



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 07:07 AM UTC

PDB ID : 7RKU / pdb_00007rku
Title : Structure of the SARS-CoV-2 receptor binding domain in complex with the human neutralizing antibody Fab fragment, C022
Authors : Jette, C.A.; Bjorkman, P.J.; Barnes, C.O.
Deposited on : 2021-07-22
Resolution : 3.20 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

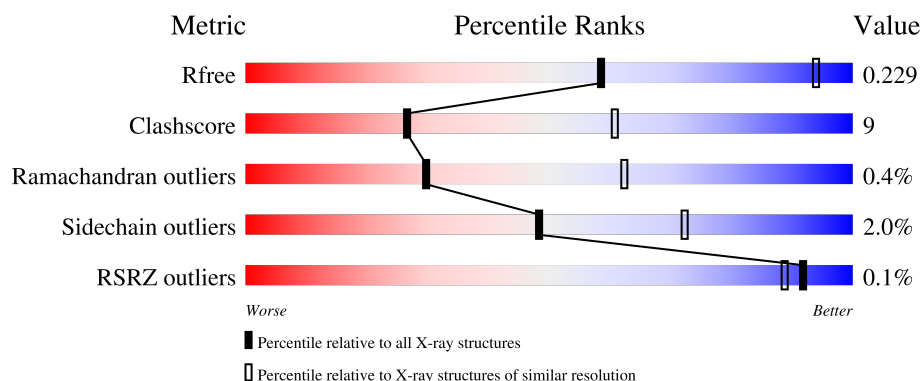
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	212	 74% 18% 8%
1	B	212	 75% 17% 8%
1	C	212	 75% 17% 8%
1	D	212	 71% 19% 8%
2	E	240	 72% 24% 8%

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Mol	Chain	Length	Quality of chain
2	G	240	
2	H	240	
2	J	240	
3	F	215	
3	I	215	
3	K	215	
3	L	215	
4	M	3	
4	N	3	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19802 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	196	Total	C	N	O	S	0	0	0
			1552	995	259	290	8			
1	B	196	Total	C	N	O	S	0	0	0
			1552	995	259	290	8			
1	C	195	Total	C	N	O	S	0	0	0
			1541	988	257	288	8			
1	D	194	Total	C	N	O	S	0	0	0
			1536	985	256	287	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
A	538	HIS	-	expression tag	UNP P0DTC2
A	539	HIS	-	expression tag	UNP P0DTC2
B	534	HIS	-	expression tag	UNP P0DTC2
B	535	HIS	-	expression tag	UNP P0DTC2
B	536	HIS	-	expression tag	UNP P0DTC2
B	537	HIS	-	expression tag	UNP P0DTC2
B	538	HIS	-	expression tag	UNP P0DTC2
B	539	HIS	-	expression tag	UNP P0DTC2
C	534	HIS	-	expression tag	UNP P0DTC2
C	535	HIS	-	expression tag	UNP P0DTC2
C	536	HIS	-	expression tag	UNP P0DTC2
C	537	HIS	-	expression tag	UNP P0DTC2
C	538	HIS	-	expression tag	UNP P0DTC2
C	539	HIS	-	expression tag	UNP P0DTC2
D	534	HIS	-	expression tag	UNP P0DTC2
D	535	HIS	-	expression tag	UNP P0DTC2
D	536	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	537	HIS	-	expression tag	UNP P0DTC2
D	538	HIS	-	expression tag	UNP P0DTC2
D	539	HIS	-	expression tag	UNP P0DTC2

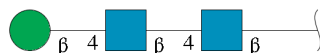
- Molecule 2 is a protein called C022 Antibody Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	231	Total	C	N	O	S	0	0	0
			1747	1112	288	343	4			
2	G	223	Total	C	N	O	S	0	0	0
			1692	1081	278	329	4			
2	H	231	Total	C	N	O	S	0	0	0
			1746	1111	288	343	4			
2	J	225	Total	C	N	O	S	0	0	0
			1703	1087	280	332	4			

- Molecule 3 is a protein called C022 Antibody Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	213	Total	C	N	O	S	0	2	0
			1654	1038	274	336	6			
3	I	214	Total	C	N	O	S	0	2	0
			1660	1041	275	337	7			
3	K	214	Total	C	N	O	S	0	2	0
			1659	1040	275	337	7			
3	L	213	Total	C	N	O	S	0	2	0
			1654	1038	274	336	6			

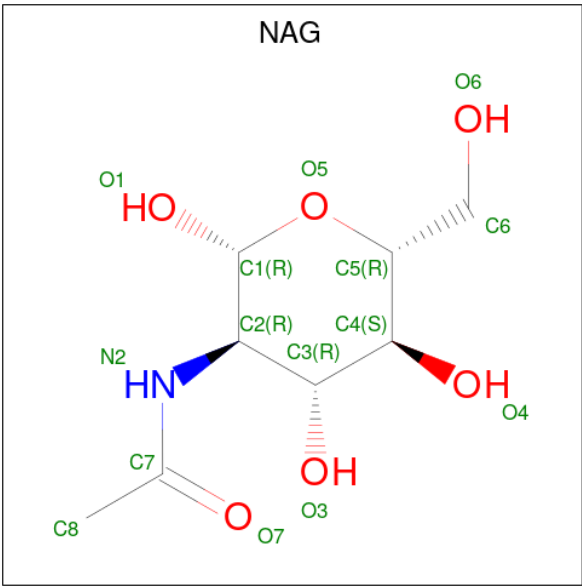
- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).

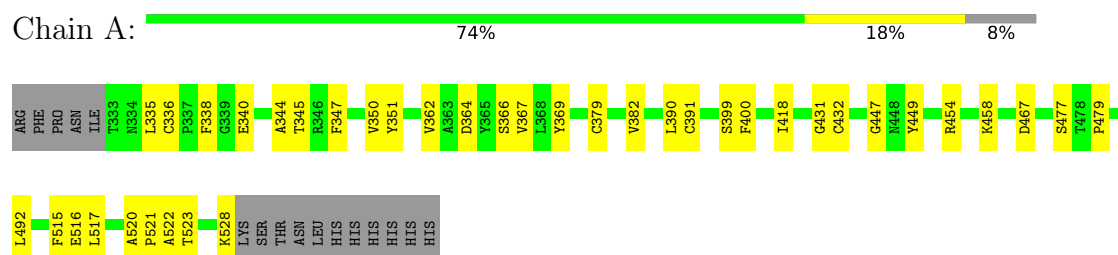


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

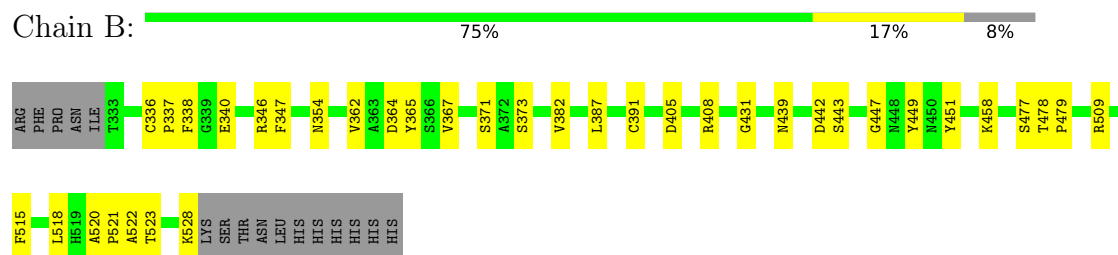
3 Residue-property plots [i](#)

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.

