



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:42 AM UTC

PDB ID : 3AST / pdb_00003ast
Title : Crystal structure of P domain Q389N mutant from Norovirus Funabashi258 stain in the complex with Lewis-b
Authors : Kubota, T.; Kumagai, A.; Itoh, H.; Furukawa, S.; Narimatsu, H.; Wakita, T.; Ishii, K.; Takeda, N.; Someya, Y.; Shirato, H.
Deposited on : 2010-12-17
Resolution : 1.40 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

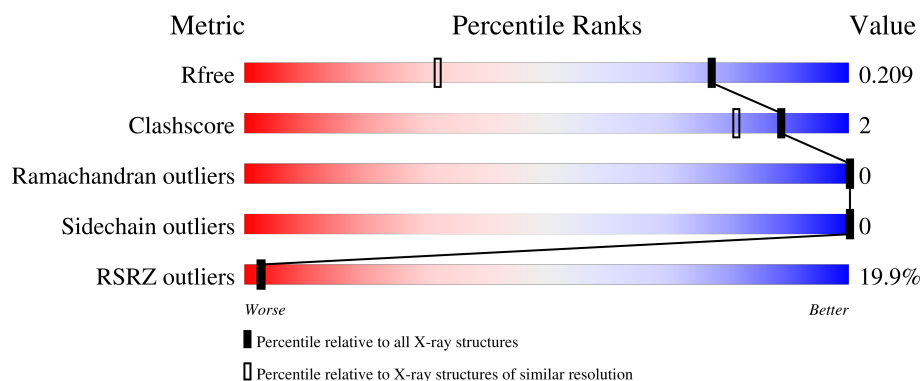
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	326	17% 91% 5%
1	B	326	20% 86% 6% 7%
2	C	4	100%
2	D	4	75% 25%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5361 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.

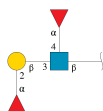
- Molecule 1 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	1	0
			2386	1526	402	449	9			
1	B	302	Total	C	N	O	S	0	3	0
			2331	1494	393	435	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	216	GLY	-	expression tag	UNP Q8JW44
A	217	PRO	-	expression tag	UNP Q8JW44
A	218	LEU	-	expression tag	UNP Q8JW44
A	219	GLY	-	expression tag	UNP Q8JW44
A	220	SER	-	expression tag	UNP Q8JW44
A	389	ASN	GLN	engineered mutation	UNP Q8JW44
B	216	GLY	-	expression tag	UNP Q8JW44
B	217	PRO	-	expression tag	UNP Q8JW44
B	218	LEU	-	expression tag	UNP Q8JW44
B	219	GLY	-	expression tag	UNP Q8JW44
B	220	SER	-	expression tag	UNP Q8JW44
B	389	ASN	GLN	engineered mutation	UNP Q8JW44

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			45	26	1	18			

Continued on next page...

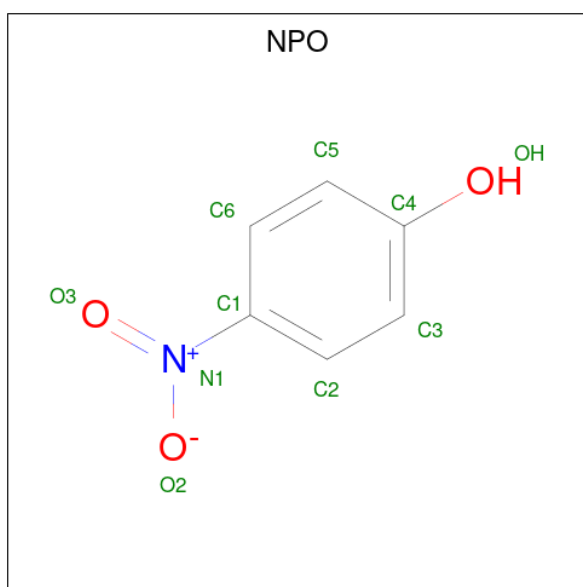
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	0	0	0
			45	26	1	18			

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is P-NITROPHENOL (CCD ID: NPO) (formula: C₆H₅NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	6	1	3		
4	B	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 5 is water.

