Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 10:11 am BST

PDB ID	:	8S0M
Title	:	Crystal structure of the HKU1 receptor binding domain in complex with TM-PRSS2 and the nanobody A01
Authors	:	Duquerroy, S.; Fernandez, I.; Rey, F.
Deposited on	:	2024-02-14
Resolution	:	3.55 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:

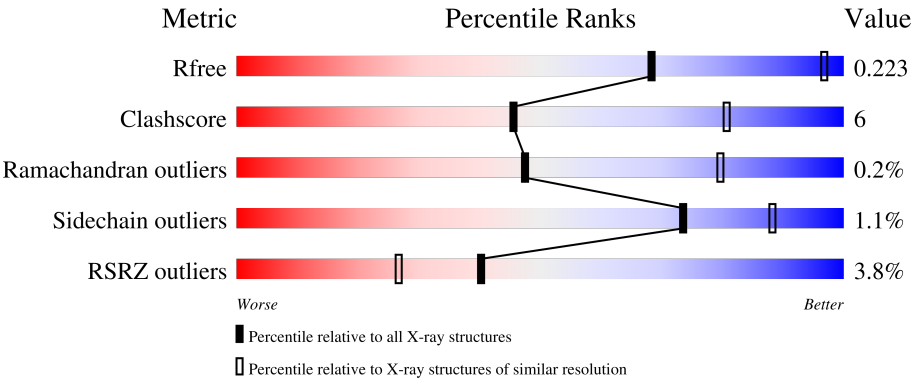
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.55 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	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)

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	B	395	3% 67% 18% • 14%
1	E	395	3% 69% 14% • 15%
2	U	136	% 81% 15% • •
2	V	136	11% 83% 11% • 5%
3	A	366	3% 82% 12% 5%

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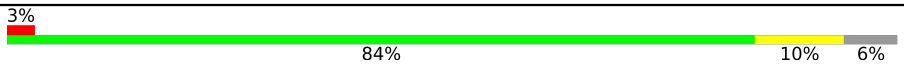
Mol	Chain	Length	Quality of chain
3	D	366	
4	F	2	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12662 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 Transmembrane protease serine 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	341	Total	C	N	O	S	0	0	0
			2662	1689	460	489	24			
1	E	334	Total	C	N	O	S	0	0	0
			2608	1655	451	478	24			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	441	ALA	SER	engineered mutation	UNP O15393
B	493	GLY	-	expression tag	UNP O15393
B	494	PRO	-	expression tag	UNP O15393
B	495	PHE	-	expression tag	UNP O15393
B	496	GLU	-	expression tag	UNP O15393
B	497	ASP	-	expression tag	UNP O15393
B	498	ASP	-	expression tag	UNP O15393
B	499	ASP	-	expression tag	UNP O15393
B	500	ASP	-	expression tag	UNP O15393
B	501	LYS	-	expression tag	UNP O15393
E	441	ALA	SER	engineered mutation	UNP O15393
E	493	GLY	-	expression tag	UNP O15393
E	494	PRO	-	expression tag	UNP O15393
E	495	PHE	-	expression tag	UNP O15393
E	496	GLU	-	expression tag	UNP O15393
E	497	ASP	-	expression tag	UNP O15393
E	498	ASP	-	expression tag	UNP O15393
E	499	ASP	-	expression tag	UNP O15393
E	500	ASP	-	expression tag	UNP O15393
E	501	LYS	-	expression tag	UNP O15393

- Molecule 2 is a protein called Nanobody A01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	U	131	Total	C	N	O	S	0	0	0
			991	616	166	203	6			
2	V	129	Total	C	N	O	S	0	0	0
			981	610	164	201	6			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	346	Total	C	N	O	S	0	0	0
			2691	1695	454	518	24			
3	D	345	Total	C	N	O	S	0	0	0
			2634	1651	447	512	24			

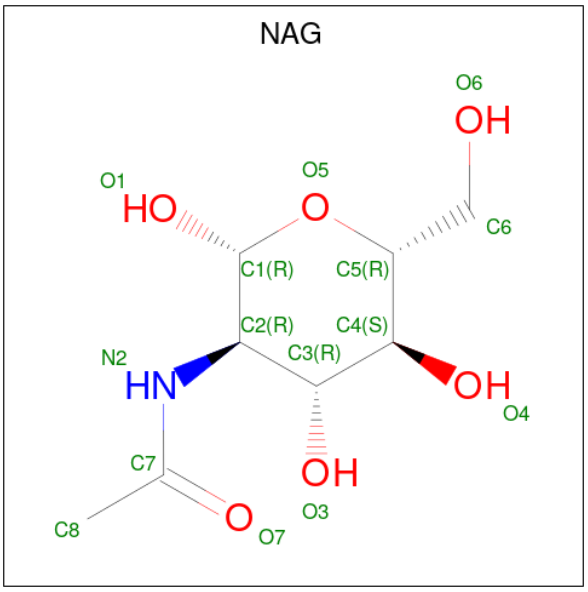
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	333	VAL	ALA	conflict	UNP Q0ZME7
D	333	VAL	ALA	conflict	UNP Q0ZME7

