



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:51 PM UTC

PDB ID : 6E4Q / pdb_00006e4q
Title : Crystal Structure of the Drosophila Melanogaster Polypeptide N-Acetylgalactosaminyl 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 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

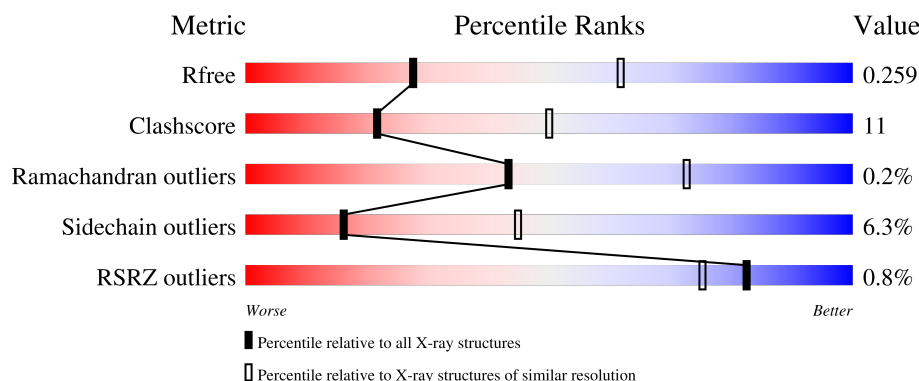
1 Overall quality at a glance

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	510	% 72% 25% ..
1	B	510	71% 25% ..
1	C	510	% 73% 24% ..
1	D	510	% 69% 26% ..

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			

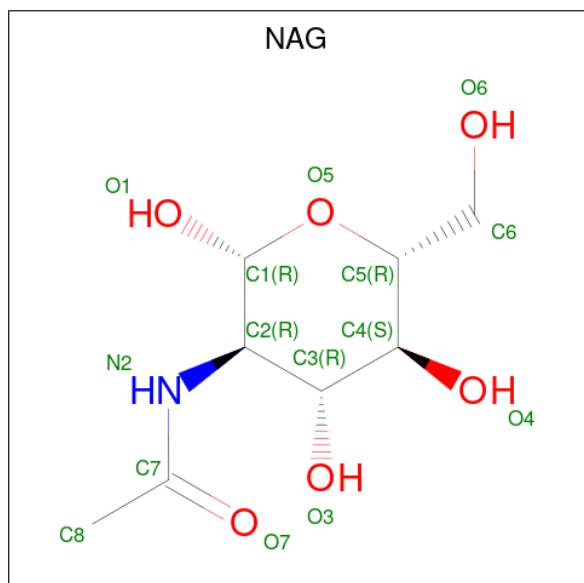
There are 20 discrepancies between the modelled and reference sequences:

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 (CCD ID: MN) (formula: Mn).

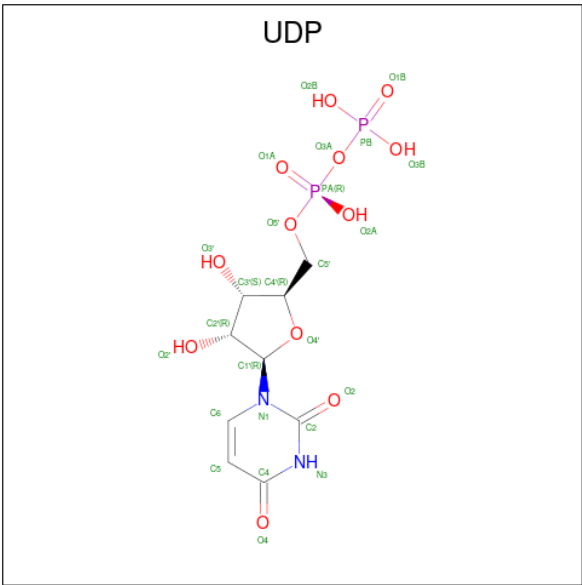
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



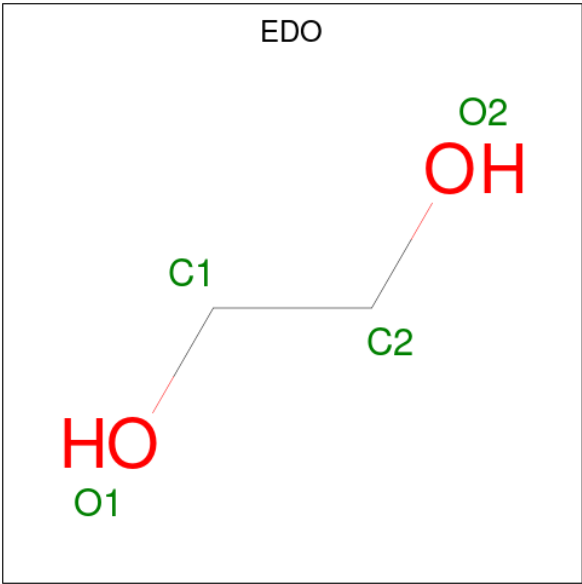
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: C₉H₁₄N₂O₁₂P₂).



