Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 01:30 PM BST

PDB ID	:	6E4Q
Title	:	Crystal Structure of the Drosophila Melanogaster Polypeptide N-Acetylgalac tosaminyl Transferase PGANT9A in Complex with UDP and Mn2+
Authors	:	Samara, N.L.; Tabak, L.A.; Ten Hagen, K.G.
Deposited on	:	2018-07-18
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 following versions of software and data (see references ⓘ) were used in the production of this report:

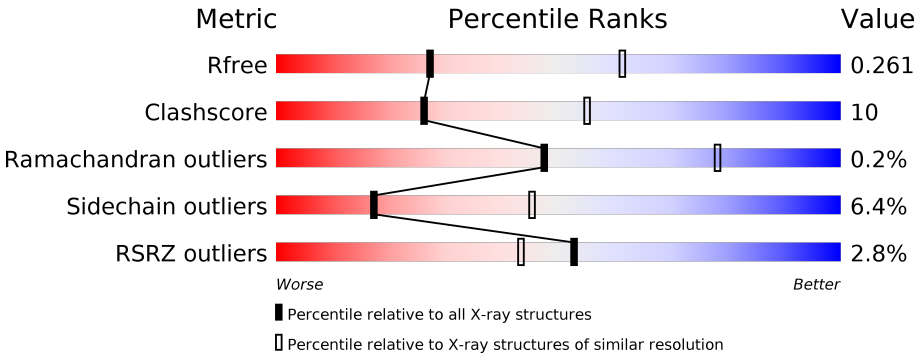
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	510	3% 72% 24%
1	B	510	2% 73% 24%
1	C	510	3% 73% 24%
1	D	510	3% 70% 25%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16632 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 polypeptide N-acetylgalactosaminyltransferase 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	0	0	0
			4074	2570	728	754	22			
1	B	503	Total	C	N	O	S	0	2	0
			4064	2563	727	752	22			
1	C	503	Total	C	N	O	S	0	2	0
			4064	2566	724	752	22			
1	D	502	Total	C	N	O	S	0	0	0
			4040	2547	720	751	22			

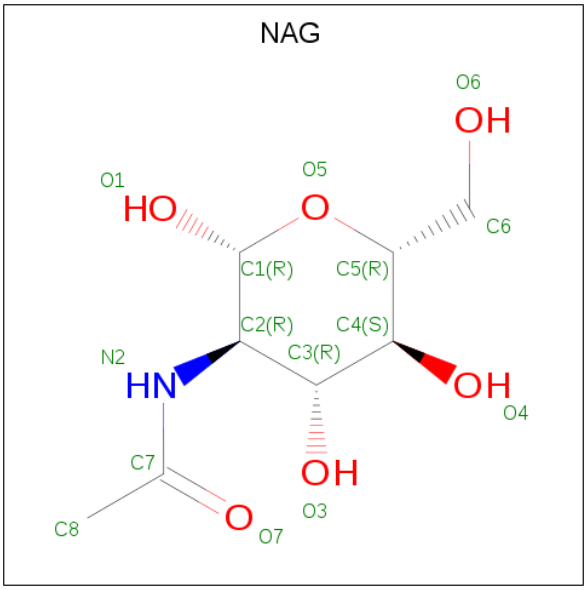
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	GLY	-	expression tag	UNP Q8MRC9
A	142	GLY	-	expression tag	UNP Q8MRC9
A	143	GLY	-	expression tag	UNP Q8MRC9
A	144	GLY	-	expression tag	UNP Q8MRC9
A	145	GLY	-	expression tag	UNP Q8MRC9
B	141	GLY	-	expression tag	UNP Q8MRC9
B	142	GLY	-	expression tag	UNP Q8MRC9
B	143	GLY	-	expression tag	UNP Q8MRC9
B	144	GLY	-	expression tag	UNP Q8MRC9
B	145	GLY	-	expression tag	UNP Q8MRC9
C	141	GLY	-	expression tag	UNP Q8MRC9
C	142	GLY	-	expression tag	UNP Q8MRC9
C	143	GLY	-	expression tag	UNP Q8MRC9
C	144	GLY	-	expression tag	UNP Q8MRC9
C	145	GLY	-	expression tag	UNP Q8MRC9
D	141	GLY	-	expression tag	UNP Q8MRC9
D	142	GLY	-	expression tag	UNP Q8MRC9
D	143	GLY	-	expression tag	UNP Q8MRC9
D	144	GLY	-	expression tag	UNP Q8MRC9
D	145	GLY	-	expression tag	UNP Q8MRC9

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

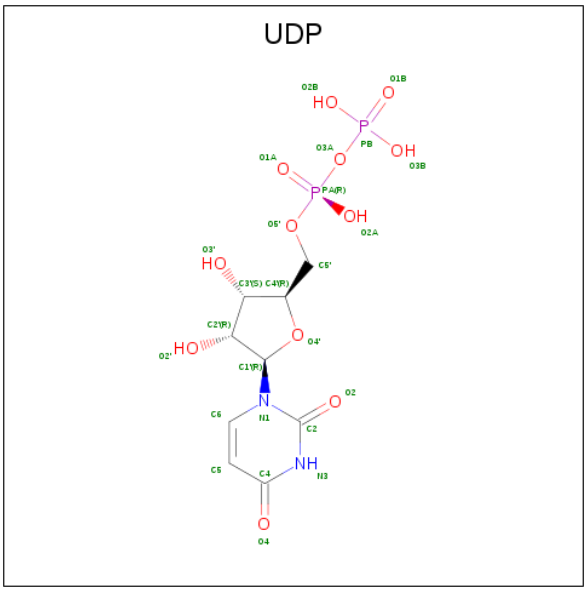
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mn 1 1	0	0
2	A	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



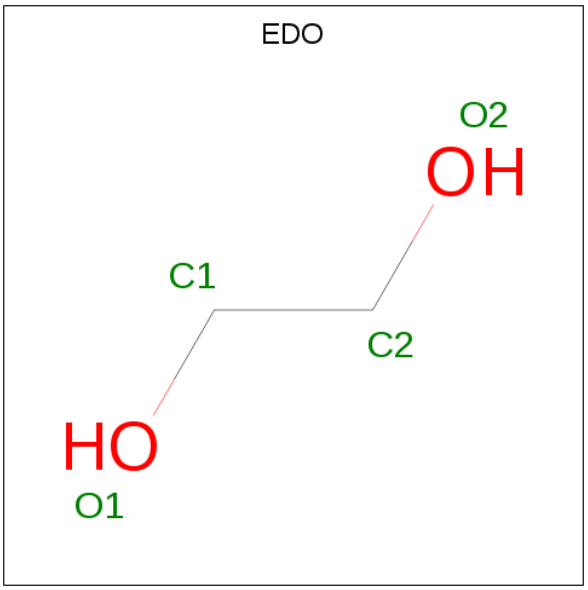
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



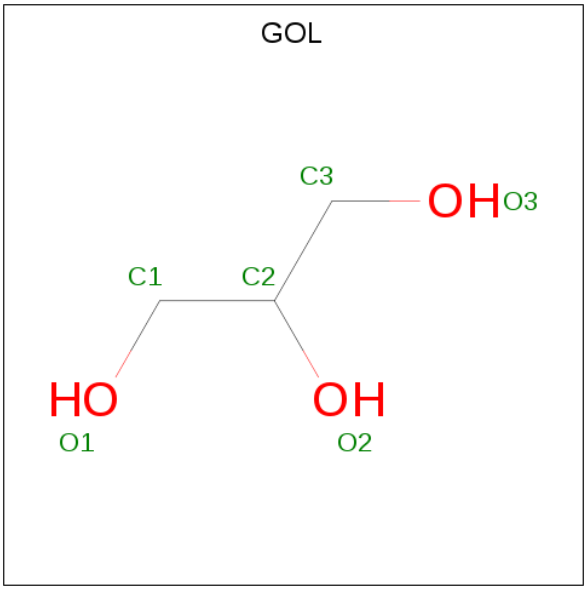
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
4	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
4	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
4	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	58	Total O 58 58	0	0
7	B	56	Total O 56 56	0	0

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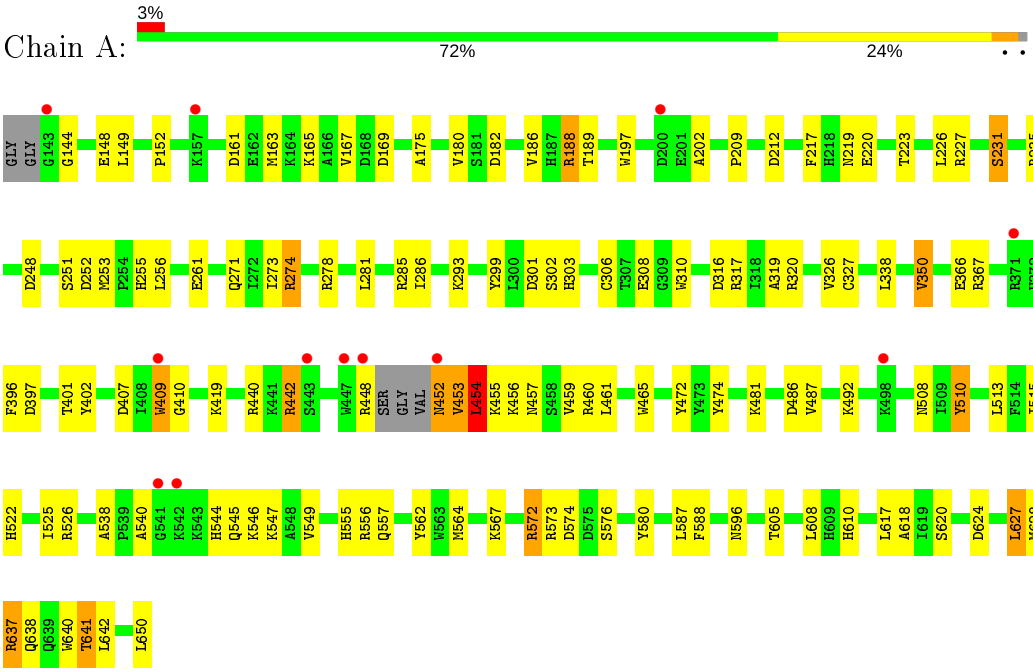
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	56	Total O 56 56	0	0
7	D	24	Total O 24 24	0	0