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

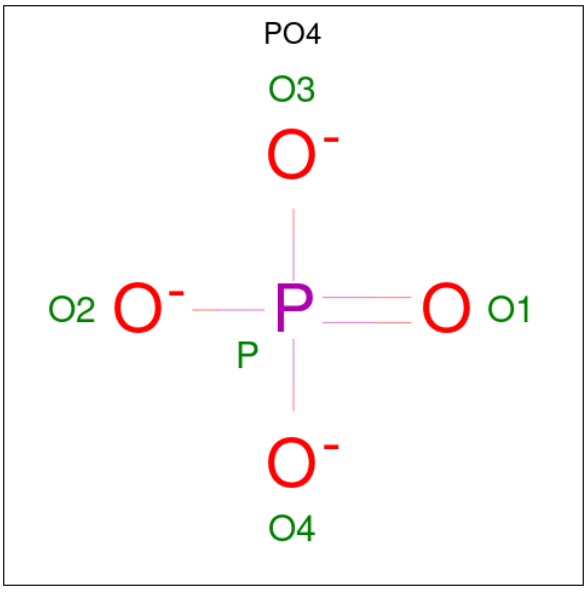
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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	B	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	D	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	D	1	Total O P 5 4 1	0	0

- Molecule 7 is water.

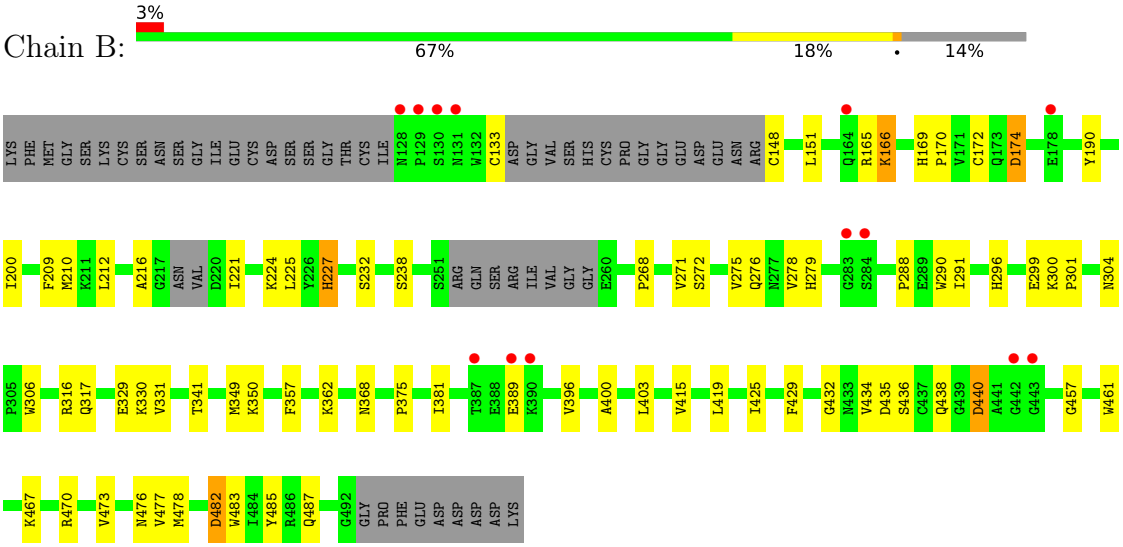
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	U	1	Total O 1 1	0	0

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.

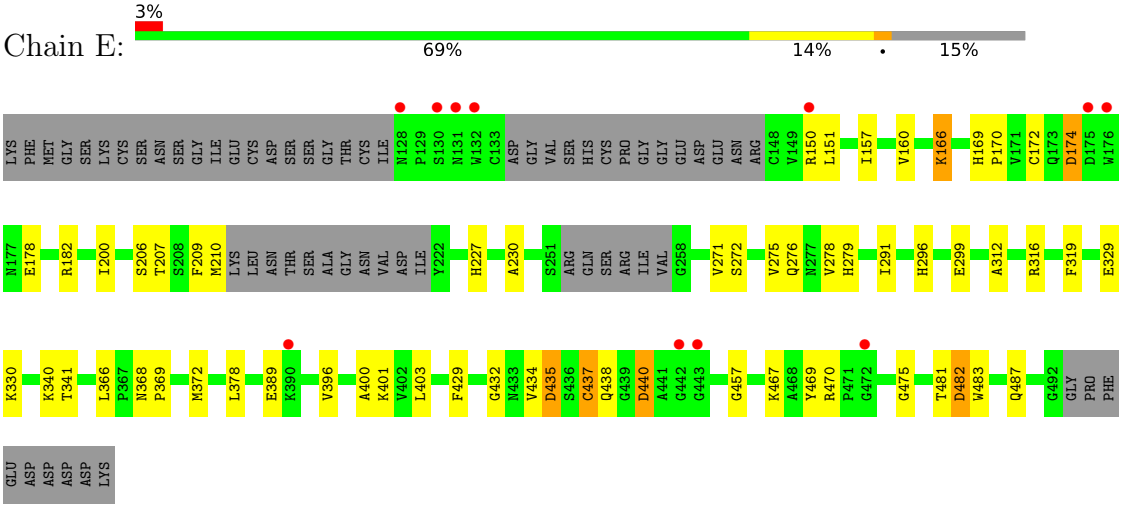
• Molecule 1: Transmembrane protease serine 2

Chain B:



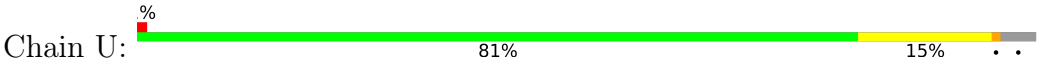
• Molecule 1: Transmembrane protease serine 2

