Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 11:09 PM EDT

PDB ID	:	7LRX
Title	:	Structure of HIV-1 Reverse Transcriptase in complex with DNA, L-dCTP, and CA(2+) ion
Authors	:	Hoang, A.; Ruiz, F.X.; Arnold, E.
Deposited on	:	2021-02-17
Resolution	:	2.90 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:

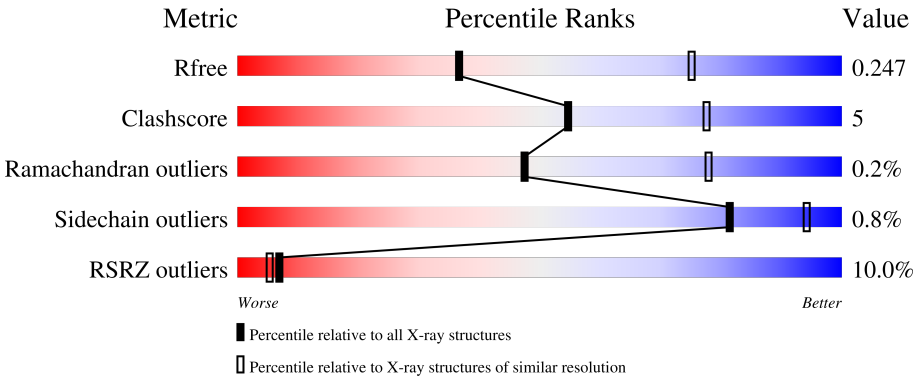
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	555	9% 84% 15%
1	C	555	18% 84% 16%
2	B	429	6% 88% 9%
2	D	429	6% 82% 14%
3	E	38	63% 24% 5% 8%

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Mol	Chain	Length	Quality of chain
3	F	38	5% 74% 16% 8%
4	H	2	100%
4	L	2	100%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 17536 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 Reverse transcriptase p66.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4504	2916	750	831	7			
1	C	553	Total	C	N	O	S	0	0	0
			4504	2916	750	831	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	engineered mutation	UNP P03366
A	498	ASN	ASP	engineered mutation	UNP P03366
C	280	SER	CYS	engineered mutation	UNP P03366
C	498	ASN	ASP	engineered mutation	UNP P03366

- Molecule 2 is a protein called Reverse transcriptase p51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	415	Total	C	N	O	S	0	0	0
			3434	2239	567	621	7			
2	D	410	Total	C	N	O	S	0	0	0
			3394	2213	561	613	7			

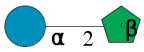
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366
D	0	GLY	-	expression tag	UNP P03366
D	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is a DNA chain called DNA/RNA (38-MER).

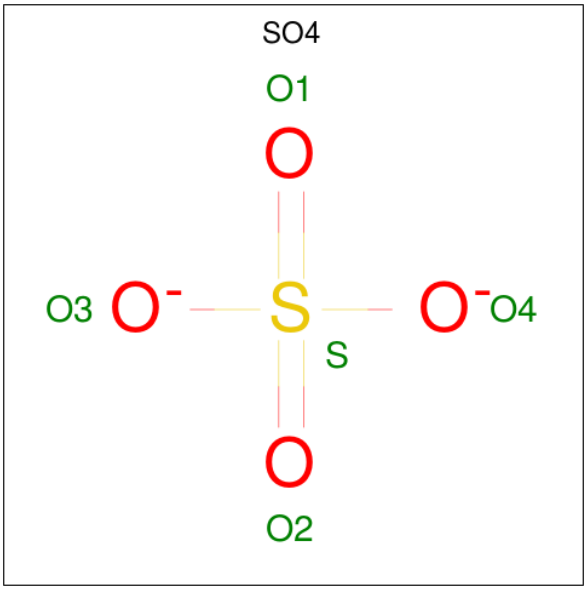
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	35	Total	C	N	O	P	0	0	0
			721	340	130	216	35			
3	E	35	Total	C	N	O	P	0	0	0
			721	340	130	216	35			

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



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

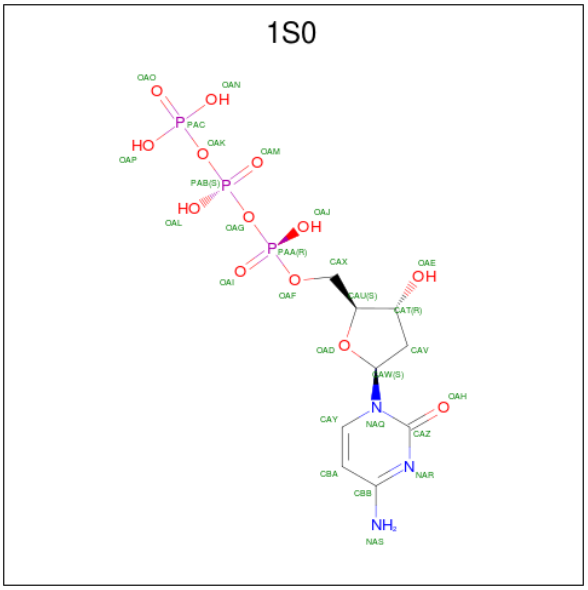
- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 4-amino-1-{2-deoxy-5-O-[(R)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]oxy}phosphoryl]-beta-L-erythro-pentofuranosyl}pyrimidin-2(1H)-one (three-letter code:

1S0) (formula: $C_9H_{16}N_3O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

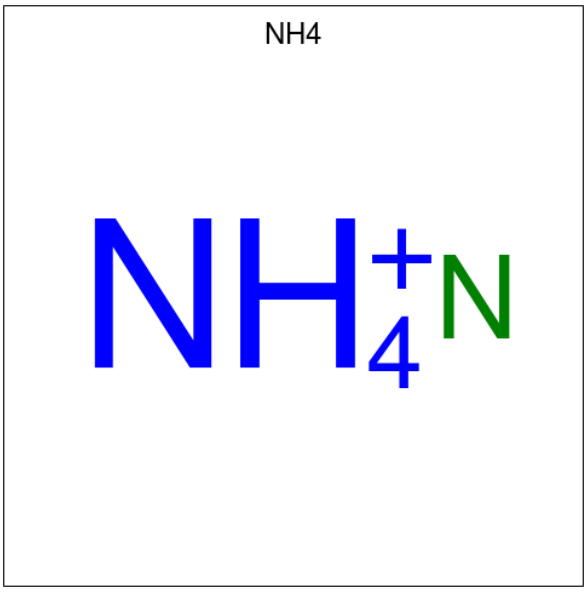


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O P 28 9 3 13 3	0	0
6	C	1	Total C N O P 28 9 3 13 3	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

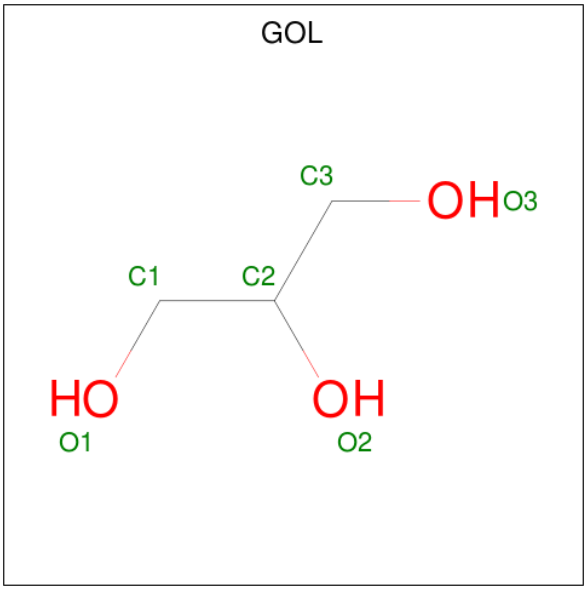
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total N 1 1	0	0
8	C	1	Total N 1 1	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 6 3 3	0	0
9	D	1	Total C O 6 3 3	0	0

- Molecule 10 is water.

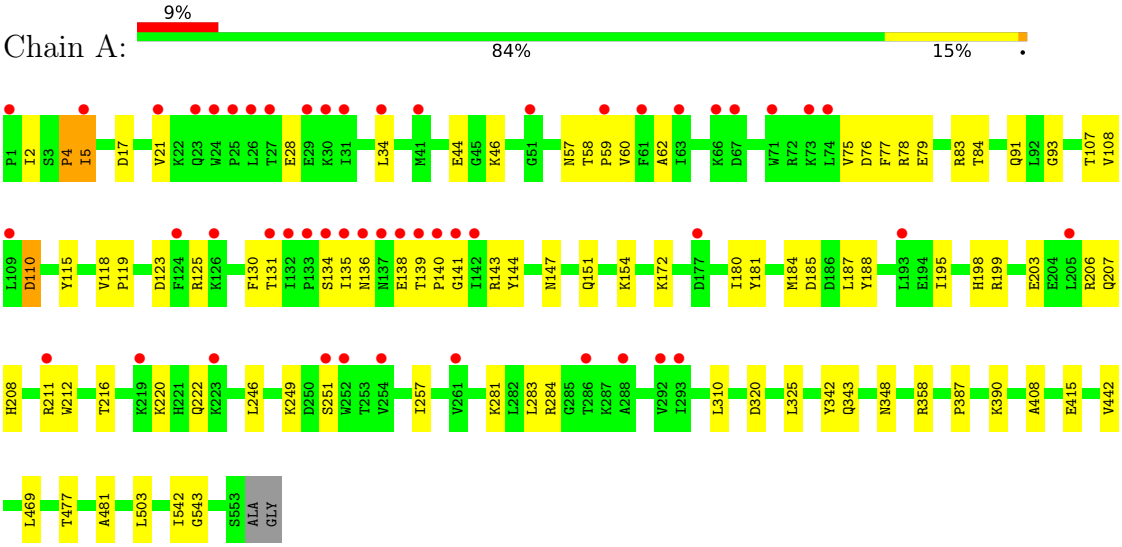
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	31	Total O 31 31	0	0
10	B	31	Total O 31 31	0	0
10	C	32	Total O 32 32	0	0
10	D	24	Total O 24 24	0	0
10	F	6	Total O 6 6	0	0
10	E	6	Total O 6 6	0	0

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.