3 Residue-property plots (i)

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

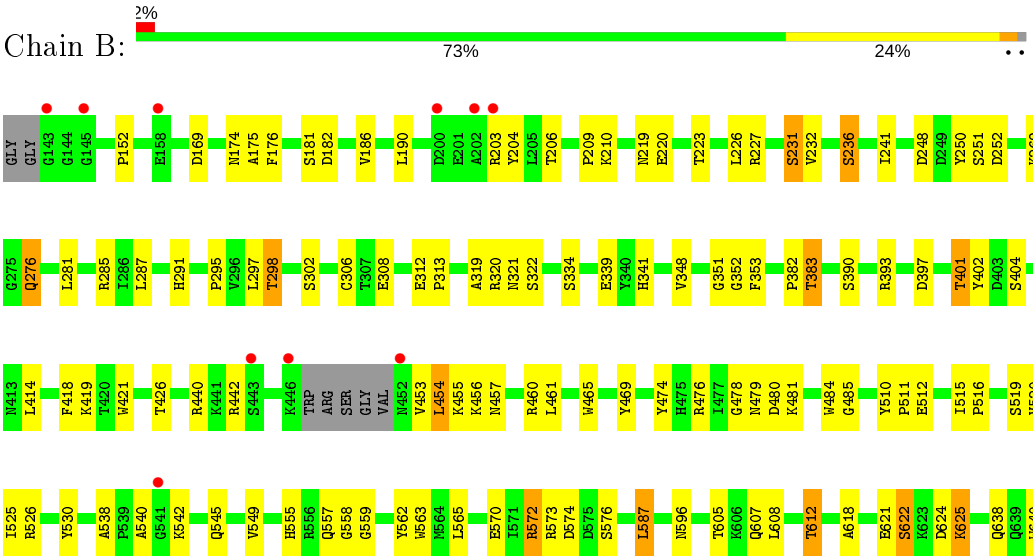
- Molecule 1: polypeptide N-acetylgalactosaminyltransferase 9

Chain A:



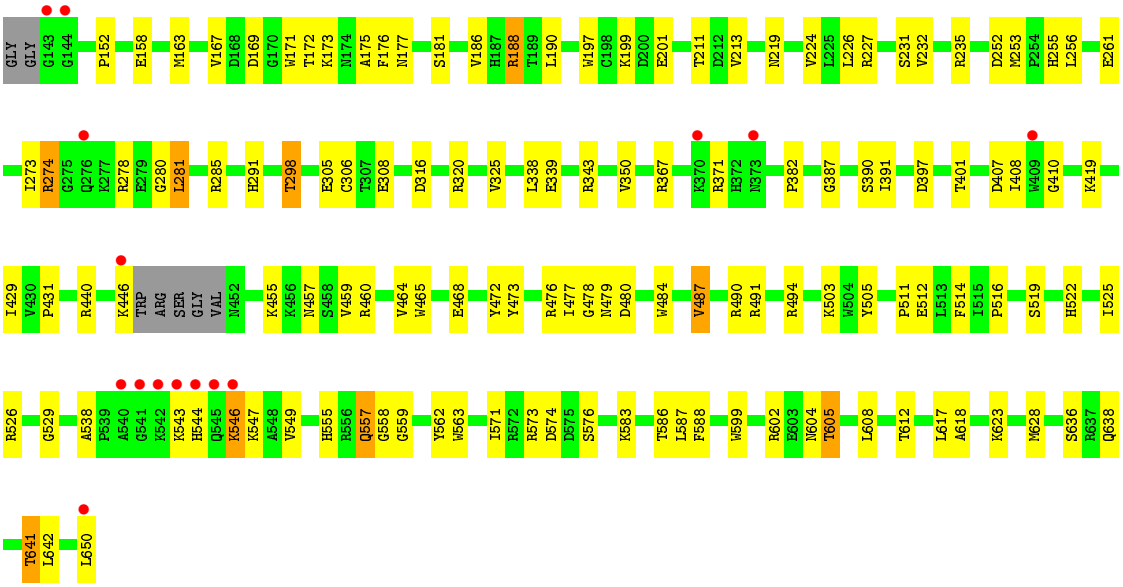
- Molecule 1: polypeptide N-acetylgalactosaminyltransferase 9

Chain B:



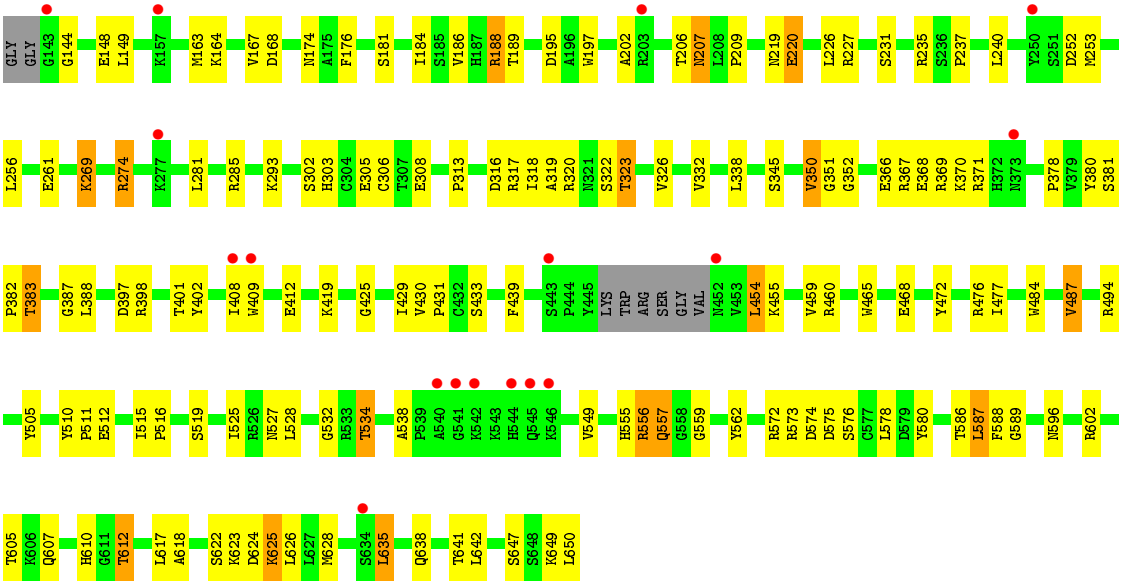
• Molecule 1: polypeptide N-acetylgalactosaminyltransferase 9

Chain C:



• Molecule 1: polypeptide N-acetylgalactosaminyltransferase 9

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	126.29Å 168.76Å 153.10Å 90.00° 106.28° 90.00°	Depositor
Resolution (Å)	19.95 – 2.80 19.95 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.0 (19.95-2.80) 94.0 (19.95-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.79Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.190 , 0.260 0.192 , 0.261	Depositor DCC
R_{free} test set	3521 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.767	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16632	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, UDP, MN, NAG, EDO

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	0.46	1/4181 (0.0%)	0.67	1/5653 (0.0%)
1	B	0.45	0/4176	0.65	1/5645 (0.0%)
1	C	0.44	0/4177	0.65	0/5647
1	D	0.44	0/4145	0.65	1/5605 (0.0%)
All	All	0.45	1/16679 (0.0%)	0.65	3/22550 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	327	CYS	CB-SG	-6.13	1.71	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	454	LEU	CA-CB-CG	7.22	131.91	115.30
1	D	454	LEU	CA-CB-CG	5.30	127.49	115.30
1	B	454	LEU	CA-CB-CG	5.00	126.81	115.30

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	4074	0	3934	85	0
1	B	4064	0	3931	72	0
1	C	4064	0	3927	82	0
1	D	4040	0	3898	97	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	14	0	13	0	0
3	B	14	0	13	1	0
3	C	14	0	13	0	0
3	D	14	0	13	0	0
4	A	25	0	11	2	0
4	B	25	0	11	1	0
4	C	25	0	11	0	0
4	D	25	0	11	4	0
5	A	8	0	12	0	0
5	B	4	0	6	0	0
5	C	8	0	12	1	0
5	D	4	0	6	0	0
6	B	6	0	8	2	0
6	D	6	0	8	3	0
7	A	58	0	0	4	0
7	B	56	0	0	0	0
7	C	56	0	0	3	0
7	D	24	0	0	1	0
All	All	16632	0	15838	336	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 10.

