



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:10 AM UTC

PDB ID : 8S0M / pdb_00008s0m
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	:	4-5-2 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

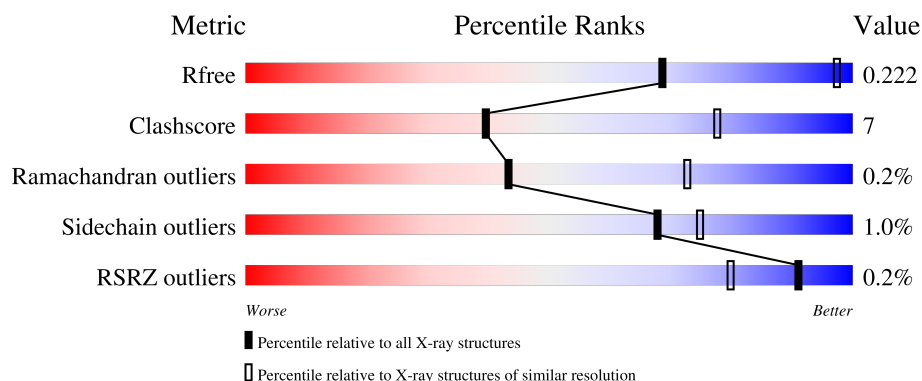
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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}	180053	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

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	B	395	
1	E	395	
2	U	136	
2	V	136	
3	A	366	

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Mol	Chain	Length	Quality of chain
3	D	366	84% 10% 6%
4	F	2	50% 50%

2 Entry composition

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:

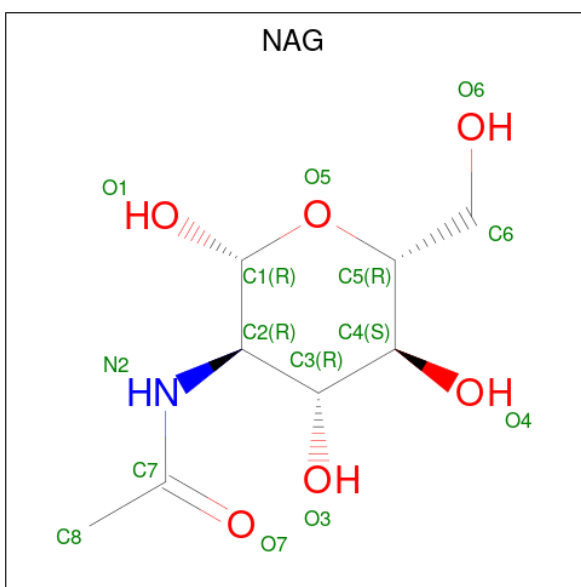
Chain	Residue	Modelled	Actual	Comment	Reference
A	333	VAL	ALA	conflict	UNP Q0ZME7
D	333	VAL	ALA	conflict	UNP Q0ZME7

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



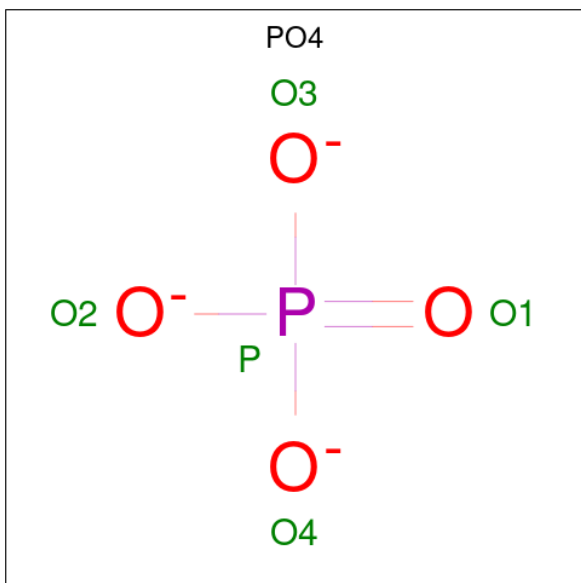
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

