



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 08:24 PM BST

PDB ID : 4YLQ
Title : Crystal Structure of a FVIIa-Trypsin Chimera (FT) in Complex with Soluble Tissue Factor
Authors : Sorensen, A.B.; Svensson, L.A.; Gandhi, P.S.
Deposited on : 2015-03-05
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
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) : 2.13.1

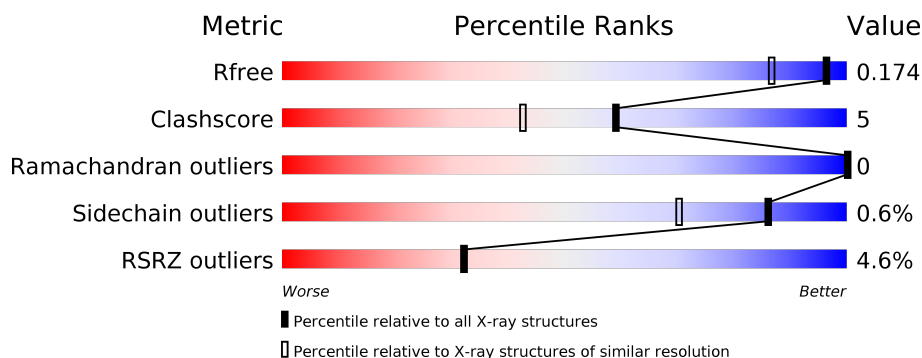
1 Overall quality at a glance

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}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (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 on 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	L	152	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>6%</div> </div> </div>
2	H	249	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
3	T	219	<div> <div>6%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>•</div> </div> </div>
4	A	3	<div> <div></div> <div>100%</div> </div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 10324 atoms, of which 4784 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 Coagulation factor VII.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	L	143	Total	C	H	N	O	S	0	3	0
			2128	697	985	189	242	15			

- Molecule 2 is a protein called Coagulation factor VII.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	249	Total	C	H	N	O	S	0	8	0
			3802	1244	1863	335	345	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	LEU	deletion	UNP P08709
H	?	-	GLN	deletion	UNP P08709
H	?	-	GLN	deletion	UNP P08709
H	?	-	SER	deletion	UNP P08709
H	?	-	ARG	deletion	UNP P08709
H	169	GLU	LYS	engineered mutation	UNP P08709
H	170	ALA	VAL	engineered mutation	UNP P08709
H	171	SER	GLY	engineered mutation	UNP P08709
H	172	PHE	ASP	engineered mutation	UNP P08709
H	173	PRO	SER	engineered mutation	UNP P08709
H	174	GLY	PRO	engineered mutation	UNP P08709
H	175	LYS	ASN	engineered mutation	UNP P08709

- Molecule 3 is a protein called Tissue factor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	T	210	Total	C	H	N	O	S	0	5	0
			3276	1065	1592	271	343	5			

- Molecule 4 is an oligosaccharide called alpha-D-xylopyranose-(1-3)-alpha-D-xylopyranose-(1

-3)-beta-D-glucopyranose.

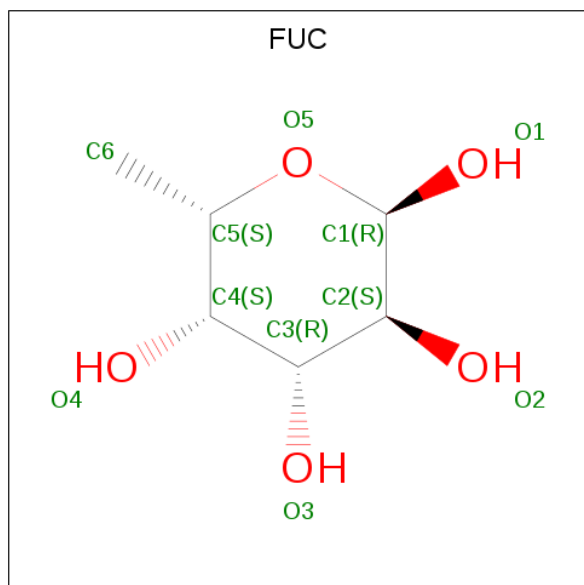


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	A	3	Total	C	H	O	0	0	0
			54	16	25	13			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