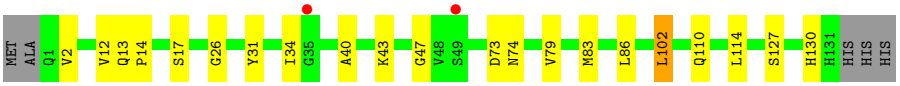
Chain E:



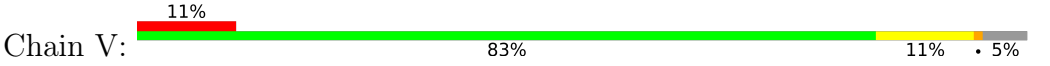
• Molecule 2: Nanobody A01

Chain U:

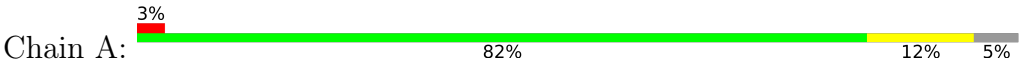


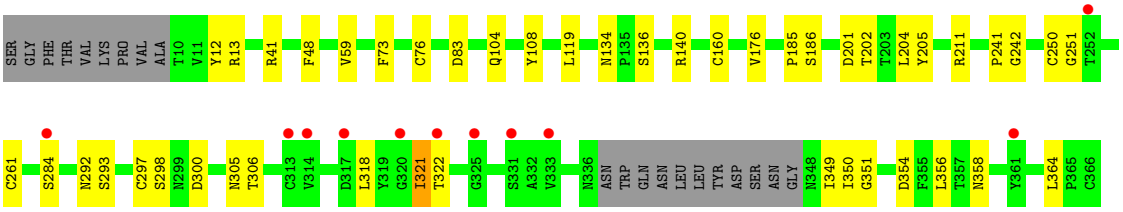


• Molecule 2: Nanobody A01

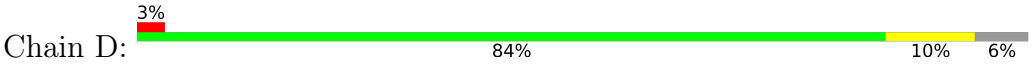


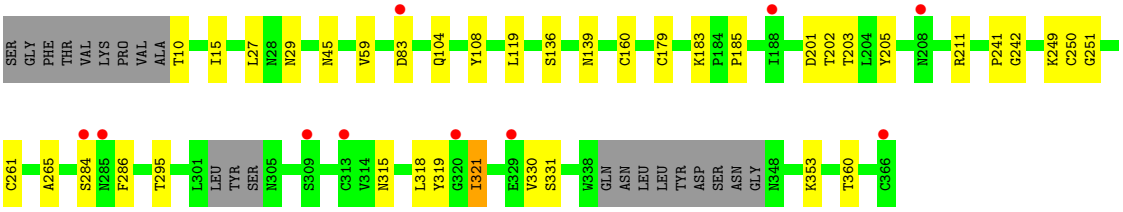
• Molecule 3: Spike protein S1





• Molecule 3: Spike protein S1





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

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	201.87Å 201.87Å 210.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.97 – 3.55 24.97 – 3.55	Depositor EDS
% Data completeness (in resolution range)	99.3 (24.97-3.55) 99.3 (24.97-3.55)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 3.54Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.193 , 0.221 0.198 , 0.223	Depositor DCC
R_{free} test set	2755 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	180.2	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 166.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.050 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12662	wwPDB-VP
Average B, all atoms (Å^2)	220.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% 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, PO4

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	B	0.31	0/2734	0.63	1/3718 (0.0%)
1	E	0.31	0/2680	0.63	1/3644 (0.0%)
2	U	0.27	0/1010	0.50	0/1369
2	V	0.27	0/1000	0.49	0/1355
3	A	0.28	0/2759	0.49	0/3756
3	D	0.26	0/2698	0.47	0/3673
All	All	0.29	0/12881	0.55	2/17515 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	225	LEU	CA-CB-CG	6.02	129.14	115.30
1	E	437	CYS	CA-CB-SG	-5.28	104.49	114.00

