	D	3	4	11,11,12	2.00	3 (27%)	15,15,17	1.97	5 (33%)

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	D	1	4	-	2/6/23/26	0/1/1/1
4	MAN	D	2	4	-	1/2/19/22	1/1/1/1
4	MAN	D	3	4	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3	MAN	C1-C2	4.07	1.61	1.52
4	D	3	MAN	O5-C1	-2.88	1.38	1.43
4	D	3	MAN	C2-C3	2.76	1.56	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	MAN	O3-C3-C2	4.56	119.37	110.05
4	D	3	MAN	C3-C4-C5	-3.98	103.01	110.23
4	D	3	MAN	O2-C2-C1	3.67	117.62	109.22
4	D	3	MAN	O5-C5-C4	-3.33	102.74	110.83
4	D	1	NAG	O4-C4-C5	-2.27	103.73	109.32
4	D	2	MAN	C1-O5-C5	2.22	115.16	112.19
4	D	3	MAN	O2-C2-C3	-2.15	105.70	110.15
4	D	1	NAG	C1-O5-C5	2.07	114.96	112.19
4	D	3	MAN	O6-C6-C5	-2.06	104.33	111.33

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	D	3	MAN	O5-C5-C6-O6
4	D	3	MAN	C4-C5-C6-O6
4	D	2	MAN	C4-C5-C6-O6

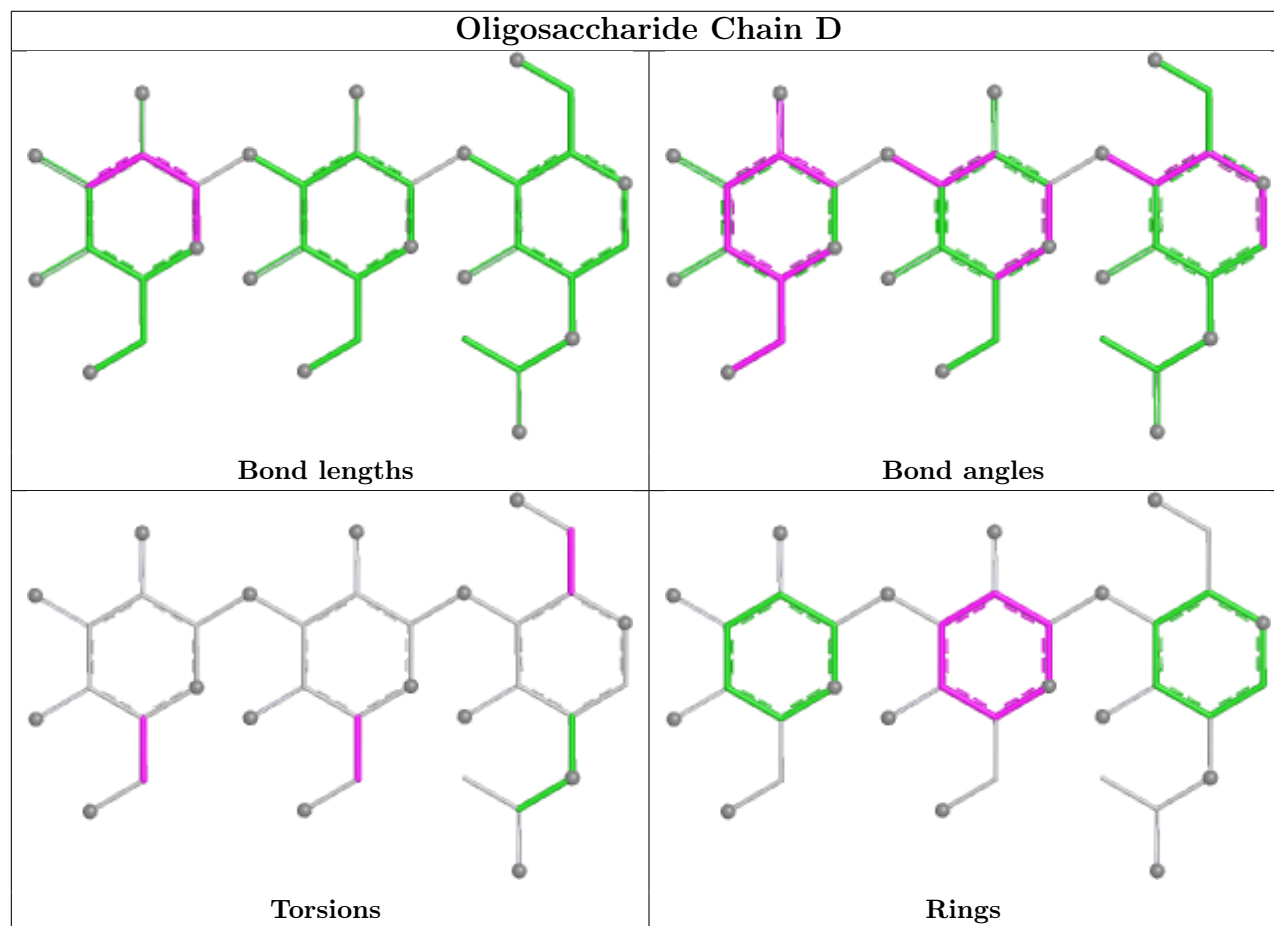
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3	MAN	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](#)

