



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:02 PM UTC

PDB ID : 8V04 / pdb_00008v04
Title : High resolution TMPRSS2 structure following acylation by nafamostat
Authors : Fraser, B.J.; Dong, A.; Kutera, M.; Seitova, A.; Li, Y.; Hutchinson, A.; Edwards, A.; Benard, F.; Levon, H.; Arrowsmith, C.
Deposited on : 2023-11-16
Resolution : 1.58 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

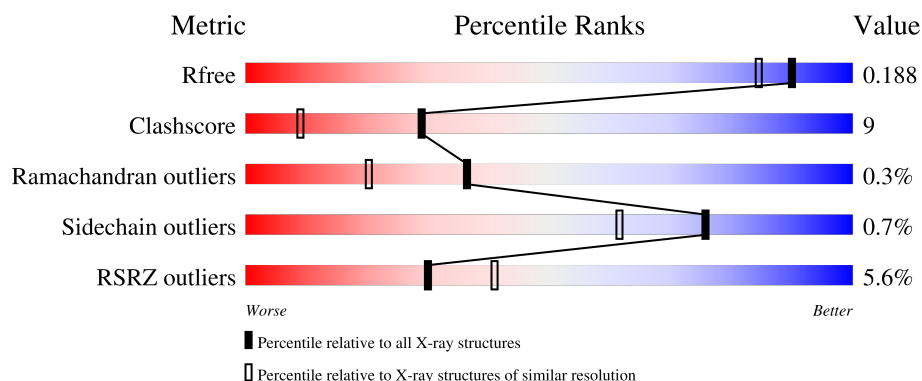
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.58 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	110	14% 74% 17% • 7%
2	B	249	2% 83% 12% •
3	C	4	50% 50%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 3228 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 non-catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	102	Total	C	N	O	S	0	9	0
			830	522	147	149	12			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	ALA	-	expression tag	UNP O15393
A	147	ALA	-	expression tag	UNP O15393
A	251	ASP	SER	engineered mutation	UNP O15393
A	252	ASP	ARG	engineered mutation	UNP O15393
A	253	ASP	GLN	engineered mutation	UNP O15393
A	254	ASP	SER	engineered mutation	UNP O15393
A	255	LYS	ARG	engineered mutation	UNP O15393

- Molecule 2 is a protein called Transmembrane protease serine 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	25	0
			1949	1262	320	346	21			

There are 12 discrepancies between the modelled and reference sequences:

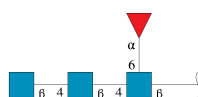
Chain	Residue	Modelled	Actual	Comment	Reference
B	493	GLU	-	expression tag	UNP O15393
B	494	PHE	-	expression tag	UNP O15393
B	495	VAL	-	expression tag	UNP O15393
B	496	GLU	-	expression tag	UNP O15393
B	497	HIS	-	expression tag	UNP O15393
B	498	HIS	-	expression tag	UNP O15393
B	499	HIS	-	expression tag	UNP O15393
B	500	HIS	-	expression tag	UNP O15393
B	501	HIS	-	expression tag	UNP O15393

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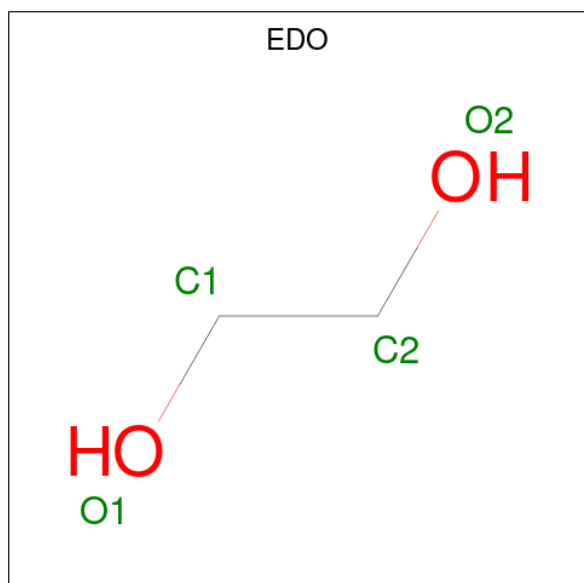
Chain	Residue	Modelled	Actual	Comment	Reference
B	502	HIS	-	expression tag	UNP O15393
B	503	HIS	-	expression tag	UNP O15393
B	504	HIS	-	expression tag	UNP O15393

