Full wwPDB X-ray Structure Validation Report ⓘ

Dec 4, 2023 – 12:47 PM EST

PDB ID	:	8F2J
Title	:	Crystal structure of antibody WRAIR-2134 in complex with SARS-CoV-2 receptor binding domain
Authors	:	Sankhala, R.S.; Joyce, M.G.
Deposited on	:	2022-11-08
Resolution	:	3.16 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:

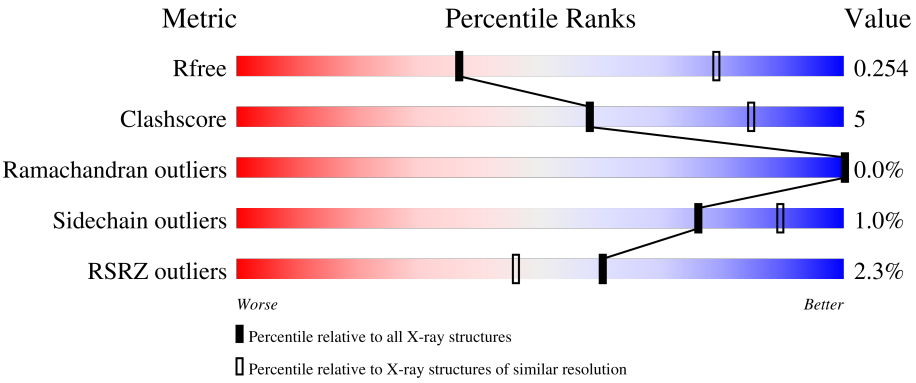
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 <=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	233	3% 83% 15%
1	D	233	2% 85% 15%
1	H	233	3% 88% 11%
1	I	233	% 86% 13%
2	B	214	5% 90% 9%

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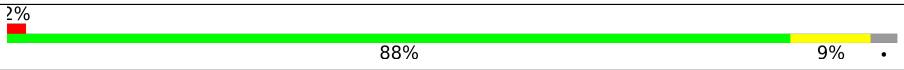
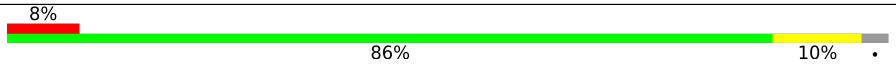
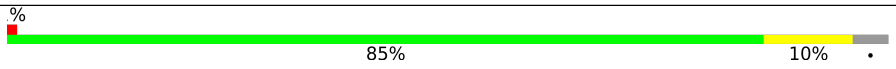
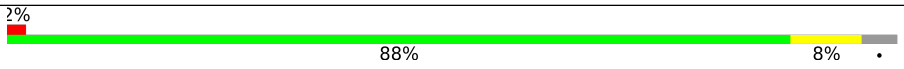
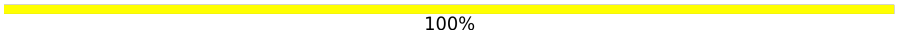
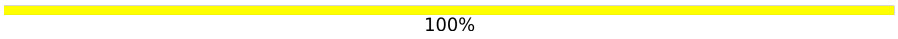
Mol	Chain	Length	Quality of chain
2	F	214	
2	J	214	
2	L	214	
3	C	205	
3	E	205	
3	G	205	
3	K	205	
4	M	2	
4	N	2	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19674 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 WRAIR-2134 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1743	1104	289	343	7			
1	D	231	Total	C	N	O	S	0	0	0
			1755	1110	291	346	8			
1	H	231	Total	C	N	O	S	0	0	0
			1755	1110	291	346	8			
1	I	230	Total	C	N	O	S	0	0	0
			1749	1107	290	345	7			

- Molecule 2 is a protein called WRAIR-2134 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1583	991	259	327	6			
2	F	211	Total	C	N	O	S	0	1	0
			1594	1001	260	327	6			
2	J	212	Total	C	N	O	S	0	0	0
			1589	994	260	329	6			
2	L	211	Total	C	N	O	S	0	0	0
			1583	991	259	327	6			

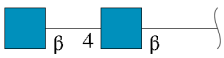
- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	199	Total	C	N	O	S	0	0	0
			1574	1006	267	293	8			
3	E	198	Total	C	N	O	S	0	0	0
			1564	1000	264	292	8			
3	G	196	Total	C	N	O	S	0	1	0
			1550	992	258	292	8			
3	K	197	Total	C	N	O	S	0	0	0
			1551	992	259	292	8			

There are 32 discrepancies between the modelled and reference sequences:

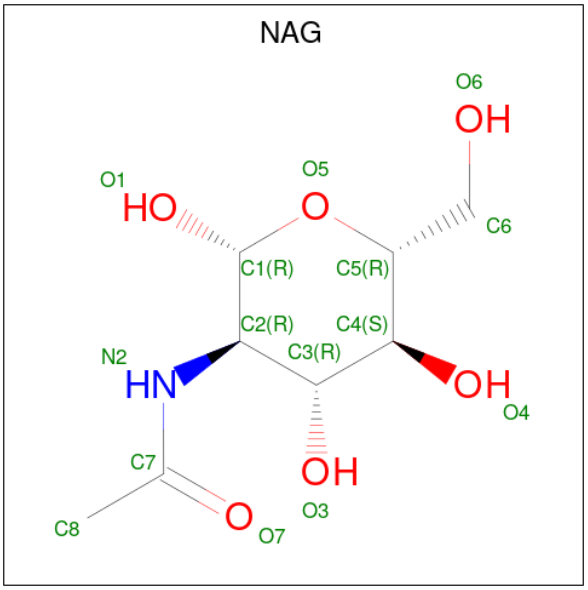
Chain	Residue	Modelled	Actual	Comment	Reference
C	528	GLY	-	expression tag	UNP P0DTC2
C	529	SER	-	expression tag	UNP P0DTC2
C	530	HIS	-	expression tag	UNP P0DTC2
C	531	HIS	-	expression tag	UNP P0DTC2
C	532	HIS	-	expression tag	UNP P0DTC2
C	533	HIS	-	expression tag	UNP P0DTC2
C	534	HIS	-	expression tag	UNP P0DTC2
C	535	HIS	-	expression tag	UNP P0DTC2
E	528	GLY	-	expression tag	UNP P0DTC2
E	529	SER	-	expression tag	UNP P0DTC2
E	530	HIS	-	expression tag	UNP P0DTC2
E	531	HIS	-	expression tag	UNP P0DTC2
E	532	HIS	-	expression tag	UNP P0DTC2
E	533	HIS	-	expression tag	UNP P0DTC2
E	534	HIS	-	expression tag	UNP P0DTC2
E	535	HIS	-	expression tag	UNP P0DTC2
G	528	GLY	-	expression tag	UNP P0DTC2
G	529	SER	-	expression tag	UNP P0DTC2
G	530	HIS	-	expression tag	UNP P0DTC2
G	531	HIS	-	expression tag	UNP P0DTC2
G	532	HIS	-	expression tag	UNP P0DTC2
G	533	HIS	-	expression tag	UNP P0DTC2
G	534	HIS	-	expression tag	UNP P0DTC2
G	535	HIS	-	expression tag	UNP P0DTC2
K	528	GLY	-	expression tag	UNP P0DTC2
K	529	SER	-	expression tag	UNP P0DTC2
K	530	HIS	-	expression tag	UNP P0DTC2
K	531	HIS	-	expression tag	UNP P0DTC2
K	532	HIS	-	expression tag	UNP P0DTC2
K	533	HIS	-	expression tag	UNP P0DTC2
K	534	HIS	-	expression tag	UNP P0DTC2
K	535	HIS	-	expression tag	UNP P0DTC2