1 ligand is 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	EDO	C	301	-	3,3,3	0.58	0	2,2,2	0.29	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
5	EDO	C	301	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	301	EDO	2	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	205/229 (89%)	0.06	9 (4%) 39 35	26, 38, 59, 79	0
2	B	225/231 (97%)	0.87	34 (15%) 5 4	27, 55, 75, 83	0
3	C	209/215 (97%)	0.88	38 (18%) 3 3	26, 50, 84, 88	0
All	All	639/675 (94%)	0.61	81 (12%) 8 7	26, 46, 80, 88	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	129	ALA	6.6
1	A	581	THR	4.8
3	C	1	GLU	4.5
3	C	192	ALA	4.4
3	C	180	LEU	4.3
3	C	208	PHE	4.0
1	A	381	VAL	3.9
3	C	207	SER	3.9
3	C	153	LEU	3.8
3	C	147	TRP	3.8
2	B	219	VAL	3.8
2	B	121	SER	3.7
3	C	130	SER	3.6
3	C	206	LYS	3.6
3	C	145	VAL	3.6
2	B	199	THR	3.5
3	C	191	TYR	3.4
3	C	149	VAL	3.4
3	C	148	LYS	3.3
3	C	114	VAL	3.3
3	C	185	TYR	3.2
3	C	189	LYS	3.2
2	B	149	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
3	C	178	LEU	3.2
3	C	150	ASP	3.1
2	B	130	PHE	3.1
1	A	459	SER	2.9
2	B	188	SER	2.9
2	B	124	THR	2.9
3	C	196	THR	2.9
2	B	62	GLN	2.9
3	C	128	THR	2.9
1	A	458	VAL	2.9
3	C	146	GLN	2.8
2	B	137	LYS	2.8
2	B	215	VAL	2.8
1	A	406	ASN	2.7
3	C	182	LYS	2.7
3	C	193	CYS	2.6
1	A	412	THR	2.6
3	C	108	THR	2.6
2	B	222	LYS	2.6
2	B	179	GLN	2.6
2	B	218	LYS	2.5
2	B	191	THR	2.5
2	B	214	LYS	2.5
3	C	201	SER	2.5
2	B	10	LYS	2.5
1	A	578	GLY	2.5
3	C	205	THR	2.5
3	C	181	SER	2.5
2	B	120	SER	2.4
2	B	123	SER	2.4
3	C	125	LYS	2.4
3	C	179	THR	2.4
2	B	138	SER	2.4
2	B	153	TYR	2.4
2	B	186	LEU	2.4
3	C	123	GLN	2.4
3	C	154	GLN	2.4
2	B	11	PRO	2.3
2	B	131	PRO	2.3
2	B	194	SER	2.3
2	B	136	SER	2.2
3	C	131	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	487	ASN	2.2
2	B	181	SER	2.2
2	B	129	VAL	2.2
1	A	583	SER	2.2
2	B	150	VAL	2.2
2	B	147	GLY	2.1
3	C	142	GLU	2.1
3	C	124	LEU	2.1
3	C	115	PHE	2.1
2	B	183	LEU	2.1
3	C	184	ASP	2.0
2	B	122	ALA	2.0
2	B	173	THR	2.0
3	C	177	THR	2.0
2	B	216	ASP	2.0
2	B	170	GLY	2.0

