



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:40 PM UTC

PDB ID : 8CM9 / pdb_00008cm9
Title : Structure of human O-GlcNAc transferase in complex with UDP and tP11
Authors : Meek, R.W.; Davies, G.J.
Deposited on : 2023-02-18
Resolution : 2.80 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

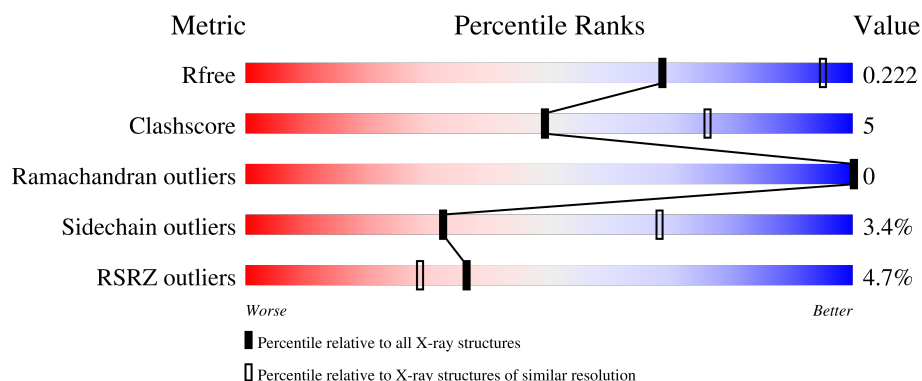
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	723	5% 83% 14% ..
1	B	723	3% 84% 12% ..
1	C	723	4% 85% 12% .
1	D	723	5% 85% 12% .
2	E	7	57% 43% 57%

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Mol	Chain	Length	Quality of chain
2	F	7	14% 57% 43%
2	G	7	43% 57% 43%
2	H	7	57% 57% 43%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22438 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 UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	704	Total	C	N	O	S	0	0	0
			5461	3467	942	1013	39			
1	B	699	Total	C	N	O	S	0	2	0
			5463	3471	942	1010	40			
1	C	704	Total	C	N	O	S	0	2	0
			5484	3483	946	1015	40			
1	D	704	Total	C	N	O	S	0	1	0
			5450	3460	945	1005	40			

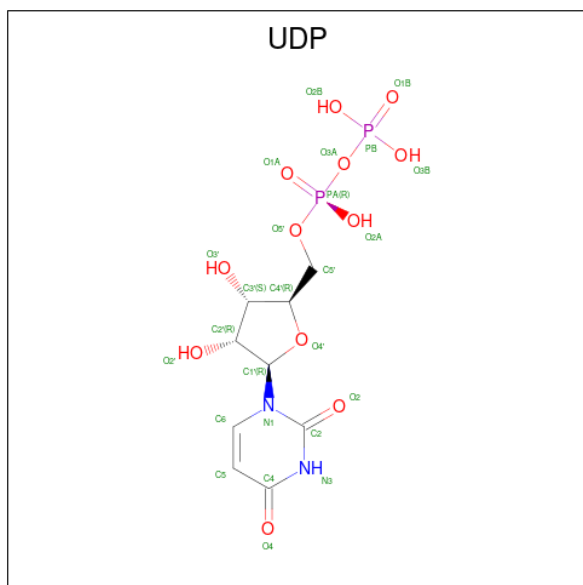
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	319	GLY	-	expression tag	UNP O15294
A	320	PRO	-	expression tag	UNP O15294
A	321	ALA	-	expression tag	UNP O15294
A	322	MET	-	expression tag	UNP O15294
B	319	GLY	-	expression tag	UNP O15294
B	320	PRO	-	expression tag	UNP O15294
B	321	ALA	-	expression tag	UNP O15294
B	322	MET	-	expression tag	UNP O15294
C	319	GLY	-	expression tag	UNP O15294
C	320	PRO	-	expression tag	UNP O15294
C	321	ALA	-	expression tag	UNP O15294
C	322	MET	-	expression tag	UNP O15294
D	319	GLY	-	expression tag	UNP O15294
D	320	PRO	-	expression tag	UNP O15294
D	321	ALA	-	expression tag	UNP O15294
D	322	MET	-	expression tag	UNP O15294

- Molecule 2 is a protein called PHE-MET-PRO-LYS-TYR-SER-ILE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	7	Total	C	N	O	S	0	0	0
			62	43	8	10	1			
2	F	7	Total	C	N	O	S	0	0	0
			62	43	8	10	1			
2	G	7	Total	C	N	O	S	0	0	0
			58	40	7	10	1			
2	H	7	Total	C	N	O	S	0	0	0
			62	43	8	10	1			

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total	O	0	0
			73	73		
4	B	55	Total	O	0	0
			55	55		

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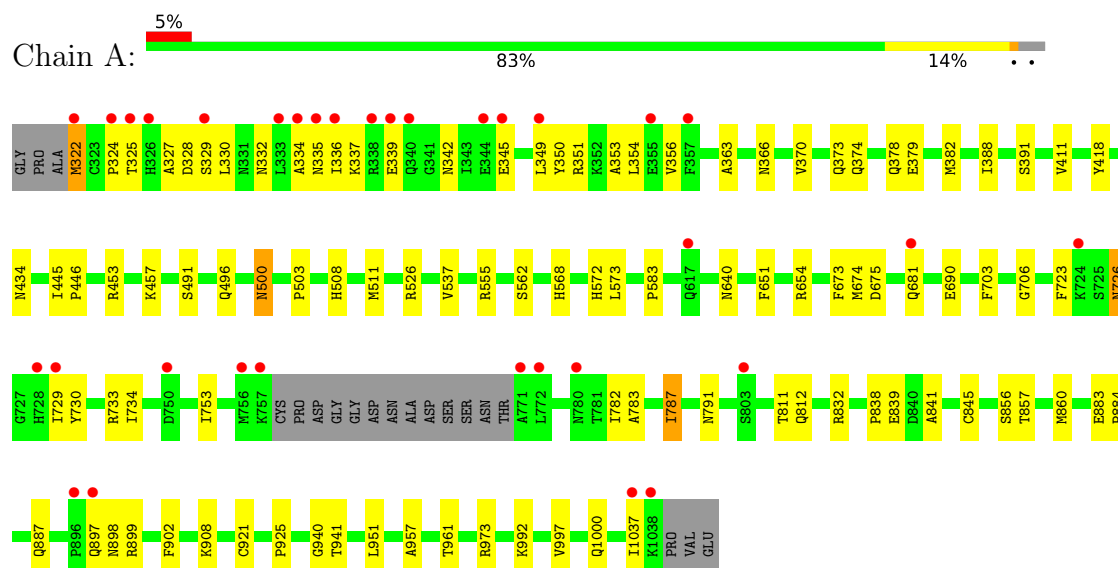
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	81	Total 81	O 81	0	0
4	D	23	Total 23	O 23	0	0
4	E	2	Total 2	O 2	0	0
4	H	2	Total 2	O 2	0	0