- Molecule 4 is an oligosaccharide called 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	2	Total C N O 28 16 2 10	0	0	0
4	N	2	Total C N O 28 16 2 10	0	0	0

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



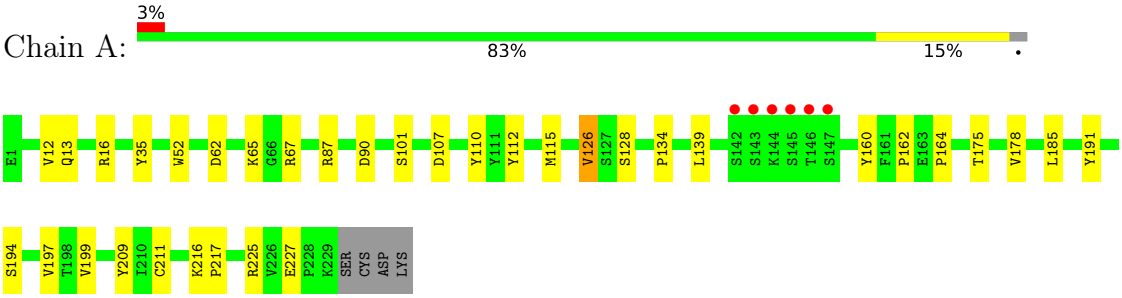
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O 14 8 1 5	0	0
5	E	1	Total C N O 14 8 1 5	0	0

3 Residue-property plots (i)

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

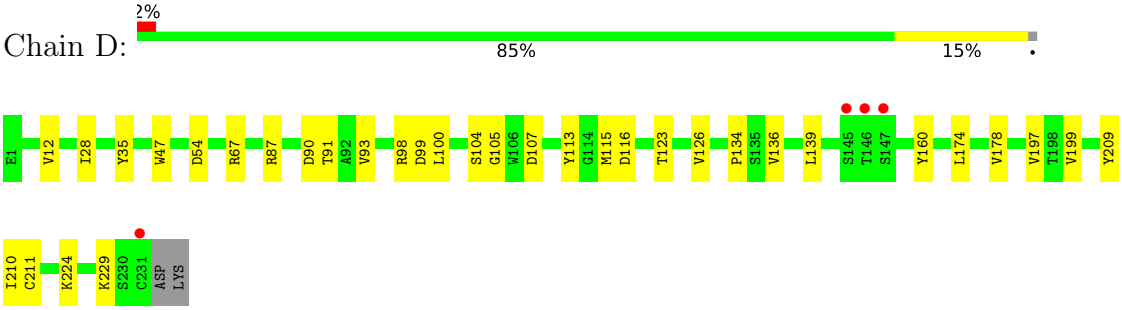
• Molecule 1: WRAIR-2134 Fab Heavy Chain

Chain A:



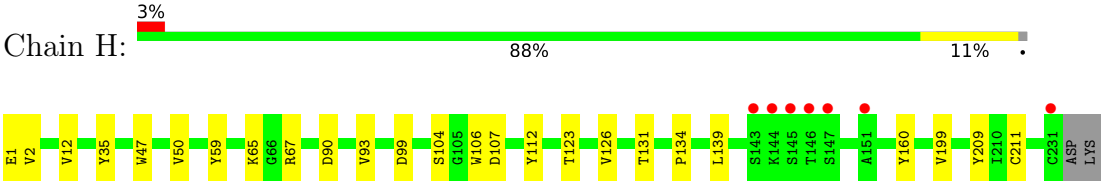
• Molecule 1: WRAIR-2134 Fab Heavy Chain

Chain D:



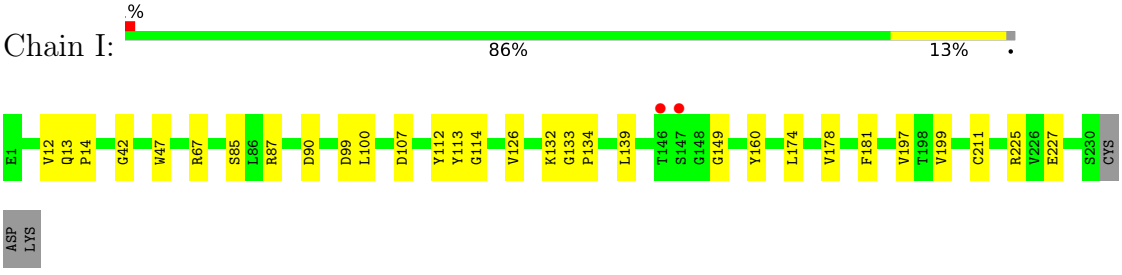
• Molecule 1: WRAIR-2134 Fab Heavy Chain

Chain H:



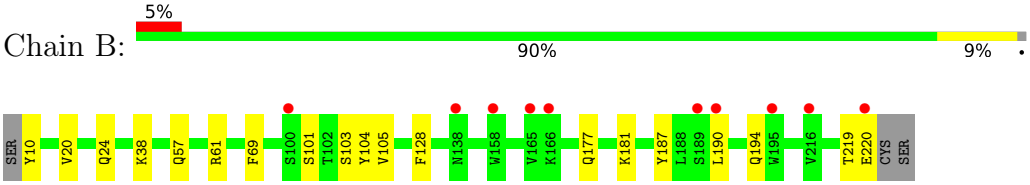
• Molecule 1: WRAIR-2134 Fab Heavy Chain

Chain I:



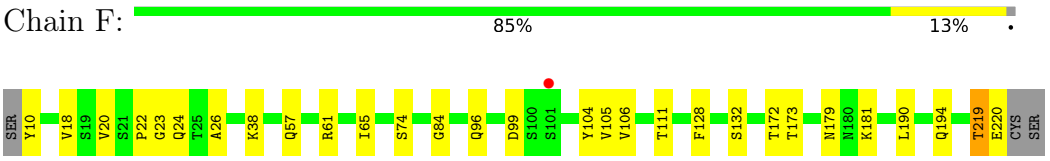
• Molecule 2: WRAIR-2134 Fab Light Chain

Chain B:



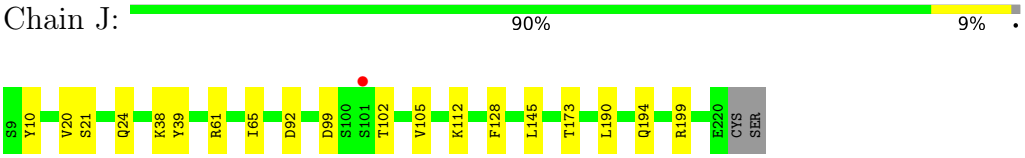
• Molecule 2: WRAIR-2134 Fab Light Chain

Chain F:



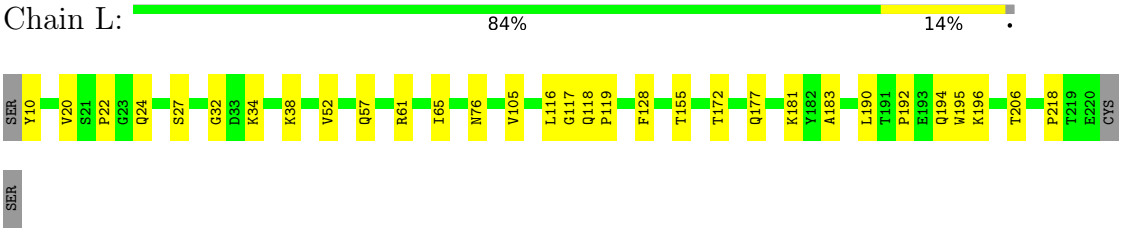
• Molecule 2: WRAIR-2134 Fab Light Chain