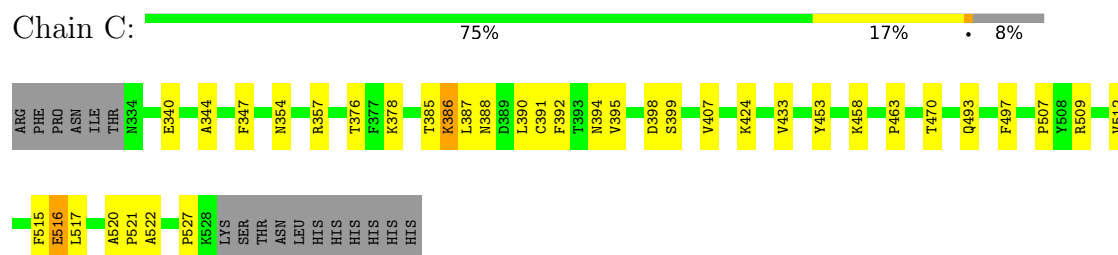
• Molecule 1: Spike protein S1



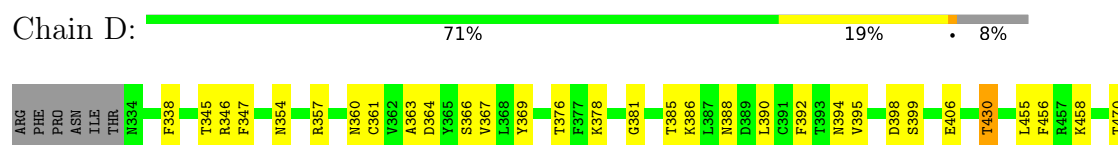
• Molecule 1: Spike protein S1

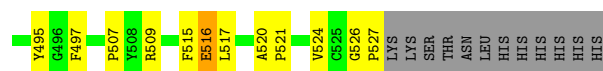


• Molecule 1: Spike protein S1

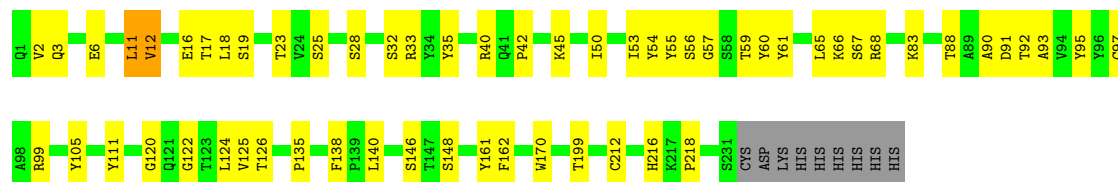


• Molecule 1: Spike protein S1

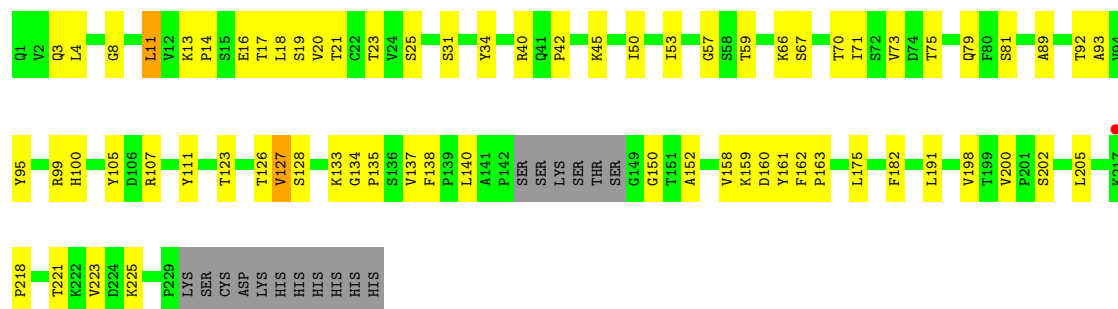




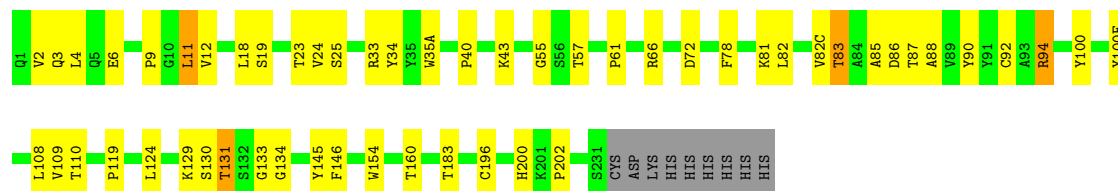
• Molecule 2: C022 Antibody Fab Heavy Chain



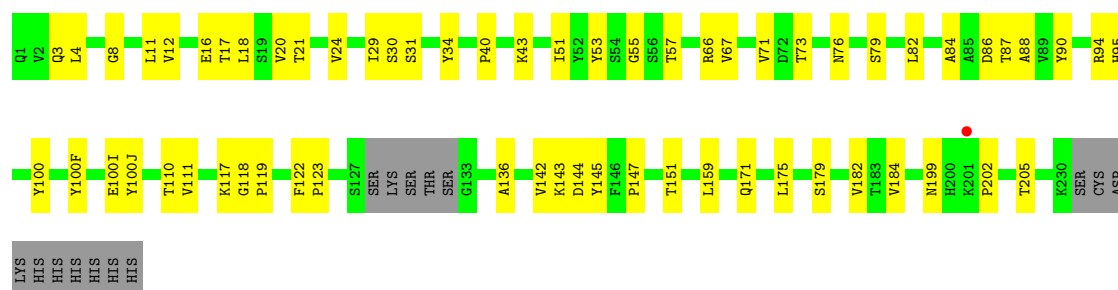
• Molecule 2: C022 Antibody Fab Heavy Chain



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• Molecule 2: C022 Antibody Fab Heavy Chain



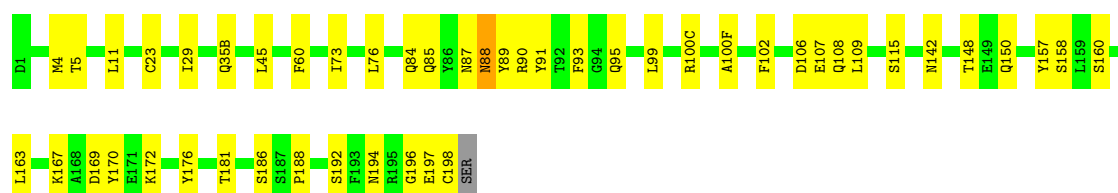
- Molecule 3: C022 Antibody Fab Light Chain

Chain F:  77% 22%



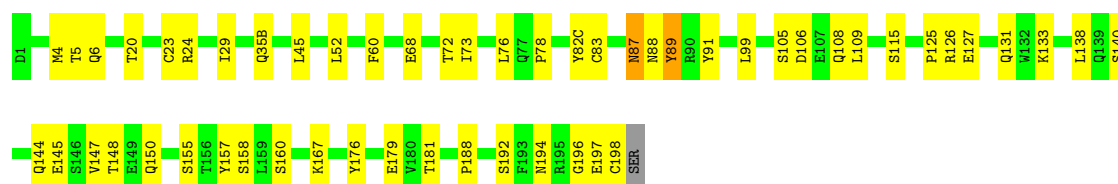
- Molecule 3: C022 Antibody Fab Light Chain

Chain I:  77% 22%



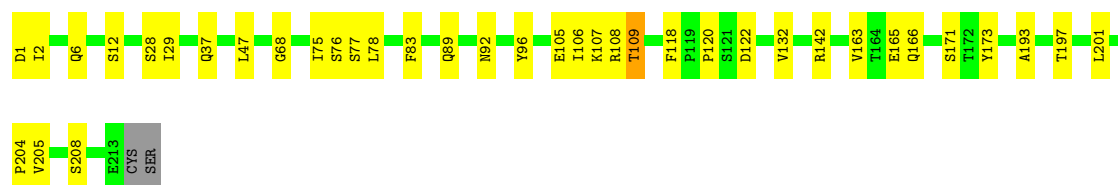
- Molecule 3: C022 Antibody Fab Light Chain

Chain K:  74% 24%



- Molecule 3: C022 Antibody Fab Light Chain

Chain L:  81% 17%



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

Chain M:  67% 33%



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

Chain N:  33% 67%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	178.38Å 178.38Å 247.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.60 – 3.20 44.60 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.60-3.20) 99.6 (44.60-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.188 , 0.231 0.190 , 0.229	Depositor DCC
R_{free} test set	3608 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	125.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 119.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.449 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19802	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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

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	0.50	0/1596	0.68	0/2172
1	B	0.49	0/1596	0.70	0/2172
1	C	0.50	0/1585	0.67	0/2158
1	D	0.51	0/1580	0.69	0/2151
2	E	0.47	0/1796	0.77	0/2453
2	G	0.46	0/1740	0.73	0/2378
2	H	0.47	0/1795	0.76	2/2451 (0.1%)
2	J	0.44	0/1751	0.72	0/2393
3	F	0.47	0/1696	0.68	0/2302
3	I	0.50	0/1702	0.71	0/2310
3	K	0.51	0/1701	0.71	0/2308
3	L	0.48	0/1696	0.71	0/2302
All	All	0.48	0/20234	0.71	2/27550 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	12	VAL	CA-C-N	-6.29	102.42	121.98
2	H	12	VAL	C-N-CA	-6.29	102.42	121.98