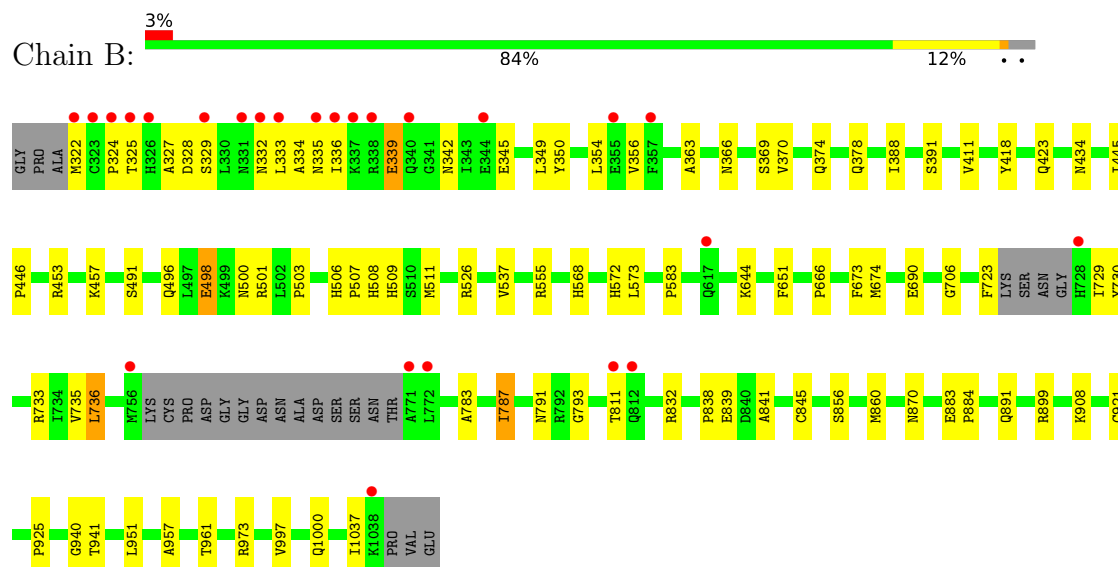
3 Residue-property plots

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

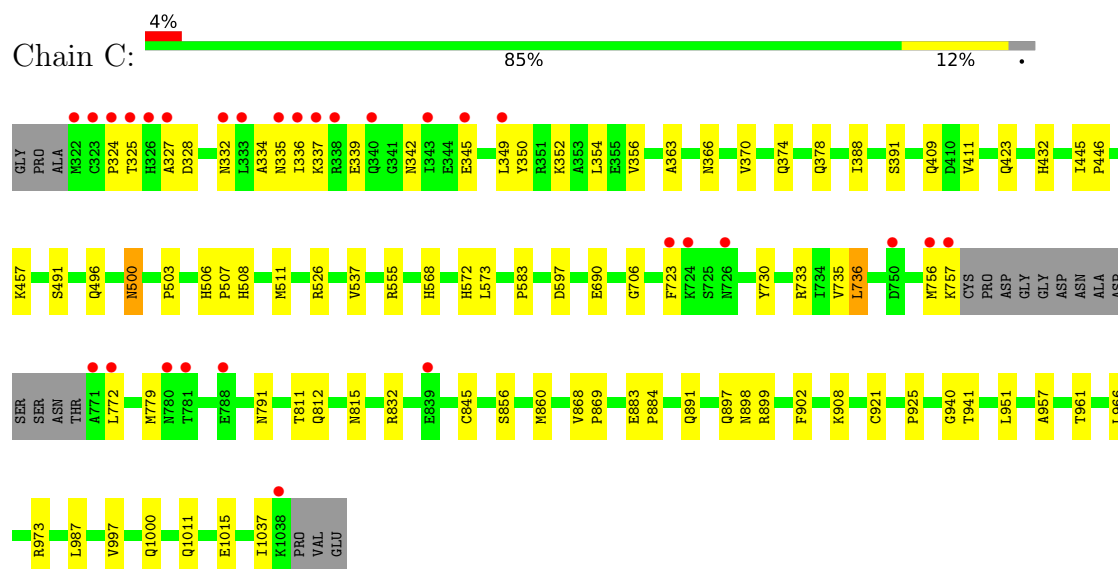
- Molecule 1: UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit



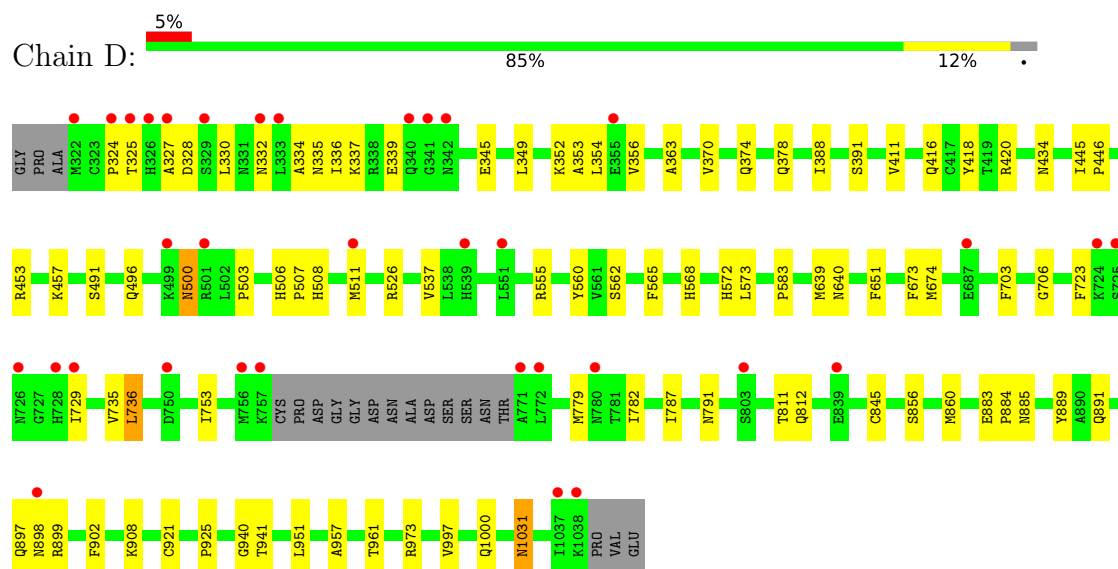
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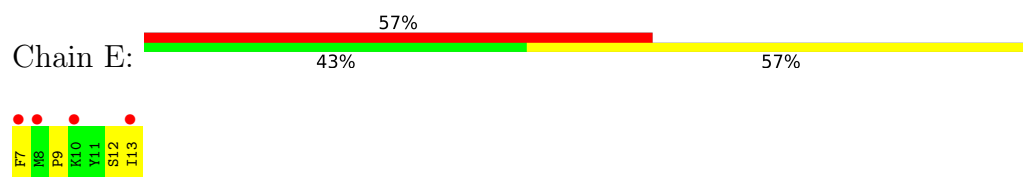
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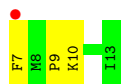


- Molecule 2: PHE-MET-PRO-LYS-TYR-SER-ILE

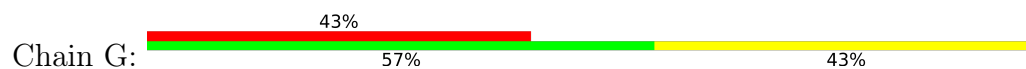


- Molecule 2: PHE-MET-PRO-LYS-TYR-SER-ILE

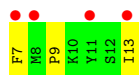




- Molecule 2: PHE-MET-PRO-LYS-TYR-SER-ILE



- Molecule 2: PHE-MET-PRO-LYS-TYR-SER-ILE



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	272.97 Å 272.97 Å 142.59 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	122.10 – 2.80 122.10 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (122.10-2.80) 100.0 (122.10-2.80)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.82 Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.196 , 0.224 0.197 , 0.222	Depositor DCC
R_{free} test set	7627 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22438	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: UDP

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	0.96	0/5589	1.33	7/7602 (0.1%)
1	B	0.96	0/5594	1.33	7/7604 (0.1%)
1	C	0.95	1/5616 (0.0%)	1.34	9/7634 (0.1%)
1	D	0.95	0/5579	1.33	9/7592 (0.1%)
2	E	1.04	0/64	1.23	0/83
2	F	1.13	0/64	1.31	0/83
2	G	1.07	0/60	1.39	0/79
2	H	0.97	0/64	1.29	0/83
All	All	0.96	1/22630 (0.0%)	1.33	32/30760 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	432	HIS	CE1-NE2	5.25	1.37	1.32

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	335	ASN	N-CA-C	-6.69	104.22	112.38
1	D	811	THR	CA-CB-OG1	-6.53	99.81	109.60
1	B	941	THR	CB-CA-C	6.42	116.53	110.17
1	C	941	THR	CB-CA-C	6.38	116.49	110.17
1	A	941	THR	CB-CA-C	6.11	116.22	110.17
1	A	335	ASN	N-CA-C	-6.10	104.94	112.38
1	D	324	PRO	N-CA-C	6.06	121.84	113.65
1	A	457	LYS	N-CA-C	-6.03	104.71	111.28
1	D	457	LYS	N-CA-C	-6.01	104.73	111.28
1	D	335	ASN	N-CA-C	-5.99	105.08	112.38
1	B	457	LYS	N-CA-C	-5.85	104.90	111.28
1	C	811	THR	CA-CB-OG1	-5.80	100.90	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	324	PRO	N-CA-C	5.77	121.44	113.65
1	C	457	LYS	N-CA-C	-5.77	104.99	111.28
1	C	335	ASN	N-CA-C	-5.75	105.37	112.38
1	D	941	THR	CB-CA-C	5.74	115.85	110.17
1	B	811	THR	CA-CB-OG1	-5.72	101.01	109.60
1	C	324	PRO	N-CA-C	5.66	121.30	113.65
1	A	324	PRO	N-CA-C	5.64	121.26	113.65
1	B	378	GLN	N-CA-C	-5.60	105.18	111.28
1	D	568	HIS	CB-CA-C	5.53	118.23	109.55
1	C	597	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	568	HIS	CB-CA-C	5.30	117.86	109.55
1	B	568	HIS	CB-CA-C	5.27	117.83	109.55
1	D	378	GLN	N-CA-C	-5.22	105.59	111.28
1	A	378	GLN	N-CA-C	-5.21	105.61	111.28
1	C	568	HIS	CB-CA-C	5.16	117.65	109.55
1	C	378	GLN	N-CA-C	-5.13	105.69	111.28
1	D	352	LYS	N-CA-C	-5.08	105.44	111.69
1	A	703	PHE	N-CA-C	-5.07	106.36	112.54
1	C	352	LYS	N-CA-C	-5.02	105.52	111.69
1	D	703	PHE	N-CA-C	-5.01	106.43	112.54