Chain J:



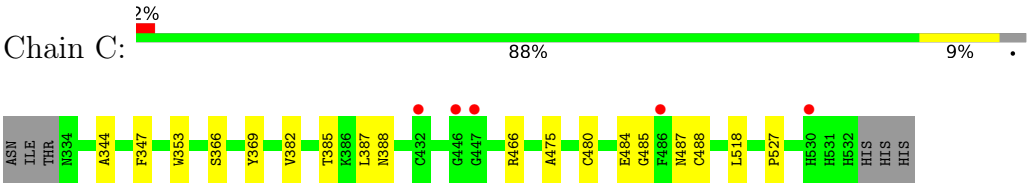
• Molecule 2: WRAIR-2134 Fab Light Chain

Chain L:



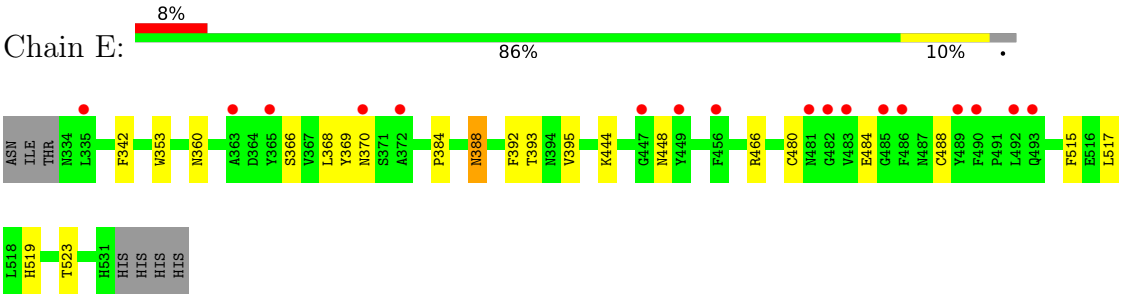
• Molecule 3: Spike protein S1

Chain C:



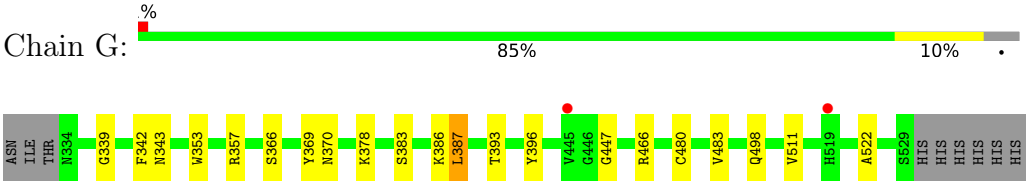
• Molecule 3: Spike protein S1

Chain E:



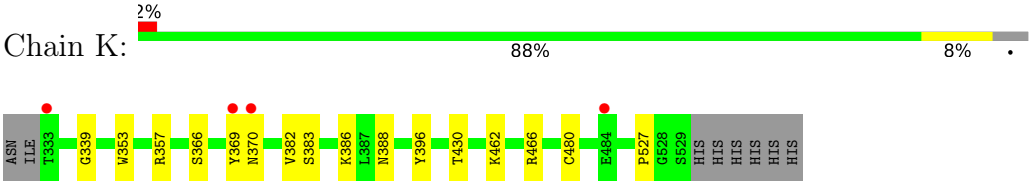
• Molecule 3: Spike protein S1

Chain G:



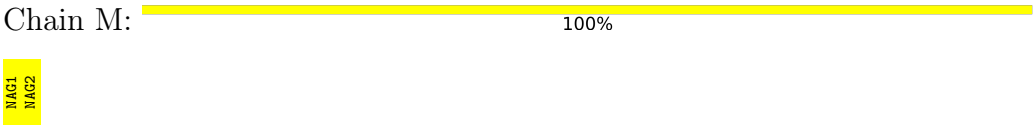
• Molecule 3: Spike protein S1

Chain K:



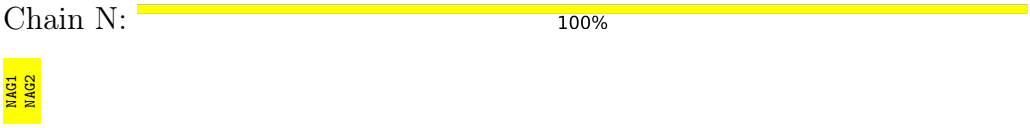
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



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

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	143.19Å 154.43Å 165.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 3.16 49.15 – 3.16	Depositor EDS
% Data completeness (in resolution range)	92.9 (19.96-3.16) 93.0 (49.15-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.209 , 0.245 0.218 , 0.254	Depositor DCC
R_{free} test set	2987 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	76.4	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 41.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	19674	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.29	0/1789	0.58	0/2438
1	D	0.28	0/1801	0.56	0/2454
1	H	0.29	0/1801	0.57	0/2454
1	I	0.27	0/1795	0.57	0/2446
2	B	0.27	0/1623	0.52	0/2218
2	F	0.33	0/1639	0.54	0/2241
2	J	0.28	0/1629	0.52	0/2226
2	L	0.29	0/1623	0.52	0/2218
3	C	0.28	0/1621	0.52	0/2205
3	E	0.29	0/1610	0.55	0/2190
3	G	0.29	0/1597	0.54	0/2172
3	K	0.30	0/1595	0.55	0/2170
All	All	0.29	0/20123	0.54	0/27432

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

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	1743	0	1680	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1755	0	1690	27	0
1	H	1755	0	1690	16	0
1	I	1749	0	1685	23	0
2	B	1583	0	1522	11	0
2	F	1594	0	1532	17	0
2	J	1589	0	1527	13	0
2	L	1583	0	1522	21	0
3	C	1574	0	1473	11	0
3	E	1564	0	1466	16	0
3	G	1550	0	1458	19	0
3	K	1551	0	1459	12	0
4	M	28	0	25	4	0
4	N	28	0	25	3	0
5	C	14	0	13	0	0
5	E	14	0	13	1	0
All	All	19674	0	18780	185	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 5.