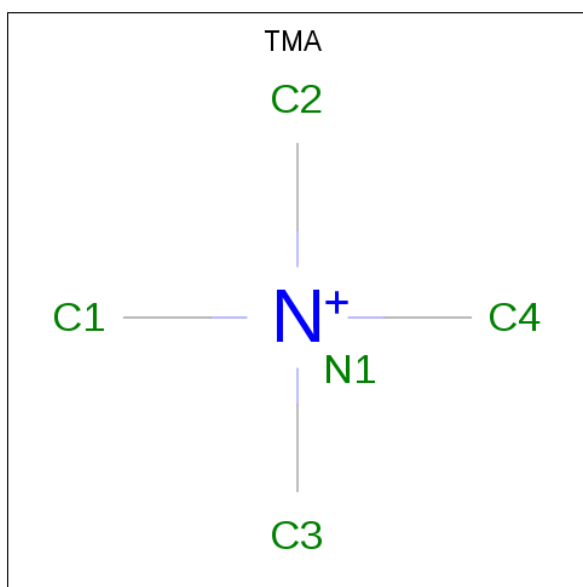
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Ca	0	0
			1	1		
5	L	8	Total	Ca	0	0
			8	8		

- Molecule 6 is alpha-L-fucopyranose (three-letter code: FUC) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	H	O	0	0
			20	6	10	4		

- Molecule 7 is TETRAMETHYLAMMONIUM ION (three-letter code: TMA) (formula: C₄H₁₂N).



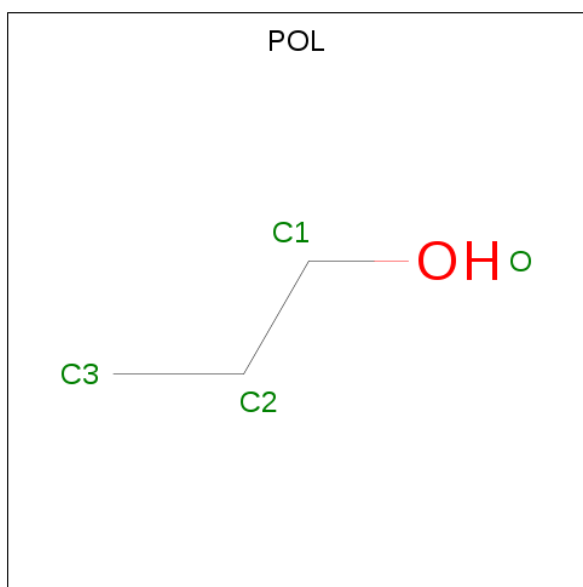
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	H	N	0	0
			17	4	12	1		
7	H	1	Total	C	H	N	0	0
			17	4	12	1		
7	H	1	Total	C	H	N	0	0
			17	4	12	1		
7	H	1	Total	C	H	N	0	0
			17	4	12	1		
7	H	1	Total	C	H	N	0	0
			17	4	12	1		
7	H	1	Total	C	H	N	0	0
			17	4	12	1		
7	H	1	Total	C	H	N	0	0
			17	4	12	1		
7	H	1	Total	C	H	N	0	0
			17	4	12	1		
7	T	1	Total	C	H	N	0	0
			17	4	12	1		
7	T	1	Total	C	H	N	0	0
			17	4	12	1		
7	T	1	Total	C	H	N	0	0
			17	4	12	1		
7	T	1	Total	C	H	N	0	0
			17	4	12	1		

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[illegible]

- [illegible]

- Molecule 9 is N-PROPANOL (three-letter code: POL) (formula: $\text{C}_3\text{H}_8\text{O}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	H	1	Total	C	H	O	0	0
			12	3	8	1		


- Molecule 10 is water.

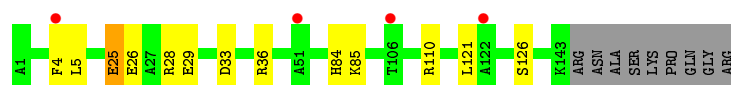
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	L	143	Total	O	0	0
			143	143		
10	H	242	Total	O	0	0
			242	242		
10	T	190	Total	O	0	0
			190	190		

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.

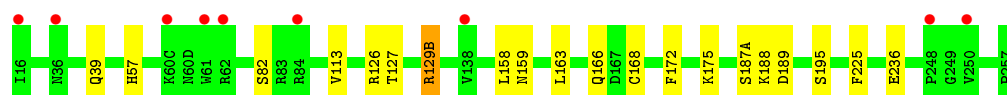
- Molecule 1: Coagulation factor VII

Chain L: 




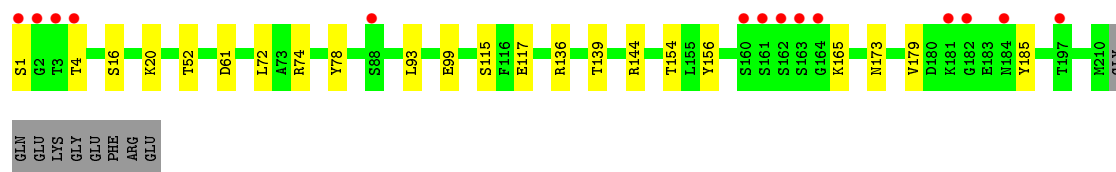
- Molecule 2: Coagulation factor VII

Chain H: 