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	5461	0	5318	61	0
1	B	5463	0	5343	65	0
1	C	5484	0	5346	52	0
1	D	5450	0	5281	62	0
2	E	62	0	62	4	0
2	F	62	0	62	2	0
2	G	58	0	51	3	0
2	H	62	0	62	3	0
3	A	25	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	25	0	11	1	0
3	C	25	0	11	1	0
3	D	25	0	11	0	0
4	A	73	0	0	0	0
4	B	55	0	0	1	0
4	C	81	0	0	2	0
4	D	23	0	0	0	0
4	E	2	0	0	0	0
4	H	2	0	0	0	0
All	All	22438	0	21569	237	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (237) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:651:PHE:CD2	1:D:674:MET:HE1	2.10	0.86
1:A:651:PHE:CD2	1:A:674:MET:HE1	2.13	0.82
1:B:651:PHE:CD1	1:B:674:MET:HE1	2.15	0.82
1:B:333:LEU:O	1:B:336:ILE:HB	1.85	0.77
1:B:651:PHE:CG	1:B:674:MET:HE1	2.20	0.76
1:A:572:HIS:ND1	1:A:908:LYS:HE3	2.04	0.73
1:A:651:PHE:CG	1:A:674:MET:HE1	2.23	0.73
1:C:572:HIS:ND1	1:C:908:LYS:HE3	2.04	0.72
1:B:572:HIS:ND1	1:B:908:LYS:HE3	2.04	0.72
1:D:651:PHE:CG	1:D:674:MET:HE1	2.26	0.71
1:D:572:HIS:ND1	1:D:908:LYS:HE3	2.05	0.70
1:A:651:PHE:HB3	1:A:674:MET:CE	2.20	0.70
1:B:651:PHE:HB3	1:B:674:MET:CE	2.21	0.70
1:D:885:ASN:O	1:D:889:TYR:HD1	1.77	0.68
1:C:772:LEU:HD23	4:C:1267:HOH:O	1.94	0.67
1:D:651:PHE:HB3	1:D:674:MET:CE	2.25	0.67
1:B:374:GLN:HB3	1:B:537:VAL:HG21	1.78	0.65
1:B:339:GLU:HA	1:B:339:GLU:OE1	1.95	0.65
1:B:333:LEU:HA	1:B:336:ILE:HD12	1.79	0.64
1:D:416:GLN:HE21	1:D:420:ARG:HH12	1.46	0.63
1:B:509:HIS:ND1	4:B:1201:HOH:O	2.31	0.61
1:D:339:GLU:HA	1:D:339:GLU:OE1	1.99	0.60
1:B:673:PHE:HD1	1:B:674:MET:HE2	1.67	0.60
1:B:651:PHE:HB3	1:B:674:MET:HE1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:GLN:HB3	1:D:537:VAL:HG21	1.85	0.59
1:C:374:GLN:HB3	1:C:537:VAL:HG21	1.84	0.59
1:C:812:GLN:HE21	2:H:7:PHE:HE2	1.50	0.59
1:C:845:CYS:SG	1:C:921:CYS:HB2	2.42	0.59
1:C:339:GLU:OE1	1:C:339:GLU:HA	2.01	0.58
1:A:845:CYS:SG	1:A:921:CYS:HB2	2.44	0.58
1:A:908:LYS:HE2	3:A:1101:UDP:O2'	2.04	0.58
1:A:374:GLN:HB3	1:A:537:VAL:HG21	1.86	0.57
1:D:845:CYS:SG	1:D:921:CYS:HB2	2.44	0.57
1:A:651:PHE:HB3	1:A:674:MET:HE1	1.85	0.57
1:B:651:PHE:CB	1:B:674:MET:HE1	2.34	0.56
1:C:791:ASN:HA	2:H:9:PRO:HG3	1.87	0.56
1:B:908:LYS:HE2	3:B:1101:UDP:O2'	2.05	0.56
1:C:327:ALA:HB2	1:C:356:VAL:HG12	1.87	0.56
1:D:334:ALA:HA	1:D:349:LEU:HD12	1.87	0.56
1:B:498:GLU:OE2	1:B:498:GLU:C	2.49	0.56
1:A:651:PHE:CB	1:A:674:MET:HE1	2.36	0.55
1:A:673:PHE:HD1	1:A:674:MET:HE2	1.71	0.55
1:A:860:MET:HE2	1:A:973:ARG:HH21	1.72	0.55
1:A:327:ALA:HB2	1:A:356:VAL:HG12	1.89	0.55
1:D:1031:ASN:N	1:D:1031:ASN:HD22	2.04	0.55
1:D:327:ALA:HB2	1:D:356:VAL:HG12	1.88	0.55
1:B:334:ALA:HA	1:B:349:LEU:HD12	1.89	0.54
1:C:334:ALA:HA	1:C:349:LEU:HD12	1.90	0.54
1:B:860:MET:HE2	1:B:973:ARG:HH21	1.73	0.54
1:B:327:ALA:HB2	1:B:356:VAL:HG12	1.90	0.54
1:B:845:CYS:SG	1:B:921:CYS:HB2	2.48	0.54
1:A:812:GLN:HE21	2:E:7:PHE:HE2	1.56	0.53
1:D:860:MET:HE2	1:D:973:ARG:HH21	1.72	0.53
1:A:812:GLN:NE2	2:E:7:PHE:HE2	2.06	0.53
1:B:733:ARG:HD2	1:B:832:ARG:HD2	1.91	0.53
1:C:883:GLU:HB3	1:C:884:PRO:HD3	1.90	0.52
1:D:735:VAL:C	1:D:736:LEU:HD23	2.35	0.52
1:D:791:ASN:HA	2:G:9:PRO:HG3	1.90	0.52
1:A:654:ARG:HH22	1:A:675:ASP:CG	2.16	0.52
1:B:791:ASN:HA	2:F:9:PRO:HG3	1.91	0.52
1:D:334:ALA:HB2	1:D:349:LEU:CB	2.40	0.52
1:A:733:ARG:HD2	1:A:832:ARG:HD2	1.91	0.52
1:C:334:ALA:HB2	1:C:349:LEU:CB	2.41	0.51
1:D:883:GLU:HB3	1:D:884:PRO:HD3	1.92	0.51
1:A:334:ALA:HB2	1:A:349:LEU:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:860:MET:HE1	1:B:925:PRO:HG2	1.93	0.51
1:D:560:TYR:HB3	1:D:639:MET:CE	2.40	0.51
1:C:860:MET:HE2	1:C:973:ARG:HH21	1.75	0.51
1:C:733:ARG:HD2	1:C:832:ARG:HD2	1.92	0.51
1:B:334:ALA:HB2	1:B:349:LEU:CB	2.41	0.51
1:B:735:VAL:C	1:B:736:LEU:HD23	2.36	0.51
1:D:736:LEU:HD23	1:D:736:LEU:N	2.26	0.50
1:A:651:PHE:CB	1:A:674:MET:CE	2.88	0.50
1:C:735:VAL:C	1:C:736:LEU:HD23	2.35	0.50
1:D:565:PHE:CZ	1:D:639:MET:HE1	2.47	0.50
1:A:883:GLU:HB3	1:A:884:PRO:HD3	1.91	0.50
1:C:736:LEU:HD23	1:C:736:LEU:N	2.27	0.50
1:A:334:ALA:HA	1:A:349:LEU:HD12	1.92	0.50
1:B:423:GLN:CD	1:C:423:GLN:HE22	2.20	0.50
1:B:354:LEU:HD21	1:B:363:ALA:HB3	1.94	0.50
1:A:783:ALA:O	1:A:787:ILE:HG13	2.12	0.50
1:B:736:LEU:HD23	1:B:736:LEU:N	2.27	0.50
1:B:883:GLU:HB3	1:B:884:PRO:HD3	1.94	0.50
1:C:328:ASP:O	1:C:332:ASN:ND2	2.45	0.49
1:C:336:ILE:O	1:C:339:GLU:N	2.44	0.49
1:A:328:ASP:O	1:A:332:ASN:ND2	2.45	0.49
1:B:651:PHE:CB	1:B:674:MET:CE	2.89	0.49
1:A:791:ASN:HA	2:E:9:PRO:HG3	1.94	0.49
1:D:651:PHE:HB3	1:D:674:MET:HE1	1.94	0.49
1:B:496:GLN:OE1	1:B:503:PRO:HA	2.12	0.49
1:D:328:ASP:O	1:D:332:ASN:ND2	2.45	0.49
1:D:812:GLN:NE2	2:G:7:PHE:HE2	2.11	0.49
1:A:734:ILE:HD11	2:E:13:ILE:HD13	1.95	0.48
1:D:673:PHE:HD1	1:D:674:MET:HE2	1.77	0.48
1:A:860:MET:HE1	1:A:925:PRO:HG2	1.94	0.48
1:A:940:GLY:HA2	1:A:997:VAL:HG12	1.95	0.48
1:D:560:TYR:HB3	1:D:639:MET:HE2	1.96	0.48
1:D:336:ILE:O	1:D:339:GLU:N	2.45	0.48
1:D:354:LEU:HD21	1:D:363:ALA:HB3	1.94	0.48
1:A:351:ARG:NH2	1:A:379:GLU:OE2	2.47	0.48
1:D:651:PHE:CB	1:D:674:MET:CE	2.92	0.48
1:D:940:GLY:HA2	1:D:997:VAL:HG12	1.95	0.47
1:C:555:ARG:HD3	1:C:583:PRO:O	2.14	0.47
1:C:908:LYS:HE2	3:C:1101:UDP:O2'	2.13	0.47
1:C:957:ALA:O	1:C:961:THR:HG23	2.14	0.47
1:B:328:ASP:O	1:B:332:ASN:ND2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LEU:HD21	1:A:363:ALA:HB3	1.96	0.47
1:D:1031:ASN:N	1:D:1031:ASN:ND2	2.62	0.47
1:C:730:TYR:CB	1:C:733:ARG:HG2	2.45	0.47
1:D:496:GLN:OE1	1:D:503:PRO:HA	2.15	0.47
1:A:496:GLN:OE1	1:A:503:PRO:HA	2.15	0.47
1:A:957:ALA:O	1:A:961:THR:HG23	2.15	0.47
1:B:783:ALA:O	1:B:787:ILE:HG13	2.14	0.47
1:B:838:PRO:HG2	1:B:841:ALA:HB3	1.96	0.47
1:D:651:PHE:CB	1:D:674:MET:HE1	2.44	0.47
1:A:345:GLU:OE1	1:A:345:GLU:HA	2.15	0.47
1:B:500:ASN:HA	1:B:526:ARG:HH22	1.80	0.47
1:C:345:GLU:OE1	1:C:345:GLU:HA	2.15	0.47
1:C:500:ASN:HA	1:C:526:ARG:NH2	2.30	0.47
1:C:860:MET:HE1	1:C:925:PRO:HG2	1.97	0.47
1:D:500:ASN:HA	1:D:526:ARG:NH2	2.31	0.47
1:D:565:PHE:HZ	1:D:639:MET:HE1	1.79	0.47
