Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2023 – 07:31 AM EDT

PDB ID	:	3PMH
Title	:	Mechanism of Sulfotyrosine-Mediated Glycoprotein Ib Interaction with Two Distinct alpha-Thrombin Sites
Authors	:	Varughese, K.I.; Celikel, R.
Deposited on	:	2010-11-16
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

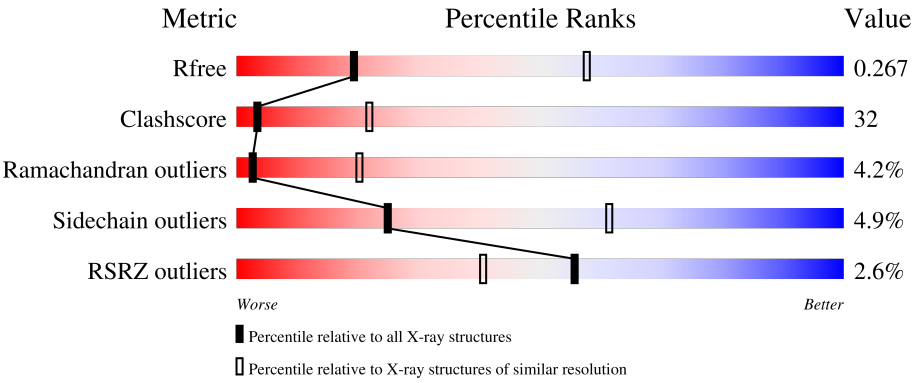
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	36	11% 47% 47% 6%
2	B	259	57% 40% .
3	G	290	4% 42% 46% 10% .
4	C	5	20% 60% 20%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4723 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 THROMBIN ALPHA-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	36	Total	C	N	O	S	0	0	0
			287	177	48	61	1			

- Molecule 2 is a protein called THROMBIN BETA-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	259	Total	C	N	O	S	0	0	0
			2093	1334	370	375	14			

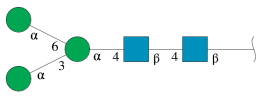
- Molecule 3 is a protein called Platelet glycoprotein Ib alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	284	Total	C	N	O	S	0	0	0
			2237	1427	363	436	11			

There is a discrepancy between the modelled and reference sequences:

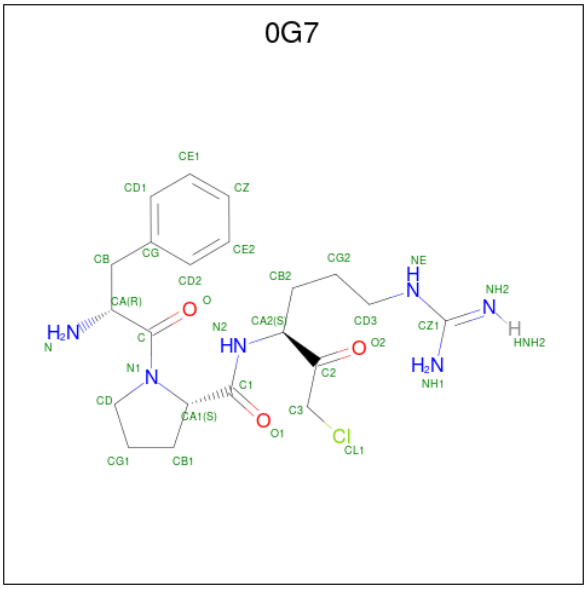
Chain	Residue	Modelled	Actual	Comment	Reference
G	65	ALA	CYS	engineered mutation	UNP P07359

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



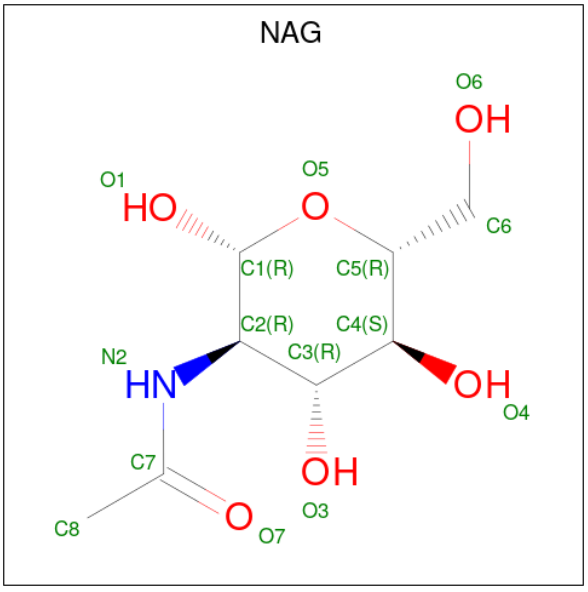
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is D-phenylalanyl-N-[(3S)-6-carbamimidamido-1-chloro-2-oxohexan-3-yl]-L-prolinamide (three-letter code: 0G7) (formula: $C_{21}H_{31}ClN_6O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
5	B	1	31	21	1	6	3	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



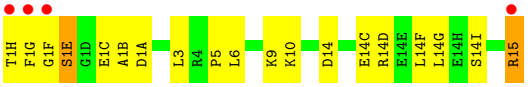
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	G	1	14	8	1	5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

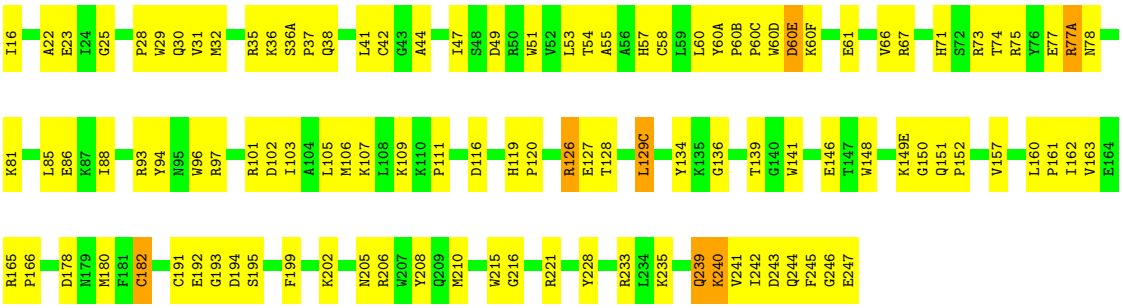
• Molecule 1: THROMBIN ALPHA-CHAIN

Chain A:



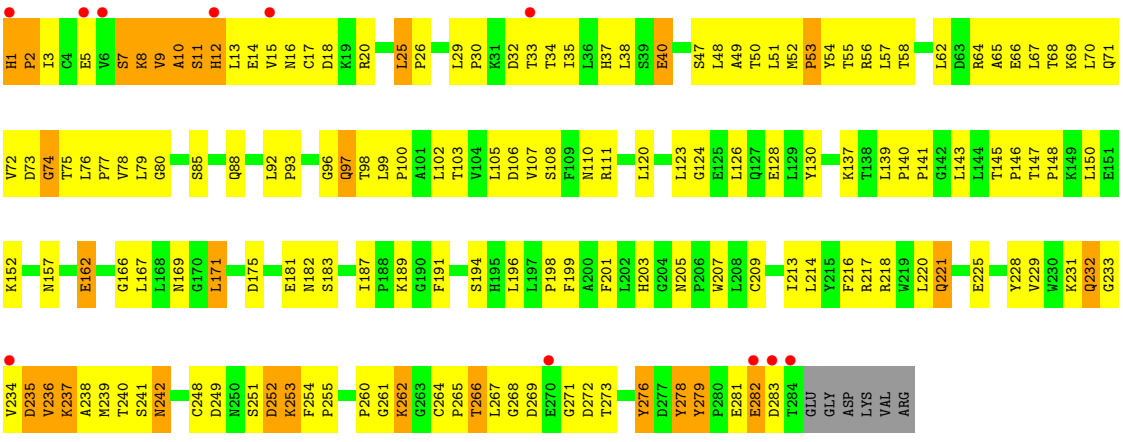
• Molecule 2: THROMBIN BETA-CHAIN

Chain B:



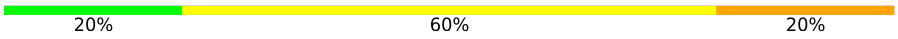
• Molecule 3: Platelet glycoprotein Ib alpha chain

Chain G:



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

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	67.66Å 67.66Å 329.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 47.34 – 3.19	Depositor EDS
% Data completeness (in resolution range)	94.2 (50.00-3.20) 88.9 (47.34-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	7.49 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.263 0.218 , 0.267	Depositor DCC
R_{free} test set	662 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	56.8	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 37.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4723	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0G7, TYS, NAG, MAN

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	0.42	0/290	0.69	0/384
2	B	0.44	0/2148	0.70	0/2903
3	G	0.37	0/2235	0.65	0/3050
All	All	0.41	0/4673	0.68	0/6337

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

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	287	0	278	32	0
2	B	2093	0	2063	110	0
3	G	2237	0	2225	179	0
4	C	61	0	52	1	0
5	B	31	0	28	20	0
6	G	14	0	13	3	0
All	All	4723	0	4659	303	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 32.

All (303) 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:126:ARG:H	2:B:126:ARG:CD	1.56	1.13
2:B:126:ARG:HD2	2:B:126:ARG:N	1.66	1.11
3:G:25:LEU:HD23	3:G:25:LEU:H	1.18	1.09
2:B:195:SER:HB3	5:B:301:0G7:O2	1.55	1.03
3:G:124:GLY:HA2	3:G:146:PRO:O	1.63	0.98
3:G:48:LEU:HD12	3:G:72:VAL:HA	1.43	0.97
3:G:25:LEU:HD21	3:G:50:THR:HG21	1.47	0.97
2:B:126:ARG:H	2:B:126:ARG:HD2	0.81	0.95
2:B:37:PRO:HG2	3:G:278:TYS:O2	1.69	0.93
2:B:193:GLY:N	5:B:301:0G7:CL1	2.39	0.92
2:B:73:ARG:HH22	3:G:282:GLU:HG2	1.32	0.91
2:B:202:LYS:HE2	2:B:205:ASN:ND2	1.84	0.91
5:B:301:0G7:N	5:B:301:0G7:HD1	1.88	0.89
5:B:301:0G7:HB	5:B:301:0G7:H29	1.53	0.89
2:B:42:CYS:SG	2:B:195:SER:OG	2.30	0.88
3:G:68:THR:HG22	3:G:88:GLN:HB2	1.56	0.88
3:G:49:ALA:HB2	3:G:73:ASP:HB2	1.53	0.87
2:B:195:SER:CB	5:B:301:0G7:O2	2.22	0.86
3:G:13:LEU:HB2	3:G:33:THR:HA	1.56	0.86
3:G:201:PHE:CE2	3:G:237:LYS:HG2	2.10	0.86
3:G:58:THR:HG22	3:G:78:VAL:HG12	1.56	0.85
1:A:15:ARG:HG2	1:A:15:ARG:HH11	1.42	0.84
3:G:17:CYS:HA	3:G:20:ARG:HE	1.45	0.81
1:A:1(C):GLU:HG2	1:A:1(B):ALA:N	1.94	0.81
3:G:14:GLU:HG3	3:G:35:ILE:HB	1.63	0.78
2:B:73:ARG:NH2	3:G:282:GLU:HG2	1.97	0.78
3:G:267:LEU:HD23	3:G:267:LEU:H	1.47	0.77
3:G:75:THR:HG22	3:G:77:PRO:HD3	1.67	0.76
2:B:85:LEU:HD11	2:B:106:MET:HE1	1.68	0.76
3:G:201:PHE:HE2	3:G:237:LYS:HG2	1.51	0.75
2:B:149(E):LYS:HG3	3:G:283:ASP:HB3	1.68	0.75
3:G:137:LYS:HE2	6:G:601:NAG:H81	1.66	0.75
3:G:17:CYS:HB2	3:G:38:LEU:HD23	1.69	0.75
5:B:301:0G7:H29	5:B:301:0G7:CB	2.17	0.74
3:G:248:CYS:HB2	3:G:254:PHE:HB3	1.70	0.74
3:G:25:LEU:H	3:G:25:LEU:CD2	1.99	0.74
3:G:52:MET:HB3	3:G:53:PRO:HD3	1.68	0.74
2:B:195:SER:HB3	5:B:301:0G7:C2	2.18	0.73
3:G:8:LYS:HD3	3:G:8:LYS:N	2.04	0.72
3:G:145:THR:HB	3:G:146:PRO:HD3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:ARG:HH12	3:G:282:GLU:HB3	1.56	0.71
3:G:25:LEU:HD21	3:G:50:THR:CG2	2.20	0.70
3:G:150:LEU:HB3	3:G:171:LEU:HD12	1.73	0.70
3:G:242:ASN:C	3:G:242:ASN:HD22	1.94	0.69
3:G:74:GLY:O	3:G:98:THR:HG23	1.93	0.69
1:A:1(C):GLU:HG2	1:A:1(B):ALA:H	1.55	0.69
3:G:40:GLU:HA	3:G:64:ARG:O	1.93	0.69
3:G:79:LEU:HD23	3:G:99:LEU:HD13	1.74	0.68
2:B:146:GLU:OE2	2:B:221:ARG:HD2	1.94	0.67
2:B:148:TRP:HA	3:G:279:TYS:O2	1.92	0.67
2:B:193:GLY:H	5:B:301:0G7:C3	2.06	0.67
5:B:301:0G7:N	5:B:301:0G7:CD1	2.57	0.67
3:G:276:TYS:HD2	3:G:278:TYS:O1	1.94	0.66