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	4	Total	C	N	O	0	0	0
			52	30	3	19			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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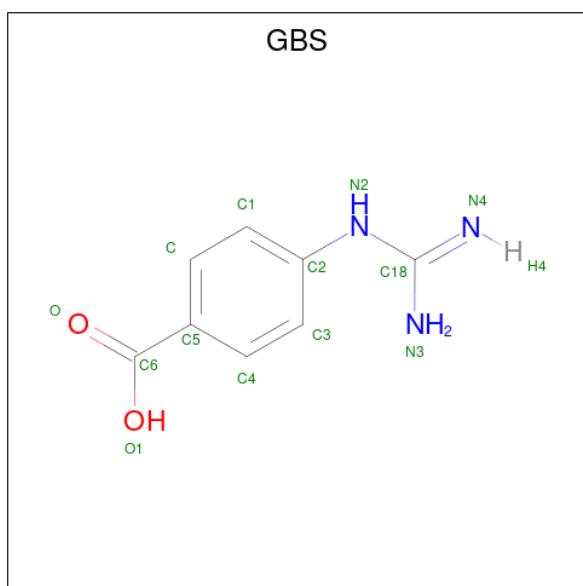
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

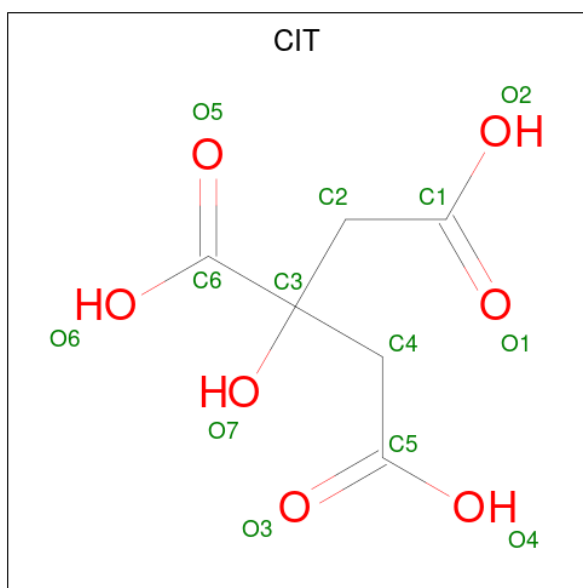
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	X	0	0
			1	1		

- Molecule 6 is 4-carbamimidamidobenzoic acid (CCD ID: GBS) (formula: C₈H₉N₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			12	8	3	1		

- Molecule 7 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).

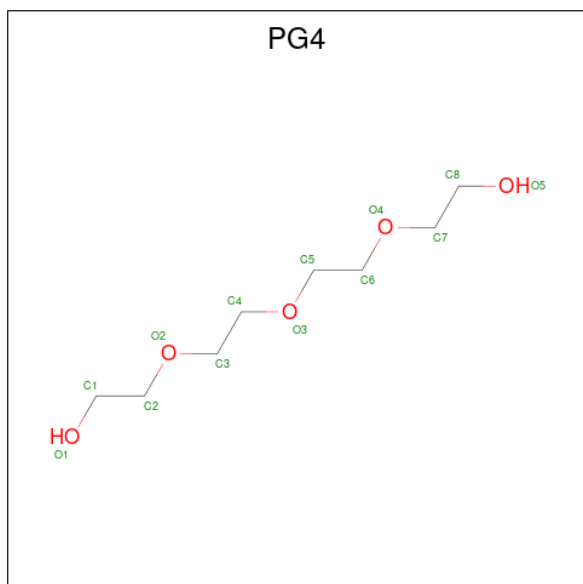


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Ca	0	0
			1	1		

- Molecule 9 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			13	8	5		

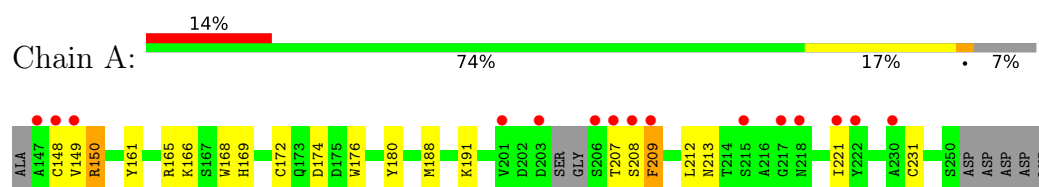
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	75	Total	O	0	0
			75	75		
10	B	245	Total	O	0	1
			246	246		