1:B:336:ILE:O	1:B:339:GLU:N	2.48	0.46
1:A:651:PHE:HB3	1:A:674:MET:HE2	1.97	0.46
1:A:951:LEU:C	1:A:951:LEU:HD23	2.41	0.46
1:B:573:LEU:HA	1:B:706:GLY:HA2	1.97	0.46
1:C:940:GLY:HA2	1:C:997:VAL:HG12	1.96	0.46
1:A:500:ASN:HA	1:A:526:ARG:NH2	2.29	0.46
1:D:951:LEU:C	1:D:951:LEU:HD23	2.41	0.46
1:D:957:ALA:O	1:D:961:THR:HG23	2.15	0.46
1:C:573:LEU:HA	1:C:706:GLY:HA2	1.97	0.46
1:A:453:ARG:HH11	1:A:453:ARG:HG2	1.81	0.46
1:B:555:ARG:HD3	1:B:583:PRO:O	2.16	0.46
1:B:951:LEU:C	1:B:951:LEU:HD23	2.40	0.46
1:C:354:LEU:HD21	1:C:363:ALA:HB3	1.96	0.46
1:D:860:MET:HE1	1:D:925:PRO:HG2	1.97	0.46
1:B:445:ILE:N	1:B:446:PRO:CD	2.79	0.46
1:B:957:ALA:O	1:B:961:THR:HG23	2.15	0.45
1:A:883:GLU:HG3	1:A:902:PHE:CD1	2.51	0.45
1:D:899:ARG:HG3	1:D:899:ARG:HH11	1.81	0.45
1:B:423:GLN:CG	1:C:423:GLN:NE2	2.80	0.45
1:B:899:ARG:HG3	1:B:899:ARG:HH11	1.81	0.45
1:D:573:LEU:HA	1:D:706:GLY:HA2	1.99	0.45
1:B:334:ALA:HB2	1:B:349:LEU:HB2	1.98	0.45
1:B:940:GLY:HA2	1:B:997:VAL:HG12	1.99	0.45
1:C:951:LEU:HD23	1:C:951:LEU:C	2.41	0.45
1:D:812:GLN:NE2	2:G:7:PHE:CE2	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:VAL:O	1:B:374:GLN:HG3	2.17	0.45
1:C:334:ALA:HB2	1:C:349:LEU:HB2	2.00	0.44
1:C:883:GLU:HG3	1:C:902:PHE:CD1	2.52	0.44
1:C:496:GLN:OE1	1:C:503:PRO:HA	2.18	0.44
1:C:508:HIS:O	1:C:511[A]:MET:HG2	2.17	0.44
1:C:973:ARG:NH1	4:C:1207:HOH:O	2.49	0.44
1:B:723:PHE:CD1	1:B:723:PHE:N	2.85	0.44
1:A:370:VAL:O	1:A:374:GLN:HG3	2.18	0.44
1:A:445:ILE:N	1:A:446:PRO:CD	2.81	0.44
1:B:651:PHE:HB3	1:B:674:MET:HE2	2.00	0.44
1:C:899:ARG:HH11	1:C:899:ARG:HG3	1.82	0.44
1:D:334:ALA:HB2	1:D:349:LEU:HB2	1.99	0.44
1:D:345:GLU:HA	1:D:345:GLU:OE1	2.16	0.44
1:A:555:ARG:HD3	1:A:583:PRO:O	2.18	0.44
1:B:729:ILE:O	1:B:729:ILE:HG22	2.18	0.44
1:D:885:ASN:O	1:D:889:TYR:CD1	2.64	0.44
1:A:573:LEU:HA	1:A:706:GLY:HA2	1.99	0.43
1:C:756:MET:O	1:C:757:LYS:CB	2.66	0.43
1:B:870:ASN:CG	1:B:870:ASN:O	2.61	0.43
1:C:812:GLN:NE2	2:H:7:PHE:HE2	2.14	0.43
1:D:555:ARG:HD3	1:D:583:PRO:O	2.18	0.43
1:A:562:SER:HA	1:A:640:ASN:HD21	1.83	0.43
1:B:508:HIS:O	1:B:511[A]:MET:HG2	2.18	0.43
1:D:508:HIS:O	1:D:511[A]:MET:HG2	2.17	0.43
1:A:334:ALA:HB2	1:A:349:LEU:HB3	2.00	0.43
1:B:345:GLU:HA	1:B:345:GLU:OE1	2.17	0.43
1:B:511[B]:MET:HE3	1:B:666:PRO:HG2	2.00	0.43
1:C:445:ILE:N	1:C:446:PRO:CD	2.82	0.43
1:D:562:SER:HB2	1:D:639:MET:HE3	1.99	0.43
1:A:730:TYR:CB	1:A:733:ARG:HG2	2.49	0.43
1:D:883:GLU:HG3	1:D:902:PHE:CD1	2.53	0.43
1:B:329:SER:HA	1:B:332:ASN:HD22	1.83	0.43
1:B:423:GLN:CG	1:C:423:GLN:HE22	2.31	0.43
1:C:860:MET:HE2	1:C:973:ARG:HE	1.82	0.43
1:D:562:SER:HA	1:D:640:ASN:HD21	1.84	0.42
1:D:445:ILE:N	1:D:446:PRO:CD	2.82	0.42
1:A:860:MET:HE2	1:A:973:ARG:HE	1.85	0.42
1:A:726:ASN:OD1	1:A:726:ASN:N	2.53	0.42
1:A:723:PHE:N	1:A:723:PHE:CD1	2.88	0.42
1:A:887:GLN:OE1	1:A:887:GLN:HA	2.20	0.42
1:C:723:PHE:CD1	1:C:723:PHE:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:418:TYR:CE1	1:D:434:ASN:HB3	2.54	0.42
1:A:336:ILE:O	1:A:337:LYS:C	2.62	0.42
1:A:1037:ILE:O	1:A:1037:ILE:HG22	2.19	0.42
1:B:506:HIS:CG	1:B:507:PRO:HD2	2.54	0.42
1:C:336:ILE:O	1:C:337:LYS:C	2.62	0.42
1:C:723:PHE:HA	1:C:779:MET:HE2	2.01	0.42
1:D:336:ILE:O	1:D:337:LYS:C	2.63	0.42
1:A:342:ASN:OD1	1:A:342:ASN:C	2.63	0.42
1:A:322:MET:HE2	1:A:322:MET:HB3	1.92	0.42
1:A:336:ILE:O	1:A:339:GLU:N	2.50	0.42
1:C:370:VAL:O	1:C:374:GLN:HG3	2.20	0.42
1:C:868:VAL:HA	1:C:869:PRO:HD2	1.89	0.42
1:D:330:LEU:HD12	1:D:353:ALA:HA	2.01	0.41
1:A:329:SER:HA	1:A:332:ASN:HD22	1.85	0.41
1:A:899:ARG:HG3	1:A:899:ARG:HH11	1.85	0.41
1:D:723:PHE:N	1:D:723:PHE:CD1	2.88	0.41
1:A:418:TYR:CE1	1:A:434:ASN:HB3	2.56	0.41
1:A:838:PRO:HG2	1:A:841:ALA:HB3	2.01	0.41
1:B:860:MET:HE2	1:B:973:ARG:HE	1.86	0.41
1:C:350:TYR:CZ	1:C:366:ASN:HB3	2.56	0.41
1:D:334:ALA:HB2	1:D:349:LEU:HB3	2.02	0.41
1:A:334:ALA:HB2	1:A:349:LEU:HB2	2.00	0.41
1:A:350:TYR:CZ	1:A:366:ASN:HB3	2.55	0.41
1:C:506:HIS:CG	1:C:507:PRO:HD2	2.55	0.41
1:D:453:ARG:HH11	1:D:453:ARG:HG2	1.86	0.41
1:A:330:LEU:HD12	1:A:353:ALA:HA	2.03	0.41
1:B:350:TYR:CZ	1:B:366:ASN:HB3	2.56	0.41
1:C:1011:GLN:O	1:C:1015:GLU:HG2	2.21	0.41
1:D:506:HIS:CG	1:D:507:PRO:HD2	2.56	0.41
1:D:860:MET:CE	1:D:973:ARG:HH21	2.34	0.41
1:B:418:TYR:CE1	1:B:434:ASN:HB3	2.56	0.41
1:C:342:ASN:OD1	1:C:342:ASN:C	2.64	0.41
1:D:860:MET:HE2	1:D:973:ARG:HE	1.86	0.41
1:B:342:ASN:C	1:B:342:ASN:OD1	2.64	0.40
1:B:418:TYR:CZ	1:B:434:ASN:HB3	2.57	0.40
1:B:1037:ILE:HG22	1:B:1037:ILE:O	2.22	0.40
1:C:334:ALA:HB2	1:C:349:LEU:HB3	2.03	0.40
1:D:370:VAL:O	1:D:374:GLN:HG3	2.20	0.40
1:C:1037:ILE:O	1:C:1037:ILE:HG22	2.21	0.40
1:D:651:PHE:HB3	1:D:674:MET:HE2	1.99	0.40
1:A:508:HIS:O	1:A:511:MET:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:THR:HA	1:A:860:MET:HE3	2.03	0.40
1:B:334:ALA:HB2	1:B:349:LEU:HB3	2.03	0.40
1:B:730:TYR:CB	1:B:733:ARG:HG2	2.51	0.40
1:B:793:GLY:O	2:F:7:PHE:N	2.54	0.40
1:D:723:PHE:HA	1:D:779:MET:HE2	2.04	0.40
1:B:332:ASN:O	1:B:336:ILE:HG13	2.21	0.40
1:B:453:ARG:HG2	1:B:453:ARG:HH11	1.87	0.40
1:D:330:LEU:HB2	1:D:353:ALA:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	700/723 (97%)	670 (96%)	30 (4%)	0	100	100
1	B	695/723 (96%)	669 (96%)	26 (4%)	0	100	100
1	C	702/723 (97%)	672 (96%)	30 (4%)	0	100	100
1	D	701/723 (97%)	670 (96%)	31 (4%)	0	100	100
2	E	5/7 (71%)	5 (100%)	0	0	100	100
2	F	5/7 (71%)	4 (80%)	1 (20%)	0	100	100
2	G	5/7 (71%)	5 (100%)	0	0	100	100
2	H	5/7 (71%)	4 (80%)	1 (20%)	0	100	100
All	All	2818/2920 (96%)	2699 (96%)	119 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	579/618 (94%)	556 (96%)	23 (4%)	28	63
1	B	583/618 (94%)	565 (97%)	18 (3%)	35	70
1	C	581/618 (94%)	564 (97%)	17 (3%)	37	73
1	D	572/618 (93%)	555 (97%)	17 (3%)	36	72
2	E	7/7 (100%)	6 (86%)	1 (14%)	3	11
2	F	7/7 (100%)	6 (86%)	1 (14%)	3	11
2	G	6/7 (86%)	5 (83%)	1 (17%)	2	8
2	H	7/7 (100%)	6 (86%)	1 (14%)	3	11
All	All	2342/2500 (94%)	2263 (97%)	79 (3%)	32	68

