Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 01:56 PM JST

PDB ID	:	5ZHP
Title	:	M3 muscarinic acetylcholine receptor in complex with a selective antagonist
Authors	:	Liu, H.; Hofmann, J.; Fish, I.; Schaake, B.; Eitel, K.; Bartuschat, A.; Kaindl, J.; Rampp, H.; Banerjee, A.; Hubner, H.; Clark, M.J.; Vincent, S.G.; Fisher, J.; Heinrich, M.; Hirata, K.; Liu, X.; Sunahara, R.K.; Shoichet, B.K.; Kobilka, B.K.; Gmeiner, P.
Deposited on	:	2018-03-13
Resolution	:	3.10 Å(reported)

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

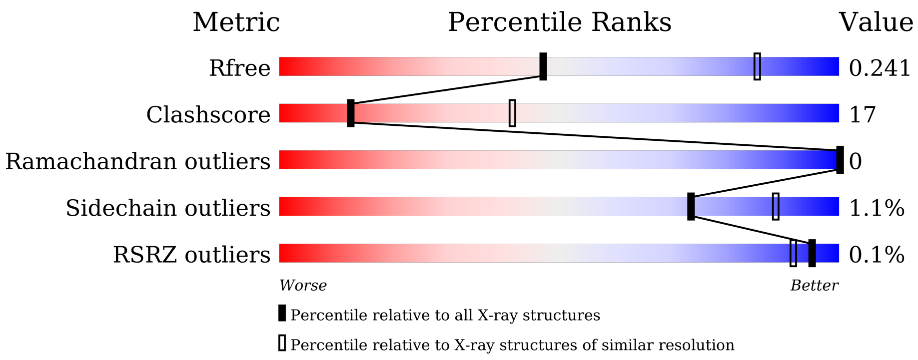
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

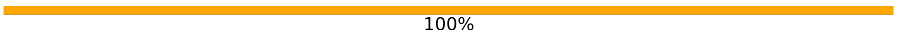
The reported resolution of this entry is 3.10 Å.

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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	418	
1	B	418	
2	C	2	

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 6324 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 Muscarinic acetylcholine receptor M3,Endolysin,Endolysin,Muscarinic acetylcholine receptor M3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total 3091	C 2028	N 505	O 537	S 21	0	0	0
1	B	394	Total 3111	C 2040	N 512	O 538	S 21	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	GLY	-	expression tag	UNP P08483
A	154	ARG	SER	engineered mutation	UNP P08483
A	1013	GLY	-	linker	UNP D9IEF7
A	1014	GLY	-	linker	UNP D9IEF7
A	1015	SER	-	linker	UNP D9IEF7
A	1016	GLY	-	linker	UNP D9IEF7
A	1017	GLY	-	linker	UNP D9IEF7
A	1054	ALA	CYS	engineered mutation	UNP D9IEF7
A	570	HIS	-	expression tag	UNP P08483
A	571	HIS	-	expression tag	UNP P08483
A	572	HIS	-	expression tag	UNP P08483
A	573	HIS	-	expression tag	UNP P08483
A	574	HIS	-	expression tag	UNP P08483
A	575	HIS	-	expression tag	UNP P08483
A	576	HIS	-	expression tag	UNP P08483
A	577	HIS	-	expression tag	UNP P08483
B	56	GLY	-	expression tag	UNP P08483
B	154	ARG	SER	engineered mutation	UNP P08483
B	1013	GLY	-	linker	UNP D9IEF7
B	1014	GLY	-	linker	UNP D9IEF7
B	1015	SER	-	linker	UNP D9IEF7
B	1016	GLY	-	linker	UNP D9IEF7
B	1017	GLY	-	linker	UNP D9IEF7
B	1054	ALA	CYS	engineered mutation	UNP D9IEF7

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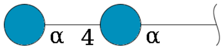
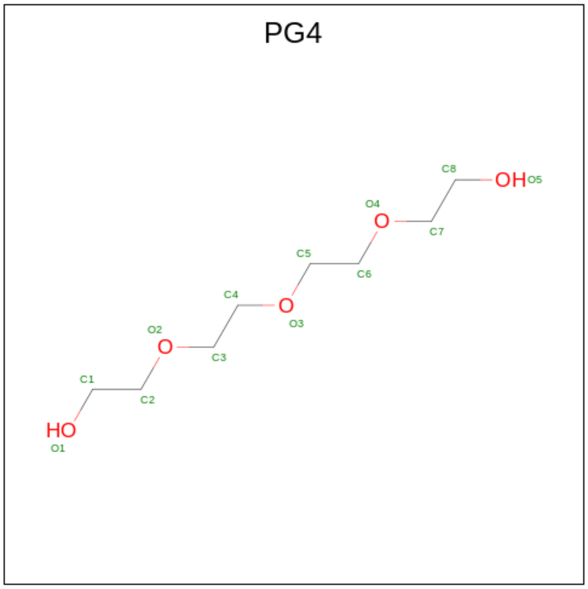
Chain	Residue	Modelled	Actual	Comment	Reference
B	570	HIS	-	expression tag	UNP P08483
B	571	HIS	-	expression tag	UNP P08483
B	572	HIS	-	expression tag	UNP P08483
B	573	HIS	-	expression tag	UNP P08483
B	574	HIS	-	expression tag	UNP P08483
B	575	HIS	-	expression tag	UNP P08483
B	576	HIS	-	expression tag	UNP P08483
B	577	HIS	-	expression tag	UNP P08483

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	C	2	Total C O 23 12 11	0	0	0

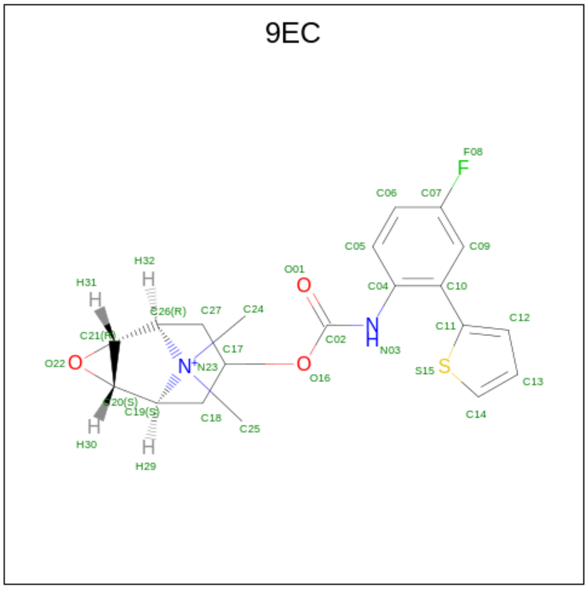
- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 8 5	0	0

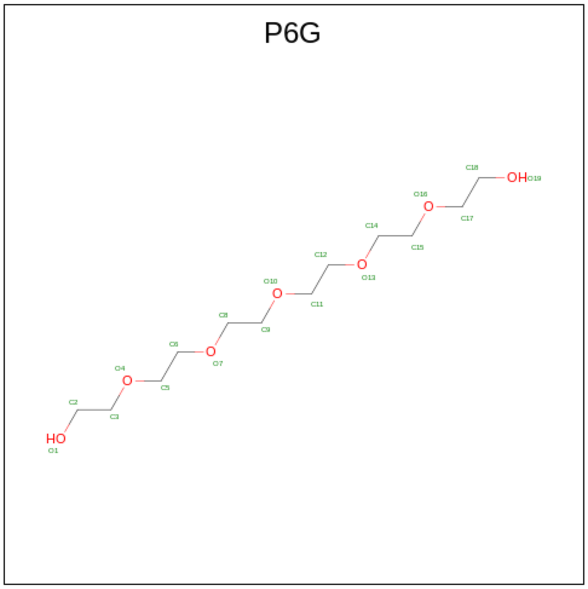
- Molecule 4 is (1R,2R,4S,5S,7s)-7-({[4-fluoro-2-(thiophen-2-yl)phenyl]carbamoyl}oxy)-9,9

-dimethyl-3-oxa-9-azatricyclo[3.3.1.0 2,4]nonan-9-ium (three-letter code: 9EC) (formula: $C_{20}H_{22}FN_2O_3S$).



