



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:12 AM UTC

PDB ID : 5TXN / pdb_00005txn
Title : STRUCTURE OF Q151M MUTANT HIV-1 REVERSE TRANSCRIPTASE (RT) TERNARY COMPLEX WITH A DOUBLE STRANDED DNA AND AN INCOMING DATP
Authors : Das, K.; Martinez, S.M.; Arnold, E.
Deposited on : 2016-11-17
Resolution : 2.55 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

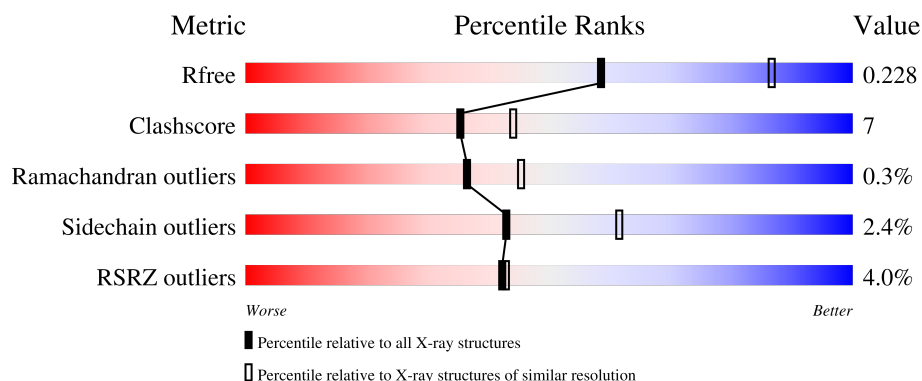
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	556	3% 81% 18% .
1	C	556	3% 78% 21% .
2	B	428	4% 81% 15% .
2	D	428	5% 82% 14% .

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Mol	Chain	Length	Quality of chain
3	E	27	37% 52% 11%
3	T	27	56% 33% 11%
4	F	21	43% 48% 5% 5%
4	P	21	5% 43% 48% 5% 5%
5	G	2	100%
5	H	2	50% 50%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 17923 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	555	Total	C	N	O	S	0	0	0
			4510	2920	750	831	9			
1	C	555	Total	C	N	O	S	0	0	0
			4510	2920	750	831	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	151	MET	GLN	engineered mutation	UNP P03366
A	258	CYS	GLN	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366
A	498	ASN	ASP	engineered mutation	UNP P03366
C	-1	MET	-	initiating methionine	UNP P03366
C	0	VAL	-	expression tag	UNP P03366
C	151	MET	GLN	engineered mutation	UNP P03366
C	258	CYS	GLN	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 HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total	C	N	O	S	0	0	0
			3400	2212	563	619	6			
2	D	412	Total	C	N	O	S	0	0	0
			3400	2212	563	619	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366
D	280	SER	CYS	engineered mutation	UNP P03366

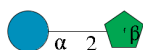
- Molecule 3 is a DNA chain called DNA (5'-D(*TP*GP*GP*TP*CP*GP*GP*CP*GP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	24	Total	C	N	O	P	0	0	0
			494	233	97	141	23			
3	E	24	Total	C	N	O	P	0	0	0
			494	233	97	141	23			

- Molecule 4 is a DNA chain called DNA (5'-D(*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	P	20	Total	C	N	O	P	S	0	0	0
			407	195	72	120	19	1			
4	F	20	Total	C	N	O	P	S	0	0	0
			407	195	72	120	19	1			

- Molecule 5 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		
6	C	2	Total	Mg	0	0
			2	2		

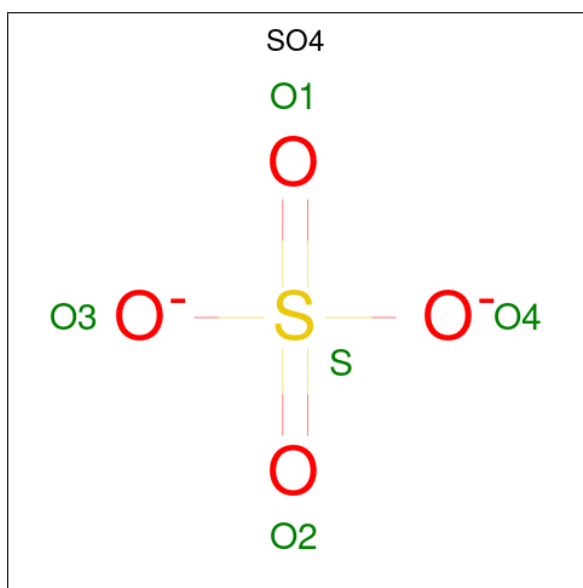
- Molecule 7 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃)



- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	O	S	0	0
			5	4	1		

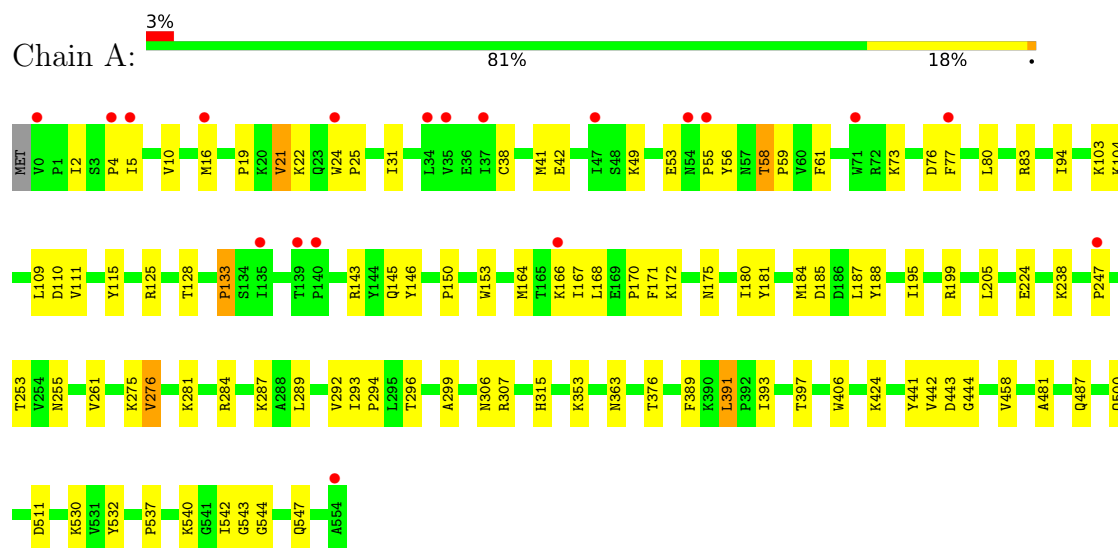
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	50	Total	O	0	0
			50	50		
10	B	42	Total	O	0	0
			42	42		
10	T	1	Total	O	0	0
			1	1		
10	P	1	Total	O	0	0
			1	1		
10	C	48	Total	O	0	0
			48	48		
10	D	33	Total	O	0	0
			33	33		
10	E	1	Total	O	0	0
			1	1		
10	F	2	Total	O	0	0
			2	2		

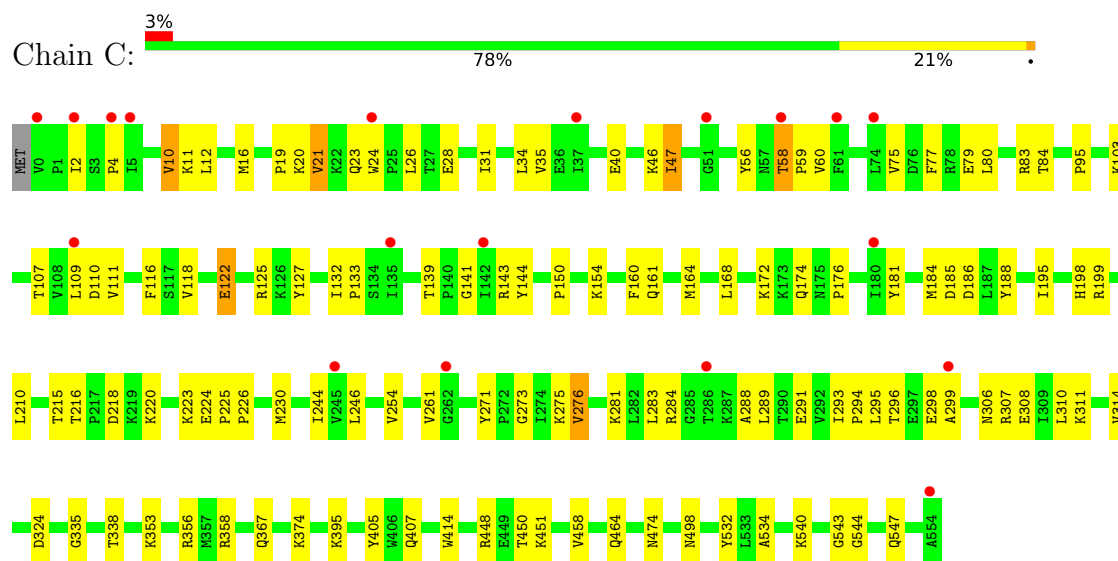
3 Residue-property plots [i](#)

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.