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	322	MET
1	A	325	THR
1	A	373	GLN
1	A	382	MET
1	A	388	ILE
1	A	391	SER
1	A	411	VAL
1	A	491	SER
1	A	500	ASN
1	A	681	GLN
1	A	690	GLU
1	A	726	ASN
1	A	729	ILE
1	A	753	ILE
1	A	782	ILE
1	A	787	ILE
1	A	811	THR
1	A	839	GLU
1	A	856	SER

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Mol	Chain	Res	Type
1	A	897	GLN
1	A	898	ASN
1	A	992	LYS
1	A	1000	GLN
1	B	322	MET
1	B	325	THR
1	B	339	GLU
1	B	369	SER
1	B	388	ILE
1	B	391	SER
1	B	411	VAL
1	B	491	SER
1	B	498	GLU
1	B	501	ARG
1	B	644	LYS
1	B	690	GLU
1	B	736	LEU
1	B	787	ILE
1	B	839	GLU
1	B	856	SER
1	B	891	GLN
1	B	1000	GLN
1	C	325	THR
1	C	388	ILE
1	C	391	SER
1	C	409	GLN
1	C	411	VAL
1	C	491	SER
1	C	500	ASN
1	C	690	GLU
1	C	736	LEU
1	C	815	ASN
1	C	856	SER
1	C	891	GLN
1	C	897	GLN
1	C	898	ASN
1	C	966	LEU
1	C	987	LEU
1	C	1000	GLN
1	D	325	THR
1	D	388	ILE
1	D	391	SER

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Mol	Chain	Res	Type
1	D	411	VAL
1	D	491	SER
1	D	500	ASN
1	D	729	ILE
1	D	736	LEU
1	D	753	ILE
1	D	782	ILE
1	D	787	ILE
1	D	856	SER
1	D	891	GLN
1	D	897	GLN
1	D	898	ASN
1	D	1000	GLN
1	D	1031	ASN
2	E	12	SER
2	F	10	LYS
2	G	12	SER
2	H	13	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	331	ASN
1	A	332	ASN
1	A	335	ASN
1	A	373	GLN
1	A	527	HIS
1	A	617	GLN
1	A	640	ASN
1	A	773	ASN
1	A	888	GLN
1	A	898	ASN
1	A	1031	ASN
1	B	332	ASN
1	B	335	ASN
1	B	416	GLN
1	B	500	ASN
1	B	527	HIS
1	B	617	GLN
1	B	773	ASN
1	B	891	GLN
1	B	897	GLN

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Mol	Chain	Res	Type
1	B	1031	ASN
1	C	331	ASN
1	C	332	ASN
1	C	366	ASN
1	C	374	GLN
1	C	409	GLN
1	C	423	GLN
1	C	539	HIS
1	C	617	GLN
1	C	794	GLN
1	C	815	ASN
1	C	891	GLN
1	C	898	ASN
1	C	974	GLN
1	C	1000	GLN
1	C	1031	ASN
1	D	331	ASN
1	D	332	ASN
1	D	366	ASN
1	D	416	GLN
1	D	527	HIS
1	D	640	ASN
1	D	794	GLN
1	D	796	GLN
1	D	863	ASN
1	D	891	GLN
1	D	892	ASN
1	D	898	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	UDP	B	1101	-	25,26,26	1.31	5 (20%)	38,40,40	1.42	6 (15%)
3	UDP	D	1101	-	25,26,26	1.37	4 (16%)	38,40,40	1.27	4 (10%)
3	UDP	C	1101	-	25,26,26	1.30	3 (12%)	38,40,40	1.60	7 (18%)
3	UDP	A	1101	-	25,26,26	1.41	4 (16%)	38,40,40	1.46	8 (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
3	UDP	B	1101	-	-	2/16/32/32	0/2/2/2
3	UDP	D	1101	-	-	2/16/32/32	0/2/2/2
3	UDP	C	1101	-	-	2/16/32/32	0/2/2/2
3	UDP	A	1101	-	-	2/16/32/32	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1101	UDP	PA-O3A	3.35	1.63	1.59
3	A	1101	UDP	C2-N1	3.08	1.43	1.38
3	D	1101	UDP	C6-C5	3.03	1.42	1.35
3	A	1101	UDP	PA-O3A	2.98	1.62	1.59
3	D	1101	UDP	PA-O3A	2.95	1.62	1.59
3	A	1101	UDP	C6-C5	2.77	1.41	1.35
3	C	1101	UDP	C6-C5	2.72	1.41	1.35
3	B	1101	UDP	PA-O3A	2.67	1.62	1.59
3	A	1101	UDP	C4-N3	-2.32	1.34	1.38
3	B	1101	UDP	C4-N3	-2.25	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1101	UDP	O4'-C4'	-2.24	1.40	1.45
3	B	1101	UDP	C6-C5	2.23	1.40	1.35
3	C	1101	UDP	O2-C2	2.06	1.26	1.23
3	D	1101	UDP	O2-C2	2.06	1.26	1.23
3	D	1101	UDP	C4-N3	-2.04	1.35	1.38
3	B	1101	UDP	C5-C4	-2.04	1.39	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1101	UDP	O3B-PB-O2B	3.98	122.74	107.80
3	D	1101	UDP	N3-C2-N1	3.86	119.92	114.89
3	B	1101	UDP	C5-C4-N3	3.63	119.89	114.80
3	A	1101	UDP	N3-C2-N1	3.56	119.53	114.89
3	C	1101	UDP	O2A-PA-O1A	3.34	128.00	112.44
3	C	1101	UDP	O2B-PB-O3A	-3.30	93.58	104.64
3	A	1101	UDP	C5-C4-N3	3.23	119.32	114.80
3	B	1101	UDP	C4-N3-C2	-3.21	122.63	126.61
3	A	1101	UDP	C4-N3-C2	-2.85	123.08	126.61
3	C	1101	UDP	N3-C2-N1	2.80	118.54	114.89
3	A	1101	UDP	O2A-PA-O1A	2.76	125.30	112.44
3	B	1101	UDP	C2'-C1'-N1	2.73	120.83	113.25
3	B	1101	UDP	N3-C2-N1	2.71	118.42	114.89
3	B	1101	UDP	O3B-PB-O2B	2.61	117.57	107.80
3	C	1101	UDP	C4-N3-C2	-2.57	123.42	126.61
3	D	1101	UDP	C4-N3-C2	-2.55	123.44	126.61
3	A	1101	UDP	O3A-PA-O1A	-2.54	103.06	110.70
3	C	1101	UDP	C5-C4-N3	2.51	118.31	114.80
3	B	1101	UDP	O3A-PB-O1B	-2.43	98.24	111.04
3	D	1101	UDP	O2B-PB-O3A	-2.38	96.67	104.64
3	A	1101	UDP	O3A-PB-O1B	-2.23	99.30	111.04
3	A	1101	UDP	C6-N1-C2	-2.19	118.33	121.00
3	D	1101	UDP	O2A-PA-O1A	2.14	122.41	112.44
3	A	1101	UDP	O2-C2-N3	-2.10	117.62	121.49
3	C	1101	UDP	C2'-C1'-N1	2.07	119.01	113.25