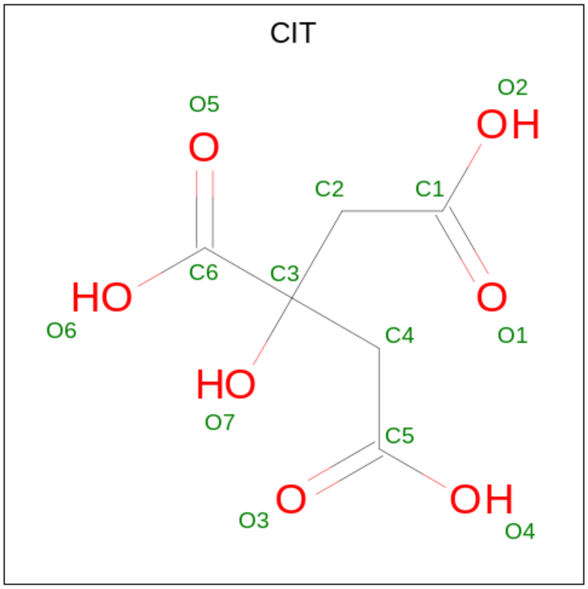
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C F N O S 27 20 1 2 3 1	0	0
4	B	1	Total C F N O S 27 20 1 2 3 1	0	0

- Molecule 5 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	19	12	7	0	0

- Molecule 6 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).

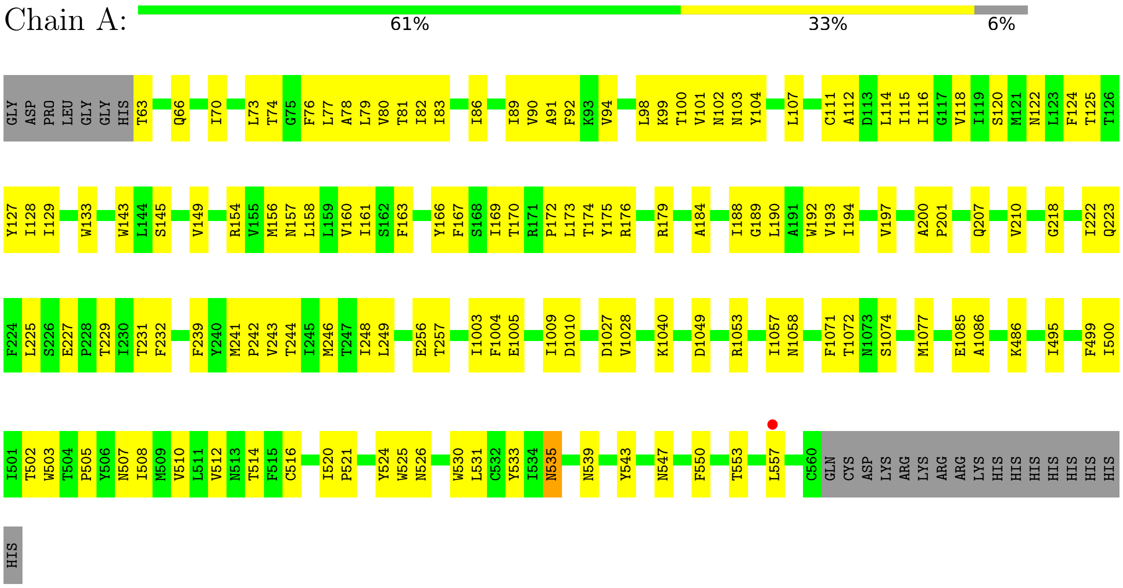


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	B	1	13	6	7	0	0

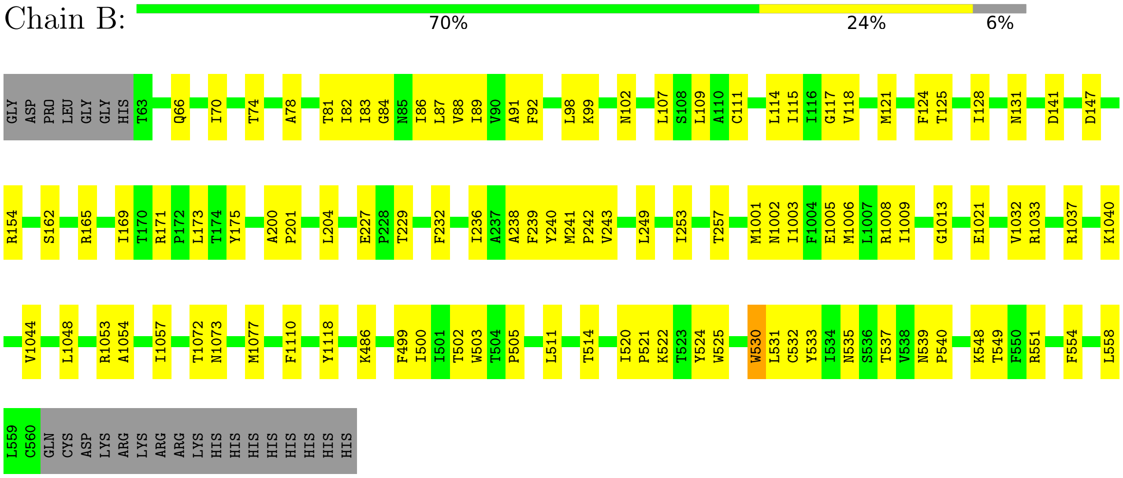
3 Residue-property plots

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.

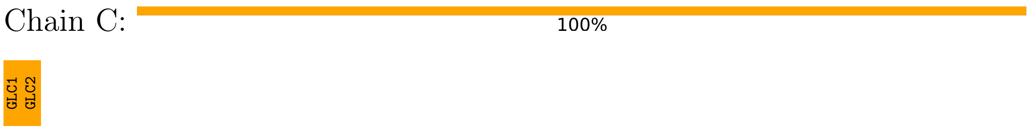
- Molecule 1: Muscarinic acetylcholine receptor M3,Endolysin,Endolysin,Muscarinic acetylcholine receptor M3



- Molecule 1: Muscarinic acetylcholine receptor M3,Endolysin,Endolysin,Muscarinic acetylcholine receptor M3



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	122.11Å 53.05Å 124.72Å 90.00° 98.70° 90.00°	Depositor
Resolution (Å)	19.98 – 3.10 48.73 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.98-3.10) 98.3 (48.73-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.229 , 0.267 0.236 , 0.241	Depositor DCC
R_{free} test set	2185 reflections (7.59%)	wwPDB-VP
Wilson B-factor (Å^2)	85.3	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 36.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.068 for l,-k,h	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6324	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: P6G, CIT, PG4, GLC, 9EC

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	0.24	0/3168	0.37	0/4330
1	B	0.24	0/3188	0.36	0/4351
All	All	0.24	0/6356	0.37	0/8681

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	3091	0	3059	125	0
1	B	3111	0	3102	74	0
2	C	23	0	21	6	0
3	A	13	0	18	1	0
4	A	27	0	0	1	0
4	B	27	0	0	1	0
5	B	19	0	26	3	0
6	B	13	0	5	1	0
All	All	6324	0	6231	208	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 17.