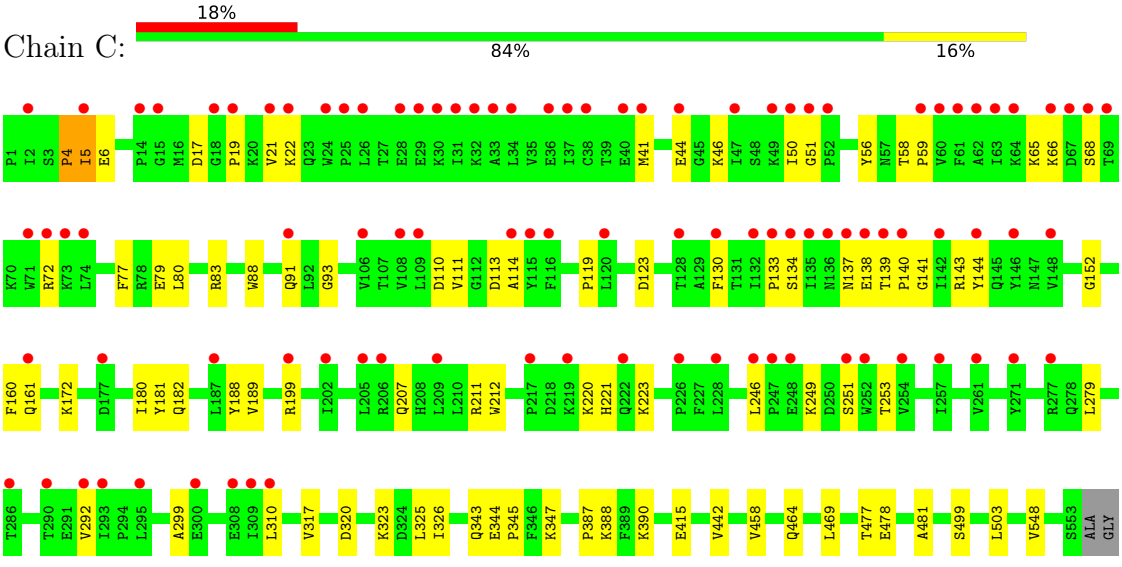
• Molecule 1: Reverse transcriptase p66

Chain A:



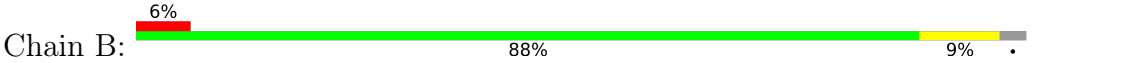
• Molecule 1: Reverse transcriptase p66

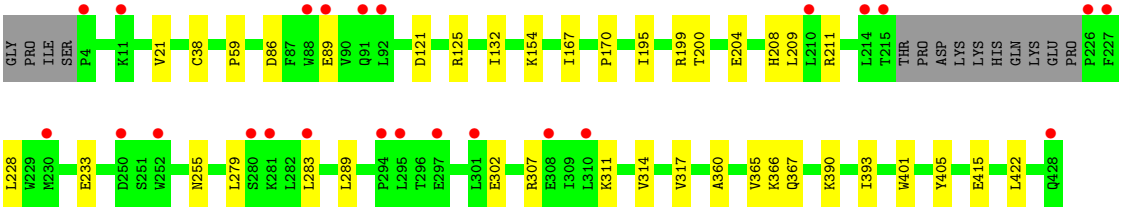
Chain C:



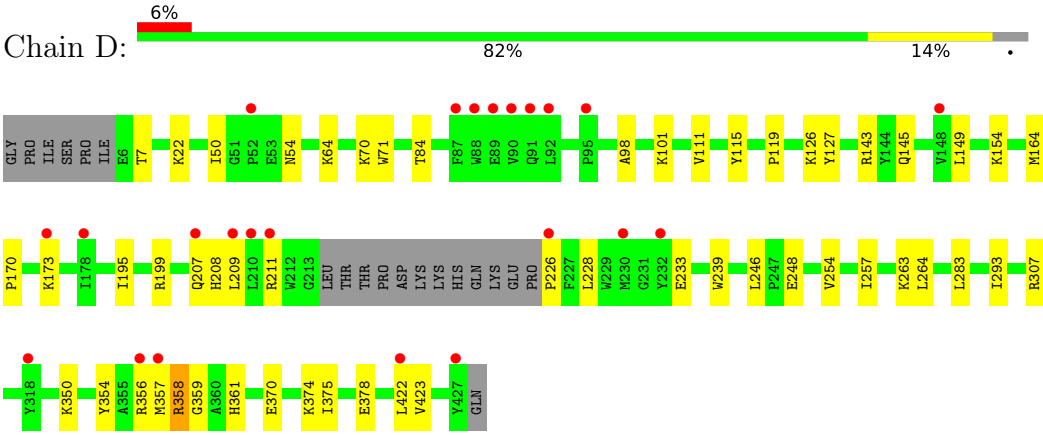
• Molecule 2: Reverse transcriptase p51

Chain B:

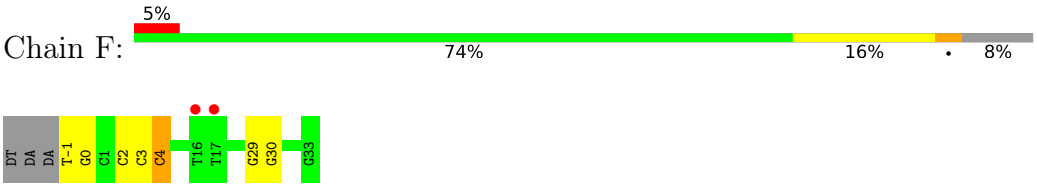




• Molecule 2: Reverse transcriptase p51

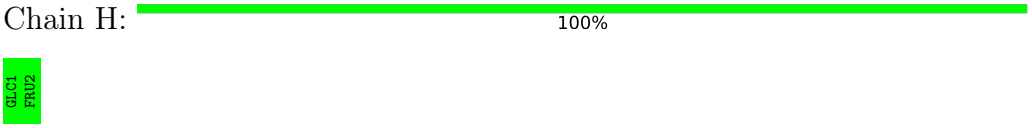


• Molecule 3: DNA/RNA (38-MER)

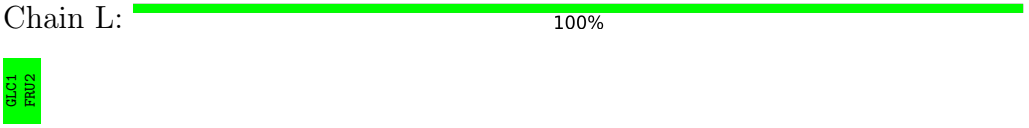


• Molecule 3: DNA/RNA (38-MER)

• Molecule 4: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



• Molecule 4: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.88Å 132.62Å 139.38Å 90.00° 97.76° 90.00°	Depositor
Resolution (Å)	73.93 – 2.90 73.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (73.93-2.90) 100.0 (73.93-2.90)	Depositor EDS
R_{merge}	0.42	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.208 , 0.247 0.208 , 0.247	Depositor DCC
R_{free} test set	1999 reflections (2.78%)	wwPDB-VP
Wilson B-factor (Å^2)	64.6	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 68.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17536	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: OMC, NH4, GLC, SO4, FRU, CA, GOL, 1S0

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	0.26	0/4622	0.44	0/6279
1	C	0.24	0/4622	0.43	0/6279
2	B	0.24	0/3534	0.43	0/4800
2	D	0.25	0/3493	0.43	0/4745
3	E	0.48	0/760	0.87	0/1172
3	F	0.51	0/760	0.85	0/1172
All	All	0.28	0/17791	0.49	0/24447