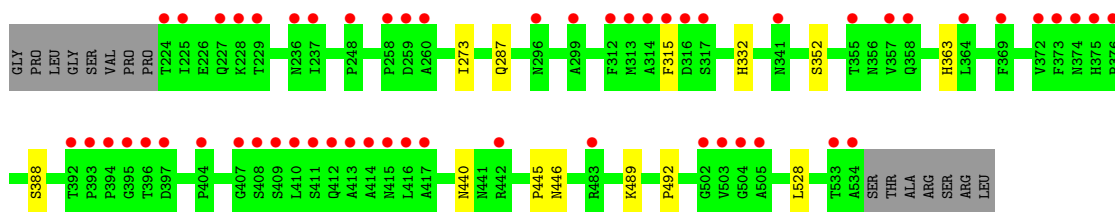
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	277	Total	O	0	0
			277	277		
5	B	255	Total	O	0	0
			255	255		

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.

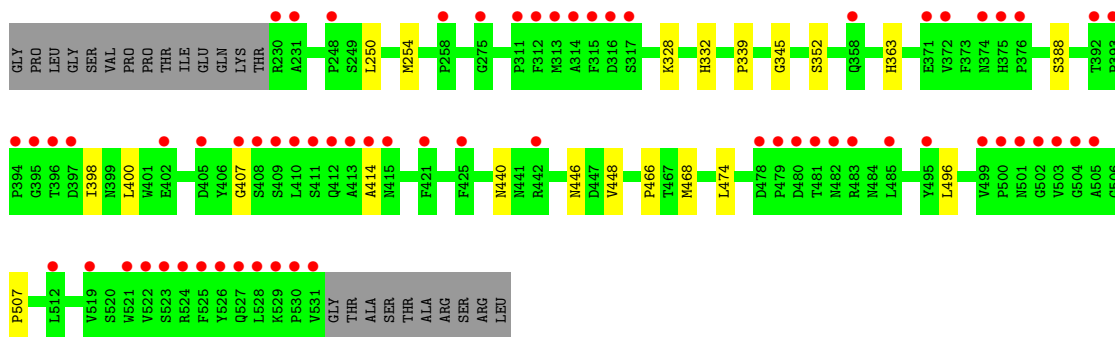
- Molecule 1: Capsid protein

Chain A: 

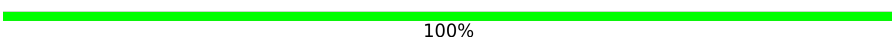


- Molecule 1: Capsid protein

Chain B: 



- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 



- Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	74.97Å 74.97Å 107.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.92 – 1.40 23.92 – 1.40	Depositor EDS
% Data completeness (in resolution range)	94.8 (23.92-1.40) 94.8 (23.92-1.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.62 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.197 , 0.212 0.194 , 0.209	Depositor DCC
R_{free} test set	6268 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	13.1	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l 0.029 for h,-h-k,-l 0.021 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5361	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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, NA, GAL, FUC, NPO

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	0.41	0/2462	0.66	0/3371
1	B	0.41	0/2414	0.67	1/3306 (0.0%)
All	All	0.41	0/4876	0.66	1/6677 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	345	GLY	N-CA-C	5.19	118.11	112.29

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2386	0	2314	8	0
1	B	2331	0	2259	12	0
2	C	45	0	40	0	0
2	D	45	0	40	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	10	0	4	0	0
4	B	10	0	4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	277	0	0	0	0
5	B	255	0	0	0	0
All	All	5361	0	4661	18	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 2.