All (208) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASN:O	1:A:125:THR:HG22	1.68	0.92
1:A:78:ALA:O	1:A:81:THR:HG22	1.76	0.86
1:B:1032:VAL:HG22	1:B:1057:ILE:HD13	1.62	0.81
1:A:172:PRO:HA	1:A:176:ARG:HB2	1.62	0.81
1:B:499:PHE:HA	1:B:535:ASN:ND2	1.98	0.78
1:A:184:ALA:O	1:A:188:ILE:HD12	1.84	0.77
1:A:200:ALA:HB3	1:A:201:PRO:HD3	1.68	0.75
2:C:2:GLC:O6	2:C:2:GLC:O4	2.01	0.74
1:B:499:PHE:HA	1:B:535:ASN:HD21	1.53	0.74
1:A:172:PRO:HA	1:A:176:ARG:CB	2.17	0.74
1:A:154:ARG:NH1	1:A:539:ASN:OD1	2.22	0.73
1:B:1003:ILE:HD13	1:B:1054:ALA:HB1	1.72	0.71
1:A:1027:ASP:CG	2:C:1:GLC:H1	2.11	0.70
1:A:553:THR:O	1:A:557:LEU:HD13	1.90	0.70
1:B:200:ALA:HB3	1:B:201:PRO:HD3	1.76	0.68
1:A:1004:PHE:CE2	1:A:1028:VAL:HG11	2.29	0.67
1:A:98:LEU:O	1:A:103:ASN:ND2	2.28	0.66
1:A:122:ASN:C	1:A:125:THR:HG22	2.16	0.66
1:A:173:LEU:HD12	1:A:174:THR:HG23	1.76	0.66
1:B:1033:ARG:HH12	1:B:1037:ARG:HH21	1.43	0.66
1:A:243:VAL:HG22	1:A:499:PHE:HE2	1.61	0.65
1:A:122:ASN:O	1:A:125:THR:CG2	2.43	0.64
1:A:227:GLU:OE2	1:A:229:THR:N	2.31	0.63
1:A:73:LEU:HD12	1:A:74:THR:N	2.13	0.63
1:A:127:TYR:CD2	1:A:133:TRP:HB2	2.34	0.62
1:A:78:ALA:O	1:A:82:ILE:HG13	1.99	0.62
1:A:70:ILE:O	1:A:74:THR:HG23	2.00	0.62
1:B:102:ASN:OD1	1:B:165:ARG:NH1	2.33	0.62
1:A:169:ILE:CG2	1:A:256:GLU:HG2	2.31	0.61
1:A:520:ILE:HB	1:A:525:TRP:NE1	2.15	0.61
1:B:502:THR:OG1	1:B:535:ASN:HB2	2.01	0.60
1:A:104:TYR:CE1	1:A:188:ILE:HD13	2.37	0.60
1:A:81:THR:HG23	1:A:82:ILE:N	2.17	0.60
1:B:74:THR:HG21	1:B:125:THR:CG2	2.31	0.60
1:A:508:ILE:O	1:A:512:VAL:HG23	2.01	0.60
1:A:257:THR:CG2	1:A:486:LYS:HG2	2.32	0.59
1:B:232:PHE:HB2	1:B:514:THR:OG1	2.01	0.59
1:B:227:GLU:OE1	1:B:229:THR:N	2.36	0.59
1:A:499:PHE:HA	1:A:535:ASN:OD1	2.02	0.58
1:A:166:TYR:O	1:A:170:THR:HG22	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ASP:OD2	1:B:533:TYR:OH	2.22	0.58
1:A:73:LEU:O	1:A:77:LEU:HG	2.03	0.58
1:A:520:ILE:HB	1:A:525:TRP:HE1	1.67	0.58
1:A:173:LEU:HD12	1:A:174:THR:N	2.19	0.57
1:B:81:THR:HG21	1:B:117:GLY:HA3	1.84	0.57
1:B:505:PRO:HG2	1:B:531:LEU:HD23	1.86	0.57
1:A:197:VAL:O	1:A:201:PRO:HD2	2.04	0.57
1:A:241:MET:HB3	1:A:242:PRO:HD3	1.87	0.56
1:A:124:PHE:HZ	1:A:526:ASN:HD22	1.52	0.56
1:B:1005:GLU:O	1:B:1009:ILE:HG13	2.05	0.56
1:B:232:PHE:O	1:B:236:ILE:HG13	2.06	0.55
1:A:83:ILE:O	1:A:86:ILE:HG22	2.06	0.55
1:A:175:TYR:O	1:A:179:ARG:HG3	2.07	0.55
1:B:111:CYS:O	1:B:115:ILE:HG13	2.06	0.55
1:A:505:PRO:HG2	1:A:531:LEU:CD2	2.37	0.55
4:A:1203:9EC:S15	4:A:1203:9EC:N03	2.80	0.55
1:A:78:ALA:O	1:A:81:THR:CG2	2.51	0.54
1:B:92:PHE:CE1	1:B:99:LYS:HA	2.42	0.54
1:B:109:LEU:CD2	1:B:154:ARG:HG3	2.38	0.54
1:B:74:THR:HG21	1:B:125:THR:HG23	1.88	0.54
1:B:554:PHE:O	1:B:558:LEU:HG	2.07	0.54
1:A:133:TRP:O	1:A:218:GLY:HA2	2.08	0.53
1:A:173:LEU:CD1	1:A:174:THR:HG23	2.38	0.53
1:A:112:ALA:HB2	1:A:192:TRP:CH2	2.44	0.53
1:A:127:TYR:HD2	1:A:133:TRP:HB2	1.74	0.53
1:B:83:ILE:O	1:B:87:LEU:HG	2.09	0.53
1:A:189:GLY:O	1:A:193:VAL:HG23	2.09	0.52
1:A:1077:MET:HB2	1:A:1086:ALA:HB2	1.91	0.52
1:B:89:ILE:HG13	1:B:107:LEU:HD11	1.92	0.52
1:A:257:THR:HG21	1:A:486:LYS:HG2	1.92	0.52
1:B:82:ILE:O	1:B:86:ILE:HG12	2.09	0.52
1:B:173:LEU:HD13	1:B:1021:GLU:HG3	1.92	0.52
1:A:547:ASN:HB3	1:A:550:PHE:HD2	1.74	0.51
1:A:92:PHE:O	1:A:99:LYS:HE2	2.09	0.51
1:A:120:SER:HB3	1:A:533:TYR:CZ	2.46	0.51
1:B:124:PHE:CE2	1:B:128:ILE:HD11	2.44	0.51
1:B:539:ASN:HB3	1:B:540:PRO:HD3	1.91	0.51
1:A:169:ILE:HG21	1:A:256:GLU:HG2	1.91	0.51
1:A:1077:MET:SD	1:A:1085:GLU:HG3	2.51	0.51
1:A:502:THR:OG1	1:A:535:ASN:HB2	2.11	0.51
1:A:222:ILE:HD12	1:A:225:LEU:HD12	1.93	0.51