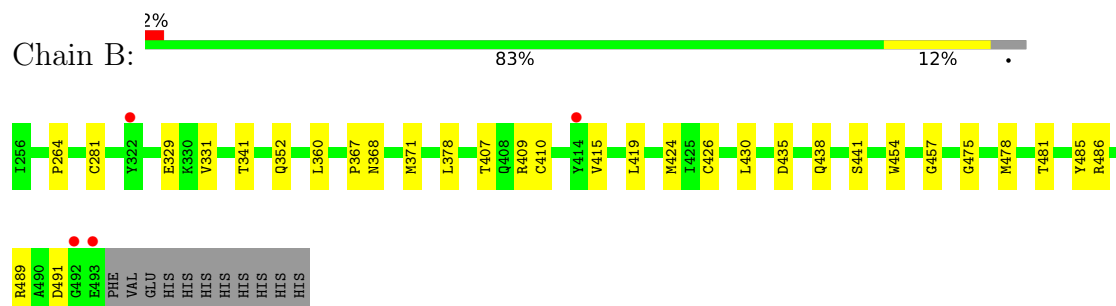
3 Residue-property plots [i](#)

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 non-catalytic chain



- Molecule 2: Transmembrane protease serine 2



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.76Å 50.50Å 64.58Å 90.00° 91.60° 90.00°	Depositor
Resolution (Å)	39.81 – 1.58 39.81 – 1.58	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.81-1.58) 99.2 (39.81-1.58)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.156 , 0.181 0.168 , 0.188	Depositor DCC
R_{free} test set	2463 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	14.0	Xtriage
Anisotropy	1.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3228	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.76% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, FUC, GBS, EDO, UNX, CIT, NAG, PG4

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	0.61	0/870	0.91	1/1172 (0.1%)
2	B	0.67	0/2076	0.95	1/2829 (0.0%)
All	All	0.66	0/2946	0.94	2/4001 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	209	PHE	CA-CB-CG	5.99	119.78	113.80
2	B	435	ASP	CA-CB-CG	5.13	117.73	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150[A]	ARG	Sidechain
1	A	150[B]	ARG	Sidechain

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	830	0	803	21	0
2	B	1949	0	1938	25	0
3	C	52	0	46	2	0
4	A	12	0	18	4	0
4	B	24	0	36	6	0
5	A	1	0	0	0	0
6	B	12	0	0	0	0
7	B	13	0	5	1	0
8	B	1	0	0	0	0
9	B	13	0	18	4	0
10	A	75	0	0	1	0
10	B	246	0	0	4	0
All	All	3228	0	2864	49	0