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	B	2662	0	2544	50	0
1	E	2608	0	2489	45	0
2	U	991	0	929	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V	981	0	925	12	0
3	A	2691	0	2535	31	0
3	D	2634	0	2431	28	0
4	F	28	0	25	2	0
5	A	28	0	26	0	0
5	B	14	0	13	1	0
5	D	14	0	12	2	0
6	A	5	0	0	0	0
6	D	5	0	0	0	0
7	U	1	0	0	0	0
All	All	12662	0	11929	158	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (158) 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)
1:B:221:ILE:HG23	1:B:224:LYS:HD2	1.63	0.80
1:B:133:CYS:SG	1:B:148:CYS:N	2.56	0.79
1:B:470:ARG:HH11	3:A:211:ARG:HD2	1.45	0.78
1:E:170:PRO:HG2	1:E:209:PHE:HD1	1.48	0.77
1:E:341:THR:HG22	3:D:205:TYR:HE2	1.52	0.74
1:B:415:VAL:O	3:A:211:ARG:NH1	2.20	0.74
1:B:470:ARG:NH1	3:A:211:ARG:HD2	2.03	0.73
1:B:165:ARG:HD3	1:B:227:HIS:CE1	2.24	0.72
1:B:467:LYS:HB3	1:B:470:ARG:HE	1.56	0.71
1:E:271:VAL:HG21	1:E:291:ILE:HD13	1.73	0.70
1:E:469:TYR:O	3:D:211:ARG:NH1	2.26	0.69
1:B:419:LEU:HD13	3:A:204:LEU:HD12	1.76	0.68
1:B:170:PRO:HG2	1:B:209:PHE:HD1	1.59	0.68
1:B:216:ALA:HB3	1:B:224:LYS:HG2	1.77	0.66
1:E:467:LYS:HB3	1:E:470:ARG:HE	1.61	0.66
1:B:329:GLU:HG3	1:B:330:LYS:HG3	1.78	0.64
3:A:41:ARG:NH2	4:F:1:NAG:O6	2.32	0.62
1:E:329:GLU:HG3	1:E:330:LYS:HG3	1.82	0.62
1:B:172:CYS:HB3	1:B:174:ASP:OD1	2.00	0.61
1:B:212:LEU:HD11	1:B:221:ILE:HG22	1.80	0.61
1:B:271:VAL:HG21	1:B:291:ILE:HD13	1.81	0.61
1:B:316:ARG:HG2	1:B:396:VAL:HG12	1.83	0.60
1:B:166:LYS:NZ	2:U:73:ASP:OD1	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:CYS:HB3	1:E:174:ASP:OD1	2.02	0.60
1:E:341:THR:HG22	3:D:205:TYR:CE2	2.34	0.59
1:B:375:PRO:HG3	2:U:114:LEU:HD21	1.83	0.59
1:B:275:VAL:O	1:B:278:VAL:HG22	2.02	0.58
1:E:432:GLY:O	1:E:434:VAL:HG23	2.04	0.58
1:E:275:VAL:O	1:E:278:VAL:HG22	2.03	0.57
3:A:13:ARG:HH22	3:A:306:THR:HA	1.68	0.57
1:E:482:ASP:HB2	2:V:31:TYR:OH	2.06	0.56
3:A:13:ARG:HB2	3:A:318:LEU:HA	1.87	0.56
2:V:2:VAL:HG22	2:V:26:GLY:HA3	1.88	0.56
5:B:601:NAG:H83	5:B:601:NAG:H3	1.88	0.56
1:B:341:THR:HG22	3:A:205:TYR:HE2	1.70	0.55
1:B:467:LYS:CB	1:B:470:ARG:HE	2.18	0.55
1:E:207:THR:HG23	2:V:56:ASP:HB3	1.89	0.54
3:A:350:ILE:HG22	3:A:351:GLY:H	1.72	0.54
1:B:268:PRO:HB2	1:B:362:LYS:N	2.22	0.54
2:V:47:GLY:HA3	2:V:110:GLN:HB2	1.90	0.54
3:D:250:CYS:HA	3:D:261:CYS:HA	1.89	0.54
3:D:59:VAL:HG22	3:D:119:LEU:HD11	1.90	0.53
1:B:400:ALA:HB2	1:B:438:GLN:HE22	1.74	0.53
3:D:185:PRO:HB2	3:D:251:GLY:HA3	1.90	0.53
3:D:353:LYS:HB3	3:D:360:THR:HG22	1.90	0.53
1:E:372:MET:HG2	2:V:104:SER:HA	1.90	0.52
3:A:12:TYR:OH	3:A:292:ASN:OD1	2.27	0.52
3:D:29:ASN:HD22	5:D:502:NAG:H61	1.74	0.52
1:E:389:GLU:OE1	1:E:467:LYS:HE3	2.10	0.51
3:D:27:LEU:HD11	3:D:286:PHE:HZ	1.74	0.51
1:B:403:LEU:HD13	1:B:429:PHE:CE1	2.45	0.51
1:B:432:GLY:O	1:B:434:VAL:HG23	2.10	0.51
1:E:470:ARG:HH11	3:D:211:ARG:HD2	1.76	0.51
3:D:318:LEU:O	3:D:321:ILE:HG12	2.10	0.51
3:A:293:SER:HB2	3:A:322:THR:HG21	1.93	0.51
2:U:2:VAL:HG22	2:U:26:GLY:HA3	1.93	0.50
3:A:318:LEU:O	3:A:321:ILE:HG12	2.11	0.50
1:E:400:ALA:HB2	1:E:438:GLN:CD	2.31	0.50
2:V:34:ILE:HG21	2:V:79:VAL:HG21	1.93	0.50
1:E:160:VAL:HB	1:E:210:MET:HG3	1.94	0.50
3:A:83:ASP:O	3:A:284:SER:HA	2.11	0.50
3:A:160:CYS:HB3	3:A:241:PRO:HD2	1.94	0.49
1:E:403:LEU:HD13	1:E:429:PHE:CE1	2.48	0.49
1:E:170:PRO:HG2	1:E:209:PHE:CD1	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:13:GLN:OE1	2:U:130:HIS:N	2.45	0.48
1:E:272:SER:OG	1:E:279:HIS:ND1	2.39	0.48
1:E:435:ASP:OD2	1:E:438:GLN:NE2	2.46	0.48
1:B:482:ASP:HB2	2:U:31:TYR:OH	2.12	0.48
3:D:160:CYS:HB3	3:D:241:PRO:HD2	1.95	0.48
1:B:304:ASN:HB3	1:B:306:TRP:CD1	2.49	0.48
1:B:389:GLU:OE1	1:B:467:LYS:HE3	2.13	0.48
3:D:29:ASN:ND2	5:D:502:NAG:H61	2.28	0.48
2:V:12:VAL:HG11	2:V:86:LEU:HD13	1.95	0.48
1:B:290:TRP:CZ3	1:B:350:LYS:HB2	2.49	0.48
3:D:136:SER:HB2	3:D:242:GLY:HA2	1.96	0.48
1:E:207:THR:H	2:V:56:ASP:HB3	1.79	0.47
1:B:300:LYS:HG2	1:B:301:PRO:HA	1.95	0.47
1:B:400:ALA:HB2	1:B:438:GLN:NE2	2.29	0.47