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:89:ILE:HD12	1:A:90:VAL:N	2.26	0.50
1:B:1003:ILE:HD13	1:B:1054:ALA:CB	2.41	0.50
4:B:2001:9EC:N03	4:B:2001:9EC:S15	2.85	0.50
1:B:109:LEU:HD21	1:B:154:ARG:HG3	1.93	0.50
1:A:78:ALA:C	1:A:81:THR:HG22	2.30	0.50
1:A:163:PHE:CE1	1:A:249:LEU:HD11	2.47	0.50
1:B:1001:MET:HG3	1:B:1002:ASN:N	2.26	0.50
1:A:244:THR:O	1:A:248:ILE:HG12	2.12	0.50
1:A:145:SER:O	1:A:149:VAL:HG23	2.12	0.49
1:B:1006:MET:HE3	1:B:1118:TYR:CE1	2.47	0.49
1:A:86:ILE:O	1:A:89:ILE:HG13	2.12	0.49
1:B:89:ILE:HA	1:B:107:LEU:CD1	2.40	0.49
1:B:91:ALA:O	1:B:98:LEU:HD11	2.13	0.49
1:B:81:THR:OG1	1:B:537:THR:OG1	2.26	0.49
1:A:101:VAL:HB	1:A:179:ARG:HH11	1.76	0.49
1:B:74:THR:HG22	1:B:530:TRP:CZ2	2.47	0.49
1:A:167:PHE:HA	1:A:170:THR:HG22	1.93	0.49
1:A:1003:ILE:HD11	1:A:1057:ILE:HB	1.94	0.49
1:A:114:LEU:O	1:A:118:VAL:HG23	2.12	0.49
1:A:521:PRO:HD2	1:A:524:TYR:CD2	2.48	0.49
1:B:114:LEU:O	1:B:118:VAL:HG23	2.12	0.49
1:A:120:SER:HB3	1:A:533:TYR:OH	2.13	0.49
1:A:100:THR:HG23	1:A:103:ASN:ND2	2.28	0.48
1:A:173:LEU:HD12	1:A:174:THR:CG2	2.43	0.48
1:B:241:MET:HB3	1:B:242:PRO:HD3	1.96	0.48
1:A:163:PHE:CZ	1:A:249:LEU:HD11	2.48	0.48
1:A:243:VAL:HA	1:A:246:MET:HE2	1.94	0.48
1:B:78:ALA:O	1:B:82:ILE:HG13	2.13	0.48
1:A:193:VAL:O	1:A:197:VAL:HG23	2.14	0.48
1:A:525:TRP:HB3	3:A:1201:PG4:H41	1.96	0.47
1:A:91:ALA:HA	1:A:94:VAL:HG12	1.95	0.47
1:A:156:MET:O	1:A:160:VAL:HG23	2.14	0.47
1:A:505:PRO:HG2	1:A:531:LEU:HD23	1.95	0.47
1:A:243:VAL:HG22	1:A:499:PHE:CE2	2.46	0.47
1:B:1032:VAL:CG2	1:B:1057:ILE:HD13	2.40	0.47
1:A:1005:GLU:O	1:A:1009:ILE:HG13	2.14	0.47
1:A:495:ILE:HD11	1:A:543:TYR:HE1	1.79	0.47
1:B:520:ILE:HB	1:B:525:TRP:NE1	2.29	0.47
5:B:2002:P6G:H92	5:B:2002:P6G:H61	1.54	0.47
1:A:157:ASN:O	1:A:161:ILE:HG13	2.15	0.47
1:B:257:THR:HG22	1:B:257:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:THR:CG2	1:A:82:ILE:N	2.78	0.46
1:A:207:GLN:HB3	1:A:223:GLN:HE22	1.80	0.46
1:B:1053:ARG:O	1:B:1057:ILE:HG13	2.16	0.46
1:A:1010:ASP:OD2	1:A:1058:ASN:ND2	2.47	0.46
1:B:84:GLY:O	1:B:88:VAL:HG23	2.14	0.46
1:B:1073:ASN:O	1:B:1077:MET:HG3	2.14	0.46
6:B:2003:CIT:O1	6:B:2003:CIT:O7	2.32	0.46
5:B:2002:P6G:H31	5:B:2002:P6G:O19	2.16	0.46
1:A:127:TYR:CE2	1:A:133:TRP:HB2	2.51	0.46
1:B:131:ASN:O	1:B:131:ASN:ND2	2.49	0.46
1:A:89:ILE:CD1	1:A:90:VAL:HG23	2.46	0.46
1:A:169:ILE:HG23	1:A:256:GLU:HG2	1.98	0.46
1:A:122:ASN:HA	1:A:125:THR:CG2	2.46	0.45
1:A:242:PRO:O	1:A:246:MET:HG3	2.16	0.45
1:A:122:ASN:CA	1:A:125:THR:HG22	2.46	0.45
1:B:1044:VAL:O	1:B:1048:LEU:HG	2.17	0.45
1:A:63:THR:N	1:A:66:GLN:HE21	2.15	0.45
1:A:122:ASN:HA	1:A:125:THR:HG22	1.99	0.45
1:B:232:PHE:CE1	1:B:511:LEU:HD13	2.51	0.45
1:A:124:PHE:HB2	1:A:143:TRP:CZ2	2.52	0.45
1:A:1040:LYS:NZ	1:A:1072:THR:HG23	2.32	0.45
1:B:243:VAL:HG13	1:B:500:ILE:CD1	2.46	0.45
1:B:81:THR:CG2	1:B:117:GLY:HA3	2.47	0.44
1:A:92:PHE:CD2	1:A:107:LEU:HD22	2.53	0.44
1:B:1033:ARG:HH12	1:B:1037:ARG:NH2	2.13	0.44
1:A:190:LEU:O	1:A:194:ILE:HG13	2.18	0.44
1:B:521:PRO:HD2	1:B:524:TYR:CD2	2.52	0.44
2:C:1:GLC:H62	2:C:2:GLC:C1	2.47	0.44
1:A:79:LEU:O	1:A:83:ILE:HG13	2.17	0.44
1:A:231:THR:HG22	1:A:510:VAL:HG13	2.00	0.44
1:A:257:THR:O	1:A:257:THR:HG22	2.17	0.44
1:B:236:ILE:HA	1:B:240:TYR:HB2	1.99	0.44
1:B:1033:ARG:NH1	1:B:1037:ARG:HH21	2.10	0.44
1:A:172:PRO:HA	1:A:176:ARG:HB3	1.99	0.44
1:A:1040:LYS:NZ	1:A:1072:THR:HA	2.33	0.43
1:A:503:TRP:O	1:A:507:ASN:ND2	2.48	0.43
1:B:239:PHE:C	1:B:242:PRO:HD2	2.38	0.43
2:C:1:GLC:C3	2:C:2:GLC:H5	2.47	0.43
1:A:173:LEU:HD12	1:A:174:THR:OG1	2.18	0.43
1:B:169:ILE:HD12	1:B:253:ILE:HG23	1.99	0.43
1:B:92:PHE:HA	1:B:98:LEU:CD1	2.49	0.43

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:B:232:PHE:CE2	1:B:236:ILE:HD11	2.53	0.43
1:B:121:MET:O	1:B:125:THR:OG1	2.24	0.43
1:B:1008:ARG:O	1:B:1013:GLY:HA2	2.19	0.43
1:A:116:ILE:HG23	1:A:533:TYR:CD1	2.54	0.43
1:A:232:PHE:HB2	1:A:514:THR:OG1	2.18	0.43
1:B:141:ASP:HB3	1:B:204:LEU:HD23	2.01	0.43
1:B:81:THR:HG1	1:B:537:THR:HG1	1.61	0.42
1:A:92:PHE:CE1	1:A:99:LYS:HA	2.54	0.42
1:A:1027:ASP:OD1	2:C:1:GLC:H1	2.18	0.42
1:A:70:ILE:CG2	1:A:129:ILE:HD11	2.50	0.42
1:A:210:VAL:HG12	1:A:210:VAL:O	2.19	0.42
1:A:1003:ILE:CD1	1:A:1057:ILE:HB	2.49	0.42
1:B:238:ALA:O	1:B:242:PRO:HG2	2.19	0.42
1:A:239:PHE:O	1:A:243:VAL:HG23	2.20	0.42
1:A:1003:ILE:HD11	1:A:1057:ILE:CG2	2.48	0.42
1:A:154:ARG:O	1:A:158:LEU:HG	2.19	0.42
1:A:163:PHE:O	1:A:167:PHE:HB2	2.19	0.42
1:A:231:THR:HG22	1:A:510:VAL:CG1	2.50	0.42
1:A:1027:ASP:HB3	2:C:1:GLC:C1	2.50	0.42
5:B:2002:P6G:H181	5:B:2002:P6G:H151	1.57	0.42
1:B:98:LEU:HD23	1:B:549:THR:HG22	2.01	0.42
1:A:101:VAL:CG1	1:A:179:ARG:HH11	2.33	0.41
1:B:66:GLN:O	1:B:70:ILE:HG13	2.19	0.41
1:B:499:PHE:CA	1:B:535:ASN:HD21	2.28	0.41
1:B:548:LYS:HA	1:B:551:ARG:HE	1.84	0.41
1:A:227:GLU:OE2	1:A:229:THR:HB	2.20	0.41
1:A:1004:PHE:CZ	1:A:1028:VAL:HG11	2.55	0.41
1:A:1071:PHE:HB3	1:A:1074:SER:HB2	2.03	0.41
1:B:257:THR:HG21	1:B:486:LYS:HA	2.01	0.41
1:B:171:ARG:O	1:B:175:TYR:HB3	2.19	0.41
1:B:503:TRP:CD1	1:B:532:CYS:HA	2.55	0.41
1:A:100:THR:HG23	1:A:103:ASN:HD22	1.85	0.41
1:A:243:VAL:HG13	1:A:500:ILE:HD11	2.02	0.41
1:A:76:PHE:O	1:A:80:VAL:HG23	2.21	0.41
1:B:87:LEU:HD11	1:B:558:LEU:HD21	2.02	0.41
1:B:162:SER:HB3	1:B:249:LEU:HD12	2.01	0.41
1:B:1040:LYS:NZ	1:B:1072:THR:OG1	2.55	0.40
1:A:111:CYS:O	1:A:115:ILE:HG13	2.22	0.40
1:A:124:PHE:O	1:A:128:ILE:HG22	2.21	0.40
1:A:173:LEU:HD12	1:A:174:THR:CB	2.51	0.40
1:A:1040:LYS:HZ1	1:A:1072:THR:HG23	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1033:ARG:O	1:B:1037:ARG:HG3	2.20	0.40
1:A:1049:ASP:O	1:A:1053:ARG:HG3	2.21	0.40
1:B:236:ILE:HA	1:B:240:TYR:HD2	1.86	0.40
1:A:94:VAL:HG22	1:A:94:VAL: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	A	392/418 (94%)	389 (99%)	3 (1%)	0	100	100
1	B	392/418 (94%)	386 (98%)	6 (2%)	0	100	100
All	All	784/836 (94%)	775 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	319/360 (89%)	315 (99%)	4 (1%)	69	87
1	B	323/360 (90%)	320 (99%)	3 (1%)	78	91
All	All	642/720 (89%)	635 (99%)	7 (1%)	73	89