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1101	UDP	C3'-C4'-C5'-O5'
3	D	1101	UDP	O4'-C4'-C5'-O5'

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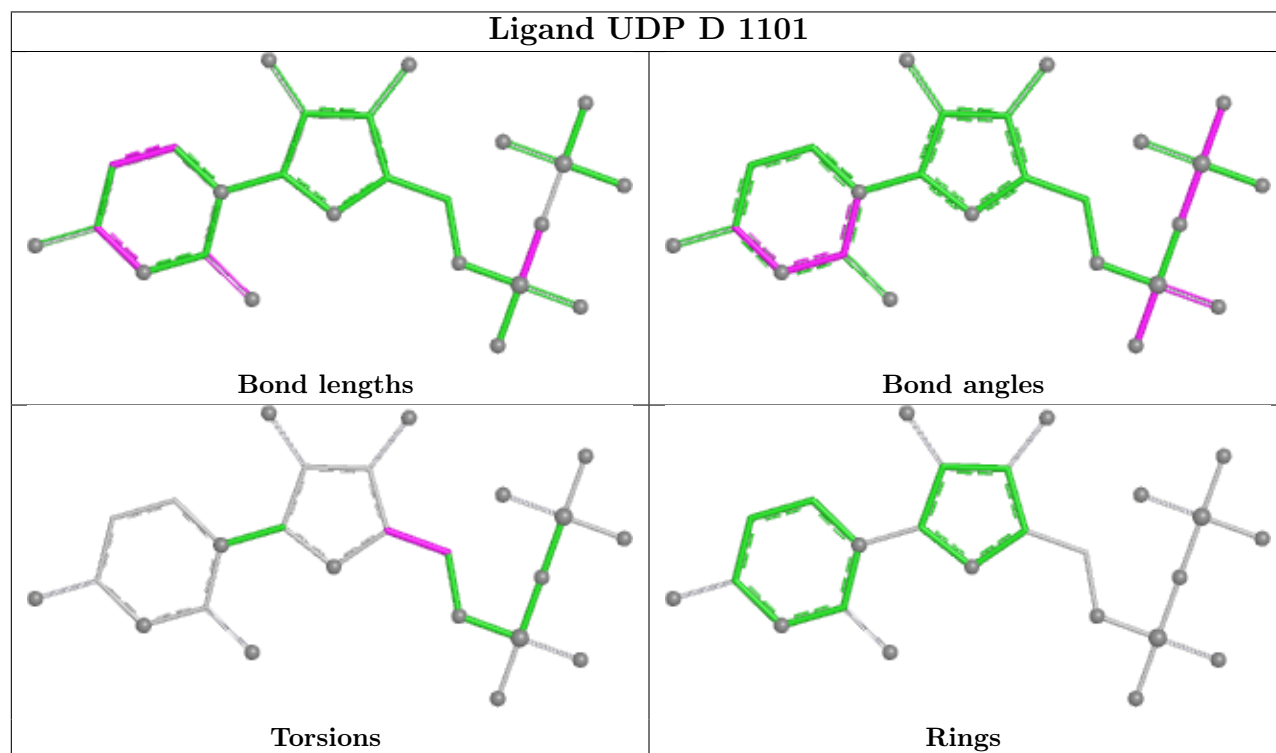
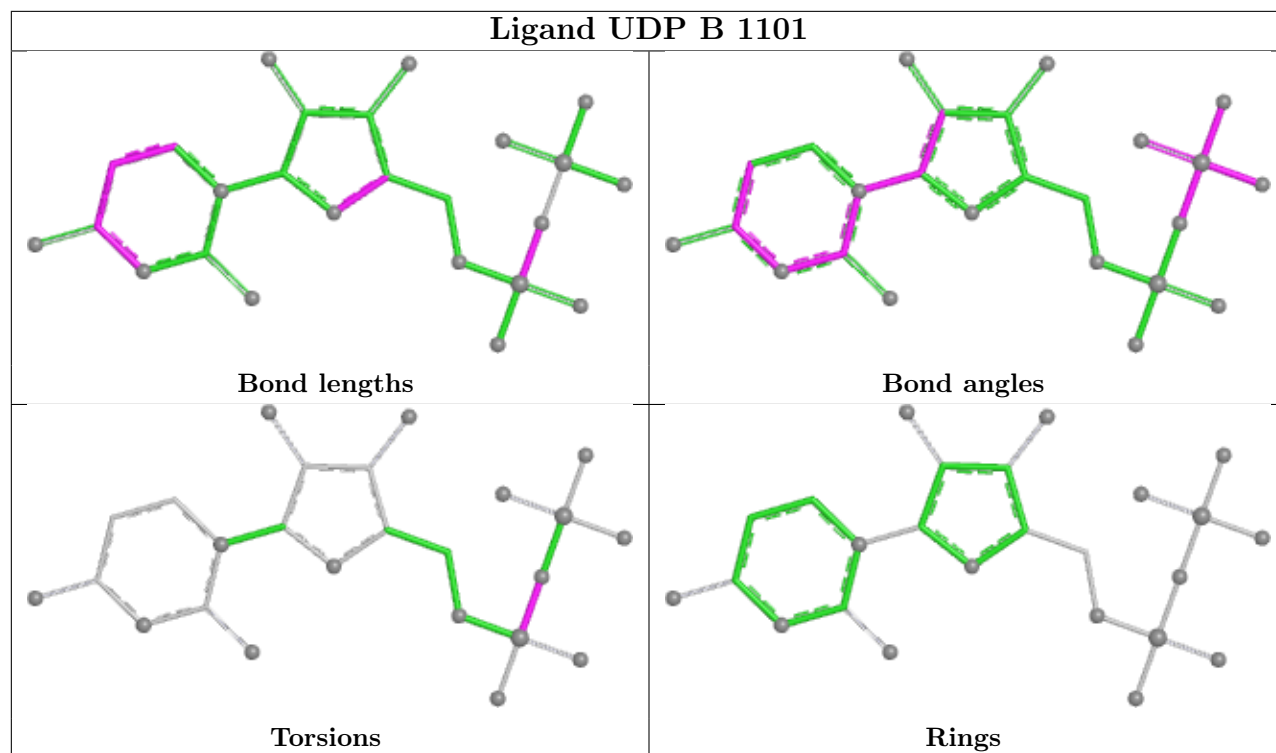
Mol	Chain	Res	Type	Atoms
3	B	1101	UDP	PB-O3A-PA-O2A
3	A	1101	UDP	O4'-C4'-C5'-O5'
3	C	1101	UDP	O4'-C4'-C5'-O5'
3	A	1101	UDP	PB-O3A-PA-O1A
3	C	1101	UDP	C3'-C4'-C5'-O5'
3	B	1101	UDP	PB-O3A-PA-O1A

