



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:04 AM UTC

PDB ID : 7DPM / pdb_00007dpm
Title : Crystal structure of SARS-CoV-2 Spike RBD in complex with MW06 Fab
Authors : Wang, J.; Jiao, S.; Wang, R.; Zhang, J.; Zhang, M.; Wang, M.
Deposited on : 2020-12-20
Resolution : 3.30 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

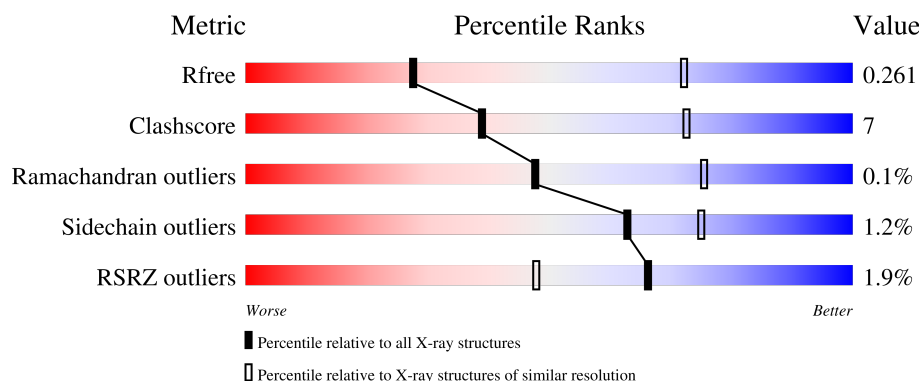
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	230	 81% 18%
1	D	230	 82% 16% ..
1	G	230	 80% 18% .
1	J	230	 9% 76% 16% 9%
2	B	214	 86% 14%

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Mol	Chain	Length	Quality of chain
2	E	214	 81% 18%
2	H	214	 83% 17%
2	K	214	 12% 82% 17%
3	C	223	 75% 13% 12%
3	F	223	 74% 13% 13%
3	I	223	 75% 11% 13%
3	L	223	 77% 10% 13%
4	M	3	 67% 33%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19571 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 heavy chain of MW06.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1714	1079	285	342	8			
1	D	228	Total	C	N	O	S	0	0	0
			1702	1073	283	339	7			
1	G	228	Total	C	N	O	S	0	0	0
			1702	1073	283	339	7			
1	J	210	Total	C	N	O	S	0	0	0
			1578	994	262	315	7			

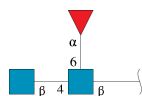
- Molecule 2 is a protein called light chain of MW06.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1646	1030	278	331	7			
2	E	214	Total	C	N	O	S	0	0	0
			1646	1030	278	331	7			
2	H	214	Total	C	N	O	S	0	0	0
			1646	1030	278	331	7			
2	K	212	Total	C	N	O	S	0	0	0
			1631	1022	276	327	6			

- Molecule 3 is a protein called Spike protein S1.

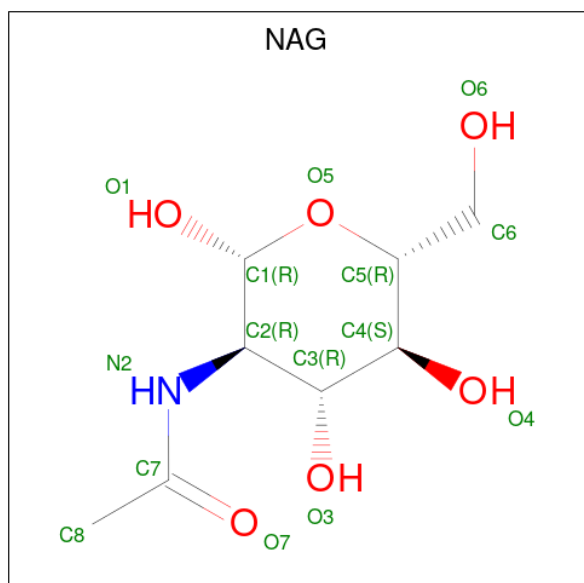
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	196	Total	C	N	O	S	0	0	0
			1552	995	259	290	8			
3	F	195	Total	C	N	O	S	0	0	0
			1543	989	257	289	8			
3	I	195	Total	C	N	O	S	0	0	0
			1543	989	257	289	8			
3	L	195	Total	C	N	O	S	0	0	0
			1543	989	257	289	8			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	10	Total	O	0	0
			10	10		

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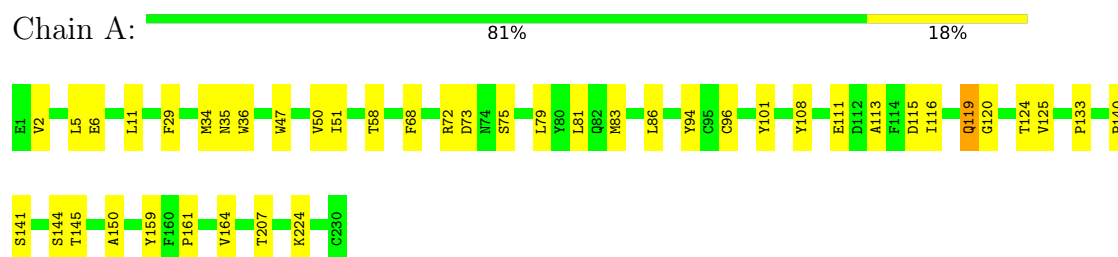
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	9	Total 9	O 9	0	0
6	C	10	Total 10	O 10	0	0
6	D	1	Total 1	O 1	0	0
6	F	6	Total 6	O 6	0	0
6	G	1	Total 1	O 1	0	0
6	H	3	Total 3	O 3	0	0
6	I	2	Total 2	O 2	0	0
6	L	3	Total 3	O 3	0	0

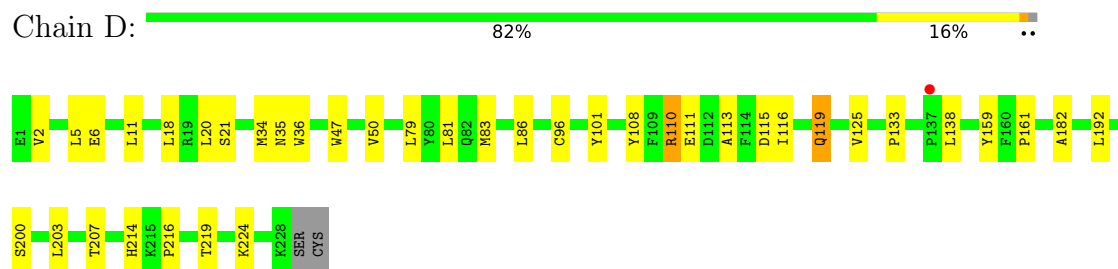
3 Residue-property plots

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.