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	4504	0	4567	61	0
1	C	4504	0	4567	53	0
2	B	3434	0	3466	24	0
2	D	3394	0	3421	36	0
3	E	721	0	397	7	0
3	F	721	0	397	5	0
4	H	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	23	0	21	0	0
5	A	5	0	0	0	0
5	C	5	0	0	0	0
6	A	28	0	14	1	0
6	C	28	0	16	3	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
9	B	6	0	8	0	0
9	D	6	0	8	0	0
10	A	31	0	0	1	0
10	B	31	0	0	1	0
10	C	32	0	0	0	0
10	D	24	0	0	1	0
10	E	6	0	0	0	0
10	F	6	0	0	0	0
All	All	17536	0	16903	177	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 (177) 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:139:THR:CG2	1:A:140:PRO:HD2	1.59	1.32
1:A:139:THR:HG23	1:A:140:PRO:HD2	1.29	1.13
1:A:139:THR:HG22	1:A:140:PRO:HD2	1.32	1.04
1:A:139:THR:HG22	1:A:140:PRO:CD	1.99	0.91
1:A:139:THR:CG2	1:A:140:PRO:CD	2.46	0.90
1:A:208:HIS:HA	1:A:211:ARG:HE	1.37	0.88
3:F:-1:DT:H2'	3:F:-1:DT:OP2	1.86	0.76
1:A:131:THR:HG22	1:A:143:ARG:HG2	1.68	0.75
1:C:390:LYS:NZ	1:C:415:GLU:OE2	2.23	0.71
1:A:5:ILE:HG22	1:A:212:TRP:HE3	1.55	0.71
2:D:170:PRO:HB2	2:D:208:HIS:HE1	1.55	0.71
1:C:323:LYS:NZ	1:C:344:GLU:OE2	2.25	0.69
1:C:503:LEU:HD23	2:D:422:LEU:HD22	1.77	0.66
1:C:113:ASP:HA	6:C:602:1S0:OAI	1.98	0.64
1:C:72:ARG:NH2	6:C:602:1S0:OAM	2.31	0.64
1:A:390:LYS:NZ	1:A:415:GLU:OE2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ILE:HD11	1:A:118:VAL:HG13	1.81	0.63
2:D:246:LEU:HD11	2:D:264:LEU:HD21	1.80	0.63
1:A:115:TYR:HD1	1:A:151:GLN:HG2	1.64	0.62
2:D:248:GLU:OE1	2:D:307:ARG:NH2	2.30	0.62
1:C:91:GLN:NE2	1:C:93:GLY:O	2.34	0.61
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.82	0.61
1:C:56:TYR:O	1:C:143:ARG:NH2	2.34	0.60
1:C:5:ILE:HG22	1:C:6:GLU:H	1.66	0.60
2:D:54:ASN:HB3	2:D:143:ARG:HH21	1.67	0.60
1:A:108:VAL:HB	1:A:222:GLN:HB2	1.84	0.59
2:D:354:TYR:HE2	2:D:375:ILE:HG13	1.66	0.59
2:D:356:ARG:NH1	2:D:374:LYS:HD2	2.17	0.59
1:A:28:GLU:OE2	1:A:136:ASN:ND2	2.30	0.58
1:A:91:GLN:NE2	1:A:93:GLY:O	2.36	0.58
1:A:543:GLY:N	2:B:283:LEU:O	2.32	0.58
1:C:50:ILE:HG22	1:C:51:GLY:N	2.18	0.58
1:A:84:THR:HB	1:A:154:LYS:HE2	1.85	0.58
1:A:503:LEU:HD23	2:B:422:LEU:HD22	1.84	0.58
1:C:21:VAL:HB	1:C:59:PRO:HD3	1.84	0.58
1:C:19:PRO:HG3	1:C:80:LEU:HB2	1.86	0.58
1:A:139:THR:HG23	1:A:140:PRO:CD	2.18	0.57
1:C:181:TYR:HB2	1:C:188:TYR:HB3	1.86	0.57
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.87	0.56
2:D:254:VAL:HG13	2:D:283:LEU:HD22	1.89	0.55
1:A:249:LYS:HG3	1:A:251:SER:H	1.71	0.55
2:B:209:LEU:HD22	2:B:228:LEU:HD22	1.90	0.54
1:C:5:ILE:HG23	1:C:212:TRP:HE3	1.70	0.54
1:A:4:PRO:HB2	1:A:119:PRO:HD3	1.88	0.54
1:A:172:LYS:HG2	1:A:180:ILE:HD12	1.89	0.54
2:D:165:THR:O	2:D:169:GLU:HG2	2.08	0.54
2:B:199:ARG:NE	2:B:233:GLU:OE2	2.42	0.53
2:D:207:GLN:O	2:D:211:ARG:HG3	2.08	0.53
1:A:135:ILE:HG13	1:A:138:GLU:HB3	1.91	0.53
1:C:5:ILE:HG23	1:C:212:TRP:CE3	2.44	0.52
1:A:206:ARG:NH2	1:A:216:THR:O	2.42	0.52
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.92	0.52
1:A:79:GLU:HG3	1:A:83:ARG:HE	1.74	0.52
2:D:7:THR:HG22	2:D:119:PRO:HB2	1.91	0.52
2:D:209:LEU:HD22	2:D:228:LEU:HD22	1.90	0.52
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.91	0.52
2:D:357:MET:O	2:D:361:HIS:CE1	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:50:ILE:HD13	2:D:145:GLN:HB3	1.92	0.52
2:D:64:LYS:HE3	2:D:71:TRP:CE2	2.45	0.52
1:C:4:PRO:HD2	1:C:119:PRO:HB3	1.92	0.52
1:C:72:ARG:NH1	6:C:602:1S0:OAM	2.43	0.51
1:C:180:ILE:HG12	1:C:189:VAL:HG22	1.93	0.51
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.92	0.51
1:A:115:TYR:CD1	1:A:151:GLN:HG2	2.43	0.51
1:A:208:HIS:HB2	1:A:211:ARG:HH21	1.76	0.51
1:C:199:ARG:HH12	1:C:223:LYS:HB3	1.74	0.51
1:A:320:ASP:O	1:A:343:GLN:NE2	2.43	0.51
1:A:257:ILE:HB	1:A:283:LEU:HD21	1.92	0.51
1:A:17:ASP:O	1:A:83:ARG:HD3	2.11	0.50
1:A:184:MET:HG3	3:E:33:DG:H1'	1.93	0.50
1:C:253:THR:HG22	1:C:292:VAL:HG22	1.94	0.49
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.93	0.49
1:A:107:THR:OG1	1:A:198:HIS:NE2	2.38	0.49
1:C:133:PRO:HB3	1:C:137:ASN:OD1	2.11	0.49
1:A:110:ASP:HB3	1:A:220:LYS:HB3	1.94	0.49
2:B:366:LYS:HG3	2:B:405:TYR:CD1	2.47	0.49
1:C:458:VAL:HG12	1:C:548:VAL:HB	1.94	0.49
2:D:239:TRP:CH2	2:D:378:GLU:HG2	2.47	0.49
2:B:390:LYS:NZ	2:B:415:GLU:OE2	2.41	0.49
2:D:356:ARG:HH11	2:D:374:LYS:HD2	1.78	0.49
3:E:23:DC:H2"	3:E:24:DG:C8	2.48	0.49
1:C:279:LEU:HD23	1:C:299:ALA:HB1	1.95	0.49
1:C:469:LEU:HD12	1:C:477:THR:HG22	1.93	0.49
1:C:246:LEU:HD11	1:C:310:LEU:HD12	1.94	0.48
2:D:164:MET:HE3	2:D:168:LEU:HD21	1.95	0.48
1:C:88:TRP:HZ2	2:D:22:LYS:HA	1.79	0.48
1:A:281:LYS:O	1:A:284:ARG:HG2	2.13	0.48
1:C:130:PHE:CZ	1:C:144:TYR:HB2	2.49	0.48
3:E:3:DC:H42	3:E:31:DG:H1	1.60	0.48
1:C:50:ILE:CG2	1:C:51:GLY:N	2.77	0.48
6:A:602:1S0:H10	6:A:602:1S0:H13	1.62	0.47
1:C:134:SER:HB3	1:C:141:GLY:HA2	1.96	0.47
1:C:17:ASP:O	1:C:83:ARG:HD3	2.15	0.47
2:D:257:ILE:HD12	2:D:293:ILE:HD11	1.95	0.47
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.96	0.47
1:A:2:ILE:HD12	1:A:2:ILE:H	1.80	0.47
1:A:76:ASP:OD2	3:E:0:DG:H4'	2.14	0.47
1:A:195:ILE:O	1:A:199:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLU:O	1:A:207:GLN:HG2	2.14	0.47
1:A:207:GLN:O	1:A:211:ARG:HG3	2.15	0.47
2:B:360:ALA:HA	2:B:367:GLN:NE2	2.30	0.47
3:F:3:DC:H2'	3:F:4:OMC:C6	2.50	0.47
3:E:1:DC:H2'	3:E:2:OMC:C6	2.49	0.47
1:A:60:VAL:HG22	1:A:75:VAL:HG13	1.96	0.47
2:B:170:PRO:HB2	2:B:208:HIS:HE1	1.80	0.47
2:B:255:ASN:HB2	2:B:289:LEU:HB3	1.97	0.47
1:C:325:LEU:HB3	1:C:387:PRO:HB3	1.97	0.47
2:B:86:ASP:OD1	2:B:154:LYS:NZ	2.48	0.46
2:D:70:LYS:HE3	2:D:226:PRO:HD2	1.97	0.46
2:D:170:PRO:HB2	2:D:208:HIS:CE1	2.43	0.46
1:C:320:ASP:O	1:C:343:GLN:NE2	2.43	0.46
1:C:478:GLU:HB3	1:C:499:SER:HB2	1.96	0.46
2:D:309:ILE:O	2:D:312:GLU:HG2	2.15	0.46
3:F:29:DG:H2'	3:F:30:DG:H8	1.81	0.46
3:E:10:DC:H2"	3:E:11:DG:C8	2.51	0.46
2:D:111:VAL:HG23	10:D:607:HOH:O	2.15	0.46
2:D:356:ARG:HD3	2:D:374:LYS:HE3	1.97	0.46
2:B:279:LEU:N	2:B:302:GLU:OE1	2.48	0.46
2:D:356:ARG:HH21	2:D:370:GLU:HB2	1.81	0.46
2:D:84:THR:HB	2:D:154:LYS:HE2	1.98	0.46
1:C:110:ASP:OD1	1:C:111:VAL:O	2.33	0.46
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.56	0.45
2:B:211:ARG:NE	10:B:602:HOH:O	2.44	0.45
2:D:354:TYR:CE2	2:D:375:ILE:HG13	2.48	0.45
1:C:44:GLU:HG2	1:C:46:LYS:HE2	1.97	0.45
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.98	0.45
2:D:126:LYS:HE2	2:D:127:TYR:CZ	2.51	0.45
1:A:139:THR:HG22	1:A:140:PRO:N	2.27	0.45
1:C:91:GLN:HB2	1:C:161:GLN:HE22	1.81	0.45
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.98	0.45
3:E:3:DC:H2'	3:E:4:OMC:C6	2.52	0.45
1:C:249:LYS:HE3	1:C:251:SER:HB3	1.98	0.45
1:A:134:SER:HB3	1:A:141:GLY:HA2	2.00	0.44
1:A:57:ASN:HB3	10:A:702:HOH:O	2.16	0.44
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.53	0.44
1:C:41:MET:HB3	1:C:46:LYS:HB2	2.00	0.44
1:A:58:THR:HG21	1:A:77:PHE:CD1	2.52	0.44
1:C:172:LYS:HD3	1:C:180:ILE:HB	2.00	0.44
1:A:408:ALA:O	2:B:393:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:GLU:CG	1:C:46:LYS:HE2	2.47	0.44
1:A:4:PRO:HD2	1:A:119:PRO:HB3	2.00	0.43
2:B:89:GLU:HG2	1:C:345:PRO:HG2	1.99	0.43
1:C:79:GLU:HG3	1:C:83:ARG:HE	1.83	0.43
1:A:76:ASP:OD2	1:A:78:ARG:NE	2.49	0.43
1:A:325:LEU:HB3	1:A:387:PRO:HB3	2.00	0.43
1:A:110:ASP:HB3	1:A:220:LYS:CB	2.48	0.43
1:C:317:VAL:HG11	1:C:347:LYS:HB3	2.00	0.43
2:B:307:ARG:O	2:B:311:LYS:HG2	2.18	0.43
1:C:114:ALA:HB1	1:C:160:PHE:CZ	2.54	0.43
1:A:342:TYR:HB3	1:A:348:ASN:HA	2.01	0.43
1:C:139:THR:HB	1:C:140:PRO:HD2	2.01	0.42
1:C:152:GLY:N	3:F:0:DG:H21	2.16	0.42
1:C:458:VAL:HG23	1:C:464:GLN:HG2	2.01	0.42
2:D:263:LYS:HA	2:D:423:VAL:HG11	2.01	0.42
2:D:358:ARG:O	2:D:361:HIS:CE1	2.73	0.42
2:D:350:LYS:HE2	2:D:378:GLU:OE2	2.19	0.42
1:A:125:ARG:HD3	1:A:147:ASN:HA	2.01	0.42
2:D:195:ILE:HD12	2:D:195:ILE:H	1.85	0.42
1:C:79:GLU:OE2	1:C:83:ARG:NH2	2.51	0.42
1:C:58:THR:HG21	1:C:77:PHE:CD1	2.54	0.41
2:D:199:ARG:NE	2:D:233:GLU:OE2	2.54	0.41
1:A:44:GLU:CG	1:A:46:LYS:HE2	2.50	0.41
1:C:207:GLN:O	1:C:211:ARG:HG3	2.20	0.41
1:C:326:ILE:HD13	1:C:388:LYS:HB2	2.02	0.41
2:B:314:VAL:O	2:B:317:VAL:HG22	2.20	0.41
2:D:98:ALA:O	2:D:101:LYS:HE2	2.21	0.41
3:F:29:DG:H2'	3:F:30:DG:C8	2.56	0.41
1:C:50:ILE:CG2	1:C:51:GLY:H	2.34	0.41
1:C:442:VAL:HB	1:C:481:ALA:HB1	2.02	0.41
2:D:115:TYR:O	2:D:149:LEU:HB2	2.21	0.41
1:A:185:ASP:OD1	1:A:185:ASP:N	2.55	0.40
2:B:167:ILE:O	2:B:208:HIS:NE2	2.53	0.40
2:B:200:THR:O	2:B:204:GLU:HG3	2.22	0.40
2:B:121:ASP:O	2:B:125:ARG:HG3	2.22	0.40
1:A:5:ILE:H	1:A:5:ILE:HG13	1.79	0.40
2:B:195:ILE:HD12	2:B:195:ILE:H	1.86	0.40
1:C:65:LYS:HB3	1:C:68:SER:HB3	2.04	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	551/555 (99%)	534 (97%)	16 (3%)	1 (0%)	47 78
1	C	551/555 (99%)	536 (97%)	13 (2%)	2 (0%)	34 66
2	B	411/429 (96%)	398 (97%)	13 (3%)	0	100 100
2	D	406/429 (95%)	389 (96%)	16 (4%)	1 (0%)	47 78
All	All	1919/1968 (98%)	1857 (97%)	58 (3%)	4 (0%)	47 78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	C	4	PRO
2	D	359	GLY
1	C	22	LYS