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

All (49) 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)
2:B:360:LEU:HD13	4:B:603:EDO:H21	1.56	0.85
2:B:407:THR:HA	2:B:410[B]:CYS:SG	2.24	0.78
2:B:438[B]:GLN:NE2	10:B:702:HOH:O	2.21	0.73
1:A:150[B]:ARG:HG2	1:A:168:TRP:CZ3	2.28	0.68
1:A:172[A]:CYS:SG	1:A:174:ASP:CG	2.76	0.68
4:B:605:EDO:H11	10:B:742:HOH:O	1.94	0.66
2:B:409:ARG:HD3	2:B:430:LEU:HD11	1.77	0.66
1:A:172[A]:CYS:SG	1:A:174:ASP:OD1	2.55	0.65
1:A:213:ASN:HD22	4:A:304:EDO:C2	2.11	0.64
2:B:409:ARG:HD3	2:B:430:LEU:CD1	2.29	0.62
1:A:209:PHE:CG	1:A:231[B]:CYS:SG	2.93	0.61
1:A:150[B]:ARG:HH21	1:A:150[B]:ARG:HB3	1.65	0.61
4:A:304:EDO:H22	3:C:1:NAG:H2	1.84	0.59
1:A:209:PHE:CD1	1:A:231[B]:CYS:SG	2.97	0.58
2:B:341:THR:O	9:B:606:PG4:H51	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:481[A]:THR:HG22	2:B:485:TYR:CE2	2.40	0.57
2:B:419:LEU:O	9:B:606:PG4:H42	2.06	0.55
1:A:150[B]:ARG:HH21	1:A:150[B]:ARG:CB	2.19	0.55
2:B:368:ASN:O	2:B:478[A]:MET:HE1	2.07	0.54
2:B:352[B]:GLN:CD	10:B:703:HOH:O	2.50	0.54
1:A:191:LYS:NZ	2:B:491:ASP:O	2.37	0.54
1:A:213:ASN:HD22	4:A:304:EDO:H22	1.74	0.53
2:B:368:ASN:O	2:B:371:MET:HG2	2.08	0.52
2:B:371:MET:HG2	2:B:478[A]:MET:HE1	1.91	0.52
2:B:281[B]:CYS:HB2	2:B:441:SER:O	2.10	0.52
1:A:165:ARG:HH11	1:A:165:ARG:HG3	1.75	0.51
1:A:176:TRP:CH2	1:A:221:ILE:HD11	2.46	0.51
1:A:169:HIS:CE1	1:A:208:SER:HB3	2.46	0.50
2:B:424:MET:HE1	9:B:606:PG4:H41	1.95	0.48
2:B:264:PRO:HB3	4:B:603:EDO:H12	1.96	0.48
2:B:367:PRO:O	2:B:481[B]:THR:HG21	2.13	0.48
1:A:191:LYS:HE3	10:B:840:HOH:O	2.14	0.47
1:A:166[B]:LYS:HE2	10:A:429:HOH:O	2.15	0.47
1:A:180:TYR:CE2	1:A:212:LEU:HD21	2.50	0.47
2:B:410[B]:CYS:CB	2:B:426:CYS:SG	3.04	0.46
1:A:188[B]:MET:HA	4:B:604:EDO:H22	1.96	0.46
1:A:172[B]:CYS:SG	1:A:209:PHE:HB3	2.56	0.45
1:A:165:ARG:HG3	1:A:165:ARG:NH1	2.31	0.45
7:B:601:CIT:O2	7:B:601:CIT:O5	2.35	0.44
2:B:329:GLU:HB2	2:B:352[B]:GLN:HG3	1.99	0.43
1:A:188[A]:MET:HA	4:B:604:EDO:H22	1.99	0.43
2:B:486:ARG:NE	2:B:489:ARG:HH11	2.15	0.43
2:B:457:GLY:HA2	2:B:475:GLY:O	2.19	0.43
1:A:148[B]:CYS:HB2	1:A:161:TYR:HB3	2.00	0.41
4:A:301:EDO:H22	3:C:1:NAG:H83	2.02	0.41
2:B:371:MET:HE1	2:B:454:TRP:CE2	2.55	0.41
2:B:341:THR:O	9:B:606:PG4:C5	2.67	0.41
2:B:331:VAL:O	4:B:608:EDO:H12	2.20	0.41

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	107/110 (97%)	104 (97%)	3 (3%)	0	100	100
2	B	261/249 (105%)	256 (98%)	4 (2%)	1 (0%)	30	12
All	All	368/359 (102%)	360 (98%)	7 (2%)	1 (0%)	36	20

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	415	VAL

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	93/95 (98%)	91 (98%)	2 (2%)	45	15
2	B	216/210 (103%)	216 (100%)	0	100	100
All	All	309/305 (101%)	307 (99%)	2 (1%)	76	65

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	VAL
1	A	207	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	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 ⓘ

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	$\# Z > 2$
3	NAG	C	1	3,1	14,14,15	0.49	0	17,19,21	0.57	0
3	NAG	C	2	3	14,14,15	0.43	0	17,19,21	0.59	0
3	NAG	C	3	3	14,14,15	0.44	0	17,19,21	1.45	1 (5%)
3	FUC	C	4	3	10,10,11	0.36	0	14,14,16	0.42	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
3	NAG	C	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	NAG	C	3	3	-	4/6/23/26	0/1/1/1
3	FUC	C	4	3	-	-	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(°)
3	C	3	NAG	O5-C1-C2	4.78	118.69	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