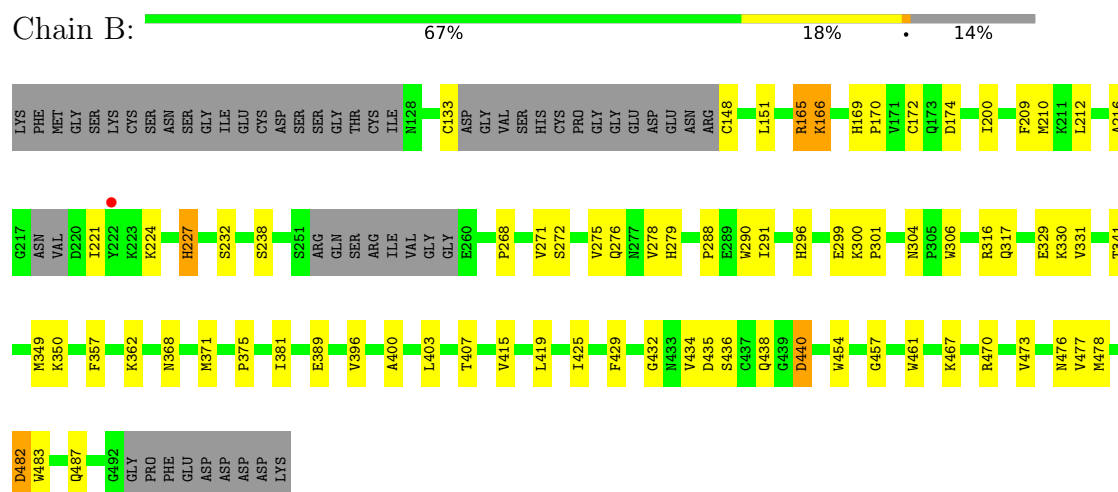
- Molecule 7 is water.

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

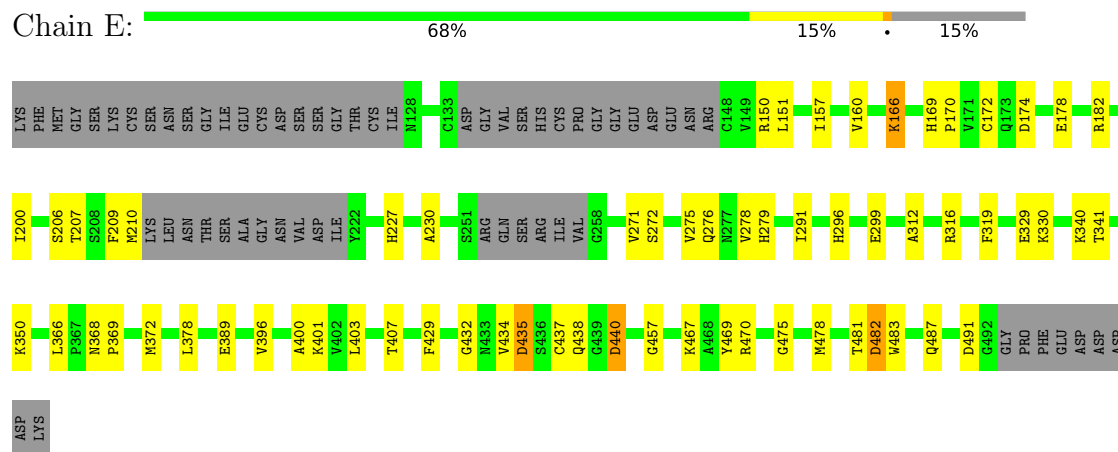
3 Residue-property plots [i](#)

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.

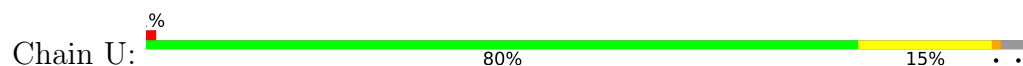
• Molecule 1: Transmembrane protease serine 2



