



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:54 AM UTC

PDB ID : 5HP1 / pdb_00005hp1
Title : STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE In COMPLEX
WITH A DNA aptamer and FOSCARNET, a Pyrophosphate analog
Authors : Das, K.; Arnold, E.
Deposited on : 2016-01-19
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

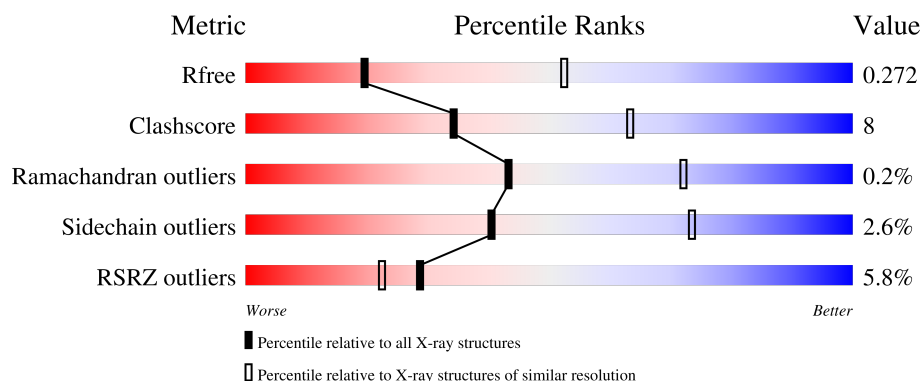
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	555	
1	C	555	
2	B	444	
2	D	444	
3	E	38	

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Mol	Chain	Length	Quality of chain
3	F	38	66% 24% 8%
4	G	2	50% 50%
4	H	2	50% 50%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 17386 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 HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4494	2909	747	831	7			
1	C	553	Total	C	N	O	S	0	0	0
			4495	2910	748	830	7			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	416	Total	C	N	O	S	0	0	0
			3430	2234	567	622	7			
2	D	410	Total	C	N	O	S	0	1	0
			3391	2212	559	614	6			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	initiating methionine	UNP P03366
B	-14	ALA	-	expression tag	UNP P03366
B	-13	HIS	-	expression tag	UNP P03366
B	-12	HIS	-	expression tag	UNP P03366
B	-11	HIS	-	expression tag	UNP P03366
B	-10	HIS	-	expression tag	UNP P03366
B	-9	HIS	-	expression tag	UNP P03366
B	-8	HIS	-	expression tag	UNP P03366
B	-7	ALA	-	expression tag	UNP P03366
B	-6	LEU	-	expression tag	UNP P03366

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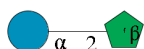
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLU	-	expression tag	UNP P03366
B	-4	VAL	-	expression tag	UNP P03366
B	-3	LEU	-	expression tag	UNP P03366
B	-2	PHE	-	expression tag	UNP P03366
B	-1	GLN	-	expression tag	UNP P03366
B	0	GLY	-	expression tag	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366
D	-15	MET	-	initiating methionine	UNP P03366
D	-14	ALA	-	expression tag	UNP P03366
D	-13	HIS	-	expression tag	UNP P03366
D	-12	HIS	-	expression tag	UNP P03366
D	-11	HIS	-	expression tag	UNP P03366
D	-10	HIS	-	expression tag	UNP P03366
D	-9	HIS	-	expression tag	UNP P03366
D	-8	HIS	-	expression tag	UNP P03366
D	-7	ALA	-	expression tag	UNP P03366
D	-6	LEU	-	expression tag	UNP P03366
D	-5	GLU	-	expression tag	UNP P03366
D	-4	VAL	-	expression tag	UNP P03366
D	-3	LEU	-	expression tag	UNP P03366
D	-2	PHE	-	expression tag	UNP P03366
D	-1	GLN	-	expression tag	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 (38-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	35	Total	C	N	O	P	0	0	0
			720	340	130	215	35			
3	E	35	Total	C	N	O	P	0	0	0
			720	340	130	215	35			

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



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

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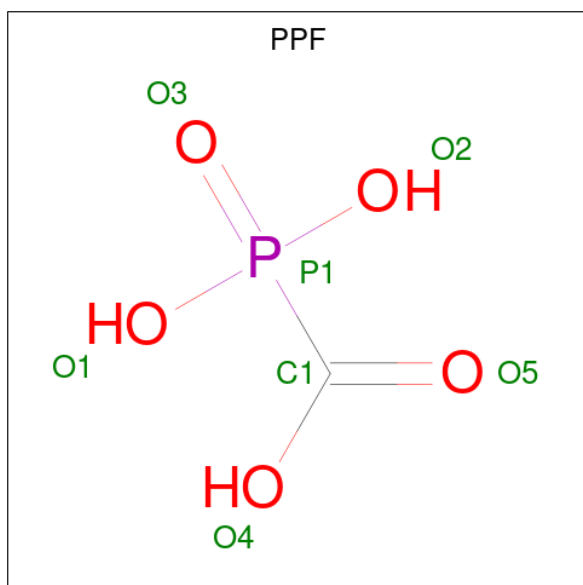
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	H	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

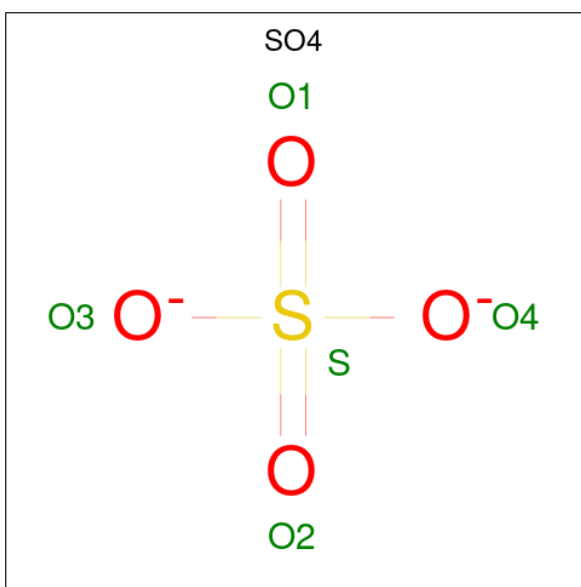
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Mg	0	0
			4	4		
5	C	4	Total	Mg	0	0
			4	4		

- Molecule 6 is PHOSPHONOFORMIC ACID (CCD ID: PPF) (formula: CH₃O₅P).



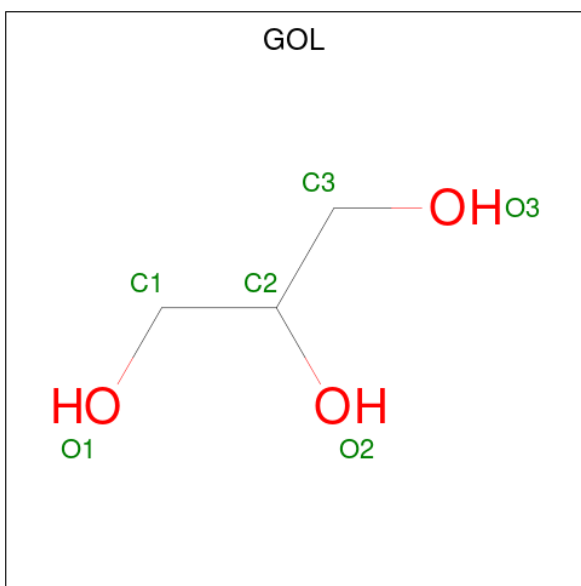
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	P	0	0
			7	1	5	1		
6	C	1	Total	C	O	P	0	0
			7	1	5	1		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



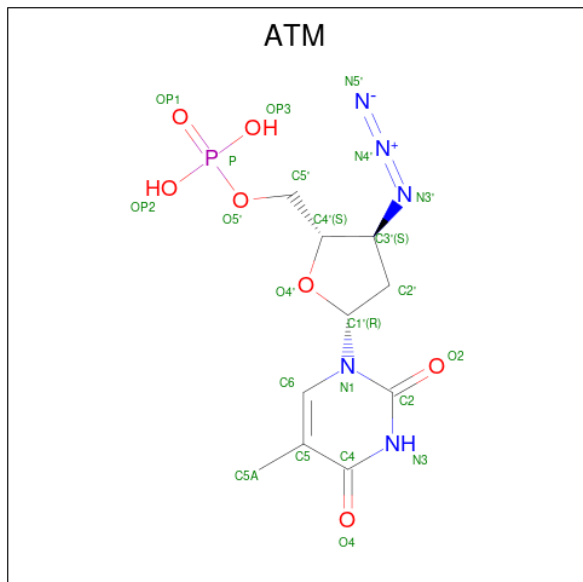
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 9 is 3'-AZIDO-3'-DEOXYTHYMIDINE-5'-MONOPHOSPHATE (CCD ID: ATM) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	F	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
9	E	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

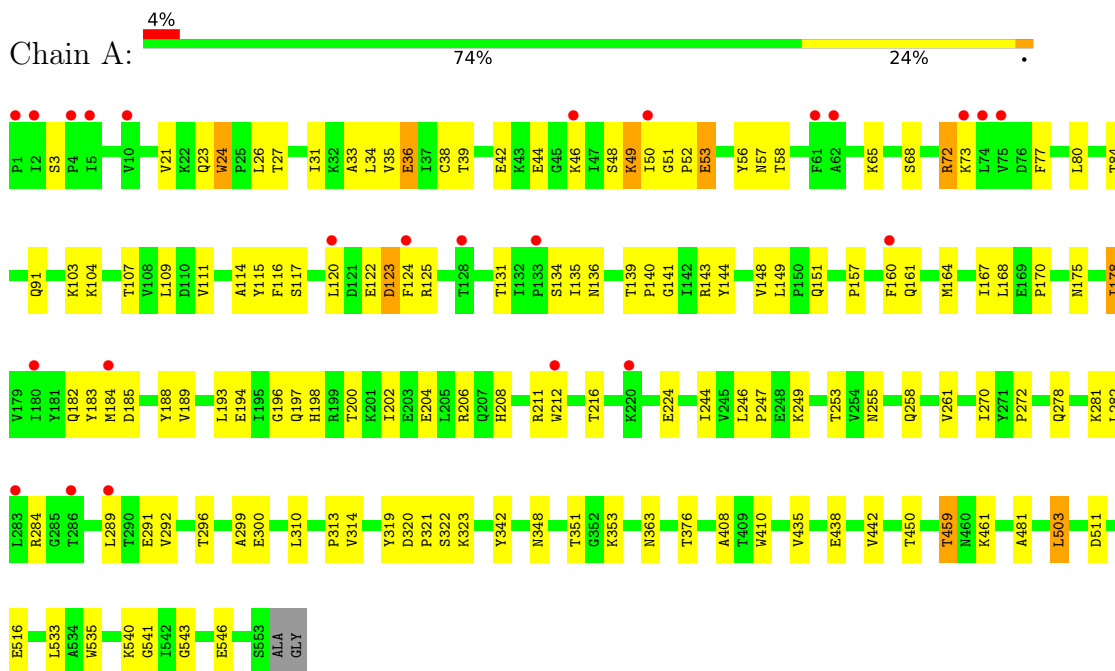
- Molecule 10 is water.