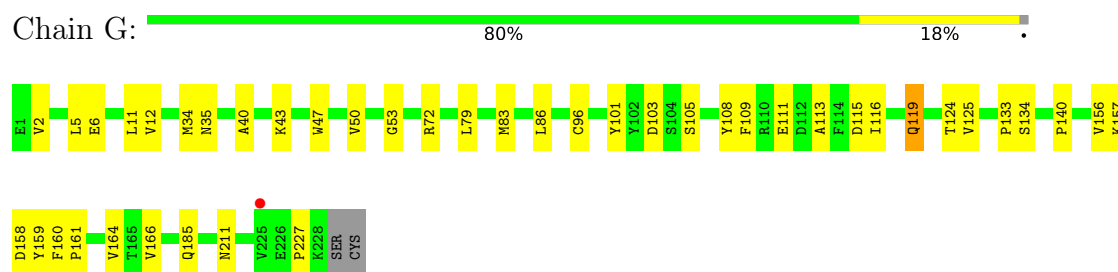
- Molecule 1: heavy chain of MW06



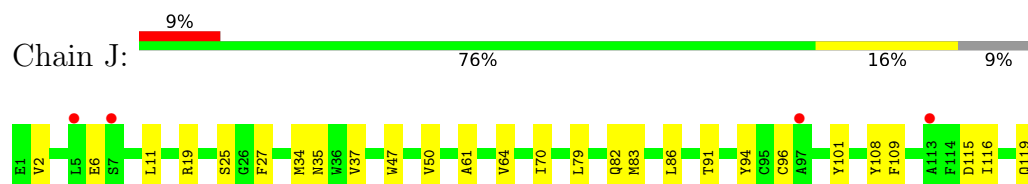
- Molecule 1: heavy chain of MW06

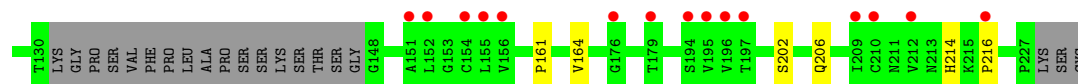


- Molecule 1: heavy chain of MW06

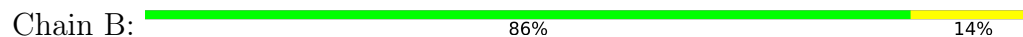


- Molecule 1: heavy chain of MW06

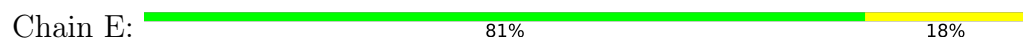




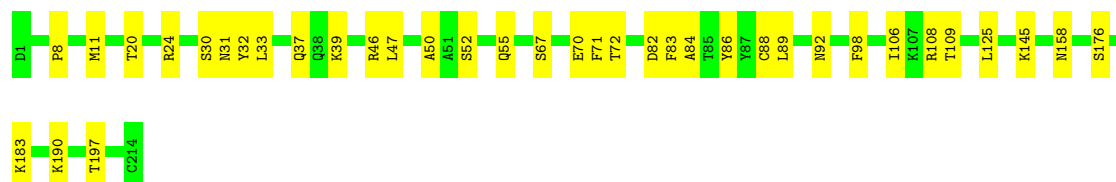
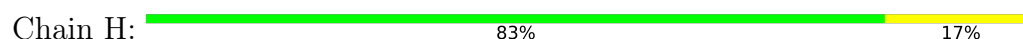
- Molecule 2: light chain of MW06



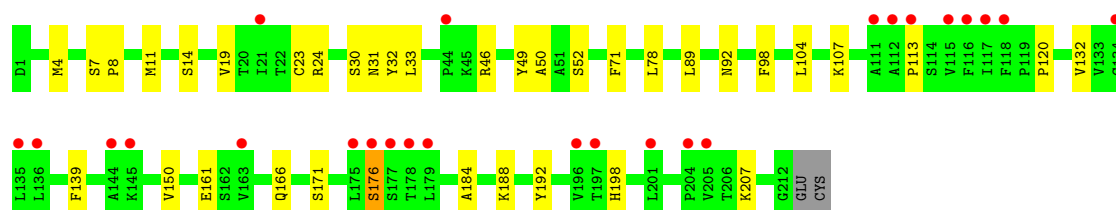
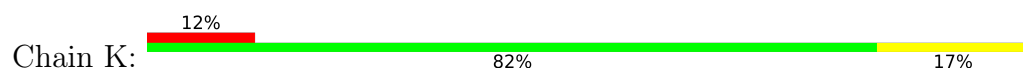
- Molecule 2: light chain of MW06



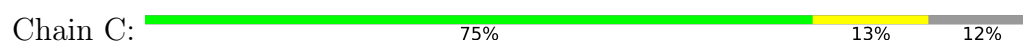
- Molecule 2: light chain of MW06

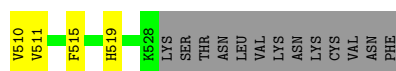


- Molecule 2: light chain of MW06



- Molecule 3: Spike protein S1





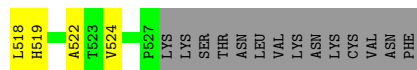
• Molecule 3: Spike protein S1

Chain F: 74% 13% 13%



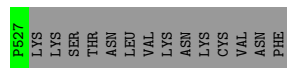
• Molecule 3: Spike protein S1

Chain I: 75% 11% 13%



• Molecule 3: Spike protein S1

Chain L: 77% 10% 13%



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

Chain M: 67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.13Å 153.83Å 172.69Å 90.00° 95.88° 90.00°	Depositor
Resolution (Å)	47.52 – 3.30 47.52 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.52-3.30) 99.2 (47.52-3.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.217 , 0.263 0.218 , 0.261	Depositor DCC
R_{free} test set	2796 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	83.8	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19571	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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, 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	0.25	0/1755	0.47	0/2387
1	D	0.19	0/1743	0.42	0/2371
1	G	0.19	0/1743	0.40	0/2371
1	J	0.17	0/1614	0.39	0/2195
2	B	0.24	0/1682	0.48	0/2281
2	E	0.18	0/1682	0.42	0/2281
2	H	0.18	0/1682	0.43	0/2281
2	K	0.18	0/1667	0.41	0/2261
3	C	0.22	0/1596	0.41	0/2172
3	F	0.20	0/1587	0.41	0/2161
3	I	0.18	0/1587	0.41	0/2161
3	L	0.17	0/1587	0.41	0/2161
All	All	0.20	0/19925	0.42	0/27083