All (336) 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:C:410:GLY:HA3	1:C:457:ASN:HD22	1.21	1.05
1:D:323:THR:HG23	1:D:425:GLY:HA2	1.41	1.03
1:B:576:SER:HB3	1:B:587:LEU:HD22	1.61	0.83
1:A:256:LEU:O	1:A:274:ARG:NH2	2.17	0.78
1:B:209:PRO:HD3	1:B:319:ALA:HB2	1.65	0.78
1:A:410:GLY:HA2	1:A:457:ASN:HD22	1.51	0.76
1:A:562:TYR:O	1:A:573:ARG:NH2	2.19	0.75
1:A:285:ARG:HD2	1:A:402:TYR:HE2	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:GLN:OE1	1:B:291[B]:HIS:NE2	2.20	0.74
1:B:540:ALA:HB3	6:B:705:GOL:H32	1.70	0.74
1:A:460:ARG:NH2	1:A:486:ASP:O	2.21	0.73
1:D:261:GLU:OE1	1:D:274:ARG:NH1	2.22	0.73
1:D:367:ARG:NH2	6:D:705:GOL:O3	2.22	0.73
1:A:303:HIS:NE2	7:A:801:HOH:O	2.22	0.72
1:C:261:GLU:OE1	1:C:274:ARG:NH1	2.22	0.72
1:D:562:TYR:O	1:D:573:ARG:NH2	2.22	0.72
1:B:248:ASP:OD2	1:B:274:ARG:NH1	2.24	0.70
1:B:401:THR:O	1:B:419:LYS:NZ	2.25	0.70
1:D:207:ASN:N	1:D:207:ASN:OD1	2.24	0.70
1:A:545:GLN:HG2	1:A:588:PHE:HB3	1.73	0.70
1:C:188:ARG:NH2	1:C:338:LEU:O	2.25	0.69
1:C:546:LYS:HA	1:C:588[A]:PHE:HE1	1.57	0.69
1:B:241:ILE:O	1:B:269:LYS:NZ	2.25	0.69
1:C:410:GLY:HA3	1:C:457:ASN:ND2	2.03	0.69
1:B:339:GLU:OE2	1:B:341:HIS:NE2	2.25	0.69
1:C:235:ARG:NH2	1:C:306:CYS:O	2.26	0.69
1:C:188:ARG:HD3	1:C:190:LEU:HD13	1.74	0.69
1:D:235:ARG:NH2	1:D:306:CYS:O	2.26	0.68
1:A:410:GLY:CA	1:A:457:ASN:HD22	2.06	0.68
1:D:149:LEU:H	1:D:189:THR:HG23	1.59	0.68
1:D:624:ASP:HB3	1:D:625:LYS:HD2	1.76	0.66
1:A:555:HIS:O	1:A:555:HIS:ND1	2.29	0.66
1:C:576:SER:HB3	1:C:587:LEU:HD22	1.77	0.66
1:C:476:ARG:NH1	1:C:574:ASP:OD2	2.26	0.66
1:A:235:ARG:NH2	1:A:306:CYS:O	2.30	0.65
1:D:186:VAL:HG11	1:D:226:LEU:HB3	1.78	0.65
1:C:525:ILE:HG12	1:C:642:LEU:HD22	1.80	0.64
1:A:572:ARG:NH2	1:A:574:ASP:O	2.30	0.64
1:C:281:LEU:HD11	1:C:285:ARG:HH11	1.63	0.64
1:A:248:ASP:OD1	1:A:251:SER:OG	2.16	0.63
1:D:555:HIS:O	1:D:555:HIS:ND1	2.31	0.63
1:B:186:VAL:HG11	1:B:226:LEU:HB3	1.79	0.63
1:C:538:ALA:O	1:C:573:ARG:NH1	2.28	0.62
1:C:186:VAL:HG11	1:C:226:LEU:HB3	1.82	0.62
1:A:186:VAL:HG11	1:A:226:LEU:HB3	1.82	0.61
1:D:538:ALA:HB2	1:D:549:VAL:HG13	1.82	0.61
1:C:555:HIS:O	1:C:555:HIS:ND1	2.33	0.61
1:C:455:LYS:HD3	1:C:480:ASP:O	2.01	0.61
1:A:525:ILE:HG12	1:A:642:LEU:HD22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:382:PRO:O	1:D:505:TYR:OH	2.18	0.61
1:D:528:LEU:HD21	1:D:641:THR:HG23	1.83	0.61
1:D:303:HIS:HE1	4:D:703:UDP:H3'	1.66	0.60
1:D:316:ASP:O	1:D:320:ARG:HG3	2.02	0.60
1:A:580:TYR:HB3	1:A:610:HIS:CD2	2.37	0.60
1:D:318:ILE:HG23	1:D:322:SER:HA	1.84	0.60
1:D:465:TRP:CZ3	1:D:494:ARG:HG3	2.37	0.59
1:A:492:LYS:NZ	7:A:803:HOH:O	2.35	0.59
1:D:610:HIS:CE1	1:D:612:THR:HG22	2.37	0.59
1:A:538:ALA:O	1:A:573:ARG:NH1	2.35	0.59
1:D:366:GLU:OE2	1:D:370:LYS:HE3	2.04	0.58
1:A:281:LEU:HD11	1:A:285:ARG:NH2	2.19	0.58
1:B:485:GLY:HA2	7:D:806:HOH:O	2.03	0.58
1:D:476:ARG:HD3	1:D:562:TYR:CD2	2.39	0.58
1:B:353:PHE:HB3	1:B:414:LEU:HD21	1.86	0.58
1:B:605:THR:HG23	1:B:607:GLN:HG3	1.86	0.58
1:C:526:ARG:HB3	1:C:641:THR:HG23	1.86	0.58
1:D:602:ARG:HB2	1:D:605:THR:HG22	1.85	0.58
1:A:567:LYS:HE3	1:A:650:LEU:C	2.24	0.58
1:B:210:LYS:O	1:B:295:PRO:HD2	2.04	0.57
1:A:455:LYS:O	1:A:459:VAL:HG23	2.04	0.57
1:A:281:LEU:HD11	1:A:285:ARG:CZ	2.35	0.57
1:D:401:THR:O	1:D:419:LYS:NZ	2.35	0.57
1:B:559:GLY:HA2	1:B:562:TYR:HB2	1.86	0.57
1:C:419:LYS:HG2	1:C:465:TRP:CZ2	2.39	0.56
1:A:350:VAL:HG22	1:A:381:SER:HB2	1.87	0.56
1:A:620:SER:HB3	1:A:627:LEU:HD21	1.87	0.56
1:C:401:THR:O	1:C:419:LYS:NZ	2.38	0.56
1:B:419:LYS:HG2	1:B:465:TRP:CZ2	2.41	0.56
1:C:503:LYS:NZ	7:C:801:HOH:O	2.38	0.56
1:D:618:ALA:HB2	1:D:638:GLN:HG2	1.88	0.56
1:D:256:LEU:O	1:D:274:ARG:NH2	2.39	0.56
1:B:555:HIS:ND1	1:B:555:HIS:O	2.39	0.55
1:D:605:THR:HG23	1:D:607:GLN:H	1.71	0.55
1:B:525:ILE:HG12	1:B:642:LEU:HD22	1.87	0.55
1:C:219:ASN:OD1	1:C:253:MET:HG3	2.07	0.55
1:D:197:TRP:CZ3	1:D:202:ALA:HB2	2.42	0.55
1:A:299:TYR:HH	1:A:396:PHE:HE2	1.56	0.54
1:A:618:ALA:HB2	1:A:638:GLN:HG2	1.89	0.54
1:D:368:GLU:OE1	1:D:371:ARG:NH1	2.40	0.54
1:A:526:ARG:HB3	1:A:641:THR:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:ALA:HB2	1:A:549:VAL:HG13	1.90	0.54
1:A:219:ASN:OD1	1:A:253:MET:HG3	2.07	0.54
1:C:188:ARG:NH1	1:C:305:GLU:OE2	2.41	0.54
1:D:368:GLU:HB2	6:D:705:GOL:H31	1.90	0.54
1:A:278:ARG:HG2	1:A:448:ARG:HH22	1.73	0.53
1:C:211:THR:OG1	1:C:298:THR:HG23	2.07	0.53
1:C:465:TRP:CZ3	1:C:494:ARG:HG3	2.42	0.53
1:A:144:GLY:HA3	1:A:148:GLU:CD	2.29	0.53
1:A:209:PRO:HD3	1:A:319:ALA:HB2	1.90	0.53
1:B:152:PRO:HG3	1:B:339:GLU:OE1	2.08	0.53
1:A:596:ASN:HA	1:A:610:HIS:HE1	1.73	0.53
1:C:316:ASP:OD2	1:C:320:ARG:NH1	2.42	0.53
1:D:617:LEU:HD13	1:D:628:MET:CE	2.38	0.53
1:D:164:LYS:HE2	1:D:168:ASP:OD2	2.09	0.53
1:B:530:TYR:CE2	1:B:621:GLU:HA	2.44	0.53
1:D:281:LEU:HD13	4:D:703:UDP:O4'	2.08	0.53
1:C:199:LYS:HA	5:C:705:EDO:H21	1.92	0.52
1:C:555:HIS:ND1	1:C:557:GLN:O	2.42	0.52
1:A:285:ARG:HD2	1:A:402:TYR:CE2	2.39	0.52
1:C:281:LEU:HD11	1:C:285:ARG:NH1	2.24	0.52
1:C:460:ARG:HG3	1:C:484:TRP:HB2	1.90	0.52
1:A:175:ALA:HB3	1:A:440:ARG:HD3	1.92	0.52
1:A:255:HIS:CD2	1:A:256:LEU:HG	2.45	0.52
1:B:181:SER:OG	1:B:227:ARG:NH1	2.41	0.52
1:C:278:ARG:HH22	1:C:446:LYS:HE3	1.75	0.52
1:A:455:LYS:NZ	7:A:807:HOH:O	2.41	0.52
1:C:188:ARG:HH22	1:C:338:LEU:HB3	1.74	0.52
1:D:538:ALA:O	1:D:573:ARG:NH1	2.43	0.52
1:A:197:TRP:CZ3	1:A:202:ALA:HB2	2.45	0.52
1:D:555:HIS:ND1	1:D:557:GLN:O	2.42	0.52
1:A:317:ARG:HB2	1:A:326:VAL:HG11	1.92	0.51
1:A:456:LYS:O	1:A:460:ARG:HG3	2.10	0.51
1:A:188:ARG:NH2	1:A:338:LEU:O	2.41	0.51
1:D:472:TYR:CG	1:D:516:PRO:HG2	2.46	0.51
1:B:460:ARG:HG2	1:B:484:TRP:HB2	1.91	0.51
1:B:298:THR:HB	1:B:390:SER:OG	2.11	0.51
1:B:524:GLU:OE2	1:B:526:ARG:NH1	2.42	0.51
1:C:181:SER:OG	1:C:227:ARG:NH1	2.44	0.51
1:A:163:MET:O	1:A:167:VAL:HG23	2.11	0.51
1:A:419:LYS:HG2	1:A:465:TRP:CZ2	2.45	0.51
1:C:472:TYR:CG	1:C:516:PRO:HG2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LEU:H	1:A:189:THR:HG23	1.76	0.51
1:C:538:ALA:HB2	1:C:549:VAL:HG13	1.93	0.51
1:D:455:LYS:HE2	1:D:477:ILE:HB	1.92	0.51
1:A:220:GLU:HG2	1:A:302:SER:HB2	1.92	0.50
1:B:281:LEU:HD13	4:B:703:UDP:O4'	2.10	0.50
1:C:186:VAL:CG1	1:C:226:LEU:HB3	2.41	0.50
1:C:171:TRP:CZ2	1:C:177:ASN:HB2	2.46	0.50
1:D:511:PRO:HD2	1:D:512:GLU:OE1	2.11	0.50
1:A:452:ASN:N	1:A:455:LYS:HE3	2.27	0.50
1:B:511:PRO:HD2	1:B:512:GLU:OE1	2.12	0.50
1:C:175:ALA:HB3	1:C:440:ARG:HD3	1.93	0.50
1:B:401:THR:OG1	1:B:402:TYR:N	2.44	0.50
1:D:186:VAL:CG1	1:D:226:LEU:HB3	2.42	0.50
1:D:351:GLY:O	1:D:382:PRO:HG2	2.12	0.50
1:D:378:PRO:HB3	1:D:430:VAL:HG22	1.93	0.49
1:A:401:THR:O	1:A:419:LYS:NZ	2.43	0.49
1:D:220:GLU:HG3	1:D:302:SER:OG	2.11	0.49
1:B:186:VAL:CG1	1:B:226:LEU:HB3	2.43	0.49
1:C:604:ASN:ND2	1:C:605:THR:HG22	2.27	0.49
1:A:454:LEU:HD22	1:A:454:LEU:H	1.77	0.49
1:C:367:ARG:NH2	1:C:371:ARG:HH12	2.10	0.49
1:D:455:LYS:O	1:D:459:VAL:HG23	2.13	0.49
1:A:261:GLU:OE1	1:A:274:ARG:NH1	2.46	0.48
1:D:401:THR:HG23	1:D:402:TYR:N	2.28	0.48
1:C:455:LYS:O	1:C:459:VAL:HG23	2.13	0.48
1:A:526:ARG:O	1:A:640:TRP:HA	2.13	0.48
1:C:464:VAL:O	1:C:494:ARG:NH1	2.46	0.48
1:D:350:VAL:HG22	1:D:381:SER:HB2	1.96	0.48
1:A:148:GLU:HG3	1:A:189:THR:CG2	2.44	0.48
1:C:455:LYS:HB2	1:C:455:LYS:HZ2	1.78	0.48
1:A:219:ASN:H	1:A:251:SER:HB3	1.77	0.48
1:D:605:THR:HG23	1:D:607:GLN:HG3	1.95	0.48
1:A:576:SER:HB3	1:A:587:LEU:HG	1.96	0.48
1:B:522:HIS:HA	1:B:563:TRP:O	2.14	0.48
1:D:195:ASP:OD2	1:D:345:SER:HB3	2.14	0.48
1:B:232:VAL:O	1:B:236:SER:OG	2.31	0.48
1:B:469:TYR:HE2	1:B:515:ILE:HD13	1.78	0.47
1:B:622:SER:HB2	1:B:624:ASP:OD1	2.14	0.47
1:C:559:GLY:HA2	1:C:562:TYR:HB2	1.95	0.47
1:B:538:ALA:HB2	1:B:549:VAL:HG13	1.95	0.47
1:C:429:ILE:O	1:C:431:PRO:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ARG:NH1	7:A:810:HOH:O	2.47	0.47
1:B:538:ALA:O	1:B:573:ARG:NH2	2.42	0.47
1:D:149:LEU:N	1:D:189:THR:HG23	2.29	0.47