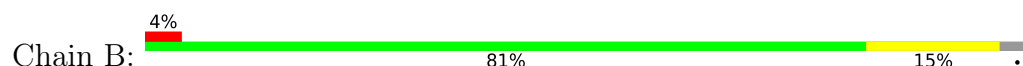
• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT

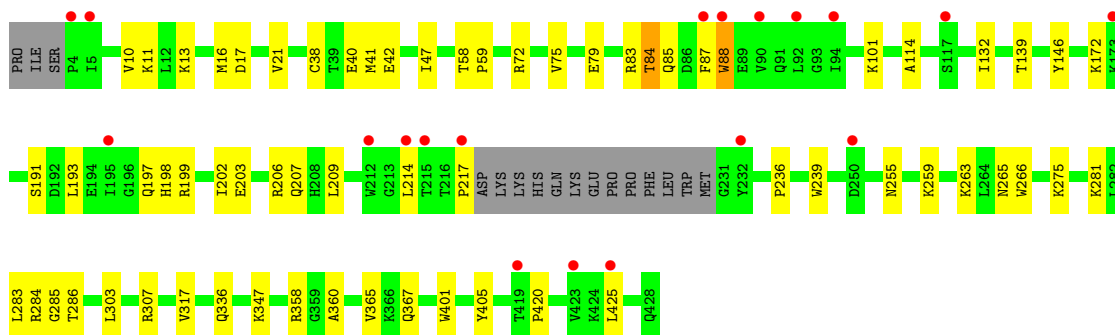


• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT

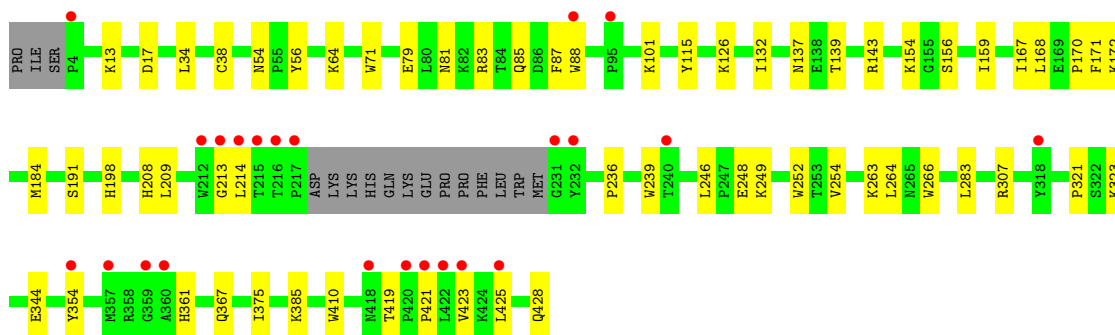
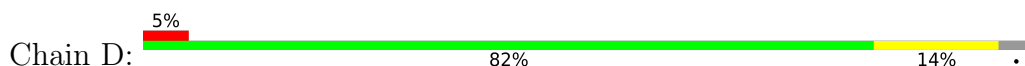


• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT





• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT



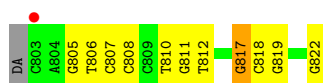
• Molecule 3: DNA (5'-D(*TP*GP*GP*TP*CP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*G)-3')



• Molecule 3: DNA (5'-D(*TP*GP*GP*TP*CP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*G)-3')



• Molecule 4: DNA (5'-D(*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*G)-3')

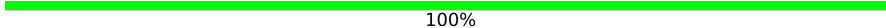


- Molecule 4: DNA (5'-D(*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*G)-3')

Chain F:  43% 48% 5% 5%



- Molecule 5: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain G:  100%



- Molecule 5: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain H:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.04Å 133.63Å 139.21Å 90.00° 97.88° 90.00°	Depositor
Resolution (Å)	33.38 – 2.55 33.38 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.2 (33.38-2.55) 98.0 (33.38-2.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.196 , 0.226 0.197 , 0.228	Depositor DCC
R_{free} test set	3101 reflections (2.84%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 68.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17923	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MRG, GLC, MG, EDO, SO4, DTP, FRU

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	0.17	0/4628	0.44	4/6288 (0.1%)
1	C	0.17	1/4628 (0.0%)	0.37	2/6288 (0.0%)
2	B	0.15	1/3497 (0.0%)	0.35	0/4751
2	D	0.17	1/3497 (0.0%)	0.36	0/4751
3	E	0.19	0/555	0.41	0/856
3	T	0.18	0/555	0.40	1/856 (0.1%)
4	F	0.24	0/424	0.53	0/649
4	P	0.25	0/424	0.54	1/649 (0.2%)
All	All	0.17	3/18208 (0.0%)	0.39	8/25088 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	172	LYS	CE-NZ	-5.36	1.33	1.49
2	D	172	LYS	CE-NZ	-5.33	1.33	1.49
1	C	172	LYS	CE-NZ	-5.32	1.33	1.49

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	LYS	N-CA-C	8.26	123.11	107.75
1	A	73	LYS	CB-CA-C	-7.41	98.86	111.31
4	P	805	DG	C5'-C4'-O4'	6.27	118.80	109.40
3	T	722	DA	C5'-C4'-O4'	5.34	117.41	109.40
1	A	224	GLU	CA-C-N	5.21	125.75	120.38
1	A	224	GLU	C-N-CA	5.21	125.75	120.38
1	C	224	GLU	CA-C-N	5.01	125.55	120.38
1	C	224	GLU	C-N-CA	5.01	125.55	120.38

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	4510	0	4571	68	0
1	C	4510	0	4571	66	0
2	B	3400	0	3433	47	0
2	D	3400	0	3433	42	0
3	E	494	0	269	9	0
3	T	494	0	269	9	0
4	F	407	0	229	13	0
4	P	407	0	229	11	0
5	G	23	0	21	0	0
5	H	23	0	21	0	0
6	A	2	0	0	0	0
6	C	2	0	0	0	0
7	A	30	0	12	2	0
7	C	30	0	12	0	0
8	B	4	0	6	0	0
8	D	4	0	6	3	0
9	D	5	0	0	0	0
10	A	50	0	0	3	0
10	B	42	0	0	2	0
10	C	48	0	0	2	0
10	D	33	0	0	4	0
10	E	1	0	0	0	0
10	F	2	0	0	0	0
10	P	1	0	0	1	0
10	T	1	0	0	0	0
All	All	17923	0	17082	253	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 7.