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	516	CYS
1	A	530	TRP
1	A	535	ASN
1	B	1110	PHE
1	B	522	LYS
1	B	530	TRP

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	103	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 ⓘ

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GLC	C	1	2	12,12,12	0.83	0	17,17,17	1.69	4 (23%)
2	GLC	C	2	2	11,11,12	1.24	2 (18%)	15,15,17	2.46	5 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	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)
2	C	2	GLC	O3-C3	-2.15	1.37	1.43
2	C	2	GLC	C4-C5	-2.01	1.48	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	GLC	O5-C5-C6	5.24	115.42	107.20
2	C	2	GLC	C1-C2-C3	-5.04	103.47	109.67
2	C	2	GLC	C3-C4-C5	-2.95	104.98	110.24
2	C	1	GLC	O5-C5-C6	2.94	113.75	106.44
2	C	1	GLC	C4-C3-C2	-2.92	105.73	110.82
2	C	1	GLC	C6-C5-C4	-2.75	106.55	113.00
2	C	2	GLC	O5-C5-C4	-2.69	104.27	110.83
2	C	1	GLC	O2-C2-C3	-2.32	104.98	110.35
2	C	2	GLC	C6-C5-C4	-2.19	107.89	113.00

There are no chirality outliers.

All (1) torsion outliers are listed below:

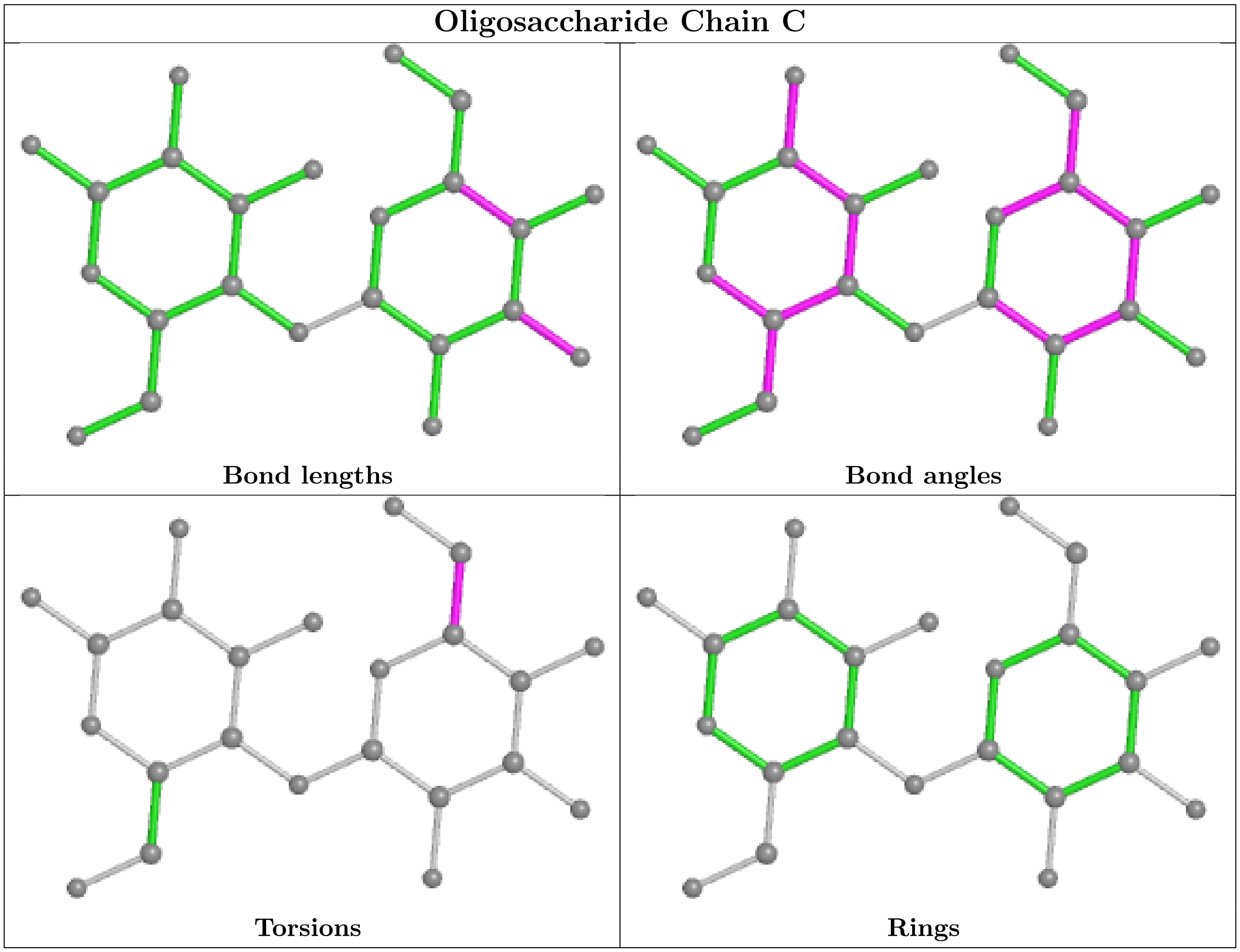
Mol	Chain	Res	Type	Atoms
2	C	2	GLC	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	GLC	3	0
2	C	1	GLC	5	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 ⓘ

5 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	$\#\|Z\| > 2$
4	9EC	B	2001	-	29,31,31	1.05	0	41,48,48	2.28	12 (29%)
3	PG4	A	1201	-	12,12,12	0.53	0	11,11,11	0.38	0
6	CIT	B	2003	-	12,12,12	1.04	0	17,17,17	1.51	1 (5%)
4	9EC	A	1203	-	29,31,31	1.05	0	41,48,48	2.27	12 (29%)
5	P6G	B	2002	-	18,18,18	0.54	0	17,17,17	0.44	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	9EC	B	2001	-	-	4/10/45/45	0/6/5/5
3	PG4	A	1201	-	-	7/10/10/10	-
6	CIT	B	2003	-	-	6/16/16/16	-
4	9EC	A	1203	-	-	4/10/45/45	0/6/5/5
5	P6G	B	2002	-	-	8/16/16/16	-