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

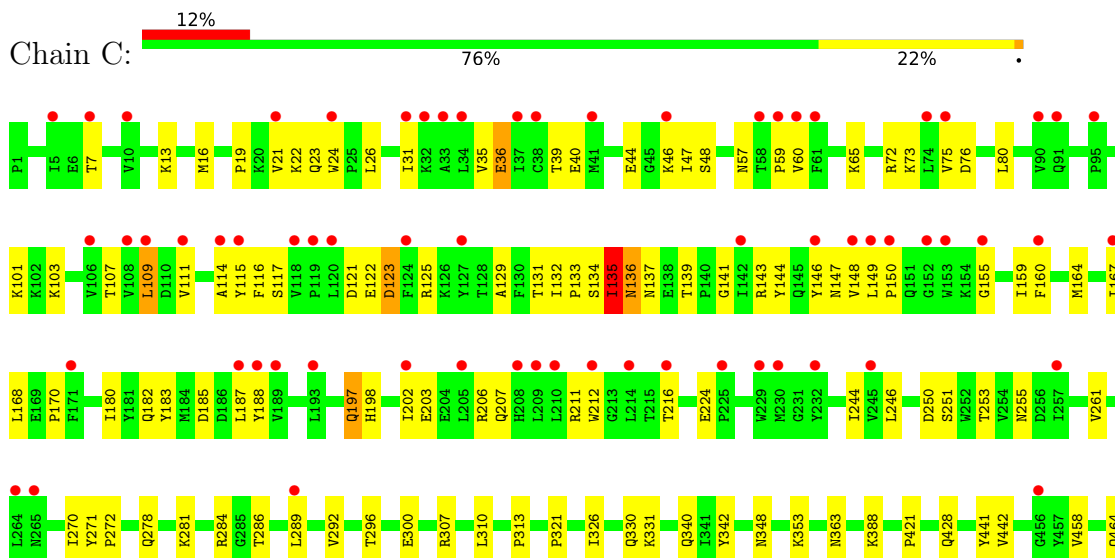
3 Residue-property plots

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: HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT

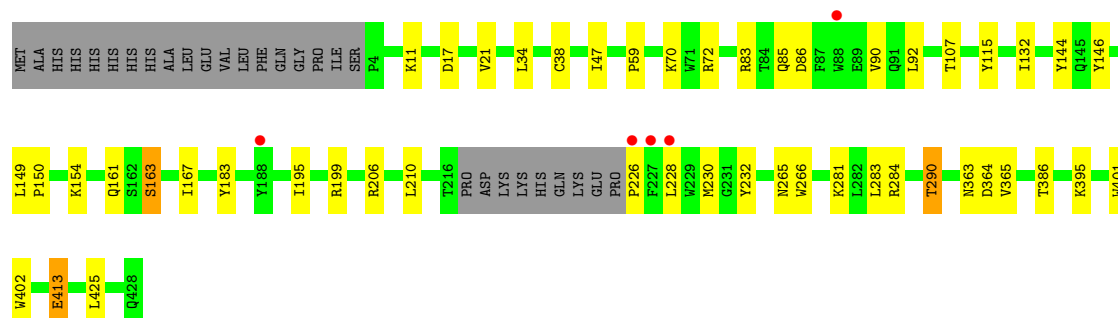
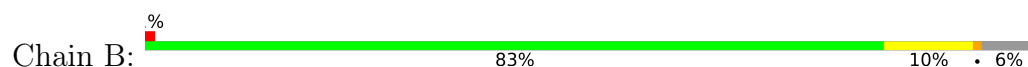


• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT

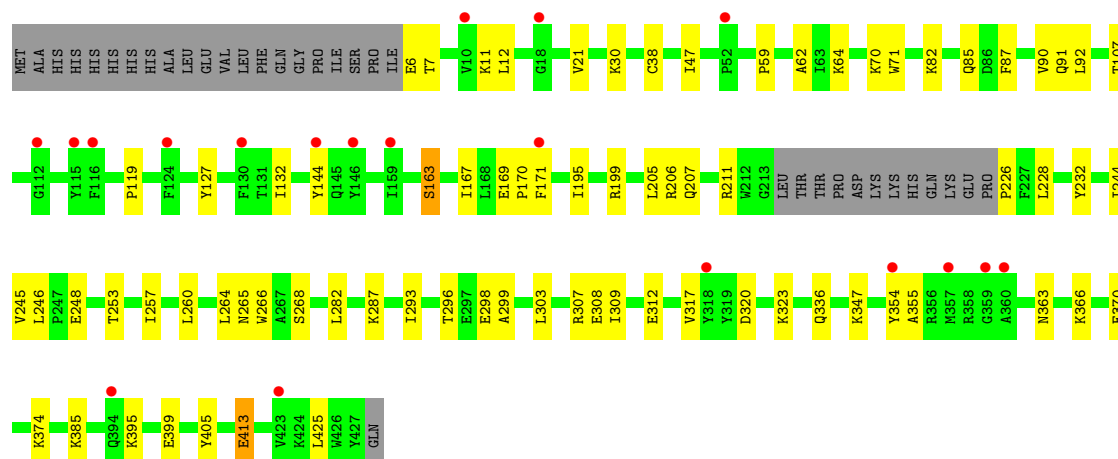
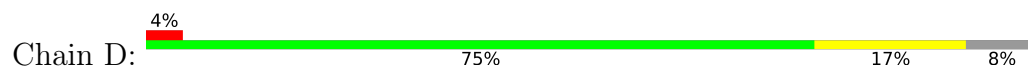




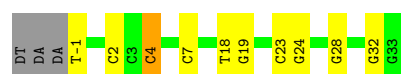
• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT



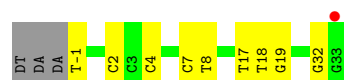
• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT



• Molecule 3: DNA (38-MER)



• Molecule 3: DNA (38-MER)



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

Chain G:  50% 50%

GLC1
FRU2

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

Chain H:  50% 50%

GLC1
FRU2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.33Å 129.07Å 131.54Å 90.00° 101.00° 90.00°	Depositor
Resolution (Å)	45.64 – 2.90 45.64 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (45.64-2.90) 96.6 (45.64-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.246 , 0.273 0.248 , 0.272	Depositor DCC
R_{free} test set	2560 reflections (3.88%)	wwPDB-VP
Wilson B-factor (Å ²)	70.7	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 67.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17386	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATM, PPF, OMC, FRU, GLC, SO4, GOL

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	0.20	0/4612	0.54	2/6268 (0.0%)
1	C	0.21	0/4613	0.61	3/6268 (0.0%)
2	B	0.18	0/3528	0.49	0/4791
2	D	0.21	1/3493 (0.0%)	0.61	1/4747 (0.0%)
3	E	0.24	0/759	0.52	0/1170
3	F	0.23	0/759	0.51	0/1170
All	All	0.20	1/17764 (0.0%)	0.56	6/24414 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	245	VAL	C-N	5.16	1.44	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	224	GLU	CA-C-N	8.72	126.03	119.66
1	C	224	GLU	C-N-CA	8.72	126.03	119.66
1	A	224	GLU	CA-C-N	7.24	124.94	119.66
1	A	224	GLU	C-N-CA	7.24	124.94	119.66
2	D	308	GLU	CA-CB-CG	6.20	126.50	114.10
1	C	141	GLY	N-CA-C	-5.23	104.19	112.66

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	4494	0	4538	93	0
1	C	4495	0	4549	83	1
2	B	3430	0	3460	37	0
2	D	3391	0	3411	49	1
3	E	720	0	396	7	0
3	F	720	0	396	8	0
4	G	23	0	21	3	0
4	H	23	0	21	1	0
5	A	4	0	0	0	0
5	C	4	0	0	0	0
6	A	7	0	0	1	0
6	C	7	0	0	1	0
7	A	5	0	0	0	0
7	C	5	0	0	0	0
8	B	12	0	16	2	0
9	E	22	0	12	1	0
9	F	22	0	12	0	0
10	A	1	0	0	0	0
10	C	1	0	0	0	0
All	All	17386	0	16832	261	1

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 8.