All (253) 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)
4:P:817:MRG:H231	4:P:817:MRG:N3	1.90	0.87
1:A:167:ILE:O	1:A:170:PRO:HD2	1.79	0.82
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.65	0.77
2:D:263:LYS:HE3	2:D:425:LEU:HA	1.69	0.75
1:A:171:PHE:CD2	1:A:205:LEU:HD13	2.24	0.71
1:A:543:GLY:O	1:A:547:GLN:NE2	2.23	0.71
1:A:111:VAL:HB	1:A:185:ASP:HB2	1.74	0.69
3:E:722:DA:H2"	3:E:723:DC:H5"	1.75	0.69
4:F:817:MRG:N3	4:F:817:MRG:C22	2.56	0.68
2:B:114:ALA:HB2	2:B:214:LEU:HD22	1.76	0.67
1:C:448:ARG:O	1:C:451:LYS:NZ	2.28	0.67
1:C:261:VAL:HG13	1:C:276:VAL:HG11	1.76	0.67
2:B:199:ARG:HA	2:B:202:ILE:HD12	1.77	0.67
2:D:56:TYR:HE2	2:D:126:LYS:HE2	1.60	0.66
2:D:421:PRO:HD3	10:D:610:HOH:O	1.95	0.66
1:C:288:ALA:HB3	1:C:291:GLU:HB2	1.77	0.66
4:F:817:MRG:N3	4:F:817:MRG:H221	2.10	0.66
1:C:543:GLY:O	1:C:547:GLN:NE2	2.28	0.65
1:A:253:THR:HA	1:A:292:VAL:HA	1.78	0.65
1:A:296:THR:HG23	1:A:299:ALA:H	1.61	0.65
1:C:276:VAL:HG23	1:C:353:LYS:HE2	1.79	0.65
1:C:498:ASN:ND2	10:C:702:HOH:O	2.30	0.64
1:C:60:VAL:HG22	1:C:75:VAL:HG13	1.79	0.64
1:A:542:ILE:HG23	2:B:283:LEU:CD1	2.28	0.64
1:C:139:THR:HG22	1:C:141:GLY:H	1.63	0.64
1:A:172:LYS:HE2	1:A:180:ILE:HB	1.80	0.63
1:A:542:ILE:CG2	2:B:283:LEU:HD13	2.27	0.63
2:B:193:LEU:HD13	2:B:197:GLN:HB3	1.80	0.63
1:C:246:LEU:HD11	1:C:310:LEU:HD22	1.80	0.63
2:B:17:ASP:O	2:B:83:ARG:NH1	2.32	0.62
2:D:191:SER:OG	2:D:198:HIS:ND1	2.25	0.62
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.82	0.61
1:A:487:GLN:NE2	10:A:705:HOH:O	2.33	0.61
2:D:137:ASN:ND2	10:D:606:HOH:O	2.34	0.61
1:C:19:PRO:HG3	1:C:80:LEU:HB2	1.83	0.61
1:C:353:LYS:O	1:C:374:LYS:NZ	2.34	0.60
1:C:16:MET:HE2	1:C:83:ARG:HH11	1.65	0.60
2:D:246:LEU:HD11	2:D:264:LEU:HD21	1.84	0.60
1:C:395:LYS:HE3	10:C:727:HOH:O	2.00	0.60
1:A:128:THR:HG21	1:A:146:TYR:HB2	1.84	0.60
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.83	0.59
1:A:110:ASP:OD1	1:A:111:VAL:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:TRP:HE3	1:A:25:PRO:HD2	1.66	0.59
1:A:164:MET:HE2	1:A:187:LEU:HD11	1.84	0.59
2:B:72:ARG:NH1	10:B:601:HOH:O	2.21	0.58
3:T:713:DC:H2'	3:T:714:DG:C8	2.38	0.58
4:F:807:DC:H2''	4:F:808:DC:H5''	1.86	0.58
1:C:107:THR:OG1	1:C:198:HIS:NE2	2.34	0.58
3:E:702:DT:H3'	3:E:703:DG:H8	1.69	0.57
3:E:720:DG:H2''	3:E:721:DG:C8	2.39	0.57
1:A:58:THR:HG21	1:A:77:PHE:HE1	1.70	0.56
2:B:209:LEU:HD22	2:B:214:LEU:HD23	1.88	0.55
2:B:203:GLU:O	2:B:207:GLN:HG2	2.07	0.55
1:A:171:PHE:CE2	1:A:205:LEU:HD13	2.41	0.55
1:C:111:VAL:HB	1:C:185:ASP:HB2	1.88	0.55
2:B:255:ASN:ND2	10:B:603:HOH:O	2.32	0.55
2:B:13:LYS:HD2	2:B:85:GLN:HB3	1.88	0.54
2:D:87:PHE:HZ	2:D:159:ILE:HG13	1.73	0.54
1:A:56:TYR:O	1:A:143:ARG:NH2	2.41	0.54
1:C:56:TYR:O	1:C:143:ARG:NH2	2.41	0.54
1:A:389:PHE:HB3	1:A:391:LEU:HD13	1.90	0.54
2:D:209:LEU:HD22	2:D:214:LEU:HD12	1.90	0.54
4:F:804:DA:H2'	4:F:805:DG:C8	2.43	0.54
2:D:168:LEU:O	2:D:171:PHE:N	2.40	0.53
1:C:181:TYR:HB2	1:C:188:TYR:HB3	1.89	0.53
2:D:64:LYS:HE3	2:D:71:TRP:CE2	2.44	0.53
2:B:266:TRP:HD1	2:B:425:LEU:HD13	1.74	0.53
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.74	0.53
2:D:184:MET:HE2	2:D:410:TRP:HB3	1.89	0.53
1:C:254:VAL:HG13	1:C:283:LEU:HD22	1.91	0.53
2:D:249:LYS:HB2	2:D:252:TRP:CE2	2.44	0.53
1:A:391:LEU:HB3	1:A:393:ILE:HG22	1.91	0.52
1:C:335:GLY:HA2	1:C:367:GLN:HE22	1.74	0.52
1:C:543:GLY:HA3	10:D:623:HOH:O	2.09	0.52
4:F:817:MRG:H2'	4:F:818:DC:C6	2.44	0.52
1:C:122:GLU:HA	1:C:125:ARG:HD2	1.92	0.52
2:B:317:VAL:HG12	2:B:347:LYS:HD3	1.92	0.52
2:D:248:GLU:HA	8:D:503:EDO:O2	2.09	0.52
1:A:166:LYS:O	1:A:170:PRO:HD3	2.10	0.52
4:F:814:DC:H2''	4:F:815:DG:C8	2.45	0.52
1:A:238:LYS:HD2	1:A:315:HIS:CG	2.45	0.52
1:C:395:LYS:NZ	1:C:414:TRP:O	2.43	0.51
1:A:31:ILE:HG23	1:A:133:PRO:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:702:DT:H3'	3:E:703:DG:C8	2.44	0.51
4:F:807:DC:H4'	4:F:808:DC:OP1	2.10	0.51
2:B:101:LYS:O	2:B:236:PRO:HB2	2.11	0.51
4:P:807:DC:H4'	4:P:808:DC:OP1	2.10	0.51
1:C:458:VAL:HG13	1:C:464:GLN:HG2	1.92	0.51
2:D:54:ASN:HB3	2:D:143:ARG:HH21	1.77	0.50
2:D:254:VAL:HG13	2:D:283:LEU:HD22	1.93	0.50
2:B:317:VAL:HG12	2:B:347:LYS:HB3	1.94	0.50
2:D:85:GLN:HA	2:D:88:TRP:CE2	2.46	0.50
2:D:213:GLY:O	2:D:214:LEU:HD23	2.11	0.50
4:F:818:DC:H2'	4:F:819:DG:C8	2.47	0.50
1:C:281:LYS:O	1:C:284:ARG:HG2	2.11	0.50
1:C:195:ILE:HD11	1:C:199:ARG:HH21	1.76	0.50
2:D:167:ILE:HD13	2:D:214:LEU:HD11	1.93	0.50
1:A:125:ARG:O	1:A:128:THR:OG1	2.23	0.50
2:B:191:SER:OG	2:B:198:HIS:ND1	2.35	0.50
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.51	0.49
1:C:356:ARG:HG2	1:C:358:ARG:HG3	1.94	0.49
2:D:249:LYS:HB2	2:D:252:TRP:CZ2	2.47	0.49
2:D:428:GLN:CD	2:D:428:GLN:H	2.19	0.49
2:B:266:TRP:NE1	2:B:425:LEU:HD22	2.28	0.49
1:C:273:GLY:HA2	1:C:338:THR:HG21	1.94	0.49
1:A:397:THR:HG21	1:A:424:LYS:HA	1.95	0.49
1:A:94:ILE:O	10:A:701:HOH:O	2.20	0.49
1:A:184:MET:HG2	4:P:822:DG:H2''	1.94	0.49
1:A:543:GLY:HA2	2:B:283:LEU:O	2.12	0.49
1:C:24:TRP:HB2	1:C:26:LEU:HG	1.94	0.49
1:C:164:MET:HE2	1:C:168:LEU:HG	1.93	0.49
2:D:38:CYS:SG	2:D:132:ILE:HD11	2.52	0.49
1:C:184:MET:HG2	4:F:822:DG:H2''	1.94	0.49
1:C:543:GLY:HA2	2:D:283:LEU:O	2.13	0.49
3:T:713:DC:H2''	3:T:714:DG:H5'	1.95	0.49
2:D:421:PRO:HB2	2:D:423:VAL:HG23	1.94	0.49
1:A:19:PRO:HD3	1:A:80:LEU:HD13	1.95	0.49
3:E:716:DA:H2''	3:E:717:DC:OP2	2.13	0.49
4:F:805:DG:H4'	4:F:806:DT:OP1	2.13	0.49
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.48	0.48
1:C:58:THR:HG21	1:C:77:PHE:CE1	2.48	0.48
1:A:276:VAL:HG23	1:A:353:LYS:HE2	1.95	0.48
1:C:47:ILE:HG12	1:C:144:TYR:HB3	1.95	0.48
1:C:296:THR:HG23	1:C:299:ALA:H	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:810:DT:H2''	4:P:811:DG:H5'	1.94	0.48
2:D:323:LYS:NZ	2:D:344:GLU:OE2	2.31	0.48
2:D:79:GLU:HG3	2:D:83:ARG:HE	1.79	0.48
1:A:10:VAL:HG11	1:A:153:TRP:CZ2	2.49	0.48
4:P:818:DC:H2'	4:P:819:DG:C8	2.49	0.48
1:A:443:ASP:OD1	1:A:444:GLY:N	2.47	0.47
2:B:84:THR:HG22	2:B:87:PHE:HB3	1.95	0.47
3:T:706:DC:H2'	3:T:707:DG:C8	2.49	0.47
2:D:354:TYR:HE2	2:D:375:ILE:HG13	1.79	0.47
8:D:503:EDO:O1	10:D:601:HOH:O	2.20	0.47
2:B:266:TRP:HE1	2:B:425:LEU:HD22	1.80	0.47
1:C:58:THR:HG21	1:C:77:PHE:HE1	1.79	0.47
1:C:307:ARG:O	1:C:311:LYS:HG3	2.14	0.47
2:D:13:LYS:HD2	2:D:85:GLN:HB3	1.97	0.47
2:D:423:VAL:HG12	2:D:423:VAL:O	2.14	0.47
4:F:806:DT:H2'	4:F:807:DC:C6	2.50	0.47
2:B:47:ILE:HG22	2:B:146:TYR:HA	1.96	0.47
1:C:308:GLU:HA	1:C:311:LYS:HE2	1.97	0.47
3:T:709:DC:H2'	3:T:710:DG:C8	2.50	0.47
1:C:95:PRO:HD2	1:C:230:MET:HE2	1.96	0.47
2:D:323:LYS:O	2:D:385:LYS:NZ	2.48	0.47
1:A:458:VAL:HG12	2:B:286:THR:HG21	1.97	0.47
1:C:79:GLU:OE1	1:C:83:ARG:NH2	2.48	0.46
3:E:709:DC:H2'	3:E:710:DG:H8	1.80	0.46
1:A:115:TYR:CD2	7:A:603:DTP:H2'1	2.51	0.46
1:C:199:ARG:NH1	1:C:223:LYS:HD2	2.30	0.46
1:C:544:GLY:HA2	1:C:547:GLN:HE21	1.81	0.46
2:B:358:ARG:NH2	2:B:405:TYR:O	2.44	0.46
1:A:406:TRP:CZ2	2:B:420:PRO:HB3	2.49	0.46
1:C:21:VAL:HG23	1:C:59:PRO:HD3	1.97	0.46
1:C:405:TYR:CE2	1:C:407:GLN:HB2	2.51	0.46
4:P:807:DC:H2''	4:P:808:DC:H5''	1.98	0.45
1:A:441:TYR:CG	1:A:544:GLY:HA3	2.51	0.45
1:C:31:ILE:O	1:C:35:VAL:HG23	2.17	0.45
1:A:247:PRO:O	1:A:307:ARG:NH2	2.50	0.45
4:P:817:MRG:H2'	4:P:818:DC:C6	2.51	0.45
1:C:275:LYS:O	1:C:306:ASN:ND2	2.43	0.45
1:C:395:LYS:HD2	1:C:414:TRP:CH2	2.52	0.45
1:C:46:LYS:HD3	1:C:116:PHE:HB3	1.97	0.45
1:A:10:VAL:HG11	1:A:153:TRP:CH2	2.51	0.45
1:A:21:VAL:HG23	1:A:59:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:ILE:HD13	1:C:133:PRO:HB2	1.98	0.45
1:A:22:LYS:HA	1:A:22:LYS:HD3	1.77	0.45
1:A:171:PHE:CE1	1:A:175:ASN:OD1	2.70	0.45
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.98	0.44
4:P:818:DC:H2'	4:P:819:DG:H8	1.81	0.44
1:C:199:ARG:HH11	1:C:223:LYS:HD2	1.81	0.44
4:F:818:DC:H2'	4:F:819:DG:H8	1.82	0.44
3:T:721:DG:H5'	3:T:721:DG:H8	1.82	0.44
1:A:376:THR:HG21	2:B:401:TRP:CH2	2.53	0.44
4:P:812:DT:OP1	10:P:901:HOH:O	2.20	0.44
1:C:103:LYS:HA	1:C:103:LYS:HD3	1.76	0.44
1:A:103:LYS:HD3	1:A:103:LYS:HA	1.84	0.44
1:A:255:ASN:HB2	1:A:289:LEU:HG	2.00	0.44
2:B:114:ALA:N	2:B:214:LEU:HD13	2.33	0.44
1:A:21:VAL:HG23	1:A:58:THR:HA	1.99	0.43
1:A:61:PHE:HE2	1:A:76:ASP:HB2	1.83	0.43
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.18	0.43
2:B:206:ARG:NH2	2:B:217:PRO:O	2.49	0.43
7:A:603:DTP:O2B	7:A:603:DTP:O1A	2.36	0.43
3:T:712:DC:H2''	3:T:713:DC:H6	1.83	0.43
1:C:110:ASP:HB3	1:C:220:LYS:HB3	1.99	0.43
1:C:174:GLN:C	1:C:176:PRO:HD3	2.44	0.43
1:A:281:LYS:O	1:A:284:ARG:HG2	2.19	0.43
1:C:161:GLN:HG3	1:C:184:MET:HE3	2.01	0.43
2:D:266:TRP:CE3	2:D:425:LEU:HG	2.53	0.43
2:D:307:ARG:HH22	8:D:503:EDO:H12	1.83	0.43
2:D:321:PRO:O	2:D:385:LYS:NZ	2.38	0.43
1:A:38:CYS:HA	1:A:41:MET:HE3	2.00	0.43
1:A:42:GLU:OE1	1:A:49:LYS:HE3	2.19	0.43
1:A:287:LYS:H	1:A:287:LYS:HG2	1.56	0.43
1:A:195:ILE:O	1:A:199:ARG:HG3	2.19	0.43
1:C:35:VAL:HG22	1:C:132:ILE:HG21	2.00	0.43
1:C:118:VAL:HG21	1:C:160:PHE:HD1	1.84	0.43
2:D:81:ASN:HB3	2:D:154:LYS:HD2	2.01	0.43
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.00	0.43
1:C:254:VAL:HG12	1:C:289:LEU:HD12	2.00	0.43
1:A:168:LEU:HD23	1:A:168:LEU:HA	1.81	0.43
2:B:266:TRP:CD1	2:B:425:LEU:HD22	2.54	0.43
2:B:42:GLU:HA	2:B:47:ILE:O	2.19	0.43
3:T:721:DG:H5'	3:T:721:DG:C8	2.54	0.43
1:A:275:LYS:O	1:A:306:ASN:ND2	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:LEU:HD11	1:C:127:TYR:CZ	2.54	0.42
1:A:532:TYR:OH	2:B:259:LYS:NZ	2.48	0.42
1:C:293:ILE:HG13	1:C:294:PRO:HD2	2.02	0.42
1:C:532:TYR:CE2	1:C:534:ALA:HB2	2.55	0.42
2:D:115:TYR:CD2	2:D:156:SER:HB3	2.54	0.42
1:A:293:ILE:HG13	1:A:294:PRO:HD2	2.01	0.42
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.01	0.42
2:B:41:MET:HB3	2:B:47:ILE:HG12	2.01	0.42
1:C:20:LYS:HG2	1:C:56:TYR:HA	2.02	0.42
1:A:53:GLU:O	1:A:55:PRO:HD3	2.19	0.42
2:B:85:GLN:HA	2:B:88:TRP:CE2	2.54	0.42
2:B:303:LEU:HD21	2:B:307:ARG:HH22	1.85	0.42
3:E:714:DG:H2''	3:E:715:DA:C8	2.55	0.42
3:T:709:DC:H2'	3:T:710:DG:H8	1.84	0.42
2:B:360:ALA:HA	2:B:367:GLN:CD	2.45	0.42
1:C:10:VAL:HG12	1:C:11:LYS:H	1.85	0.42
1:C:225:PRO:HA	1:C:226:PRO:C	2.44	0.42
3:T:712:DC:O2	4:P:817:MRG:H212	2.20	0.42
2:B:263:LYS:HE3	2:B:425:LEU:HA	2.02	0.42
2:D:170:PRO:HB2	2:D:208:HIS:CE1	2.55	0.42
3:E:711:DC:H2'	3:E:712:DC:C6	2.55	0.42
1:A:145:GLN:O	1:A:145:GLN:HG3	2.19	0.41
2:B:281:LYS:O	2:B:284:ARG:HG3	2.20	0.41
4:P:806:DT:H2'	4:P:807:DC:C6	2.55	0.41
2:D:361:HIS:H	2:D:367:GLN:NE2	2.18	0.41
4:F:807:DC:H2''	4:F:808:DC:C5'	2.50	0.41
1:C:271:TYR:CE2	1:C:310:LEU:HA	2.55	0.41
1:C:84:THR:HB	1:C:154:LYS:HE2	2.03	0.41
2:B:275:LYS:HA	2:B:275:LYS:HD3	1.80	0.41
3:E:709:DC:H2'	3:E:710:DG:C8	2.54	0.41
1:A:543:GLY:HA2	2:B:285:GLY:O	2.20	0.41
2:D:34:LEU:HD23	2:D:34:LEU:HA	1.91	0.41
2:D:101:LYS:O	2:D:236:PRO:HB2	2.21	0.41
2:D:419:THR:O	2:D:421:PRO:HD3	2.21	0.41
1:C:540:LYS:HD3	1:C:540:LYS:HA	1.82	0.41
1:A:537:PRO:HG2	1:A:540:LYS:HG3	2.03	0.40
2:B:88:TRP:CD1	2:B:88:TRP:H	2.39	0.40
1:C:271:TYR:CE2	1:C:310:LEU:HG	2.55	0.40
2:D:17:ASP:O	2:D:83:ARG:HD3	2.21	0.40
1:A:530:LYS:NZ	10:A:710:HOH:O	2.48	0.40
1:A:540:LYS:HD3	1:A:540:LYS:HA	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:VAL:O	2:B:11:LYS:HD2	2.21	0.40
2:D:87:PHE:CZ	2:D:159:ILE:HG13	2.54	0.40
1:A:16:MET:HG2	1:A:83:ARG:HD3	2.03	0.40
1:A:540:LYS:HE3	2:B:265:ASN:OD1	2.22	0.40
2:D:236:PRO:HA	2:D:239:TRP:CE2	2.57	0.40
1:A:104:LYS:HE3	1:A:104:LYS:HB2	1.86	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	553/556 (100%)	533 (96%)	17 (3%)	3 (0%)	24	34
1	C	553/556 (100%)	534 (97%)	17 (3%)	2 (0%)	30	39
2	B	408/428 (95%)	399 (98%)	9 (2%)	0	100	100
2	D	408/428 (95%)	394 (97%)	14 (3%)	0	100	100
All	All	1922/1968 (98%)	1860 (97%)	57 (3%)	5 (0%)	36	45