All (185) 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:339:GLY:HA2	4:N:1:NAG:O7	1.54	1.08
3:G:387:LEU:H	3:G:387:LEU:HD12	1.17	1.07
2:L:117:GLY:O	2:L:118:GLN:HG2	1.71	0.90
4:M:1:NAG:H83	4:M:1:NAG:H3	1.58	0.86
3:C:382:VAL:HB	3:C:387:LEU:HD11	1.63	0.81
1:D:67:ARG:NH2	1:D:90:ASP:OD2	2.15	0.79
1:A:13:GLN:HB3	1:D:28:ILE:HD13	1.64	0.77
1:H:107:ASP:OD2	3:E:466:ARG:NH1	2.19	0.75
3:G:387:LEU:H	3:G:387:LEU:CD1	1.96	0.74
2:F:219:THR:HG23	2:F:220:GLU:HG3	1.69	0.74
2:L:118:GLN:HB2	2:L:119:PRO:HD2	1.68	0.73
2:F:22:PRO:O	2:L:27:SER:OG	2.06	0.72
4:M:1:NAG:H83	4:M:1:NAG:C3	2.18	0.72
1:D:93:VAL:HG22	1:D:123:THR:HG22	1.73	0.71
1:I:67:ARG:NH2	1:I:90:ASP:OD2	2.22	0.71
1:I:100:LEU:HD21	1:I:113:TYR:HB2	1.72	0.71
1:H:67:ARG:NH2	1:H:90:ASP:OD2	2.24	0.71
2:J:20:VAL:HG22	2:J:24:GLN:HG3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ARG:NH2	1:A:90:ASP:OD2	2.24	0.70
1:D:107:ASP:OD2	3:G:466:ARG:NH1	2.22	0.70
5:E:601:NAG:H3	5:E:601:NAG:H82	1.74	0.70
1:D:100:LEU:HD21	1:D:113:TYR:HB2	1.74	0.68
1:A:134:PRO:HB3	1:A:160:TYR:HB3	1.75	0.68
2:B:219:THR:HG23	2:B:220:GLU:HG2	1.77	0.66
1:H:93:VAL:HG22	1:H:123:THR:HG22	1.77	0.66
1:I:149:GLY:H	2:L:34:LYS:HE3	1.60	0.66
1:H:1:GLU:HG2	1:H:2:VAL:H	1.61	0.65
1:D:104:SER:OG	1:D:107:ASP:OD1	2.14	0.64
3:C:485:GLY:H	3:C:488:CYS:HB2	1.62	0.62
1:A:101:SER:O	1:A:110:TYR:OH	2.13	0.61
1:H:104:SER:HG	1:H:106:TRP:HD1	1.49	0.61
3:C:388:ASN:OD1	3:C:527:PRO:HD2	2.02	0.60
3:E:353:TRP:CE2	3:E:466:ARG:HB2	2.36	0.60
3:K:353:TRP:CE2	3:K:466:ARG:HB2	2.36	0.60
1:I:85:SER:HB3	1:I:87:ARG:NH2	2.17	0.60
3:G:353:TRP:CE2	3:G:466:ARG:HB2	2.37	0.60
3:G:387:LEU:HD12	3:G:387:LEU:N	2.02	0.60
1:H:99:ASP:OD2	1:H:112:TYR:HA	2.01	0.59
1:D:87:ARG:O	1:D:126:VAL:HG21	2.03	0.58
3:K:339:GLY:CA	4:N:1:NAG:O7	2.42	0.58
1:D:229:LYS:NZ	2:F:132:SER:H	2.02	0.58
1:H:104:SER:OG	1:H:106:TRP:HD1	1.87	0.58
1:A:35:TYR:CE1	1:A:115:MET:HG2	2.39	0.57
3:E:484:GLU:HA	3:E:488:CYS:O	2.04	0.57
1:I:225:ARG:NE	1:I:227:GLU:OE2	2.34	0.57
1:A:194:SER:HG	2:B:187:TYR:HE2	1.52	0.57
1:A:13:GLN:HB3	1:D:28:ILE:CD1	2.34	0.56
1:D:12:VAL:HG13	1:D:126:VAL:HG12	1.88	0.55
3:C:366:SER:HA	3:C:369:TYR:CZ	2.43	0.54
3:E:444:LYS:HE2	3:E:448:ASN:HA	1.90	0.54
2:F:10:TYR:CZ	2:F:38:LYS:HE3	2.43	0.54
1:A:216:LYS:HB2	1:A:217:PRO:HD3	1.89	0.54
1:I:87:ARG:O	1:I:126:VAL:HG11	2.09	0.53
1:I:139:LEU:HB3	2:J:128:PHE:CD2	2.43	0.53
1:I:42:GLY:HA3	2:J:173:THR:HG21	1.91	0.53
2:L:10:TYR:CZ	2:L:38:LYS:HE3	2.44	0.53
3:G:366:SER:HA	3:G:369:TYR:CZ	2.44	0.53
3:E:366:SER:HA	3:E:369:TYR:CZ	2.44	0.53
2:B:20:VAL:HG22	2:B:24:GLN:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:134:PRO:HB3	1:I:160:TYR:HB3	1.90	0.52
3:E:353:TRP:NE1	3:E:466:ARG:HB2	2.24	0.52
1:A:62:ASP:HA	1:A:65:LYS:HD3	1.92	0.52
3:C:353:TRP:CE2	3:C:466:ARG:HB2	2.44	0.52
3:C:484:GLU:HG3	3:C:488:CYS:O	2.09	0.52
1:I:99:ASP:OD2	1:I:112:TYR:HA	2.10	0.52
2:J:99:ASP:HB3	2:J:102:THR:O	2.10	0.52
3:G:383:SER:O	3:G:387:LEU:HD11	2.10	0.51
3:G:393:THR:HA	3:G:522:ALA:HA	1.92	0.51
3:K:366:SER:HA	3:K:369:TYR:CZ	2.44	0.51
1:A:52:TRP:HD1	1:A:112:TYR:HH	1.58	0.51
1:A:107:ASP:OD2	3:C:466:ARG:NH2	2.44	0.51
1:D:91:THR:OG1	1:D:126:VAL:HG22	2.10	0.51
2:B:10:TYR:CZ	2:B:38:LYS:HE3	2.47	0.50
1:D:229:LYS:HZ1	2:F:132:SER:H	1.58	0.50
1:A:12:VAL:O	1:A:126:VAL:HA	2.11	0.50
2:B:61:ARG:NH1	2:B:69:PHE:O	2.43	0.50
3:E:342:PHE:CE2	3:E:368:LEU:HD11	2.47	0.49
2:F:18:VAL:HG23	2:F:111:THR:CG2	2.43	0.49
2:L:155:THR:OG1	2:L:206:THR:HB	2.12	0.49
3:K:353:TRP:NE1	3:K:466:ARG:HB2	2.27	0.49
1:I:149:GLY:N	2:L:34:LYS:HE3	2.25	0.49
1:H:35:TYR:HE2	2:L:105:VAL:HG21	1.78	0.49
3:C:475:ALA:HB3	3:C:487:ASN:HB3	1.93	0.49
1:D:134:PRO:HB3	1:D:160:TYR:HB3	1.95	0.48
3:K:383:SER:HB2	3:K:386:LYS:HB2	1.95	0.48
1:A:35:TYR:HE2	2:B:105:VAL:HG21	1.78	0.48
1:I:13:GLN:HG2	1:I:14:PRO:HD2	1.95	0.48
2:J:92:ASP:OD1	2:J:112:LYS:HG3	2.14	0.48
2:F:20:VAL:HG21	2:F:26:ALA:HB2	1.95	0.48
3:K:388:ASN:OD1	3:K:527:PRO:HD2	2.14	0.48
1:A:178:VAL:HG22	1:A:197:VAL:HB	1.95	0.48
1:H:134:PRO:HB3	1:H:160:TYR:HB3	1.94	0.48
1:H:50:VAL:HG12	1:H:59:TYR:HB2	1.96	0.48
1:I:132:LYS:HG2	1:I:133:GLY:N	2.28	0.48
3:G:353:TRP:NE1	3:G:466:ARG:HB2	2.29	0.48
3:E:392:PHE:HA	3:E:517:LEU:CD1	2.44	0.47
3:E:360:ASN:HA	3:E:523:THR:HB	1.97	0.47
3:E:395:VAL:HG22	3:E:515:PHE:HD1	1.80	0.47
4:N:1:NAG:H61	4:N:2:NAG:N2	2.30	0.47
1:I:181:PHE:CE1	2:J:145:LEU:HD13	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:10:TYR:CZ	2:J:38:LYS:HE3	2.50	0.47