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	1714	0	1659	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1702	0	1650	30	0
1	G	1702	0	1650	38	0
1	J	1578	0	1517	27	1
2	B	1646	0	1599	18	0
2	E	1646	0	1600	24	0
2	H	1646	0	1600	21	0
2	K	1631	0	1589	24	0
3	C	1552	0	1472	16	0
3	F	1543	0	1459	19	0
3	I	1543	0	1461	19	0
3	L	1543	0	1459	13	0
4	M	38	0	34	0	0
5	F	14	0	13	0	0
5	I	14	0	13	0	0
5	L	14	0	13	0	0
6	A	10	0	0	0	0
6	B	9	0	0	0	0
6	C	10	0	0	0	0
6	D	1	0	0	0	0
6	F	6	0	0	0	0
6	G	1	0	0	0	0
6	H	3	0	0	0	0
6	I	2	0	0	0	0
6	L	3	0	0	0	0
All	All	19571	0	18788	259	1

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 7.

All (259) 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:384:PRO:HA	3:C:387:LEU:HD23	1.52	0.92
2:E:142:ARG:HH22	2:E:163:VAL:HG11	1.44	0.83
1:A:5:LEU:HA	1:A:119:GLN:HE22	1.50	0.77
1:A:11:LEU:HD11	1:A:161:PRO:HG3	1.73	0.71
2:H:32:TYR:HD2	2:H:92:ASN:HA	1.57	0.69
3:F:468:ILE:HD11	2:H:158:ASN:HB3	1.75	0.68
1:J:108:TYR:HA	3:L:376:THR:HG23	1.76	0.68
1:G:5:LEU:HA	1:G:119:GLN:HE22	1.60	0.67
1:D:5:LEU:HA	1:D:119:GLN:HE22	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:LEU:HD11	1:G:161:PRO:HG3	1.79	0.65
2:B:32:TYR:HD2	2:B:92:ASN:HA	1.62	0.64
3:L:393:THR:HA	3:L:522:ALA:HA	1.78	0.64
1:D:83:MET:HE2	1:D:86:LEU:HD21	1.79	0.64
2:E:24:ARG:HG2	2:E:70:GLU:HG3	1.80	0.64
1:A:207:THR:HG23	1:A:224:LYS:HE3	1.79	0.63
1:G:133:PRO:HB3	1:G:159:TYR:HB3	1.81	0.63
1:A:108:TYR:HA	3:C:376:THR:HG23	1.80	0.62
1:G:108:TYR:HA	3:I:376:THR:HG23	1.79	0.62
1:A:145:THR:HG22	1:A:150:ALA:HB2	1.82	0.62
1:G:108:TYR:HB2	3:I:378:LYS:HE3	1.82	0.62
1:J:161:PRO:O	1:J:214:HIS:NE2	2.27	0.61
1:J:37:VAL:HG22	1:J:47:TRP:HA	1.83	0.60
1:D:133:PRO:HB3	1:D:159:TYR:HB3	1.83	0.60
1:A:133:PRO:HB3	1:A:159:TYR:HB3	1.83	0.59
1:D:6:GLU:OE2	1:D:96:CYS:N	2.36	0.58
3:I:388:ASN:OD1	3:I:388:ASN:N	2.35	0.58
2:H:108:ARG:NH1	2:H:109:THR:O	2.38	0.57
1:D:108:TYR:O	3:F:376:THR:OG1	2.22	0.57
3:F:431:GLY:HA2	3:F:515:PHE:CE2	2.40	0.57
1:G:111:GLU:HG3	2:H:32:TYR:CE1	2.40	0.57
3:I:382:VAL:HG11	3:I:387:LEU:HD13	1.87	0.57
1:A:113:ALA:O	2:B:46:ARG:NH1	2.38	0.57
1:J:2:VAL:HG11	1:J:116:ILE:HD13	1.87	0.56
1:A:73:ASP:OD1	1:A:75:SER:OG	2.23	0.56
3:C:392:PHE:CD1	3:C:515:PHE:HB3	2.41	0.56
1:J:91:THR:HG23	1:J:124:THR:HA	1.86	0.56
3:L:388:ASN:O	3:L:526:GLY:HA3	2.04	0.56
2:K:46:ARG:HD3	2:K:49:TYR:HB3	1.86	0.56
2:E:142:ARG:NH2	2:E:163:VAL:HG11	2.19	0.56
3:L:520:ALA:HB1	3:L:521:PRO:HD2	1.88	0.55
1:D:2:VAL:HG11	1:D:116:ILE:HD13	1.88	0.55
1:G:11:LEU:HD23	1:G:124:THR:HB	1.87	0.55
2:E:32:TYR:HD2	2:E:92:ASN:HA	1.71	0.54
3:I:384:PRO:HA	3:I:387:LEU:HB2	1.89	0.54
3:I:393:THR:HA	3:I:522:ALA:HA	1.88	0.54
1:J:108:TYR:O	3:L:376:THR:OG1	2.24	0.54
1:G:108:TYR:CD2	1:G:109:PHE:HB2	2.43	0.54
1:D:207:THR:HG23	1:D:224:LYS:HE3	1.89	0.54
1:G:158:ASP:OD1	1:G:185:GLN:NE2	2.35	0.54
2:H:39:LYS:HD3	2:H:84:ALA:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:32:TYR:HD2	2:K:92:ASN:HA	1.71	0.54
1:D:11:LEU:HD21	1:D:161:PRO:HG3	1.89	0.53
1:A:6:GLU:OE2	1:A:96:CYS:N	2.41	0.53
1:A:86:LEU:HB3	1:A:125:VAL:HG21	1.89	0.53
1:D:47:TRP:CZ2	1:D:50:VAL:HG23	2.44	0.53
3:C:350:VAL:HG22	3:C:422:ASN:HB3	1.90	0.53
2:E:33:LEU:HD22	2:E:71:PHE:CG	2.44	0.53
2:K:120:PRO:HD3	2:K:132:VAL:HG22	1.91	0.52
1:A:11:LEU:HD23	1:A:124:THR:HB	1.90	0.52
1:A:47:TRP:CZ2	1:A:50:VAL:HG23	2.44	0.52
1:J:101:TYR:HB3	1:J:108:TYR:HB3	1.91	0.52
1:G:156:VAL:HG11	1:G:164:VAL:HG11	1.91	0.52
1:A:94:TYR:O	1:A:120:GLY:HA2	2.10	0.52
2:E:8:PRO:HG3	2:E:11:MET:HE3	1.91	0.52
2:H:37:GLN:HB2	2:H:47:LEU:HD11	1.91	0.52
1:J:47:TRP:CZ2	1:J:50:VAL:HG23	2.45	0.52
2:K:78:LEU:HD21	2:K:104:LEU:HD21	1.91	0.51
2:K:14:SER:HB3	2:K:107:LYS:HB3	1.92	0.51
2:K:33:LEU:HD22	2:K:71:PHE:CG	2.46	0.51
2:K:161:GLU:HA	2:K:176:SER:O	2.11	0.51
3:C:398:ASP:O	3:C:511:VAL:HA	2.11	0.51
1:D:111:GLU:HG3	2:E:32:TYR:CD1	2.45	0.51
1:D:34:MET:HB3	1:D:79:LEU:HD22	1.92	0.51
1:A:119:GLN:H	1:A:119:GLN:NE2	2.09	0.50
1:J:6:GLU:OE2	1:J:96:CYS:N	2.42	0.50
3:I:359:SER:HA	3:I:524:VAL:HG22	1.92	0.50