All (261) 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:206:ARG:NH2	2:B:230:MET:O	2.02	0.94
2:B:70:LYS:HG3	2:B:226:PRO:HD2	1.53	0.90
1:C:134:SER:HG	1:C:139:THR:HG1	1.18	0.83
1:C:122:GLU:HA	1:C:125:ARG:HE	1.41	0.83
1:C:330:GLN:HE22	1:C:340:GLN:HE22	1.24	0.83
1:A:134:SER:OG	1:A:139:THR:OG1	1.96	0.81
1:A:56:TYR:O	1:A:143:ARG:NH1	2.15	0.77
1:A:91:GLN:OE1	1:A:161:GLN:NE2	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:GLN:HG2	1:C:133:PRO:HD3	1.65	0.76
1:C:22:LYS:O	1:C:59:PRO:HG3	1.86	0.76
1:A:131:THR:HG22	1:A:143:ARG:HG2	1.69	0.75
2:B:195:ILE:HD11	2:B:199:ARG:HE	1.52	0.74
1:C:73:LYS:HD3	1:C:73:LYS:H	1.53	0.73
2:B:402:TRP:HE1	8:B:2003:GOL:H32	1.54	0.72
2:D:320:ASP:HB3	2:D:323:LYS:HE2	1.72	0.72
2:D:246:LEU:HD11	2:D:264:LEU:HD21	1.71	0.70
3:F:18:DT:H4'	3:F:19:DG:C8	2.29	0.68
2:D:206:ARG:HG3	2:D:228:LEU:HG	1.76	0.68
1:A:459:THR:HG22	1:A:461:LYS:H	1.59	0.67
2:D:85:GLN:HE21	2:D:90:VAL:HG21	1.60	0.66
1:A:73:LYS:O	1:A:151:GLN:NE2	2.29	0.66
1:C:26:LEU:HD22	1:C:132:ILE:HG13	1.79	0.64
1:A:65:LYS:HB2	1:A:68:SER:HB3	1.80	0.64
1:A:65:LYS:HE2	1:A:72:ARG:NH1	2.13	0.64
1:C:206:ARG:NH2	1:C:216:THR:O	2.30	0.63
1:A:122:GLU:HA	1:A:125:ARG:HE	1.62	0.63
1:A:116:PHE:HA	1:A:148:VAL:HG21	1.81	0.62
1:C:123:ASP:N	1:C:123:ASP:OD1	2.33	0.61
2:B:206:ARG:NH2	2:B:228:LEU:O	2.29	0.61
1:C:21:VAL:O	1:C:57:ASN:ND2	2.34	0.61
2:D:266:TRP:CE3	2:D:425:LEU:HD22	2.35	0.61
1:A:206:ARG:NH2	1:A:216:THR:O	2.34	0.60
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.83	0.60
1:C:134:SER:OG	1:C:139:THR:OG1	1.99	0.60
1:C:65:LYS:NZ	6:C:601:PPF:O5	2.28	0.60
1:A:123:ASP:N	1:A:123:ASP:OD1	2.34	0.60
2:D:64:LYS:HE3	2:D:71:TRP:CE2	2.37	0.60
1:A:31:ILE:O	1:A:35:VAL:HG23	2.03	0.59
1:C:65:LYS:HB2	1:C:72:ARG:HG3	1.85	0.59
1:C:111:VAL:HB	1:C:185:ASP:HB2	1.84	0.59
2:D:195:ILE:HD11	2:D:199:ARG:HE	1.67	0.59
1:A:410:TRP:CD1	2:B:363:ASN:HA	2.39	0.58
1:C:278:GLN:OE1	1:C:281:LYS:NZ	2.36	0.58
1:C:40:GLU:O	1:C:44:GLU:HG2	2.04	0.57
2:D:70:LYS:HG3	2:D:226:PRO:HD2	1.86	0.57
1:A:52:PRO:HG2	1:A:53:GLU:HG2	1.85	0.57
1:A:178:ILE:HD11	1:A:189:VAL:HG13	1.87	0.57
1:A:3:SER:HB2	1:A:211:ARG:HH22	1.71	0.56
1:C:203:GLU:O	1:C:207:GLN:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.45	0.56
2:D:246:LEU:HD13	2:D:260:LEU:HD11	1.88	0.56
1:C:47:ILE:HG22	1:C:146:TYR:HA	1.87	0.56
2:D:363:ASN:ND2	2:D:405:TYR:OH	2.39	0.56
1:A:164:MET:HE2	1:A:168:LEU:HG	1.88	0.56
1:C:23:GLN:OE1	1:C:59:PRO:HA	2.06	0.55
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.87	0.55
2:B:92:LEU:O	2:B:161:GLN:NE2	2.39	0.55
1:C:331:LYS:HD3	1:C:421:PRO:HG2	1.89	0.55
1:A:175:ASN:O	1:A:178:ILE:HG22	2.07	0.55
1:A:49:LYS:H	1:A:49:LYS:HD3	1.72	0.54
1:C:65:LYS:HE3	1:C:72:ARG:NH2	2.22	0.54
1:A:459:THR:CG2	1:A:461:LYS:H	2.21	0.54
2:B:281:LYS:O	2:B:284:ARG:HG3	2.07	0.54
2:D:207:GLN:O	2:D:211:ARG:HG3	2.08	0.54
1:A:51:GLY:O	1:A:143:ARG:HD2	2.07	0.54
1:A:272:PRO:HG3	1:A:351:THR:HG21	1.91	0.53
1:C:164:MET:HE3	1:C:168:LEU:HD11	1.89	0.53
1:A:134:SER:HB3	1:A:141:GLY:HA2	1.90	0.53
4:G:1:GLC:H62	4:G:2:FRU:H61	1.90	0.53
1:A:278:GLN:OE1	1:A:281:LYS:NZ	2.41	0.53
1:C:73:LYS:H	1:C:73:LYS:CD	2.21	0.53
1:C:146:TYR:CG	1:C:150:PRO:HB3	2.44	0.53
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.91	0.52
2:D:6:GLU:N	2:D:6:GLU:OE1	2.42	0.52
1:C:65:LYS:HE3	1:C:72:ARG:HH21	1.75	0.52
2:D:395:LYS:HE2	2:D:399:GLU:OE2	2.10	0.52
1:C:115:TYR:CZ	9:E:101:ATM:H1'	2.45	0.52
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.45	0.52
2:D:82:LYS:NZ	2:D:413:GLU:OE2	2.28	0.52
2:D:296:THR:HG23	2:D:299:ALA:H	1.75	0.51
2:B:266:TRP:CE3	2:B:425:LEU:HD21	2.45	0.51
2:B:402:TRP:NE1	8:B:2003:GOL:H32	2.24	0.51
1:C:428:GLN:OE1	1:C:509:GLN:NE2	2.43	0.51
3:E:17:DT:C5'	3:E:17:DT:H6	2.24	0.51
3:E:18:DT:H4'	3:E:19:DG:C8	2.45	0.51
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.93	0.51
1:A:38:CYS:O	1:A:42:GLU:HG3	2.10	0.51
1:A:247:PRO:HB3	1:A:249:LYS:HE3	1.93	0.51
1:C:31:ILE:HG23	1:C:132:ILE:HD11	1.93	0.51
1:C:31:ILE:O	1:C:35:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ILE:HD11	1:A:189:VAL:CG1	2.42	0.50
1:C:115:TYR:HB3	1:C:149:LEU:HB2	1.94	0.50
2:B:163:SER:O	2:B:167:ILE:HG13	2.11	0.50
2:D:309:ILE:O	2:D:312:GLU:HG2	2.12	0.50
1:A:51:GLY:H	1:A:52:PRO:CD	2.25	0.49
1:C:131:THR:HG22	1:C:143:ARG:HG2	1.94	0.49
2:D:87:PHE:HB3	2:D:92:LEU:HB2	1.94	0.49
2:D:38:CYS:SG	2:D:132:ILE:HD11	2.52	0.49
1:C:129:ALA:HA	1:C:144:TYR:O	2.11	0.49
2:D:244:ILE:HD11	2:D:425:LEU:HD21	1.94	0.49
1:A:3:SER:CB	1:A:211:ARG:HH12	2.26	0.49
1:C:183:TYR:OH	3:E:32:DG:N3	2.45	0.49
1:A:200:THR:O	1:A:204:GLU:HG3	2.13	0.49
2:D:47:ILE:HD12	2:D:144:TYR:CD2	2.48	0.49
1:A:3:SER:HB2	1:A:211:ARG:NH2	2.28	0.48
1:A:23:GLN:HE21	1:A:26:LEU:HD11	1.78	0.48
1:C:469:LEU:HD11	1:C:480:GLN:HG2	1.95	0.48
2:D:253:THR:O	2:D:257:ILE:HD12	2.12	0.48
1:A:42:GLU:OE2	1:A:144:TYR:OH	2.25	0.48
1:C:65:LYS:HG3	1:C:72:ARG:HE	1.77	0.48
2:D:11:LYS:O	2:D:85:GLN:HB3	2.13	0.48
1:A:167:ILE:O	1:A:170:PRO:HD2	2.14	0.48
1:A:281:LYS:O	1:A:284:ARG:HG2	2.13	0.48
2:D:257:ILE:HD13	2:D:293:ILE:HD11	1.95	0.48
2:B:266:TRP:CZ3	2:B:425:LEU:HD21	2.48	0.48
1:C:442:VAL:HB	1:C:481:ALA:HB1	1.95	0.48
2:D:7:THR:HG22	2:D:119:PRO:HB2	1.95	0.48
1:A:438:GLU:OE2	1:A:459:THR:HG21	2.14	0.48
1:C:458:VAL:HG23	1:C:464:GLN:HG2	1.96	0.48
1:A:24:TRP:CZ2	3:F:-1:DT:H2'	2.50	0.47
1:C:363:ASN:HA	1:C:511:ASP:OD1	2.13	0.47
1:C:540:LYS:HE3	2:D:265:ASN:OD1	2.14	0.47
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.96	0.47
1:A:541:GLY:HA2	1:A:546:GLU:HB2	1.95	0.47
2:B:17:ASP:O	2:B:83:ARG:HD3	2.13	0.47
1:C:73:LYS:HD3	1:C:73:LYS:N	2.24	0.47
1:C:353:LYS:NZ	3:E:7:DC:OP1	2.47	0.47
1:A:107:THR:OG1	1:A:198:HIS:NE2	2.35	0.47
1:C:101:LYS:HE2	1:C:321:PRO:HG3	1.97	0.47