1:B:220:GLU:HG2	1:B:302:SER:HB2	1.96	0.47
1:B:312:GLU:N	1:B:312:GLU:OE1	2.40	0.47
1:D:460:ARG:HG3	1:D:484:TRP:HB2	1.96	0.47
1:A:281:LEU:HD21	1:A:285:ARG:HH21	1.79	0.47
1:D:580:TYR:CD1	1:D:628:MET:HG3	2.49	0.47
1:B:572:ARG:NH1	1:B:574:ASP:O	2.47	0.47
1:B:526:ARG:O	1:B:640:TRP:HA	2.14	0.47
1:C:278:ARG:NH2	1:C:446:LYS:HE3	2.30	0.47
1:D:527:ASN:O	1:D:532:GLY:HA2	2.15	0.47
1:A:596:ASN:HA	1:A:610:HIS:CE1	2.50	0.46
1:C:571:ILE:HD11	1:C:608:LEU:HD22	1.96	0.46
1:C:618:ALA:HB2	1:C:638:GLN:HG2	1.96	0.46
1:A:617:LEU:HD13	1:A:628:MET:HE1	1.96	0.46
1:A:227:ARG:O	1:A:231:SER:HB3	2.15	0.46
1:C:169:ASP:OD2	1:C:173:LYS:HE3	2.15	0.46
1:D:556:ARG:HB3	1:D:556:ARG:HH21	1.81	0.46
1:C:516:PRO:O	1:C:519:SER:OG	2.26	0.46
1:C:543:LYS:HE3	1:C:543:LYS:HB2	1.64	0.46
1:D:380:TYR:HB2	6:D:705:GOL:H2	1.98	0.46
1:C:472:TYR:CD1	1:C:516:PRO:HG2	2.50	0.46
1:D:622:SER:OG	1:D:624:ASP:HB2	2.16	0.46
1:A:182:ASP:HA	1:A:223:THR:HG21	1.98	0.46
1:B:321:ASN:ND2	3:B:702:NAG:H62	2.30	0.46
1:D:578:LEU:HD23	1:D:587:LEU:HD23	1.98	0.46
1:D:303:HIS:CE1	4:D:703:UDP:H3'	2.50	0.46
1:A:243:LYS:HG2	1:A:271:GLN:OE1	2.16	0.46
1:A:580:TYR:CE1	1:A:628:MET:HG3	2.51	0.46
1:B:182:ASP:HA	1:B:223:THR:HG21	1.98	0.46
1:D:559:GLY:HA2	1:D:562:TYR:HB2	1.97	0.46
1:A:306:CYS:HB3	1:A:310:TRP:CD1	2.51	0.46
1:D:352:GLY:O	1:D:383:THR:HG21	2.16	0.46
1:C:410:GLY:CA	1:C:457:ASN:HD22	2.08	0.46
1:B:418:PHE:HE2	1:B:461:LEU:HD11	1.81	0.45
1:C:176:PHE:CZ	1:C:224:VAL:HG21	2.51	0.45
1:C:382:PRO:O	1:C:505:TYR:OH	2.30	0.45
1:C:529:GLY:HA2	1:C:636:SER:HB3	1.97	0.45
1:D:401:THR:HG23	1:D:402:TYR:H	1.81	0.45
1:D:460:ARG:NH2	1:D:487:VAL:HG23	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:HIS:CE1	4:D:703:UDP:O1A	2.69	0.45
1:C:273:ILE:HD11	1:C:291[B]:HIS:CE1	2.51	0.45
1:C:623:LYS:NZ	7:C:804:HOH:O	2.49	0.45
1:D:209:PRO:HD3	1:D:319:ALA:HB2	1.98	0.45
1:D:617:LEU:HD13	1:D:628:MET:HE2	1.98	0.45
1:A:301:ASP:OD2	4:A:703:UDP:H5'1	2.17	0.45
1:A:545:GLN:O	1:A:546:LYS:HG2	2.16	0.45
1:B:474:TYR:CZ	1:B:481:LYS:HE3	2.52	0.45
1:A:617:LEU:HD13	1:A:628:MET:CE	2.47	0.45
1:B:538:ALA:CB	1:B:549:VAL:HG13	2.46	0.45
1:D:184:ILE:HD12	1:D:338:LEU:HD22	1.98	0.45
1:B:618:ALA:HB2	1:B:638:GLN:HG2	1.99	0.45
1:C:602:ARG:HB2	1:C:605:THR:HG23	1.98	0.45
1:A:580:TYR:HB3	1:A:610:HIS:NE2	2.32	0.45
1:D:402:TYR:CD1	1:D:412:GLU:HB2	2.51	0.45
1:D:635:LEU:HA	1:D:635:LEU:HD12	1.61	0.45
1:A:472:TYR:CG	1:A:516:PRO:HG2	2.52	0.45
1:B:175:ALA:HB3	1:B:440:ARG:HD3	1.99	0.44
1:C:188:ARG:NH2	1:C:338:LEU:HB3	2.33	0.44
1:A:629:GLU:OE1	1:A:637:ARG:HD2	2.17	0.44
1:D:419:LYS:HG2	1:D:465:TRP:CZ2	2.52	0.44
1:B:352:GLY:O	1:B:383:THR:HG21	2.17	0.44
1:B:219:ASN:H	1:B:251:SER:HB3	1.82	0.44
1:D:237:PRO:HG2	1:D:240:LEU:HD12	2.00	0.44
1:D:617:LEU:HD13	1:D:628:MET:HE1	2.00	0.44
1:A:608:LEU:HA	1:A:608:LEU:HD23	1.90	0.44
1:B:174:ASN:HB3	1:B:176:PHE:CZ	2.53	0.44
1:B:402:TYR:CD1	1:B:412:GLU:HB2	2.52	0.44
1:C:152:PRO:HG3	1:C:339:GLU:CD	2.37	0.44
1:C:197:TRP:CD1	1:C:201:GLU:HB2	2.52	0.44
1:B:297:LEU:HD21	1:B:393:ARG:HG3	1.99	0.44
1:C:617:LEU:HD13	1:C:628:MET:HE1	1.99	0.44
1:C:163:MET:O	1:C:167:VAL:HG23	2.18	0.44
1:C:544:HIS:HB3	1:C:547:LYS:HD3	2.00	0.43
1:B:525:ILE:HG22	1:B:640:TRP:CE3	2.53	0.43
1:D:350:VAL:HG13	1:D:382:PRO:HD2	2.00	0.43
1:C:586:THR:HB	1:C:588[A]:PHE:CE1	2.53	0.43
1:B:624:ASP:OD1	1:B:625:LYS:N	2.52	0.43
1:D:285:ARG:HD2	1:D:402:TYR:HE2	1.83	0.43
1:D:588:PHE:CD2	1:D:589:GLY:N	2.87	0.43
1:B:204:TYR:OH	1:B:313:PRO:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:SER:OG	1:B:306:CYS:N	2.39	0.43
1:C:175:ALA:HB3	1:C:440:ARG:CD	2.48	0.43
1:A:367:ARG:NH2	1:A:508:ASN:O	2.52	0.43
1:B:190:LEU:HD12	1:B:190:LEU:HA	1.80	0.43
1:C:255:HIS:CD2	1:C:256:LEU:HG	2.53	0.43
1:A:516:PRO:O	1:A:519:SER:OG	2.35	0.42
1:C:213:VAL:HG21	1:C:232:VAL:HG11	2.02	0.42
1:D:285:ARG:NH2	1:D:387:GLY:HA2	2.34	0.42
1:B:421:TRP:CZ3	1:B:426:THR:HG22	2.55	0.42
1:B:516:PRO:O	1:B:519:SER:OG	2.23	0.42
1:D:602:ARG:HB2	1:D:605:THR:CG2	2.48	0.42
1:D:647:SER:O	1:D:650:LEU:HB2	2.20	0.42
1:A:510:TYR:CE2	1:A:513:LEU:HD13	2.54	0.42
1:A:555:HIS:C	1:A:557:GLN:H	2.22	0.42
1:B:418:PHE:CE2	1:B:461:LEU:HD11	2.53	0.42
1:C:325:VAL:HG22	1:C:391:ILE:HG13	2.01	0.42
1:C:522:HIS:HA	1:C:563:TRP:O	2.19	0.42
1:C:490:ARG:NH1	7:C:803:HOH:O	2.45	0.42
1:D:174:ASN:HB3	1:D:176:PHE:CZ	2.55	0.42
1:D:281:LEU:HD11	1:D:285:ARG:HE	1.83	0.42
1:A:212:ASP:OD1	1:A:243:LYS:N	2.45	0.42
1:B:476:ARG:HH11	6:B:705:GOL:H12	1.85	0.42
1:C:285:ARG:NH1	1:C:387:GLY:HA2	2.34	0.42
1:A:522:HIS:HB3	1:A:564:MET:HG2	2.00	0.42
1:B:542:LYS:HA	1:B:545:GLN:HG3	2.02	0.42
1:C:407:ASP:O	1:C:457:ASN:ND2	2.49	0.42
1:D:317:ARG:HB2	1:D:326:VAL:HG11	2.01	0.42
1:B:478:GLY:CA	1:B:558:GLY:H	2.33	0.42
1:D:332:VAL:HG22	1:D:439:PHE:CD2	2.55	0.42
1:B:287:LEU:HD12	1:B:287:LEU:HA	1.79	0.42
1:B:476:ARG:HD3	1:B:562:TYR:CD2	2.55	0.42
1:D:163:MET:O	1:D:167:VAL:HG23	2.19	0.42
1:A:544:HIS:HA	1:A:547:LYS:HD2	2.02	0.41
1:B:596:ASN:OD1	1:B:612:THR:HG21	2.20	0.41
1:C:587:LEU:HA	1:C:587:LEU:HD23	1.91	0.41
1:D:534:THR:HG21	1:D:623:LYS:HB3	2.01	0.41
1:D:596:ASN:OD1	1:D:612:THR:HG21	2.20	0.41
1:B:276:GLN:CD	1:B:276:GLN:H	2.19	0.41
1:B:281:LEU:HD11	1:B:285:ARG:HH11	1.84	0.41
1:D:387:GLY:C	1:D:388:LEU:HD12	2.39	0.41
1:D:269:LYS:HG2	1:D:269:LYS:H	1.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:429:ILE:O	1:D:431:PRO:HD3	2.20	0.41
1:B:455:LYS:HD3	1:B:480:ASP:O	2.20	0.41
1:C:478:GLY:CA	1:C:558:GLY:H	2.34	0.41
1:C:511:PRO:HD2	1:C:512:GLU:OE1	2.20	0.41
1:A:513:LEU:O	1:A:515:ILE:HD12	2.21	0.41
1:B:419:LYS:HG2	1:B:465:TRP:CH2	2.56	0.41
1:C:256:LEU:O	1:C:274:ARG:NH2	2.54	0.41
1:D:181:SER:OG	1:D:227:ARG:NH1	2.53	0.41
1:A:180:VAL:HG12	1:A:338:LEU:HD13	2.03	0.41
1:A:316:ASP:O	1:A:320:ARG:HG3	2.20	0.41
1:B:565:LEU:HA	1:B:570:GLU:O	2.21	0.41
1:C:473:TYR:CE2	1:C:477:ILE:HD13	2.56	0.41
1:C:599:TRP:CH2	1:C:628:MET:HE1	2.55	0.41
1:D:269:LYS:HB3	1:D:269:LYS:HE3	1.72	0.41
1:A:217:PHE:HA	4:A:703:UDP:O2'	2.21	0.41
1:C:280:GLY:HA3	1:C:408:ILE:HG22	2.03	0.41
1:D:476:ARG:NH1	1:D:574:ASP:OD2	2.42	0.41
1:A:245:ILE:HG23	1:A:273:ILE:HD13	2.03	0.41
1:A:540:ALA:O	1:A:544:HIS:HD2	2.04	0.41
1:D:574:ASP:O	1:D:575:ASP:HB2	2.20	0.41
1:D:144:GLY:HA3	1:D:148:GLU:OE1	2.20	0.41
1:C:460:ARG:NH2	1:C:487:VAL:HG23	2.37	0.41
1:D:219:ASN:OD1	1:D:253:MET:HG3	2.20	0.41
1:A:409:TRP:CD1	1:A:453:VAL:HG13	2.56	0.40
1:B:351:GLY:O	1:B:382:PRO:HD2	2.21	0.40
1:B:410:GLY:O	1:B:457:ASN:ND2	2.35	0.40
1:D:519:SER:O	1:D:649:LYS:HD3	2.21	0.40
1:A:165:LYS:O	1:A:169:ASP:HB2	2.22	0.40
1:D:313:PRO:HG2	1:D:433:SER:HB2	2.04	0.40
1:D:538:ALA:CB	1:D:549:VAL:HG13	2.50	0.40
1:A:286:ILE:HD11	1:A:402:TYR:HB2	2.04	0.40
1:B:608:LEU:HA	1:B:608:LEU:HD23	1.89	0.40
1:C:190:LEU:HA	1:C:190:LEU:HD12	1.80	0.40
1:C:298:THR:HB	1:C:390:SER:OG	2.22	0.40
1:D:188:ARG:NH2	1:D:305:GLU:OE2	2.54	0.40
1:D:366:GLU:HA	1:D:369:ARG:HB2	2.02	0.40
1:D:580:TYR:CE1	1:D:628:MET:HG3	2.57	0.40
1:A:474:TYR:CZ	1:A:481:LYS:HE3	2.56	0.40
1:B:520:VAL:HG21	1:B:650:LEU:HD23	2.03	0.40
1:D:576:SER:HB3	1:D:587:LEU:HD13	2.02	0.40
1:D:525:ILE:HG12	1:D:642:LEU:HD22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	501/510 (98%)	482 (96%)	17 (3%)	2 (0%)	34 66
1	B	501/510 (98%)	484 (97%)	17 (3%)	0	100 100
1	C	501/510 (98%)	486 (97%)	15 (3%)	0	100 100
1	D	498/510 (98%)	480 (96%)	17 (3%)	1 (0%)	47 78
All	All	2001/2040 (98%)	1932 (97%)	66 (3%)	3 (0%)	47 81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	408	ILE
1	A	556	ARG
1	A	409	TRP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	439/441 (100%)	413 (94%)	26 (6%)	19 49
1	B	439/441 (100%)	408 (93%)	31 (7%)	14 39
1	C	439/441 (100%)	415 (94%)	24 (6%)	21 52
1	D	436/441 (99%)	405 (93%)	31 (7%)	14 39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1753/1764 (99%)	1641 (94%)	112 (6%)	17 45