1:A:1(G):PHE:CE2	1:A:1(E):SER:HB2	2.30	0.66
3:G:75:THR:HG22	3:G:77:PRO:CD	2.26	0.66
2:B:57:HIS:NE2	5:B:301:0G7:O2	2.24	0.66
3:G:49:ALA:HB2	3:G:73:ASP:CB	2.25	0.64
3:G:25:LEU:HD23	3:G:25:LEU:N	2.02	0.64
1:A:1(C):GLU:C	1:A:1(A):ASP:H	1.99	0.64
3:G:34:THR:HA	3:G:56:ARG:O	1.98	0.64
3:G:214:LEU:O	3:G:217:ARG:HB3	1.98	0.63
3:G:218:ARG:NH2	3:G:273:THR:HB	2.13	0.63
5:B:301:0G7:H29	5:B:301:0G7:CD2	2.29	0.63
3:G:218:ARG:HH21	3:G:273:THR:HB	1.62	0.63
3:G:124:GLY:CA	3:G:146:PRO:O	2.45	0.62
1:A:6:LEU:HD21	2:B:116:ASP:HB3	1.80	0.62
3:G:67:LEU:HD23	3:G:68:THR:N	2.15	0.62
3:G:232:GLN:N	3:G:232:GLN:HE21	1.97	0.62
3:G:97:GLN:H	3:G:97:GLN:NE2	1.98	0.62
5:B:301:0G7:HB	5:B:301:0G7:CD	2.27	0.62
2:B:136:GLY:HA3	2:B:199:PHE:CZ	2.36	0.61
2:B:202:LYS:CE	2:B:205:ASN:ND2	2.61	0.61
3:G:137:LYS:HE2	6:G:601:NAG:C8	2.31	0.61
1:A:1(H):THR:HA	2:B:243:ASP:HA	1.82	0.60
3:G:228:TYR:CD2	3:G:241:SER:HA	2.35	0.60
3:G:120:LEU:HD12	3:G:143:LEU:O	2.00	0.60
1:A:1(G):PHE:HE2	1:A:1(E):SER:HB2	1.66	0.60
3:G:17:CYS:HA	3:G:20:ARG:NE	2.16	0.60
1:A:1(H):THR:HA	2:B:243:ASP:CA	2.32	0.59
2:B:235:LYS:O	2:B:239:GLN:HG2	2.02	0.59
2:B:77(A):ARG:HG3	2:B:78:ASN:OD1	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:ARG:HB2	2:B:166:PRO:HD3	1.83	0.59
2:B:246:GLY:O	2:B:247:GLU:HB3	2.03	0.59
3:G:128:GLU:HG2	3:G:152:LYS:HB2	1.84	0.59
2:B:96:TRP:CZ3	2:B:97:ARG:HG3	2.37	0.59
3:G:25:LEU:HD11	3:G:50:THR:HG22	1.84	0.58
3:G:75:THR:O	3:G:76:LEU:HD23	2.03	0.58
3:G:209:CYS:HA	3:G:213:ILE:HG21	1.85	0.58
3:G:80:GLY:O	3:G:102:LEU:HD12	2.04	0.58
3:G:13:LEU:HD12	3:G:32:ASP:C	2.24	0.57
3:G:9:VAL:O	3:G:10:ALA:HB3	2.05	0.57
2:B:150:GLY:N	3:G:281:GLU:HG3	2.20	0.57
3:G:228:TYR:CE2	3:G:241:SER:HA	2.39	0.57
1:A:1(F):GLY:O	1:A:1(E):SER:HB3	2.05	0.57
3:G:29:LEU:HB2	3:G:54:TYR:HE2	1.69	0.57
3:G:267:LEU:H	3:G:267:LEU:CD2	2.16	0.57
3:G:15:VAL:HG11	3:G:29:LEU:HD13	1.86	0.57
2:B:150:GLY:H	3:G:281:GLU:HG3	1.69	0.57
2:B:35:ARG:HB2	2:B:41:LEU:HD21	1.85	0.57
1:A:6:LEU:HD12	2:B:25:GLY:HA3	1.86	0.56
2:B:163:VAL:HB	2:B:182:CYS:SG	2.45	0.56
1:A:15:ARG:HG2	1:A:15:ARG:NH1	2.13	0.56
2:B:93:ARG:HB3	2:B:101:ARG:NH1	2.21	0.56
2:B:31:VAL:CG1	2:B:66:VAL:HG13	2.35	0.56
3:G:1:HIS:N	3:G:2:PRO:CD	2.69	0.55
1:A:5:PRO:HA	1:A:9:LYS:HD2	1.89	0.55
2:B:191:CYS:O	2:B:194:ASP:HB2	2.05	0.55
3:G:67:LEU:HD11	3:G:70:LEU:HD13	1.88	0.55
2:B:178:ASP:O	2:B:233:ARG:HD3	2.07	0.55
1:A:1(H):THR:HA	2:B:243:ASP:O	2.07	0.55
3:G:7:SER:C	3:G:8:LYS:HD3	2.26	0.55
3:G:12:HIS:C	3:G:12:HIS:CD2	2.80	0.55
2:B:105:LEU:HD12	2:B:241:VAL:HG21	1.88	0.55
3:G:157:ASN:HD21	3:G:181:GLU:HG3	1.71	0.55
1:A:14(C):GLU:O	1:A:14(G):LEU:HD23	2.07	0.55
2:B:57:HIS:O	2:B:60(F):LYS:HE3	2.07	0.55
3:G:97:GLN:H	3:G:97:GLN:CD	2.10	0.55
3:G:218:ARG:HD2	3:G:271:GLY:H	1.72	0.54
2:B:126:ARG:CD	2:B:126:ARG:N	2.40	0.54
2:B:85:LEU:HD11	2:B:106:MET:CE	2.37	0.53
1:A:1(C):GLU:CG	1:A:1(B):ALA:N	2.69	0.53
2:B:202:LYS:NZ	2:B:205:ASN:HD21	2.05	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:LYS:HE2	2:B:205:ASN:HD22	1.72	0.53
3:G:217:ARG:HH12	3:G:221:GLN:HE22	1.57	0.53
3:G:126:LEU:HD23	3:G:147:THR:HG21	1.91	0.53
3:G:9:VAL:HG12	3:G:12:HIS:NE2	2.24	0.53
3:G:68:THR:HG22	3:G:88:GLN:CB	2.35	0.53
2:B:127:GLU:HA	2:B:127:GLU:OE1	2.09	0.52
3:G:236:VAL:O	3:G:238:ALA:N	2.32	0.52
2:B:150:GLY:HA3	3:G:281:GLU:HG3	1.90	0.52
1:A:14(C):GLU:OE2	2:B:202:LYS:NZ	2.36	0.52
2:B:22:ALA:HB2	2:B:157:VAL:CG2	2.40	0.52
3:G:67:LEU:HD23	3:G:69:LYS:N	2.25	0.52
3:G:47:SER:HB3	3:G:50:THR:OG1	2.10	0.51
2:B:60(A):TYR:CE2	2:B:60(C):PRO:HB2	2.45	0.51
3:G:146:PRO:C	3:G:148:PRO:HD3	2.31	0.51
2:B:86:GLU:HB2	2:B:109:LYS:HA	1.92	0.51
3:G:253:LYS:C	3:G:255:PRO:HD3	2.30	0.51