• Molecule 1: Transmembrane protease serine 2

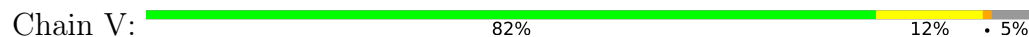


• Molecule 2: Nanobody A01

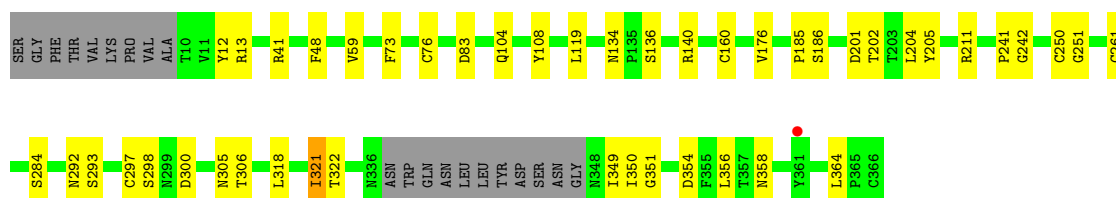
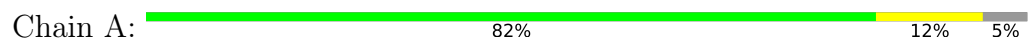




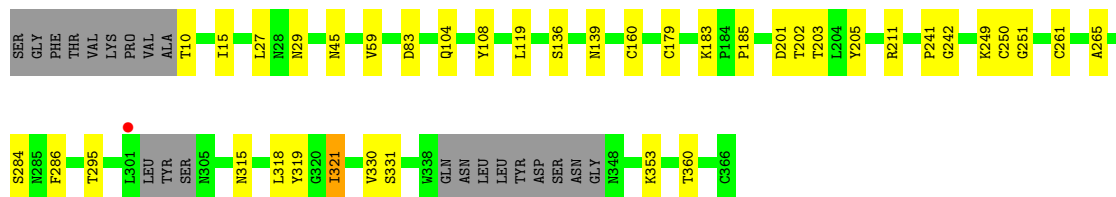
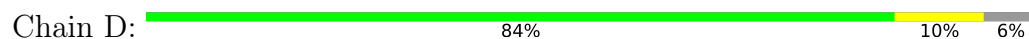
• Molecule 2: Nanobody A01



• 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

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) 99.0 (24.97-3.55)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 3.54Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.193 , 0.221 0.195 , 0.222	Depositor DCC
R_{free} test set	2898 reflections (4.74%)	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)	0.33 , 186.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	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.*

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, 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	0.21	0/2734	0.65	0/3718
1	E	0.20	0/2680	0.64	0/3644
2	U	0.13	0/1010	0.32	0/1369
2	V	0.12	0/1000	0.31	0/1355
3	A	0.14	0/2759	0.33	0/3756
3	D	0.13	0/2698	0.30	0/3673
All	All	0.17	0/12881	0.48	0/17515

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2662	0	2544	52	0
1	E	2608	0	2489	48	0
2	U	991	0	929	14	0
2	V	981	0	925	13	0
3	A	2691	0	2535	33	0
3	D	2634	0	2431	28	0
4	F	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	165	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 7.

All (165) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:400:ALA:HB2	1:E:438:GLN:CD	2.31	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
1:B:368:ASN:O	1:B:478:MET:HE2	2.08	0.53
1:B:478:MET:HE1	2:U:102:LEU:HA	1.90	0.53
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
1:B:272:SER:OG	1:B:279:HIS:ND1	2.37	0.50
3:A:318:LEU:O	3:A:321:ILE:HG12	2.11	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
2:U:14:PRO:HD3	2:U:127:SER:C	2.37	0.49
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: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
1:E:272:SER:OG	1:E:279:HIS:ND1	2.39	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:350:LYS:NZ	1:E:491:ASP:OD2	2.42	0.47
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:E:407:THR:HB	2:V:116:ASP:CG	2.42	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
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:B:407:THR:HB	2:U:116:ASP:CG	2.42	0.44
1:E:316:ARG:HB2	1:E:319:PHE:HD1	1.83	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
3:D:201:ASP:OD2	3:D:203:THR:OG1	2.27	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
1:E:368:ASN:O	1:E:478:MET:HE2	2.18	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:A:185:PRO:HB2	3:A:251:GLY:C	2.44	0.43
3:D:249:LYS:HB2	3:D:265:ALA:HB2	2.01	0.43
1:B:371:MET:HE1	1:B:454:TRP:CE2	2.54	0.42
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: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
3:A:185:PRO:C	3:A:251:GLY:HA3	2.44	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	333/395 (84%)	313 (94%)	19 (6%)	1 (0%)	36	65
1	E	326/395 (82%)	307 (94%)	17 (5%)	2 (1%)	21	54
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%)	43	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	435	ASP
1	B	227	HIS
1	E	227	HIS