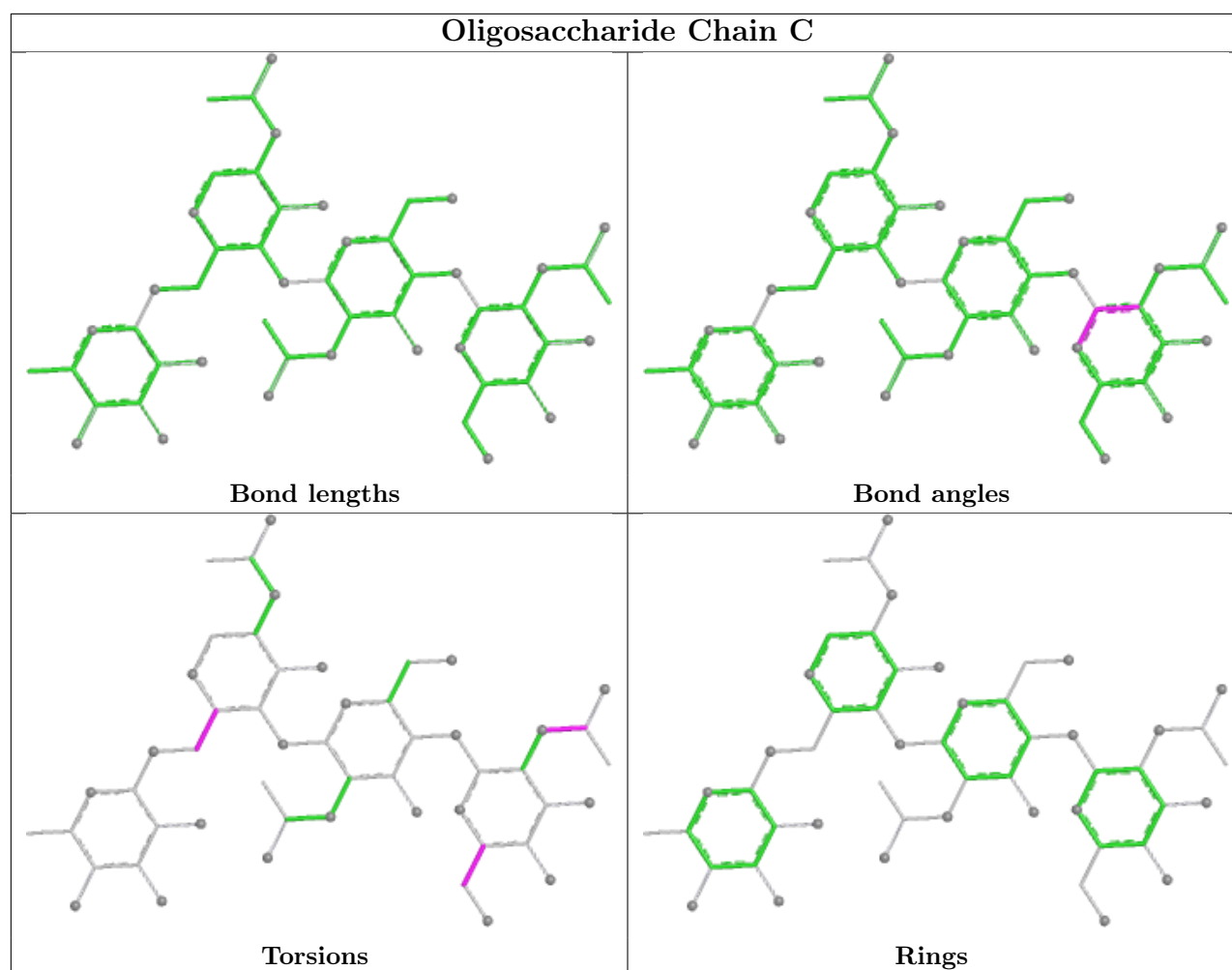
Mol	Chain	Res	Type	Atoms
3	C	3	NAG	C8-C7-N2-C2
3	C	3	NAG	O7-C7-N2-C2
3	C	3	NAG	C4-C5-C6-O6
3	C	3	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	2	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](#)