2:D:296:THR:CG2	2:D:299:ALA:H	2.28	0.47
2:B:47:ILE:HD12	2:B:144:TYR:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:LYS:O	2:B:85:GLN:HB3	2.14	0.47
2:D:303:LEU:O	2:D:307:ARG:HG3	2.15	0.47
1:A:120:LEU:H	1:A:148:VAL:HA	1.79	0.47
1:C:253:THR:HA	1:C:292:VAL:HA	1.97	0.47
1:C:76:ASP:OD2	3:E:-1:DT:H2''	2.14	0.47
2:D:248:GLU:OE1	2:D:307:ARG:NH2	2.48	0.47
1:A:21:VAL:O	1:A:57:ASN:ND2	2.47	0.46
1:A:111:VAL:HB	1:A:185:ASP:HB2	1.97	0.46
2:B:85:GLN:HE21	2:B:90:VAL:HG21	1.80	0.46
1:C:107:THR:OG1	1:C:198:HIS:NE2	2.42	0.46
1:C:246:LEU:HD11	1:C:310:LEU:HD12	1.98	0.46
2:D:12:LEU:HD11	2:D:127:TYR:CZ	2.51	0.46
2:B:72:ARG:HG2	2:B:226:PRO:HB3	1.98	0.46
2:B:413:GLU:HG3	4:G:1:GLC:O6	2.15	0.46
1:A:198:HIS:O	1:A:202:ILE:HG12	2.16	0.46
1:A:296:THR:O	1:A:300:GLU:HG2	2.16	0.46
2:D:30:LYS:NZ	2:D:62:ALA:O	2.47	0.46
1:A:540:LYS:HE3	2:B:265:ASN:OD1	2.16	0.45
1:C:109:LEU:HD12	1:C:187:LEU:HB2	1.98	0.45
3:F:4:OMC:HM23	3:F:4:OMC:H1'	1.74	0.45
2:D:163:SER:O	2:D:167:ILE:HG13	2.15	0.45
1:C:60:VAL:HG22	1:C:75:VAL:HG13	1.97	0.45
1:A:182:GLN:O	1:A:182:GLN:HG3	2.16	0.45
1:C:136:ASN:OD1	1:C:136:ASN:N	2.49	0.45
3:E:17:DT:H6	3:E:17:DT:H5'	1.81	0.45
1:A:46:LYS:HD2	1:A:116:PHE:O	2.16	0.45
1:A:202:ILE:O	1:A:206:ARG:HG3	2.17	0.45
1:C:255:ASN:ND2	1:C:289:LEU:HD13	2.31	0.45
1:C:131:THR:HG22	1:C:143:ARG:CG	2.47	0.45
1:C:326:ILE:HD13	1:C:388:LYS:HB2	1.98	0.45
1:A:49:LYS:H	1:A:49:LYS:CD	2.30	0.45
2:D:366:LYS:O	2:D:370:GLU:HG3	2.16	0.45
1:A:320:ASP:OD1	1:A:322:SER:OG	2.20	0.45
1:C:180:ILE:HA	1:C:188:TYR:O	2.17	0.45
2:D:354:TYR:CE1	2:D:374:LYS:HD2	2.52	0.45
1:A:319:TYR:CZ	1:A:321:PRO:HA	2.52	0.44
1:A:49:LYS:HA	1:A:144:TYR:CD1	2.53	0.44
1:A:103:LYS:HA	1:A:103:LYS:HD3	1.84	0.44
1:A:543:GLY:N	2:B:283:LEU:O	2.49	0.44
1:C:511:ASP:OD1	1:C:512:LYS:NZ	2.48	0.44
1:A:58:THR:HG21	1:A:77:PHE:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:TYR:HB3	1:A:149:LEU:O	2.18	0.44
1:A:157:PRO:HB3	1:A:184:MET:HE1	2.00	0.44
1:A:255:ASN:HD22	1:A:289:LEU:HD13	1.81	0.44
1:C:13:LYS:HB3	1:C:16:MET:HE3	1.99	0.44
3:F:23:DC:H2''	3:F:24:DG:C8	2.52	0.44
2:B:115:TYR:O	2:B:149:LEU:HB2	2.18	0.44
1:C:36:GLU:O	1:C:40:GLU:HG2	2.18	0.44
1:A:435:VAL:HG13	2:B:290:THR:HG21	2.00	0.43
1:C:133:PRO:HB3	1:C:137:ASN:H	1.82	0.43
1:A:24:TRP:CH2	3:F:-1:DT:H2'	2.53	0.43
2:D:320:ASP:CB	2:D:323:LYS:HE2	2.46	0.43
2:D:336:GLN:OE1	2:D:355:ALA:HB2	2.19	0.43
1:A:353:LYS:NZ	3:F:7:DC:OP1	2.51	0.43
2:B:183:TYR:OH	2:B:386:THR:HG23	2.18	0.43
1:C:296:THR:O	1:C:300:GLU:HG2	2.19	0.43
1:A:116:PHE:HA	1:A:148:VAL:CG2	2.46	0.43
2:D:323:LYS:O	2:D:385:LYS:NZ	2.51	0.43
1:C:198:HIS:O	1:C:202:ILE:HG12	2.18	0.43
1:A:27:THR:O	1:A:31:ILE:HG13	2.18	0.43
1:A:50:ILE:HG23	1:A:52:PRO:HD2	2.01	0.43
1:A:51:GLY:N	1:A:52:PRO:CD	2.82	0.43
1:A:26:LEU:O	1:A:31:ILE:HD11	2.18	0.43
1:A:503:LEU:HD12	1:A:503:LEU:HA	1.70	0.43
1:A:26:LEU:HD23	1:A:34:LEU:CD1	2.49	0.42
1:C:19:PRO:HG3	1:C:80:LEU:HB2	2.02	0.42
1:C:182:GLN:O	1:C:182:GLN:HG3	2.18	0.42
2:B:34:LEU:HD23	2:B:34:LEU:HA	1.86	0.42
1:C:134:SER:C	1:C:135:ILE:HG12	2.45	0.42
2:D:298:GLU:OE1	2:D:298:GLU:N	2.45	0.42
1:A:270:ILE:O	1:A:272:PRO:HD3	2.19	0.42
1:C:441:TYR:OH	2:D:287:LYS:O	2.34	0.42
1:A:51:GLY:HA3	1:A:143:ARG:HB2	2.01	0.42
2:B:395:LYS:NZ	4:G:2:FRU:O4	2.50	0.42
2:D:70:LYS:HB2	2:D:70:LYS:HE2	1.77	0.42
2:D:413:GLU:HG3	4:H:1:GLC:O6	2.19	0.42
1:A:33:ALA:O	1:A:36:GLU:HG3	2.19	0.42
2:B:210:LEU:HD12	2:B:210:LEU:O	2.19	0.42
1:A:503:LEU:CD2	1:A:535:TRP:HB2	2.50	0.41
1:A:183:TYR:OH	3:F:32:DG:N3	2.41	0.41
1:A:253:THR:HA	1:A:292:VAL:HA	2.01	0.41
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.56	0.41
1:C:167:ILE:O	1:C:170:PRO:HD2	2.20	0.41
1:C:503:LEU:CD2	1:C:535:TRP:HB2	2.51	0.41
2:D:171:PHE:CD2	2:D:205:LEU:HD13	2.54	0.41
1:A:282:LEU:HD11	1:A:299:ALA:HB1	2.02	0.41
1:C:211:ARG:HG2	1:C:212:TRP:CD1	2.55	0.41
2:B:266:TRP:CE3	2:B:425:LEU:HD11	2.56	0.41
1:C:197:GLN:H	1:C:197:GLN:HG3	1.71	0.41
1:C:342:TYR:HB3	1:C:348:ASN:HA	2.02	0.41
2:D:169:GLU:HB3	2:D:170:PRO:HD3	2.02	0.41
2:B:86:ASP:OD1	2:B:154:LYS:NZ	2.53	0.41
1:C:121:ASP:O	1:C:125:ARG:HG3	2.20	0.41
1:A:320:ASP:OD2	1:A:323:LYS:HE3	2.20	0.41
1:C:270:ILE:O	1:C:272:PRO:HD3	2.21	0.41
1:C:300:GLU:HG2	1:C:300:GLU:H	1.65	0.41
1:A:408:ALA:HB1	2:B:364:ASP:HB3	2.02	0.41
1:A:503:LEU:HD11	1:A:533:LEU:HB3	2.03	0.41
2:B:107:THR:HA	2:B:232:TYR:O	2.20	0.41
1:A:139:THR:HB	1:A:140:PRO:HD2	2.03	0.41
1:C:46:LYS:O	1:C:147:ASN:HB2	2.20	0.41
1:C:103:LYS:HA	1:C:103:LYS:HD3	1.82	0.41
1:A:72:ARG:NH2	6:A:602:PPF:O1	2.49	0.41
1:A:80:LEU:HD11	1:A:124:PHE:CZ	2.55	0.41
1:A:376:THR:HG21	2:B:401:TRP:CH2	2.56	0.41
2:B:11:LYS:HE3	2:B:11:LYS:HB3	1.80	0.41
1:C:114:ALA:HB1	1:C:160:PHE:CZ	2.56	0.41
1:C:271:TYR:CD2	1:C:310:LEU:HD23	2.55	0.41
2:D:12:LEU:HD11	2:D:127:TYR:CE1	2.55	0.41
2:D:265:ASN:O	2:D:268:SER:OG	2.34	0.41
1:C:475:GLN:HB3	1:C:501:TYR:CE2	2.55	0.41
2:D:317:VAL:HG12	2:D:347:LYS:HB3	2.03	0.41
1:A:208:HIS:O	1:A:212:TRP:HD1	2.04	0.40
1:A:258:GLN:OE1	3:F:28:DG:H2"	2.21	0.40
1:A:342:TYR:HB3	1:A:348:ASN:HA	2.02	0.40
2:B:72:ARG:HB2	2:B:226:PRO:HD3	2.02	0.40
1:C:155:GLY:O	1:C:159:ILE:HG12	2.21	0.40
1:C:503:LEU:HD12	1:C:503:LEU:HA	1.76	0.40
2:D:107:THR:HA	2:D:232:TYR:O	2.20	0.40
1:A:104:LYS:HD2	1:A:193:LEU:O	2.21	0.40
2:D:260:LEU:HD21	2:D:303:LEU:HD21	2.03	0.40
1:C:44:GLU:HB2	1:C:46:LYS:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:282:LEU:HD21	2:D:296:THR:HG22	2.02	0.40
1:C:246:LEU:HD13	1:C:307:ARG:HD3	2.04	0.40
1:C:284:ARG:HG2	3:E:8:DT:H5"	2.03	0.40
1:A:80:LEU:O	1:A:84:THR:OG1	2.31	0.40
1:A:194:GLU:CD	1:A:196:GLY:H	2.30	0.40
1:C:116:PHE:HA	1:C:148:VAL:HG21	2.02	0.40
1:C:250:ASP:OD1	1:C:251:SER:N	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:GLN:NE2	2:D:91:GLN:OE1[2_657]	2.06	0.14