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	1552	0	1472	22	0
1	B	1552	0	1472	20	0
1	C	1541	0	1454	26	0
1	D	1536	0	1452	29	0
2	E	1747	0	1702	37	0
2	G	1692	0	1643	46	0
2	H	1746	0	1698	31	0
2	J	1703	0	1650	39	0
3	F	1654	0	1610	34	0
3	I	1660	0	1615	31	0
3	K	1659	0	1611	38	0
3	L	1654	0	1610	28	0
4	M	39	0	34	0	0
4	N	39	0	34	0	0
5	C	14	0	13	0	0
5	D	14	0	11	0	0
All	All	19802	0	19081	361	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (361) 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:K:126:ARG:HH12	3:K:147[B]:VAL:HG21	1.24	0.99
3:F:142:ARG:HH12	3:F:163[B]:VAL:HG21	1.44	0.82
2:G:92:THR:HG23	2:G:126:THR:HA	1.67	0.77
3:L:142:ARG:HH12	3:L:163[B]:VAL:HG21	1.51	0.76
2:G:23:THR:HG22	2:G:79:GLN:HG2	1.66	0.75
2:E:42:PRO:HG2	2:E:45:LYS:HB2	1.69	0.75
2:J:87:THR:HG23	2:J:110:THR:HA	1.67	0.75
3:K:181:THR:HG22	3:K:188:PRO:HB3	1.69	0.74
3:F:6:GLN:HE22	3:F:87:TYR:HA	1.52	0.74
2:G:16:GLU:HG2	2:G:17:THR:H	1.53	0.74
3:L:29:ILE:HA	3:L:92:ASN:HD22	1.51	0.72
2:G:89:ALA:HA	2:G:127:VAL:HG11	1.71	0.72
2:H:40:PRO:HG2	2:H:43:LYS:HB2	1.71	0.70
3:K:24:ARG:HG3	3:K:24:ARG:HH11	1.58	0.69
2:J:84:ALA:HA	2:J:111:VAL:HG11	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:35(B):GLN:HB2	3:I:45:LEU:HD11	1.73	0.69
3:K:35(B):GLN:HB2	3:K:45:LEU:HD11	1.75	0.68
2:G:175:LEU:HD21	2:G:198:VAL:HG21	1.75	0.68
3:L:89:GLN:NE2	3:L:96:TYR:HD2	1.92	0.68
3:K:126:ARG:NH1	3:K:147[B]:VAL:HG21	2.04	0.67
2:E:35:TYR:CE1	2:E:54:TYR:HD2	2.12	0.67
2:G:42:PRO:HG2	2:G:45:LYS:HB2	1.76	0.66
2:H:3:GLN:HG3	2:H:25:SER:HB2	1.76	0.66
2:G:53:ILE:HD13	2:G:73:VAL:HG13	1.78	0.65
2:H:200:HIS:CD2	2:H:202:PRO:HD2	2.31	0.65
2:J:16:GLU:HG2	2:J:17:THR:H	1.62	0.65
1:D:360:ASN:HB3	2:E:146:SER:HB3	1.80	0.64
2:E:216:HIS:CD2	2:E:218:PRO:HD2	2.33	0.63
3:K:6:GLN:HE22	3:K:82(C):TYR:HA	1.64	0.63
2:H:2:VAL:HG21	2:H:94:ARG:HH21	1.63	0.63
2:J:119:PRO:HB3	2:J:145:TYR:HB3	1.80	0.62
2:G:21:THR:HG22	2:G:81:SER:HB3	1.81	0.62
2:G:133:LYS:NZ	2:G:160:ASP:O	2.31	0.62
1:C:391:CYS:HB3	1:C:522:ALA:HB1	1.81	0.62
3:I:181:THR:HG22	3:I:188:PRO:HB3	1.81	0.62
2:J:40:PRO:HG2	2:J:43:LYS:HB2	1.81	0.61
2:E:135:PRO:HB3	2:E:161:TYR:HB3	1.82	0.61
2:J:51:ILE:HD13	2:J:71:VAL:HG13	1.81	0.61
2:G:93:ALA:HB3	2:G:95:TYR:CE1	2.36	0.61
2:G:99:ARG:HD2	2:G:100:HIS:O	2.01	0.60
3:I:5:THR:HA	3:I:95:GLN:HE22	1.66	0.60
3:F:89:GLN:NE2	3:F:96:TYR:HD2	2.00	0.59
3:I:109:LEU:HD22	3:I:167:LYS:HG3	1.83	0.59
1:C:520:ALA:HB1	1:C:521:PRO:HD2	1.84	0.59
2:G:3:GLN:HG3	2:G:25:SER:HB2	1.85	0.59
2:H:87:THR:HG23	2:H:110:THR:HA	1.85	0.59
1:C:388:ASN:HB3	1:C:527:PRO:HD2	1.83	0.59
2:E:54:TYR:HE1	2:E:55:TYR:CE2	2.20	0.59
1:D:357:ARG:NH1	1:D:394:ASN:OD1	2.35	0.59
3:F:76:SER:OG	3:F:77:SER:N	2.34	0.59
2:G:13:LYS:HA	2:G:128:SER:O	2.02	0.59
1:C:395:VAL:HG22	1:C:515:PHE:HD1	1.68	0.59
2:G:34:TYR:CG	2:G:99:ARG:HD3	2.38	0.59
2:J:66:ARG:NH1	2:J:86:ASP:OD2	2.25	0.59
3:I:85:GLN:NE2	3:I:90:ARG:O	2.36	0.59
2:G:135:PRO:HD2	2:G:221:THR:HG21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:135:PRO:HB3	2:G:161:TYR:HB3	1.84	0.58
1:A:364:ASP:O	1:A:367:VAL:HG12	2.03	0.58
2:E:2:VAL:HG21	2:E:99:ARG:NH1	2.18	0.58
3:I:194:ASN:HB2	3:I:198:CYS:C	2.29	0.58
3:K:133:LYS:HG2	3:K:138:LEU:HD23	1.86	0.58
2:E:6:GLU:OE2	2:E:97:CYS:SG	2.63	0.57
1:C:386:LYS:O	1:C:390:LEU:HD13	2.04	0.57
2:J:159:LEU:HD21	2:J:182:VAL:HG21	1.86	0.57
1:C:385:THR:HG22	1:C:386:LYS:HG3	1.87	0.57
2:E:57:GLY:O	2:E:59:THR:HG23	2.05	0.57
2:J:117:LYS:NZ	2:J:118:GLY:O	2.38	0.57
1:D:376:THR:HG23	1:D:378:LYS:HE3	1.88	0.56
2:E:19:SER:HB3	2:E:83:LYS:HG2	1.88	0.56
1:C:517:LEU:HD12	1:C:517:LEU:O	2.05	0.56
1:D:366:SER:HA	1:D:369:TYR:HB3	1.87	0.56
2:J:21:THR:HG22	2:J:79:SER:HB3	1.87	0.56
1:B:364:ASP:O	1:B:367:VAL:HG12	2.06	0.55
2:H:11:LEU:HD21	2:H:146:PHE:CE1	2.41	0.55
3:K:87:ASN:OD1	3:K:88:ASN:N	2.39	0.55
2:H:11:LEU:HD21	2:H:146:PHE:HE1	1.71	0.55
1:B:439:ASN:O	1:B:443:SER:OG	2.24	0.55
3:F:6:GLN:NE2	3:F:88:CYS:H	2.04	0.55
1:A:391:CYS:HB3	1:A:522:ALA:HB1	1.89	0.55
2:E:3:GLN:HB2	2:E:25:SER:HB2	1.89	0.55
2:E:11:LEU:HD21	2:E:162:PHE:CE1	2.41	0.55
2:J:94:ARG:HD2	2:J:95:HIS:O	2.07	0.55
1:B:391:CYS:HB3	1:B:522:ALA:HB1	1.88	0.54
2:G:160:ASP:HB3	2:G:191:LEU:HD12	1.89	0.54
1:C:354:ASN:O	1:C:398:ASP:HA	2.08	0.54
2:J:143:LYS:HE3	3:K:115:SER:OG	2.08	0.54
1:D:388:ASN:HB3	1:D:527:PRO:HD2	1.89	0.54
3:F:108:ARG:NH1	3:F:109:THR:HG23	2.22	0.54
2:J:88:ALA:HB3	2:J:90:TYR:CE1	2.43	0.54
3:L:166:GLN:HE21	3:L:171:SER:HB3	1.73	0.54
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.90	0.54
1:D:455:LEU:HD22	1:D:456:PHE:CE2	2.43	0.54
3:K:24:ARG:NH1	3:K:68:GLU:OE2	2.34	0.54
1:B:382:VAL:HG12	1:C:470:THR:OG1	2.08	0.53
1:D:395:VAL:HG22	1:D:515:PHE:HD1	1.73	0.53
3:F:37:GLN:HB2	3:F:47:LEU:HD11	1.89	0.53
3:L:89:GLN:NE2	3:L:96:TYR:CD2	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:517:LEU:HD12	1:D:517:LEU:O	2.07	0.53
3:F:108:ARG:HG2	3:F:109:THR:H	1.73	0.53
2:J:100:TYR:CE1	2:J:100(F):TYR:HD1	2.26	0.53
3:K:29:ILE:HA	3:K:87:ASN:HD22	1.74	0.53
3:I:176:TYR:O	3:I:192:SER:HB2	2.09	0.53
2:H:55:GLY:O	2:H:57:THR:HG23	2.09	0.53
1:D:520:ALA:HB1	1:D:521:PRO:HD2	1.91	0.52
1:A:369:TYR:O	2:G:107:ARG:HD2	2.09	0.52
2:H:88:ALA:HB3	2:H:90:TYR:CE2	2.44	0.52
3:K:4:MET:HE3	3:K:23:CYS:SG	2.49	0.52
1:D:392:PHE:HD1	1:D:517:LEU:HD23	1.74	0.52
2:H:66:ARG:NH1	2:H:82:LEU:HD21	2.23	0.52
2:J:24:VAL:HG23	2:J:76:ASN:ND2	2.25	0.52
3:F:166:GLN:HE21	3:F:171:SER:HB3	1.74	0.52
1:B:447:GLY:HA3	1:B:449:TYR:CE1	2.44	0.52
3:K:194:ASN:HB2	3:K:198:CYS:C	2.34	0.52
3:K:89:TYR:HA	3:K:91:TYR:HE1	1.74	0.52
1:B:405:ASP:OD1	1:B:408:ARG:NH1	2.42	0.52
1:D:386:LYS:O	1:D:390:LEU:HD13	2.10	0.52
2:E:6:GLU:OE2	2:E:120:GLY:HA3	2.09	0.52