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	C	4	PRO
1	A	150	PRO
1	A	133	PRO
1	C	150	PRO

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	495/497 (100%)	487 (98%)	8 (2%)	55	73
1	C	495/497 (100%)	471 (95%)	24 (5%)	23	35
2	B	374/390 (96%)	366 (98%)	8 (2%)	47	66
2	D	374/390 (96%)	373 (100%)	1 (0%)	86	92
All	All	1738/1774 (98%)	1697 (98%)	41 (2%)	43	61

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	5	ILE
1	A	21	VAL
1	A	58	THR
1	A	109	LEU
1	A	276	VAL
1	A	391	LEU
1	A	500	GLN
2	B	16	MET
2	B	40	GLU
2	B	58	THR
2	B	75	VAL
2	B	84	THR
2	B	88	TRP
2	B	139	THR
2	B	336	GLN
1	C	2	ILE
1	C	10	VAL
1	C	21	VAL
1	C	23	GLN
1	C	28	GLU
1	C	34	LEU
1	C	40	GLU
1	C	47	ILE

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Mol	Chain	Res	Type
1	C	58	THR
1	C	109	LEU
1	C	122	GLU
1	C	186	ASP
1	C	210	LEU
1	C	215	THR
1	C	216	THR
1	C	218	ASP
1	C	244	ILE
1	C	276	VAL
1	C	295	LEU
1	C	298	GLU
1	C	314	VAL
1	C	324	ASP
1	C	450	THR
1	C	474	ASN
2	D	139	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	A	174	GLN
2	B	255	ASN
1	C	367	GLN
1	C	487	GLN
1	C	509	GLN
1	C	539	HIS
1	C	545	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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
4	MRG	P	817	1,4,3	25,28,29	2.72	7 (28%)	32,39,42	2.26	12 (37%)
4	MRG	F	817	1,4,3	25,28,29	2.68	7 (28%)	32,39,42	2.19	12 (37%)

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	MRG	P	817	1,4,3	-	3/12/26/27	0/3/3/3
4	MRG	F	817	1,4,3	-	2/12/26/27	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	817	MRG	C2-N2	7.03	1.49	1.34
4	F	817	MRG	C2-N2	6.87	1.49	1.34
4	P	817	MRG	C2-N3	6.79	1.45	1.32
4	F	817	MRG	C2-N3	6.67	1.44	1.32
4	P	817	MRG	C4-N3	4.97	1.45	1.34
4	F	817	MRG	C4-N3	4.86	1.45	1.34
4	F	817	MRG	C2-N1	4.40	1.43	1.36
4	P	817	MRG	C2-N1	4.36	1.43	1.36
4	P	817	MRG	C2'-C3'	-3.42	1.44	1.52
4	F	817	MRG	C2'-C3'	-3.38	1.44	1.52
4	F	817	MRG	O4'-C4'	-2.67	1.39	1.45
4	F	817	MRG	O3'-C3'	-2.63	1.37	1.43
4	P	817	MRG	O3'-C3'	-2.60	1.37	1.43
4	P	817	MRG	O4'-C4'	-2.59	1.39	1.45

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	817	MRG	C2-N3-C4	6.86	120.59	112.00
4	F	817	MRG	C2-N3-C4	6.58	120.24	112.00
4	P	817	MRG	C5-C4-N3	-5.28	119.99	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	817	MRG	C5-C4-N3	-5.12	120.25	128.39
4	F	817	MRG	C2-N1-C6	-3.78	119.98	124.55
4	P	817	MRG	C2-N1-C6	-3.60	120.20	124.55
4	P	817	MRG	N9-C4-N3	3.34	132.64	125.95
4	P	817	MRG	C22-C21-N2	3.10	120.89	112.20
4	F	817	MRG	N9-C4-N3	3.08	132.11	125.95
4	P	817	MRG	O4'-C1'-N9	3.00	113.19	107.86
4	F	817	MRG	O4'-C1'-N9	2.89	113.00	107.86
4	P	817	MRG	C5-C6-N1	2.69	120.09	113.25
4	F	817	MRG	C5-C6-N1	2.63	119.95	113.25
4	P	817	MRG	N1-C2-N3	-2.56	119.37	123.68
4	F	817	MRG	O6-C6-C5	-2.49	119.95	126.53
4	P	817	MRG	O6-C6-C5	-2.47	120.02	126.53
4	F	817	MRG	N1-C2-N3	-2.30	119.80	123.68
4	F	817	MRG	N9-C8-N7	-2.29	109.15	113.40
4	F	817	MRG	C22-C21-N2	2.29	118.62	112.20
4	P	817	MRG	N9-C8-N7	-2.24	109.25	113.40
4	F	817	MRG	C4-C5-N7	-2.21	107.16	110.67
4	F	817	MRG	C8-N7-C5	2.12	108.04	104.26
4	P	817	MRG	C4-C5-N7	-2.08	107.38	110.67
4	P	817	MRG	C8-N7-C5	2.07	107.96	104.26