1:E:296:HIS:HA	1:E:299:GLU:HG3	1.96	0.47
1:E:271:VAL:HG12	1:E:312:ALA:HB2	1.97	0.47
1:B:440:ASP:OD1	1:B:440:ASP:N	2.48	0.46
3:D:45:ASN:OD1	3:D:295:THR:OG1	2.32	0.46
3:A:136:SER:HB2	3:A:242:GLY:HA2	1.96	0.46
3:A:250:CYS:HA	3:A:261:CYS:HA	1.98	0.46
3:D:15:ILE:HG12	3:D:319:TYR:HB3	1.98	0.46
3:D:201:ASP:OD1	3:D:202:THR:N	2.48	0.45
4:F:1:NAG:H5	4:F:2:NAG:O5	2.16	0.45
3:D:330:VAL:HG12	3:D:331:SER:N	2.32	0.45
1:B:276:GLN:O	1:B:278:VAL:HG13	2.16	0.45
1:E:157:ILE:HG12	1:E:200:ILE:HD11	1.97	0.45
2:U:34:ILE:HG21	2:U:79:VAL:HG21	1.98	0.45
1:B:272:SER:OG	1:B:279:HIS:ND1	2.37	0.45
1:E:166:LYS:HG2	2:V:74:ASN:HB2	1.98	0.45
3:A:201:ASP:OD1	3:A:202:THR:N	2.49	0.45
3:A:354:ASP:O	3:A:358:ASN:N	2.48	0.45
1:E:467:LYS:CB	1:E:470:ARG:HE	2.28	0.45
2:U:14:PRO:HD3	2:U:127:SER:C	2.37	0.45
3:D:179:CYS:HB2	3:D:183:LYS:HG3	1.99	0.45
1:E:178:GLU:HB3	1:E:182:ARG:NH1	2.33	0.44
1:B:483:TRP:O	1:B:487:GLN:HG2	2.17	0.44
1:E:316:ARG:HG2	1:E:396:VAL:HG12	1.98	0.44
2:U:12:VAL:HG11	2:U:86:LEU:HD13	1.99	0.44
3:A:59:VAL:HG22	3:A:119:LEU:HD11	1.98	0.44
1:E:316:ARG:HB2	1:E:319:PHE:HD1	1.83	0.44
1:B:190:TYR:HH	1:B:485:TYR:HE1	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:134:ASN:O	3:A:140:ARG:NH1	2.50	0.44
1:B:279:HIS:HB2	1:B:317:GLN:OE1	2.18	0.44
1:E:440:ASP:OD1	1:E:440:ASP:N	2.50	0.44
3:D:83:ASP:O	3:D:284:SER:HA	2.18	0.43
1:B:288:PRO:HG3	1:B:357:PHE:CE2	2.54	0.43
3:A:13:ARG:NH2	3:A:305:ASN:O	2.51	0.43
1:B:151:LEU:O	1:B:368:ASN:HB3	2.17	0.43
2:U:40:ALA:HB3	2:U:43:LYS:HB2	2.00	0.43
1:E:206:SER:HA	2:V:56:ASP:HB2	2.00	0.43
2:U:47:GLY:HA3	2:U:110:GLN:HB2	2.00	0.43
3:D:136:SER:HB3	3:D:139:ASN:HB2	2.00	0.43
1:B:268:PRO:HB2	1:B:362:LYS:H	1.82	0.43
3:A:321:ILE:HG12	3:A:321:ILE:H	1.64	0.43
1:B:200:ILE:HD13	1:B:238:SER:HB2	2.00	0.43
2:V:67:ARG:NH1	2:V:85:SER:O	2.51	0.43
1:B:169:HIS:HB2	1:B:210:MET:HG2	2.01	0.43
3:D:249:LYS:HB2	3:D:265:ALA:HB2	2.01	0.43
3:A:48:PHE:CZ	3:A:298:SER:HB2	2.54	0.42
3:A:185:PRO:HB2	3:A:251:GLY:CA	2.48	0.42
1:B:478:MET:HE3	2:U:102:LEU:HD23	2.01	0.42
1:E:166:LYS:HD3	2:V:73:ASP:HA	2.01	0.42
1:B:425:ILE:HD11	1:B:476:ASN:OD1	2.18	0.42
3:A:104:GLN:HA	3:A:108:TYR:O	2.19	0.42
1:E:483:TRP:O	1:E:487:GLN:HG2	2.20	0.42
3:A:176:VAL:HG21	3:A:186:SER:HB3	2.01	0.42
3:A:349:ILE:HG12	3:A:364:LEU:HD23	2.02	0.42
3:D:201:ASP:OD2	3:D:203:THR:OG1	2.27	0.42
3:A:306:THR:HG22	3:A:356:LEU:HD13	2.02	0.42
1:B:461:TRP:CZ2	1:B:473:VAL:HG21	2.55	0.42
1:E:209:PHE:CE2	1:E:230:ALA:HA	2.55	0.42
1:B:296:HIS:O	1:B:299:GLU:HG2	2.20	0.41
1:E:340:LYS:O	3:D:205:TYR:HD2	2.03	0.41
2:U:17:SER:HA	2:U:83:MET:O	2.19	0.41
1:E:169:HIS:HB2	1:E:210:MET:HG2	2.02	0.41
1:E:378:LEU:HD11	1:E:401:LYS:HD2	2.01	0.41
1:B:457:GLY:HA2	1:B:477:VAL:HG23	2.01	0.41
1:E:366:LEU:HD13	1:E:481:THR:HG23	2.03	0.41
3:A:73:PHE:HD2	3:A:300:ASP:CB	2.33	0.41
3:D:185:PRO:HB2	3:D:251:GLY:CA	2.50	0.41
1:E:150:ARG:HD2	1:E:369:PRO:HG3	2.01	0.41
1:E:470:ARG:NH1	3:D:211:ARG:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:10:THR:HA	3:D:315:ASN:O	2.21	0.41
1:B:331:VAL:HG22	1:B:349:MET:HG2	2.02	0.41
3:A:76:CYS:HA	3:A:297:CYS:HA	2.02	0.41
3:A:350:ILE:HG22	3:A:351:GLY:N	2.35	0.41
1:E:276:GLN:O	1:E:278:VAL:HG13	2.21	0.41
1:B:166:LYS:HG2	2:U:74:ASN:H	1.85	0.41
1:E:457:GLY:HA2	1:E:475:GLY:O	2.21	0.41
1:E:178:GLU:HB3	1:E:182:ARG:HH12	1.85	0.40
3:D:104:GLN:HA	3:D:108:TYR:O	2.21	0.40
1:B:174:ASP:OD2	1:B:232:SER:HB2	2.20	0.40
1:B:381:ILE:HD11	1:B:436:SER:HB2	2.02	0.40
1:E:151:LEU:O	1:E:368:ASN:HB3	2.20	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	B	333/395 (84%)	313 (94%)	19 (6%)	1 (0%)	41 74
1	E	326/395 (82%)	307 (94%)	17 (5%)	2 (1%)	25 64
2	U	129/136 (95%)	127 (98%)	2 (2%)	0	100 100
2	V	127/136 (93%)	126 (99%)	1 (1%)	0	100 100
3	A	342/366 (93%)	332 (97%)	10 (3%)	0	100 100
3	D	339/366 (93%)	328 (97%)	11 (3%)	0	100 100
All	All	1596/1794 (89%)	1533 (96%)	60 (4%)	3 (0%)	47 80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	435	ASP