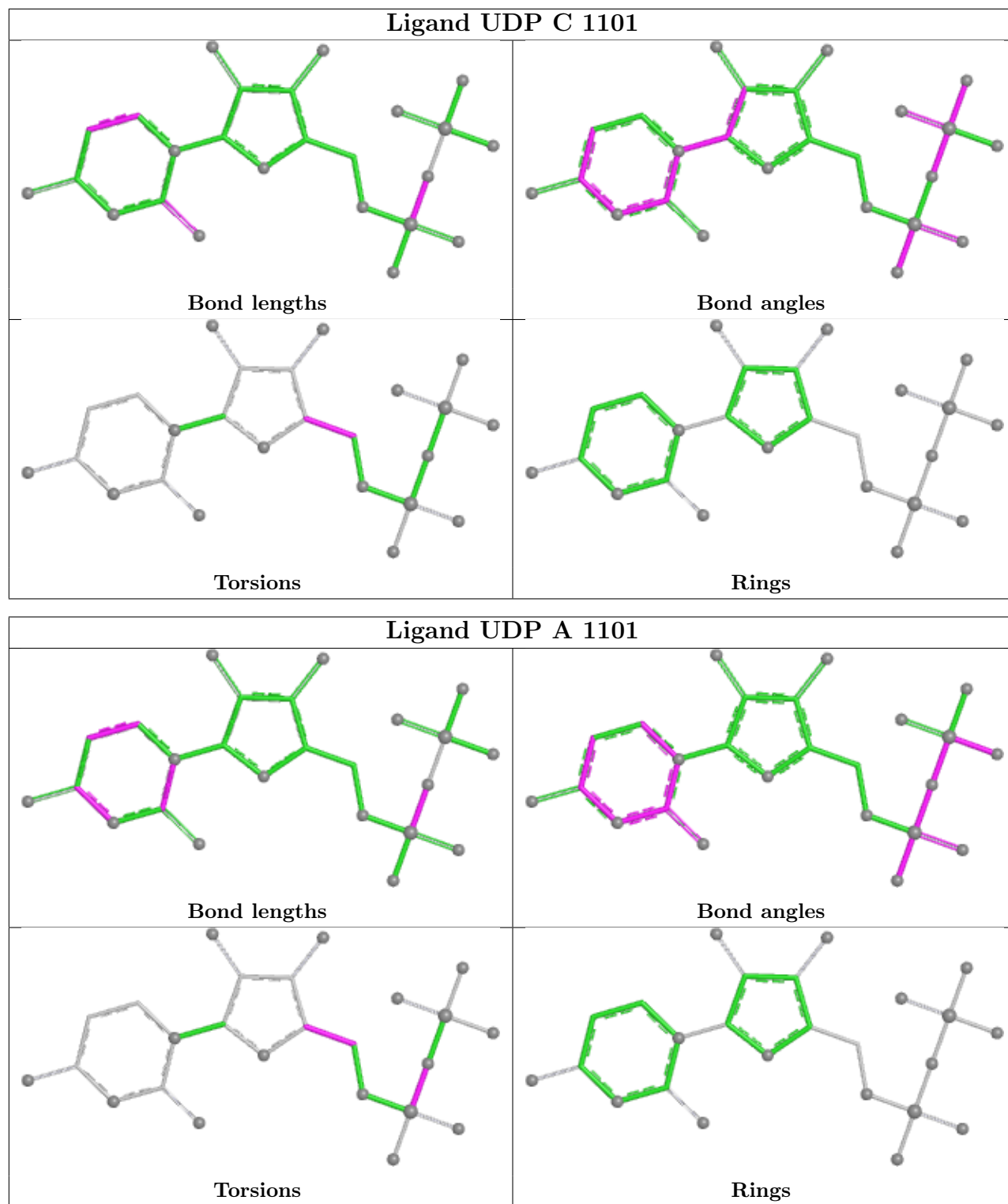
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1101	UDP	1	0
3	C	1101	UDP	1	0
3	A	1101	UDP	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 ⓘ

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	704/723 (97%)	-0.00	33 (4%)	36	29	40, 56, 98, 142	0
1	B	699/723 (96%)	0.02	25 (3%)	46	37	24, 55, 93, 135	2 (0%)
1	C	704/723 (97%)	-0.01	29 (4%)	41	33	26, 57, 94, 133	2 (0%)
1	D	704/723 (97%)	0.23	34 (4%)	35	28	35, 68, 101, 140	1 (0%)
2	E	7/7 (100%)	1.89	4 (57%)	0	0	87, 92, 107, 111	0
2	F	7/7 (100%)	2.17	1 (14%)	6	5	85, 107, 110, 120	0
2	G	7/7 (100%)	2.10	3 (42%)	0	0	106, 109, 120, 128	0
2	H	7/7 (100%)	2.43	4 (57%)	0	0	110, 111, 115, 125	0
All	All	2839/2920 (97%)	0.08	133 (4%)	36	29	24, 59, 103, 142	5 (0%)

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	7	PHE	6.3
1	C	325	THR	5.6
1	C	324	PRO	5.2
2	H	7	PHE	5.2
1	D	771	ALA	5.0
1	A	322	MET	5.0
1	B	322	MET	4.7
1	A	1038	LYS	4.6
1	D	772	LEU	4.5
1	A	325	THR	4.4
1	D	729	ILE	4.3
1	B	325	THR	4.2
1	D	324	PRO	4.1
1	C	772	LEU	4.0
1	D	728	HIS	4.0
1	C	757	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
2	E	7	PHE	4.0
2	H	13	ILE	4.0
1	D	726	ASN	4.0
1	B	772	LEU	4.0
1	D	757	LYS	4.0
1	A	333	LEU	3.8
1	C	322	MET	3.8
1	D	325	THR	3.8
1	D	1038	LYS	3.7
1	A	772	LEU	3.7
1	C	771	ALA	3.5
1	B	357	PHE	3.5
1	C	343	ILE	3.5
1	A	771	ALA	3.5
1	D	756	MET	3.4
1	C	323	CYS	3.4
1	D	341	GLY	3.3
1	D	687	GLU	3.3
1	A	729	ILE	3.3
1	C	726	ASN	3.2
1	D	511[A]	MET	3.2
1	A	756	MET	3.2
1	D	329	SER	3.2
1	D	322	MET	3.2
1	C	1038	LYS	3.1
2	G	10	LYS	3.1
1	C	756	MET	3.1
1	A	357	PHE	3.1
1	D	355	GLU	3.1
1	B	771	ALA	3.1
1	A	780	ASN	3.1
1	A	617	GLN	3.1
1	B	323	CYS	3.0
1	A	340	GLN	3.0
1	A	335	ASN	3.0
1	A	329	SER	3.0
1	B	333	LEU	3.0
1	A	728	HIS	3.0
2	G	7	PHE	3.0
1	B	338	ARG	3.0
1	D	340	GLN	3.0
1	D	539	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	337	LYS	2.9
1	B	336	ILE	2.9
1	C	839	GLU	2.9
1	D	724	LYS	2.9
1	C	326	HIS	2.9
1	D	780	ASN	2.8
1	B	617	GLN	2.8
1	A	1037	ILE	2.8
1	D	501	ARG	2.7
1	B	331	ASN	2.7
1	D	750	ASP	2.7
1	A	344	GLU	2.7
1	C	336	ILE	2.7
1	D	332	ASN	2.7
1	A	324	PRO	2.7
1	D	725	SER	2.7
1	D	898	ASN	2.7
1	B	1038	LYS	2.6
1	D	326	HIS	2.6
1	B	728	HIS	2.6
1	A	724	LYS	2.6
1	D	333	LEU	2.6
1	C	338	ARG	2.6
1	D	342	ASN	2.6
1	C	327	ALA	2.5
1	B	324	PRO	2.5
1	A	897	GLN	2.5
1	B	326	HIS	2.5
1	A	345	GLU	2.4
1	B	756	MET	2.4
1	A	338	ARG	2.4
1	C	340	GLN	2.4
1	B	344	GLU	2.4
1	A	326	HIS	2.4
1	D	499	LYS	2.4
1	C	781	THR	2.4
2	E	8	MET	2.4
2	G	11	TYR	2.4
1	C	333	LEU	2.3
1	A	896	PRO	2.3
1	B	332	ASN	2.3
1	C	332	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	803	SER	2.3
1	D	1037	ILE	2.3
1	A	355	GLU	2.3
1	A	339	GLU	2.3
2	H	8	MET	2.3
1	A	681	GLN	2.2
1	B	812	GLN	2.2
1	C	345	GLU	2.2
1	C	724	LYS	2.2
1	C	780	ASN	2.2
1	C	788	GLU	2.2
1	C	335	ASN	2.2
1	D	839	GLU	2.2
1	C	750	ASP	2.2
1	A	757	LYS	2.2
1	A	336	ILE	2.1
2	E	13	ILE	2.1
1	A	349	LEU	2.1
1	C	349	LEU	2.1
1	B	329	SER	2.1
1	B	355	GLU	2.1
1	B	340	GLN	2.1
2	E	10	LYS	2.1
1	D	551	LEU	2.1
2	H	11	TYR	2.1
1	C	337	LYS	2.0
1	B	811	THR	2.0
1	A	334	ALA	2.0
1	D	327	ALA	2.0
1	A	803	SER	2.0
1	B	335	ASN	2.0
1	C	723	PHE	2.0
1	A	750	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