5:B:301:0G7:H29	5:B:301:0G7:CG	2.40	0.51
3:G:34:THR:O	3:G:57:LEU:HD12	2.10	0.51
3:G:225:GLU:O	3:G:225:GLU:HG2	2.10	0.51
3:G:18:ASP:O	3:G:20:ARG:HG3	2.11	0.51
2:B:60:LEU:HG	2:B:60(B):PRO:HD3	1.93	0.50
2:B:73:ARG:NH1	3:G:282:GLU:HB3	2.24	0.50
3:G:53:PRO:HB2	3:G:54:TYR:CD1	2.46	0.50
2:B:51:TRP:CZ2	2:B:107:LYS:HD3	2.46	0.50
2:B:73:ARG:HG3	2:B:141:TRP:HB3	1.93	0.50
3:G:33:THR:HG22	3:G:54:TYR:HD2	1.75	0.50
1:A:1(C):GLU:CG	1:A:1(B):ALA:H	2.23	0.50
3:G:167:LEU:HB3	3:G:191:PHE:HE1	1.76	0.50
3:G:9:VAL:O	3:G:9:VAL:HG13	2.11	0.50
1:A:15:ARG:NH1	1:A:15:ARG:CG	2.75	0.50
1:A:1(C):GLU:C	1:A:1(A):ASP:N	2.66	0.49
3:G:106:ASP:HA	3:G:130:TYR:HB2	1.94	0.49
3:G:12:HIS:HD2	3:G:12:HIS:O	1.94	0.49
3:G:76:LEU:HD12	3:G:79:LEU:HD22	1.94	0.49
2:B:60(D):TRP:O	2:B:60(E):ASP:C	2.51	0.49
3:G:175:ASP:HA	3:G:198:PRO:HD2	1.95	0.49
1:A:1(H):THR:CA	2:B:243:ASP:HA	2.42	0.49
1:A:5:PRO:O	1:A:10:LYS:HG3	2.11	0.49
3:G:187:ILE:HG13	3:G:216:PHE:CD1	2.48	0.49
3:G:231:LYS:O	3:G:232:GLN:HB3	2.12	0.49
3:G:232:GLN:HG2	3:G:233:GLY:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:162:GLU:O	3:G:162:GLU:HG3	2.12	0.49
2:B:22:ALA:HB2	2:B:157:VAL:HG23	1.95	0.49
2:B:67:ARG:HH12	3:G:196:LEU:CD2	2.26	0.48
2:B:75:ARG:O	2:B:77:GLU:HG3	2.14	0.48
2:B:73:ARG:NH1	2:B:152:PRO:O	2.40	0.48
3:G:218:ARG:NH1	3:G:272:ASP:OD1	2.46	0.48
1:A:1(H):THR:N	2:B:245:PHE:O	2.47	0.48
2:B:58:CYS:SG	2:B:195:SER:OG	2.63	0.48
3:G:157:ASN:ND2	3:G:181:GLU:HB2	2.28	0.48
3:G:171:LEU:HD22	3:G:171:LEU:N	2.29	0.48
3:G:12:HIS:CD2	3:G:12:HIS:O	2.66	0.48
3:G:65:ALA:C	3:G:66:GLU:HG2	2.34	0.47
2:B:22:ALA:O	2:B:71:HIS:HE1	1.96	0.47
2:B:30:GLN:NE2	2:B:139:THR:OG1	2.40	0.47
3:G:187:ILE:HB	3:G:216:PHE:HB2	1.96	0.47
2:B:150:GLY:CA	3:G:281:GLU:HG3	2.45	0.47
3:G:198:PRO:HB2	3:G:199:PHE:CD1	2.50	0.47
2:B:202:LYS:HZ3	2:B:205:ASN:HD21	1.63	0.47
2:B:67:ARG:NH1	3:G:196:LEU:CD2	2.77	0.47
3:G:248:CYS:O	3:G:251:SER:HB3	2.13	0.47
2:B:134:TYR:O	2:B:162:ILE:HG13	2.15	0.47
2:B:239:GLN:HE21	2:B:239:GLN:HA	1.79	0.47
3:G:137:LYS:NZ	6:G:601:NAG:O7	2.37	0.47
2:B:36:LYS:NZ	3:G:194:SER:HB2	2.30	0.47
3:G:78:VAL:HG12	3:G:78:VAL:O	2.14	0.47
3:G:254:PHE:N	3:G:255:PRO:HD3	2.30	0.47
3:G:5:GLU:HA	3:G:5:GLU:OE1	2.15	0.47
3:G:171:LEU:HD22	3:G:171:LEU:H	1.79	0.47
3:G:38:LEU:HB2	3:G:62:LEU:HD23	1.97	0.47
3:G:64:ARG:HG3	3:G:64:ARG:HH11	1.80	0.47
5:B:301:0G7:H29	5:B:301:0G7:HD2	1.97	0.46
3:G:203:HIS:CD2	3:G:229:VAL:HA	2.50	0.46
3:G:102:LEU:HD21	3:G:105:LEU:HD13	1.96	0.46
2:B:16:ILE:N	2:B:194:ASP:OD2	2.48	0.46
1:A:1(F):GLY:O	2:B:49:ASP:OD1	2.34	0.46
1:A:3:LEU:HD21	2:B:206:ARG:HG2	1.97	0.45
1:A:1(C):GLU:O	1:A:1(B):ALA:HB3	2.15	0.45
3:G:267:LEU:HD23	3:G:267:LEU:N	2.25	0.45
3:G:58:THR:HA	3:G:79:LEU:HA	1.98	0.45
3:G:249:ASP:C	3:G:251:SER:H	2.20	0.45
1:A:14:ASP:HB2	2:B:23:GLU:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:261:GLY:O	3:G:264:CYS:SG	2.75	0.45
2:B:57:HIS:ND1	2:B:102:ASP:OD2	2.50	0.45
2:B:105:LEU:HD12	2:B:241:VAL:CG2	2.47	0.44
3:G:92:LEU:HA	3:G:93:PRO:HD3	1.86	0.44
3:G:107:VAL:HG12	3:G:107:VAL:O	2.17	0.44
1:A:1(B):ALA:C	2:B:206:ARG:HH12	2.21	0.44
2:B:28:PRO:HG2	2:B:29:TRP:CE3	2.52	0.44
3:G:139:LEU:HA	3:G:140:PRO:HD3	1.79	0.44
3:G:16:ASN:HD22	3:G:37:HIS:HB2	1.83	0.44
3:G:282:GLU:H	3:G:282:GLU:CD	2.21	0.44
2:B:35:ARG:O	2:B:38:GLN:HA	2.18	0.44
3:G:20:ARG:HG2	3:G:20:ARG:HH11	1.83	0.44
2:B:61:GLU:HG3	2:B:88:ILE:HG13	1.99	0.44
2:B:208:TYR:HB2	2:B:210:MET:HE1	2.00	0.44
5:B:301:0G7:CB	5:B:301:0G7:CD	2.86	0.44
3:G:11:SER:O	3:G:56:ARG:NH2	2.50	0.44
3:G:53:PRO:O	3:G:54:TYR:C	2.56	0.44
3:G:106:ASP:OD2	3:G:108:SER:HB2	2.17	0.44
3:G:205:ASN:HB2	3:G:207:TRP:NE1	2.33	0.44