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	B	288/335 (86%)	283 (98%)	5 (2%)	53	69
1	E	282/335 (84%)	278 (99%)	4 (1%)	59	71
2	U	106/113 (94%)	105 (99%)	1 (1%)	70	76
2	V	106/113 (94%)	104 (98%)	2 (2%)	50	67
3	A	316/337 (94%)	315 (100%)	1 (0%)	86	82
3	D	303/337 (90%)	302 (100%)	1 (0%)	86	82
All	All	1401/1570 (89%)	1387 (99%)	14 (1%)	68	75

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	165	ARG
1	B	166	LYS
1	B	435	ASP
1	B	440	ASP
1	B	482	ASP
1	E	166	LYS
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. All (17)

such sidechains are listed below:

Mol	Chain	Res	Type
1	B	131	ASN
1	B	249	ASN
1	B	327	GLN
1	B	336	ASN
1	E	159	GLN
1	E	336	ASN
1	E	344	ASN
1	E	398	ASN
2	U	39	GLN
2	U	82	GLN
2	U	84	ASN
3	A	197	HIS
3	D	197	HIS
3	D	253	GLN
3	D	289	ASN
2	V	82	GLN
2	V	84	ASN

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](#)

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	0.73	1 (7%)	17,19,21	1.17	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	F	2	4	14,14,15	0.51	0	17,19,21	0.67	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	-	3/6/23/26	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	2.22	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	C1-O5-C5	4.53	118.25	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

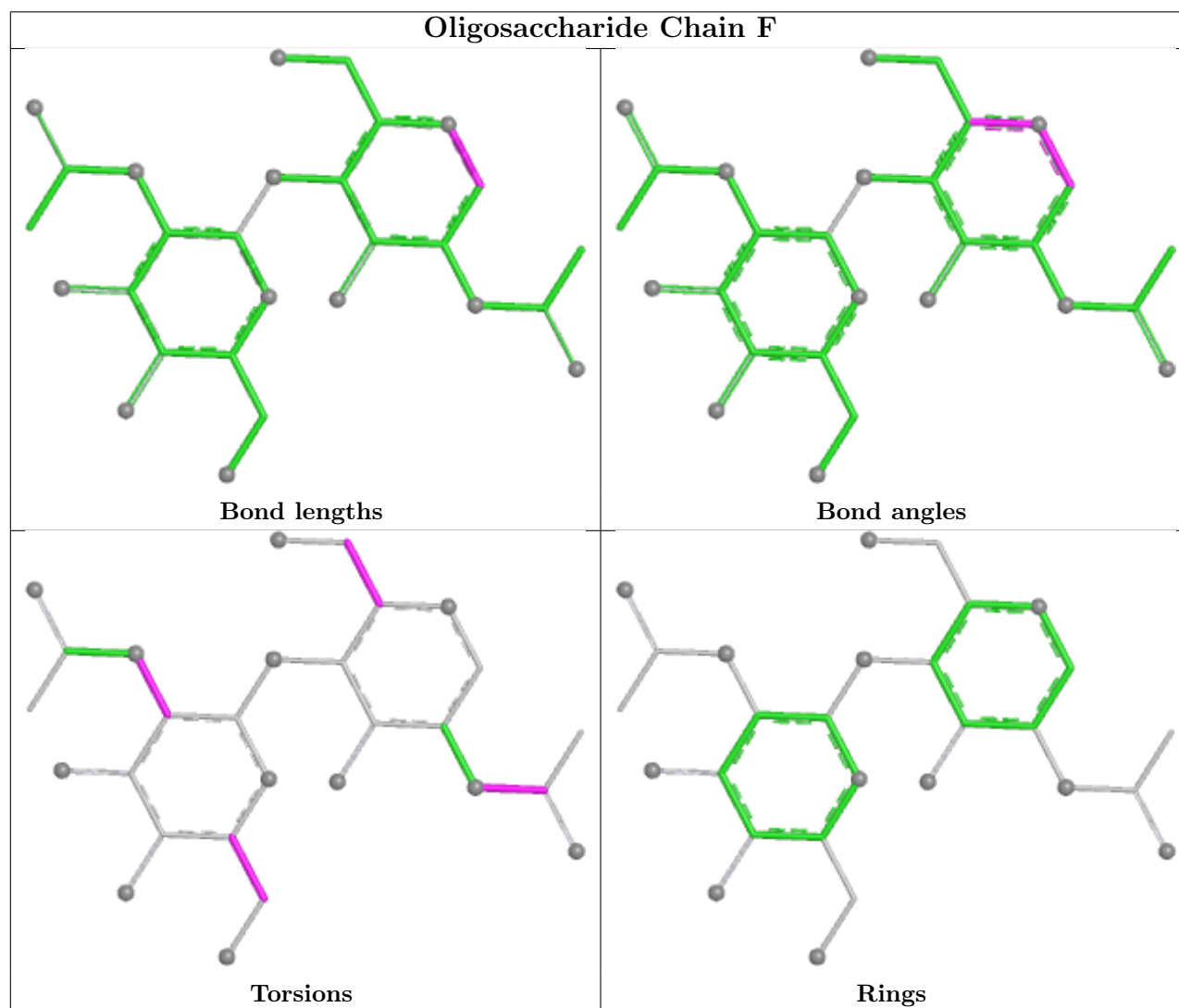
Mol	Chain	Res	Type	Atoms
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	F	1	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C3-C2-N2-C7
4	F	1	NAG	C4-C5-C6-O6
4	F	2	NAG	C1-C2-N2-C7