2:G:66:LYS:O	2:G:67:SER:OG	2.19	0.52
2:J:34:TYR:CG	2:J:94:ARG:HD3	2.45	0.52
1:B:371:SER:OG	1:B:373:SER:HB3	2.09	0.51
1:C:453:TYR:CE1	1:C:493:GLN:HB3	2.45	0.51
3:I:4:MET:HE3	3:I:23:CYS:SG	2.50	0.51
1:C:347:PHE:CD1	1:C:509:ARG:NH1	2.78	0.51
2:H:6:GLU:OE2	2:H:92:CYS:SG	2.68	0.51
3:I:148:THR:HG23	3:I:158:SER:O	2.09	0.51
2:J:12:VAL:HG21	2:J:18:LEU:HB3	1.92	0.51
3:K:24:ARG:HG3	3:K:24:ARG:NH1	2.25	0.51
1:A:521:PRO:O	1:A:523:THR:HG23	2.10	0.51
3:K:176:TYR:O	3:K:192:SER:HB2	2.11	0.51
3:I:150:GLN:HG3	3:I:157:TYR:CE1	2.45	0.51
1:A:382:VAL:HG12	1:D:470:THR:OG1	2.11	0.51
2:J:100:TYR:CE1	2:J:100(F):TYR:CD1	2.99	0.51
3:K:76:LEU:HD11	3:K:99:LEU:HD21	1.93	0.51
3:L:75:ILE:HG21	3:L:78:LEU:HD12	1.93	0.51
1:C:376:THR:HG23	1:C:378:LYS:HE3	1.93	0.50
3:I:87:ASN:O	3:I:88:ASN:HB2	2.11	0.50
3:F:89:GLN:NE2	3:F:96:TYR:CD2	2.78	0.50
2:H:4:LEU:HD21	2:H:35(A):TRP:HZ3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:66:LYS:O	2:E:67:SER:OG	2.17	0.50
2:E:12:VAL:HG12	2:E:16:GLU:HB2	1.94	0.50
3:K:148:THR:HG23	3:K:158:SER:O	2.11	0.50
3:K:150:GLN:HG3	3:K:157:TYR:CE1	2.46	0.50
2:J:117:LYS:NZ	2:J:144:ASP:O	2.40	0.50
1:C:385:THR:O	1:C:386:LYS:HB2	2.12	0.50
3:F:142:ARG:NH1	3:F:163[B]:VAL:HG21	2.21	0.50
2:E:54:TYR:HD1	2:E:56:SER:H	1.58	0.49
2:G:89:ALA:HA	2:G:127:VAL:CG1	2.42	0.49
2:G:105:TYR:CE1	2:G:111:TYR:HD1	2.30	0.49
2:H:40:PRO:HA	2:H:88:ALA:HA	1.94	0.49
3:L:166:GLN:NE2	3:L:171:SER:HB3	2.27	0.49
2:H:18:LEU:HB2	2:H:82(C):VAL:HG11	1.93	0.49
3:F:75:ILE:HG21	3:F:78:LEU:HD12	1.93	0.49
1:C:433:VAL:HG22	1:C:512:VAL:HG22	1.94	0.49
2:J:24:VAL:HG21	2:J:29:ILE:HG13	1.95	0.49
3:L:106:ILE:HB	3:L:166:GLN:HE22	1.77	0.49
3:K:150:GLN:HG3	3:K:157:TYR:CZ	2.48	0.49
3:L:193:ALA:HB2	3:L:208:SER:HB2	1.95	0.49
2:H:61:PRO:HG2	3:L:1:ASP:OD1	2.13	0.49
3:I:170:TYR:O	3:I:176:TYR:OH	2.30	0.49
1:C:347:PHE:CE2	1:C:399:SER:HB2	2.48	0.49
2:J:30:SER:HB2	2:J:73:THR:HG23	1.95	0.49
2:E:60:TYR:CE2	3:F:94:TYR:CD2	3.01	0.48
3:K:125:PRO:HB2	3:K:127:GLU:OE1	2.13	0.48
3:K:6:GLN:NE2	3:K:83:CYS:H	2.12	0.48
3:F:193:ALA:HB2	3:F:208:SER:HB2	1.95	0.48
2:G:225:LYS:HE3	3:I:107:GLU:OE1	2.13	0.48
3:L:83:PHE:CE2	3:L:106:ILE:HG12	2.49	0.48
1:A:477:SER:O	1:A:479:PRO:HD3	2.13	0.48
1:B:347:PHE:CE2	1:B:509:ARG:HB3	2.49	0.48
2:J:144:ASP:HB3	2:J:175:LEU:HD12	1.96	0.48
3:L:89:GLN:HE22	3:L:96:TYR:HD2	1.60	0.48
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.96	0.48
2:E:105:TYR:CE1	2:E:111:TYR:CD1	3.02	0.48
3:F:166:GLN:NE2	3:F:171:SER:HB3	2.28	0.48
2:E:11:LEU:HD21	2:E:162:PHE:HE1	1.78	0.47
3:F:6:GLN:HE21	3:F:88:CYS:H	1.62	0.47
2:H:100:TYR:CE1	2:H:100(F):TYR:CD1	3.02	0.47
2:J:136:ALA:HB3	2:J:184:VAL:HG23	1.96	0.47
3:L:29:ILE:HA	3:L:92:ASN:ND2	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:PHE:HB3	1:C:516:GLU:O	2.14	0.47
1:D:406:GLU:OE1	1:D:495:TYR:OH	2.25	0.47
2:E:170:TRP:CZ3	2:E:212:CYS:HB3	2.49	0.47
1:B:521:PRO:O	1:B:523:THR:HG23	2.13	0.47
2:G:105:TYR:CE1	2:G:111:TYR:CD1	3.01	0.47
2:E:6:GLU:OE1	2:E:122:GLY:N	2.44	0.47
2:J:3:GLN:C	2:J:4:LEU:HD12	2.39	0.47
3:F:29:ILE:HA	3:F:92:ASN:HD22	1.79	0.47
2:G:152:ALA:HB1	2:G:205:LEU:HD21	1.96	0.47
1:C:395:VAL:HG22	1:C:515:PHE:CD1	2.49	0.47
3:F:197:THR:HG22	3:F:204:PRO:HB3	1.97	0.47
1:B:520:ALA:HB1	1:B:521:PRO:HD2	1.96	0.47
2:G:21:THR:HG22	2:G:81:SER:CB	2.45	0.47
3:I:84:GLN:HB2	3:I:93:PHE:CD2	2.49	0.47
2:J:67:VAL:HG12	2:J:82:LEU:HG	1.95	0.47
1:B:336:CYS:O	1:B:338:PHE:N	2.44	0.47
1:D:338:PHE:CE2	1:D:363:ALA:HB1	2.49	0.47
2:H:83:THR:HB	2:H:85:ALA:H	1.80	0.47
1:C:392:PHE:HD1	1:C:517:LEU:HD23	1.79	0.47
1:D:364:ASP:O	1:D:367:VAL:HG12	2.14	0.47
1:A:351:TYR:CE2	1:A:492:LEU:HD21	2.50	0.47
2:E:124:LEU:HG	2:E:125:VAL:N	2.30	0.47
3:I:89:TYR:HA	3:I:91:TYR:HE1	1.80	0.47
2:J:119:PRO:HD2	2:J:205:THR:HG21	1.96	0.47
1:D:357:ARG:HH12	1:D:394:ASN:CG	2.22	0.46
2:H:18:LEU:HD11	2:H:109:VAL:HG11	1.97	0.46
3:I:76:LEU:HD12	3:I:76:LEU:HA	1.72	0.46
1:A:336:CYS:O	1:A:338:PHE:N	2.41	0.46
1:B:431:GLY:HA2	1:B:515:PHE:CD2	2.51	0.46
3:I:142:ASN:HB2	3:I:163:LEU:HD11	1.97	0.46
3:L:28:SER:HA	3:L:68:GLY:O	2.14	0.46
3:K:60:PHE:CE1	3:K:73:ILE:HG12	2.50	0.46
1:A:366:SER:HA	1:A:369:TYR:CE1	2.50	0.46
3:F:2:ILE:HD13	3:F:29:ILE:HG22	1.97	0.46
2:G:11:LEU:HD22	2:G:162:PHE:HE1	1.80	0.46
2:E:42:PRO:HA	2:E:93:ALA:HA	1.98	0.46
2:G:135:PRO:HB2	2:G:158:VAL:HG13	1.96	0.46
2:H:154:TRP:CZ3	2:H:196:CYS:HB3	2.51	0.46
1:C:497:PHE:CD2	1:C:507:PRO:HB3	2.50	0.46
3:L:76:SER:OG	3:L:77:SER:N	2.48	0.46
1:A:520:ALA:HB1	1:A:521:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2:VAL:HG21	2:H:94:ARG:NH2	2.29	0.46
3:I:29:ILE:HA	3:I:87:ASN:HD22	1.81	0.46
3:K:131:GLN:HB3	3:K:179:GLU:HB3	1.99	0.45
3:L:105:GLU:HB3	3:L:166:GLN:OE1	2.16	0.45
2:E:68:ARG:NH2	2:E:91:ASP:OD1	2.48	0.45
2:E:140:LEU:HB3	3:F:118:PHE:CD1	2.52	0.45
2:G:133:LYS:NZ	2:G:134:GLY:O	2.46	0.45
3:I:91:TYR:HD1	3:I:91:TYR:N	2.15	0.45
3:K:89:TYR:CD1	3:K:89:TYR:N	2.83	0.45
3:I:76:LEU:HD11	3:I:99:LEU:HD21	1.98	0.45
2:J:151:THR:OG1	2:J:199:ASN:HB3	2.17	0.45
3:I:60:PHE:CE1	3:I:73:ILE:HG12	2.51	0.45
3:I:169:ASP:HA	3:I:172:LYS:HD3	1.97	0.45
1:A:379:CYS:HA	1:A:432:CYS:HA	1.99	0.45
3:K:87:ASN:CG	3:K:88:ASN:H	2.25	0.45
1:A:447:GLY:HA3	1:A:449:TYR:CE1	2.52	0.45
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.99	0.45
2:E:92:THR:HG23	2:E:126:THR:HA	1.99	0.45
2:E:105:TYR:CE1	2:E:111:TYR:HD1	2.35	0.45
2:H:131:THR:HG22	2:H:133:GLY:H	1.81	0.45
1:B:442:ASP:HB3	1:B:451:TYR:HE2	1.81	0.44
2:E:40:ARG:HB3	2:E:50:ILE:HD11	1.99	0.44
2:E:53:ILE:HG13	2:E:59:THR:HG22	1.98	0.44
2:G:140:LEU:HB3	3:I:102:PHE:CD2	2.52	0.44
1:D:347:PHE:CD2	1:D:509:ARG:NH1	2.85	0.44
1:D:381:GLY:HA3	1:D:430:THR:HG22	1.98	0.44
2:G:16:GLU:HG2	2:G:17:THR:N	2.29	0.44