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 (CCD ID: EDO) (formula: C₂H₆O₂).



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 (CCD ID: 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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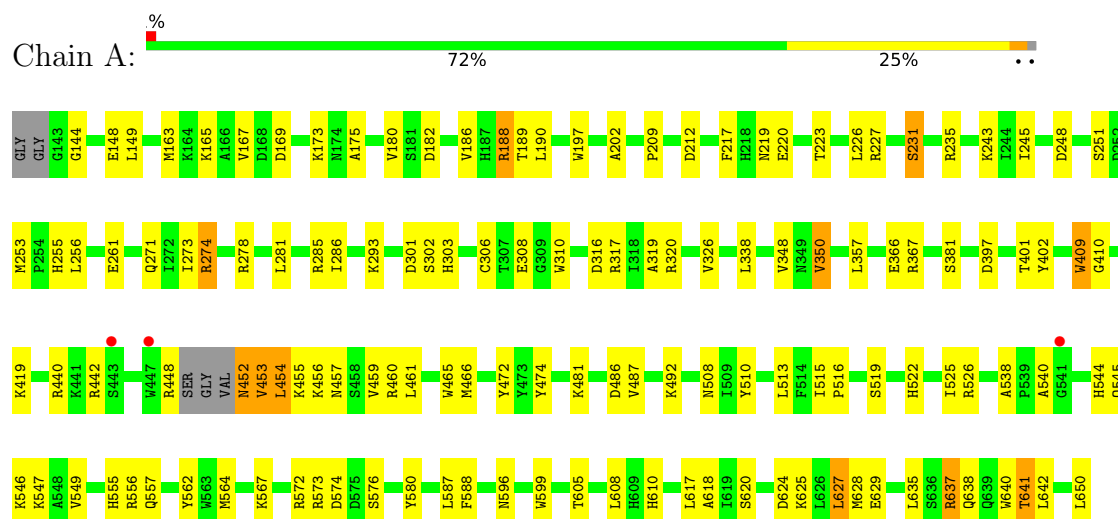
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	56	Total	O	0	0
			56	56		
7	D	24	Total	O	0	0
			24	24		

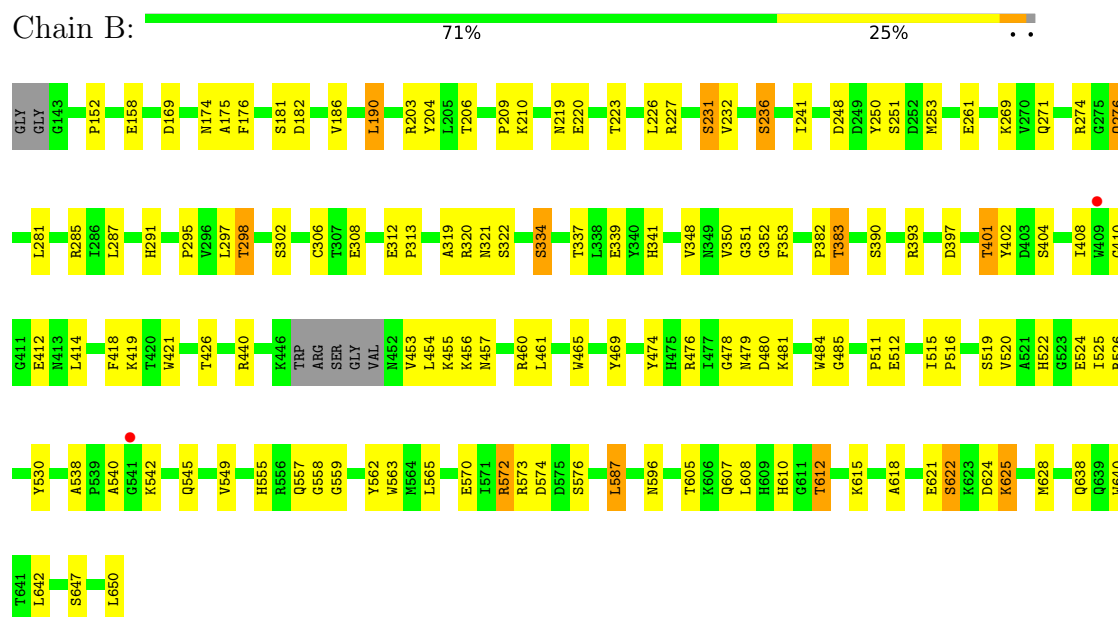
3 Residue-property plots

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.