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	495/495 (100%)	490 (99%)	5 (1%)	76 92
1	C	495/495 (100%)	488 (99%)	7 (1%)	67 89
2	B	377/390 (97%)	377 (100%)	0	100 100
2	D	372/390 (95%)	370 (100%)	2 (0%)	88 96
All	All	1739/1770 (98%)	1725 (99%)	14 (1%)	81 94

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	110	ASP
1	A	123	ASP
1	A	187	LEU
1	A	358	ARG
1	C	5	ILE
1	C	66	LYS
1	C	123	ASP
1	C	138	GLU
1	C	182	GLN
1	C	220	LYS
1	C	221	HIS
2	D	173	LYS
2	D	358	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	373	GLN
1	C	161	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	OMC	F	2	3	19,22,23	3.06	7 (36%)	26,31,34	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	OMC	F	4	3	19,22,23	3.07	7 (36%)	26,31,34	0.71	0
3	OMC	E	2	3	19,22,23	3.07	7 (36%)	26,31,34	0.71	0
3	OMC	E	4	3	19,22,23	3.07	7 (36%)	26,31,34	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	F	2	3	-	0/9/27/28	0/2/2/2
3	OMC	F	4	3	-	0/9/27/28	0/2/2/2
3	OMC	E	2	3	-	0/9/27/28	0/2/2/2
3	OMC	E	4	3	-	0/9/27/28	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	OMC	C2-N3	6.53	1.49	1.36
3	F	4	OMC	C2-N3	6.52	1.49	1.36
3	E	4	OMC	C6-C5	6.48	1.50	1.35
3	F	2	OMC	C6-C5	6.47	1.50	1.35
3	E	2	OMC	C2-N3	6.47	1.49	1.36
3	F	4	OMC	C6-C5	6.44	1.50	1.35
3	E	2	OMC	C6-C5	6.43	1.50	1.35
3	F	2	OMC	C2-N3	6.39	1.49	1.36
3	E	2	OMC	C4-N3	6.19	1.46	1.34
3	F	4	OMC	C4-N3	6.14	1.46	1.34
3	E	4	OMC	C4-N3	6.11	1.46	1.34
3	F	2	OMC	C4-N3	6.10	1.46	1.34
3	E	4	OMC	C4-N4	4.10	1.43	1.33
3	F	4	OMC	C4-N4	4.08	1.43	1.33
3	E	2	OMC	C4-N4	4.07	1.43	1.33
3	F	2	OMC	C4-N4	4.02	1.43	1.33
3	E	4	OMC	C2-N1	3.95	1.48	1.40
3	F	2	OMC	C2-N1	3.93	1.48	1.40
3	F	4	OMC	C2-N1	3.91	1.48	1.40
3	E	2	OMC	C2-N1	3.90	1.48	1.40
3	F	2	OMC	C6-N1	3.80	1.47	1.38
3	E	2	OMC	C6-N1	3.73	1.47	1.38
3	E	4	OMC	C6-N1	3.71	1.46	1.38
3	F	4	OMC	C6-N1	3.70	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	OMC	O2-C2	-2.73	1.18	1.23
3	F	4	OMC	O2-C2	-2.73	1.18	1.23
3	E	4	OMC	O2-C2	-2.73	1.18	1.23
3	F	2	OMC	O2-C2	-2.69	1.18	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	4	OMC	1	0
3	E	2	OMC	1	0
3	E	4	OMC	1	0

5.5 Carbohydrates (i)

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GLC	H	1	4	11,11,12	0.52	0	15,15,17	0.69	0
4	FRU	H	2	4	11,12,12	0.60	0	10,18,18	0.66	0
4	GLC	L	1	4	11,11,12	0.61	0	15,15,17	0.60	0
4	FRU	L	2	4	11,12,12	0.51	0	10,18,18	0.90	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	GLC	H	1	4	-	0/2/19/22	0/1/1/1
4	FRU	H	2	4	-	1/5/24/24	0/1/1/1
4	GLC	L	1	4	-	0/2/19/22	0/1/1/1
4	FRU	L	2	4	-	0/5/24/24	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