3:I:366:SER:HB2	3:I:388:ASN:ND2	2.27	0.50
2:H:89:LEU:HB2	2:H:98:PHE:CD1	2.47	0.50
2:E:6:GLN:O	2:E:100:GLN:NE2	2.43	0.50
2:K:113:PRO:HD3	2:K:198:HIS:ND1	2.27	0.50
1:J:94:TYR:O	1:J:120:GLY:HA2	2.12	0.50
1:A:108:TYR:O	3:C:376:THR:OG1	2.25	0.50
2:H:24:ARG:NH2	2:H:70:GLU:OE2	2.42	0.50
2:K:7:SER:OG	2:K:24:ARG:NH1	2.44	0.50
3:F:392:PHE:CD1	3:F:515:PHE:HB3	2.47	0.49
1:J:34:MET:HB3	1:J:79:LEU:HD22	1.94	0.49
3:C:398:ASP:OD2	3:C:423:TYR:OH	2.28	0.49
1:D:108:TYR:HA	3:F:376:THR:HG23	1.94	0.49
1:A:36:TRP:NE1	1:A:81:LEU:HB2	2.28	0.49
1:G:47:TRP:CZ2	1:G:50:VAL:HG23	2.47	0.49
1:G:6:GLU:OE2	1:G:96:CYS:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:PRO:HG3	2:B:11:MET:HE3	1.94	0.49
1:G:34:MET:HB3	1:G:79:LEU:HD22	1.94	0.48
1:A:47:TRP:HE1	1:A:50:VAL:HG23	1.77	0.48
2:E:50:ALA:C	2:E:52:SER:H	2.21	0.48
1:D:20:LEU:HD12	1:D:81:LEU:HD23	1.96	0.48
3:I:518:LEU:HG	3:I:519:HIS:H	1.79	0.48
2:K:50:ALA:C	2:K:52:SER:H	2.22	0.48
1:A:115:ASP:N	1:A:115:ASP:OD1	2.44	0.48
1:D:35:ASN:CG	1:D:50:VAL:HG22	2.39	0.48
2:B:67:SER:HA	2:B:71:PHE:CE2	2.48	0.48
1:G:2:VAL:HG11	1:G:116:ILE:HD13	1.94	0.48
1:J:115:ASP:OD1	1:J:115:ASP:N	2.45	0.48
2:K:184:ALA:O	2:K:188:LYS:HG3	2.14	0.48
1:A:144:SER:HA	2:B:116:PHE:HD2	1.79	0.47
1:J:83:MET:HE2	1:J:86:LEU:HD21	1.96	0.47
2:B:191:VAL:HG22	2:B:210:ASN:OD1	2.14	0.47
1:D:110:ARG:NH2	3:F:374:PHE:O	2.32	0.47
2:E:37:GLN:HB2	2:E:47:LEU:HD11	1.95	0.47
2:H:50:ALA:C	2:H:52:SER:H	2.22	0.47
2:K:78:LEU:HD23	2:K:78:LEU:HA	1.68	0.47
2:H:33:LEU:HD22	2:H:71:PHE:CG	2.49	0.47
3:C:443:SER:HB3	3:C:499:PRO:HD3	1.96	0.47
3:F:366:SER:HB2	3:F:388:ASN:ND2	2.30	0.47
1:J:108:TYR:CD2	1:J:109:PHE:HB2	2.50	0.47
3:F:359:SER:HB3	3:F:394:ASN:OD1	2.15	0.47
1:G:101:TYR:HB3	1:G:108:TYR:HB3	1.97	0.47
1:A:2:VAL:HG11	1:A:116:ILE:HD13	1.97	0.47
1:D:113:ALA:O	2:E:46:ARG:NH1	2.47	0.47
1:G:40:ALA:HB3	1:G:43:LYS:HB2	1.96	0.47
3:L:412:PRO:HG3	3:L:429:PHE:HB3	1.96	0.47
3:L:502:GLY:O	3:L:506:GLN:HG3	2.15	0.46
1:D:47:TRP:HZ2	1:D:50:VAL:HG23	1.81	0.46
2:H:8:PRO:HG3	2:H:11:MET:HE3	1.98	0.46
3:I:401:VAL:HG22	3:I:509:ARG:HG2	1.98	0.46
2:B:161:GLU:HA	2:B:176:SER:O	2.15	0.46
1:D:101:TYR:HB3	1:D:108:TYR:HB3	1.98	0.46
3:L:401:VAL:HG22	3:L:509:ARG:HG2	1.96	0.46
1:G:101:TYR:CE1	1:G:103:ASP:HB2	2.51	0.46
3:C:366:SER:HB2	3:C:388:ASN:ND2	2.31	0.46
1:D:36:TRP:CE2	1:D:81:LEU:HB2	2.51	0.46
1:D:182:ALA:HA	1:D:192:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:ASP:OD1	1:G:115:ASP:N	2.47	0.46
3:C:365:TYR:CG	3:C:387:LEU:HD11	2.51	0.46
3:C:431:GLY:HA2	3:C:515:PHE:CE2	2.51	0.46
1:G:140:PRO:HG2	1:G:227:PRO:HB3	1.97	0.46
1:J:2:VAL:HG13	1:J:27:PHE:CD1	2.50	0.46
1:J:11:LEU:HD11	1:J:126:SER:HB3	1.98	0.46
2:B:124:GLN:O	2:B:127:SER:OG	2.23	0.45
1:G:12:VAL:HG13	1:G:125:VAL:HG22	1.99	0.45
1:D:119:GLN:NE2	1:D:119:GLN:H	2.14	0.45
1:G:83:MET:HE2	1:G:86:LEU:HD21	1.97	0.45
2:B:145:LYS:HB3	2:B:197:THR:OG1	2.16	0.45
3:F:476:GLY:N	3:F:487:ASN:HB3	2.32	0.45
2:K:166:GLN:HE21	2:K:171:SER:HB3	1.81	0.45
3:C:454:ARG:NH2	3:C:467:ASP:O	2.48	0.45
2:E:142:ARG:HB3	2:E:173:TYR:CG	2.52	0.45
1:G:35:ASN:ND2	1:G:50:VAL:HG22	2.32	0.45
1:A:111:GLU:HG3	2:B:32:TYR:CE1	2.52	0.45
1:D:214:HIS:CD2	1:D:216:PRO:HD2	2.52	0.45
3:C:412:PRO:HG3	3:C:429:PHE:HB3	1.98	0.45
1:G:108:TYR:O	3:I:376:THR:OG1	2.31	0.45
1:J:161:PRO:HD2	1:J:216:PRO:HB2	1.99	0.44
2:E:134:CYS:HB2	2:E:148:TRP:CH2	2.51	0.44
3:F:354:ASN:O	3:F:398:ASP:HA	2.17	0.44
2:H:125:LEU:O	2:H:183:LYS:HD2	2.17	0.44
2:K:8:PRO:HG3	2:K:11:MET:HE3	1.99	0.44
3:L:398:ASP:OD2	3:L:423:TYR:OH	2.30	0.44
2:B:33:LEU:HD22	2:B:71:PHE:CD2	2.53	0.44
3:F:357:ARG:NH2	2:H:190:LYS:HD3	2.32	0.44
1:G:113:ALA:O	2:H:46:ARG:NH1	2.50	0.44
3:F:412:PRO:HG3	3:F:429:PHE:HB3	1.99	0.44
1:A:36:TRP:CE2	1:A:81:LEU:HB2	2.53	0.44
2:B:78:LEU:HD23	2:B:78:LEU:HA	1.81	0.44
2:E:89:LEU:HB2	2:E:98:PHE:CD2	2.53	0.44
2:H:82:ASP:O	2:H:86:TYR:OH	2.25	0.44
1:A:35:ASN:CG	1:A:50:VAL:HG22	2.43	0.44
3:F:350:VAL:HG22	3:F:422:ASN:HB3	1.99	0.44
1:A:47:TRP:HZ2	1:A:50:VAL:HG23	1.83	0.44