All (18) 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:466:PRO:HG2	1:B:468:MET:HE3	1.74	0.70
1:B:440:ASN:HD22	1:B:446:ASN:ND2	1.95	0.64
1:B:363[A]:HIS:CE1	1:B:414:ALA:H	2.15	0.63
1:B:254:MET:HG2	1:B:507:PRO:HB2	1.81	0.62
1:B:332:HIS:HE1	1:B:388:SER:OG	1.84	0.60
1:A:332:HIS:HE1	1:A:388:SER:OG	1.84	0.60
1:A:315:PHE:HA	1:A:363:HIS:CE1	2.43	0.53
1:A:287:GLN:HG3	1:B:250:LEU:HD11	1.90	0.53
1:A:440:ASN:HD22	1:A:446:ASN:ND2	2.07	0.52
1:A:273:ILE:HG12	1:A:492:PRO:HA	1.93	0.51
1:A:445:PRO:HG3	1:B:339:PRO:HB2	1.95	0.49
1:B:363[B]:HIS:CD2	1:B:407:GLY:HA2	2.48	0.49
1:A:332:HIS:HD2	1:A:352:SER:OG	1.98	0.46
1:B:332:HIS:HD2	1:B:352:SER:OG	1.99	0.45
1:B:474:LEU:HD12	1:B:496:LEU:HD21	1.99	0.44
1:A:489:LYS:HG3	1:A:528:LEU:HD21	2.02	0.41
1:B:328:LYS:O	1:B:398:ILE:HA	2.21	0.40
1:B:400:LEU:HD13	1:B:448:VAL:HG22	2.04	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	A	310/326 (95%)	307 (99%)	3 (1%)	0	100	100
1	B	303/326 (93%)	300 (99%)	3 (1%)	0	100	100
All	All	613/652 (94%)	607 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	266/277 (96%)	266 (100%)	0	100	100
1	B	261/277 (94%)	261 (100%)	0	100	100
All	All	527/554 (95%)	527 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	GLN
1	A	287	GLN
1	A	296	ASN
1	A	332	HIS
1	A	363	HIS
1	A	389	ASN
1	A	415	ASN
1	A	446	ASN
1	A	527	GLN
1	B	296	ASN
1	B	303	ASN
1	B	332	HIS
1	B	354	GLN
1	B	415	ASN
1	B	446	ASN
1	B	484	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 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	$\# Z > 2$
2	NAG	C	1	2,4	14,14,15	0.50	0	17,19,21	0.79	0
2	GAL	C	2	2	11,11,12	0.57	0	15,15,17	0.53	0
2	FUC	C	3	2	10,10,11	0.59	0	14,14,16	0.44	0
2	FUC	C	4	2	10,10,11	0.58	0	14,14,16	0.38	0
2	NAG	D	1	2,4	14,14,15	0.52	0	17,19,21	0.68	0
2	GAL	D	2	2	11,11,12	0.57	0	15,15,17	0.71	1 (6%)
2	FUC	D	3	2	10,10,11	0.60	0	14,14,16	0.45	0
2	FUC	D	4	2	10,10,11	0.57	0	14,14,16	0.52	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
2	NAG	C	1	2,4	-	0/6/23/26	0/1/1/1
2	GAL	C	2	2	-	0/2/19/22	0/1/1/1
2	FUC	C	3	2	-	-	0/1/1/1
2	FUC	C	4	2	-	-	0/1/1/1
2	NAG	D	1	2,4	-	0/6/23/26	0/1/1/1
2	GAL	D	2	2	-	0/2/19/22	0/1/1/1
2	FUC	D	3	2	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FUC	D	4	2	-	-	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GAL	C1-O5-C5	2.15	115.07	112.19