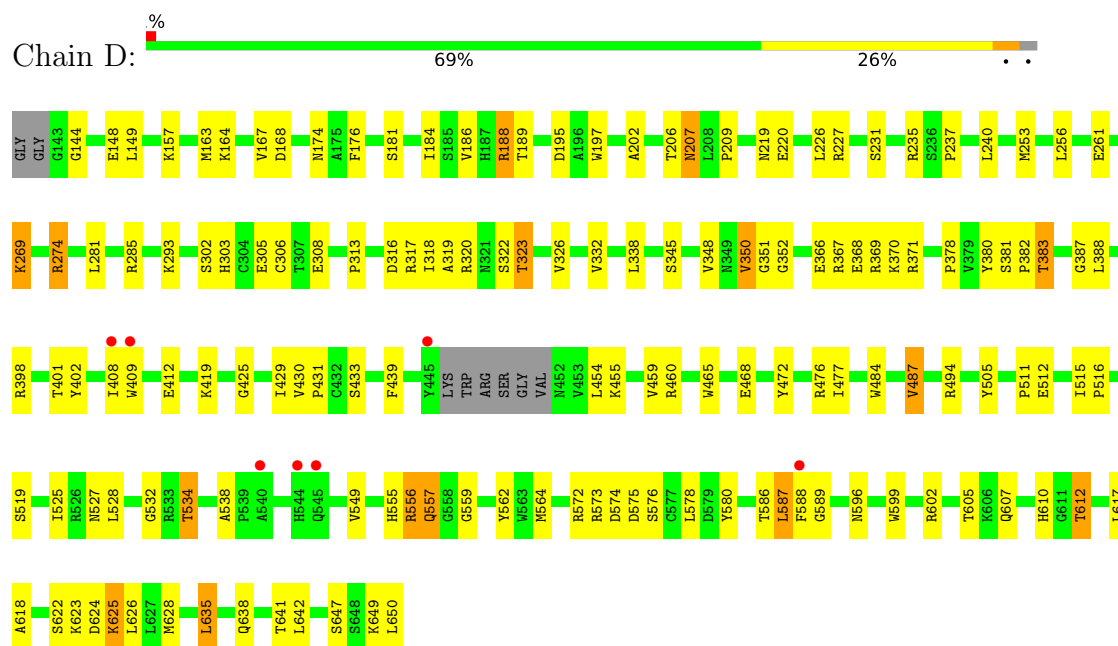
- Molecule 1: polypeptide N-acetylgalactosaminyltransferase 9



- Molecule 1: polypeptide N-acetylgalactosaminyltransferase 9



- Molecule 1: polypeptide N-acetylgalactosaminyltransferase 9



4 Data and refinement statistics

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) 93.8 (19.95-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.79Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.190 , 0.260 0.193 , 0.259	Depositor DCC
R_{free} test set	3521 reflections (4.65%)	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)	0.30 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

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: EDO, UDP, NAG, GOL, MN

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	0.40	0/4181	0.64	0/5653
1	B	0.39	0/4176	0.64	0/5645
1	C	0.38	0/4177	0.63	0/5647
1	D	0.39	0/4145	0.64	0/5605
All	All	0.39	0/16679	0.64	0/22550

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	88	0
1	B	4064	0	3931	77	0
1	C	4064	0	3927	85	0
1	D	4040	0	3898	100	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	0
7	B	56	0	0	0	0
7	C	56	0	0	2	0
7	D	24	0	0	1	0
All	All	16632	0	15838	350	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 11.