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	PRO
1	A	161	ASP
1	A	188	ARG
1	A	231	SER
1	A	252	ASP
1	A	274	ARG
1	A	293	LYS
1	A	308	GLU
1	A	350	VAL
1	A	366	GLU
1	A	397	ASP
1	A	407	ASP
1	A	442	ARG
1	A	452	ASN
1	A	453	VAL
1	A	454	LEU
1	A	461	LEU
1	A	487	VAL
1	A	510	TYR
1	A	572	ARG
1	A	605	THR
1	A	624	ASP
1	A	627	LEU
1	A	635	LEU
1	A	637	ARG
1	A	641	THR
1	B	169	ASP
1	B	203	ARG
1	B	206	THR
1	B	231	SER
1	B	236	SER
1	B	250	TYR
1	B	252	ASP
1	B	276	GLN
1	B	298	THR
1	B	308	GLU
1	B	320	ARG

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Mol	Chain	Res	Type
1	B	322	SER
1	B	334	SER
1	B	348	VAL
1	B	383	THR
1	B	397	ASP
1	B	401	THR
1	B	404	SER
1	B	442	ARG
1	B	453	VAL
1	B	454	LEU
1	B	456	LYS
1	B	479	ASN
1	B	510	TYR
1	B	557	GLN
1	B	572	ARG
1	B	587	LEU
1	B	612	THR
1	B	622	SER
1	B	625	LYS
1	B	647	SER
1	C	158	GLU
1	C	172	THR
1	C	188	ARG
1	C	231	SER
1	C	252	ASP
1	C	274	ARG
1	C	281	LEU
1	C	298	THR
1	C	308	GLU
1	C	343	ARG
1	C	350	VAL
1	C	397	ASP
1	C	468	GLU
1	C	479	ASN
1	C	487	VAL
1	C	491	ARG
1	C	514	PHE
1	C	546	LYS
1	C	557	GLN
1	C	583	LYS
1	C	605	THR
1	C	612	THR