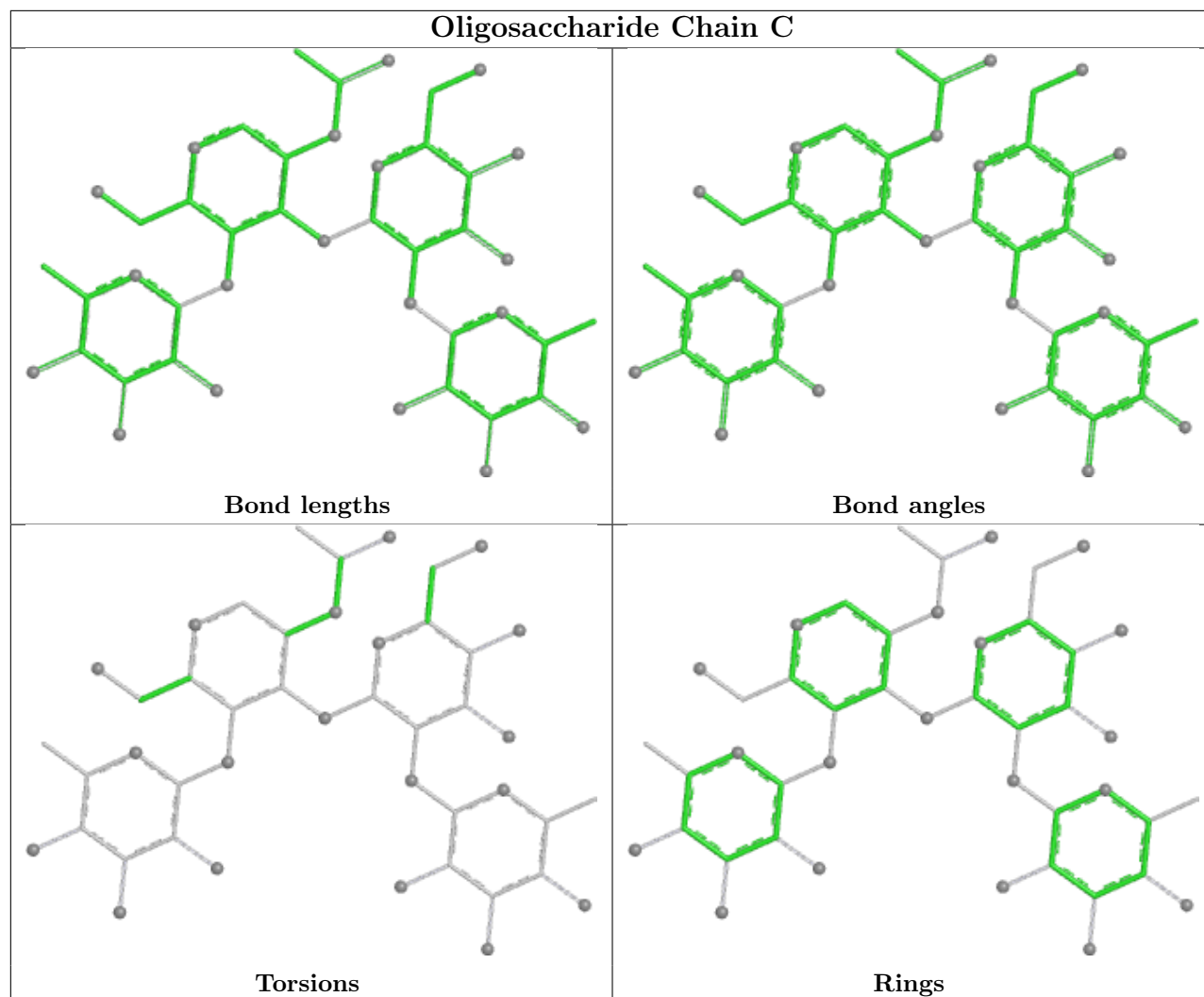
There are no chirality outliers.