2:G:182:PHE:CE2	3:I:160:SER:HB3	2.51	0.44
2:G:225:LYS:HD2	2:G:225:LYS:HA	1.71	0.44
3:K:20:THR:HG22	3:K:72:THR:OG1	2.17	0.44
2:E:59:THR:HG1	2:E:61:TYR:HE2	1.61	0.44
2:H:4:LEU:HD22	2:H:24:VAL:HG22	1.99	0.44
1:A:335:LEU:HD23	1:A:336:CYS:N	2.32	0.44
1:A:458:LYS:HA	1:A:458:LYS:HD2	1.59	0.44
1:C:424:LYS:HB3	1:C:463:PRO:HA	1.98	0.44
3:F:83:PHE:CE2	3:F:106:ILE:HG12	2.52	0.44
3:F:90:GLN:HG2	3:F:91:TYR:N	2.32	0.44
2:H:35(A):TRP:HB3	2:H:78:PHE:CZ	2.53	0.44
1:A:350:VAL:HA	1:A:400:PHE:HB2	1.99	0.44
1:B:346:ARG:HH12	1:B:354:ASN:ND2	2.16	0.44
3:F:125:LEU:HD22	3:F:183:LYS:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:28:SER:O	2:E:32:SER:OG	2.35	0.44
3:F:108:ARG:HG2	3:F:109:THR:N	2.31	0.44
2:G:18:LEU:HD23	2:G:19:SER:N	2.32	0.44
3:L:166:GLN:HG3	3:L:173:TYR:CZ	2.53	0.44
3:L:197:THR:HG22	3:L:204:PRO:HB3	1.99	0.44
1:B:458:LYS:HA	1:B:458:LYS:HD2	1.69	0.44
2:G:152:ALA:HB3	2:G:200:VAL:HG23	1.99	0.44
3:I:91:TYR:N	3:I:91:TYR:CD1	2.85	0.44
3:F:201:LEU:HD13	3:F:205:VAL:HG23	2.00	0.43
1:B:408:ARG:NH2	3:K:52:LEU:O	2.51	0.43
3:I:150:GLN:HG3	3:I:157:TYR:CZ	2.53	0.43
2:J:122:PHE:CG	3:K:108:GLN:HB2	2.53	0.43
3:F:105:GLU:HB3	3:F:166:GLN:OE1	2.18	0.43
3:K:109:LEU:HD22	3:K:167:LYS:HG3	2.00	0.43
3:L:201:LEU:HD13	3:L:205:VAL:HG23	2.00	0.43
1:C:340:GLU:O	1:C:344:ALA:HB2	2.18	0.43
2:G:163:PRO:HD2	2:G:218:PRO:CB	2.49	0.43
1:A:390:LEU:HD21	1:D:470:THR:HG21	2.00	0.43
2:H:34:TYR:CG	2:H:94:ARG:HD3	2.54	0.43
2:J:87:THR:OG1	2:J:111:VAL:HG12	2.18	0.43
2:G:138:PHE:CG	3:I:108:GLN:HB2	2.54	0.43
2:H:108:LEU:HG	2:H:109:VAL:N	2.33	0.43
1:D:354:ASN:O	1:D:398:ASP:HA	2.18	0.43
2:G:14:PRO:HD3	2:G:128:SER:O	2.19	0.43
3:L:108:ARG:NH2	3:L:109:THR:HG23	2.34	0.43
1:C:357:ARG:NH1	1:C:394:ASN:OD1	2.52	0.43
2:E:65:LEU:HD23	2:E:65:LEU:HA	1.81	0.43
1:A:347:PHE:CE2	1:A:399:SER:HB2	2.54	0.43
2:G:150:GLY:HA2	2:G:202:SER:OG	2.19	0.43
3:I:11:LEU:HD23	3:I:99:LEU:HD13	2.00	0.43
3:K:91:TYR:HD1	3:K:91:TYR:N	2.17	0.43
3:K:126:ARG:HB3	3:K:157:TYR:CD2	2.54	0.43
1:A:431:GLY:HA2	1:A:515:PHE:CD2	2.54	0.42
3:F:141:PRO:HB2	3:F:143:GLU:OE1	2.19	0.42
3:L:108:ARG:HH21	3:L:109:THR:HG23	1.84	0.42
1:D:392:PHE:HB3	1:D:516:GLU:O	2.18	0.42
2:J:11:LEU:HA	2:J:110:THR:O	2.18	0.42
2:E:18:LEU:HD11	2:E:125:VAL:HG11	2.00	0.42
3:K:196:GLY:O	3:K:197:GLU:HB3	2.19	0.42
1:D:455:LEU:O	1:D:455:LEU:HD23	2.18	0.42
2:E:138:PHE:HB3	3:F:121:SER:OG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:166:GLN:HG3	3:F:173:TYR:CZ	2.54	0.42
2:J:119:PRO:HB2	2:J:142:VAL:HG13	2.01	0.42
2:G:71:ILE:HD13	2:G:71:ILE:HG21	1.78	0.42
2:J:123:PRO:O	3:K:105:SER:HB3	2.19	0.42
3:L:2:ILE:H	3:L:2:ILE:HG13	1.63	0.42
1:B:337:PRO:O	1:B:340:GLU:HB2	2.19	0.42
2:E:54:TYR:CE1	2:E:55:TYR:CD2	3.07	0.42
3:F:106:ILE:HB	3:F:166:GLN:HE22	1.85	0.42
2:G:159:LYS:HE3	3:I:115:SER:OG	2.20	0.42
1:B:365:TYR:CD2	1:B:387:LEU:HB3	2.55	0.42
3:F:94:TYR:CD1	3:F:94:TYR:N	2.87	0.42
3:F:165:GLU:HA	3:F:165:GLU:OE1	2.20	0.42
2:J:171:GLN:HA	3:K:144:GLN:HE22	1.83	0.42
1:A:418:ILE:HD13	1:A:418:ILE:HA	1.87	0.42
1:C:347:PHE:HD1	1:C:509:ARG:NH1	2.17	0.42
1:D:361:CYS:O	1:D:524:VAL:HA	2.20	0.42
1:D:385:THR:O	1:D:386:LYS:HB2	2.19	0.42
3:F:124:GLN:HG2	3:F:129:THR:O	2.20	0.42
3:L:12:SER:HB3	3:L:107:LYS:HB2	2.01	0.42
2:J:8:GLY:HA3	2:J:20:VAL:HG12	2.02	0.42
1:D:388:ASN:O	1:D:526:GLY:HA3	2.20	0.41
2:G:8:GLY:HA3	2:G:20:VAL:HG12	2.01	0.41
2:H:19:SER:HB3	2:H:81:LYS:HD3	2.02	0.41
1:C:387:LEU:HD23	1:C:387:LEU:HA	1.81	0.41
1:D:369:TYR:CE1	1:D:385:THR:HG22	2.55	0.41
1:D:458:LYS:HD2	1:D:458:LYS:HA	1.82	0.41
2:E:93:ALA:HB3	2:E:95:TYR:CE1	2.55	0.41
1:B:518:LEU:HD23	1:B:518:LEU:HA	1.78	0.41
2:E:88:THR:HB	2:E:90:ALA:H	1.85	0.41
2:G:137:VAL:HG21	2:G:223:VAL:HB	2.03	0.41
2:J:12:VAL:HG21	2:J:18:LEU:CB	2.51	0.41
3:K:91:TYR:N	3:K:91:TYR:CD1	2.88	0.41
3:L:193:ALA:HB2	3:L:208:SER:CB	2.49	0.41
2:H:66:ARG:HH11	2:H:82:LEU:HD21	1.85	0.41
1:B:477:SER:O	1:B:479:PRO:HD3	2.20	0.41
3:K:78:PRO:HB3	3:K:155:SER:OG	2.20	0.41
1:C:458:LYS:HD2	1:C:458:LYS:HA	1.89	0.41
3:L:165:GLU:OE1	3:L:165:GLU:HA	2.19	0.41
1:A:517:LEU:HD12	1:A:517:LEU:O	2.21	0.41
1:D:497:PHE:CD2	1:D:507:PRO:HB3	2.56	0.41
3:F:21:ILE:HG12	3:F:102:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3:GLN:C	2:G:4:LEU:HD12	2.46	0.41
2:G:163:PRO:HD2	2:G:218:PRO:HB2	2.02	0.41
2:H:124:LEU:HB3	3:L:118:PHE:CD1	2.55	0.41
2:J:55:GLY:O	2:J:57:THR:HG23	2.21	0.41
2:J:31:SER:HA	2:J:53:TYR:CE2	2.56	0.41
1:A:454:ARG:NH2	1:A:467:ASP:O	2.51	0.40
2:G:40:ARG:HB3	2:G:50:ILE:HD11	2.02	0.40
3:I:100(C):ARG:NH2	3:I:100(F):ALA:HB2	2.36	0.40
2:J:147:PRO:HD2	2:J:202:PRO:CB	2.52	0.40
1:C:385:THR:O	1:C:386:LYS:CB	2.69	0.40
2:G:57:GLY:O	2:G:59:THR:HG23	2.21	0.40
1:D:347:PHE:CE1	1:D:399:SER:HB2	2.56	0.40
2:H:9:PRO:HD3	2:H:19:SER:O	2.21	0.40
3:I:196:GLY:O	3:I:197:GLU:HB3	2.21	0.40
2:J:100(I):GLU:HB3	2:J:100(J):TYR:H	1.69	0.40
3:K:145:GLU:HA	3:K:160:SER:O	2.21	0.40
1:A:340:GLU:O	1:A:344:ALA:HB2	2.21	0.40
2:H:66:ARG:NH1	2:H:86:ASP:OD2	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	194/212 (92%)	183 (94%)	11 (6%)	0	100	100
1	B	194/212 (92%)	184 (95%)	10 (5%)	0	100	100
1	C	193/212 (91%)	181 (94%)	11 (6%)	1 (0%)	24	59
1	D	192/212 (91%)	183 (95%)	9 (5%)	0	100	100
2	E	229/240 (95%)	217 (95%)	11 (5%)	1 (0%)	30	62
2	G	219/240 (91%)	203 (93%)	15 (7%)	1 (0%)	24	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	229/240 (95%)	215 (94%)	11 (5%)	3 (1%)	9	40
2	J	221/240 (92%)	210 (95%)	11 (5%)	0	100	100
3	F	213/215 (99%)	199 (93%)	14 (7%)	0	100	100
3	I	214/215 (100%)	202 (94%)	11 (5%)	1 (0%)	24	59
3	K	214/215 (100%)	202 (94%)	10 (5%)	2 (1%)	14	47
3	L	213/215 (99%)	199 (93%)	14 (7%)	0	100	100
All	All	2525/2668 (95%)	2378 (94%)	138 (6%)	9 (0%)	30	62