3:G:357:ARG:HD3	3:G:396:TYR:CE2	2.50	0.47
2:F:179:ASN:C	2:F:181:LYS:H	2.17	0.46
3:E:369:TYR:CD2	3:E:384:PRO:HB2	2.50	0.46
1:D:136:VAL:O	1:D:224:LYS:HE2	2.15	0.46
1:D:12:VAL:O	1:D:126:VAL:HA	2.16	0.46
1:I:100:LEU:HD21	1:I:113:TYR:CB	2.45	0.46
1:I:197:VAL:HG22	1:I:199:VAL:HG13	1.97	0.46
1:A:62:ASP:OD1	2:B:104:TYR:OH	2.30	0.46
2:L:32:GLY:O	2:L:76:ASN:HB3	2.16	0.46
4:M:1:NAG:H3	4:M:1:NAG:C8	2.37	0.46
1:H:199:VAL:HG21	1:H:209:TYR:CZ	2.51	0.45
1:A:199:VAL:HG21	1:A:209:TYR:CZ	2.51	0.45
3:G:383:SER:HB2	3:G:386:LYS:HB2	1.99	0.45
1:D:210:ILE:HG13	1:D:224:LYS:C	2.37	0.45
1:D:35:TYR:HE1	1:D:99:ASP:HB2	1.81	0.45
1:D:174:LEU:HD21	1:D:197:VAL:HG21	1.99	0.45
2:B:177:GLN:HG2	2:B:181:LYS:O	2.17	0.45
1:D:139:LEU:HB3	2:F:128:PHE:CD2	2.51	0.45
1:A:62:ASP:HA	1:A:65:LYS:CD	2.47	0.45
1:D:126:VAL:HG23	1:D:126:VAL:O	2.17	0.45
2:F:190:LEU:HB3	2:F:194:GLN:HG3	1.97	0.45
2:J:39:TYR:CE2	3:K:462:LYS:HD3	2.53	0.44
2:L:22:PRO:HD3	2:L:116:LEU:O	2.17	0.44
4:M:2:NAG:O7	4:M:2:NAG:H3	2.17	0.44
1:A:225:ARG:HE	1:A:227:GLU:CD	2.20	0.44
1:D:54:ASP:OD2	3:G:357:ARG:NH2	2.50	0.44
3:G:339:GLY:O	3:G:343:ASN:HB2	2.18	0.44
2:B:101:SER:C	2:B:103:SER:H	2.20	0.44
1:A:162:PRO:HG2	1:A:217:PRO:HG2	1.99	0.44
1:I:107:ASP:OD2	3:K:466:ARG:NH1	2.44	0.44
3:G:378:LYS:HA	3:G:378:LYS:HD2	1.77	0.44
3:E:366:SER:O	3:E:370:ASN:HB2	2.18	0.44
3:G:447:GLY:HA2	3:G:498:GLN:HG3	2.00	0.43
2:L:61:ARG:HD2	2:L:65:ILE:O	2.18	0.43
1:I:100:LEU:HD22	1:I:114:GLY:O	2.18	0.43
3:E:393:THR:H	3:E:517:LEU:HD12	1.83	0.43
3:C:518:LEU:O	3:G:483:VAL:HG21	2.18	0.43
3:K:366:SER:O	3:K:370:ASN:HB2	2.19	0.43
1:H:65:LYS:HE3	3:E:519:HIS:HB2	1.99	0.43
2:L:177:GLN:OE1	2:L:183:ALA:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:344:ALA:HB3	3:C:347:PHE:CE1	2.53	0.43
2:F:172:THR:HG22	2:F:173:THR:O	2.18	0.43
2:J:190:LEU:HB3	2:J:194:GLN:HG3	2.01	0.43
1:D:35:TYR:CE1	1:D:115:MET:HG2	2.53	0.43
1:A:185:LEU:HD13	1:A:191:TYR:CE1	2.54	0.42
2:L:195:TRP:CZ2	2:L:218:PRO:HA	2.54	0.42
1:D:199:VAL:HG21	1:D:209:TYR:CZ	2.54	0.42
1:I:12:VAL:O	1:I:126:VAL:HA	2.18	0.42
2:L:190:LEU:HB3	2:L:194:GLN:HG3	2.01	0.42
2:F:74:SER:OG	2:J:199:ARG:NH2	2.53	0.42
3:G:357:ARG:HD3	3:G:396:TYR:CZ	2.55	0.42
2:J:61:ARG:HD2	2:J:65:ILE:O	2.20	0.42
1:D:47:TRP:CG	2:F:105:VAL:HB	2.54	0.42
1:D:178:VAL:HG22	1:D:197:VAL:HB	2.01	0.42
1:H:139:LEU:HB3	2:L:128:PHE:CD2	2.55	0.42
1:D:98:ARG:NH2	1:D:116:ASP:OD2	2.42	0.42
1:I:225:ARG:HG2	1:I:227:GLU:HG2	2.02	0.42
3:G:342:PHE:CZ	3:G:511:VAL:HG11	2.55	0.42
1:H:47:TRP:CG	2:L:105:VAL:HB	2.55	0.41
2:F:61:ARG:HD2	2:F:65:ILE:O	2.20	0.41
1:H:104:SER:OG	1:H:106:TRP:CD1	2.69	0.41
2:F:96:GLN:HA	2:F:106:VAL:O	2.21	0.41
1:A:16:ARG:NH2	1:D:105:GLY:HA2	2.35	0.41
1:A:87:ARG:O	1:A:126:VAL:HG11	2.20	0.41
1:I:178:VAL:HG22	1:I:197:VAL:HB	2.01	0.41
2:J:21:SER:O	2:J:24:GLN:HG2	2.20	0.41
2:F:23:GLY:O	2:F:84:GLY:HA2	2.21	0.41
1:H:12:VAL:O	1:H:126:VAL:HA	2.21	0.41
1:I:47:TRP:CG	2:J:105:VAL:HB	2.56	0.41
2:L:118:GLN:HE22	2:L:181:LYS:HG2	1.85	0.41
2:L:192:PRO:O	2:L:196:LYS:HG3	2.19	0.41
2:F:99:ASP:HB2	2:F:104:TYR:HB3	2.03	0.41
2:L:20:VAL:HG22	2:L:24:GLN:HB2	2.02	0.41
3:G:366:SER:O	3:G:370:ASN:HB2	2.21	0.41
3:K:357:ARG:HD3	3:K:396:TYR:CZ	2.56	0.41
3:E:388:ASN:HD22	3:E:388:ASN:HA	1.62	0.40
1:A:139:LEU:HB3	2:B:128:PHE:CD2	2.56	0.40
1:I:174:LEU:HD21	1:I:197:VAL:HG21	2.02	0.40
2:L:117:GLY:O	2:L:118:GLN:CG	2.55	0.40
3:C:369:TYR:CZ	3:C:385:THR:HG22	2.56	0.40
3:E:395:VAL:HG22	3:E:515:PHE:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:382:VAL:HG13	3:K:430:THR:HG23	2.03	0.40
2:L:118:GLN:HB2	2:L:119:PRO:CD	2.43	0.40
2:B:190:LEU:HB3	2:B:194:GLN:HG3	2.04	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	227/233 (97%)	214 (94%)	12 (5%)	1 (0%)	34	68
1	D	229/233 (98%)	221 (96%)	8 (4%)	0	100	100
1	H	229/233 (98%)	221 (96%)	8 (4%)	0	100	100
1	I	228/233 (98%)	220 (96%)	8 (4%)	0	100	100
2	B	209/214 (98%)	201 (96%)	8 (4%)	0	100	100
2	F	210/214 (98%)	201 (96%)	9 (4%)	0	100	100
2	J	210/214 (98%)	199 (95%)	11 (5%)	0	100	100
2	L	209/214 (98%)	199 (95%)	10 (5%)	0	100	100
3	C	197/205 (96%)	181 (92%)	16 (8%)	0	100	100
3	E	196/205 (96%)	181 (92%)	15 (8%)	0	100	100
3	G	195/205 (95%)	179 (92%)	16 (8%)	0	100	100
3	K	195/205 (95%)	181 (93%)	14 (7%)	0	100	100
All	All	2534/2608 (97%)	2398 (95%)	135 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	PRO