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	551/555 (99%)	526 (96%)	24 (4%)	1 (0%)	43	72
1	C	551/555 (99%)	526 (96%)	23 (4%)	2 (0%)	30	59
2	B	412/444 (93%)	399 (97%)	13 (3%)	0	100	100
2	D	407/444 (92%)	396 (97%)	11 (3%)	0	100	100
All	All	1921/1998 (96%)	1847 (96%)	71 (4%)	3 (0%)	43	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	PRO
1	C	313	PRO
1	C	135	ILE

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	492/495 (99%)	468 (95%)	24 (5%)	22	54
1	C	493/495 (100%)	477 (97%)	16 (3%)	34	68
2	B	376/403 (93%)	373 (99%)	3 (1%)	73	90
2	D	371/403 (92%)	369 (100%)	2 (0%)	81	93
All	All	1732/1796 (96%)	1687 (97%)	45 (3%)	40	73

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TRP
1	A	36	GLU
1	A	39	THR
1	A	44	GLU
1	A	48	SER
1	A	49	LYS
1	A	53	GLU
1	A	72	ARG
1	A	109	LEU
1	A	117	SER
1	A	123	ASP
1	A	135	ILE
1	A	136	ASN
1	A	178	ILE
1	A	188	TYR
1	A	197	GLN
1	A	244	ILE
1	A	261	VAL
1	A	291	GLU
1	A	314	VAL
1	A	450	THR
1	A	459	THR
1	A	503	LEU
1	A	516	GLU

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Mol	Chain	Res	Type
2	B	163	SER
2	B	290	THR
2	B	413	GLU
1	C	7	THR
1	C	24	TRP
1	C	36	GLU
1	C	39	THR
1	C	48	SER
1	C	109	LEU
1	C	117	SER
1	C	123	ASP
1	C	135	ILE
1	C	136	ASN
1	C	197	GLN
1	C	244	ILE
1	C	261	VAL
1	C	286	THR
1	C	503	LEU
1	C	516	GLU
2	D	163	SER
2	D	413	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	ASN
2	B	96	HIS
2	B	147	ASN
2	B	151	GLN
2	B	161	GLN
2	B	269	GLN
1	C	151	GLN
1	C	161	GLN
1	C	330	GLN
1	C	394	GLN
1	C	428	GLN
1	C	464	GLN
1	C	471	ASN
1	C	509	GLN
2	D	137	ASN
2	D	151	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	E	2	3	19,22,23	2.72	6 (31%)	25,31,34	0.79	0
3	OMC	F	4	3	19,22,23	2.72	6 (31%)	25,31,34	0.69	0
3	OMC	E	4	3	19,22,23	2.68	6 (31%)	25,31,34	0.70	0
3	OMC	F	2	3	19,22,23	2.70	6 (31%)	25,31,34	0.79	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	E	2	3	-	0/9/27/28	0/2/2/2
3	OMC	F	4	3	-	1/9/27/28	0/2/2/2
3	OMC	E	4	3	-	1/9/27/28	0/2/2/2
3	OMC	F	2	3	-	1/9/27/28	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4	OMC	C6-C5	6.01	1.49	1.35
3	F	2	OMC	C6-C5	5.95	1.48	1.35
3	E	2	OMC	C6-C5	5.94	1.48	1.35
3	E	4	OMC	C6-C5	5.92	1.48	1.35
3	F	4	OMC	C2-N3	5.86	1.48	1.36
3	E	2	OMC	C2-N3	5.84	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	OMC	C2-N3	5.83	1.47	1.36
3	E	4	OMC	C2-N3	5.71	1.47	1.36
3	E	2	OMC	C4-N3	5.36	1.45	1.34
3	F	4	OMC	C4-N3	5.33	1.45	1.34
3	E	4	OMC	C4-N3	5.31	1.45	1.34
3	F	2	OMC	C4-N3	5.29	1.45	1.34
3	F	4	OMC	C2-N1	4.18	1.48	1.40
3	F	2	OMC	C2-N1	4.16	1.48	1.40
3	E	4	OMC	C2-N1	4.14	1.48	1.40
3	E	2	OMC	C2-N1	4.14	1.48	1.40
3	F	2	OMC	C4-N4	3.27	1.41	1.33
3	F	4	OMC	C4-N4	3.25	1.41	1.33
3	E	2	OMC	C4-N4	3.23	1.41	1.33
3	E	4	OMC	C4-N4	3.22	1.41	1.33
3	E	2	OMC	C6-N1	3.17	1.45	1.38
3	F	4	OMC	C6-N1	3.07	1.45	1.38
3	F	2	OMC	C6-N1	3.05	1.45	1.38
3	E	4	OMC	C6-N1	3.02	1.45	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	OMC	C1'-C2'-O2'-CM2
3	F	4	OMC	C1'-C2'-O2'-CM2
3	E	4	OMC	C1'-C2'-O2'-CM2

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates ⓘ

4 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GLC	G	1	4	11,11,12	0.53	0	15,15,17	0.80	1 (6%)
4	FRU	G	2	4	11,12,12	0.52	0	10,18,18	0.70	0
4	GLC	H	1	4	11,11,12	0.56	0	15,15,17	0.62	0
4	FRU	H	2	4	11,12,12	0.51	0	10,18,18	0.64	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	G	1	4	-	2/2/19/22	0/1/1/1
4	FRU	G	2	4	-	4/5/24/24	0/1/1/1
4	GLC	H	1	4	-	0/2/19/22	0/1/1/1
4	FRU	H	2	4	-	2/5/24/24	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	GLC	C1-O5-C5	2.08	114.97	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

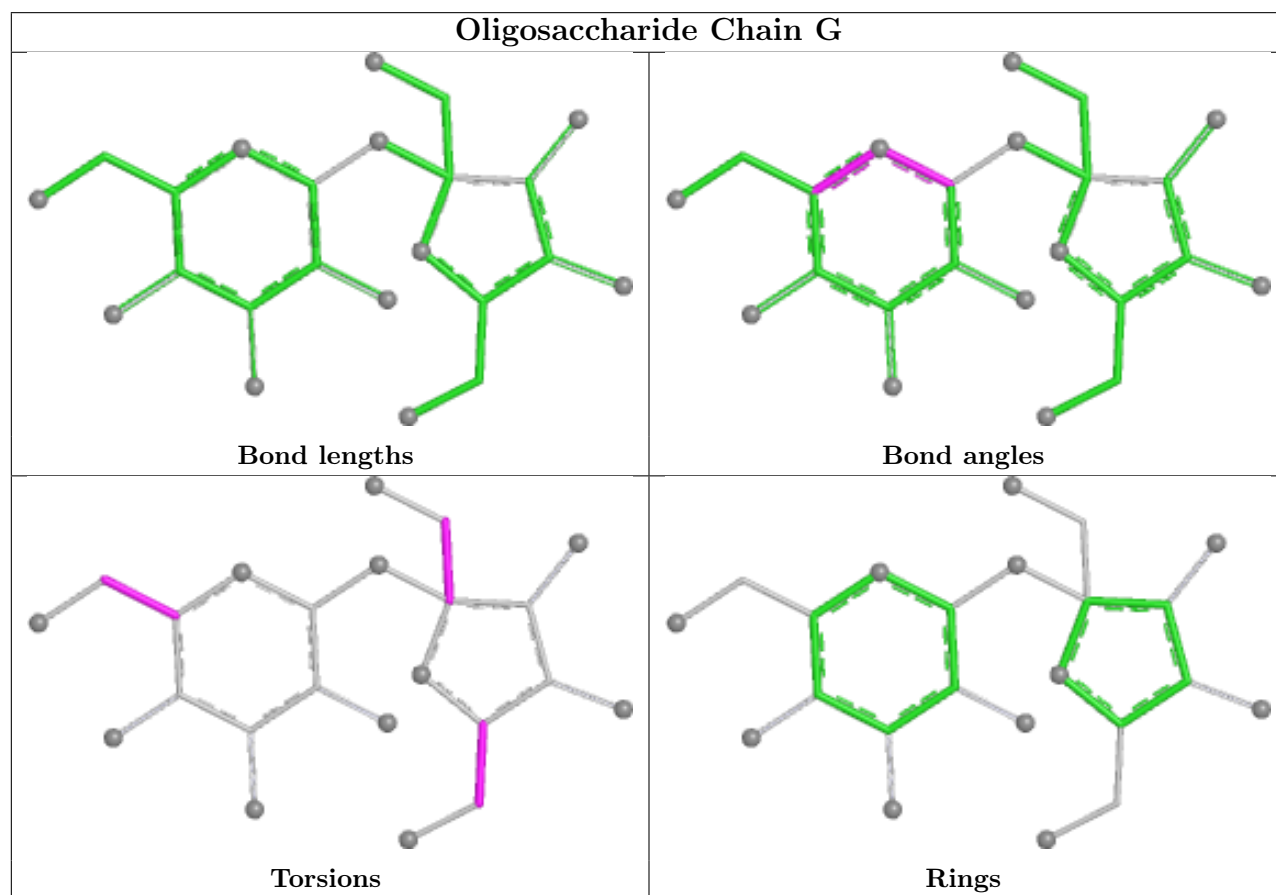
Mol	Chain	Res	Type	Atoms
4	H	2	FRU	O5-C5-C6-O6
4	H	2	FRU	C4-C5-C6-O6
4	G	2	FRU	C4-C5-C6-O6
4	G	2	FRU	O5-C5-C6-O6
4	G	2	FRU	O1-C1-C2-C3
4	G	2	FRU	O1-C1-C2-O2
4	G	1	GLC	C4-C5-C6-O6
4	G	1	GLC	O5-C5-C6-O6

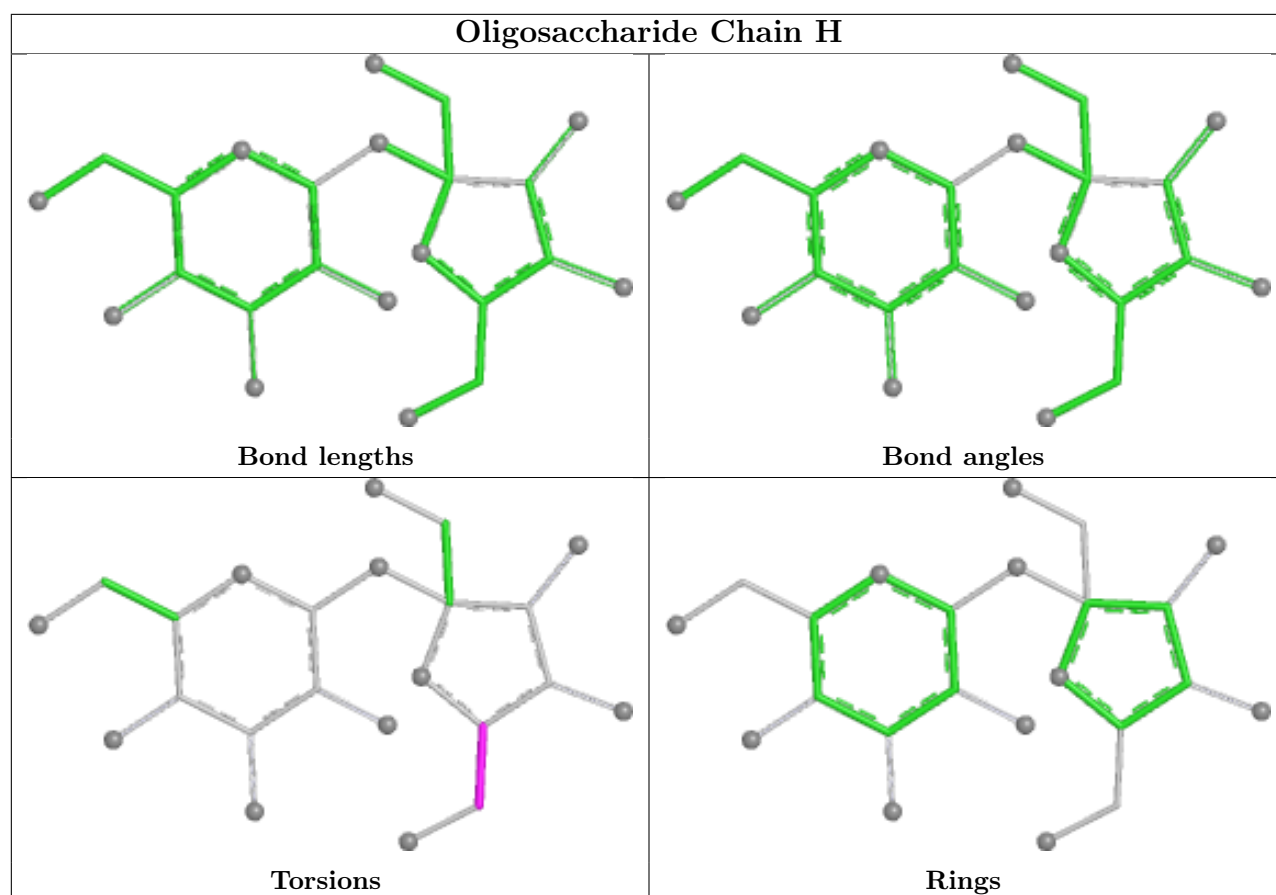
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	FRU	2	0
4	H	1	GLC	1	0
4	G	1	GLC	2	0