- Molecule 3: Tissue factor

Chain T: 



- Molecule 4: alpha-D-xylopyranose-(1-3)-alpha-D-xylopyranose-(1-3)-beta-D-glucopyranose

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.31Å 80.04Å 123.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.25 – 1.40 40.31 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.25-1.40) 99.8 (40.31-1.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 1.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.140 , 0.174 0.141 , 0.174	Depositor DCC
R_{free} test set	6918 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	15.3	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	10324	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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: BGC, 0Z7, TMA, POL, XYS, FUC, CGU, CA

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	L	0.73	0/1048	0.81	0/1403
2	H	0.85	2/2008 (0.1%)	0.91	3/2737 (0.1%)
3	T	0.83	1/1735 (0.1%)	0.85	2/2364 (0.1%)
All	All	0.82	3/4791 (0.1%)	0.87	5/6504 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	39	GLN	CB-CG	-6.44	1.35	1.52
3	T	117	GLU	CD-OE1	5.32	1.31	1.25
2	H	113	VAL	CB-CG2	-5.06	1.42	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	189	ASP	CB-CG-OD1	6.58	124.22	118.30
3	T	74	ARG	NE-CZ-NH2	-5.47	117.56	120.30
3	T	144	ARG	NE-CZ-NH2	5.39	122.99	120.30
2	H	126	ARG	NE-CZ-NH2	-5.19	117.70	120.30
2	H	129(B)	ARG	NE-CZ-NH2	-5.17	117.72	120.30

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	L	1143	985	992	5	0
2	H	1939	1863	1906	17	0
3	T	1684	1592	1637	18	0
4	A	29	25	24	0	0
5	H	1	0	0	0	0
5	L	8	0	0	0	0
6	L	10	10	10	0	0
7	H	45	108	108	8	0
7	L	5	12	12	0	0
7	T	60	144	144	9	0
8	H	37	37	31	0	0
9	H	4	8	8	0	0
10	H	242	0	0	7	0
10	L	143	0	0	0	0
10	T	190	0	0	6	0
All	All	5540	4784	4872	46	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (46) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:173[B]:ASN:OD1	10:T:401:HOH:O	1.86	0.92
3:T:78:TYR:OH	7:T:302:TMA:H12	1.81	0.80
3:T:165:LYS:HE3	7:T:309:TMA:C3	2.15	0.76
3:T:165:LYS:HE3	7:T:309:TMA:H33	1.72	0.70
2:H:129(B):ARG:NH2	10:H:601:HOH:O	2.25	0.69
2:H:82:SER:OG	7:H:503:TMA:H33	1.93	0.67
3:T:1:SER:HG	3:T:4:THR:HG1	1.42	0.67
3:T:115:SER:OG	7:T:304:TMA:H12	1.96	0.65
7:H:503:TMA:H32	10:H:811:HOH:O	2.02	0.59
3:T:165:LYS:HE3	7:T:309:TMA:H31	1.85	0.59
7:H:510:TMA:H32	10:H:728:HOH:O	2.04	0.58
3:T:52:THR:OG1	7:T:312:TMA:H33	2.05	0.57
7:H:510:TMA:H31	10:H:784:HOH:O	2.04	0.56
3:T:173[B]:ASN:ND2	10:T:402:HOH:O	2.28	0.56
2:H:166:GLN:HE21	7:H:511:TMA:H31	1.73	0.54
2:H:159:ASN:HD22	7:H:506:TMA:H32	1.73	0.54
2:H:158:LEU:HD11	2:H:188:LYS:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:156:TYR:HD1	3:T:165:LYS:HD3	1.77	0.49
2:H:158:LEU:HD11	2:H:188:LYS:HE3	1.94	0.49
7:T:310:TMA:H32	10:T:569:HOH:O	2.13	0.49
3:T:156:TYR:CD1	3:T:165:LYS:HD3	2.49	0.48
2:H:127:THR:HB	10:H:700:HOH:O	2.12	0.48
3:T:1:SER:OG	3:T:4:THR:OG1	2.20	0.47
1:L:85:LYS:NZ	3:T:61:ASP:OD2	2.46	0.46
3:T:154[A]:THR:HG21	10:T:541:HOH:O	2.15	0.46
3:T:16:SER:HA	3:T:20:LYS:O	2.15	0.46
2:H:187(A):SER:C	2:H:188:LYS:HG3	2.35	0.46
7:T:301:TMA:H32	10:T:412:HOH:O	2.15	0.46
2:H:163:LEU:HD22	2:H:168[B]:CYS:HB3	1.99	0.45
2:H:158:LEU:CD1	2:H:188:LYS:HE3	2.46	0.45
2:H:172[A]:PHE:HB3	2:H:175:LYS:HB2	1.98	0.44
2:H:127:THR:HG21	2:H:129(B):ARG:CZ	2.48	0.44
2:H:163:LEU:HD21	2:H:225:PHE:CZ	2.52	0.44
1:L:4[B]:PHE:CZ	1:L:5:LEU:CD1	3.01	0.43
1:L:25:CGU:OE22	1:L:28:ARG:NH2	2.39	0.43
2:H:166:GLN:HE21	7:H:511:TMA:C3	2.30	0.43
1:L:121:LEU:HD12	1:L:126:SER:HB2	2.02	0.42
3:T:179:VAL:HB	3:T:185:TYR:CE1	2.55	0.42
3:T:72:LEU:CD2	3:T:99:GLU:HG2	2.50	0.42
2:H:57:HIS:CE1	2:H:195:SER:OG	2.74	0.41
3:T:136:ARG:O	3:T:139:THR:HG22	2.21	0.41
2:H:236:GLU:HG2	10:H:699:HOH:O	2.20	0.41
2:H:127:THR:CG2	2:H:129(B):ARG:CZ	2.99	0.41
1:L:33:ASP:HB3	1:L:36:ARG:HD2	2.03	0.41
7:T:301:TMA:H31	10:T:548:HOH:O	2.20	0.40
7:H:504:TMA:H12	10:H:612:HOH:O	2.21	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	L	134/152 (88%)	129 (96%)	5 (4%)	0	100	100
2	H	253/249 (102%)	248 (98%)	5 (2%)	0	100	100
3	T	213/219 (97%)	208 (98%)	5 (2%)	0	100	100
All	All	600/620 (97%)	585 (98%)	15 (2%)	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	L	112/122 (92%)	109 (97%)	3 (3%)	44	13
2	H	208/210 (99%)	208 (100%)	0	100	100
3	T	195/200 (98%)	194 (100%)	1 (0%)	88	74
All	All	515/532 (97%)	511 (99%)	4 (1%)	86	62