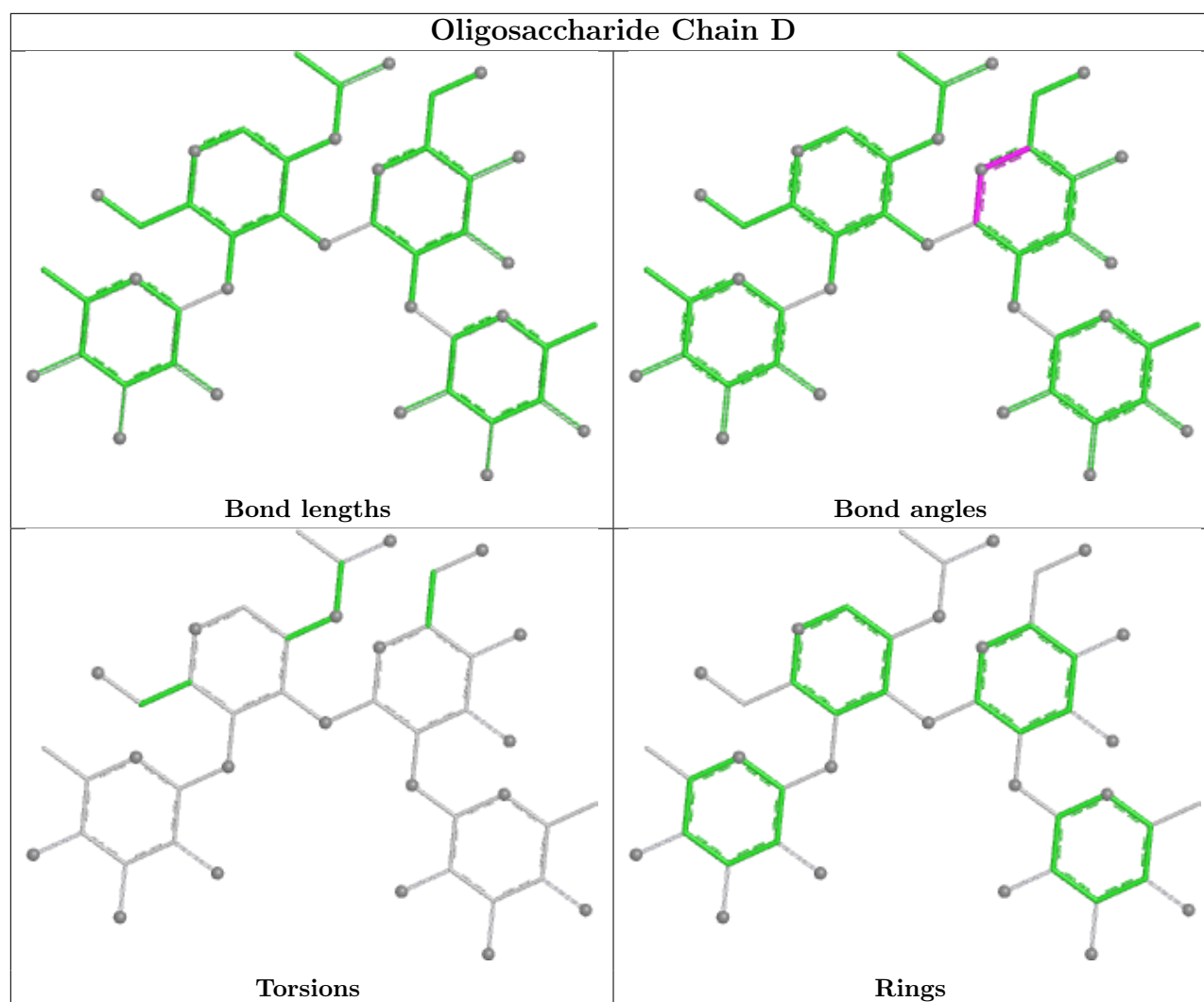
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	NPO	B	1001	2	10,10,10	0.97	0	11,13,13	0.42	0
4	NPO	A	1001	2	10,10,10	0.95	0	11,13,13	0.54	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	NPO	B	1001	2	-	2/2/4/4	0/1/1/1
4	NPO	A	1001	2	-	0/2/4/4	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1001	NPO	C2-C1-N1-O3
4	B	1001	NPO	C6-C1-N1-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	311/326 (95%)	1.27	56 (18%)	3 4	9, 14, 26, 35	1 (0%)
1	B	302/326 (92%)	1.25	66 (21%)	2 2	8, 14, 27, 30	3 (0%)
All	All	613/652 (94%)	1.26	122 (19%)	3 3	8, 14, 27, 35	4 (0%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	314	ALA	8.1
1	A	315	PHE	7.9
1	B	410	LEU	7.0
1	A	503	VAL	7.0
1	B	505	ALA	6.8
1	A	407	GLY	6.8
1	B	504	GLY	6.1
1	B	314	ALA	6.1
1	A	317	SER	6.0
1	B	503	VAL	5.9
1	A	409	SER	5.7
1	A	408	SER	5.6
1	A	394	PRO	5.5
1	A	316	ASP	5.3
1	A	411	SER	5.1
1	B	525	PHE	5.1
1	A	413	ALA	5.0
1	A	414	ALA	4.9
1	B	409	SER	4.9
1	B	411	SER	4.8
1	B	313	MET	4.7
1	A	410	LEU	4.7
1	A	393	PRO	4.6
1	B	397	ASP	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	502	GLY	4.5
1	B	531	VAL	4.5
1	B	501	ASN	4.5
1	A	504	GLY	4.4
1	B	425	PHE	4.4
1	B	528	LEU	4.4
1	B	394	PRO	4.4
1	B	395	GLY	4.4
1	A	395	GLY	4.3
1	B	315	PHE	4.3
1	A	412	GLN	4.1
1	A	248	PRO	4.1
1	A	397	ASP	4.0
1	A	225	ILE	4.0
1	A	533	THR	3.8
1	B	481	THR	3.8
1	B	312	PHE	3.8
1	A	396	THR	3.7
1	B	230	ARG	3.7