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





5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\# Z > 2$
8	GOL	B	2003	-	5,5,5	0.41	0	5,5,5	0.23	0
6	PPF	A	602	5	4,6,6	1.15	0	3,9,9	0.83	0
6	PPF	C	601	5	4,6,6	1.12	0	3,9,9	0.97	0
9	ATM	E	101	3,5	20,23,24	1.21	2 (10%)	26,32,35	2.37	9 (34%)
8	GOL	B	2002	-	5,5,5	0.38	0	5,5,5	0.19	0
7	SO4	A	606	-	4,4,4	0.23	0	6,6,6	0.09	0
9	ATM	F	101	3,5	20,23,24	1.30	2 (10%)	26,32,35	2.47	9 (34%)
7	SO4	C	605	-	4,4,4	0.25	0	6,6,6	0.08	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	PPF	A	602	5	-	0/0/6/6	-
6	PPF	C	601	5	-	0/0/6/6	-
9	ATM	E	101	3,5	-	0/10/24/25	0/2/2/2
8	GOL	B	2002	-	-	2/4/4/4	-
9	ATM	F	101	3,5	-	0/10/24/25	0/2/2/2
8	GOL	B	2003	-	-	4/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	101	ATM	C6-C5	3.22	1.39	1.34
9	F	101	ATM	C4-C5	-3.19	1.39	1.44
9	E	101	ATM	C4-C5	-3.03	1.39	1.44
9	E	101	ATM	C6-C5	2.92	1.39	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	101	ATM	C4-N3-C2	-5.91	119.60	127.34
9	E	101	ATM	C4-N3-C2	-5.88	119.63	127.34
9	E	101	ATM	C5-C4-N3	5.67	120.25	115.32
9	F	101	ATM	C5-C4-N3	5.62	120.21	115.32
9	F	101	ATM	O4-C4-C5	-4.21	120.10	124.92
9	E	101	ATM	O4-C4-C5	-4.20	120.11	124.92
9	F	101	ATM	N3-C2-N1	4.11	120.24	114.89
9	E	101	ATM	N3-C2-N1	3.63	119.62	114.89
9	F	101	ATM	C5-C6-N1	-3.40	119.62	123.31
9	E	101	ATM	C5-C6-N1	-3.38	119.64	123.31
9	F	101	ATM	O4'-C1'-N1	3.12	113.40	107.86
9	F	101	ATM	C6-C5-C4	2.94	120.44	118.02
9	E	101	ATM	C6-C5-C4	2.70	120.25	118.02
9	E	101	ATM	C5A-C5-C6	-2.49	119.49	122.85
9	E	101	ATM	C2'-C1'-N1	-2.30	108.06	113.81
9	F	101	ATM	O2-C2-N1	-2.22	119.90	122.80
9	E	101	ATM	O2-C2-N1	-2.22	119.91	122.80
9	F	101	ATM	C5A-C5-C6	-2.09	120.02	122.85

There are no chirality outliers.

All (6) torsion outliers are listed below:

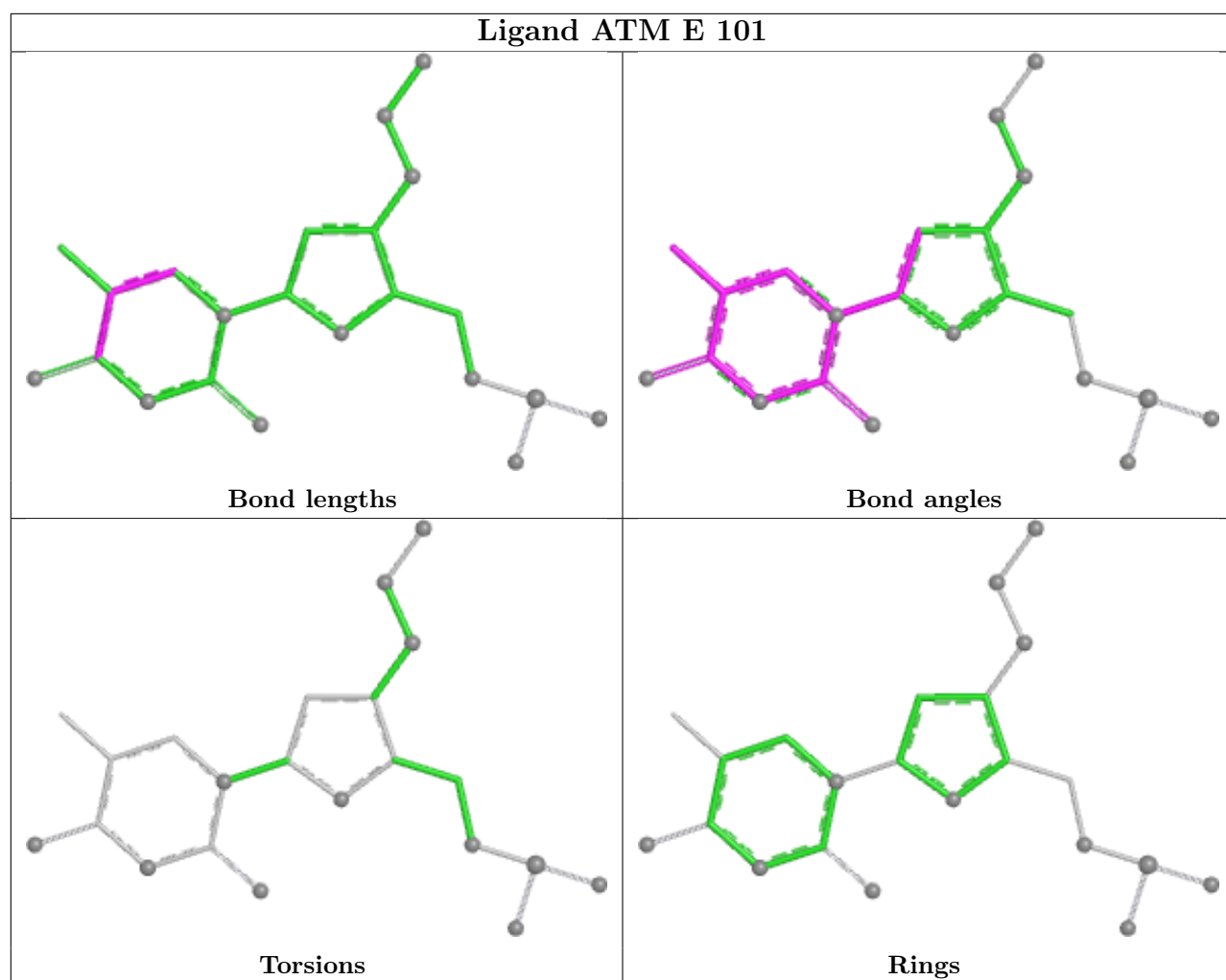
Mol	Chain	Res	Type	Atoms
8	B	2002	GOL	O1-C1-C2-C3
8	B	2003	GOL	O1-C1-C2-C3
8	B	2003	GOL	C1-C2-C3-O3
8	B	2003	GOL	O1-C1-C2-O2
8	B	2002	GOL	O1-C1-C2-O2
8	B	2003	GOL	O2-C2-C3-O3