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	817	MRG	N3-C2-N2-C21
4	P	817	MRG	N1-C2-N2-C21
4	P	817	MRG	C21-C22-C23-S24
4	F	817	MRG	C22-C21-N2-C2
4	F	817	MRG	C21-C22-C23-S24

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	817	MRG	3	0
4	F	817	MRG	3	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	$\# Z > 2$
5	GLC	G	1	5	11,11,12	0.30	0	15,15,17	0.74	0
5	FRU	G	2	5	11,12,12	0.49	0	10,18,18	0.53	0
5	GLC	H	1	5	11,11,12	0.20	0	15,15,17	1.07	2 (13%)
5	FRU	H	2	5	11,12,12	0.47	0	10,18,18	0.63	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
5	GLC	G	1	5	-	0/2/19/22	0/1/1/1
5	FRU	G	2	5	-	3/5/24/24	0/1/1/1
5	GLC	H	1	5	-	1/2/19/22	0/1/1/1
5	FRU	H	2	5	-	3/5/24/24	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1	GLC	C1-O5-C5	2.30	115.26	112.19
5	H	1	GLC	C6-C5-C4	-2.07	107.94	113.02

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	2	FRU	O1-C1-C2-C3
5	G	2	FRU	O1-C1-C2-O2

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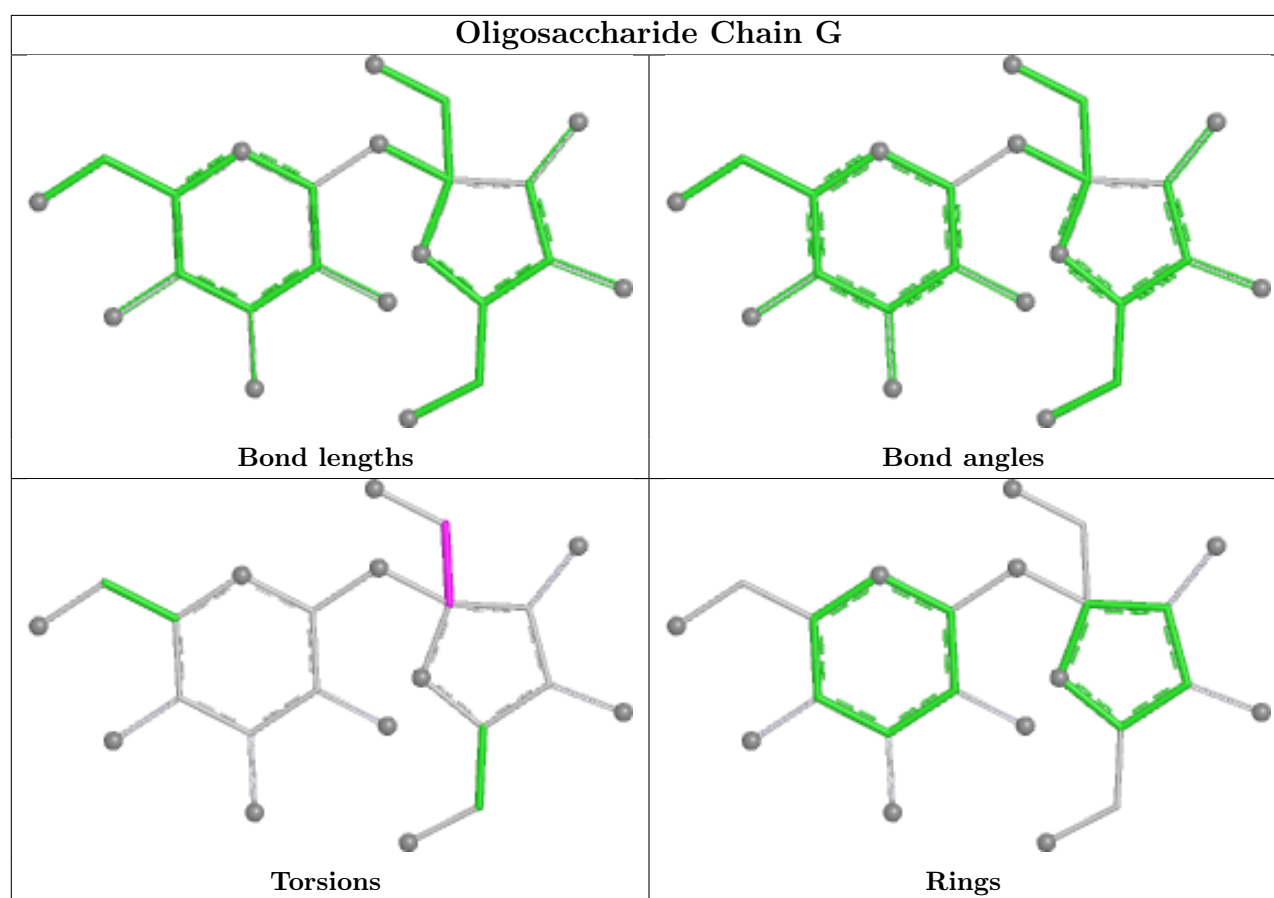
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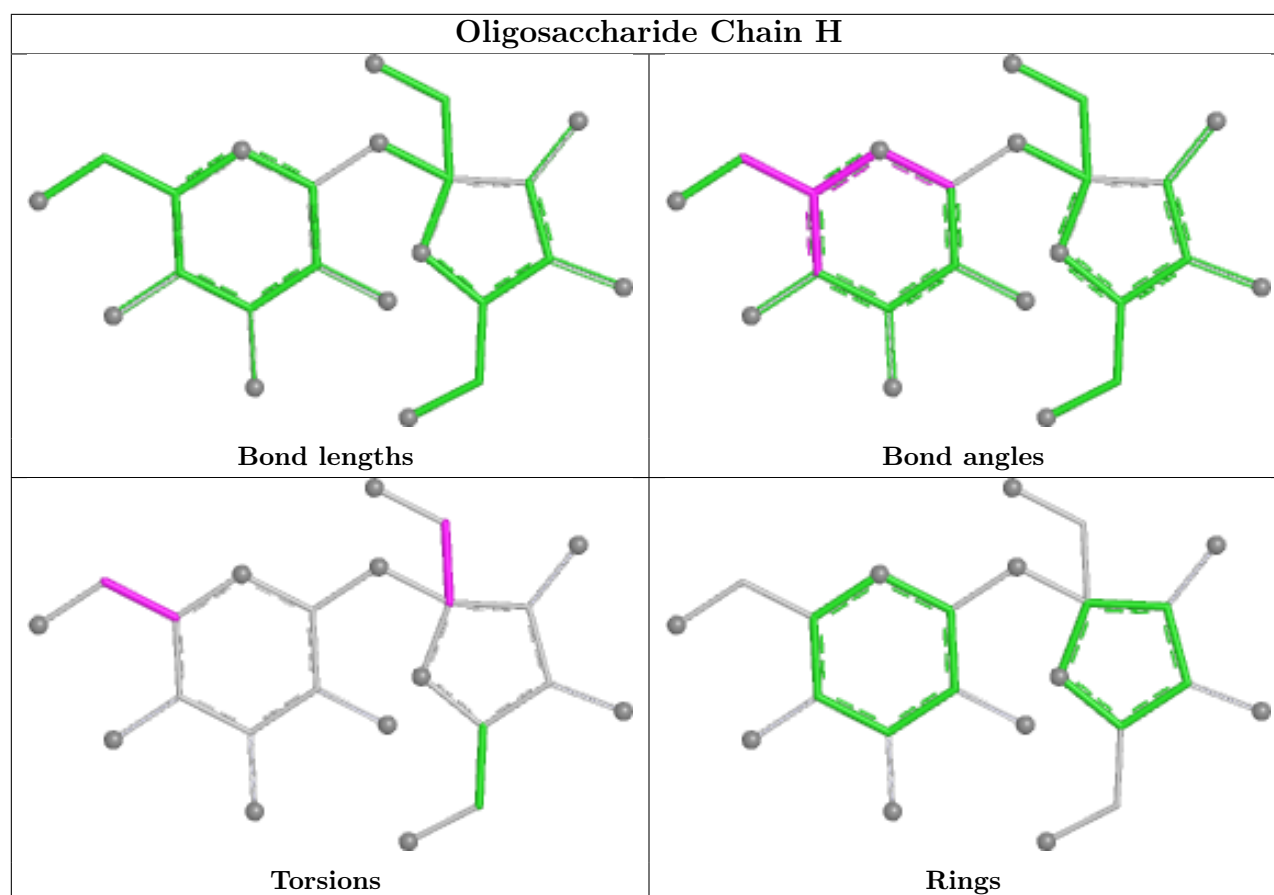
Mol	Chain	Res	Type	Atoms
5	H	2	FRU	O1-C1-C2-O2
5	G	2	FRU	O1-C1-C2-O5
5	H	2	FRU	O1-C1-C2-C3
5	H	1	GLC	C4-C5-C6-O6
5	H	2	FRU	O1-C1-C2-O5

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.