Of 14 ligands modelled in this entry, 1 is unknown and 1 is monoatomic - leaving 12 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	EDO	A	303	-	3,3,3	0.06	0	2,2,2	0.28	0
4	EDO	B	605	-	3,3,3	0.41	0	2,2,2	0.60	0
4	EDO	A	301	-	3,3,3	0.26	0	2,2,2	0.78	0
4	EDO	B	604	-	3,3,3	0.28	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GBS	B	600	2	12,12,13	0.78	0	14,15,17	0.92	0
9	PG4	B	606	-	12,12,12	0.34	0	11,11,11	0.37	0
7	CIT	B	601	-	12,12,12	1.27	1 (8%)	17,17,17	1.05	1 (5%)
4	EDO	A	304	-	3,3,3	0.33	0	2,2,2	0.25	0
4	EDO	B	607	-	3,3,3	0.11	0	2,2,2	0.03	0
4	EDO	B	608	-	3,3,3	0.07	0	2,2,2	0.13	0
4	EDO	B	609	-	3,3,3	0.08	0	2,2,2	0.04	0
4	EDO	B	603	-	3,3,3	0.42	0	2,2,2	0.37	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	EDO	A	303	-	-	1/1/1/1	-
4	EDO	B	605	-	-	1/1/1/1	-
4	EDO	A	301	-	-	1/1/1/1	-
4	EDO	B	604	-	-	1/1/1/1	-
6	GBS	B	600	2	-	2/6/6/8	0/1/1/1
9	PG4	B	606	-	-	5/10/10/10	-
7	CIT	B	601	-	-	5/16/16/16	-
4	EDO	A	304	-	-	1/1/1/1	-
4	EDO	B	607	-	-	1/1/1/1	-
4	EDO	B	608	-	-	0/1/1/1	-
4	EDO	B	609	-	-	0/1/1/1	-
4	EDO	B	603	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	601	CIT	C3-C6	2.38	1.55	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	601	CIT	O3-C5-C4	-2.24	116.61	122.95

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	601	CIT	C2-C3-C6-O5
7	B	601	CIT	C2-C3-C6-O6
7	B	601	CIT	O7-C3-C6-O5
7	B	601	CIT	O7-C3-C6-O6
9	B	606	PG4	O3-C5-C6-O4
9	B	606	PG4	C5-C6-O4-C7
9	B	606	PG4	O4-C7-C8-O5
9	B	606	PG4	O2-C3-C4-O3
4	A	303	EDO	O1-C1-C2-O2
4	B	604	EDO	O1-C1-C2-O2
4	B	607	EDO	O1-C1-C2-O2
6	B	600	GBS	C4-C5-C6-O
4	B	603	EDO	O1-C1-C2-O2
4	B	605	EDO	O1-C1-C2-O2
6	B	600	GBS	C-C5-C6-O
9	B	606	PG4	C8-C7-O4-C6
4	A	304	EDO	O1-C1-C2-O2
7	B	601	CIT	O7-C3-C4-C5
4	A	301	EDO	O1-C1-C2-O2