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	84[A]	HIS
1	L	84[B]	HIS
1	L	110	ARG
3	T	93	LEU

Some 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 ⓘ

10 non-standard protein/DNA/RNA residues 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
1	CGU	L	7	1,5	3,11,12	1.23	0	1,14,16	0.29	0
1	CGU	L	16	1,5	3,11,12	0.85	0	1,14,16	0.25	0
1	CGU	L	35	1	3,11,12	0.88	0	1,14,16	0.80	0
1	CGU	L	29	1,5	3,11,12	1.99	1 (33%)	1,14,16	0.12	0
1	CGU	L	6	1,5	3,11,12	1.18	0	1,14,16	1.19	0
1	CGU	L	26	1,5	3,11,12	1.74	1 (33%)	1,14,16	1.81	0
1	CGU	L	14	1,5	3,11,12	1.42	0	1,14,16	1.00	0
1	CGU	L	19	1,5	3,11,12	1.03	0	1,14,16	0.52	0
1	CGU	L	25	1,5	3,11,12	1.93	1 (33%)	1,14,16	1.31	0
1	CGU	L	20	1,5	3,11,12	1.13	0	1,14,16	0.27	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
1	CGU	L	7	1,5	-	0/5/14/16	-
1	CGU	L	16	1,5	-	0/5/14/16	-
1	CGU	L	35	1	-	4/5/14/16	-
1	CGU	L	29	1,5	-	0/5/14/16	-
1	CGU	L	6	1,5	-	2/5/14/16	-
1	CGU	L	26	1,5	-	0/5/14/16	-
1	CGU	L	14	1,5	-	0/5/14/16	-
1	CGU	L	19	1,5	-	0/5/14/16	-
1	CGU	L	25	1,5	-	2/5/14/16	-
1	CGU	L	20	1,5	-	0/5/14/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	29	CGU	CB-CG	-2.47	1.48	1.53
1	L	25	CGU	CB-CG	2.46	1.58	1.53
1	L	26	CGU	CB-CG	-2.39	1.48	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	L	35	CGU	N-CA-CB-CG
1	L	35	CGU	C-CA-CB-CG
1	L	35	CGU	CA-CB-CG-CD1
1	L	35	CGU	CA-CB-CG-CD2
1	L	6	CGU	CA-CB-CG-CD1
1	L	6	CGU	CA-CB-CG-CD2
1	L	25	CGU	CA-CB-CG-CD2
1	L	25	CGU	CA-CB-CG-CD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L	25	CGU	1	0