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1203	9EC	C19-C20-C21	-5.91	103.83	107.46
4	B	2001	9EC	C19-C20-C21	-5.83	103.89	107.46
4	B	2001	9EC	C26-C21-C20	-5.34	104.18	107.46
4	A	1203	9EC	C26-C21-C20	-5.30	104.21	107.46
4	A	1203	9EC	C20-C19-N23	4.79	106.52	103.54
4	B	2001	9EC	C20-C19-N23	4.78	106.51	103.54
4	A	1203	9EC	C21-C26-N23	4.77	106.51	103.54
4	B	2001	9EC	C21-C26-N23	4.51	106.34	103.54
6	B	2003	CIT	O6-C6-C3	4.15	120.26	113.05
4	A	1203	9EC	C18-C19-N23	3.93	111.29	108.82
4	B	2001	9EC	C18-C19-N23	3.90	111.27	108.82
4	B	2001	9EC	C13-C14-S15	-3.71	109.97	112.98
4	A	1203	9EC	C13-C14-S15	-3.66	110.01	112.98
4	B	2001	9EC	C27-C26-N23	3.40	110.96	108.82
4	A	1203	9EC	O22-C20-C19	3.26	120.16	117.11
4	B	2001	9EC	O22-C21-C26	3.24	120.14	117.11
4	B	2001	9EC	O22-C20-C19	3.21	120.11	117.11
4	A	1203	9EC	C27-C26-N23	2.98	110.69	108.82
4	A	1203	9EC	O22-C21-C26	2.94	119.86	117.11
4	A	1203	9EC	C06-C07-C09	-2.58	119.94	123.29
4	B	2001	9EC	C06-C07-C09	-2.54	120.00	123.29
4	A	1203	9EC	C27-C26-C21	-2.16	105.25	107.04
4	B	2001	9EC	O16-C17-C18	2.11	112.86	107.79
4	A	1203	9EC	C09-C10-C04	2.07	119.81	118.46
4	B	2001	9EC	C09-C10-C04	2.02	119.78	118.46

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	2003	CIT	C2-C3-C4-C5
6	B	2003	CIT	O7-C3-C4-C5
6	B	2003	CIT	C6-C3-C4-C5
5	B	2002	P6G	C9-C8-O7-C6
4	A	1203	9EC	O01-C02-N03-C04
4	A	1203	9EC	O16-C02-N03-C04
3	A	1201	PG4	O2-C3-C4-O3
5	B	2002	P6G	O4-C5-C6-O7
4	B	2001	9EC	O16-C02-N03-C04
4	B	2001	9EC	O01-C02-N03-C04
3	A	1201	PG4	O4-C7-C8-O5
5	B	2002	P6G	C18-C17-O16-C15
6	B	2003	CIT	C1-C2-C3-O7
6	B	2003	CIT	C1-C2-C3-C6
5	B	2002	P6G	O1-C2-C3-O4
6	B	2003	CIT	C1-C2-C3-C4
5	B	2002	P6G	O16-C17-C18-O19
5	B	2002	P6G	O7-C8-C9-O10
5	B	2002	P6G	C6-C5-O4-C3
3	A	1201	PG4	C5-C6-O4-C7
3	A	1201	PG4	C1-C2-O2-C3
4	A	1203	9EC	C05-C04-N03-C02
4	B	2001	9EC	C05-C04-N03-C02
4	A	1203	9EC	C10-C04-N03-C02
4	B	2001	9EC	C10-C04-N03-C02
3	A	1201	PG4	O3-C5-C6-O4
3	A	1201	PG4	C4-C3-O2-C2
3	A	1201	PG4	O1-C1-C2-O2
5	B	2002	P6G	C14-C15-O16-C17

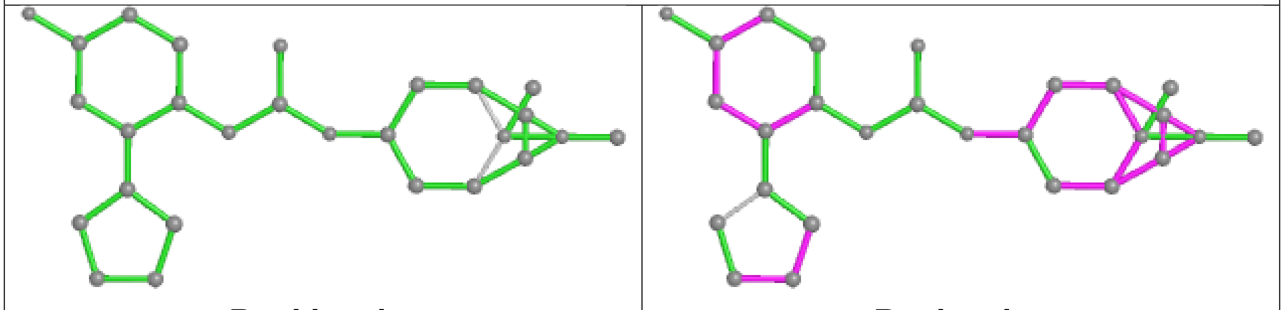
There are no ring outliers.

5 monomers are involved in 7 short contacts:

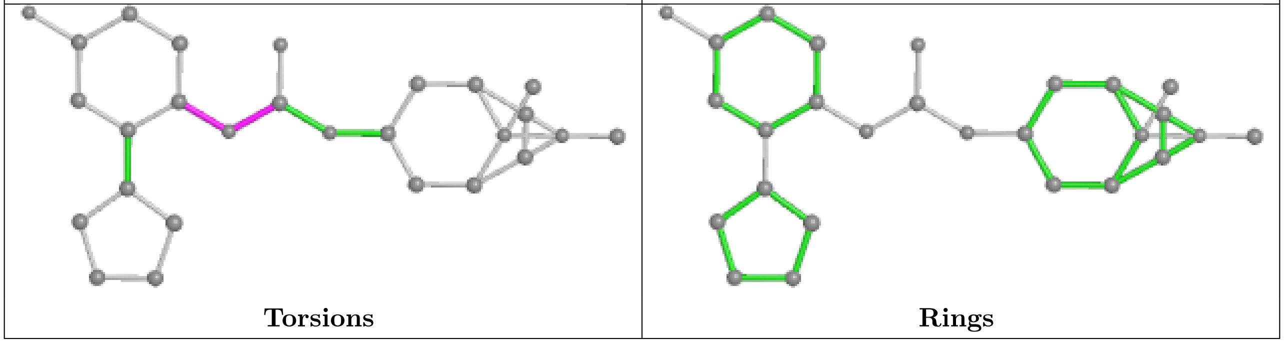
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2001	9EC	1	0
3	A	1201	PG4	1	0
6	B	2003	CIT	1	0
4	A	1203	9EC	1	0
5	B	2002	P6G	3	0