3:G:3:ILE:HG22	3:G:20:ARG:HD3	2.00	0.43
3:G:252:ASP:O	3:G:254:PHE:N	2.50	0.43
2:B:37:PRO:CG	3:G:278:TYS:O2	2.54	0.43
2:B:85:LEU:CD1	2:B:106:MET:CE	2.95	0.43
2:B:216:GLY:O	5:B:301:0G7:N	2.51	0.43
3:G:79:LEU:HD23	3:G:99:LEU:HD22	1.99	0.43
3:G:166:GLY:CA	3:G:169:ASN:ND2	2.82	0.43
3:G:9:VAL:O	3:G:10:ALA:CB	2.66	0.43
3:G:47:SER:HB3	3:G:50:THR:HG1	1.83	0.43
3:G:218:ARG:HD2	3:G:271:GLY:N	2.34	0.43
2:B:160:LEU:HA	2:B:161:PRO:HD3	1.94	0.43
3:G:1:HIS:H3	3:G:2:PRO:HD3	1.84	0.43
3:G:157:ASN:ND2	3:G:181:GLU:CB	2.81	0.43
2:B:53:LEU:HD11	2:B:103:ILE:HD11	2.00	0.43
1:A:14(F):LEU:O	1:A:14(I):SER:HB2	2.19	0.43
2:B:215:TRP:HB2	5:B:301:0G7:O	2.19	0.43
3:G:265:PRO:O	3:G:266:THR:O	2.37	0.43
2:B:85:LEU:HD13	2:B:106:MET:HE2	2.01	0.43
2:B:228:TYR:CD1	2:B:228:TYR:N	2.86	0.43
3:G:242:ASN:O	3:G:242:ASN:ND2	2.50	0.43
2:B:246:GLY:O	2:B:247:GLU:CB	2.67	0.43
3:G:76:LEU:N	3:G:77:PRO:HD3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:79:LEU:HD23	3:G:99:LEU:CD1	2.46	0.43
3:G:196:LEU:O	3:G:198:PRO:HD3	2.19	0.42
2:B:31:VAL:HG13	2:B:66:VAL:HG13	2.00	0.42
3:G:218:ARG:HD2	3:G:271:GLY:HA2	2.01	0.42
1:A:1(E):SER:HB3	2:B:49:ASP:OD1	2.20	0.42
2:B:215:TRP:HA	5:B:301:0G7:HG2	2.01	0.42
3:G:85:SER:HA	3:G:108:SER:O	2.19	0.42
1:A:1(F):GLY:O	1:A:1(E):SER:CB	2.66	0.42
3:G:49:ALA:CB	3:G:73:ASP:HB2	2.37	0.42
2:B:32:MET:HB3	2:B:67:ARG:HB2	2.02	0.42
3:G:25:LEU:HD11	3:G:50:THR:CG2	2.49	0.42
3:G:140:PRO:HA	3:G:141:PRO:HD3	1.96	0.42
2:B:31:VAL:HB	2:B:44:ALA:HB3	2.02	0.42
3:G:106:ASP:OD2	3:G:108:SER:CB	2.67	0.42
3:G:98:THR:C	3:G:100:PRO:HD3	2.40	0.42
3:G:182:ASN:HB3	3:G:183:SER:H	1.68	0.42
2:B:36(A):SER:HA	2:B:37:PRO:C	2.39	0.42
2:B:109:LYS:HE3	2:B:109:LYS:HB2	1.89	0.42
2:B:139:THR:HG22	2:B:157:VAL:HG13	2.02	0.42
3:G:15:VAL:HG23	3:G:33:THR:OG1	2.19	0.42
3:G:33:THR:CG2	3:G:54:TYR:HD2	2.33	0.42
3:G:8:LYS:O	3:G:9:VAL:HB	2.19	0.41
3:G:14:GLU:HG3	3:G:35:ILE:CB	2.43	0.41
2:B:81:LYS:HA	2:B:81:LYS:HD3	1.88	0.41
3:G:8:LYS:HB2	3:G:9:VAL:H	1.66	0.41
3:G:25:LEU:CD2	3:G:25:LEU:N	2.74	0.41
2:B:195:SER:OG	5:B:301:0G7:O2	2.38	0.41
3:G:48:LEU:HD12	3:G:72:VAL:HG13	2.02	0.41
2:B:193:GLY:N	5:B:301:0G7:C3	2.77	0.41
3:G:29:LEU:O	3:G:30:PRO:C	2.58	0.41
3:G:128:GLU:HB3	3:G:130:TYR:CE1	2.55	0.41
2:B:241:VAL:HG23	2:B:242:ILE:N	2.35	0.41
3:G:29:LEU:HB2	3:G:54:TYR:CE2	2.50	0.41
3:G:51:LEU:O	3:G:52:MET:C	2.59	0.41
3:G:201:PHE:CZ	3:G:237:LYS:HG2	2.52	0.41
1:A:1(C):GLU:O	1:A:1(A):ASP:N	2.54	0.41
2:B:49:ASP:O	2:B:111:PRO:HA	2.19	0.41
3:G:110:ASN:HB3	3:G:111:ARG:H	1.76	0.41
2:B:47:ILE:HG12	2:B:51:TRP:O	2.21	0.41
3:G:47:SER:HA	3:G:71:GLN:HB2	2.03	0.41
3:G:102:LEU:HD23	3:G:123:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:233:GLY:C	3:G:235:ASP:H	2.23	0.41
2:B:240:LYS:O	2:B:244:GLN:HB2	2.21	0.41
3:G:97:GLN:NE2	3:G:97:GLN:N	2.68	0.41
3:G:216:PHE:O	3:G:220:LEU:HG	2.21	0.41
3:G:225:GLU:O	3:G:225:GLU:CG	2.68	0.41
3:G:260:PRO:C	3:G:262:LYS:H	2.25	0.41
4:C:2:NAG:O3	4:C:3:MAN:C1	2.69	0.41
2:B:54:THR:OG1	2:B:55:ALA:N	2.54	0.40
2:B:94:TYR:CZ	2:B:96:TRP:HB3	2.56	0.40
3:G:201:PHE:CD1	3:G:201:PHE:N	2.89	0.40
3:G:218:ARG:HD2	3:G:271:GLY:CA	2.52	0.40
2:B:119:HIS:HA	2:B:120:PRO:HD3	1.81	0.40
2:B:128:THR:HG23	2:B:129(C):LEU:HD22	2.04	0.40
3:G:102:LEU:HD23	3:G:123:LEU:CD1	2.52	0.40
3:G:103:THR:C	3:G:126:LEU:HD12	2.41	0.40
3:G:12:HIS:C	3:G:12:HIS:HD2	2.24	0.40
3:G:88:GLN:OE1	3:G:111:ARG:HD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	34/36 (94%)	28 (82%)	5 (15%)	1 (3%)	4 28
2	B	257/259 (99%)	240 (93%)	15 (6%)	2 (1%)	19 58
3	G	279/290 (96%)	209 (75%)	49 (18%)	21 (8%)	1 7
All	All	570/585 (97%)	477 (84%)	69 (12%)	24 (4%)	3 20