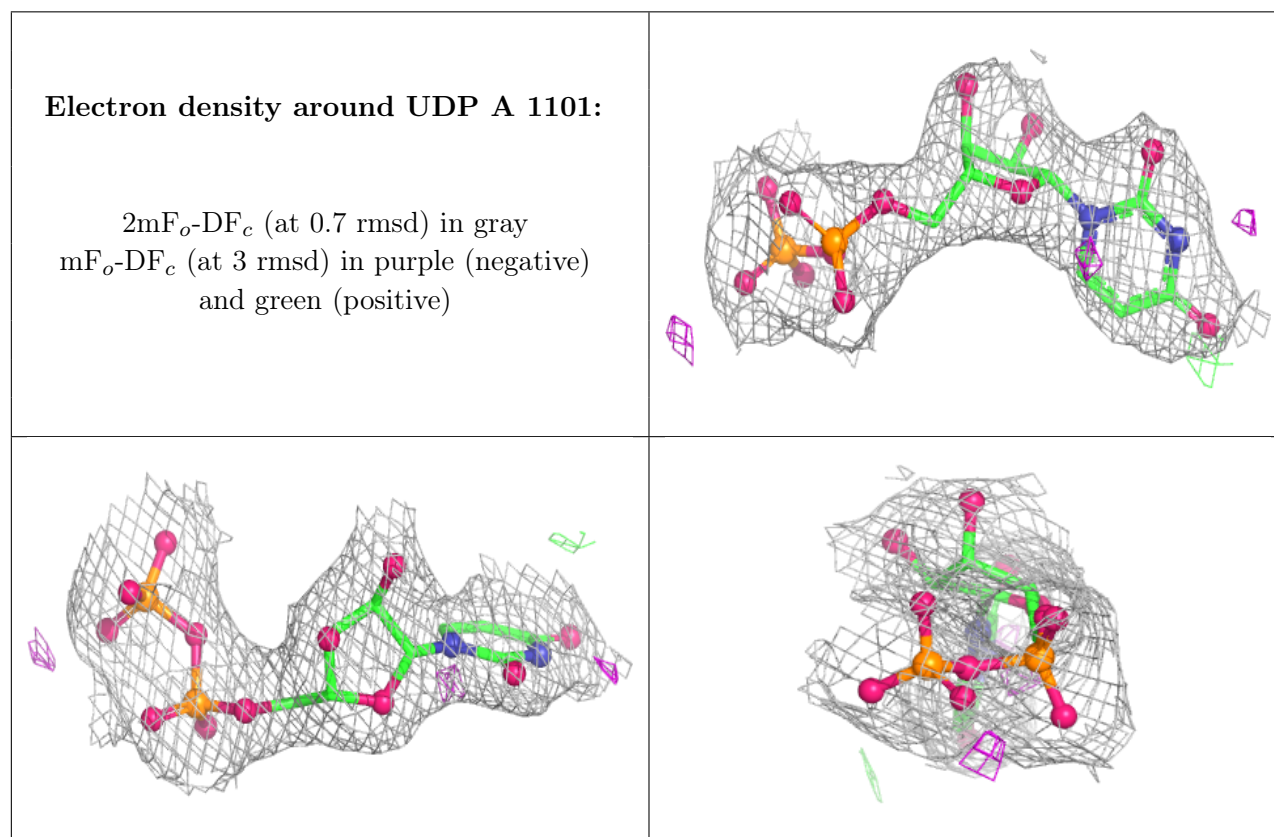
There are no oligosaccharides in this entry.

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.

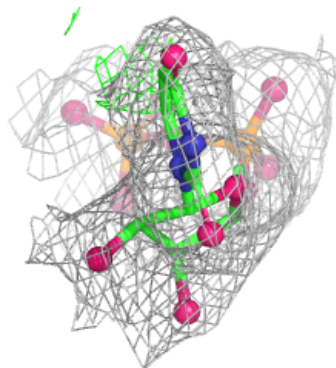
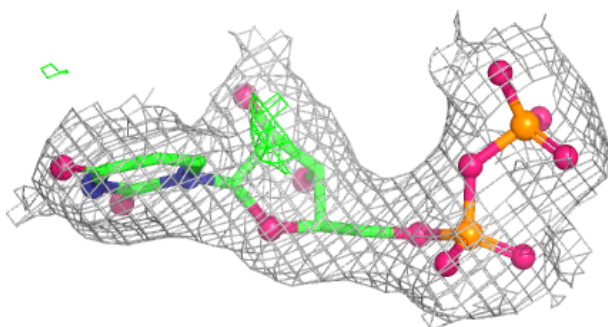
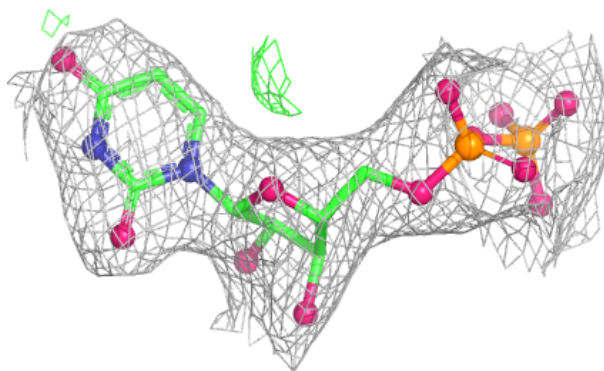
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	UDP	A	1101	25/25	0.98	0.06	39,47,52,54	0
3	UDP	B	1101	25/25	0.98	0.06	38,45,60,65	0
3	UDP	C	1101	25/25	0.98	0.05	39,49,55,57	0
3	UDP	D	1101	25/25	0.98	0.06	50,59,64,75	0

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

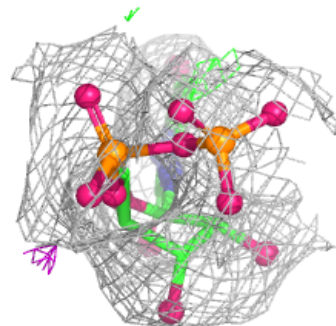
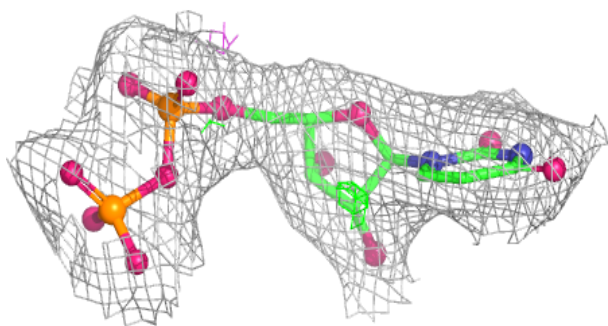
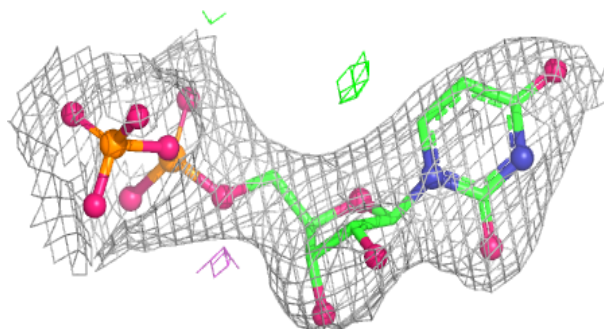


Electron density around UDP B 1101:

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

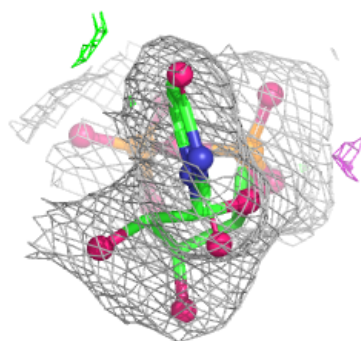
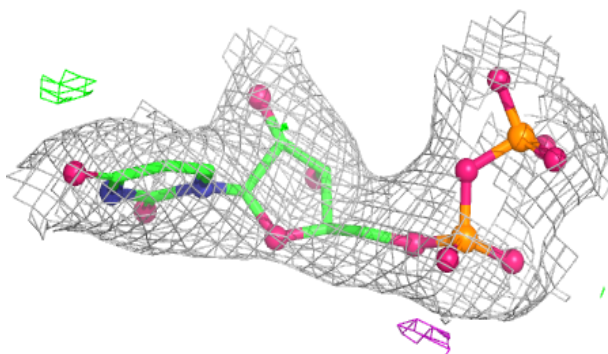
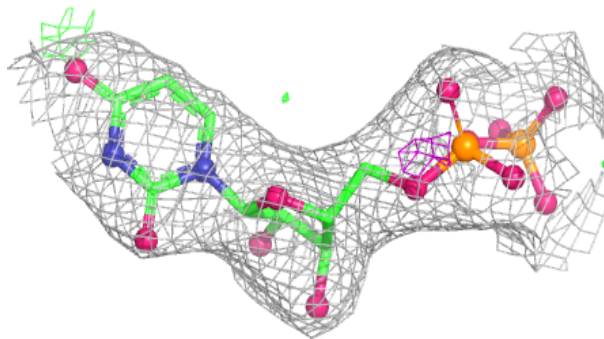
**Electron density around UDP C 1101:**

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



Electron density around UDP D 1101:

$2mF_o-DF_c$ (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.