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Mol	Chain	Res	Type
1	C	641	THR
1	C	650	LEU
1	D	188	ARG
1	D	206	THR
1	D	207	ASN
1	D	220	GLU
1	D	231	SER
1	D	252	ASP
1	D	269	LYS
1	D	274	ARG
1	D	293	LYS
1	D	308	GLU
1	D	323	THR
1	D	350	VAL
1	D	383	THR
1	D	397	ASP
1	D	398	ARG
1	D	409	TRP
1	D	454	LEU
1	D	468	GLU
1	D	487	VAL
1	D	510	TYR
1	D	515	ILE
1	D	534	THR
1	D	556	ARG
1	D	557	GLN
1	D	572	ARG
1	D	586	THR
1	D	587	LEU
1	D	612	THR
1	D	625	LYS
1	D	626	LEU
1	D	635	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	HIS
1	A	610	HIS
1	D	271	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
5	EDO	A	705	-	3,3,3	0.50	0	2,2,2	0.41	0
4	UDP	D	703	2	20,26,26	1.06	1 (5%)	25,40,40	1.16	1 (4%)
5	EDO	A	704	-	3,3,3	0.53	0	2,2,2	0.45	0
4	UDP	B	703	2	20,26,26	1.08	1 (5%)	25,40,40	0.98	1 (4%)
3	NAG	A	702	1	14,14,15	0.75	1 (7%)	17,19,21	1.88	3 (17%)
5	EDO	B	704	-	3,3,3	0.64	0	2,2,2	0.28	0
5	EDO	C	704	-	3,3,3	0.62	0	2,2,2	0.13	0
6	GOL	D	705	-	5,5,5	0.32	0	5,5,5	0.66	0
5	EDO	D	704	-	3,3,3	0.49	0	2,2,2	0.38	0
6	GOL	B	705	-	5,5,5	0.38	0	5,5,5	0.51	0
3	NAG	D	702	1	14,14,15	0.55	0	17,19,21	2.20	1 (5%)
4	UDP	C	703	2	20,26,26	1.12	1 (5%)	25,40,40	1.07	1 (4%)
4	UDP	A	703	2	20,26,26	1.05	1 (5%)	25,40,40	1.16	4 (16%)
3	NAG	B	702	1	14,14,15	0.66	0	17,19,21	1.40	1 (5%)
5	EDO	C	705	-	3,3,3	0.53	0	2,2,2	0.16	0
3	NAG	C	702	1	14,14,15	0.44	0	17,19,21	0.91	1 (5%)

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	EDO	A	705	-	-	1/1/1/1	-
4	UDP	D	703	2	-	4/14/32/32	0/2/2/2
5	EDO	A	704	-	-	1/1/1/1	-
4	UDP	B	703	2	-	4/14/32/32	0/2/2/2
3	NAG	A	702	1	-	3/6/23/26	0/1/1/1
5	EDO	B	704	-	-	0/1/1/1	-
5	EDO	C	704	-	-	0/1/1/1	-
6	GOL	D	705	-	-	0/4/4/4	-
5	EDO	D	704	-	-	0/1/1/1	-
6	GOL	B	705	-	-	4/4/4/4	-
3	NAG	D	702	1	-	1/6/23/26	0/1/1/1
4	UDP	C	703	2	-	6/14/32/32	0/2/2/2
4	UDP	A	703	2	-	2/14/32/32	0/2/2/2
3	NAG	B	702	1	-	2/6/23/26	0/1/1/1
5	EDO	C	705	-	-	1/1/1/1	-
3	NAG	C	702	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	703	UDP	C4-N3	3.33	1.38	1.33
4	D	703	UDP	C4-N3	3.11	1.38	1.33
4	A	703	UDP	C4-N3	3.10	1.38	1.33
4	B	703	UDP	C4-N3	3.06	1.38	1.33
3	A	702	NAG	O5-C1	2.55	1.47	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	702	NAG	C1-O5-C5	8.49	123.70	112.19
3	A	702	NAG	C1-O5-C5	5.44	119.57	112.19
3	B	702	NAG	C1-O5-C5	4.72	118.58	112.19
3	A	702	NAG	C1-C2-N2	3.68	116.77	110.49
4	D	703	UDP	PA-O3A-PB	-3.50	120.83	132.83
4	C	703	UDP	PA-O3A-PB	-3.48	120.90	132.83
3	A	702	NAG	C2-N2-C7	3.19	127.45	122.90
4	A	703	UDP	PA-O3A-PB	-3.03	122.43	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	703	UDP	PA-O3A-PB	-2.66	123.70	132.83
3	C	702	NAG	C1-O5-C5	2.54	115.64	112.19
4	A	703	UDP	C5-C4-N3	-2.35	118.13	123.31
4	A	703	UDP	C6-N1-C2	-2.28	117.58	121.20
4	A	703	UDP	C2'-C3'-C4'	2.06	106.65	102.64

There are no chirality outliers.

All (29) torsion outliers are listed below:

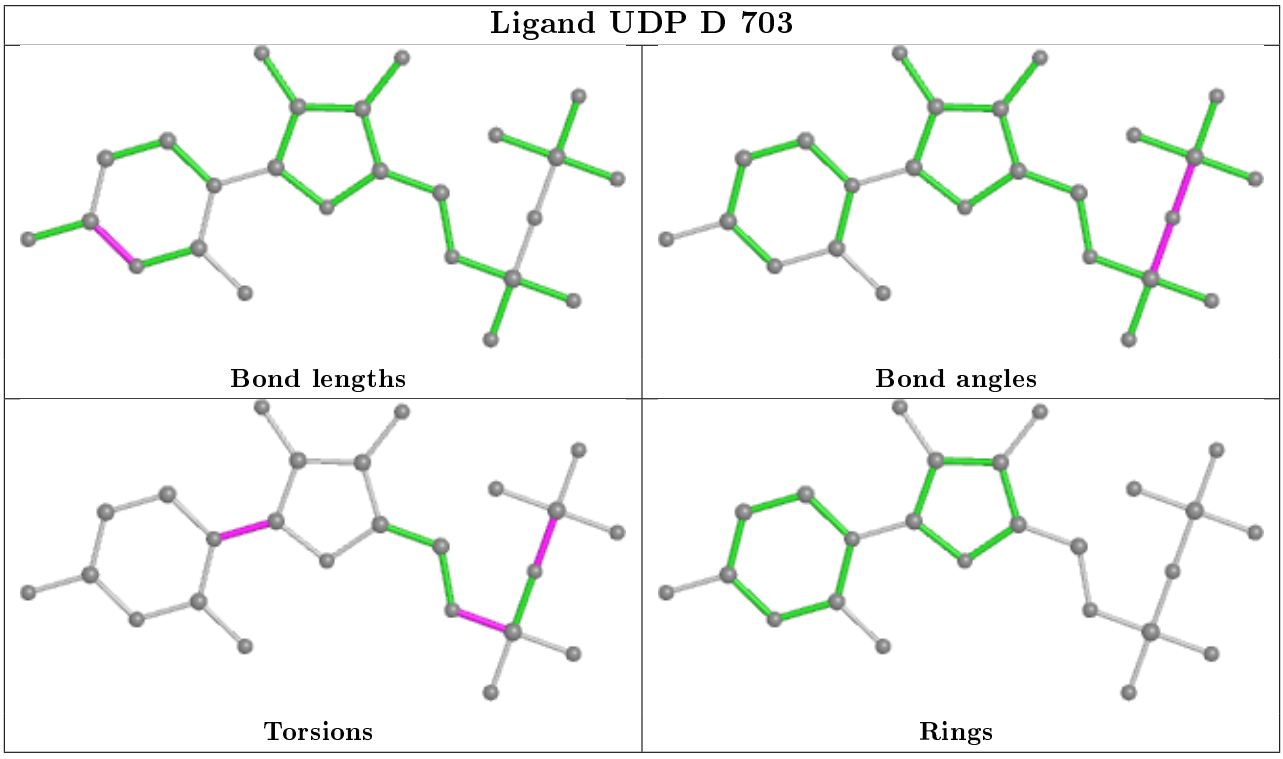
Mol	Chain	Res	Type	Atoms
4	D	703	UDP	C2'-C1'-N1-C6
4	D	703	UDP	O4'-C1'-N1-C6
4	D	703	UDP	PA-O3A-PB-O2B
4	B	703	UDP	C2'-C1'-N1-C6
4	B	703	UDP	O4'-C1'-N1-C6
6	B	705	GOL	O1-C1-C2-C3
6	B	705	GOL	C1-C2-C3-O3
4	C	703	UDP	C5'-O5'-PA-O1A
4	C	703	UDP	C5'-O5'-PA-O2A
4	C	703	UDP	C5'-O5'-PA-O3A
4	C	703	UDP	PA-O3A-PB-O2B
4	A	703	UDP	C2'-C1'-N1-C6
4	A	703	UDP	O4'-C1'-N1-C6
3	B	702	NAG	C4-C5-C6-O6
3	A	702	NAG	C4-C5-C6-O6
3	A	702	NAG	O5-C5-C6-O6
3	B	702	NAG	O5-C5-C6-O6
4	B	703	UDP	C3'-C4'-C5'-O5'
3	A	702	NAG	C1-C2-N2-C7
4	B	703	UDP	O4'-C4'-C5'-O5'
6	B	705	GOL	O1-C1-C2-O2
5	A	704	EDO	O1-C1-C2-O2
6	B	705	GOL	O2-C2-C3-O3
4	C	703	UDP	PA-O3A-PB-O3B
3	D	702	NAG	C4-C5-C6-O6
5	A	705	EDO	O1-C1-C2-O2
5	C	705	EDO	O1-C1-C2-O2
4	C	703	UDP	PA-O3A-PB-O1B
4	D	703	UDP	C5'-O5'-PA-O1A

There are no ring outliers.