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	77(A)	ARG
3	G	2	PRO
3	G	9	VAL
3	G	189	LYS
3	G	234	VAL
3	G	240	THR
3	G	252	ASP
3	G	253	LYS
3	G	266	THR
3	G	10	ALA
3	G	55	THR
3	G	74	GLY
3	G	237	LYS
1	A	1(E)	SER
2	B	60(E)	ASP
3	G	53	PRO
3	G	171	LEU
3	G	262	LYS
3	G	40	GLU
3	G	269	ASP
3	G	236	VAL
3	G	26	PRO
3	G	96	GLY
3	G	268	GLY

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	31/31 (100%)	29 (94%)	2 (6%)	17 51
2	B	225/225 (100%)	216 (96%)	9 (4%)	31 66
3	G	251/256 (98%)	237 (94%)	14 (6%)	21 57
All	All	507/512 (99%)	482 (95%)	25 (5%)	25 61

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14(D)	ARG
1	A	15	ARG
2	B	74	THR
2	B	126	ARG
2	B	129(C)	LEU
2	B	151	GLN
2	B	180	MET
2	B	182	CYS
2	B	192	GLU
2	B	239	GLN
2	B	240	LYS
3	G	1	HIS
3	G	7	SER
3	G	8	LYS
3	G	11	SER
3	G	12	HIS
3	G	25	LEU
3	G	97	GLN
3	G	162	GLU
3	G	221	GLN
3	G	232	GLN
3	G	235	ASP
3	G	239	MET
3	G	242	ASN
3	G	282	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	30	GLN
2	B	38	GLN
2	B	71	HIS
2	B	151	GLN
2	B	205	ASN
2	B	209	GLN
2	B	239	GLN
3	G	12	HIS
3	G	16	ASN
3	G	37	HIS
3	G	61	ASN
3	G	71	GLN
3	G	86	HIS
3	G	97	GLN

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Mol	Chain	Res	Type
3	G	127	GLN
3	G	169	ASN
3	G	195	HIS
3	G	223	ASN
3	G	226	ASN
3	G	232	GLN
3	G	242	ASN
3	G	247	GLN
3	G	250	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

3 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	$\#\|Z\| > 2$
3	TYS	G	276	3	15,16,17	1.31	2 (13%)	18,22,24	1.12	1 (5%)
3	TYS	G	278	-	15,16,17	0.97	1 (6%)	18,22,24	1.00	1 (5%)
3	TYS	G	279	3	15,16,17	1.10	2 (13%)	18,22,24	1.08	1 (5%)

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	TYS	G	276	3	-	3/10/11/13	0/1/1/1
3	TYS	G	278	-	-	3/10/11/13	0/1/1/1
3	TYS	G	279	3	-	4/10/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	276	TYS	OH-S	-3.68	1.52	1.58
3	G	279	TYS	OH-S	-2.79	1.54	1.58
3	G	276	TYS	OH-CZ	-2.74	1.38	1.42
3	G	278	TYS	OH-S	-2.46	1.54	1.58
3	G	279	TYS	OH-CZ	-2.46	1.38	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	276	TYS	OH-CZ-CE1	2.84	124.22	118.64
3	G	279	TYS	OH-CZ-CE1	2.72	123.98	118.64
3	G	278	TYS	OH-CZ-CE1	2.29	123.14	118.64

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	276	TYS	CE2-CZ-OH-S
3	G	278	TYS	O-C-CA-CB
3	G	278	TYS	CE1-CZ-OH-S
3	G	279	TYS	C-CA-CB-CG
3	G	279	TYS	CE2-CZ-OH-S
3	G	279	TYS	N-CA-CB-CG
3	G	276	TYS	CE1-CZ-OH-S
3	G	278	TYS	CE2-CZ-OH-S
3	G	279	TYS	CE1-CZ-OH-S
3	G	276	TYS	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	276	TYS	1	0
3	G	278	TYS	3	0
3	G	279	TYS	1	0

5.5 Carbohydrates (i)

5 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	C	1	2,4	14,14,15	1.74	2 (14%)	17,19,21	2.14	6 (35%)
4	NAG	C	2	4	14,14,15	0.67	0	17,19,21	1.07	1 (5%)
4	MAN	C	3	4	11,11,12	0.92	0	15,15,17	0.78	0
4	MAN	C	4	4	11,11,12	0.66	0	15,15,17	0.53	0
4	MAN	C	5	4	11,11,12	0.79	0	15,15,17	0.71	1 (6%)

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	C	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	0/1/1/1
4	MAN	C	3	4	-	0/2/19/22	0/1/1/1
4	MAN	C	4	4	-	1/2/19/22	0/1/1/1
4	MAN	C	5	4	-	1/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1	NAG	C1-C2	5.07	1.59	1.52
4	C	1	NAG	C8-C7	2.59	1.55	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1	NAG	C1-O5-C5	4.45	118.22	112.19
4	C	1	NAG	C8-C7-N2	4.24	123.27	116.10
4	C	1	NAG	O5-C5-C6	-3.16	102.25	107.20
4	C	1	NAG	C1-C2-N2	2.96	115.55	110.49
4	C	1	NAG	C2-N2-C7	-2.75	118.99	122.90
4	C	5	MAN	C1-O5-C5	2.45	115.51	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1	NAG	O7-C7-C8	-2.40	117.60	122.06
4	C	2	NAG	C4-C3-C2	-2.13	107.90	111.02

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2	NAG	C4-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
4	C	1	NAG	C4-C5-C6-O6
4	C	4	MAN	C4-C5-C6-O6
4	C	5	MAN	C4-C5-C6-O6

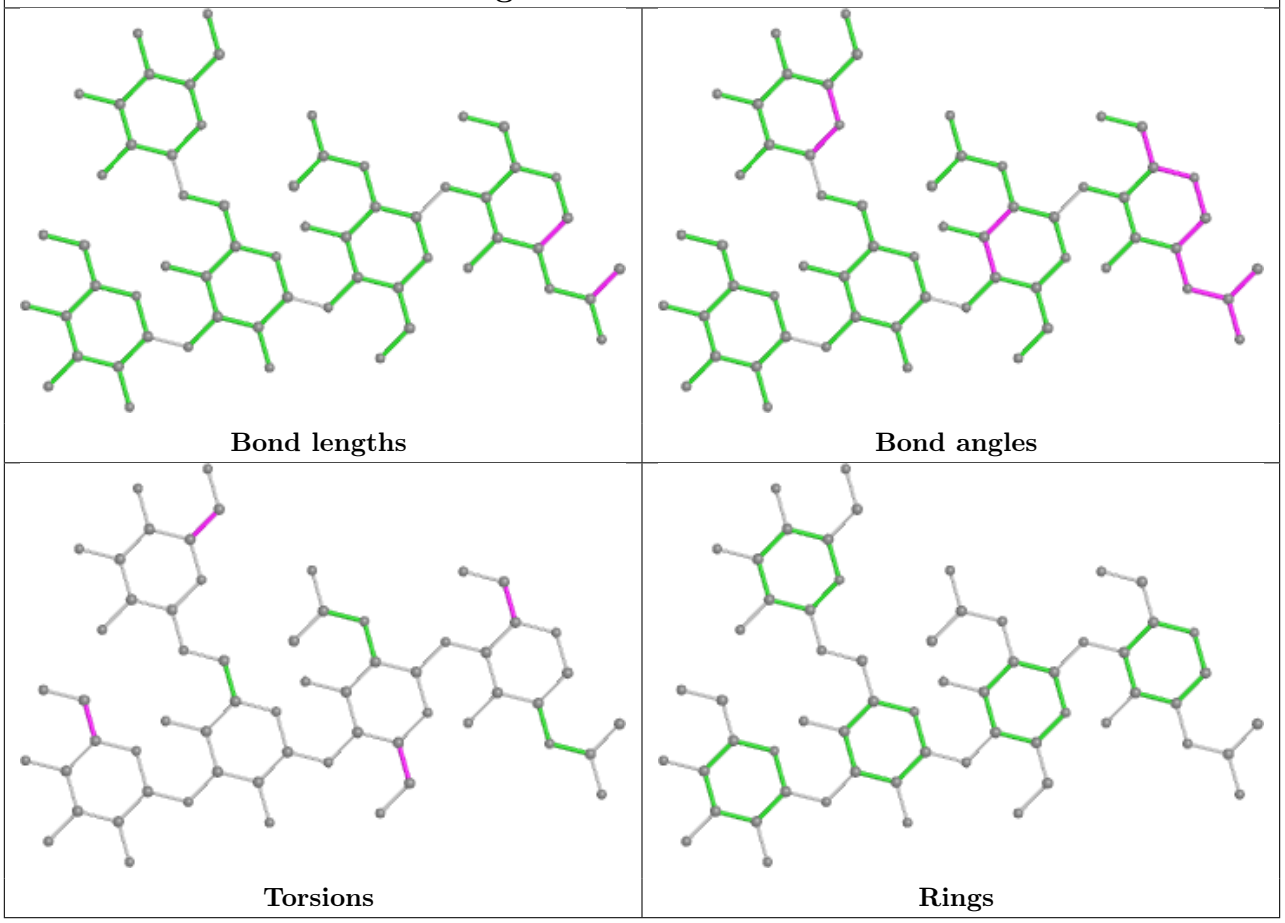
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3	MAN	1	0
4	C	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.