5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	EDO	B	502	-	3,3,3	0.34	0	2,2,2	0.47	0
8	EDO	D	503	-	3,3,3	0.42	0	2,2,2	0.26	0
7	DTP	A	603	6	31,32,32	1.85	7 (22%)	46,50,50	1.94	10 (21%)
9	SO4	D	502	-	4,4,4	0.23	0	6,6,6	0.08	0
7	DTP	C	601	6	31,32,32	1.85	7 (22%)	46,50,50	1.94	10 (21%)

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
7	DTP	A	603	6	-	4/22/34/34	0/3/3/3
8	EDO	B	502	-	-	0/1/1/1	-
8	EDO	D	503	-	-	1/1/1/1	-
7	DTP	C	601	6	-	1/22/34/34	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	603	DTP	PB-O3A	-5.18	1.53	1.59
7	C	601	DTP	PB-O3A	-5.16	1.53	1.59
7	C	601	DTP	C6-N6	4.98	1.46	1.34
7	A	603	DTP	C6-N6	4.96	1.46	1.34
7	A	603	DTP	C5'-C4'	-3.23	1.41	1.51
7	C	601	DTP	C5'-C4'	-3.22	1.41	1.51
7	A	603	DTP	C2'-C3'	-2.71	1.46	1.52
7	C	601	DTP	C2'-C3'	-2.71	1.46	1.52
7	C	601	DTP	O5'-C5'	-2.53	1.35	1.44
7	A	603	DTP	O5'-C5'	-2.52	1.35	1.44
7	C	601	DTP	O3'-C3'	-2.37	1.38	1.43
7	A	603	DTP	O3'-C3'	-2.36	1.38	1.43
7	C	601	DTP	C3'-C4'	-2.29	1.47	1.53
7	A	603	DTP	C3'-C4'	-2.28	1.47	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	603	DTP	C5-C4-N3	-5.62	118.98	126.72
7	C	601	DTP	C5-C4-N3	-5.57	119.04	126.72
7	C	601	DTP	N3-C2-N1	-4.46	121.83	128.58
7	A	603	DTP	N3-C4-N9	4.44	134.72	127.17
7	A	603	DTP	N3-C2-N1	-4.40	121.92	128.58
7	C	601	DTP	N3-C4-N9	4.36	134.58	127.17
7	C	601	DTP	N9-C8-N7	-4.12	108.09	113.94
7	A	603	DTP	N9-C8-N7	-4.11	108.11	113.94
7	C	601	DTP	C2-N3-C4	3.72	120.91	111.83
7	A	603	DTP	C2-N3-C4	3.71	120.88	111.83
7	A	603	DTP	C4-N9-C8	3.68	109.60	105.74
7	C	601	DTP	C4-N9-C8	3.64	109.56	105.74
7	C	601	DTP	C5-N7-C8	3.39	108.78	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	603	DTP	C5-N7-C8	3.32	108.67	103.45
7	A	603	DTP	O4'-C1'-N9	3.15	113.62	107.96
7	C	601	DTP	O4'-C1'-N9	3.05	113.45	107.96
7	C	601	DTP	C4-C5-N7	-2.96	107.20	110.58
7	A	603	DTP	C4-C5-N7	-2.85	107.32	110.58
7	A	603	DTP	O5'-C5'-C4'	2.33	116.92	108.99
7	C	601	DTP	O5'-C5'-C4'	2.32	116.91	108.99

There are no chirality outliers.

All (6) torsion outliers are listed below:

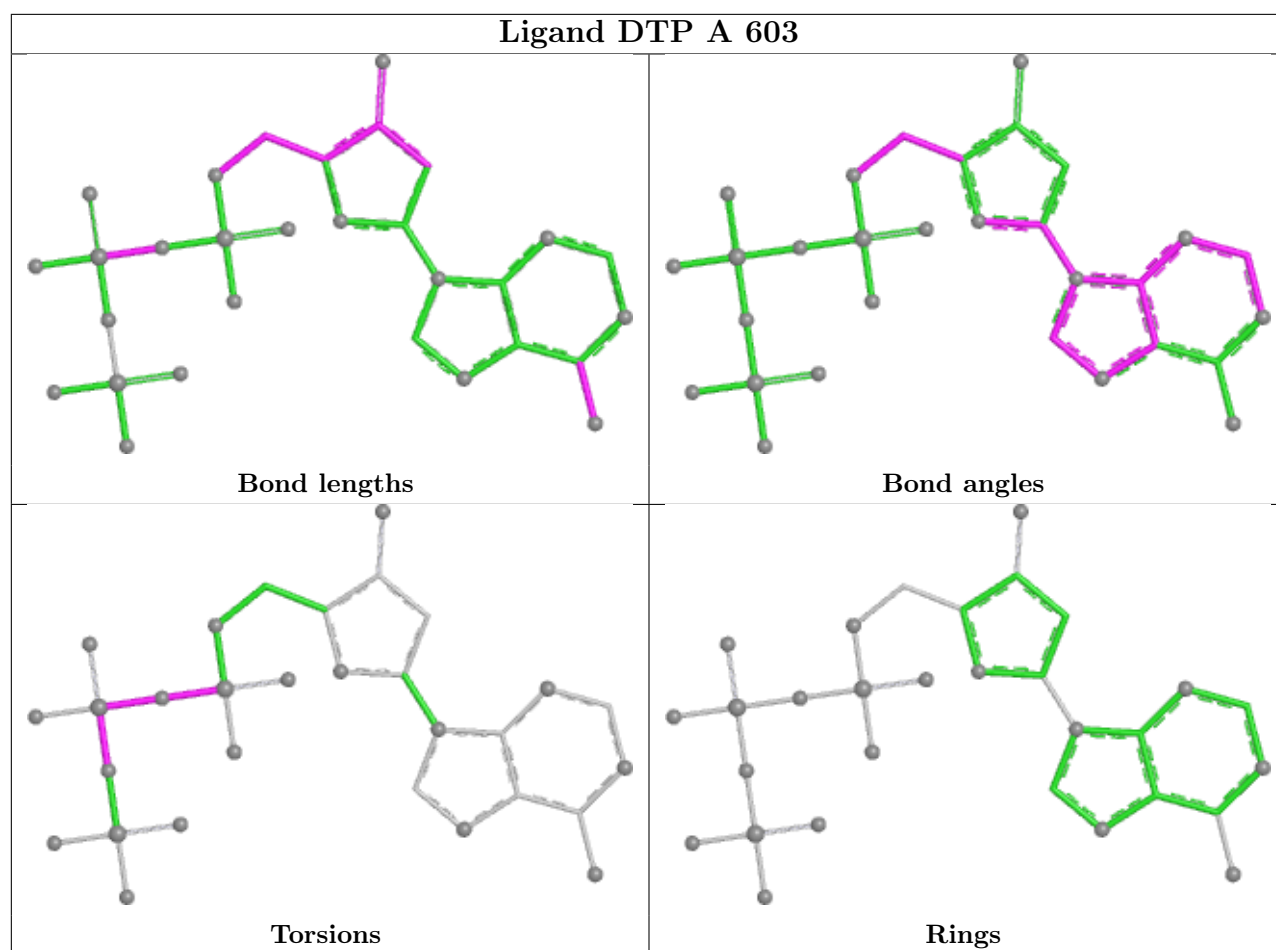
Mol	Chain	Res	Type	Atoms
7	C	601	DTP	PA-O3A-PB-O2B
7	A	603	DTP	PA-O3A-PB-O2B
7	A	603	DTP	PG-O3B-PB-O1B
8	D	503	EDO	O1-C1-C2-O2
7	A	603	DTP	PA-O3A-PB-O1B
7	A	603	DTP	PB-O3A-PA-O2A