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Mol	Chain	Res	Type
1	B	227	HIS
1	E	227	HIS

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	B	288/335 (86%)	283 (98%)	5 (2%)	60	83
1	E	282/335 (84%)	277 (98%)	5 (2%)	59	81
2	U	106/113 (94%)	105 (99%)	1 (1%)	78	90
2	V	106/113 (94%)	104 (98%)	2 (2%)	57	80
3	A	316/337 (94%)	315 (100%)	1 (0%)	92	97
3	D	303/337 (90%)	302 (100%)	1 (0%)	92	97
All	All	1401/1570 (89%)	1386 (99%)	15 (1%)	73	88

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	166	LYS
1	B	174	ASP
1	B	435	ASP
1	B	440	ASP
1	B	482	ASP
1	E	166	LYS
1	E	174	ASP
1	E	437	CYS
1	E	440	ASP
1	E	482	ASP
2	U	102	LEU
3	A	321	ILE
3	D	321	ILE
2	V	56	ASP
2	V	102	LEU

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

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

2 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	F	1	4,3	14,14,15	0.74	1 (7%)	17,19,21	1.16	1 (5%)
4	NAG	F	2	4	14,14,15	0.51	0	17,19,21	0.63	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	F	1	4,3	-	4/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	NAG	O5-C1	2.32	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	1	NAG	C1-O5-C5	4.47	118.25	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