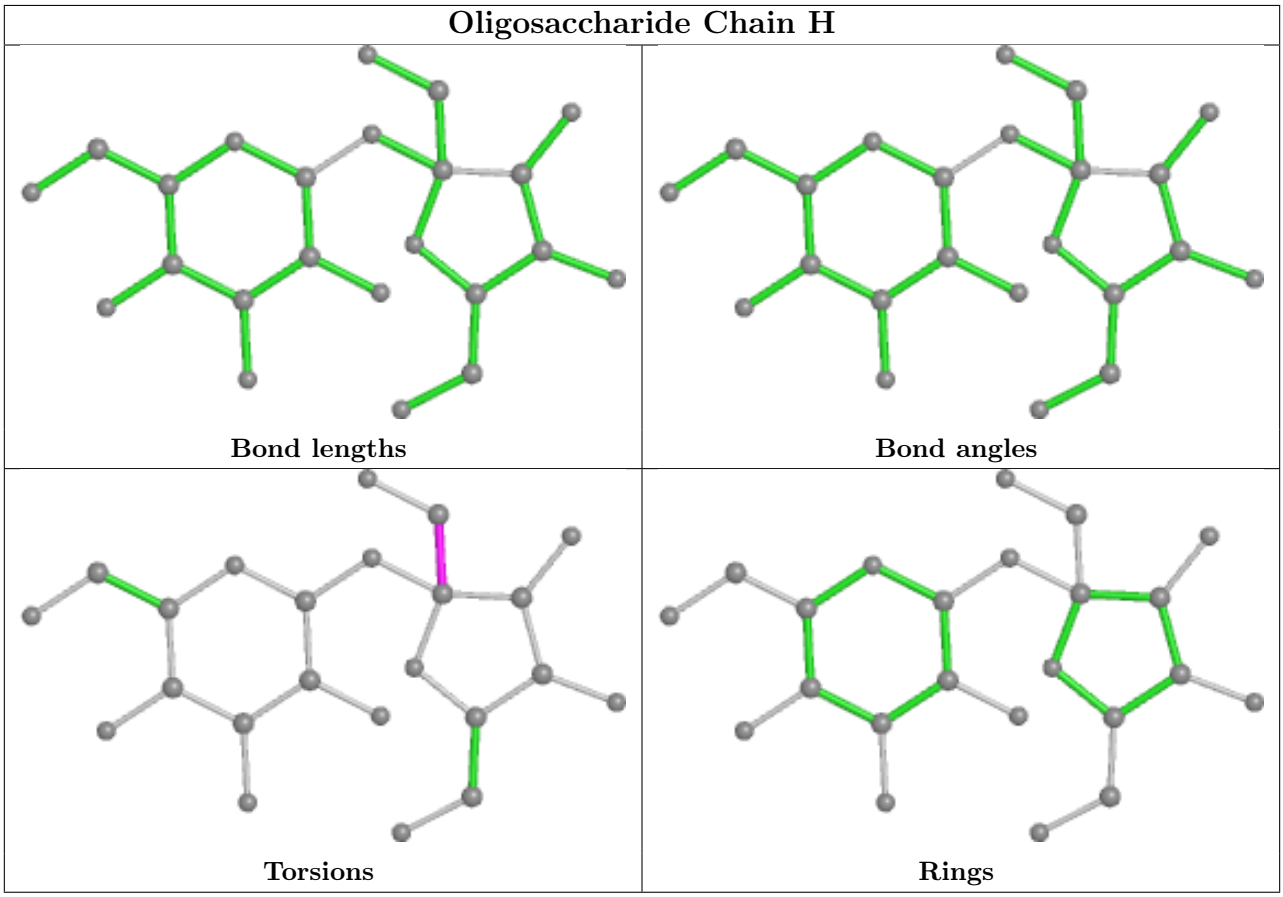
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	2	FRU	O1-C1-C2-C3

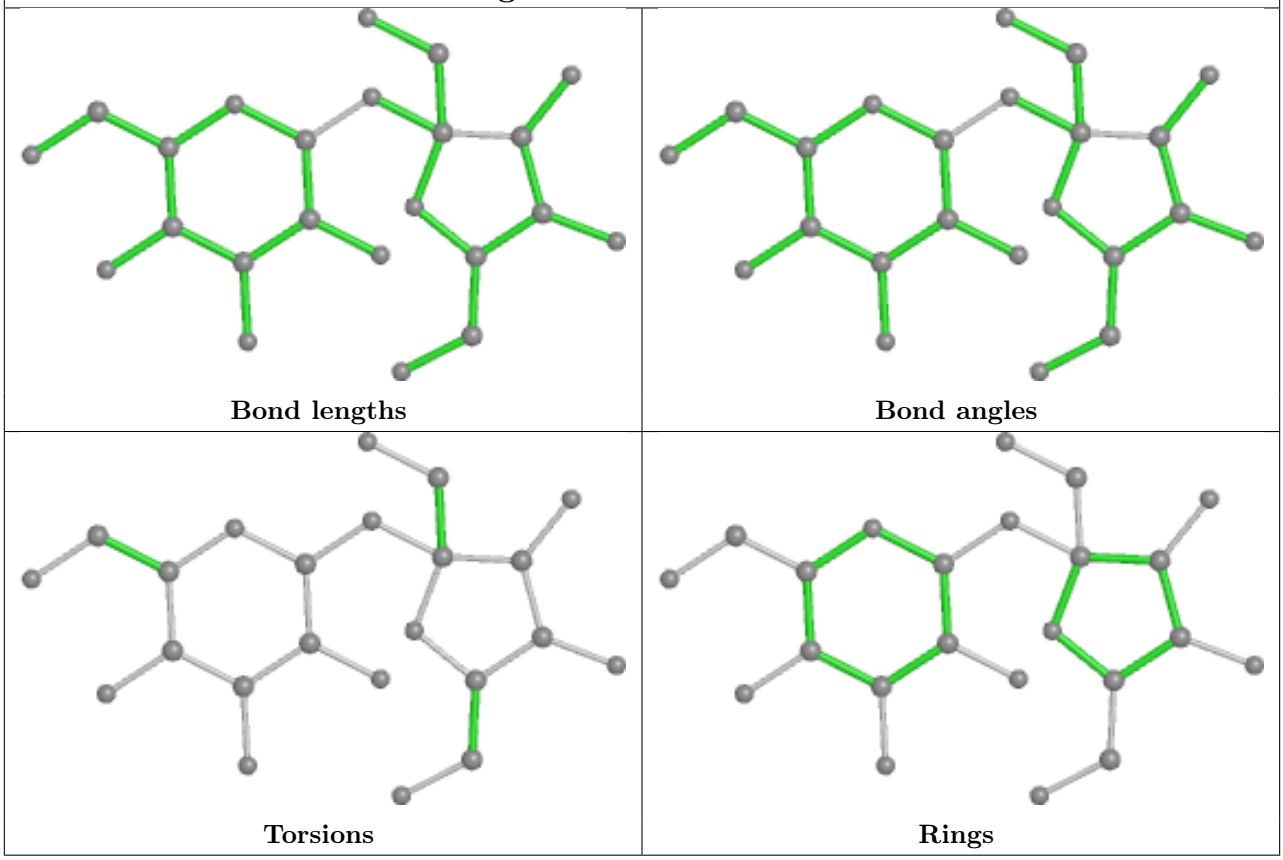
There are no ring outliers.

No monomer is involved in short contacts.

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



Oligosaccharide Chain L



5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 2 are monoatomic and 2 are modelled with single atom - leaving 6 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	$\#\|Z\| > 2$
6	1S0	C	602	7	25,29,29	0.49	0	37,45,45	0.55	0
5	SO4	A	601	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	C	601	-	4,4,4	0.14	0	6,6,6	0.07	0
9	GOL	B	501	-	5,5,5	0.93	0	5,5,5	0.97	0
9	GOL	D	501	-	5,5,5	0.93	0	5,5,5	0.98	0
6	1S0	A	602	7	25,29,29	1.01	3 (12%)	37,45,45	0.53	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
6	1S0	C	602	7	-	8/22/34/34	0/2/2/2
9	GOL	D	501	-	-	0/4/4/4	-
6	1S0	A	602	7	-	14/22/34/34	0/2/2/2
9	GOL	B	501	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	602	1S0	PAC-OAO	-2.70	1.41	1.50
6	A	602	1S0	PAC-OAN	-2.53	1.45	1.54
6	A	602	1S0	PAA-OAJ	-2.12	1.45	1.55

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	602	1S0	PAB-OAK-PAC-OAP
6	A	602	1S0	CAX-OAF-PAA-OAG
6	C	602	1S0	CAX-OAF-PAA-OAJ
6	A	602	1S0	CAT-CAU-CAX-OAF
6	A	602	1S0	OAD-CAU-CAX-OAF
6	A	602	1S0	CAV-CAW-NAQ-CAY
9	B	501	GOL	O1-C1-C2-C3
6	A	602	1S0	CAV-CAW-NAQ-CAZ
6	C	602	1S0	PAC-OAK-PAB-OAM
6	A	602	1S0	OAD-CAW-NAQ-CAY
6	C	602	1S0	PAB-OAG-PAA-OAF
6	A	602	1S0	OAD-CAW-NAQ-CAZ
6	C	602	1S0	CAX-OAF-PAA-OAG
6	A	602	1S0	PAC-OAK-PAB-OAL
6	A	602	1S0	CAX-OAF-PAA-OAJ
6	A	602	1S0	CAX-OAF-PAA-OAI
6	C	602	1S0	CAX-OAF-PAA-OAI
6	C	602	1S0	PAB-OAG-PAA-OAI
6	A	602	1S0	PAB-OAK-PAC-OAO
9	B	501	GOL	O1-C1-C2-O2