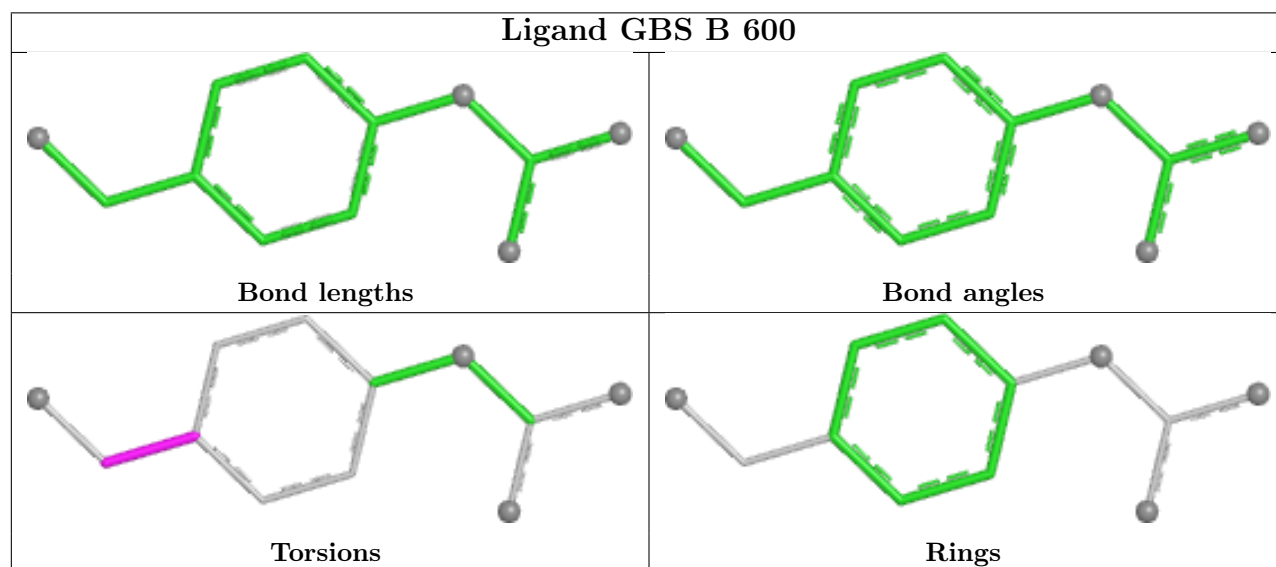
There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	605	EDO	1	0
4	A	301	EDO	1	0
4	B	604	EDO	2	0
9	B	606	PG4	4	0
7	B	601	CIT	1	0
4	A	304	EDO	3	0
4	B	608	EDO	1	0
4	B	603	EDO	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	A	102/110 (92%)	0.86	15 (14%) 6 10	11, 26, 54, 75	9 (8%)
2	B	238/249 (95%)	-0.13	4 (1%) 69 78	8, 15, 29, 59	25 (10%)
All	All	340/359 (94%)	0.16	19 (5%) 30 41	8, 18, 42, 75	34 (10%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	147	ALA	5.9
1	A	149	VAL	4.4
2	B	492	GLY	4.2
1	A	207	THR	4.1
2	B	322	TYR	3.9
1	A	218	ASN	3.7
1	A	208	SER	3.6
1	A	203	ASP	3.5
1	A	148[A]	CYS	3.0
1	A	206	SER	3.0
2	B	493	GLU	2.9
1	A	222	TYR	2.9
1	A	209	PHE	2.9
2	B	414	TYR	2.7
1	A	217	GLY	2.5
1	A	201	VAL	2.5
1	A	230	ALA	2.3
1	A	221	ILE	2.2
1	A	215[A]	SER	2.1

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

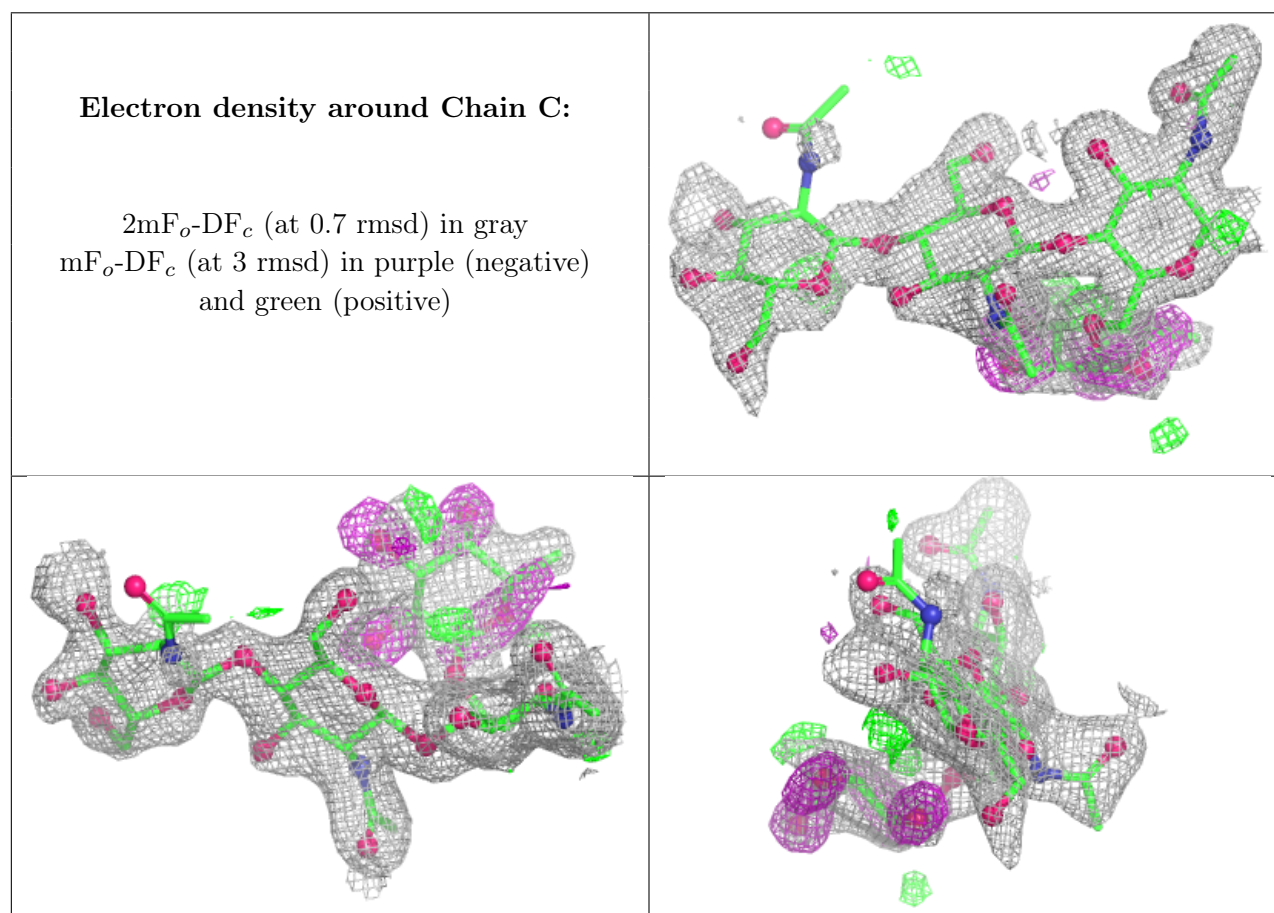
There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
3	NAG	C	3	14/15	0.67	0.16	55,62,81,81	0
3	FUC	C	4	10/11	0.73	0.19	30,30,30,30	0
3	NAG	C	1	14/15	0.90	0.09	22,26,31,32	0
3	NAG	C	2	14/15	0.91	0.10	35,43,53,53	0