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 9EC B 2001

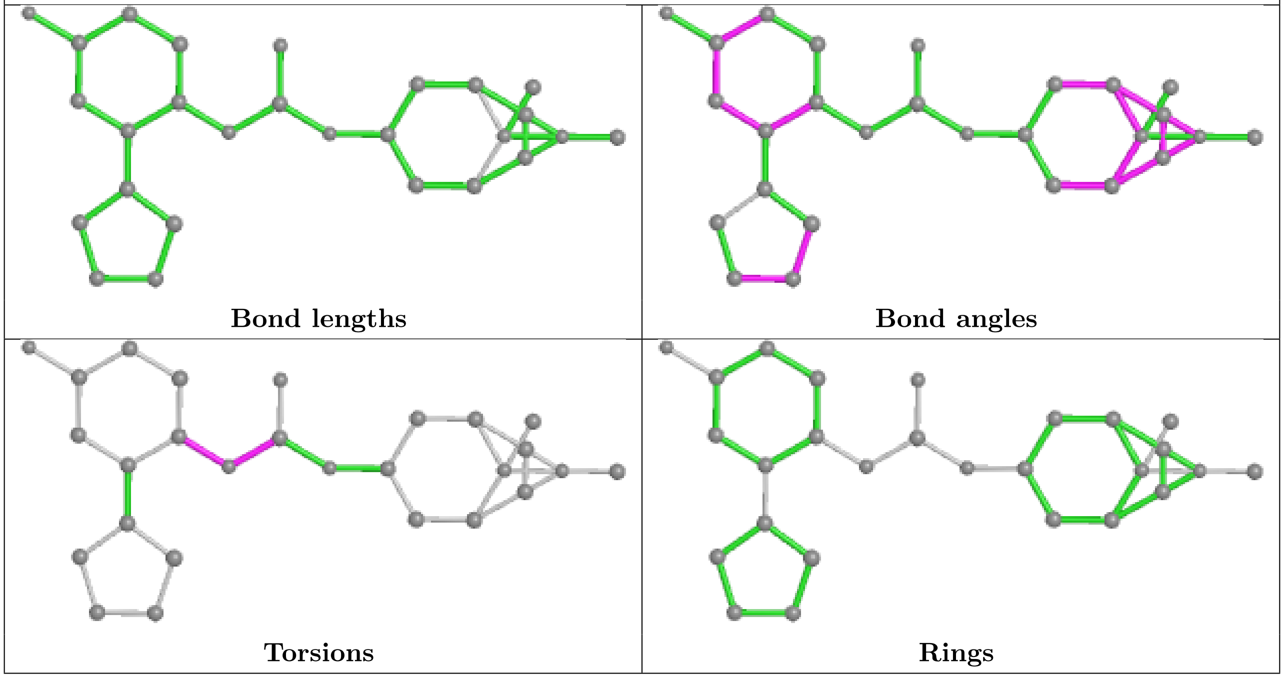


Bond lengths **Bond angles**



Torsions **Rings**

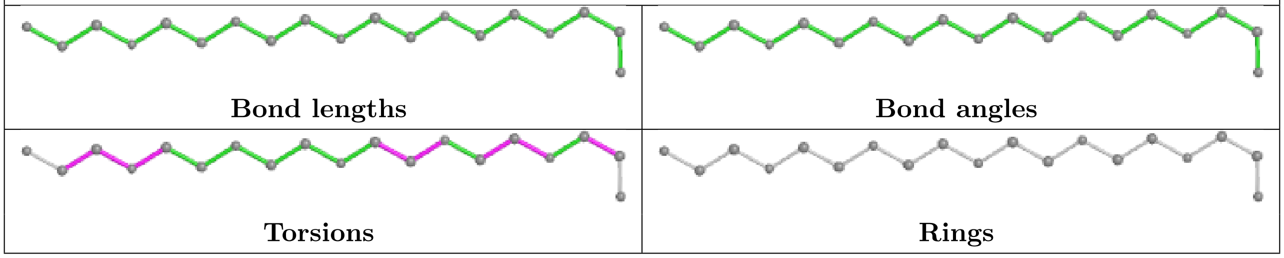
Ligand 9EC A 1203



Bond lengths Bond angles

Torsions Rings

Ligand P6G B 2002



Bond lengths Bond angles

Torsions Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	394/418 (94%)	-0.32	1 (0%)	94	88	56, 88, 120, 144	0
1	B	394/418 (94%)	-0.32	0	100	100	54, 75, 98, 122	0
All	All	788/836 (94%)	-0.32	1 (0%)	95	92	54, 80, 116, 144	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	557	LEU	2.5

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

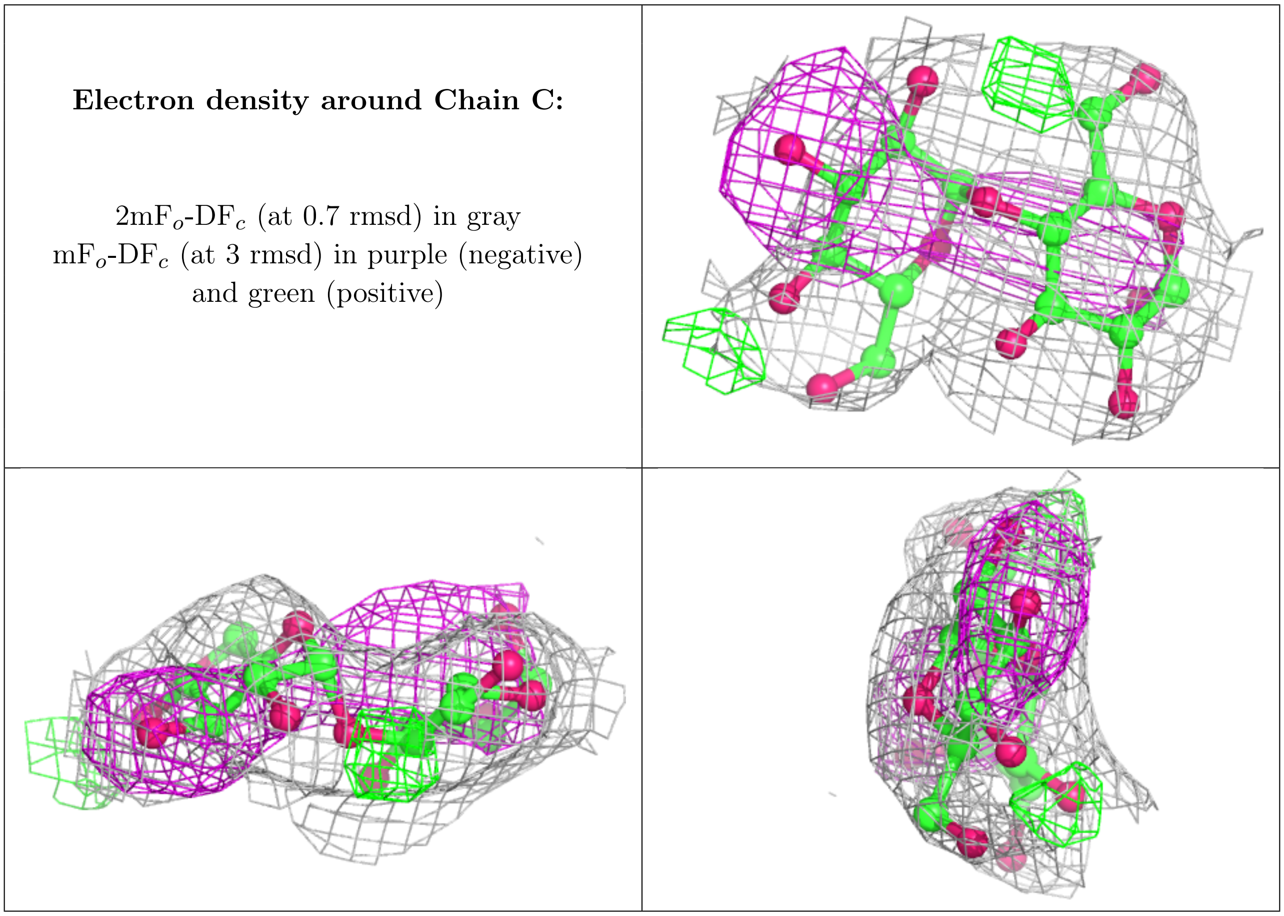
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	C	2	11/12	0.78	0.38	94,103,107,108	0
2	GLC	C	1	12/12	0.83	0.31	80,91,96,100	0

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



Electron density around Chain C:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.4 Ligands ⓘ

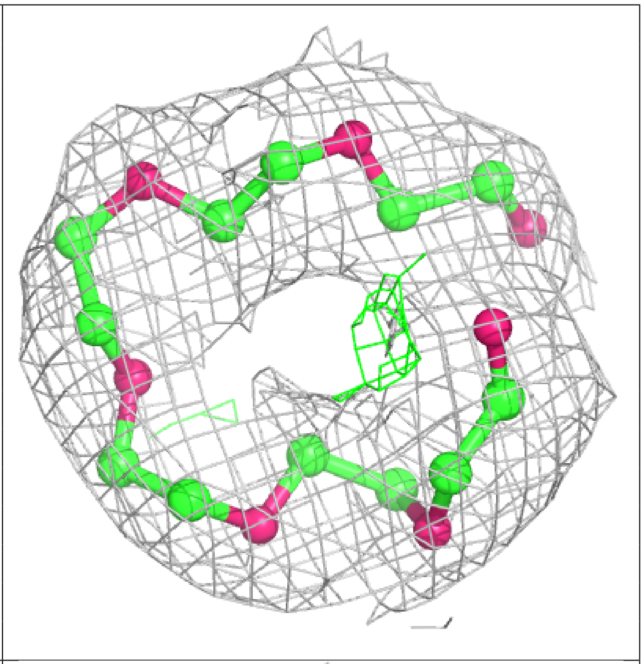
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