1	B	483	ARG	3.7
1	B	248	PRO	3.7
1	B	480	ASP	3.7
1	B	316	ASP	3.6
1	B	311	PRO	3.5
1	B	414	ALA	3.5
1	A	236	ASN	3.5
1	A	415	ASN	3.5
1	B	482	ASN	3.5
1	A	224	THR	3.4
1	A	416	LEU	3.4
1	A	534	ALA	3.3
1	A	502	GLY	3.3
1	A	392	THR	3.3
1	B	412	GLN	3.2
1	B	526	TYR	3.2
1	B	500	PRO	3.1
1	B	407	GLY	3.1
1	A	372	VAL	3.0
1	A	260	ALA	3.0
1	B	413	ALA	3.0
1	A	229	THR	3.0
1	A	376	PRO	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	317	SER	3.0
1	B	530	PRO	2.9
1	A	375	HIS	2.9
1	B	529	LYS	2.9
1	B	231	ALA	2.8
1	B	358	GLN	2.8
1	A	374	ASN	2.8
1	A	312	PHE	2.8
1	B	376	PRO	2.8
1	B	372	VAL	2.7
1	B	408	SER	2.7
1	A	417	ALA	2.7
1	B	527	GLN	2.7
1	A	373	PHE	2.6
1	B	392	THR	2.6
1	A	228	LYS	2.6
1	B	371	GLU	2.6
1	B	275	GLY	2.6
1	B	478	ASP	2.6
1	B	393	PRO	2.5
1	B	522	VAL	2.5
1	B	523	SER	2.5
1	A	358	GLN	2.5
1	A	364	LEU	2.4
1	B	519	VAL	2.3
1	B	374	ASN	2.3
1	A	313	MET	2.3
1	A	258	PRO	2.3
1	B	396	THR	2.3
1	A	237	ILE	2.3
1	A	227	GLN	2.3
1	B	479	PRO	2.3
1	B	405	ASP	2.2
1	A	442	ARG	2.2
1	B	375	HIS	2.2
1	A	357	VAL	2.2
1	B	521	TRP	2.2
1	A	483	ARG	2.2
1	A	404	PRO	2.2
1	B	258	PRO	2.2
1	B	524	ARG	2.2
1	A	259	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	485	LEU	2.2
1	B	512	LEU	2.2
1	A	355	THR	2.2
1	A	341	ASN	2.2
1	B	415	ASN	2.1
1	B	495	TYR	2.1
1	B	402	GLU	2.1
1	B	421	PHE	2.1
1	A	505	ALA	2.1
1	B	442	ARG	2.1
1	A	369	PHE	2.0
1	B	499	VAL	2.0
1	A	299	ALA	2.0
1	A	296	ASN	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](#)