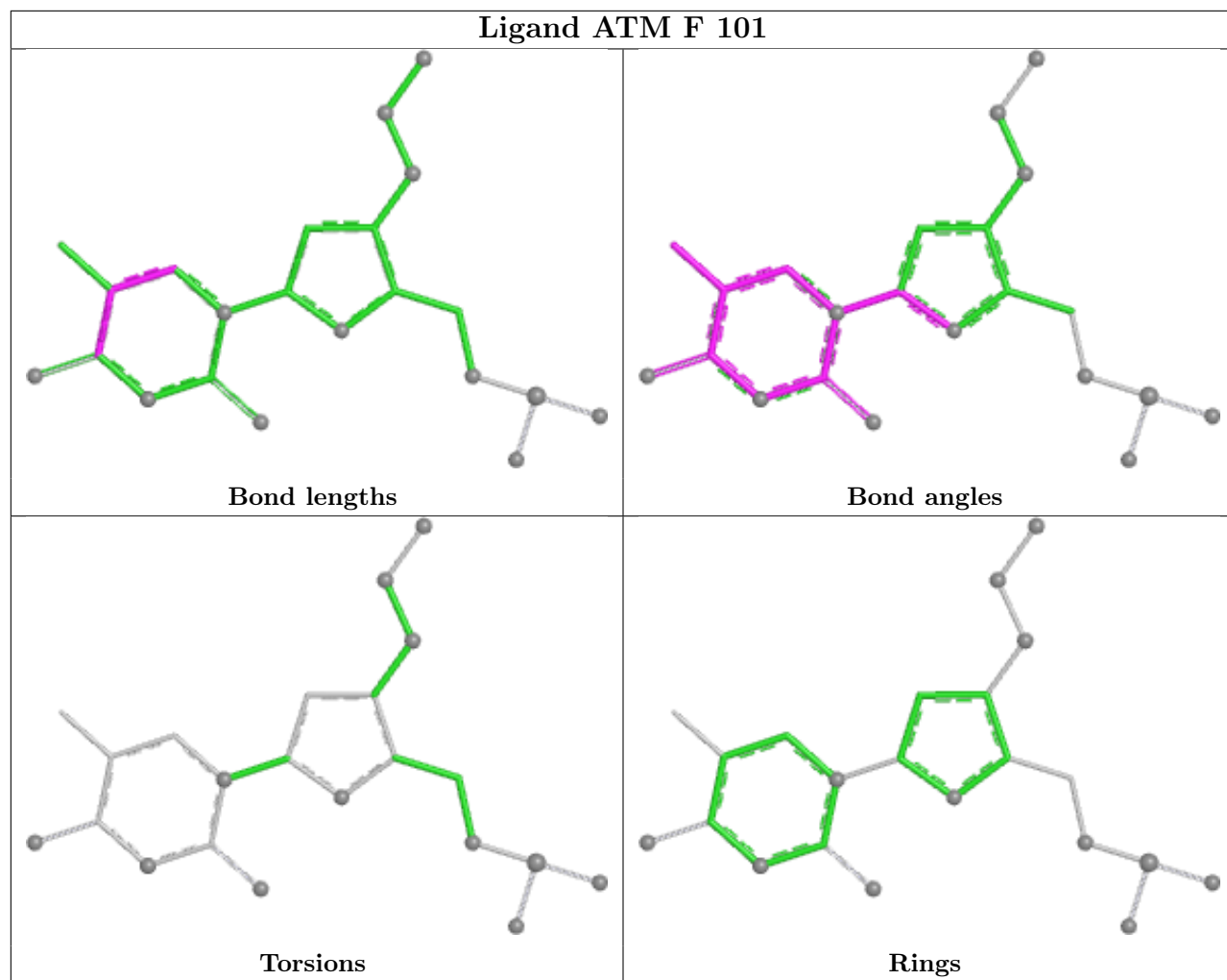
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	2003	GOL	2	0
6	A	602	PPF	1	0
6	C	601	PPF	1	0
9	E	101	ATM	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	553/555 (99%)	0.35	24 (4%) 40 31	35, 103, 171, 223	0
1	C	553/555 (99%)	0.61	67 (12%) 8 7	35, 121, 215, 263	0
2	B	416/444 (93%)	0.07	5 (1%) 76 69	42, 82, 149, 195	0
2	D	410/444 (92%)	0.47	19 (4%) 37 29	37, 98, 167, 238	1 (0%)
3	E	33/38 (86%)	0.14	1 (3%) 52 43	80, 118, 143, 210	0
3	F	33/38 (86%)	-0.29	0 100 100	71, 103, 134, 175	0
All	All	1998/2074 (96%)	0.38	116 (5%) 29 22	35, 99, 191, 263	1 (0%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	111	VAL	6.0
1	C	205	LEU	4.4
1	C	229	TRP	4.3
2	D	146	TYR	4.3
1	C	232	TYR	4.3
1	C	114	ALA	3.9
1	C	187	LEU	3.9
1	C	38	CYS	3.9
1	C	153	TRP	3.8
1	A	2	ILE	3.8
1	A	184	MET	3.8
1	A	124	PHE	3.6
1	C	60	VAL	3.5
2	D	360	ALA	3.5
1	C	124	PHE	3.4
1	C	188	TYR	3.3
1	C	150	PRO	3.3
2	D	423	VAL	3.3
1	A	73	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	160	PHE	3.2
1	C	142	ILE	3.2
2	D	116	PHE	3.2
2	D	10	VAL	3.1
2	D	115	TYR	3.1
1	A	4	PRO	3.1
1	C	214	LEU	3.1
1	C	75	VAL	3.0
1	C	109	LEU	3.0
1	C	74	LEU	3.0
1	C	41	MET	3.0
1	C	90	VAL	2.9
2	D	112	GLY	2.9
1	C	209	LEU	2.8
2	D	359	GLY	2.8
1	A	5	ILE	2.8
1	C	225	PRO	2.7
1	C	189	VAL	2.7
1	C	95	PRO	2.7
2	D	159	ILE	2.6
1	C	33	ALA	2.6
1	C	146	TYR	2.6
2	B	88	TRP	2.6
2	D	144	TYR	2.6
1	A	120	LEU	2.6
1	A	283	LEU	2.6
1	C	120	LEU	2.6
1	C	10	VAL	2.6
1	C	32	LYS	2.5
1	C	46	LYS	2.5
1	C	265	ASN	2.5
1	C	37	ILE	2.5
1	A	212	TRP	2.5
1	C	212	TRP	2.5
1	A	128	THR	2.5
1	A	133	PRO	2.4
1	C	108	VAL	2.4
1	A	220	LYS	2.4
2	D	354	TYR	2.4
1	C	216	THR	2.4
1	C	210	LEU	2.4
1	C	289	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1	PRO	2.4
3	E	33	DG	2.4
1	C	230	MET	2.4
1	A	74	LEU	2.4
1	C	167	ILE	2.4
1	C	21	VAL	2.4
1	C	115	TYR	2.4
2	D	52	PRO	2.4
1	C	149	LEU	2.3
1	A	180	ILE	2.3
1	C	7	THR	2.3
1	C	59	PRO	2.3
2	D	124	PHE	2.3
1	A	62	ALA	2.3
1	C	551	LEU	2.3
1	C	456	GLY	2.3
1	C	264	LEU	2.2
1	C	24	TRP	2.2
1	C	245	VAL	2.2
1	C	34	LEU	2.2
1	A	10	VAL	2.2
1	C	193	LEU	2.2
1	C	106	VAL	2.2
1	A	61	PHE	2.2
1	C	127	TYR	2.2
1	C	208	HIS	2.1
2	B	188	TYR	2.1
2	D	318	TYR	2.1
1	C	31	ILE	2.1
1	C	202	ILE	2.1
1	A	46	LYS	2.1
1	C	58	THR	2.1
1	C	152	GLY	2.1
1	C	155	GLY	2.1
1	C	91	GLN	2.1
2	D	18	GLY	2.1
1	C	5	ILE	2.1
2	D	394[A]	GLN	2.1
2	D	357	MET	2.1
2	B	228	LEU	2.1
1	A	160	PHE	2.1
1	C	171	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	171	PHE	2.1
1	C	257	ILE	2.1
1	C	119	PRO	2.0
2	B	226	PRO	2.0
1	A	289	LEU	2.0
2	B	227	PHE	2.0
2	D	130	PHE	2.0
1	A	50	ILE	2.0
1	A	286	THR	2.0
1	A	75	VAL	2.0
1	C	61	PHE	2.0
1	C	118	VAL	2.0
1	C	148	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OMC	E	2	21/22	0.78	0.13	104,117,125,132	0
3	OMC	E	4	21/22	0.86	0.10	86,101,112,115	0
3	OMC	F	2	21/22	0.90	0.10	88,97,105,106	0
3	OMC	F	4	21/22	0.93	0.09	64,73,78,83	0

6.3 Carbohydrates [i](#)

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

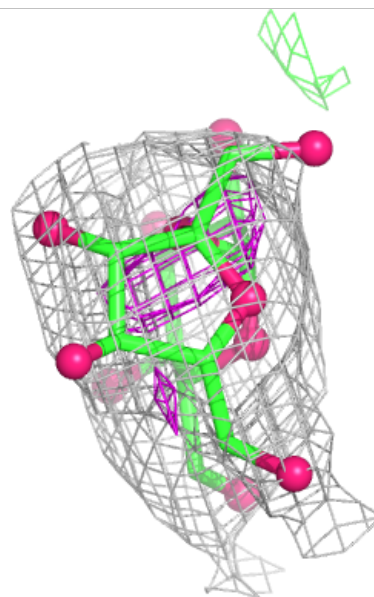
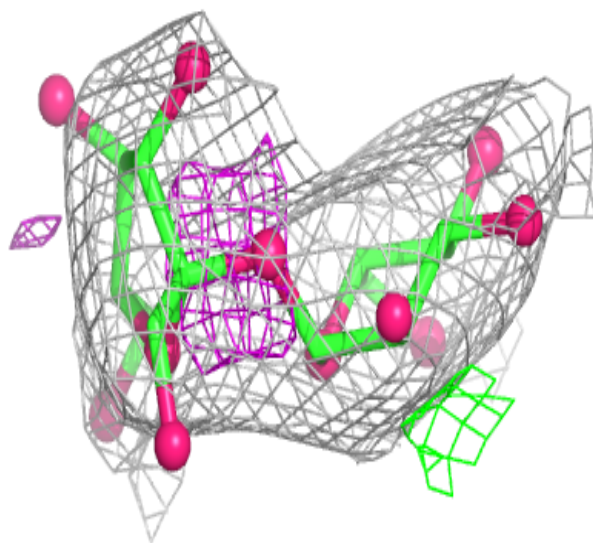
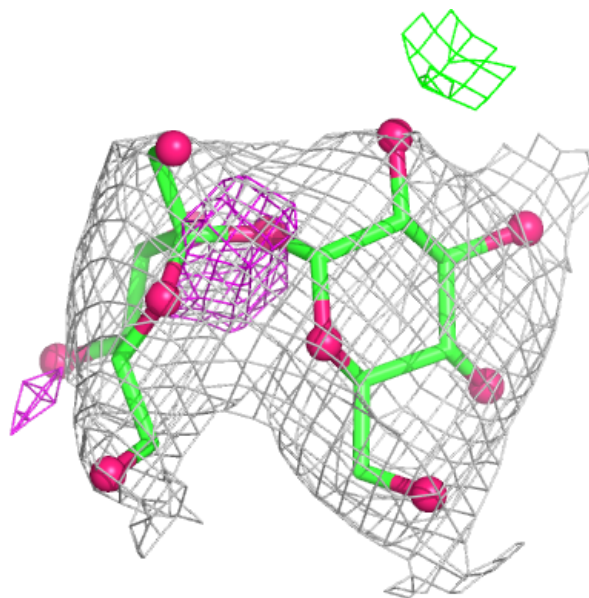
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GLC	H	1	11/12	0.79	0.14	81,90,98,100	0
4	FRU	G	2	12/12	0.84	0.14	69,85,92,94	0
4	FRU	H	2	12/12	0.85	0.10	87,93,97,101	0
4	GLC	G	1	11/12	0.88	0.11	64,74,82,83	0