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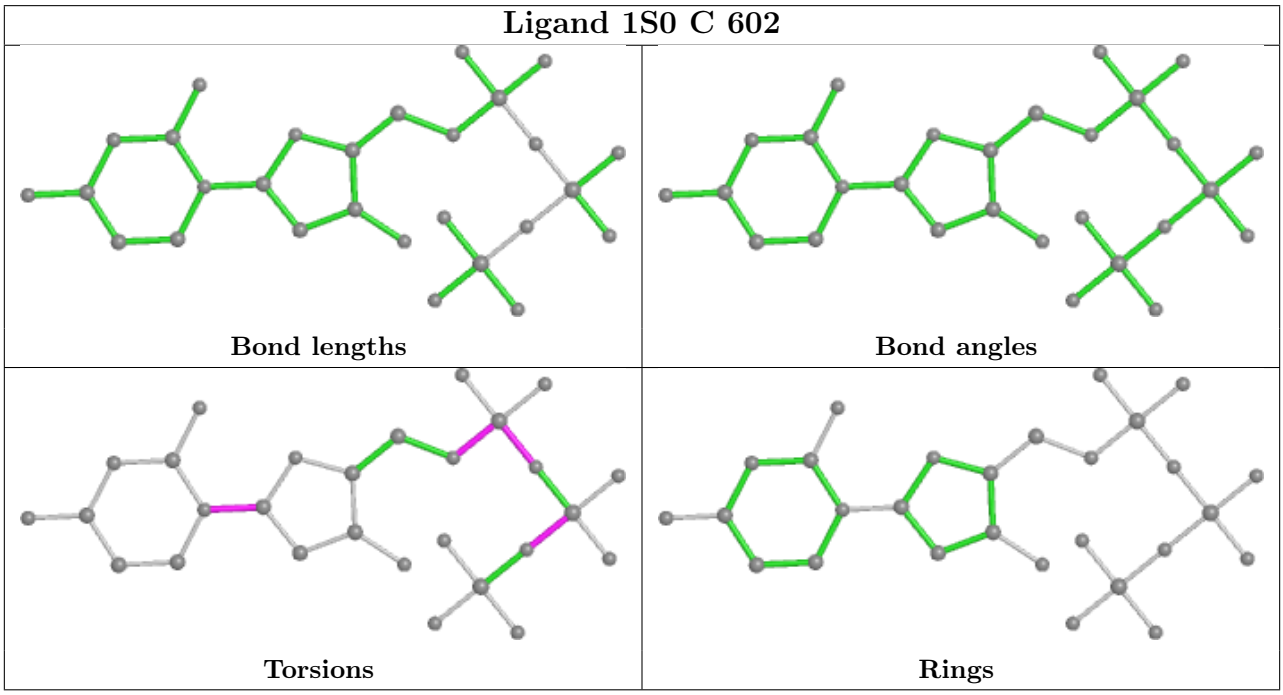
Mol	Chain	Res	Type	Atoms
6	A	602	1S0	PAA-OAG-PAB-OAL
6	A	602	1S0	PAC-OAK-PAB-OAM
6	C	602	1S0	OAD-CAW-NAQ-CAY
6	C	602	1S0	PAC-OAK-PAB-OAG

There are no ring outliers.

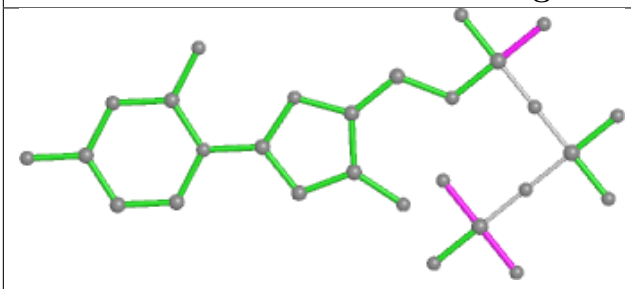
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	602	1S0	3	0
6	A	602	1S0	1	0

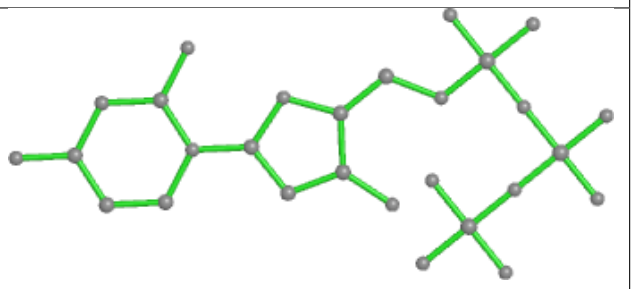
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



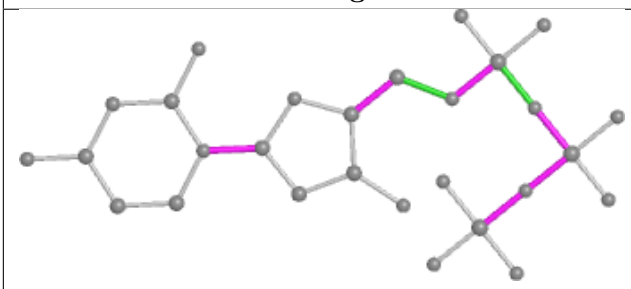
Ligand 1S0 A 602



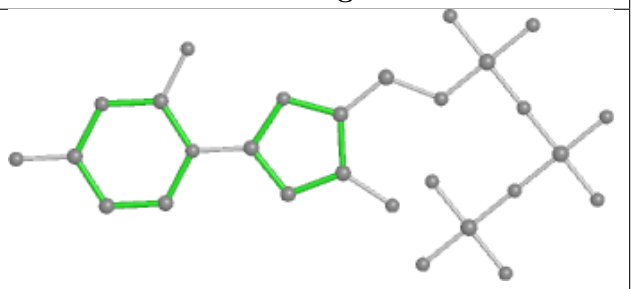
Bond lengths



Bond angles



Torsions



Rings

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	553/555 (99%)	0.63	51 (9%) 9 6	36, 94, 189, 322	0
1	C	553/555 (99%)	0.98	98 (17%) 1 1	33, 100, 208, 309	0
2	B	415/429 (96%)	0.38	24 (5%) 23 19	34, 76, 146, 225	0
2	D	410/429 (95%)	0.44	24 (5%) 22 18	43, 89, 162, 222	0
3	E	33/38 (86%)	-0.33	0 100 100	67, 103, 143, 189	0
3	F	33/38 (86%)	-0.07	2 (6%) 21 17	82, 117, 180, 234	0
All	All	1997/2044 (97%)	0.61	199 (9%) 7 5	33, 89, 188, 322	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	133	PRO	13.7
1	A	137	ASN	12.0
1	C	26	LEU	11.4
1	A	134	SER	10.3
1	C	67	ASP	9.6
1	C	61	PHE	9.3
1	C	63	ILE	9.2
1	C	136	ASN	9.1
1	A	136	ASN	8.9
1	C	34	LEU	8.8
1	A	132	ILE	8.7
1	A	133	PRO	8.6
1	C	137	ASN	8.5
1	C	74	LEU	8.3
1	C	132	ILE	8.1
2	D	226	PRO	8.0
2	B	214	LEU	7.5
1	C	138	GLU	7.4
1	A	24	TRP	7.1