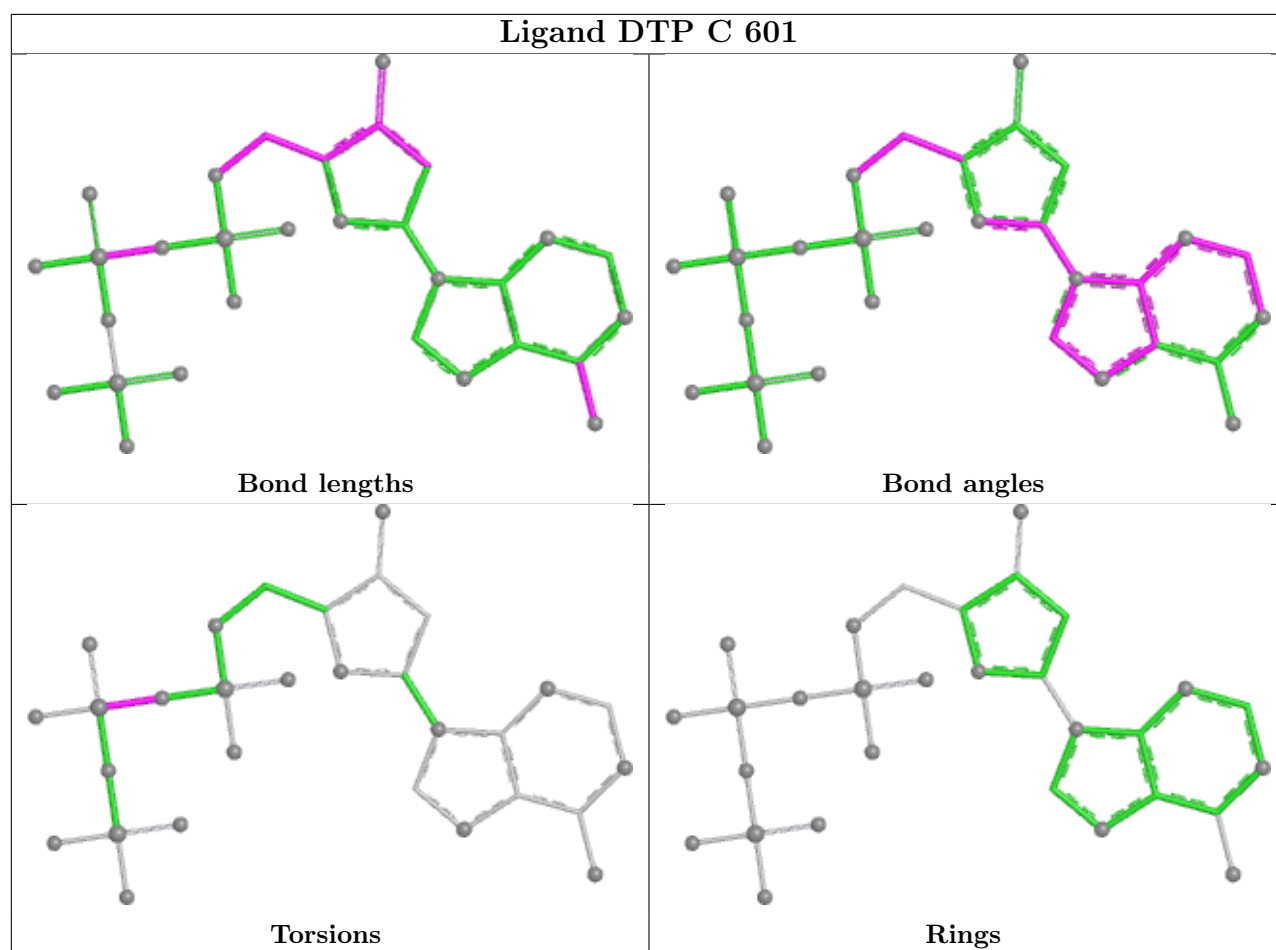
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	503	EDO	3	0
7	A	603	DTP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	555/556 (99%)	0.15	19 (3%)	48	49	33, 84, 169, 230	0
1	C	555/556 (99%)	0.19	19 (3%)	48	49	36, 91, 160, 232	0
2	B	412/428 (96%)	0.04	19 (4%)	37	38	35, 70, 124, 162	0
2	D	412/428 (96%)	0.23	23 (5%)	30	29	37, 82, 142, 174	0
3	E	24/27 (88%)	0.09	0	100	100	76, 116, 193, 231	0
3	T	24/27 (88%)	0.18	0	100	100	76, 110, 203, 249	0
4	F	19/21 (90%)	0.18	0	100	100	62, 99, 182, 186	0
4	P	19/21 (90%)	0.04	1 (5%)	32	31	69, 100, 158, 180	0
All	All	2020/2064 (97%)	0.15	81 (4%)	42	43	33, 81, 156, 249	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	214	LEU	6.4
2	D	423	VAL	4.6
2	B	90	VAL	4.5
2	D	217	PRO	4.5
2	D	360	ALA	4.4
2	B	217	PRO	4.2
2	B	423	VAL	3.9
2	B	232	TYR	3.8
1	C	74	LEU	3.8
2	D	214	LEU	3.8
2	D	425	LEU	3.7
2	D	418	ASN	3.6
2	B	215	THR	3.4
1	A	37	ILE	3.4
2	D	232	TYR	3.4
2	D	88	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	88	TRP	3.3
2	D	95	PRO	3.3
2	B	92	LEU	3.2
2	B	5	ILE	3.2
2	B	425	LEU	3.1
2	D	357	MET	3.1
2	D	422	LEU	3.0
2	D	420	PRO	3.0
2	B	117	SER	3.0
1	A	54	ASN	3.0
2	D	359	GLY	3.0
1	A	135	ILE	2.9
1	C	2	ILE	2.9
2	B	87	PHE	2.9
2	D	354	TYR	2.9
2	D	240	THR	2.8
2	B	4	PRO	2.7
1	C	286	THR	2.7
2	B	195	ILE	2.6
1	A	35	VAL	2.6
2	D	212	TRP	2.6
1	A	77	PHE	2.6
2	D	231	GLY	2.5
1	C	58	THR	2.5
1	C	554	ALA	2.5
1	C	262	GLY	2.5
2	D	421	PRO	2.4
1	A	24	TRP	2.4
1	A	55	PRO	2.4
1	C	4	PRO	2.4
2	B	250	ASP	2.4
1	C	0	VAL	2.4
1	A	140	PRO	2.4
1	C	142	ILE	2.4
1	A	16	MET	2.4
1	C	51	GLY	2.4
1	C	37	ILE	2.4
1	C	109	LEU	2.4
2	D	216	THR	2.3
1	A	554	ALA	2.3
1	A	139	THR	2.3
2	D	213	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	299	ALA	2.3
1	C	135	ILE	2.3
1	C	245	VAL	2.3
1	A	4	PRO	2.3
2	D	318	TYR	2.2
2	B	212	TRP	2.2
1	A	34	LEU	2.2
1	A	0	VAL	2.1
2	B	419	THR	2.1
1	C	5	ILE	2.1
2	B	94	ILE	2.1
1	C	24	TRP	2.1
1	C	61	PHE	2.1
1	A	47	ILE	2.1
2	D	4	PRO	2.1
1	A	166	LYS	2.1
2	D	215	THR	2.1
1	A	5	ILE	2.1
1	C	180	ILE	2.1
4	P	803	DC	2.0
1	A	247	PRO	2.0
2	B	173	LYS	2.0
1	A	71	TRP	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.

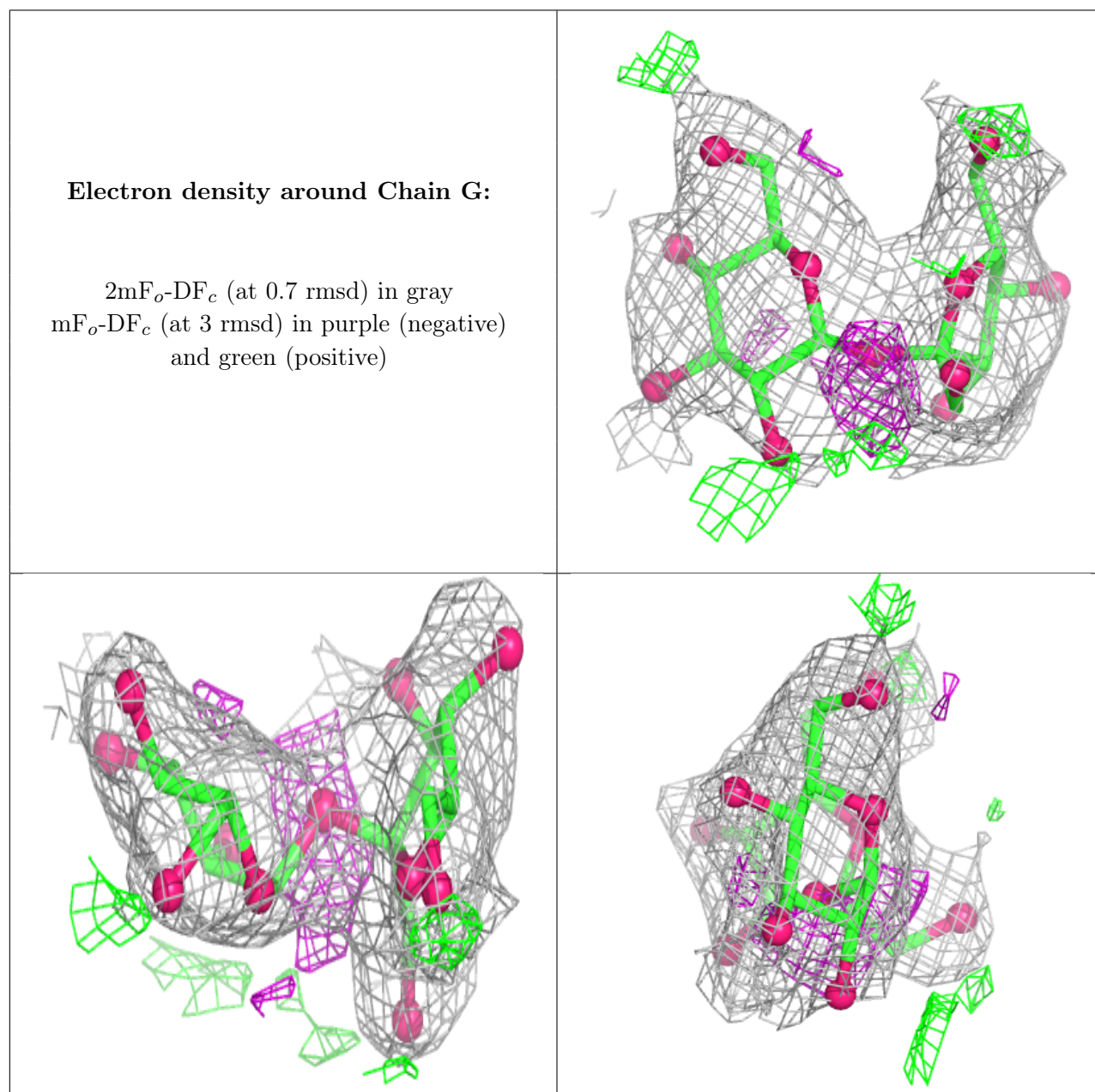
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MRG	P	817	26/27	0.88	0.11	90,114,145,155	0
4	MRG	F	817	26/27	0.88	0.13	105,119,149,157	0