5.5 Carbohydrates ⓘ

3 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	BGC	A	1	1,4	11,11,12	2.32	3 (27%)	15,15,17	1.84	3 (20%)
4	XYS	A	2	4	9,9,10	1.07	1 (11%)	10,12,14	1.70	2 (20%)
4	XYS	A	3	4	9,9,10	0.75	0	10,12,14	2.12	4 (40%)

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	BGC	A	1	1,4	-	0/2/19/22	0/1/1/1
4	XYS	A	2	4	-	-	0/1/1/1
4	XYS	A	3	4	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	BGC	O5-C1	6.01	1.53	1.43
4	A	2	XYS	O5-C1	-2.71	1.37	1.42
4	A	1	BGC	O5-C5	2.32	1.48	1.43
4	A	1	BGC	O4-C4	2.03	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	BGC	O5-C1-C2	-5.31	102.57	110.77
4	A	3	XYS	O4-C4-C3	3.60	117.34	110.14
4	A	2	XYS	C5-O5-C1	3.41	116.77	111.52
4	A	3	XYS	C5-O5-C1	3.37	116.71	111.52
4	A	1	BGC	C6-C5-C4	-2.57	106.99	113.00
4	A	2	XYS	C1-C2-C3	2.55	112.80	109.67
4	A	3	XYS	O3-C3-C4	2.42	114.62	109.99
4	A	1	BGC	C3-C4-C5	2.25	114.25	110.24
4	A	3	XYS	O3-C3-C2	-2.02	106.13	109.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 9 are monoatomic - leaving 25 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	$\# Z > 2$
7	TMA	H	505	-	4,4,4	1.21	0	6,6,6	0.20	0
6	FUC	L	212	1	10,10,11	1.03	1 (10%)	14,14,16	0.66	0
7	TMA	H	503	-	4,4,4	1.50	1 (25%)	6,6,6	0.36	0
7	TMA	T	301	-	4,4,4	1.17	0	6,6,6	0.53	0
7	TMA	L	213	-	4,4,4	1.11	0	6,6,6	0.34	0
7	TMA	T	302	-	4,4,4	1.45	1 (25%)	6,6,6	0.52	0
7	TMA	H	506	-	4,4,4	1.15	0	6,6,6	0.23	0
7	TMA	T	303	-	4,4,4	1.21	0	6,6,6	0.28	0
7	TMA	T	307	-	4,4,4	1.22	0	6,6,6	0.18	0
7	TMA	T	304	-	4,4,4	1.22	0	6,6,6	0.39	0
7	TMA	H	507	-	4,4,4	1.28	0	6,6,6	0.34	0
7	TMA	H	504	-	4,4,4	1.28	0	6,6,6	0.30	0
9	POL	H	509	-	3,3,3	0.42	0	2,2,2	0.46	0
7	TMA	H	512	-	4,4,4	1.13	0	6,6,6	0.24	0
7	TMA	H	508	-	4,4,4	1.30	0	6,6,6	0.14	0
7	TMA	T	305	-	4,4,4	1.25	0	6,6,6	0.26	0
7	TMA	T	312	-	4,4,4	1.15	0	6,6,6	0.36	0
7	TMA	T	311	-	4,4,4	0.92	0	6,6,6	0.38	0
7	TMA	T	309	-	4,4,4	1.18	0	6,6,6	0.25	0
7	TMA	T	306	-	4,4,4	1.25	0	6,6,6	0.65	0
7	TMA	H	511	-	4,4,4	1.21	0	6,6,6	0.17	0
7	TMA	T	310	-	4,4,4	0.89	0	6,6,6	0.42	0
8	0Z7	H	501	2	37,38,39	3.53	12 (32%)	45,49,50	1.90	8 (17%)
7	TMA	H	510	-	4,4,4	0.88	0	6,6,6	0.36	0
7	TMA	T	308	-	4,4,4	1.27	0	6,6,6	0.21	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
9	POL	H	509	-	-	0/1/1/1	-
8	0Z7	H	501	2	-	10/39/39/41	0/2/2/2
6	FUC	L	212	1	-	-	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	501	0Z7	C27-C26	-15.56	1.18	1.50
8	H	501	0Z7	C26-N1	-7.56	1.08	1.34
8	H	501	0Z7	C25-N4	5.16	1.43	1.33
8	H	501	0Z7	C5-N2	4.92	1.44	1.34
8	H	501	0Z7	C3-N3	4.77	1.44	1.34
8	H	501	0Z7	C13-N2	-4.45	1.36	1.45
8	H	501	0Z7	C14-C13	-3.54	1.45	1.54
8	H	501	0Z7	C6-C4	-3.39	1.45	1.54
8	H	501	0Z7	C4-N1	-3.21	1.39	1.45
7	H	503	TMA	C3-N1	-2.45	1.36	1.48
6	L	212	FUC	O5-C1	-2.36	1.39	1.43
7	T	302	TMA	C1-N1	-2.26	1.37	1.48
8	H	501	0Z7	C21-N3	-2.22	1.42	1.46
8	H	501	0Z7	C4-C5	-2.19	1.47	1.52
8	H	501	0Z7	C13-C3	-2.11	1.47	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	501	0Z7	C27-C26-N1	6.92	127.81	116.10
8	H	501	0Z7	O4-C26-C27	-5.93	111.05	122.06
8	H	501	0Z7	C22-C21-N3	-3.37	105.89	110.33
8	H	501	0Z7	C23-C24-N4	-2.86	104.03	112.21
8	H	501	0Z7	C15-C14-C13	2.70	120.83	113.39
8	H	501	0Z7	C4-N1-C26	2.50	128.90	121.48
8	H	501	0Z7	O1-C5-N2	-2.44	118.42	122.93
8	H	501	0Z7	O1-C5-C4	2.13	124.94	120.45