5.3.2 Protein sidechains (i)

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	193/197 (98%)	189 (98%)	4 (2%)	53 78
1	D	195/197 (99%)	194 (100%)	1 (0%)	88 95
1	H	195/197 (99%)	193 (99%)	2 (1%)	76 89
1	I	194/197 (98%)	193 (100%)	1 (0%)	88 95
2	B	179/182 (98%)	178 (99%)	1 (1%)	86 94
2	F	180/182 (99%)	177 (98%)	3 (2%)	60 82
2	J	180/182 (99%)	180 (100%)	0	100 100
2	L	179/182 (98%)	176 (98%)	3 (2%)	60 82
3	C	171/177 (97%)	170 (99%)	1 (1%)	86 94
3	E	170/177 (96%)	168 (99%)	2 (1%)	71 87
3	G	169/177 (96%)	167 (99%)	2 (1%)	71 87
3	K	169/177 (96%)	168 (99%)	1 (1%)	86 94
All	All	2174/2224 (98%)	2153 (99%)	21 (1%)	76 89

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	VAL
1	A	128	SER
1	A	175	THR
1	A	211	CYS
2	B	57	GLN
1	D	211	CYS
2	F	24	GLN
2	F	57	GLN
2	F	219	THR
1	H	131	THR
1	H	211	CYS
1	I	211	CYS
2	L	52	VAL
2	L	57	GLN

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Mol	Chain	Res	Type
2	L	172	THR
3	C	480	CYS
3	E	388	ASN
3	E	480	CYS
3	G	387	LEU
3	G	480	CYS
3	K	480	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

4 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	0.29	0	17,19,21	0.63	0
4	NAG	M	2	4	14,14,15	0.31	0	17,19,21	0.72	0
4	NAG	N	1	3,4	14,14,15	0.47	0	17,19,21	0.83	0
4	NAG	N	2	4	14,14,15	0.30	0	17,19,21	0.96	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	-	5/6/23/26	0/1/1/1
4	NAG	M	2	4	-	4/6/23/26	0/1/1/1
4	NAG	N	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	1	NAG	C3-C2-N2-C7
4	M	1	NAG	C8-C7-N2-C2
4	M	1	NAG	O7-C7-N2-C2
4	M	2	NAG	O7-C7-N2-C2
4	N	1	NAG	C8-C7-N2-C2
4	N	1	NAG	O7-C7-N2-C2
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	M	2	NAG	C8-C7-N2-C2
4	M	1	NAG	O5-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	M	2	NAG	C1-C2-N2-C7
4	M	2	NAG	C3-C2-N2-C7

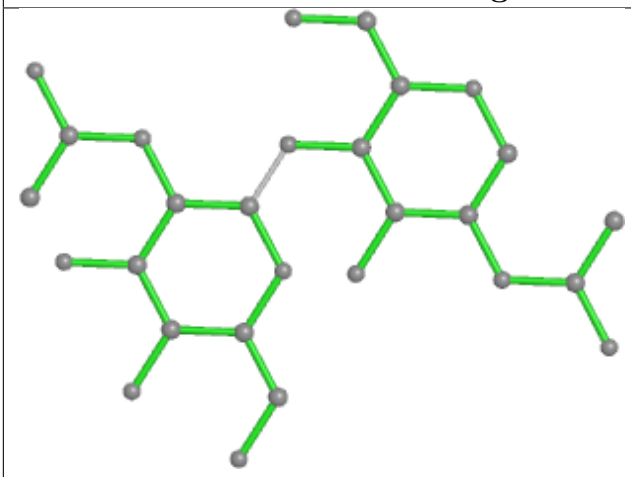
There are no ring outliers.

4 monomers are involved in 7 short contacts:

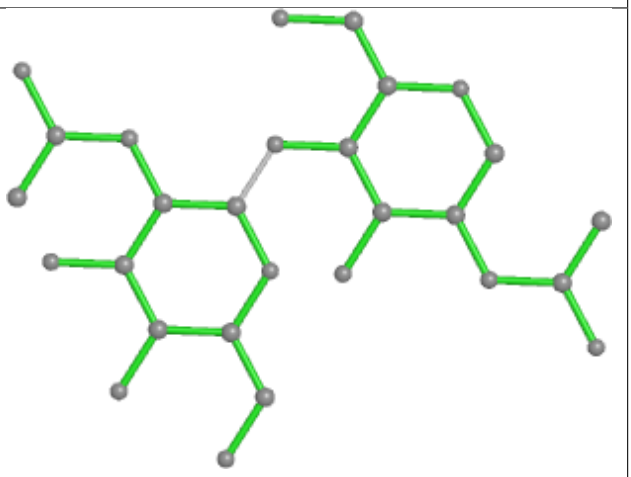
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	1	NAG	3	0
4	M	2	NAG	1	0
4	N	1	NAG	3	0
4	N	2	NAG	1	0