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	$\# Z > 2$
5	NAG	D	502	3	14,14,15	0.85	1 (7%)	17,19,21	1.18	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	402	3	14,14,15	0.23	0	17,19,21	0.47	0
5	NAG	A	401	3	14,14,15	0.41	0	17,19,21	0.52	0
5	NAG	B	601	1	14,14,15	0.50	0	17,19,21	1.39	2 (11%)
6	PO4	A	403	-	4,4,4	0.94	0	6,6,6	0.50	0
6	PO4	D	501	-	4,4,4	0.97	0	6,6,6	0.41	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	A	402	3	-	0/6/23/26	0/1/1/1
5	NAG	B	601	1	-	4/6/23/26	0/1/1/1
5	NAG	A	401	3	-	0/6/23/26	0/1/1/1
5	NAG	D	502	3	-	4/6/23/26	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	2.35	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	601	NAG	C2-N2-C7	4.65	129.13	122.90
5	D	502	NAG	C1-O5-C5	4.36	118.03	112.19
5	B	601	NAG	C1-C2-N2	2.14	113.81	110.43

There are no chirality outliers.

All (8) 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	C1-C2-N2-C7
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 [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	B	341/395 (86%)	-0.45	1 (0%) 90 74	140, 198, 284, 357	0
1	E	334/395 (84%)	-0.42	0 100 100	170, 227, 312, 358	0
2	U	131/136 (96%)	-0.37	1 (0%) 82 58	166, 196, 239, 275	0
2	V	129/136 (94%)	-0.28	0 100 100	215, 286, 330, 348	0
3	A	346/366 (94%)	-0.40	1 (0%) 90 74	145, 191, 286, 361	0
3	D	345/366 (94%)	-0.39	1 (0%) 90 74	155, 210, 282, 358	0
All	All	1626/1794 (90%)	-0.40	4 (0%) 91 80	140, 209, 305, 361	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	301	LEU	2.5
1	B	222	TYR	2.3
3	A	361	TYR	2.2
2	U	100	SER	2.1