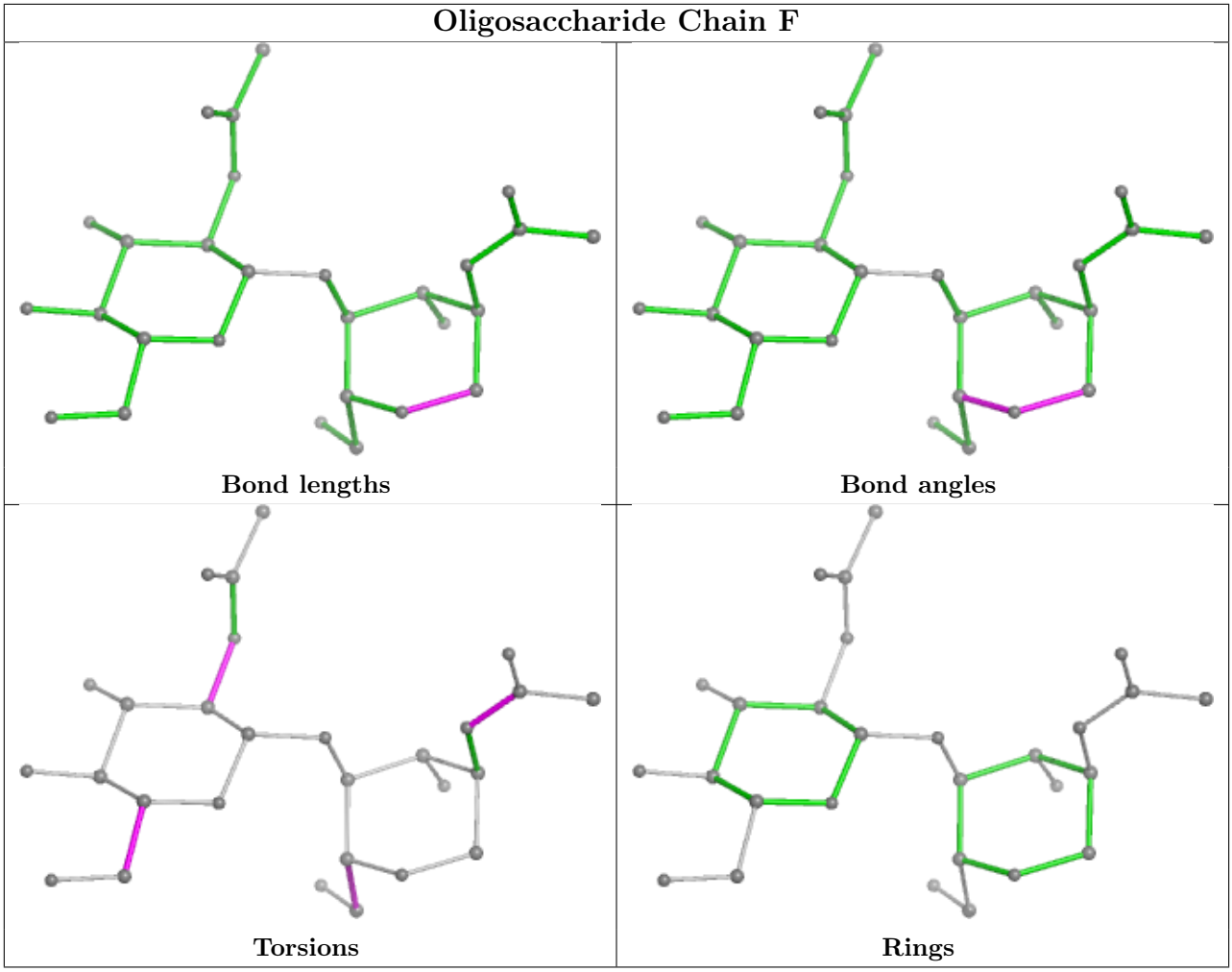
Mol	Chain	Res	Type	Atoms
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	F	1	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C3-C2-N2-C7
4	F	1	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	2	0
4	F	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.



5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
6	PO4	A	403	-	4,4,4	0.89	0	6,6,6	0.47	0
5	NAG	A	402	3	14,14,15	0.22	0	17,19,21	0.45	0
5	NAG	D	502	3	14,14,15	0.82	1 (7%)	17,19,21	1.17	1 (5%)
6	PO4	D	501	-	4,4,4	0.92	0	6,6,6	0.38	0
5	NAG	B	601	1	14,14,15	0.47	0	17,19,21	1.31	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	A	401	3	14,14,15	0.39	0	17,19,21	0.50	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	D	502	3	-	4/6/23/26	0/1/1/1
5	NAG	B	601	1	-	3/6/23/26	0/1/1/1
5	NAG	A	401	3	-	0/6/23/26	0/1/1/1
5	NAG	A	402	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	502	NAG	C1-C2	2.15	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	601	NAG	C2-N2-C7	4.37	129.13	122.90
5	D	502	NAG	C1-O5-C5	4.31	118.03	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	502	NAG	O5-C5-C6-O6
5	D	502	NAG	C4-C5-C6-O6
5	B	601	NAG	C8-C7-N2-C2
5	B	601	NAG	O7-C7-N2-C2
5	D	502	NAG	C8-C7-N2-C2
5	D	502	NAG	O7-C7-N2-C2
5	B	601	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	502	NAG	2	0
5	B	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	B	341/395 (86%)	0.02	13 (3%) 40 27	140, 198, 284, 357	0
1	E	334/395 (84%)	0.09	11 (3%) 46 32	170, 227, 312, 358	0
2	U	131/136 (96%)	-0.19	2 (1%) 73 59	166, 196, 239, 275	0
2	V	129/136 (94%)	0.64	15 (11%) 4 4	215, 286, 330, 348	0
3	A	346/366 (94%)	-0.11	11 (3%) 47 32	145, 191, 286, 361	0
3	D	345/366 (94%)	-0.08	10 (2%) 51 35	155, 210, 282, 358	0
All	All	1626/1794 (90%)	0.02	62 (3%) 40 27	140, 209, 305, 361	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	V	35	GLY	6.1
2	V	10	GLY	4.9
2	V	16	GLY	4.8
3	D	366	CYS	4.5
1	E	175	ASP	4.0
3	D	284	SER	3.9
1	B	284	SER	3.8
1	B	389	GLU	3.8
3	A	320	GLY	3.6
2	V	60	TYR	3.6
3	D	309	SER	3.6
2	V	11	LEU	3.5
3	A	361	TYR	3.5
1	B	390	LYS	3.4
3	A	314	VAL	3.4
2	V	125	THR	3.4
1	E	130	SER	3.4
1	B	443	GLY	3.3
1	E	131	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
3	D	285	ASN	3.3
2	V	129	HIS	3.2
1	E	128	ASN	3.2
2	V	49	SER	3.1
1	B	128	ASN	3.0
2	V	128	SER	2.9
1	B	283	GLY	2.9
1	E	443	GLY	2.8
2	V	33	ALA	2.8
2	U	35	GLY	2.8
2	V	15	GLY	2.8
2	V	17	SER	2.7
1	B	178	GLU	2.7
1	B	387	THR	2.7
1	E	150	ARG	2.7
1	B	131	ASN	2.6
3	A	313	CYS	2.6
3	D	313	CYS	2.6
3	A	325	GLY	2.6
3	D	320	GLY	2.6
3	D	208	ASN	2.5
1	B	130	SER	2.5
1	B	129	PRO	2.5
3	D	329	GLU	2.4
1	E	390	LYS	2.4
1	B	164	GLN	2.3
1	B	442	GLY	2.3
3	A	317	ASP	2.3
3	A	322	THR	2.3
2	U	49	SER	2.2
1	E	132	TRP	2.2
2	V	85	SER	2.2
3	D	83	ASP	2.1
1	E	442	GLY	2.1
2	V	124	VAL	2.1
3	D	188	ILE	2.1
1	E	176	TRP	2.1
1	E	472	GLY	2.1
3	A	284	SER	2.0
3	A	333	VAL	2.0
3	A	252	THR	2.0
3	A	331	SER	2.0