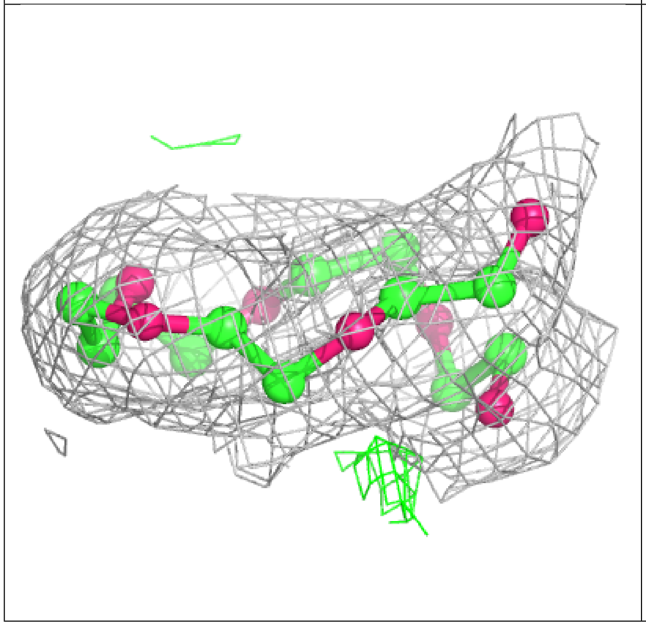
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CIT	B	2003	13/13	0.89	0.35	89,105,113,115	0
3	PG4	A	1201	13/13	0.91	0.17	80,84,91,92	0
5	P6G	B	2002	19/19	0.95	0.20	66,76,87,89	0
4	9EC	A	1203	27/27	0.97	0.21	70,74,81,84	0
4	9EC	B	2001	27/27	0.98	0.20	61,67,72,80	0

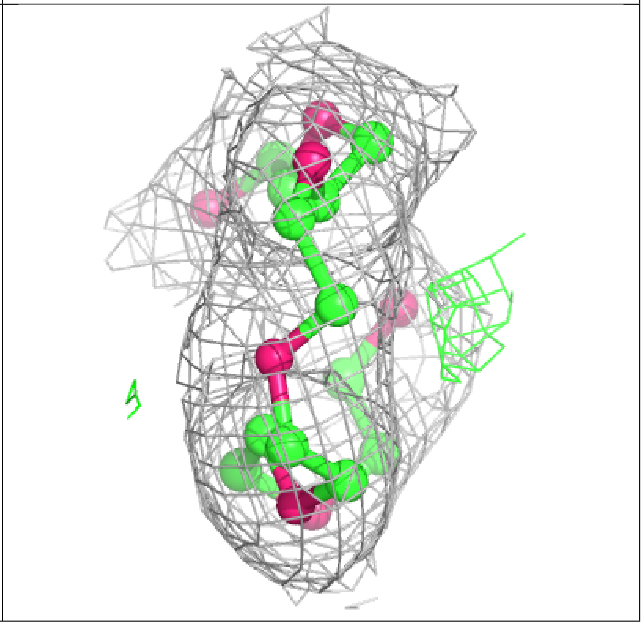
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P6G B 2002:

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

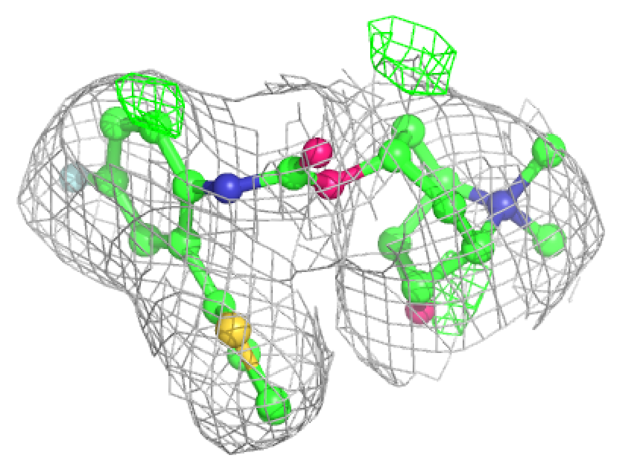


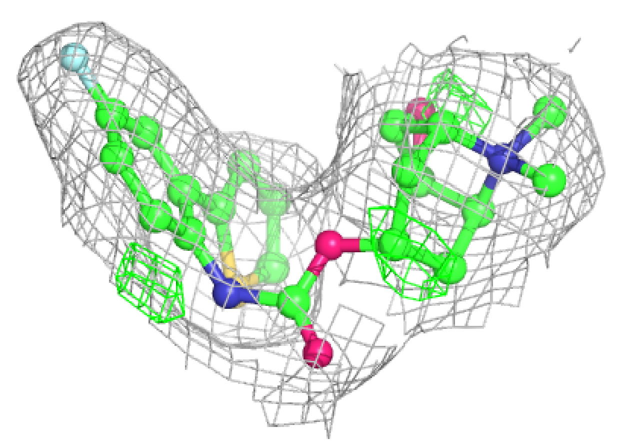


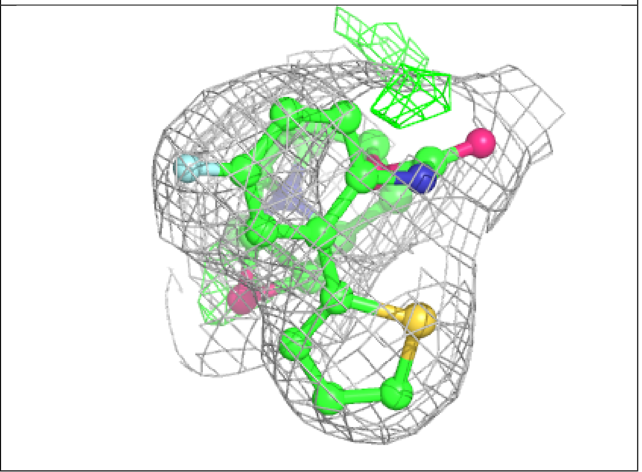


Electron density around 9EC A 1203:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

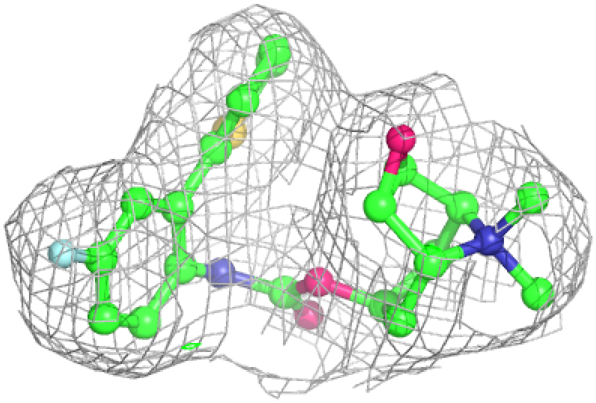


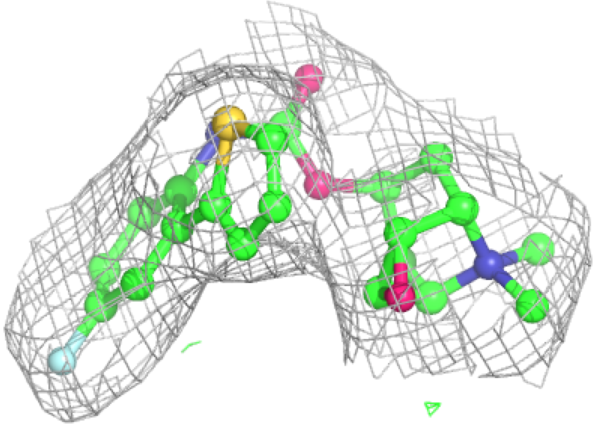


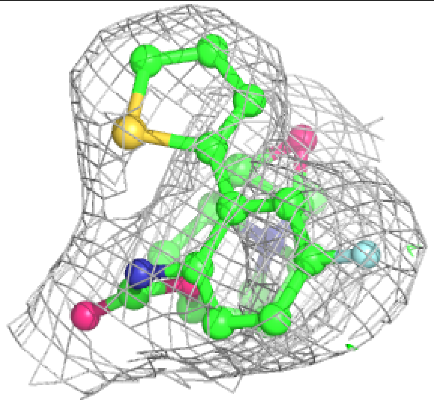


Electron density around 9EC B 2001:

$2mF_o$-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 ⓘ

There are no such residues in this entry.