1:A:101:TYR:HB3	1:A:108:TYR:HB3	1.99	0.44
2:H:33:LEU:HD11	2:H:88:CYS:HB2	2.00	0.44
1:J:2:VAL:HG12	1:J:116:ILE:HG21	2.00	0.44
2:K:113:PRO:HB3	2:K:139:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:398:ASP:O	3:F:511:VAL:HA	2.18	0.43
1:J:115:ASP:HB3	2:K:46:ARG:NH1	2.33	0.43
1:D:6:GLU:HA	1:D:21:SER:O	2.19	0.43
1:J:35:ASN:CG	1:J:50:VAL:HG22	2.43	0.43
2:B:50:ALA:C	2:B:52:SER:H	2.26	0.43
1:G:86:LEU:HB3	1:G:125:VAL:HG21	2.00	0.43
2:H:30:SER:OG	2:H:31:ASN:N	2.50	0.43
3:I:439:ASN:O	3:I:443:SER:HB2	2.18	0.43
1:J:47:TRP:HZ2	1:J:50:VAL:HG23	1.82	0.43
1:D:200:SER:HA	1:D:203:LEU:HG	2.00	0.43
1:J:202:SER:HB2	1:J:206:GLN:HG2	1.99	0.43
3:L:443:SER:HB3	3:L:499:PRO:HD3	1.99	0.43
3:C:355:ARG:HD3	3:C:396:TYR:CD1	2.54	0.43
2:H:145:LYS:HB3	2:H:197:THR:OG1	2.19	0.43
1:J:70:ILE:HD11	1:J:79:LEU:HD11	2.00	0.43
2:K:11:MET:SD	2:K:19:VAL:HG13	2.58	0.43
3:F:431:GLY:HA2	3:F:515:PHE:CD2	2.54	0.43
2:H:67:SER:HA	2:H:71:PHE:CE2	2.54	0.43
3:I:354:ASN:O	3:I:398:ASP:HA	2.19	0.43
1:D:115:ASP:OD1	1:D:115:ASP:N	2.47	0.43
2:H:83:PHE:CE2	2:H:106:ILE:HG12	2.53	0.43
3:I:390:LEU:HD12	3:I:390:LEU:HA	1.80	0.43
2:E:125:LEU:O	2:E:183:LYS:HD2	2.18	0.43
1:A:111:GLU:HG3	2:B:32:TYR:CD1	2.54	0.42
2:H:20:THR:HG23	2:H:72:THR:HG23	2.01	0.42
1:G:35:ASN:CG	1:G:50:VAL:HG22	2.45	0.42
3:I:502:GLY:O	3:I:506:GLN:HG3	2.18	0.42
3:F:349:SER:OG	3:F:451:TYR:HA	2.19	0.42
1:J:61:ALA:HB3	1:J:64:VAL:HG22	2.02	0.42
3:L:365:TYR:HD2	3:L:388:ASN:HB3	1.84	0.42
1:G:105:SER:HB2	3:I:379:CYS:O	2.20	0.42
3:I:444:LYS:HB2	3:I:448:ASN:HB2	2.02	0.42
1:A:68:PHE:HB3	1:A:81:LEU:HD11	2.02	0.42
1:A:140:PRO:HA	1:A:144:SER:OG	2.20	0.42
1:A:141:SER:O	1:A:145:THR:HG23	2.20	0.42
2:E:145:LYS:HD3	2:E:145:LYS:HA	1.91	0.42
1:G:157:LYS:NZ	1:G:185:GLN:OE1	2.52	0.42
1:G:166:VAL:HA	1:G:211:ASN:O	2.20	0.42
1:J:47:TRP:HE1	1:J:50:VAL:HG23	1.85	0.42
2:K:166:GLN:NE2	2:K:171:SER:HB3	2.35	0.42
3:F:502:GLY:O	3:F:506:GLN:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:164:VAL:HG22	1:J:214:HIS:HB2	2.01	0.42
1:A:47:TRP:NE1	1:A:50:VAL:HG23	2.34	0.41
2:B:2:ILE:HD13	2:B:29:ILE:HG22	2.01	0.41
2:K:30:SER:OG	2:K:31:ASN:N	2.52	0.41
3:L:485:GLY:H	3:L:488:CYS:HB2	1.85	0.41
1:D:47:TRP:HE1	1:D:50:VAL:HG23	1.85	0.41
1:D:133:PRO:HD2	1:D:219:THR:HG21	2.03	0.41
2:E:4:MET:HE3	2:E:23:CYS:SG	2.60	0.41
1:G:53:GLY:HA2	1:G:72:ARG:NH1	2.35	0.41
3:I:359:SER:HA	3:I:524:VAL:CG2	2.50	0.41
1:G:47:TRP:HE1	1:G:50:VAL:HG23	1.85	0.41
2:B:78:LEU:HD21	2:B:104:LEU:HD21	2.02	0.41
1:D:18:LEU:HD12	1:D:18:LEU:HA	1.94	0.41
1:G:160:PHE:HA	1:G:161:PRO:HA	1.85	0.41
3:L:338:PHE:HE2	3:L:363:ALA:HB1	1.85	0.41
1:A:83:MET:HE2	1:A:86:LEU:HD21	2.02	0.41
2:E:20:THR:HG23	2:E:72:THR:HG23	2.03	0.41
1:A:51:ILE:HG13	1:A:58:THR:HG22	2.03	0.41
2:E:9:SER:O	2:E:102:THR:HA	2.20	0.41
2:E:107:LYS:HA	2:E:140:TYR:OH	2.20	0.41
2:E:161:GLU:HA	2:E:176:SER:O	2.20	0.41
3:F:399:SER:HA	3:F:510:VAL:O	2.20	0.41
1:J:19:ARG:HG3	1:J:82:GLN:HG2	2.03	0.41
3:C:401:VAL:HG22	3:C:509:ARG:HG2	2.03	0.41
3:F:401:VAL:HG22	3:F:509:ARG:HG2	2.03	0.41
1:G:12:VAL:O	1:G:125:VAL:HA	2.20	0.41
1:G:47:TRP:HZ2	1:G:50:VAL:HG23	1.86	0.41
1:G:119:GLN:H	1:G:119:GLN:HE21	1.69	0.41
2:K:4:MET:HE3	2:K:23:CYS:SG	2.61	0.41
1:D:138:LEU:HB3	2:E:118:PHE:CD1	2.56	0.41
1:A:34:MET:HB3	1:A:79:LEU:HD22	2.03	0.40
2:E:124:GLN:HG2	2:E:129:THR:O	2.21	0.40
1:G:5:LEU:HD23	1:G:119:GLN:HE22	1.86	0.40
2:K:46:ARG:NH2	2:K:49:TYR:HB3	2.36	0.40
2:K:166:GLN:HG2	2:K:171:SER:HA	2.03	0.40
2:B:108:ARG:NH1	2:B:109:THR:O	2.54	0.40
3:C:399:SER:HA	3:C:510:VAL:O	2.21	0.40
2:B:89:LEU:HB2	2:B:98:PHE:CD1	2.56	0.40
1:D:86:LEU:HB3	1:D:125:VAL:HG21	2.01	0.40
1:G:133:PRO:CB	1:G:159:TYR:HB3	2.51	0.40
2:K:89:LEU:HB2	2:K:98:PHE:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:150:VAL:HG22	2:K:192:TYR:CD1	2.57	0.40
1:A:29:PHE:O	1:A:72:ARG:NH2	2.54	0.40
2:E:145:LYS:HB2	2:E:197:THR:OG1	2.21	0.40
1:G:111:GLU:OE1	3:I:375:SER:HB2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:25:SER:OG	1:J:25:SER:OG[2_656]	2.06	0.14