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



6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

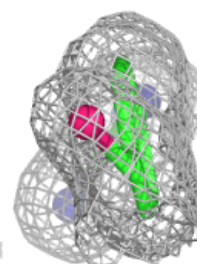
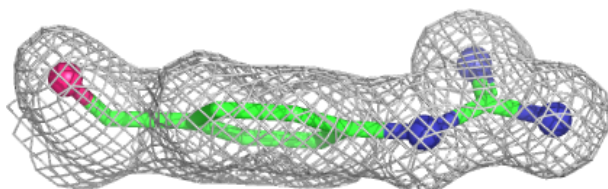
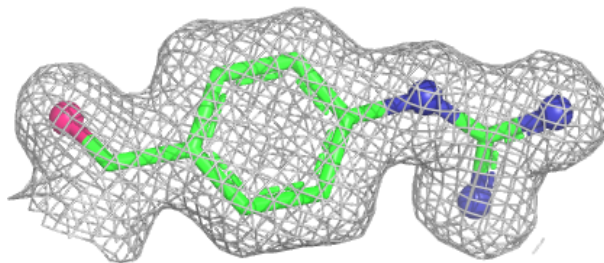
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	A	304	4/4	0.65	0.20	42,47,48,52	0
9	PG4	B	606	13/13	0.76	0.18	33,53,59,59	0
8	CA	B	602	1/1	0.77	0.13	83,83,83,83	0
4	EDO	B	608	4/4	0.78	0.16	52,54,56,60	0
4	EDO	B	607	4/4	0.79	0.14	63,63,65,67	0
4	EDO	B	605	4/4	0.79	0.14	41,44,44,45	0
4	EDO	B	604	4/4	0.80	0.17	46,49,51,53	0
4	EDO	B	609	4/4	0.80	0.20	58,63,63,67	0
4	EDO	A	303	4/4	0.83	0.14	42,48,48,49	0
4	EDO	B	603	4/4	0.84	0.14	34,37,39,39	0
5	UNX	A	302	1/1	0.85	0.13	32,32,32,32	0
4	EDO	A	301	4/4	0.87	0.13	34,39,39,41	0
7	CIT	B	601	13/13	0.95	0.07	21,24,35,40	0
6	GBS	B	600	12/13	0.97	0.04	15,16,17,19	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GBS B 600:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.