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

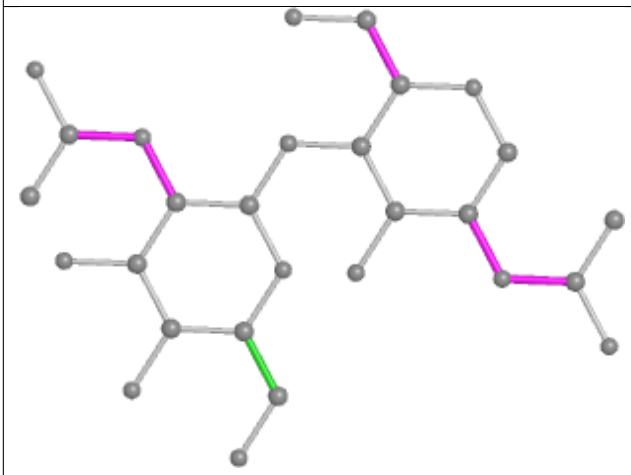
Oligosaccharide Chain M



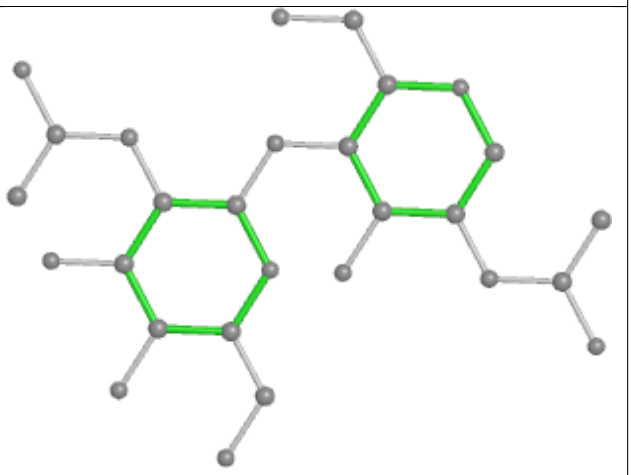
Bond lengths



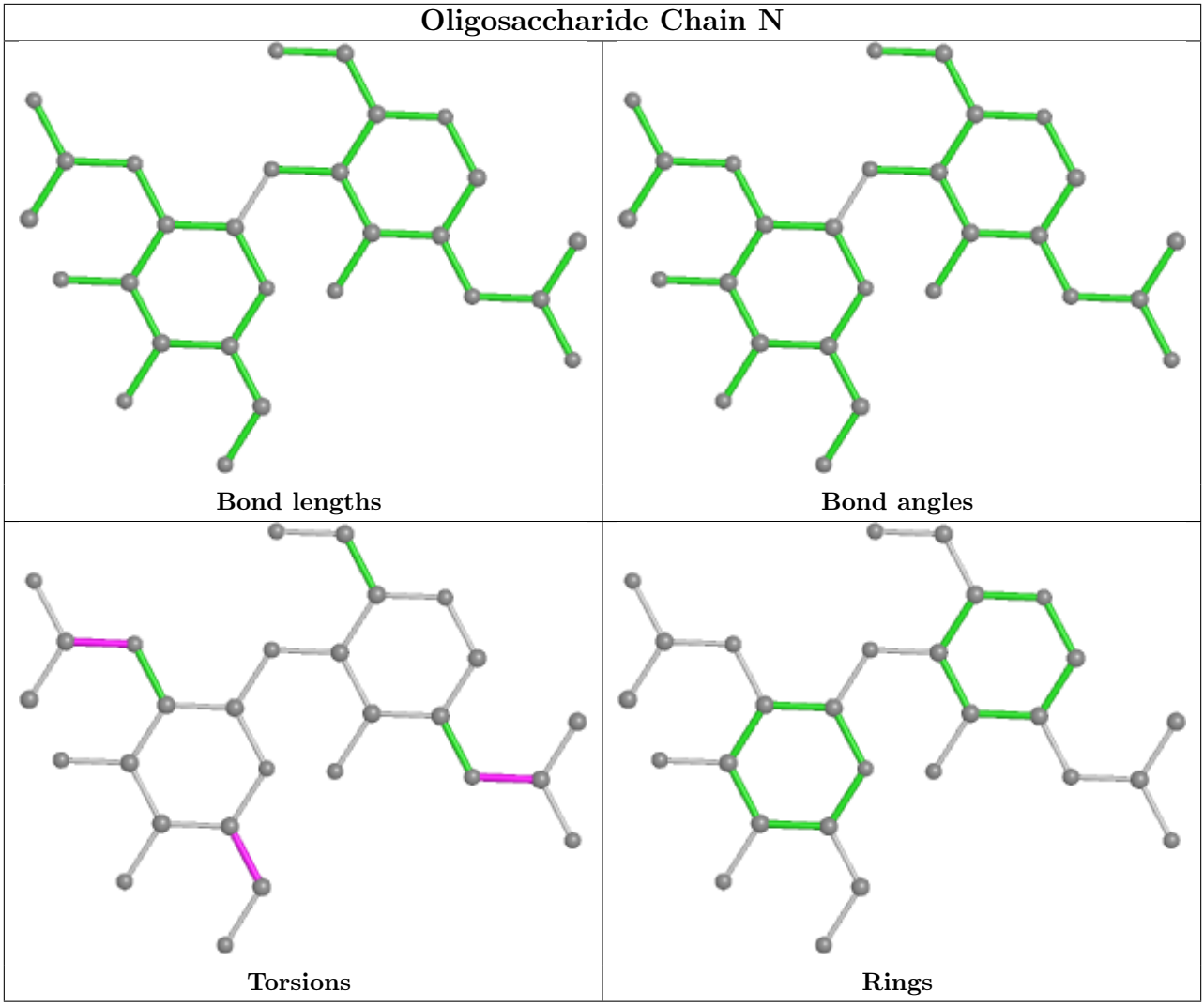
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	C	601	3	14,14,15	0.29	0	17,19,21	0.84	0
5	NAG	E	601	3	14,14,15	0.28	0	17,19,21	0.71	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	C	601	3	-	4/6/23/26	0/1/1/1
5	NAG	E	601	3	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	601	NAG	C8-C7-N2-C2
5	E	601	NAG	O7-C7-N2-C2
5	E	601	NAG	O5-C5-C6-O6
5	C	601	NAG	C8-C7-N2-C2
5	C	601	NAG	O5-C5-C6-O6
5	E	601	NAG	C1-C2-N2-C7
5	C	601	NAG	O7-C7-N2-C2
5	C	601	NAG	C3-C2-N2-C7
5	E	601	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	601	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	229/233 (98%)	0.02	6 (2%) 56 40	55, 78, 123, 212	0
1	D	231/233 (99%)	-0.07	4 (1%) 70 57	44, 69, 114, 208	0
1	H	231/233 (99%)	-0.08	7 (3%) 50 33	43, 62, 104, 198	0
1	I	230/233 (98%)	0.05	2 (0%) 84 75	44, 73, 138, 247	0
2	B	211/214 (98%)	0.28	10 (4%) 31 17	57, 92, 140, 160	0
2	F	211/214 (98%)	-0.14	1 (0%) 91 86	47, 63, 94, 138	0
2	J	212/214 (99%)	-0.13	1 (0%) 91 86	44, 65, 101, 178	0
2	L	211/214 (98%)	-0.01	0 100 100	49, 79, 123, 143	0
3	C	199/205 (97%)	0.31	5 (2%) 57 42	69, 107, 154, 217	0
3	E	198/205 (96%)	0.49	17 (8%) 10 5	64, 114, 174, 216	0
3	G	196/205 (95%)	0.05	2 (1%) 82 73	59, 89, 145, 196	0
3	K	197/205 (96%)	-0.05	4 (2%) 65 50	48, 69, 124, 153	0
All	All	2556/2608 (98%)	0.05	59 (2%) 60 46	43, 77, 140, 247	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	486	PHE	6.1
1	H	146	THR	5.8
1	A	143	SER	5.5
1	A	142	SER	5.0
1	A	146	THR	4.9
1	A	147	SER	4.9
3	C	530	HIS	4.6
1	H	145	SER	4.4
3	E	489	TYR	4.2
3	E	493	GLN	4.1
3	E	492	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	145	SER	3.8
1	H	144	LYS	3.8
3	G	445	VAL	3.8
3	E	485	GLY	3.8
1	I	147	SER	3.8
1	D	147	SER	3.6
1	A	144	LYS	3.5
3	K	484	GLU	3.4
3	E	486	PHE	3.3
3	E	482	GLY	3.2
1	H	147	SER	3.2
3	E	372	ALA	3.0
3	K	333	THR	3.0
3	C	447	GLY	2.9
2	B	166	LYS	2.9
1	D	146	THR	2.8
2	B	195	TRP	2.8
3	C	446	GLY	2.7
1	D	231	CYS	2.7
1	D	145	SER	2.7
2	J	101	SER	2.7
2	F	101	SER	2.6
3	E	447	GLY	2.6
3	E	370	ASN	2.5
3	E	335	LEU	2.5
1	H	143	SER	2.5
1	I	146	THR	2.5
3	G	519	HIS	2.4
1	H	151	ALA	2.4
2	B	165	VAL	2.4
3	E	449	TYR	2.4
3	K	370	ASN	2.4
2	B	100	SER	2.3
2	B	216	VAL	2.3
2	B	189	SER	2.3
3	E	456	PHE	2.3
2	B	158	TRP	2.2
3	E	481	ASN	2.2
3	C	432	CYS	2.2
3	E	490	PHE	2.1
3	K	369	TYR	2.0
1	H	231	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
3	E	363	ALA	2.0
2	B	138	ASN	2.0
2	B	190	LEU	2.0
2	B	220	GLU	2.0
3	E	365	TYR	2.0
3	E	483	VAL	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)