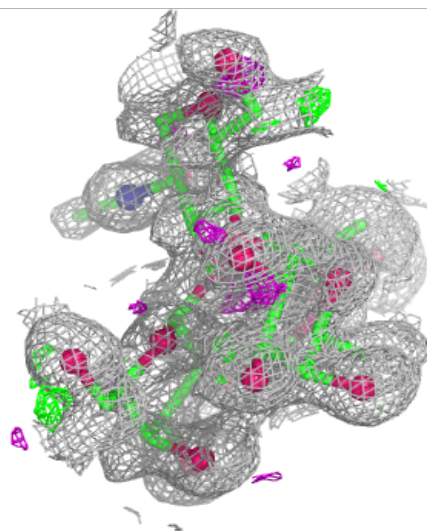
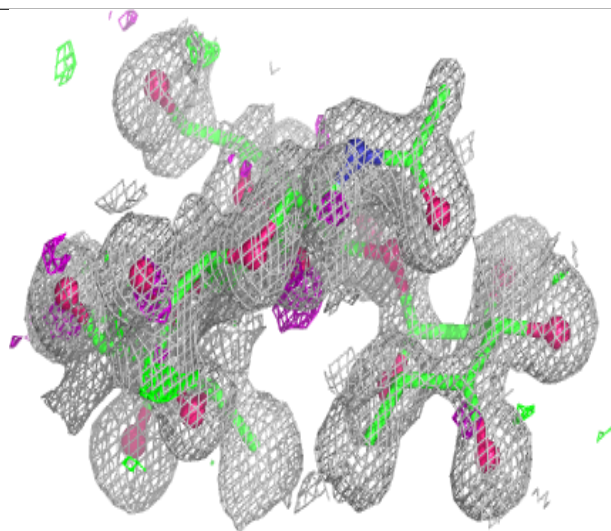
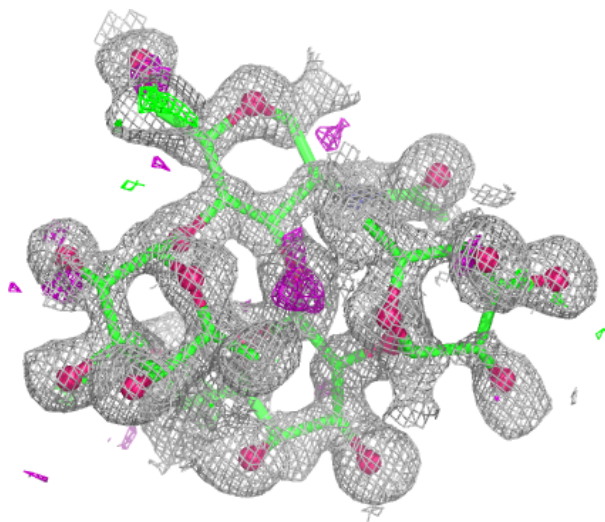
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