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	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	D	226/230 (98%)	214 (95%)	12 (5%)	0	100	100
1	G	226/230 (98%)	218 (96%)	8 (4%)	0	100	100
1	J	206/230 (90%)	201 (98%)	5 (2%)	0	100	100
2	B	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
2	E	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
2	H	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
2	K	210/214 (98%)	202 (96%)	8 (4%)	0	100	100
3	C	194/223 (87%)	180 (93%)	14 (7%)	0	100	100
3	F	193/223 (86%)	179 (93%)	14 (7%)	0	100	100
3	I	193/223 (86%)	181 (94%)	12 (6%)	0	100	100
3	L	193/223 (86%)	176 (91%)	15 (8%)	2 (1%)	12	40
All	All	2505/2668 (94%)	2379 (95%)	124 (5%)	2 (0%)	48	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	385	THR
3	L	522	ALA

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	191/191 (100%)	189 (99%)	2 (1%)	68	76
1	D	189/191 (99%)	187 (99%)	2 (1%)	65	76
1	G	189/191 (99%)	187 (99%)	2 (1%)	65	76
1	J	174/191 (91%)	173 (99%)	1 (1%)	78	81
2	B	187/187 (100%)	184 (98%)	3 (2%)	55	72
2	E	187/187 (100%)	184 (98%)	3 (2%)	55	72
2	H	187/187 (100%)	185 (99%)	2 (1%)	65	76
2	K	185/187 (99%)	183 (99%)	2 (1%)	65	76
3	C	169/196 (86%)	166 (98%)	3 (2%)	51	70
3	F	168/196 (86%)	166 (99%)	2 (1%)	63	75
3	I	168/196 (86%)	165 (98%)	3 (2%)	51	70
3	L	168/196 (86%)	167 (99%)	1 (1%)	78	81
All	All	2162/2296 (94%)	2136 (99%)	26 (1%)	63	75

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	164	VAL
2	B	70	GLU
2	B	142	ARG
2	B	190	LYS
3	C	354	ASN
3	C	403	ARG