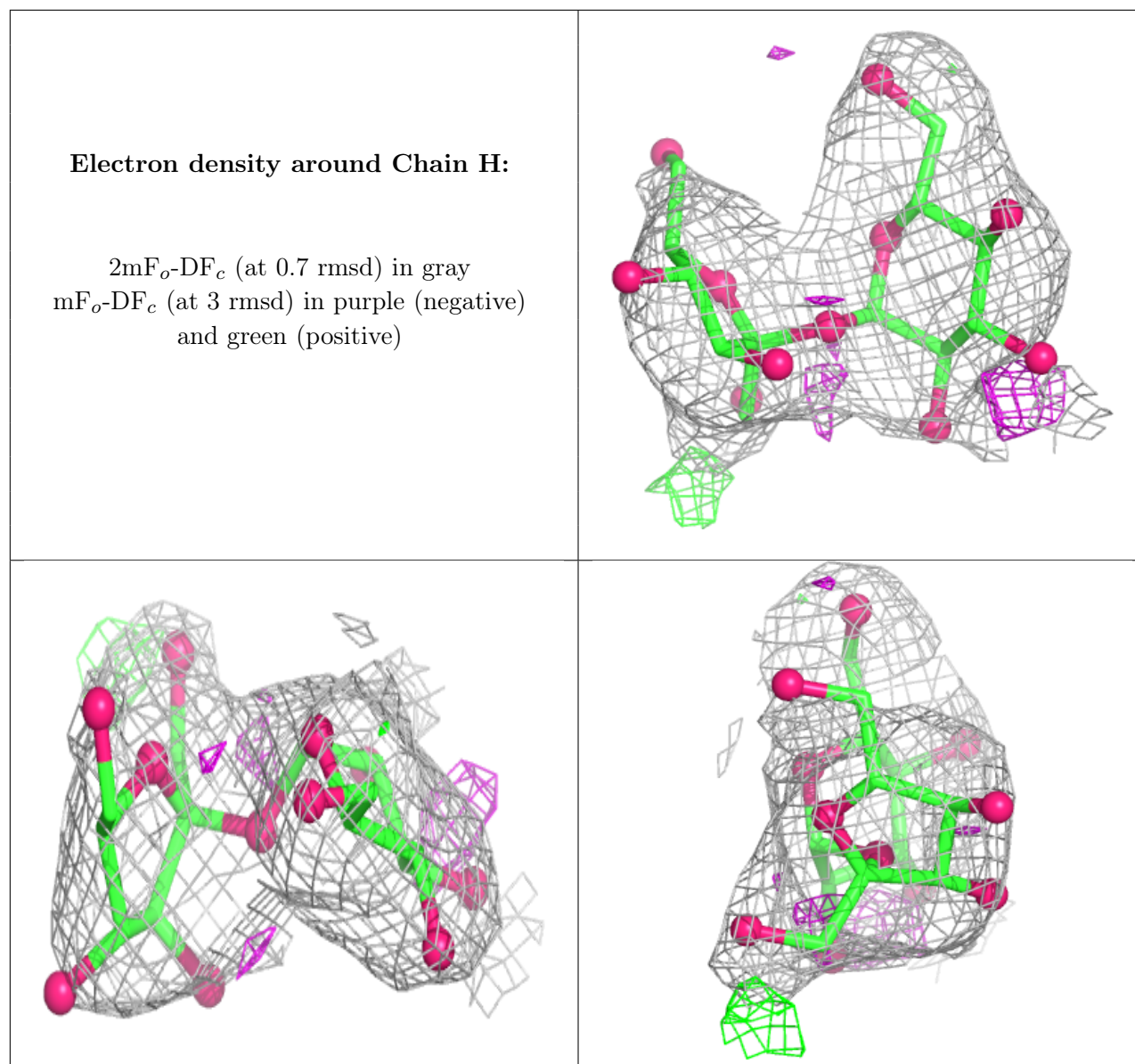
6.3 Carbohydrates [i](#)

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($\text{\AA}^2$)	Q<0.9
5	GLC	G	1	11/12	-	-	69,91,106,110	0
5	FRU	G	2	12/12	-	-	102,114,119,121	0
5	GLC	H	1	11/12	-	-	79,102,114,114	0
5	FRU	H	2	12/12	-	-	95,115,120,123	0

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





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

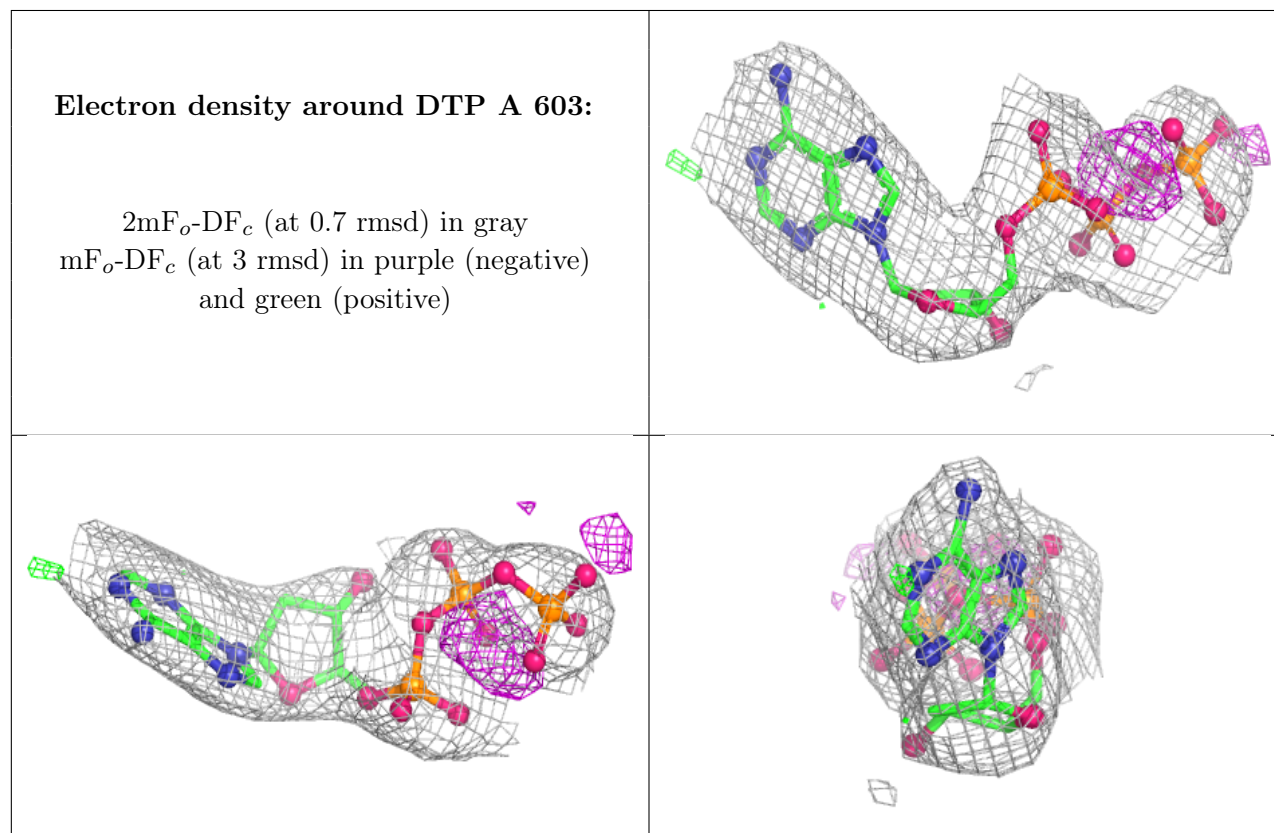
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	A	602	1/1	0.45	0.23	85,85,85,85	0
6	MG	C	603	1/1	0.81	0.16	96,96,96,96	0
8	EDO	D	503	4/4	0.85	0.16	70,74,74,77	0
7	DTP	A	603	30/30	0.88	0.10	73,104,136,139	0
8	EDO	B	502	4/4	0.89	0.14	59,66,71,79	0

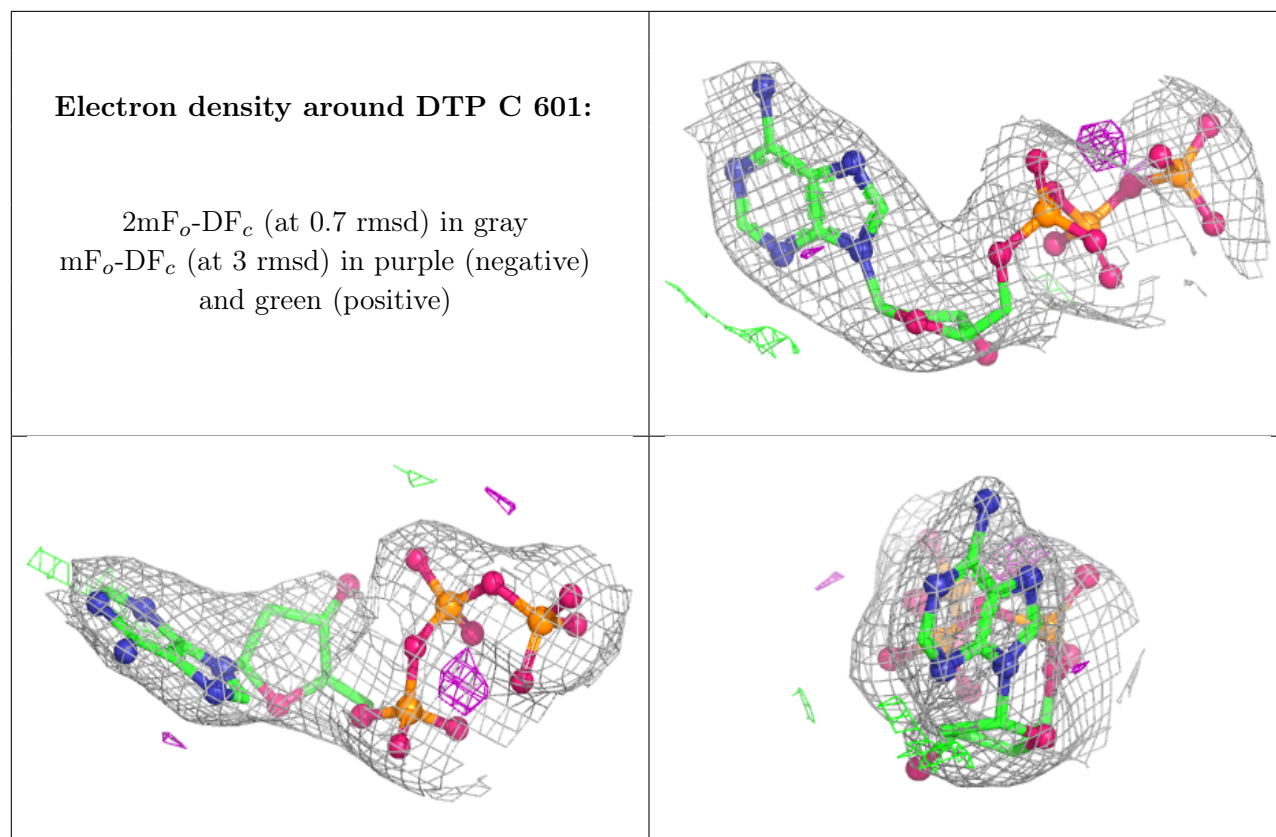
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	SO4	D	502	5/5	0.90	0.16	160,162,164,165	0
7	DTP	C	601	30/30	0.91	0.09	76,97,131,138	0
6	MG	A	601	1/1	0.94	0.08	95,95,95,95	0
6	MG	C	602	1/1	0.95	0.07	80,80,80,80	0

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.