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	89	TYR
2	H	129	LYS
2	H	131	THR
3	I	88	ASN
2	E	148	SER
2	H	134	GLY
3	K	87	ASN
1	C	386	LYS
2	G	31	SER

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	169/185 (91%)	165 (98%)	4 (2%)	43	70
1	B	169/185 (91%)	166 (98%)	3 (2%)	51	74
1	C	167/185 (90%)	165 (99%)	2 (1%)	63	79
1	D	167/185 (90%)	163 (98%)	4 (2%)	43	70
2	E	197/207 (95%)	191 (97%)	6 (3%)	36	66
2	G	189/207 (91%)	184 (97%)	5 (3%)	40	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	197/207 (95%)	188 (95%)	9 (5%)	24	58
2	J	190/207 (92%)	189 (100%)	1 (0%)	81	85
3	F	190/190 (100%)	187 (98%)	3 (2%)	55	75
3	I	191/190 (100%)	189 (99%)	2 (1%)	68	80
3	K	191/190 (100%)	188 (98%)	3 (2%)	55	75
3	L	190/190 (100%)	187 (98%)	3 (2%)	55	75
All	All	2207/2328 (95%)	2162 (98%)	45 (2%)	48	72

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	345	THR
1	A	362	VAL
1	A	516	GLU
1	A	528	LYS
1	B	362	VAL
1	B	478	THR
1	B	528	LYS
1	C	407	VAL
1	C	516	GLU
1	D	345	THR
1	D	346	ARG
1	D	430	THR
1	D	516	GLU
2	E	11	LEU
2	E	12	VAL
2	E	17	THR
2	E	23	THR
2	E	33	ARG
2	E	199	THR
3	F	31	SER
3	F	107	LYS
3	F	122	ASP
2	G	11	LEU
2	G	70	THR
2	G	75	THR
2	G	123	THR
2	G	127	VAL
2	H	11	LEU
2	H	23	THR

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Mol	Chain	Res	Type
2	H	33	ARG
2	H	72	ASP
2	H	83	THR
2	H	94	ARG
2	H	130	SER
2	H	160	THR
2	H	183	THR
3	I	106	ASP
3	I	186	SER
2	J	179	SER
3	K	5	THR
3	K	106	ASP
3	K	140	SER
3	L	6	GLN
3	L	109	THR
3	L	122	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	450	ASN
1	C	360	ASN
1	C	370	ASN
1	D	360	ASN
1	D	370	ASN
2	E	180	HIS
3	F	6	GLN
3	F	138	ASN
2	G	41	GLN
2	G	118	HIS
2	H	39	GLN
3	I	36	GLN
3	I	136	ASN
2	J	164	HIS
3	K	6	GLN
3	K	121	ASN
3	L	38	GLN
3	L	198	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 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	1,4	14,14,15	0.37	0	17,19,21	0.81	0
4	NAG	M	2	4	14,14,15	0.24	0	17,19,21	0.61	0
4	BMA	M	3	4	11,11,12	2.37	3 (27%)	15,15,17	1.83	5 (33%)
4	NAG	N	1	1,4	14,14,15	0.70	1 (7%)	17,19,21	0.89	1 (5%)
4	NAG	N	2	4	14,14,15	0.30	0	17,19,21	0.49	0
4	BMA	N	3	4	11,11,12	1.47	3 (27%)	15,15,17	1.06	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
4	NAG	M	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	BMA	M	3	4	-	2/2/19/22	0/1/1/1
4	NAG	N	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	BMA	N	3	4	-	2/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	3	BMA	C4-C3	4.63	1.64	1.52
4	M	3	BMA	C4-C5	4.44	1.62	1.53
4	M	3	BMA	C1-C2	3.61	1.60	1.52
4	N	1	NAG	O5-C1	2.44	1.47	1.43
4	N	3	BMA	O5-C1	2.34	1.47	1.43
4	N	3	BMA	C2-C3	2.17	1.55	1.52
4	N	3	BMA	O5-C5	2.01	1.47	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	3	BMA	C3-C4-C5	4.47	118.33	110.23
4	M	3	BMA	O2-C2-C1	3.08	116.27	109.22
4	N	3	BMA	C1-O5-C5	2.99	116.19	112.19
4	M	3	BMA	C2-C3-C4	2.89	115.94	110.86
4	N	1	NAG	C1-O5-C5	2.35	115.34	112.19
4	M	3	BMA	C1-O5-C5	-2.32	109.08	112.19
4	M	3	BMA	C1-C2-C3	-2.18	106.47	109.64

There are no chirality outliers.