Oligosaccharide Chain C



5.6 Ligand geometry (i)

2 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	0G7	B	301	-	32,32,32	2.82	3 (9%)	38,42,42	2.18	4 (10%)
6	NAG	G	601	3	14,14,15	1.35	3 (21%)	17,19,21	1.12	1 (5%)

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	0G7	B	301	-	-	7/32/43/43	0/2/2/2
6	NAG	G	601	3	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	301	0G7	C3-C2	-15.35	1.25	1.51
6	G	601	NAG	C1-C2	3.13	1.57	1.52
5	B	301	0G7	O2-C2	2.87	1.26	1.21
6	G	601	NAG	C3-C2	2.30	1.57	1.52
6	G	601	NAG	C4-C3	2.14	1.57	1.52
5	B	301	0G7	C3-CL1	2.13	1.83	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	301	0G7	C2-C3-CL1	11.81	127.04	113.08
5	B	301	0G7	O2-C2-C3	-3.57	118.59	123.49
5	B	301	0G7	CB-CA-C	2.65	115.61	109.27
5	B	301	0G7	CB-CA-N	-2.24	102.76	111.46
6	G	601	NAG	O5-C1-C2	-2.04	108.06	111.29

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	301	0G7	O-C-CA-CB
5	B	301	0G7	N1-C-CA-CB
5	B	301	0G7	CA2-C2-C3-CL1
5	B	301	0G7	O2-C2-C3-CL1
5	B	301	0G7	CA-CB-CG-CD1
5	B	301	0G7	NE-CD3-CG2-CB2
5	B	301	0G7	CA-CB-CG-CD2

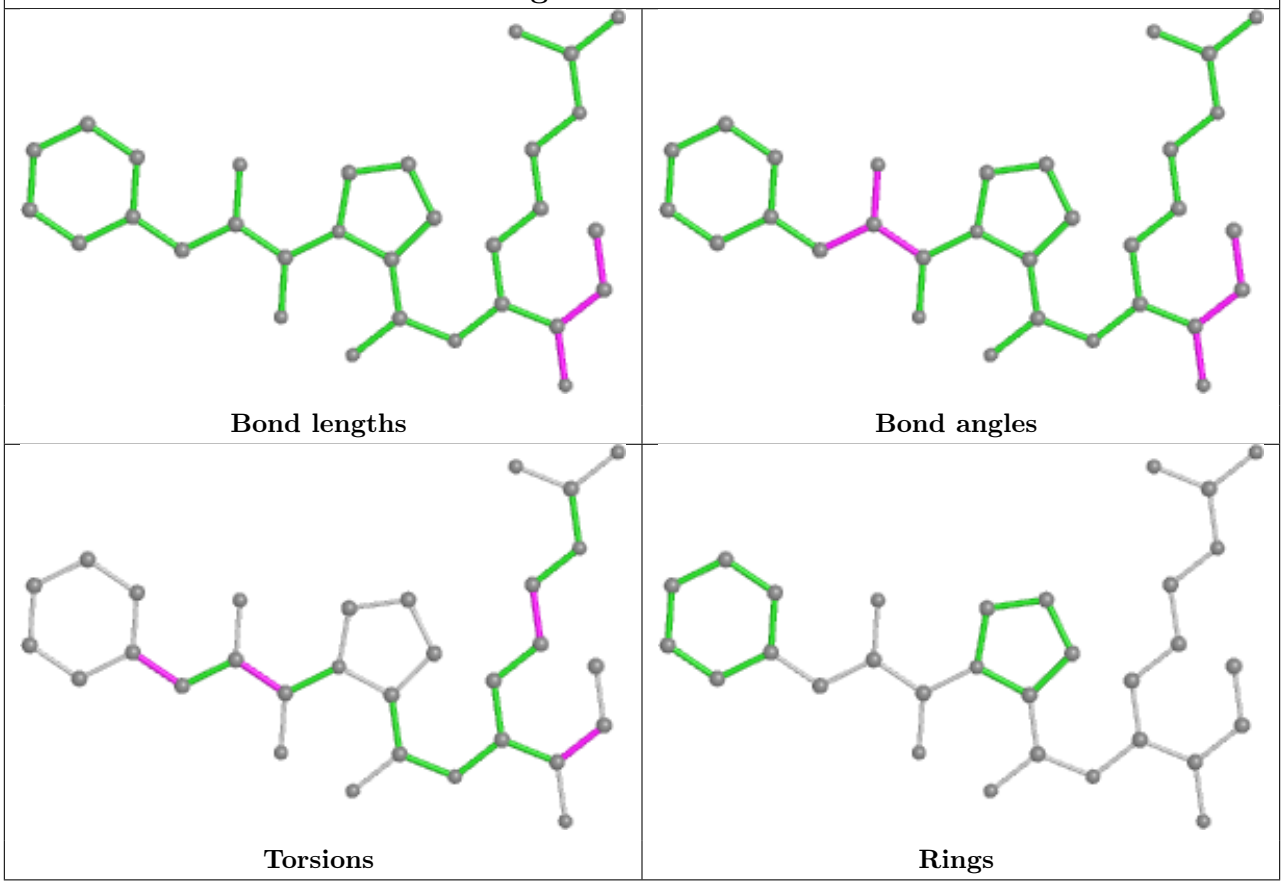
There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	301	0G7	20	0
6	G	601	NAG	3	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 then 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.