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

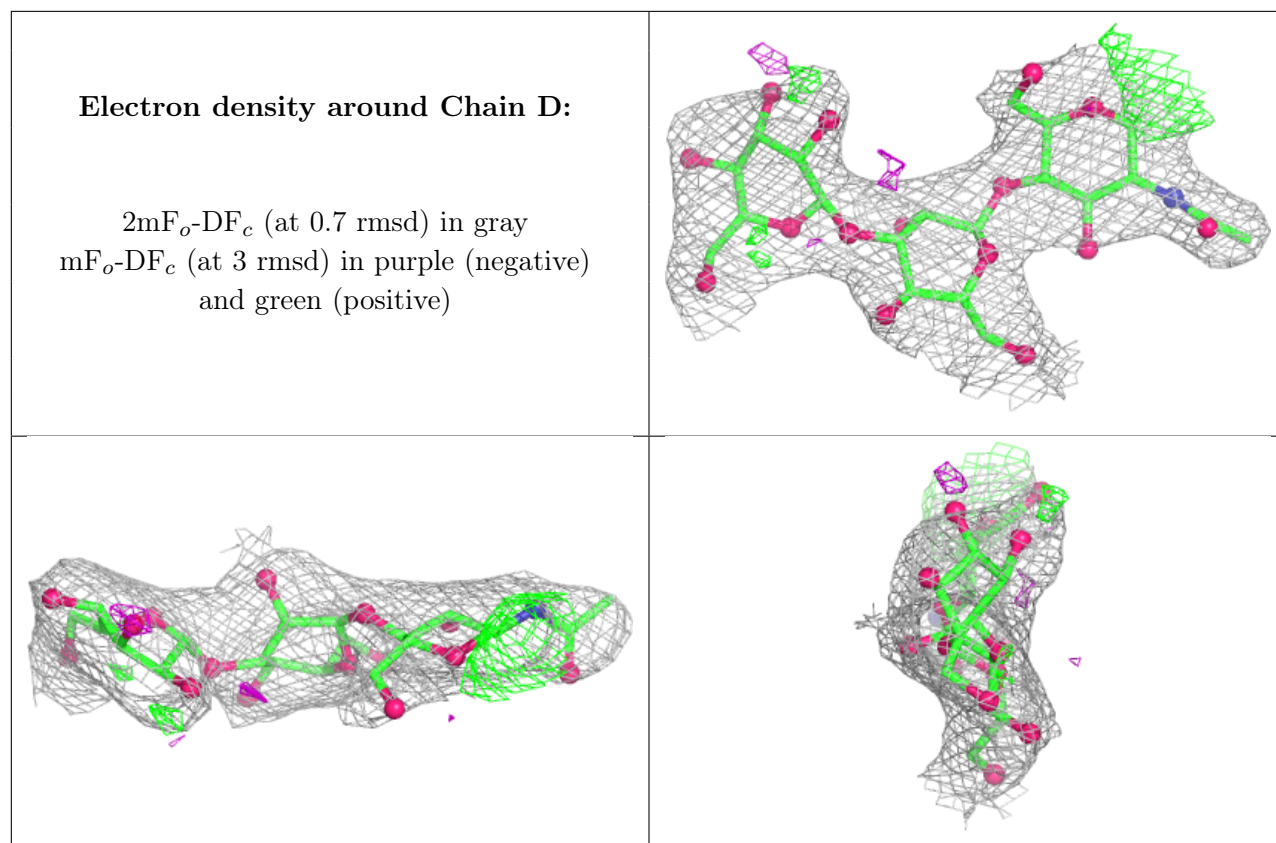
There are no non-standard protein/DNA/RNA residues in this entry.

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	NAG	D	1	14/15	0.71	0.19	54,60,64,65	0
4	MAN	D	3	11/12	0.81	0.15	52,54,59,64	0
4	MAN	D	2	11/12	0.84	0.12	52,54,61,70	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
5	EDO	C	301	4/4	0.83	0.25	33,33,39,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.