There are no chirality outliers.

All (10) torsion outliers are listed below:

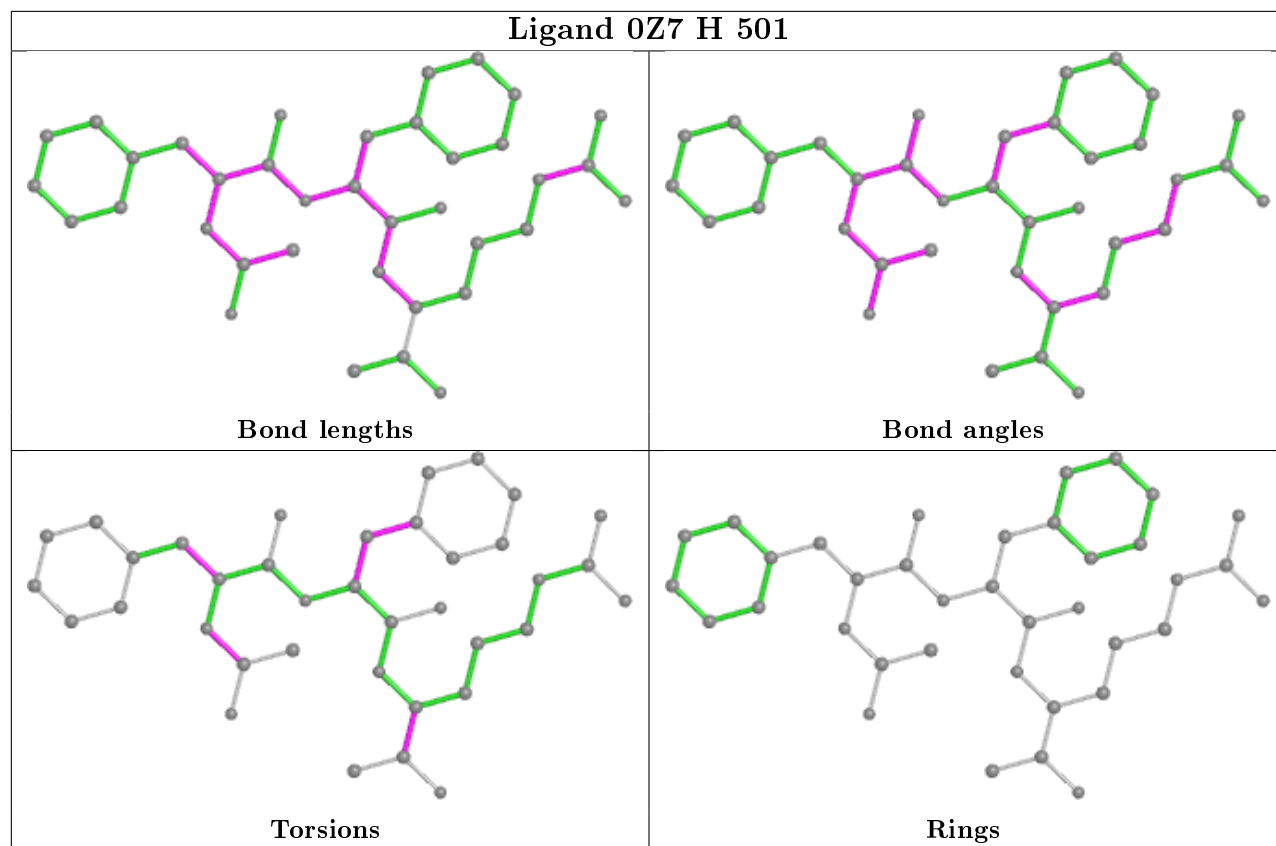
Mol	Chain	Res	Type	Atoms
8	H	501	0Z7	O3-C2-C21-C22
8	H	501	0Z7	O4-C26-N1-C4
8	H	501	0Z7	C27-C26-N1-C4
8	H	501	0Z7	N2-C13-C14-C15
8	H	501	0Z7	C3-C13-C14-C15
8	H	501	0Z7	C13-C14-C15-C16
8	H	501	0Z7	C1-C2-C21-C22
8	H	501	0Z7	C1-C2-C21-N3
8	H	501	0Z7	C13-C14-C15-C17
8	H	501	0Z7	N1-C4-C6-C7