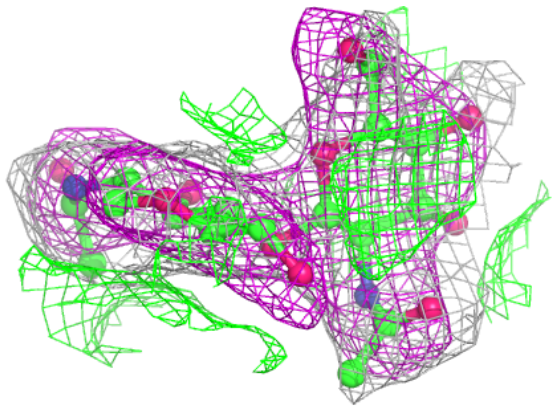
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

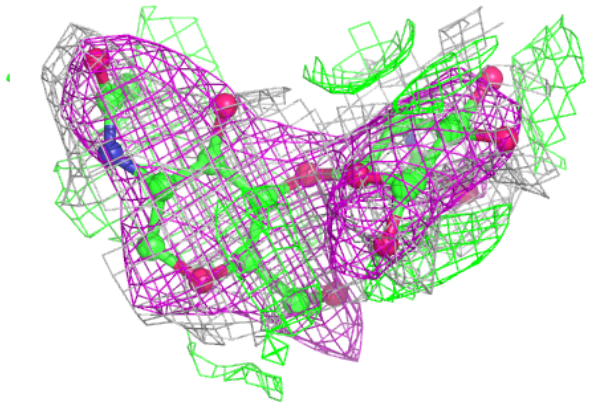
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	M	2	14/15	0.63	0.37	30,30,30,30	0
4	NAG	N	2	14/15	0.81	0.39	30,30,30,30	0
4	NAG	M	1	14/15	0.84	0.37	30,30,30,30	0
4	NAG	N	1	14/15	0.93	0.28	30,30,30,30	0

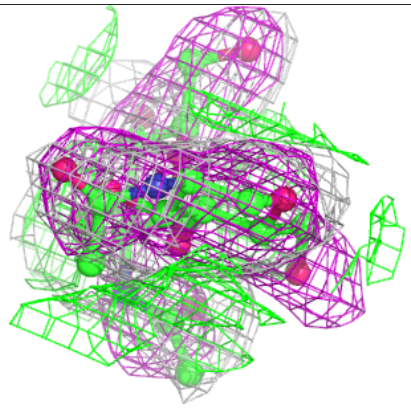
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain M:

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

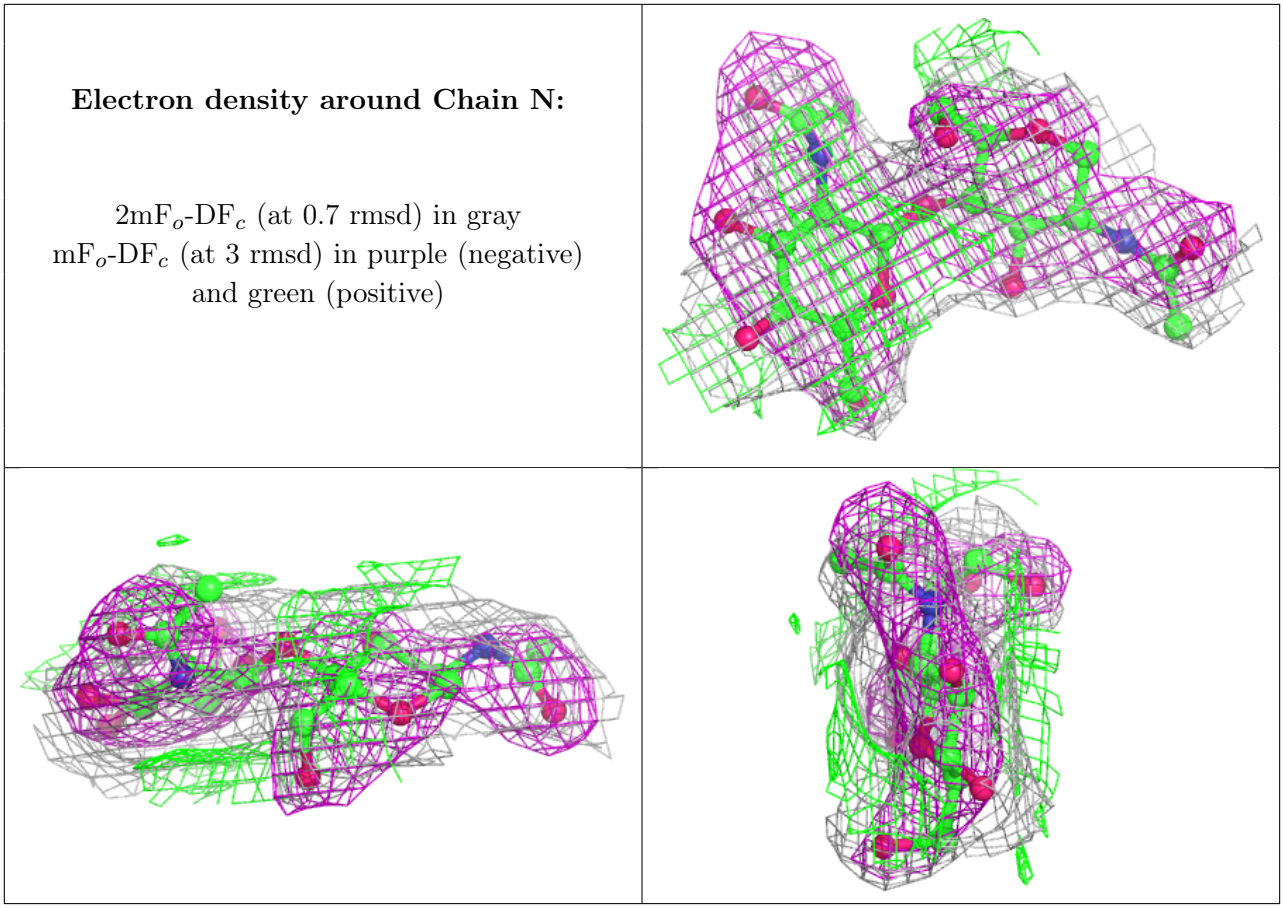






Electron density around Chain N:

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



6.4 Ligands

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, 95^{th} 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	C	601	14/15	0.85	0.45	30,30,30,30	0
5	NAG	E	601	14/15	0.90	0.43	30,30,30,30	0

6.5 Other polymers

There are no such residues in this entry.