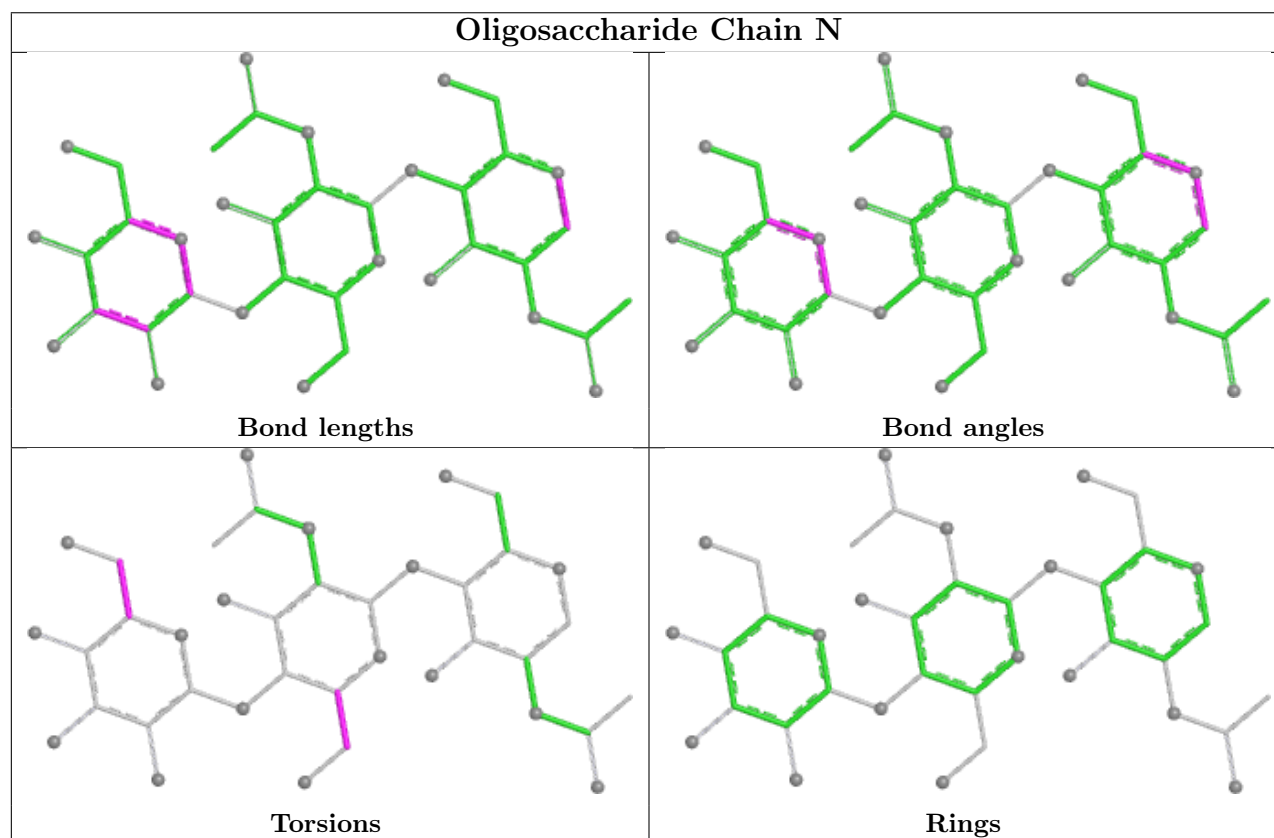
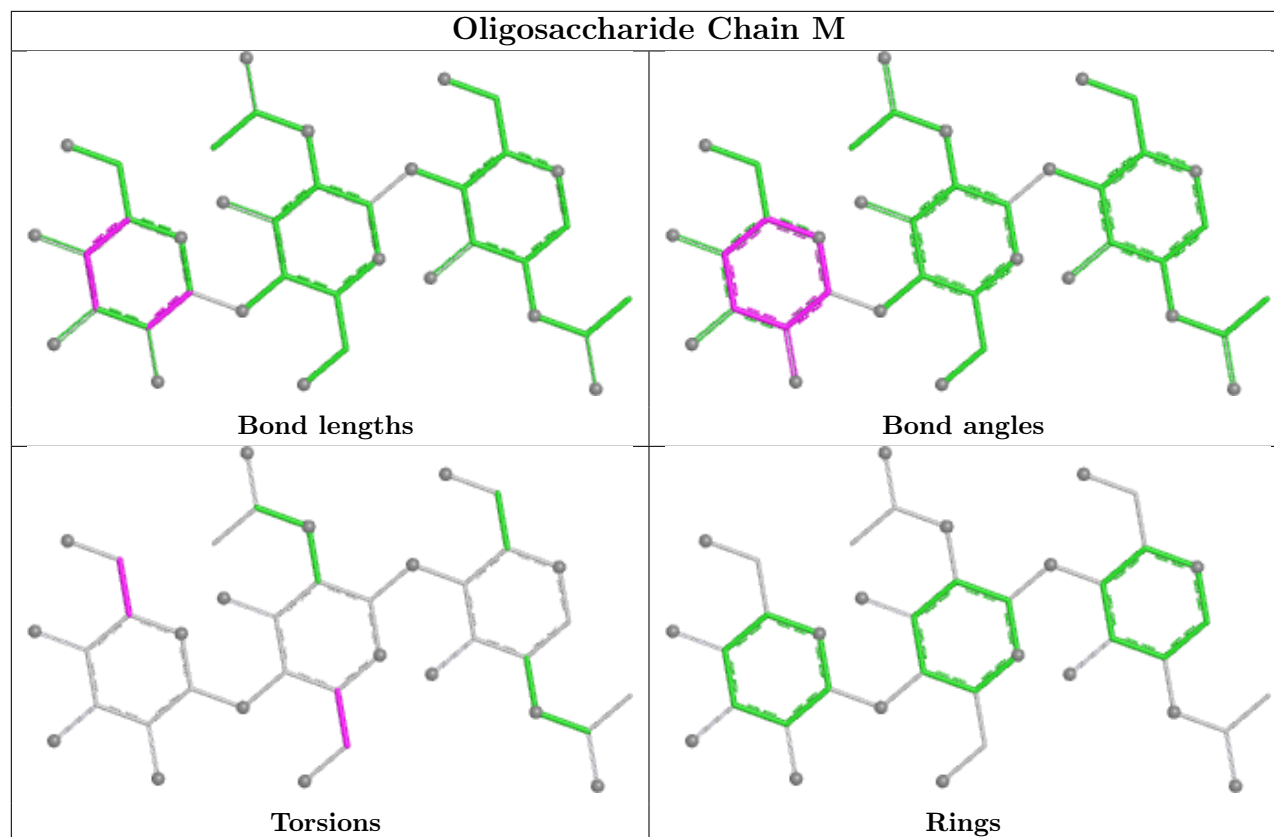
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	3	BMA	C4-C5-C6-O6
4	M	3	BMA	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	N	3	BMA	O5-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	N	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

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
5	NAG	D	601	1	14,14,15	1.43	1 (7%)	17,19,21	0.96	1 (5%)
5	NAG	C	601	1	14,14,15	1.06	1 (7%)	17,19,21	0.67	1 (5%)