There are no ring outliers.

11 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	503	TMA	2	0
7	T	301	TMA	2	0
7	T	302	TMA	1	0
7	H	506	TMA	1	0
7	T	304	TMA	1	0
7	H	504	TMA	1	0
7	T	312	TMA	1	0
7	T	309	TMA	3	0
7	H	511	TMA	2	0
7	T	310	TMA	1	0
7	H	510	TMA	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 ⓘ

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	L	133/152 (87%)	-0.07	4 (3%)	50	49	15, 28, 41, 56	0
2	H	249/249 (100%)	0.02	9 (3%)	42	42	10, 15, 38, 53	0
3	T	210/219 (95%)	-0.25	14 (6%)	17	16	12, 20, 44, 62	0
All	All	592/620 (95%)	-0.10	27 (4%)	32	32	10, 20, 41, 62	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	T	161	SER	5.4
3	T	1	SER	5.2
2	H	61	TRP	4.9
3	T	2	GLY	4.7
3	T	3	THR	4.6
2	H	36	ASN	3.8
2	H	62	ARG	3.6
3	T	163	SER	3.3
3	T	182	GLY	3.2
1	L	122	ALA	3.1
1	L	106	THR	3.0
2	H	248	PRO	3.0
3	T	160	SER	3.0
3	T	162	SER	2.7
2	H	60(C)	LYS	2.7
3	T	197	THR	2.6
3	T	184	ASN	2.6
1	L	4[A]	PHE	2.5
1	L	51	ALA	2.5
3	T	4	THR	2.5
2	H	16	ILE	2.5
3	T	181	LYS	2.4
3	T	88	SER	2.4

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Mol	Chain	Res	Type	RSRZ
3	T	164	GLY	2.4
2	H	84	ARG	2.1
2	H	138[A]	VAL	2.1
2	H	250	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CGU	L	35	12/13	0.89	0.18	31,58,63,68	0
1	CGU	L	25	12/13	0.92	0.09	22,30,36,36	0
1	CGU	L	14	12/13	0.94	0.14	26,39,43,46	0
1	CGU	L	19	12/13	0.95	0.12	32,41,46,49	0
1	CGU	L	20	12/13	0.96	0.10	26,30,35,36	0
1	CGU	L	29	12/13	0.97	0.06	21,24,29,30	0
1	CGU	L	6	12/13	0.97	0.06	20,24,28,29	0
1	CGU	L	7	12/13	0.98	0.06	18,19,23,23	0
1	CGU	L	26	12/13	0.98	0.05	20,23,26,28	0
1	CGU	L	16	12/13	0.98	0.06	18,21,24,25	0

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
4	XYS	A	3	9/10	0.82	0.23	41,43,51,52	0
4	XYS	A	2	9/10	0.91	0.16	40,43,51,52	0
4	BGC	A	1	11/12	0.96	0.09	38,45,55,57	0