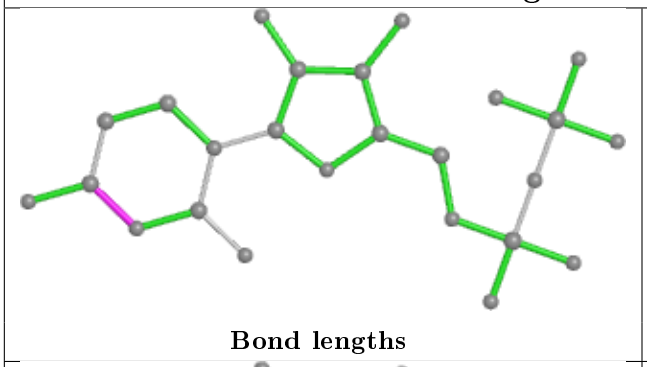
7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	703	UDP	4	0
4	B	703	UDP	1	0
6	D	705	GOL	3	0
6	B	705	GOL	2	0
4	A	703	UDP	2	0
3	B	702	NAG	1	0
5	C	705	EDO	1	0

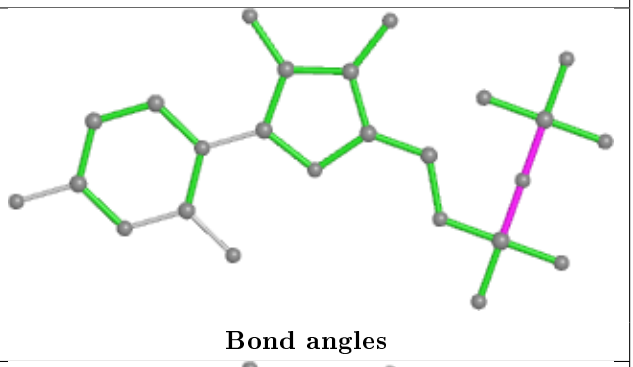
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



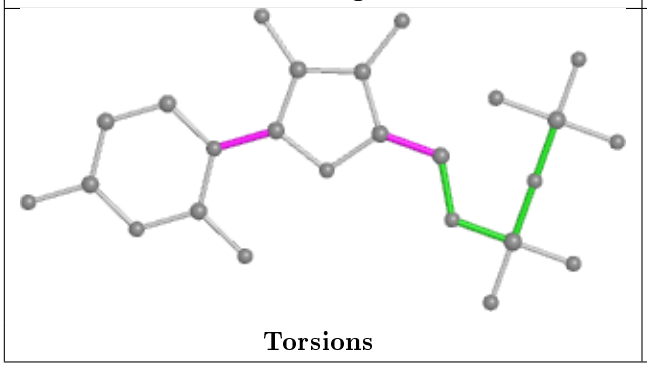
Ligand UDP B 703



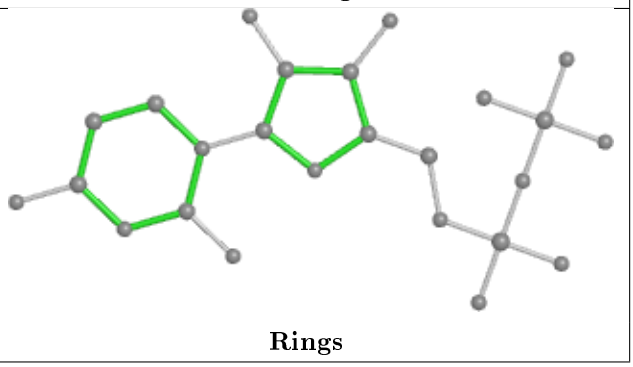
Bond lengths



Bond angles

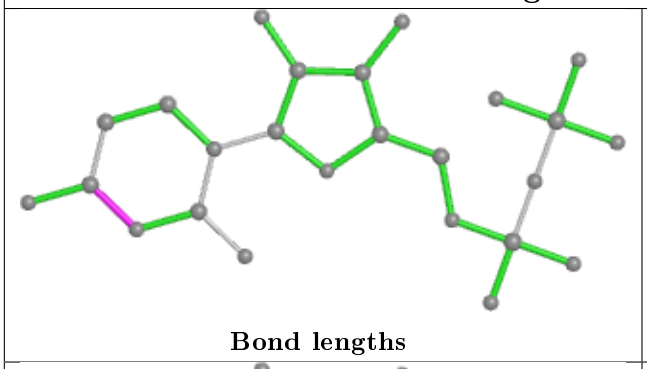


Torsions

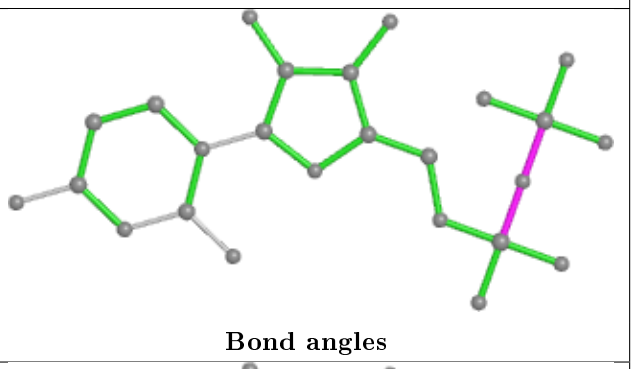


Rings

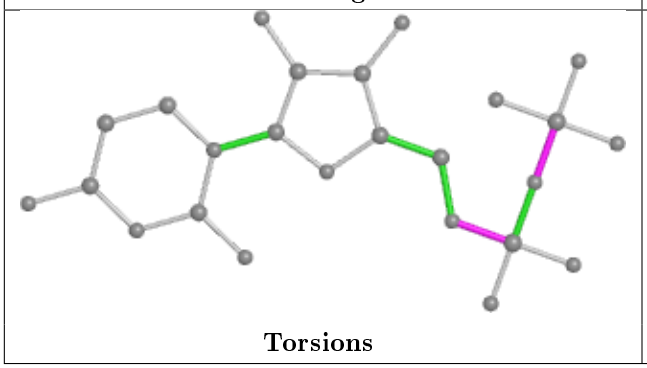
Ligand UDP C 703



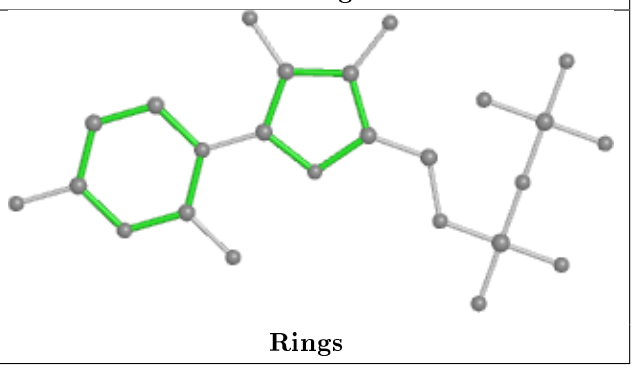
Bond lengths



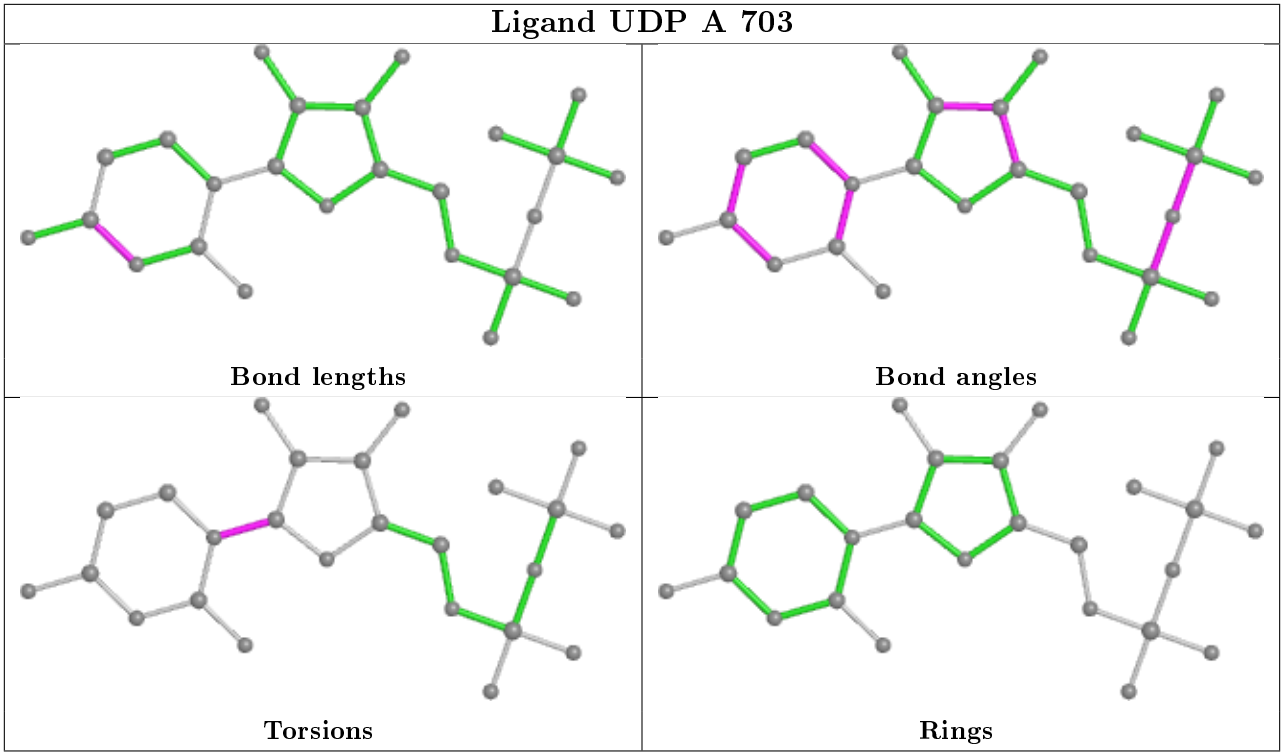
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	505/510 (99%)	-0.31	13 (2%)	56	46	31, 48, 77, 142	0
1	B	503/510 (98%)	-0.31	11 (2%)	62	52	30, 50, 81, 109	0
1	C	503/510 (98%)	-0.29	15 (2%)	50	40	32, 50, 81, 143	0
1	D	502/510 (98%)	-0.24	17 (3%)	45	35	35, 53, 85, 139	0
All	All	2013/2040 (98%)	-0.29	56 (2%)	53	43	30, 50, 82, 143	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	544	HIS	6.3
1	A	447	TRP	4.7
1	B	143	GLY	4.4
1	B	446	LYS	4.2
1	B	409	TRP	4.1
1	B	541	GLY	3.9
1	C	409	TRP	3.6
1	D	373	ASN	3.6
1	C	143	GLY	3.5
1	C	541	GLY	3.4
1	C	540	ALA	3.4
1	D	542	LYS	3.3
1	D	409	TRP	3.3
1	A	143	GLY	3.3
1	A	409	TRP	3.3
1	D	143	GLY	3.1
1	C	446	LYS	3.1
1	D	203	ARG	3.1
1	D	540	ALA	3.0
1	A	542	LYS	2.9
1	D	544	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	373	ASN	2.9
1	B	200	ASP	2.9
1	A	541	GLY	2.9
1	A	498	LYS	2.8
1	C	543	LYS	2.8
1	A	452	ASN	2.8
1	C	545	GLN	2.7
1	C	546	LYS	2.6
1	B	202	ALA	2.5
1	D	541	GLY	2.5
1	C	542	LYS	2.5
1	D	452	ASN	2.5
1	A	200	ASP	2.5
1	A	443	SER	2.5
1	D	634	SER	2.5
1	A	448	ARG	2.4
1	A	157	LYS	2.4
1	D	443	SER	2.4
1	B	443	SER	2.3
1	D	277	LYS	2.3
1	A	371	ARG	2.3
1	B	158	GLU	2.3
1	D	545	GLN	2.3
1	D	546	LYS	2.3
1	C	370	LYS	2.3
1	D	408	ILE	2.2
1	D	250	TYR	2.2
1	B	145	GLY	2.2
1	C	144	GLY	2.2
1	D	157	LYS	2.1
1	A	373	ASN	2.1
1	C	650	LEU	2.1
1	B	203	ARG	2.0
1	C	276	GLN	2.0
1	B	452	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