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Mol	Chain	Res	Type	RSRZ
1	C	62	ALA	6.9
1	A	25	PRO	6.8
2	B	91	GLN	6.8
1	C	37	ILE	6.8
1	C	24	TRP	6.7
1	C	25	PRO	6.5
1	C	71	TRP	6.4
1	C	33	ALA	6.1
1	A	140	PRO	6.0
1	A	73	LYS	5.8
1	C	38	CYS	5.7
1	A	30	LYS	5.7
1	A	142	ILE	5.6
1	C	69	THR	5.6
1	C	19	PRO	5.5
1	C	68	SER	5.3
1	A	26	LEU	5.3
1	A	27	THR	5.2
1	C	144	TYR	5.2
1	A	139	THR	5.2
1	C	21	VAL	5.0
1	C	64	LYS	4.9
1	C	52	PRO	4.8
2	B	215	THR	4.8
2	B	226	PRO	4.8
1	A	193	LEU	4.7
1	A	74	LEU	4.7
2	D	87	PHE	4.6
1	A	21	VAL	4.6
2	B	89	GLU	4.6
1	C	146	TYR	4.5
1	C	44	GLU	4.5
2	D	357	MET	4.4
2	D	232	TYR	4.4
1	C	142	ILE	4.3
1	C	73	LYS	4.3
1	C	72	ARG	4.2
1	A	66	LYS	4.2
1	C	134	SER	4.2
1	C	202	ILE	4.1
2	D	91	GLN	4.0
2	D	92	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	138	GLU	4.0
1	A	131	THR	3.9
1	C	286	THR	3.9
1	C	30	LYS	3.9
1	A	286	THR	3.8
2	B	252	TRP	3.8
1	C	50	ILE	3.8
1	C	130	PHE	3.8
2	D	89	GLU	3.8
2	D	209	LEU	3.8
1	A	124	PHE	3.8
1	C	29	GLU	3.7
1	C	15	GLY	3.7
1	A	29	GLU	3.5
1	C	66	LYS	3.4
1	A	177	ASP	3.4
1	C	49	LYS	3.4
1	C	206	ARG	3.4
1	C	108	VAL	3.4
1	C	247	PRO	3.3
1	A	288	ALA	3.3
1	A	254	VAL	3.3
1	C	32	LYS	3.3
1	C	254	VAL	3.3
1	C	41	MET	3.3
2	B	295	LEU	3.3
1	C	219	LYS	3.3
1	C	252	TRP	3.3
1	A	205	LEU	3.2
2	D	90	VAL	3.2
1	C	257	ILE	3.2
1	C	140	PRO	3.2
2	B	4	PRO	3.2
1	C	177	ASP	3.1
1	C	246	LEU	3.1
1	C	59	PRO	3.1
3	F	16	DT	3.0
1	C	209	LEU	3.0
1	A	63	ILE	3.0
1	C	5	ILE	3.0
2	B	227	PHE	3.0
2	D	88	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	22	LYS	3.0
2	D	210	LEU	2.9
2	B	88	TRP	2.9
1	C	261	VAL	2.9
2	B	230	MET	2.9
1	C	28	GLU	2.9
1	C	115	TYR	2.9
1	A	71	TRP	2.9
1	A	67	ASP	2.9
1	C	60	VAL	2.9
1	C	116	PHE	2.9
1	A	1	PRO	2.8
1	C	128	THR	2.8
1	A	252	TRP	2.8
1	C	47	ILE	2.8
1	C	135	ILE	2.8
1	C	293	ILE	2.8
1	C	295	LEU	2.8
1	A	251	SER	2.7
1	C	248	GLU	2.7
2	B	280	SER	2.7
1	C	290	THR	2.7
1	C	187	LEU	2.6
1	C	251	SER	2.6
1	A	31	ILE	2.6
2	B	310	LEU	2.6
1	A	34	LEU	2.6
2	D	427	TYR	2.6
1	C	271	TYR	2.5
1	C	217	PRO	2.5
1	C	222	GLN	2.5
2	B	250	ASP	2.5
1	A	5	ILE	2.5
2	B	210	LEU	2.5
1	C	292	VAL	2.5
1	C	139	THR	2.5
1	A	135	ILE	2.5
2	D	178	ILE	2.5
1	C	40	GLU	2.5
2	B	294	PRO	2.4
2	B	297	GLU	2.4
2	D	230	MET	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	281	LYS	2.4
2	D	318	TYR	2.4
2	B	283	LEU	2.4
1	C	226	PRO	2.4
1	C	309	ILE	2.4
1	C	308	GLU	2.4
1	A	61	PHE	2.3
2	B	308	GLU	2.3
1	C	2	ILE	2.3
1	C	109	LEU	2.3
1	A	211	ARG	2.3
1	A	41	MET	2.3
1	C	18	GLY	2.3
1	C	51	GLY	2.3
1	C	205	LEU	2.3
1	A	109	LEU	2.3
1	A	51	GLY	2.2
1	A	59	PRO	2.2
1	C	199	ARG	2.2
1	C	31	ILE	2.2
2	D	207	GLN	2.2
1	C	106	VAL	2.2
2	D	211	ARG	2.2
1	C	277	ARG	2.2
2	B	428	GLN	2.2
2	D	168	LEU	2.2
1	A	141	GLY	2.2
1	A	292	VAL	2.2
1	C	114	ALA	2.2
1	A	261	VAL	2.2
1	C	228	LEU	2.2
2	D	173	LYS	2.2
2	D	52	PRO	2.2
2	D	356	ARG	2.1
2	B	11	LYS	2.1
2	B	301	LEU	2.1
3	F	17	DT	2.1
1	C	36	GLU	2.1
2	D	422	LEU	2.1
1	C	300	GLU	2.1
1	C	148	VAL	2.1
1	A	293	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	14	PRO	2.1
2	D	95	PRO	2.1
1	C	91	GLN	2.1
1	C	161	GLN	2.1
1	C	120	LEU	2.0
1	A	126	LYS	2.0
2	D	148	VAL	2.0
1	A	23	GLN	2.0
1	C	310	LEU	2.0
2	B	92	LEU	2.0
1	A	223	LYS	2.0
1	A	219	LYS	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, 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	OMC	F	2	21/22	0.93	0.17	102,114,124,132	0
3	OMC	E	2	21/22	0.96	0.17	81,93,102,108	0
3	OMC	F	4	21/22	0.97	0.17	69,85,98,103	0
3	OMC	E	4	21/22	0.97	0.18	60,68,82,89	0

6.3 Carbohydrates (i)

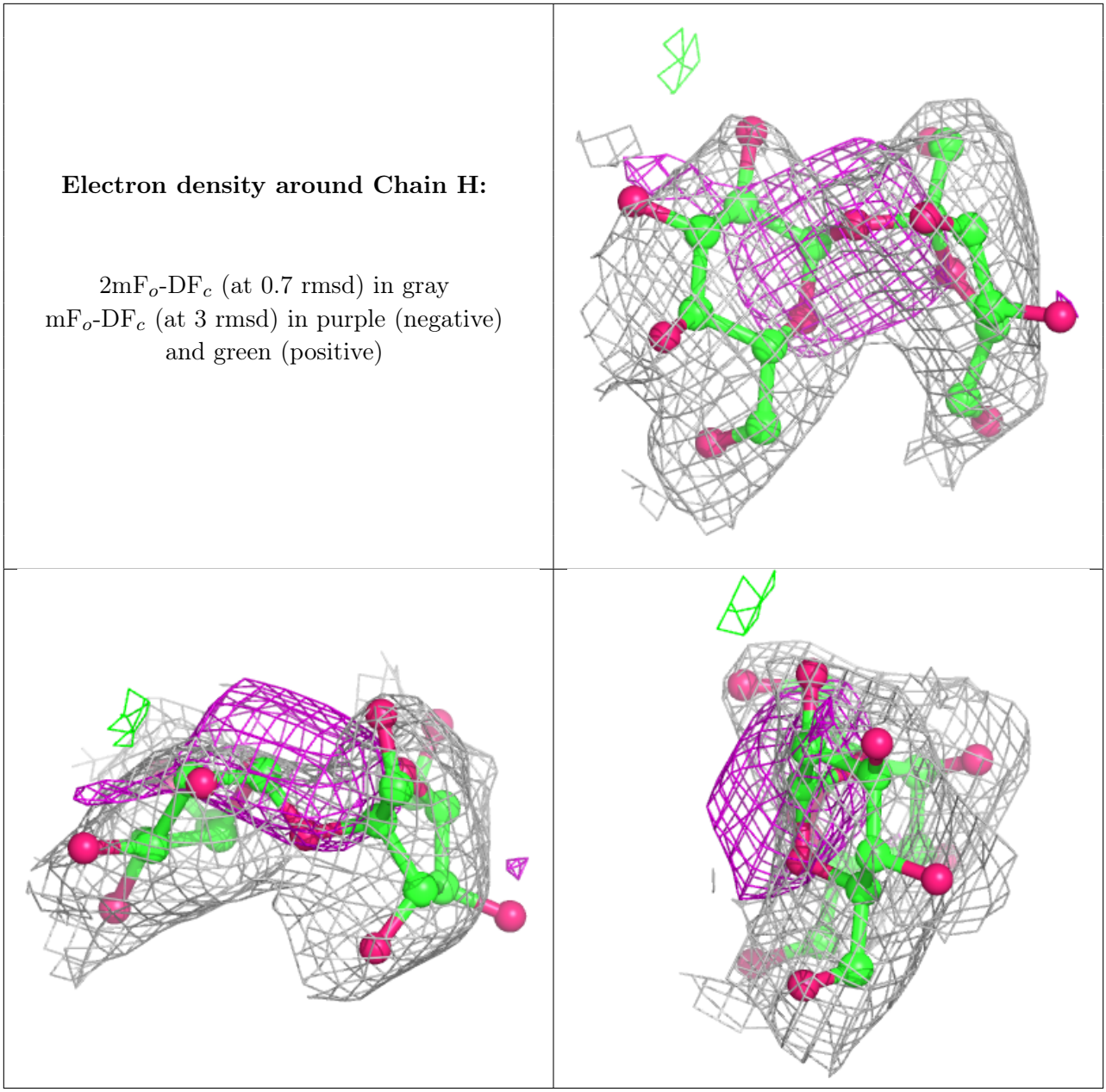
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	FRU	H	2	12/12	0.83	0.28	68,93,102,109	0
4	GLC	H	1	11/12	0.85	0.25	52,76,84,97	0
4	GLC	L	1	11/12	0.88	0.19	62,87,93,94	0
4	FRU	L	2	12/12	0.90	0.18	71,89,105,105	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.

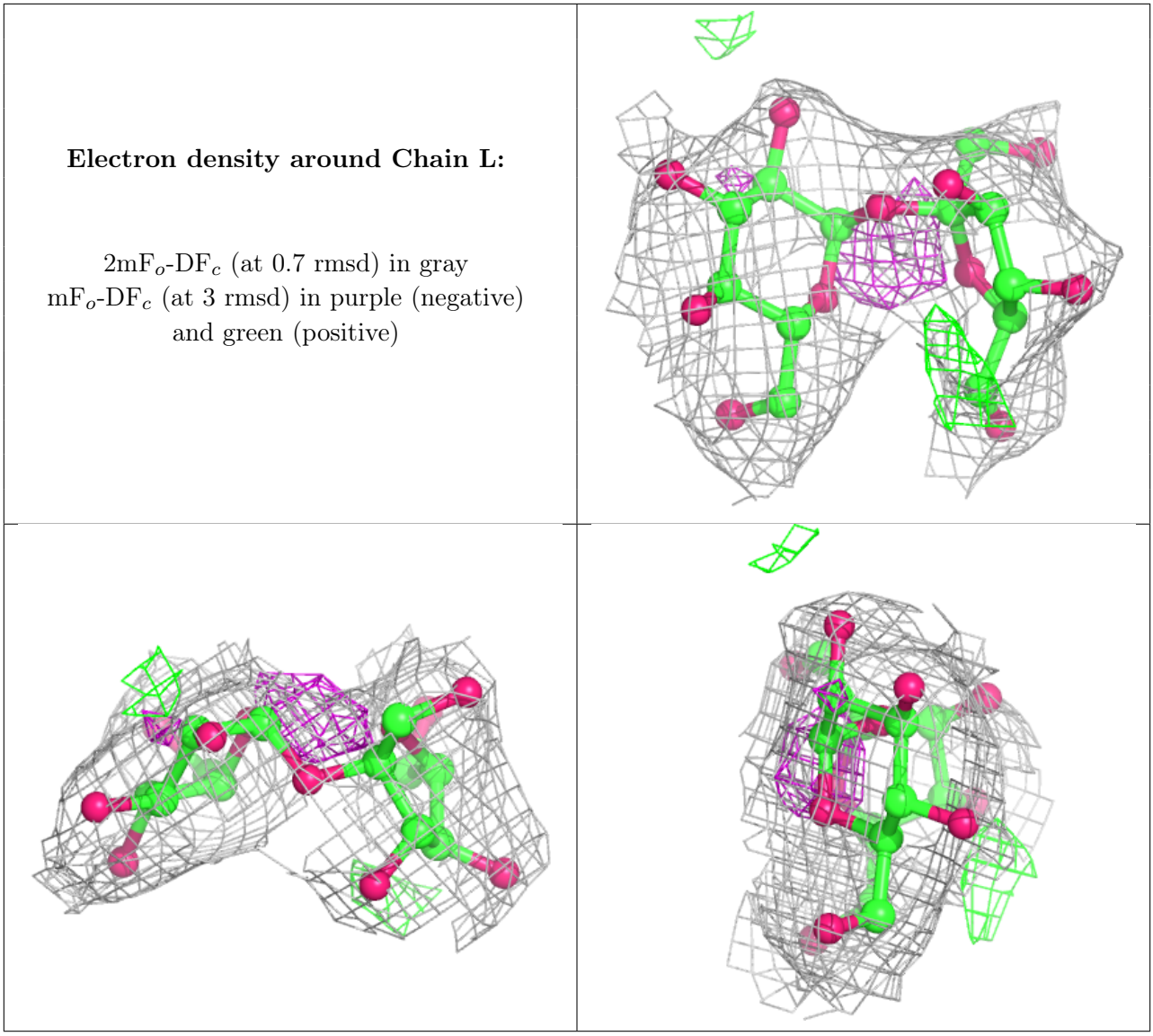
Electron density around Chain H:

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



Electron density around Chain L:

$2mF_o$-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, 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
7	CA	A	603	1/1	0.83	0.14	130,130,130,130	0
7	CA	C	603	1/1	0.87	0.12	148,148,148,148	0
9	GOL	D	501	6/6	0.87	0.24	61,73,81,85	0
9	GOL	B	501	6/6	0.88	0.32	51,62,68,79	0
5	SO4	A	601	5/5	0.90	0.21	97,108,136,139	0
6	1S0	C	602	28/28	0.90	0.17	108,133,170,185	0

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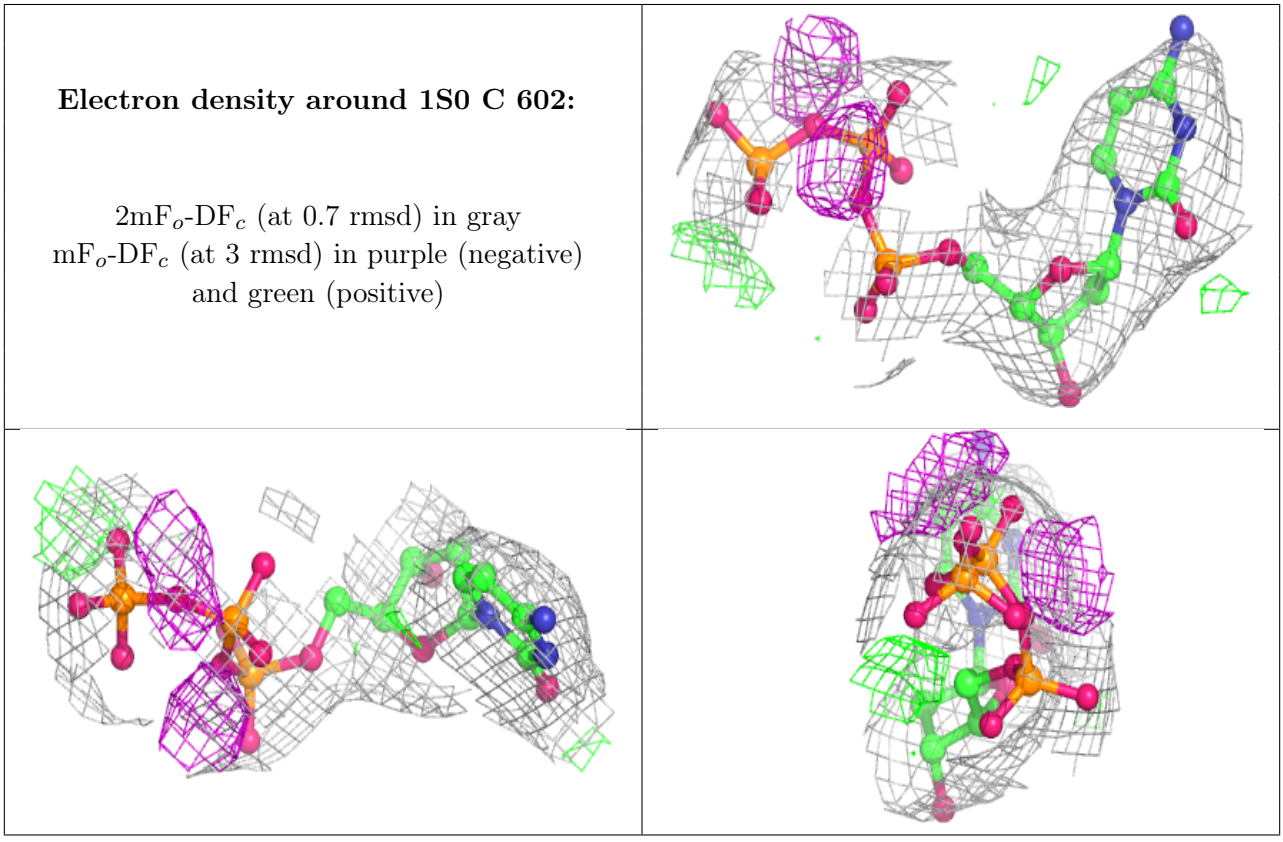
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	1S0	A	602	28/28	0.91	0.16	96,125,148,152	0
8	NH4	C	604	1/1	0.91	0.54	29,29,29,29	0
5	SO4	C	601	5/5	0.93	0.14	91,91,117,126	0
8	NH4	A	604	1/1	0.98	0.29	41,41,41,41	0

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.

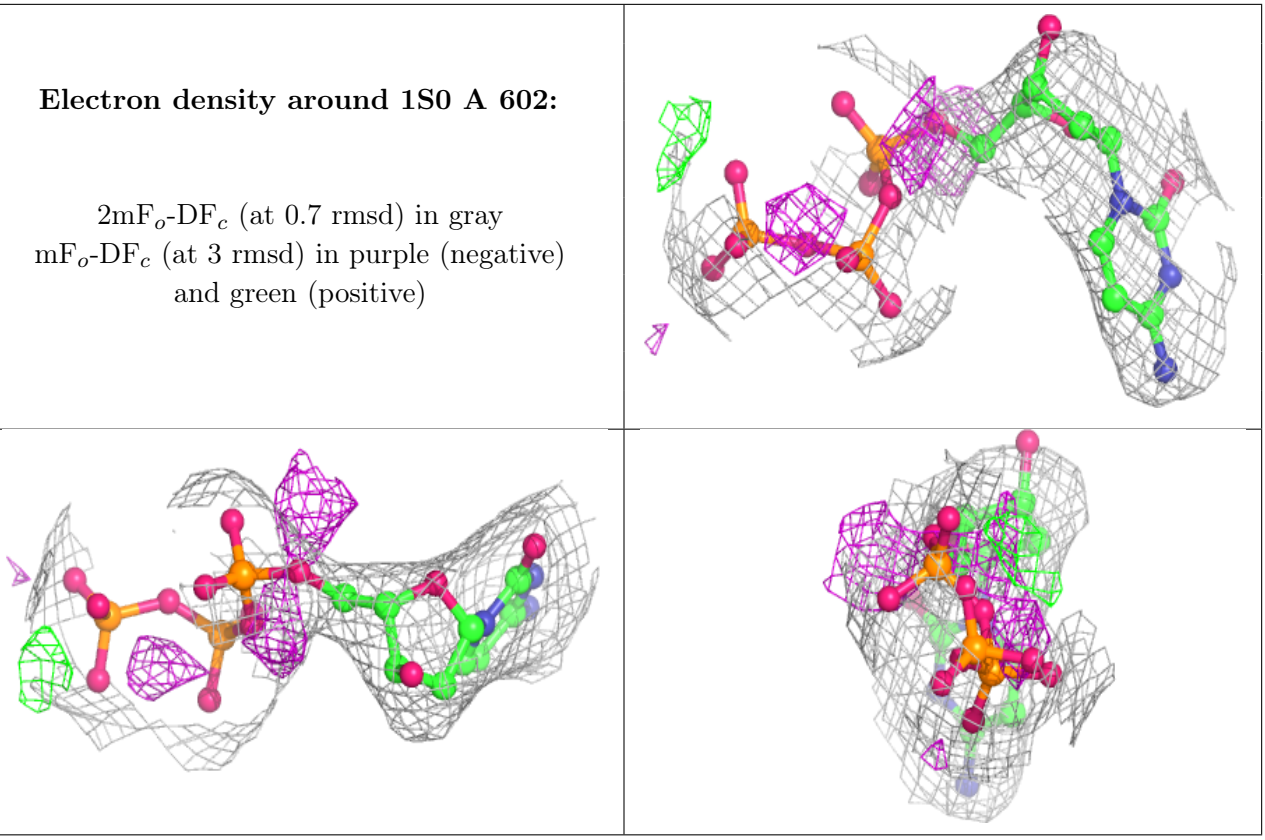
Electron density around 1S0 C 602:

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



Electron density around 1S0 A 602:

$2mF_o$-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.