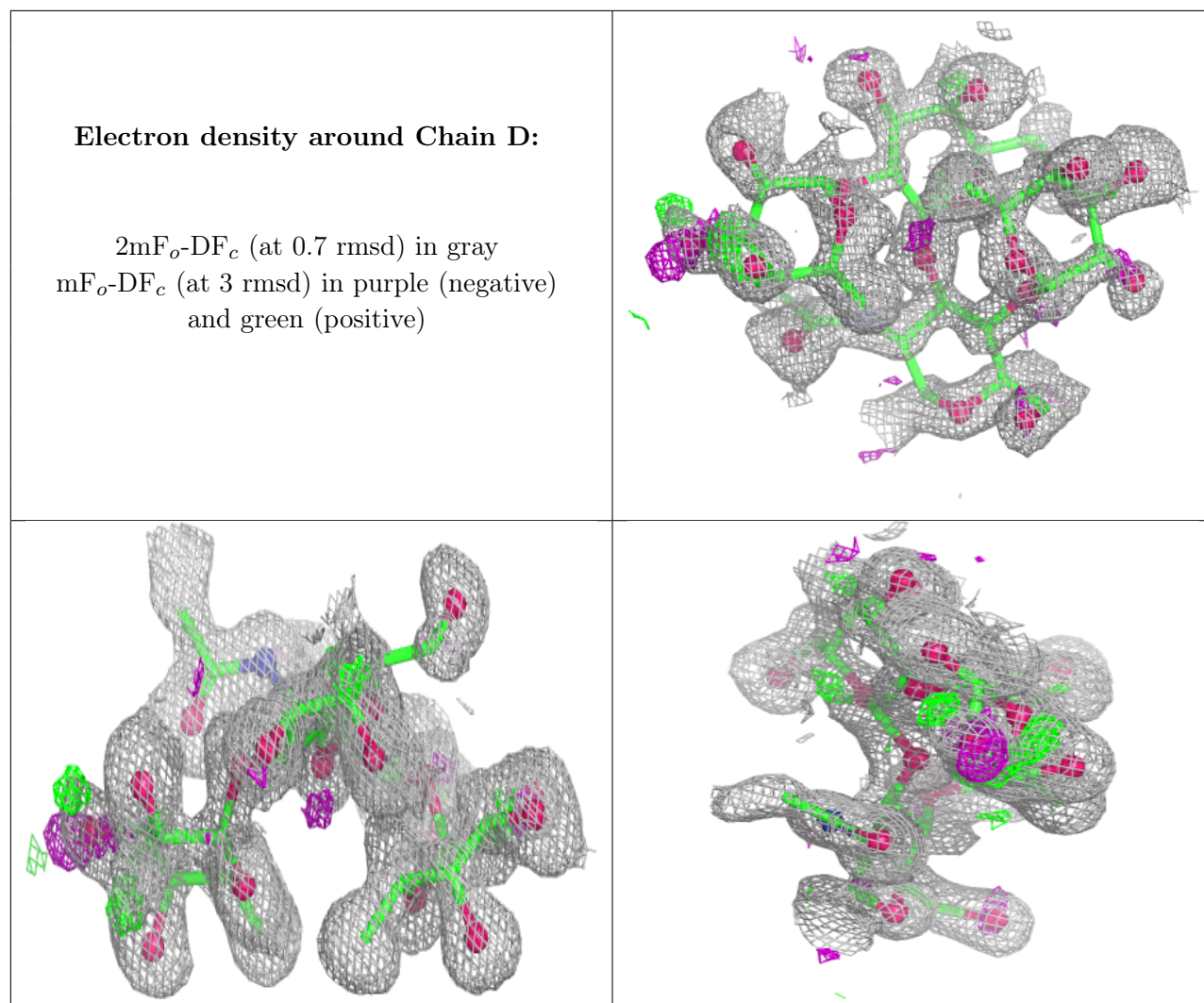
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	1	14/15	0.90	0.14	18,22,23,24	0
2	FUC	D	3	10/11	0.91	0.13	17,18,20,20	0
2	NAG	C	1	14/15	0.94	0.11	13,15,17,18	0
2	FUC	C	4	10/11	0.95	0.10	13,15,16,16	0
2	FUC	D	4	10/11	0.95	0.11	17,18,19,19	0
2	FUC	C	3	10/11	0.96	0.09	13,14,15,16	0
2	GAL	D	2	11/12	0.96	0.10	14,16,17,17	0
2	GAL	C	2	11/12	0.97	0.08	13,13,14,16	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 C:

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





6.4 Ligands [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	NPO	B	1001	10/10	0.71	0.21	28,32,34,34	0
4	NPO	A	1001	10/10	0.84	0.16	19,23,26,26	0
3	NA	A	701	1/1	0.88	0.16	34,34,34,34	0
3	NA	B	701	1/1	0.98	0.07	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.