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	D	601	1	-	1/6/23/26	0/1/1/1
5	NAG	C	601	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	601	NAG	O5-C1	5.16	1.52	1.43
5	C	601	NAG	O5-C1	3.70	1.49	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	601	NAG	C4-C3-C2	-2.44	107.45	111.02
5	C	601	NAG	C1-O5-C5	2.07	114.97	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	601	NAG	O5-C5-C6-O6
5	D	601	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	196/212 (92%)	-1.40	0 100 100	82, 112, 158, 176	0
1	B	196/212 (92%)	-1.43	0 100 100	79, 113, 157, 169	0
1	C	195/212 (91%)	-1.36	0 100 100	90, 121, 157, 173	0
1	D	194/212 (91%)	-1.33	0 100 100	93, 121, 159, 177	0
2	E	231/240 (96%)	-1.42	0 100 100	85, 110, 150, 187	0
2	G	223/240 (92%)	-1.29	1 (0%) 88 79	79, 141, 196, 215	0
2	H	231/240 (96%)	-1.43	0 100 100	87, 109, 148, 178	0
2	J	225/240 (93%)	-1.28	1 (0%) 88 79	79, 141, 201, 222	0
3	F	213/215 (99%)	-1.43	0 100 100	72, 114, 143, 156	2 (0%)
3	I	214/215 (99%)	-1.31	0 100 100	77, 131, 205, 216	2 (0%)
3	K	214/215 (99%)	-1.31	0 100 100	77, 128, 206, 216	2 (0%)
3	L	213/215 (99%)	-1.40	0 100 100	73, 114, 140, 156	2 (0%)
All	All	2545/2668 (95%)	-1.37	2 (0%) 92 89	72, 117, 192, 222	8 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	217	LYS	2.2
2	J	201	LYS	2.2

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

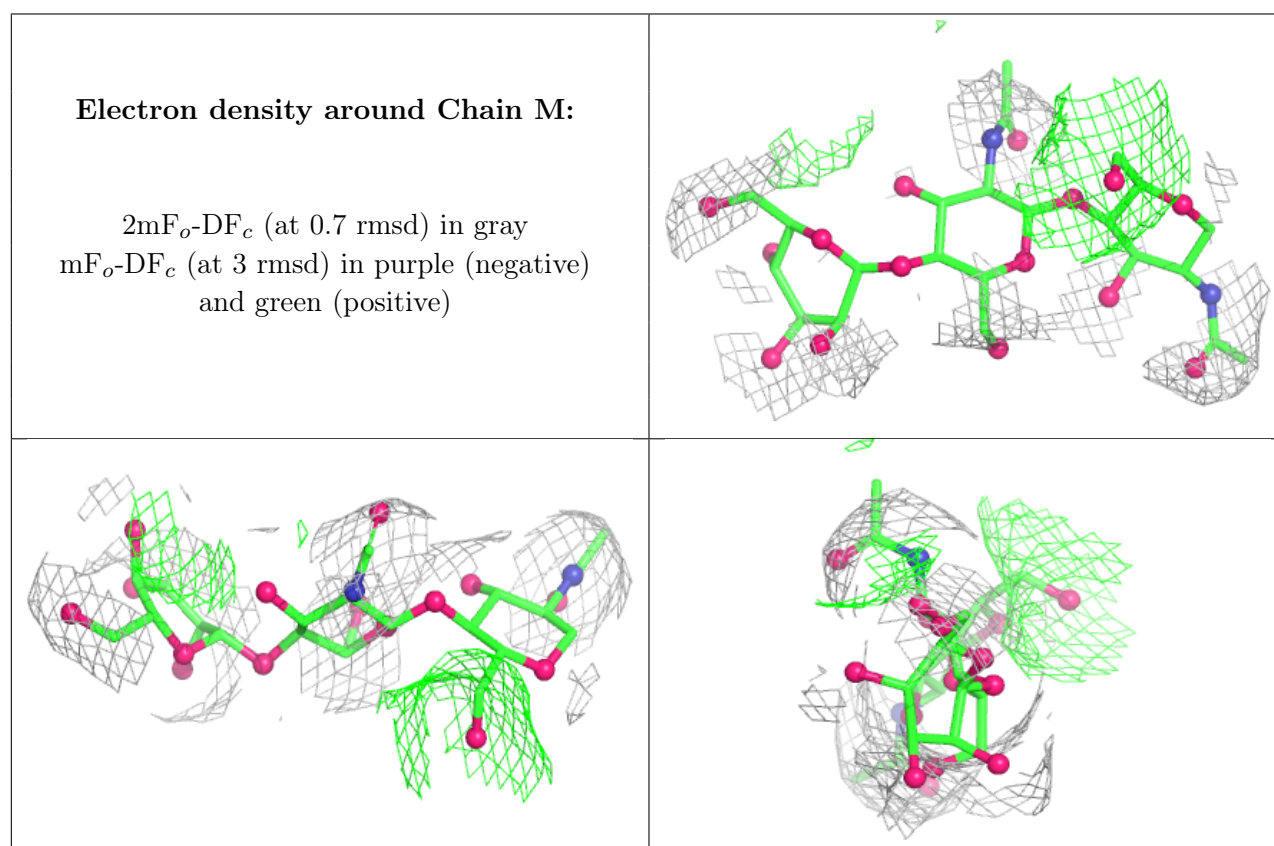
There are no non-standard protein/DNA/RNA residues in this entry.

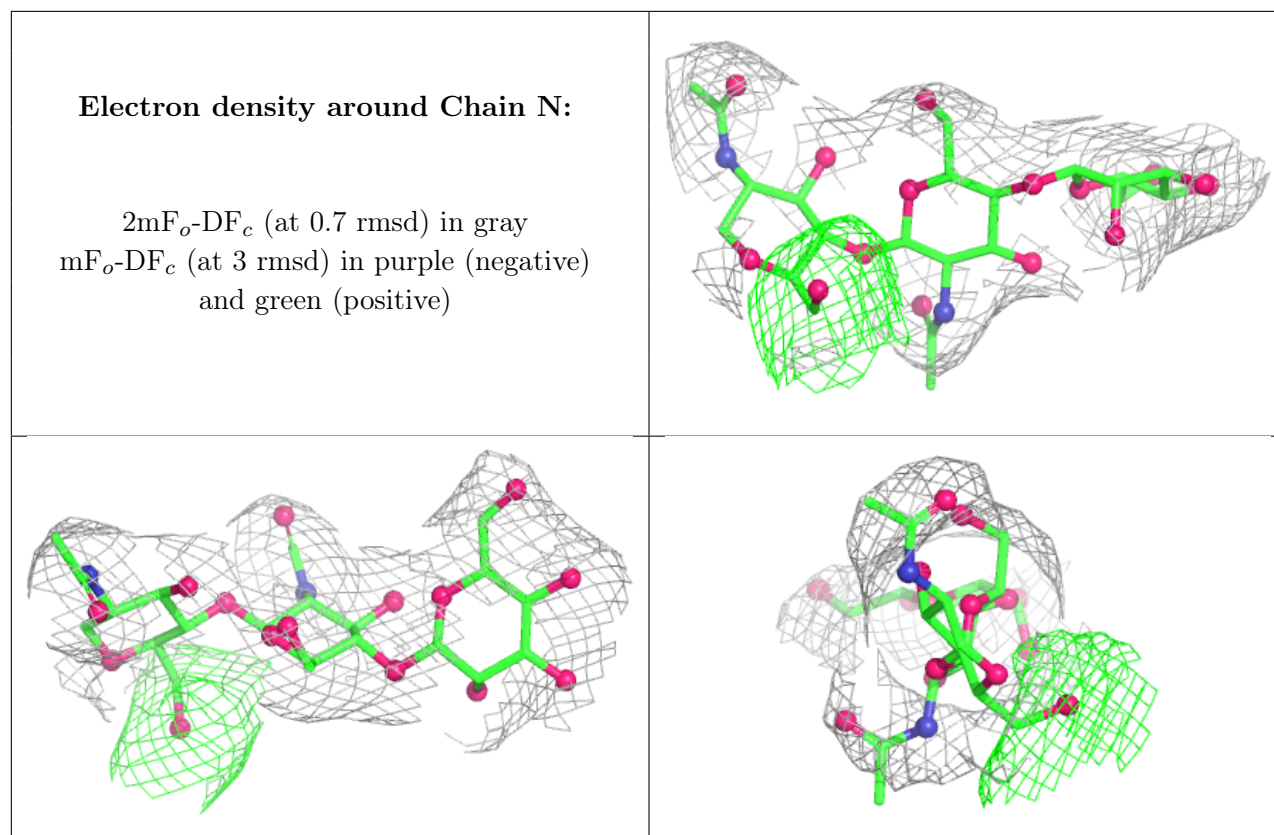
6.3 Carbohydrates [i](#)

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	BMA	N	3	11/12	0.89	0.05	152,176,185,189	0
4	BMA	M	3	11/12	0.94	0.04	157,172,174,175	0
4	NAG	N	2	14/15	0.97	0.05	149,165,179,185	0
4	NAG	M	2	14/15	0.97	0.05	145,161,169,172	0
4	NAG	M	1	14/15	0.98	0.05	113,137,151,154	0
4	NAG	N	1	14/15	0.98	0.04	114,136,149,157	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	D	601	14/15	0.96	0.06	133,148,154,155	0
5	NAG	C	601	14/15	0.97	0.06	138,148,164,166	0

6.5 Other polymers [i](#)

There are no such residues in this entry.