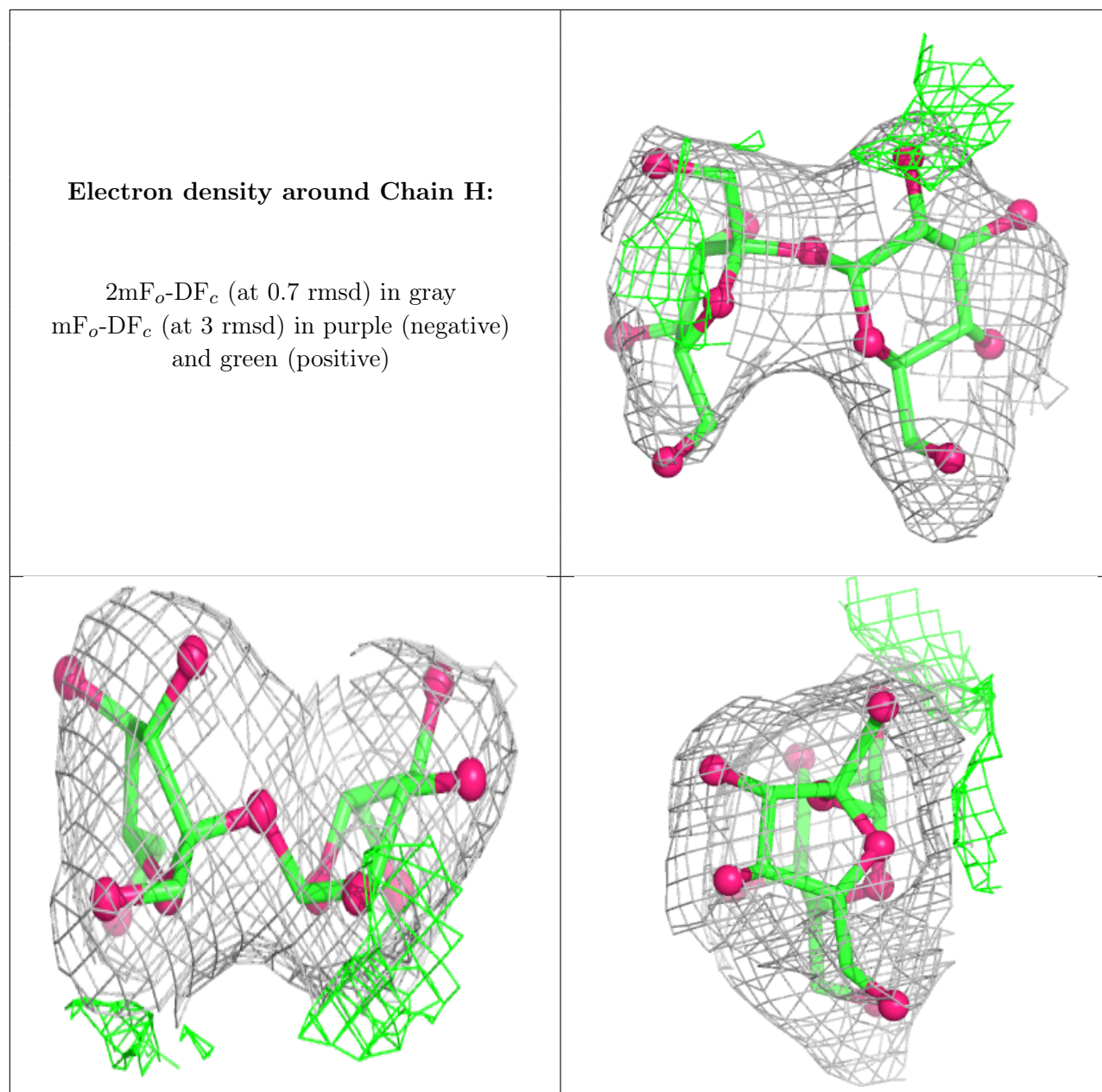
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PPF	C	601	7/7	0.61	0.11	150,162,172,189	0
6	PPF	A	602	7/7	0.66	0.10	124,142,159,169	0
5	MG	A	601	1/1	0.67	0.15	80,80,80,80	0

Continued on next page...

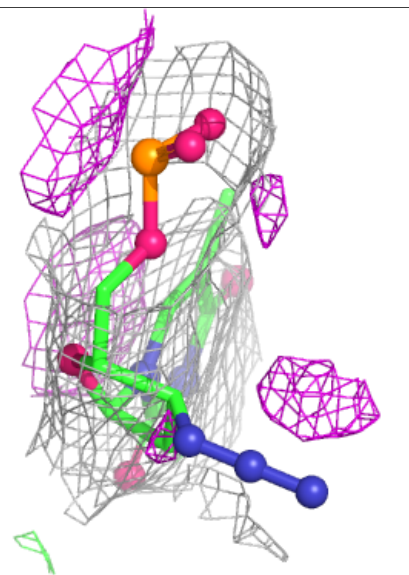
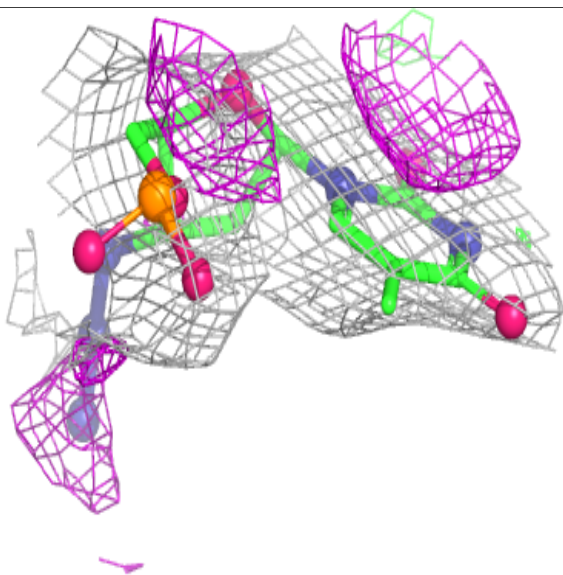
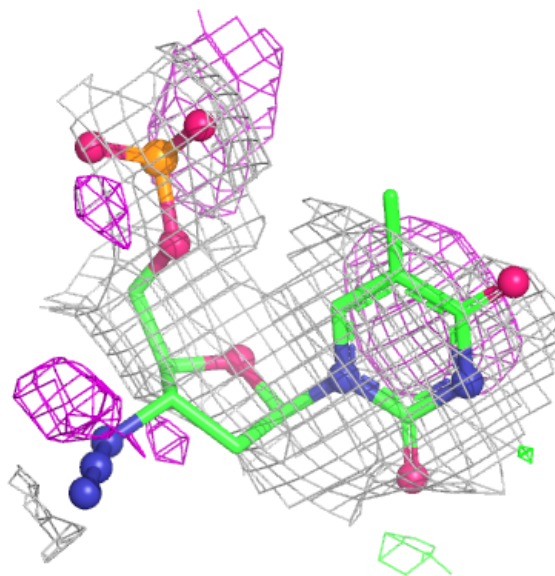
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	GOL	B	2002	6/6	0.70	0.18	71,79,80,81	0
7	SO4	A	606	5/5	0.71	0.13	95,108,116,127	0
7	SO4	C	605	5/5	0.72	0.11	102,108,113,123	0
5	MG	C	602	1/1	0.75	0.18	62,62,62,62	0
9	ATM	E	101	22/23	0.77	0.14	121,134,156,168	0
8	GOL	B	2003	6/6	0.83	0.14	60,64,68,73	0
5	MG	A	605	1/1	0.83	0.14	80,80,80,80	0
5	MG	C	604	1/1	0.85	0.08	166,166,166,166	0
9	ATM	F	101	22/23	0.88	0.11	141,148,164,171	0
5	MG	A	604	1/1	0.90	0.07	130,130,130,130	0
5	MG	C	603	1/1	0.93	0.07	156,156,156,156	0
5	MG	C	606	1/1	0.93	0.07	63,63,63,63	0
5	MG	A	603	1/1	0.97	0.03	133,133,133,133	1

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.

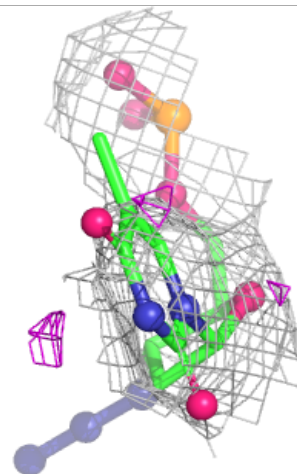
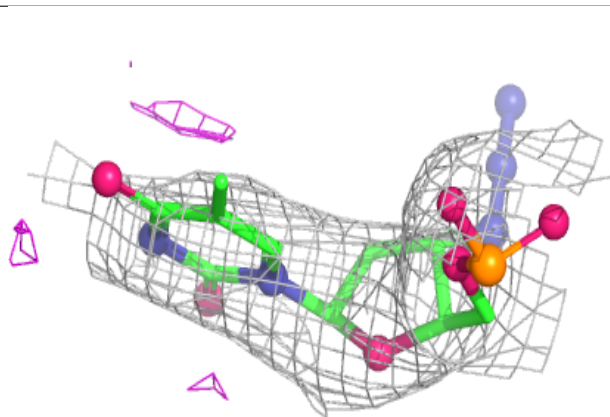
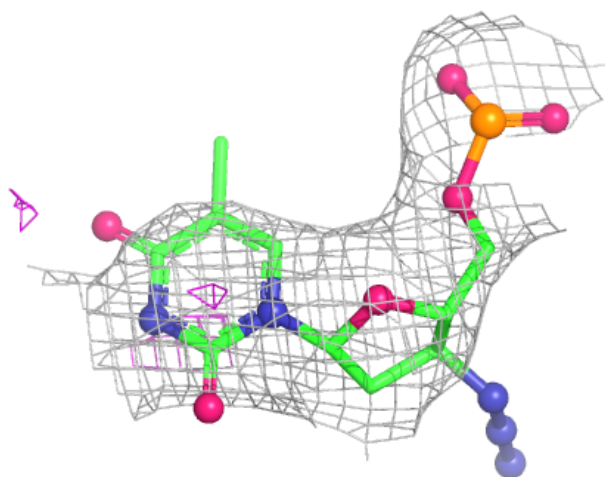
Electron density around ATM E 101:

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



Electron density around ATM F 101:

$2mF_o-DF_c$ (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.