All (350) 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
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:D:219:ASN:HB3	1:D:253:MET:HE3	1.68	0.73
1:C:219:ASN:HB3	1:C:253:MET:HE3	1.70	0.73
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD1	1:D:207:ASN:N	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:B:219:ASN:HB3	1:B:253:MET:HE3	1.74	0.68
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:A:219:ASN:HB3	1:A:253:MET:HE3	1.79	0.64
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:ND1	1:D:555:HIS:O	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:A:567:LYS:HE3	1:A:650:LEU:C	2.24	0.62
1:C:186:VAL:HG11	1:C:226:LEU:HB3	1.82	0.62
1:D:617:LEU:HD13	1:D:628:MET:HE2	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:401:THR:O	1:D:419:LYS:NZ	2.35	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:A:144:GLY:HA3	1:A:148:GLU:CD	2.29	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: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: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:C:401:THR:O	1:C:419:LYS:NZ	2.38	0.56
1:A:620:SER:HB3	1:A:627:LEU:HD21	1.87	0.56
1:A:599:TRP:CH2	1:A:628:MET:HE1	2.41	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:O	1:B:555:HIS:ND1	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:618:ALA:HB2	1:A:638:GLN:HG2	1.89	0.54
1:C:599:TRP:CH2	1:C:628:MET:HE1	2.43	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
1:A:538:ALA:HB2	1:A:549:VAL:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:164:LYS:HE2	1:D:168:ASP:OD2	2.09	0.53
1:D:617:LEU:HD13	1:D:628:MET:CE	2.38	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:599:TRP:HH2	1:A:628:MET:HE1	1.76	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:C:382:PRO:O	1:C:505:TYR:OH	2.30	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:B:401:THR:OG1	1:B:402:TYR:N	2.44	0.49
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:H	1:A:454:LEU:HD22	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:C:152:PRO:HG3	1:C:339:GLU:CD	2.37	0.48
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:A:219:ASN:H	1:A:251:SER:HB3	1.77	0.48
1:B:610:HIS:HB2	1:B:628:MET:HE1	1.94	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:276:GLN:H	1:B:276:GLN:CD	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:429:ILE:O	1:C:431:PRO:HD3	2.14	0.47
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:OE1	1:B:312:GLU:N	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:A:357:LEU:HD21	1:A:466:MET:HE1	1.96	0.47
1:A:555:HIS:C	1:A:557:GLN:H	2.22	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: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:387:GLY:C	1:D:388:LEU:HD12	2.39	0.46
1:D:556:ARG:HH21	1:D:556:ARG:HB3	1.81	0.46
1:C:516:PRO:O	1:C:519:SER:OG	2.26	0.46
1:C:543:LYS:HB2	1:C:543:LYS:HE3	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:303:HIS:CE1	4:D:703:UDP:H3'	2.50	0.46
1:D:578:LEU:HD23	1:D:587:LEU:HD23	1.98	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:529:GLY:HA2	1:C:636:SER:HB3	1.97	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: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
1:C:273:ILE:HD11	1:C:291[B]:HIS:CE1	2.51	0.45
1:A:617:LEU:HD13	1:A:628:MET:HE2	1.98	0.45
1:D:209:PRO:HD3	1:D:319:ALA:HB2	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:HD12	1:D:635:LEU:HA	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:C:599:TRP:HH2	1:C:628:MET:HE1	1.82	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:B:615:LYS:HB2	1:B:628:MET:HE3	2.00	0.44
1:D:237:PRO:HG2	1:D:240:LEU:HD12	2.00	0.44
1:A:608:LEU:HD23	1:A:608:LEU:HA	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: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:163:MET:O	1:C:167:VAL:HG23	2.18	0.44
1:C:169:ASP:CG	1:C:173:LYS:HE3	2.43	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:387:GLY:C	1:C:388:LEU:HD12	2.43	0.43
1:C:586:THR:HB	1:C:588[A]:PHE:CE1	2.53	0.43
1:D:599:TRP:CZ3	1:D:628:MET:HE1	2.53	0.43
1:B:624:ASP:OD1	1:B:625:LYS:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:617:LEU:CD1	1:D:628:MET:HE2	2.46	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
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:C:579:ASP:CG	1:C:588[B]:PHE:HE2	2.27	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: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:D:564:MET:HE3	1:D:564:MET:HB2	1.99	0.42
1:A:169:ASP:CG	1:A:173:LYS:HE3	2.45	0.41
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:HD23	1:C:587:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:281:LEU:HD11	1:B:285:ARG:HH11	1.84	0.41
1:D:269:LYS:H	1:D:269:LYS:HG2	1.49	0.41
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:C:564:MET:HE3	1:C:564:MET:HB2	1.94	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:334:SER:HG	1:B:337:THR:H	1.67	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:D:269:LYS:HE3	1:D:269:LYS:HB3	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:B:261:GLU:CD	1:B:274:ARG:HH21	2.29	0.41
1:D:144:GLY:HA3	1:D:148:GLU:OE1	2.20	0.41
1:D:574:ASP:O	1:D:575:ASP:HB2	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:HD23	1:B:608:LEU:HA	1.89	0.40
1:C:190:LEU:HD12	1:C:190:LEU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:525:ILE:HG12	1:D:642:LEU:HD22	2.04	0.40
1:D:576:SER:HB3	1:D:587:LEU:HD13	2.02	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%)	30	60
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%)	43	72
All	All	2001/2040 (98%)	1932 (97%)	66 (3%)	3 (0%)	43	77