Ligand 0G7 B 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	36/36 (100%)	0.11	4 (11%) 5 3	40, 63, 136, 153	0
2	B	259/259 (100%)	-0.44	0 100 100	26, 49, 76, 101	0
3	G	281/290 (96%)	0.14	11 (3%) 39 25	38, 81, 127, 139	0
All	All	576/585 (98%)	-0.12	15 (2%) 56 40	26, 62, 122, 153	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1(H)	THR	8.5
3	G	15	VAL	3.4
3	G	234	VAL	3.4
3	G	270	GLU	3.0
3	G	33	THR	2.9
1	A	1(G)	PHE	2.9
3	G	6	VAL	2.7
3	G	283	ASP	2.5
3	G	282	GLU	2.5
3	G	284	THR	2.4
1	A	1(F)	GLY	2.3
3	G	12	HIS	2.2
3	G	1	HIS	2.2
3	G	5	GLU	2.1
1	A	15	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

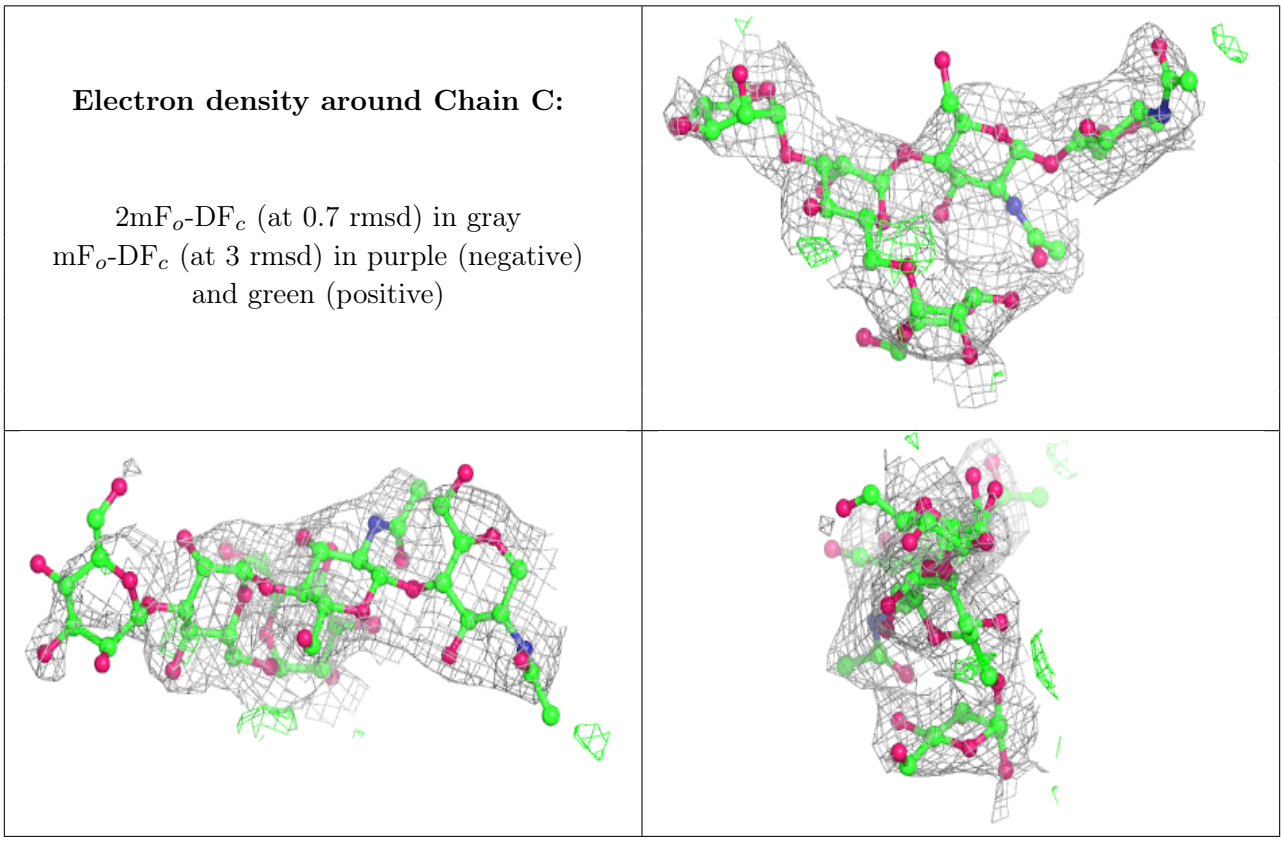
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TYS	G	276	16/17	0.84	0.33	97,103,120,122	4
3	TYS	G	278	16/17	0.87	0.24	84,94,100,101	4
3	TYS	G	279	16/17	0.94	0.21	67,75,87,89	0

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	C	4	11/12	0.55	0.37	128,134,137,139	0
4	MAN	C	5	11/12	0.72	0.28	78,90,98,99	0
4	MAN	C	3	11/12	0.81	0.20	104,112,116,118	0
4	NAG	C	2	14/15	0.85	0.20	99,104,108,112	0
4	NAG	C	1	14/15	0.92	0.19	93,101,107,118	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)

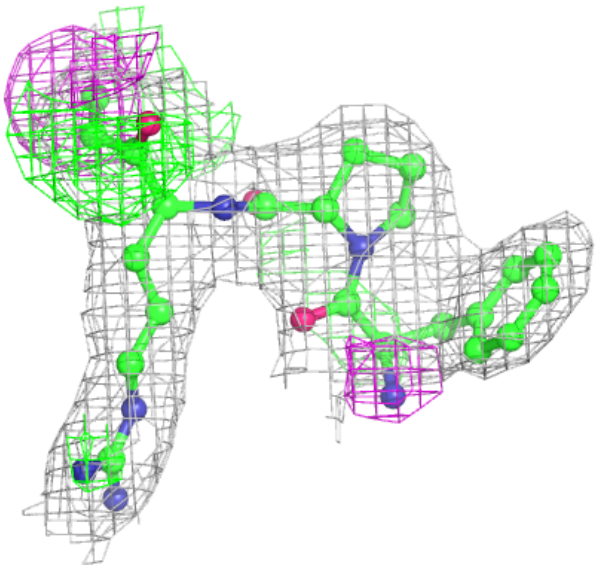
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

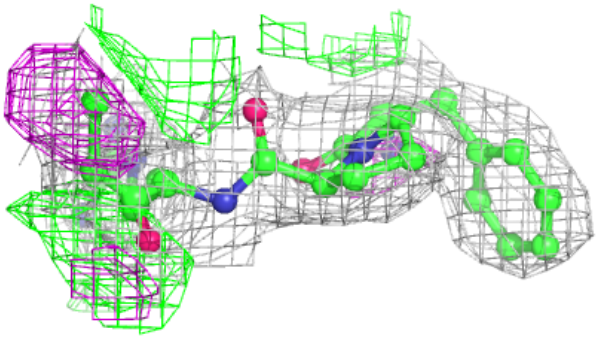
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	G	601	14/15	0.82	0.17	86,102,107,112	0
5	0G7	B	301	31/31	0.86	0.25	20,36,44,56	0

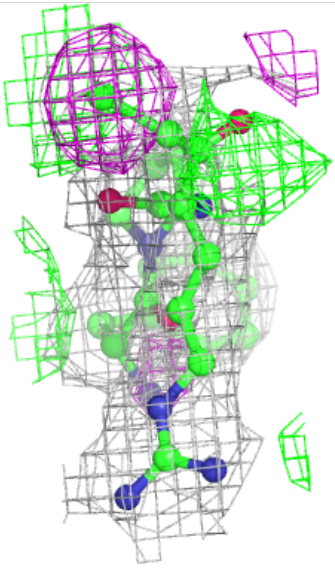
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 0G7 B 301:

$2mF_o$-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.