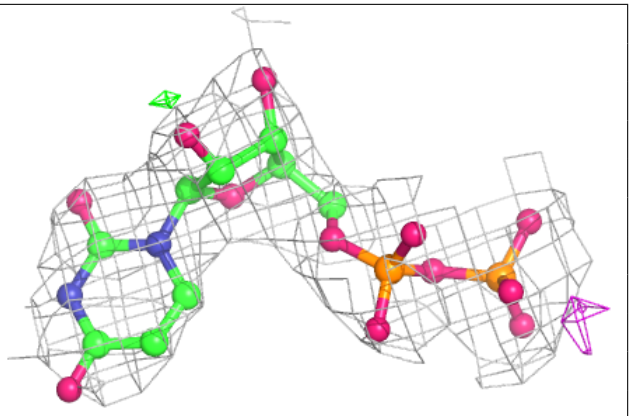
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

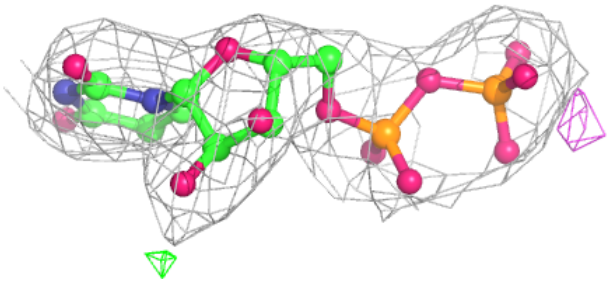
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	C	704	4/4	0.82	0.29	62,68,70,71	0
6	GOL	B	705	6/6	0.89	0.19	52,64,67,68	0
5	EDO	A	704	4/4	0.90	0.13	43,50,58,62	0
6	GOL	D	705	6/6	0.92	0.23	52,52,57,58	0
5	EDO	B	704	4/4	0.92	0.18	36,42,43,48	0
5	EDO	A	705	4/4	0.93	0.17	45,56,61,62	0
5	EDO	D	704	4/4	0.94	0.14	54,54,60,63	0
3	NAG	B	702	14/15	0.94	0.19	39,51,73,79	0
3	NAG	D	702	14/15	0.94	0.16	46,64,73,77	0
3	NAG	A	702	14/15	0.95	0.20	37,56,73,77	0
4	UDP	C	703	25/25	0.95	0.13	53,82,87,88	0
4	UDP	B	703	25/25	0.96	0.14	41,78,97,98	0
4	UDP	D	703	25/25	0.96	0.13	43,80,103,104	0
3	NAG	C	702	14/15	0.96	0.15	28,49,58,59	0
4	UDP	A	703	25/25	0.97	0.12	35,68,96,97	0
5	EDO	C	705	4/4	0.97	0.23	55,55,56,56	0
2	MN	C	701	1/1	0.98	0.07	54,54,54,54	0
2	MN	B	701	1/1	0.98	0.03	55,55,55,55	0
2	MN	D	701	1/1	0.99	0.04	51,51,51,51	0
2	MN	A	701	1/1	0.99	0.02	46,46,46,46	0

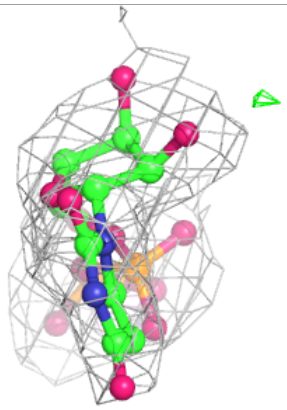
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UDP C 703:

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

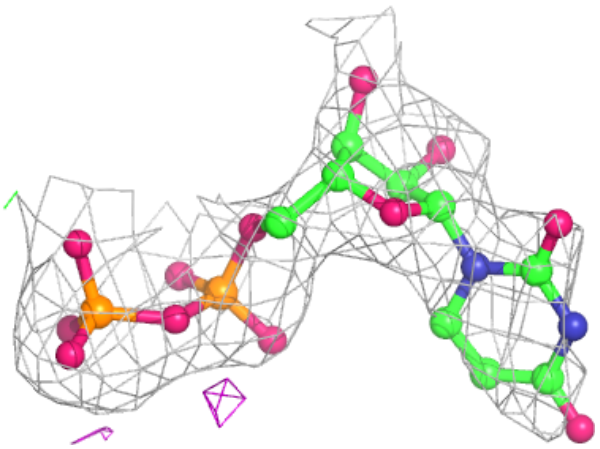


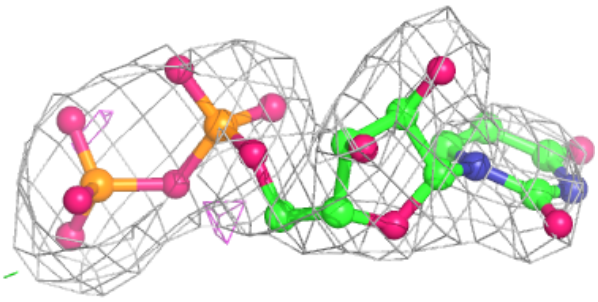


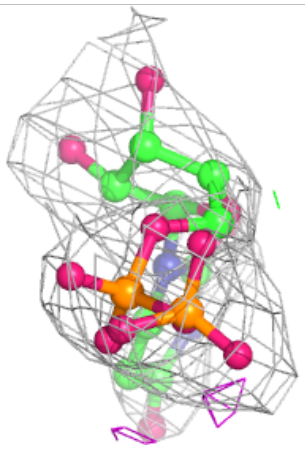


Electron density around UDP B 703:

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

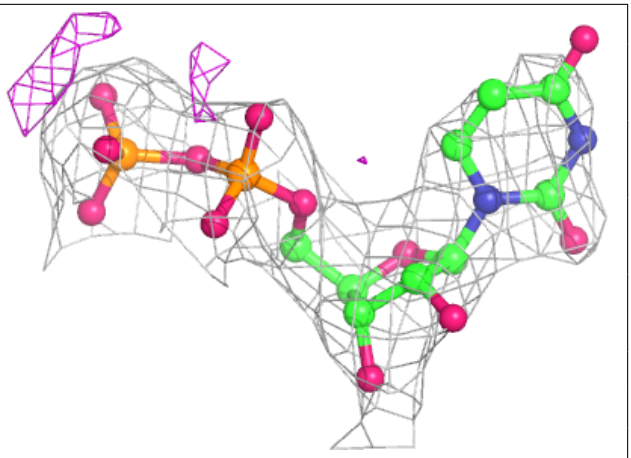


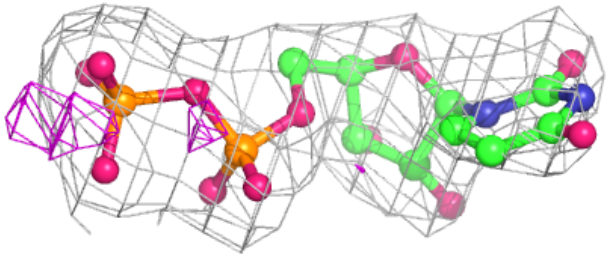


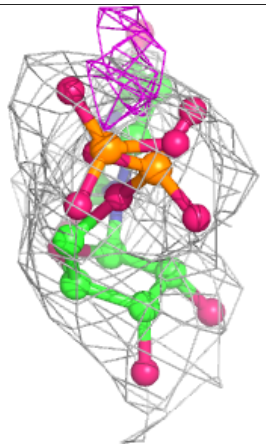


Electron density around UDP D 703:

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

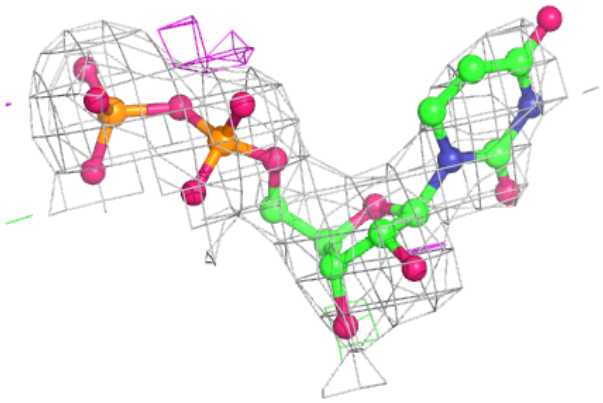


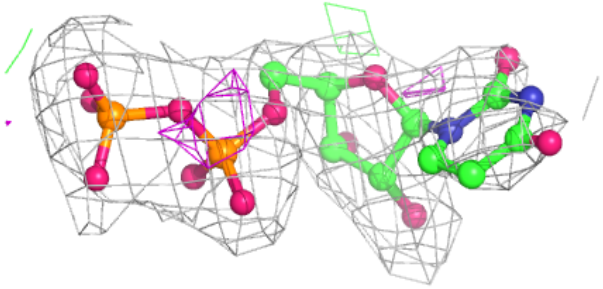


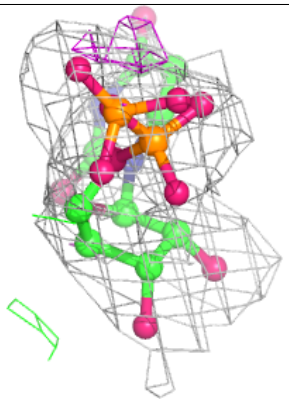


Electron density around UDP A 703:

$2mF_o$-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.