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Mol	Chain	Res	Type
3	C	519	HIS
1	D	110	ARG
1	D	119	GLN
2	E	53	SER
2	E	142	ARG
2	E	176	SER
3	F	408	ARG
3	F	519	HIS
1	G	119	GLN
1	G	134	SER
2	H	55	GLN
2	H	176	SER
3	I	388	ASN
3	I	390	LEU
3	I	484	GLU
1	J	119	GLN
2	K	176	SER
2	K	207	LYS
3	L	498	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	119	GLN
3	C	334	ASN
3	C	370	ASN
3	C	498	GLN
1	D	77	ASN
1	D	119	GLN
1	D	178	HIS
3	F	334	ASN
3	F	498	GLN
3	F	501	ASN
1	G	77	ASN
1	G	119	GLN
2	H	160	GLN
1	J	77	ASN
1	J	178	HIS
2	K	38	GLN
2	K	138	ASN
3	L	334	ASN

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Mol	Chain	Res	Type
3	L	501	ASN

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	M	1	3,4	14,14,15	0.32	0	17,19,21	0.82	1 (5%)
4	NAG	M	2	4	14,14,15	0.43	0	17,19,21	0.51	0
4	FUC	M	3	4	10,10,11	0.89	0	14,14,16	0.77	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	M	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	1/6/23/26	0/1/1/1
4	FUC	M	3	4	-	-	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1	NAG	C1-O5-C5	2.99	116.20	112.19

There are no chirality outliers.

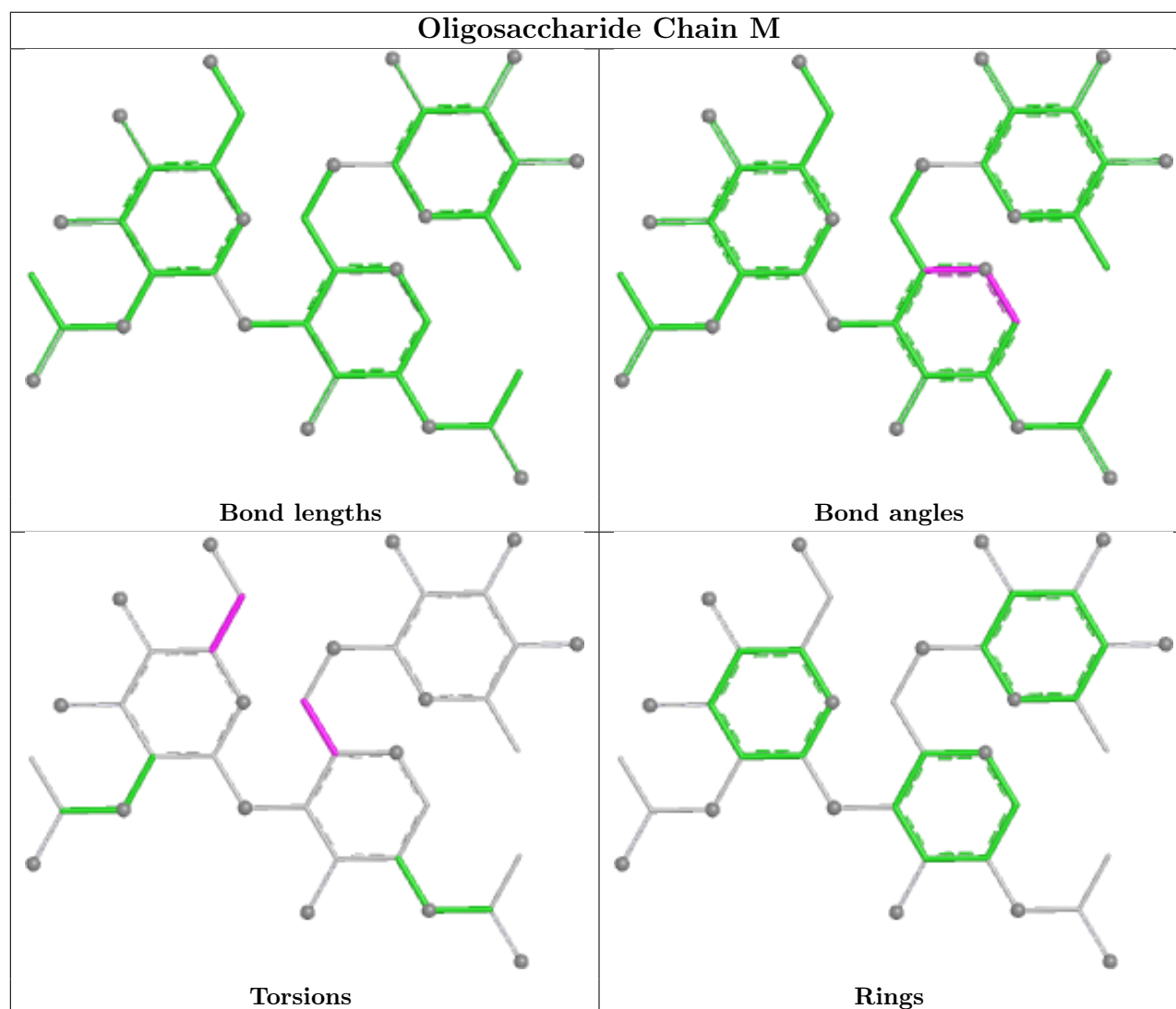
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	1	NAG	O5-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	M	2	NAG	O5-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

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	$\# Z > 2$
5	NAG	I	601	3	14,14,15	0.47	0	17,19,21	0.59	0
5	NAG	F	601	3	14,14,15	0.41	0	17,19,21	0.57	0
5	NAG	L	601	3	14,14,15	0.31	0	17,19,21	0.49	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	NAG	I	601	3	-	2/6/23/26	0/1/1/1
5	NAG	F	601	3	-	2/6/23/26	0/1/1/1
5	NAG	L	601	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	601	NAG	O5-C5-C6-O6
5	I	601	NAG	O5-C5-C6-O6
5	F	601	NAG	C4-C5-C6-O6
5	I	601	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	230/230 (100%)	-0.32	0 100 100	35, 55, 94, 141	0
1	D	228/230 (99%)	-0.10	1 (0%) 88 79	62, 80, 128, 165	0
1	G	228/230 (99%)	-0.06	1 (0%) 88 79	67, 88, 115, 124	0
1	J	210/230 (91%)	0.85	20 (9%) 14 11	94, 168, 190, 199	0
2	B	214/214 (100%)	-0.28	0 100 100	42, 59, 74, 117	0
2	E	214/214 (100%)	0.01	1 (0%) 87 76	66, 97, 141, 150	0
2	H	214/214 (100%)	-0.15	0 100 100	64, 81, 98, 118	0
2	K	212/214 (99%)	0.91	25 (11%) 9 8	100, 157, 188, 195	0
3	C	196/223 (87%)	-0.13	0 100 100	49, 68, 91, 126	0
3	F	195/223 (87%)	-0.15	0 100 100	57, 78, 108, 125	0
3	I	195/223 (87%)	0.06	1 (0%) 87 76	74, 96, 150, 167	0
3	L	195/223 (87%)	0.08	0 100 100	78, 102, 143, 157	0
All	All	2531/2668 (94%)	0.06	49 (1%) 66 48	35, 86, 175, 199	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	144	ALA	5.0
1	J	196	VAL	4.9
2	K	197	THR	4.6
1	J	195	VAL	4.1
2	K	196	VAL	4.1
2	K	205	VAL	3.8
2	K	177	SER	3.8
2	K	176	SER	3.8
2	K	134	CYS	3.4
1	J	152	LEU	3.4
1	J	197	THR	3.3