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Mol	Chain	Res	Type	RSRZ
2	V	57	LYS	2.0

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

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

6.3 Carbohydrates (i)

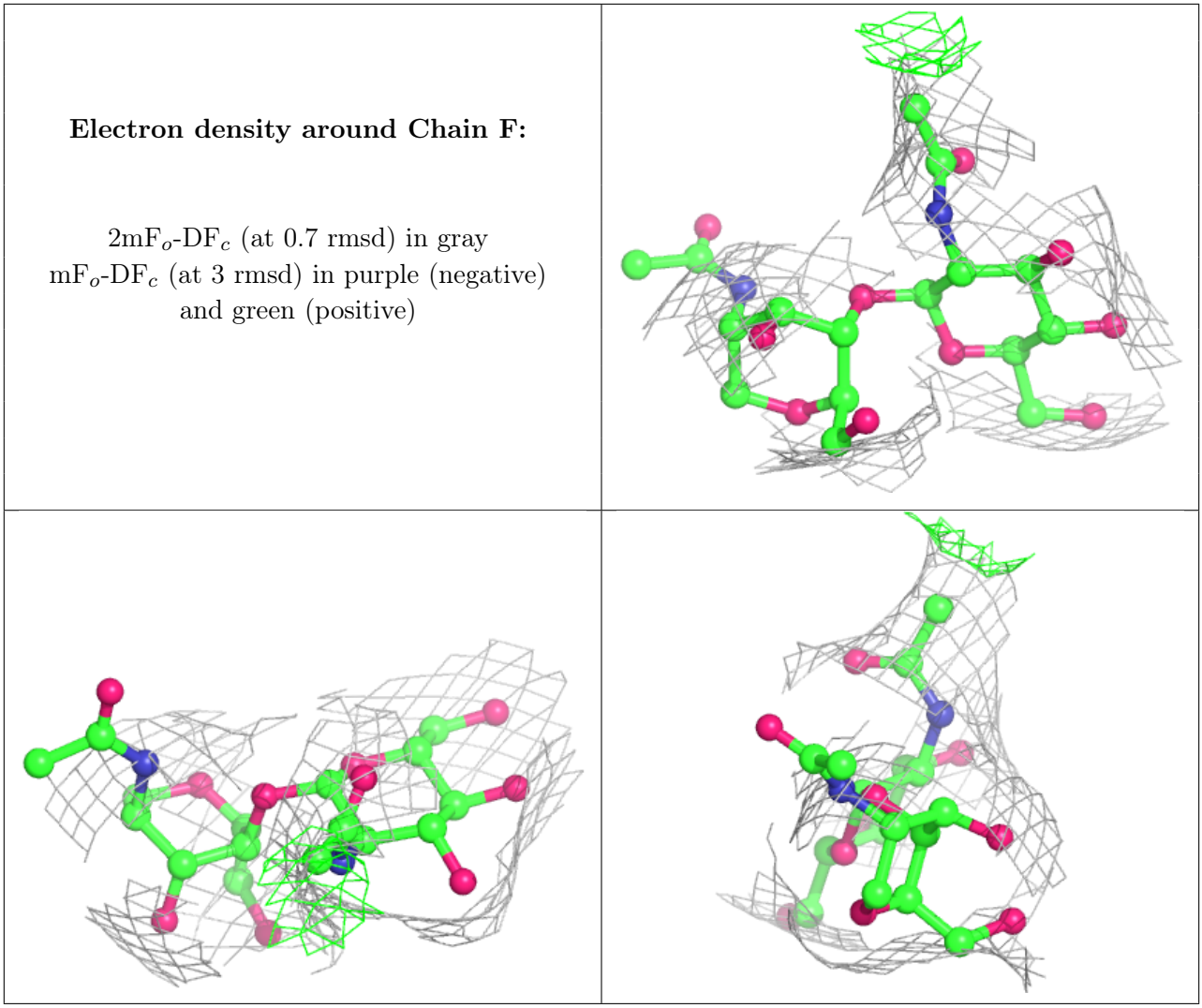
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	F	2	14/15	0.84	0.50	161,290,318,331	0
4	NAG	F	1	14/15	0.85	0.46	213,279,309,311	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 F:

$2mF_o$-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	A	401	14/15	0.78	0.36	196,246,279,292	0
5	NAG	B	601	14/15	0.81	0.30	193,262,289,293	0
6	PO4	D	501	5/5	0.84	0.19	225,230,257,258	0
5	NAG	A	402	14/15	0.86	0.45	203,285,307,309	0
5	NAG	D	502	14/15	0.87	0.33	192,259,309,317	0
6	PO4	A	403	5/5	0.90	0.09	189,212,234,272	0

6.5 Other polymers (i)

There are no such residues in this entry.