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

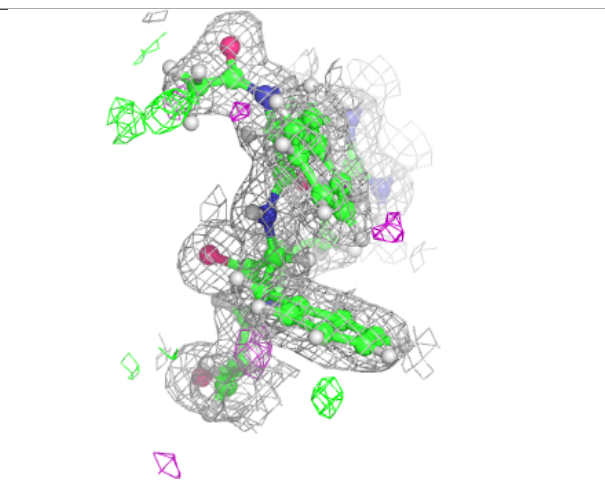
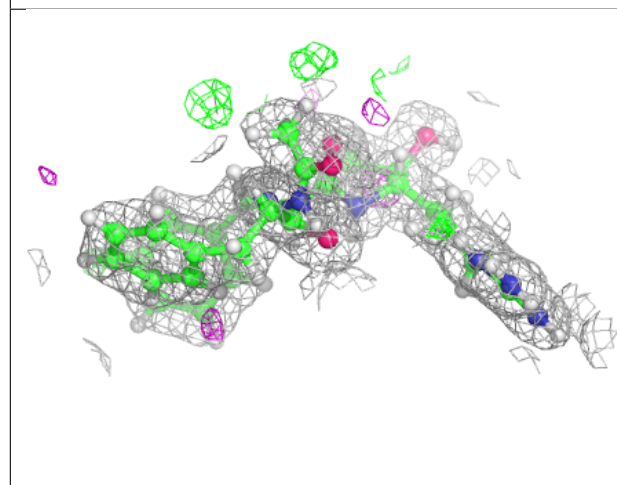
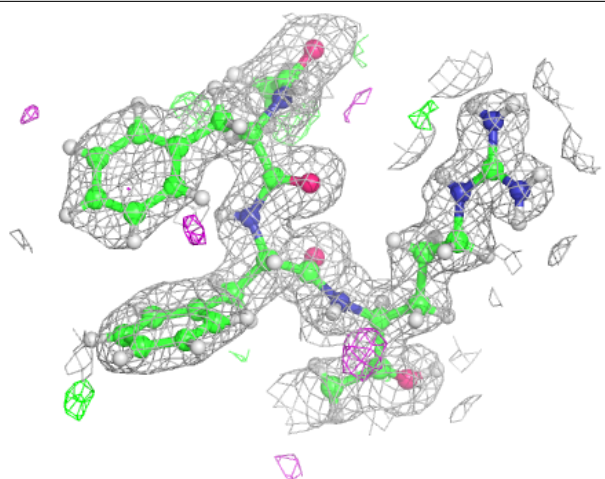
labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	POL	H	509	4/4	0.61	0.15	55,66,68,70	0
7	TMA	H	512	5/5	0.64	0.18	66,79,80,80	0
7	TMA	T	301	5/5	0.76	0.20	50,61,64,64	0
7	TMA	T	308	5/5	0.77	0.19	69,83,84,84	0
7	TMA	H	506	5/5	0.78	0.19	61,74,74,74	0
7	TMA	H	510	5/5	0.79	0.20	37,44,49,49	0
7	TMA	H	511	5/5	0.79	0.21	55,67,68,68	0
7	TMA	T	306	5/5	0.81	0.20	48,58,61,61	0
7	TMA	T	311	5/5	0.81	0.30	41,49,53,53	0
7	TMA	T	312	5/5	0.85	0.15	37,44,48,48	0
7	TMA	T	304	5/5	0.86	0.18	40,48,57,57	0
7	TMA	L	213	5/5	0.86	0.17	63,76,77,77	0
7	TMA	T	307	5/5	0.86	0.30	51,62,63,63	0
7	TMA	T	310	5/5	0.89	0.19	38,46,47,47	0
7	TMA	T	303	5/5	0.90	0.18	56,68,68,68	0
7	TMA	H	507	5/5	0.91	0.22	58,70,71,71	0
7	TMA	T	309	5/5	0.92	0.19	42,50,52,52	0
7	TMA	H	504	5/5	0.93	0.18	36,43,47,47	0
7	TMA	T	305	5/5	0.94	0.20	50,60,61,61	0
7	TMA	H	505	5/5	0.94	0.09	44,53,55,55	0
7	TMA	T	302	5/5	0.94	0.09	27,33,39,39	0
7	TMA	H	508	5/5	0.94	0.09	55,66,68,68	0
8	0Z7	H	501	37/38	0.96	0.08	15,20,29,32	0
6	FUC	L	212	10/11	0.98	0.04	33,38,43,46	0
7	TMA	H	503	5/5	0.98	0.08	14,23,27,27	0
5	CA	L	206	1/1	0.99	0.04	35,35,35,35	0
5	CA	L	208	1/1	0.99	0.05	27,27,27,27	0
5	CA	L	207	1/1	0.99	0.07	44,44,44,44	0
5	CA	L	205	1/1	1.00	0.06	25,25,25,25	0
5	CA	H	502	1/1	1.00	0.09	13,13,13,13	0
5	CA	L	201	1/1	1.00	0.04	28,28,28,28	0
5	CA	L	203	1/1	1.00	0.05	19,19,19,19	0
5	CA	L	202	1/1	1.00	0.07	22,22,22,22	0
5	CA	L	204	1/1	1.00	0.06	20,20,20,20	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 0Z7 H 501:

$2mF_o-DF_c$ (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.