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Mol	Chain	Res	Type	RSRZ
2	K	175	LEU	3.3
1	J	212	VAL	3.3
1	J	151	ALA	3.1
2	K	135	LEU	2.9
2	K	112	ALA	2.9
2	K	115	VAL	2.8
2	K	136	LEU	2.8
2	K	113	PRO	2.6
1	D	137	PRO	2.6
1	J	155	LEU	2.5
2	K	201	LEU	2.5
2	K	117	ILE	2.5
2	K	163	VAL	2.5
2	K	178	THR	2.5
1	J	154	CYS	2.5
1	J	216	PRO	2.4
1	J	210	CYS	2.4
1	J	209	ILE	2.4
1	J	97	ALA	2.4
1	J	179	THR	2.4
2	K	204	PRO	2.4
1	J	176	GLY	2.4
1	J	156	VAL	2.4
2	K	179	LEU	2.3
2	K	44	PRO	2.3
1	J	126	SER	2.3
1	J	194	SER	2.3
1	J	5	LEU	2.2
3	I	482	GLY	2.2
2	K	116	PHE	2.2
2	K	21	ILE	2.2
1	J	7	SER	2.1
2	K	111	ALA	2.1
2	K	118	PHE	2.1
2	K	145	LYS	2.1
1	G	225	VAL	2.0
2	E	11	MET	2.0
1	J	113	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

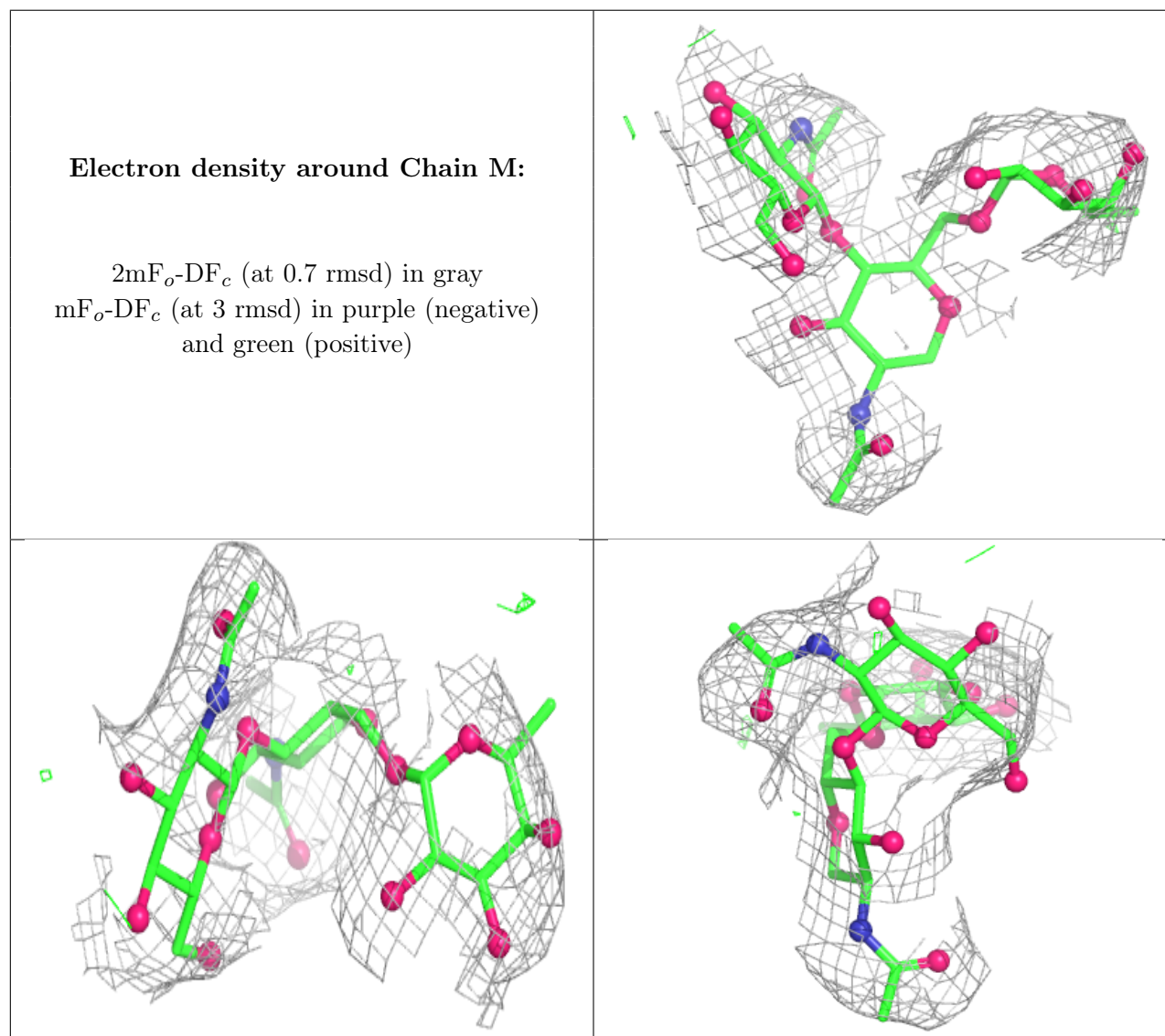
There are no non-standard protein/DNA/RNA residues in this entry.

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. 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	FUC	M	3	10/11	0.71	0.11	101,113,115,116	0
4	NAG	M	2	14/15	0.77	0.10	95,104,111,113	0
4	NAG	M	1	14/15	0.92	0.07	68,90,101,105	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
5	NAG	I	601	14/15	0.66	0.12	106,109,115,116	0
5	NAG	L	601	14/15	0.76	0.10	111,120,126,127	0
5	NAG	F	601	14/15	0.85	0.10	83,86,93,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.