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

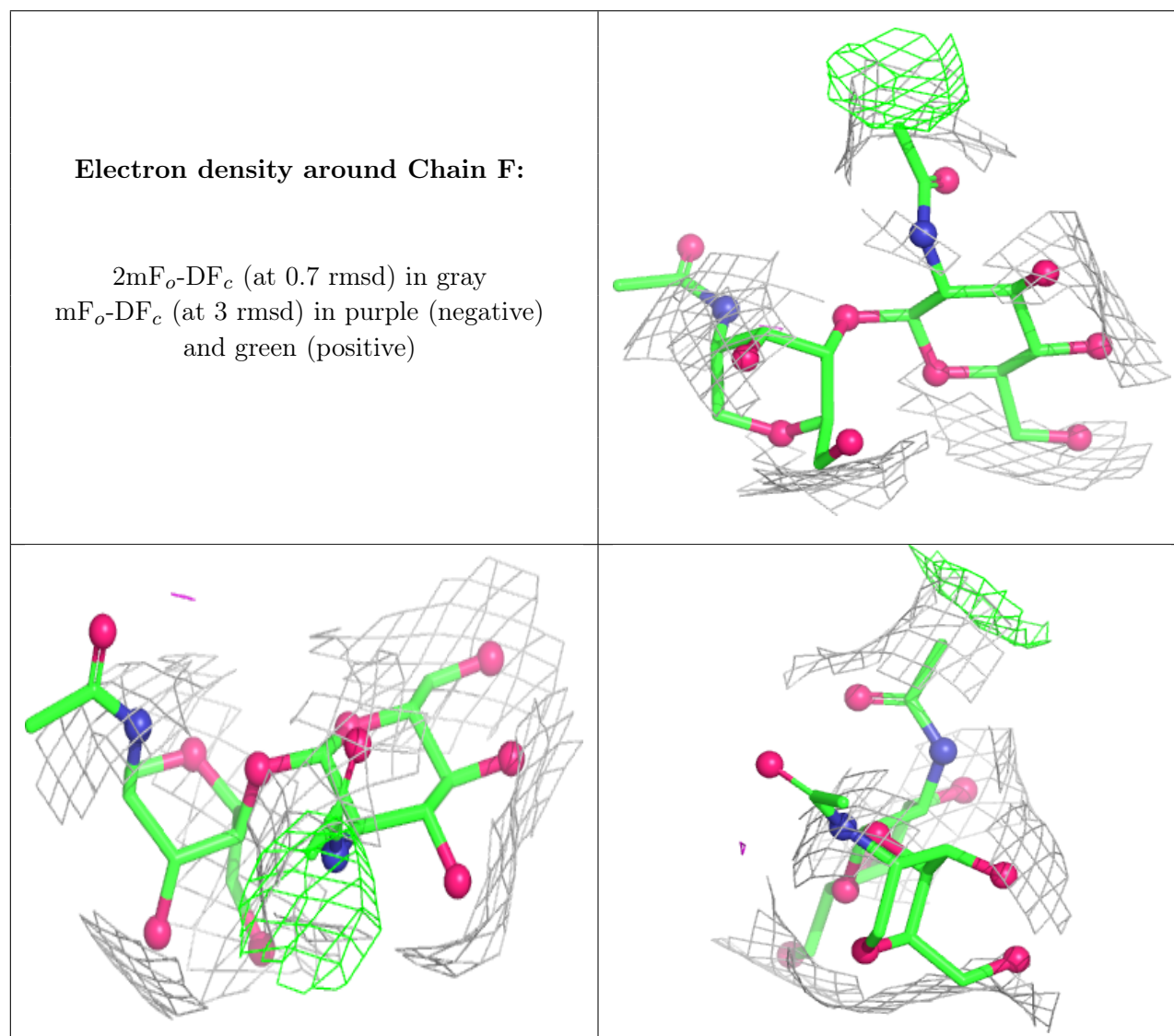
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
4	NAG	F	1	14/15	-	-	213,279,309,311	0
4	NAG	F	2	14/15	-	-	161,290,318,331	0

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	A	402	14/15	0.62	0.07	203,285,307,309	0
5	NAG	B	601	14/15	0.79	0.06	193,262,289,293	0
5	NAG	A	401	14/15	0.86	0.08	196,246,279,292	0
5	NAG	D	502	14/15	0.86	0.08	192,259,309,317	0
6	PO4	D	501	5/5	0.89	0.09	225,230,257,258	0
6	PO4	A	403	5/5	0.95	0.07	189,212,234,272	0

6.5 Other polymers [i](#)

There are no such residues in this entry.