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%)	417 (95%)	22 (5%)	22	54
1	B	439/441 (100%)	407 (93%)	32 (7%)	13	38
1	C	439/441 (100%)	411 (94%)	28 (6%)	16	44
1	D	436/441 (99%)	407 (93%)	29 (7%)	15	42
All	All	1753/1764 (99%)	1642 (94%)	111 (6%)	16	45

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	ARG
1	A	190	LEU
1	A	231	SER
1	A	274	ARG
1	A	293	LYS
1	A	308	GLU
1	A	348	VAL
1	A	350	VAL
1	A	366	GLU
1	A	397	ASP
1	A	452	ASN
1	A	453	VAL
1	A	454	LEU
1	A	461	LEU
1	A	487	VAL
1	A	605	THR
1	A	624	ASP
1	A	625	LYS
1	A	627	LEU
1	A	635	LEU
1	A	637	ARG
1	A	641	THR
1	B	158	GLU
1	B	169	ASP
1	B	190	LEU
1	B	203	ARG
1	B	206	THR
1	B	231	SER
1	B	236	SER
1	B	250	TYR

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Mol	Chain	Res	Type
1	B	276	GLN
1	B	298	THR
1	B	308	GLU
1	B	320	ARG
1	B	322	SER
1	B	334	SER
1	B	348	VAL
1	B	350	VAL
1	B	383	THR
1	B	397	ASP
1	B	401	THR
1	B	404	SER
1	B	408	ILE
1	B	453	VAL
1	B	454	LEU
1	B	456	LYS
1	B	479	ASN
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	190	LEU
1	C	231	SER
1	C	274	ARG
1	C	281	LEU
1	C	298	THR
1	C	308	GLU
1	C	343	ARG
1	C	348	VAL
1	C	350	VAL
1	C	383	THR
1	C	397	ASP
1	C	446	LYS
1	C	455	LYS
1	C	468	GLU
1	C	479	ASN

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Mol	Chain	Res	Type
1	C	487	VAL
1	C	491	ARG
1	C	542	LYS
1	C	546	LYS
1	C	557	GLN
1	C	583	LYS
1	C	605	THR
1	C	612	THR
1	C	641	THR
1	C	650	LEU
1	D	157	LYS
1	D	188	ARG
1	D	206	THR
1	D	207	ASN
1	D	231	SER
1	D	269	LYS
1	D	274	ARG
1	D	293	LYS
1	D	308	GLU
1	D	323	THR
1	D	348	VAL
1	D	350	VAL
1	D	383	THR
1	D	398	ARG
1	D	409	TRP
1	D	454	LEU
1	D	468	GLU
1	D	487	VAL
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	HIS
1	A	434	HIS
1	A	609	HIS
1	A	610	HIS
1	B	174	ASN
1	B	178	GLN
1	B	349	ASN
1	C	358	GLN
1	C	508	ASN
1	C	609	HIS
1	D	271	GLN
1	D	508	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 ⓘ

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	D	704	-	3,3,3	0.45	0	2,2,2	0.42	0
4	UDP	C	703	2	25,26,26	0.93	0	38,40,40	1.71	6 (15%)
5	EDO	A	704	-	3,3,3	0.49	0	2,2,2	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	UDP	D	703	2	25,26,26	0.89	0	38,40,40	1.61	5 (13%)
5	EDO	B	704	-	3,3,3	0.61	0	2,2,2	0.25	0
5	EDO	C	705	-	3,3,3	0.50	0	2,2,2	0.21	0
3	NAG	D	702	1	14,14,15	0.56	0	17,19,21	2.22	1 (5%)
5	EDO	C	704	-	3,3,3	0.58	0	2,2,2	0.16	0
4	UDP	B	703	2	25,26,26	1.00	1 (4%)	38,40,40	1.59	6 (15%)
3	NAG	B	702	1	14,14,15	0.67	0	17,19,21	1.42	2 (11%)
4	UDP	A	703	2	25,26,26	0.94	2 (8%)	38,40,40	1.63	9 (23%)
3	NAG	C	702	1	14,14,15	0.42	0	17,19,21	0.91	1 (5%)
6	GOL	B	705	-	5,5,5	0.40	0	5,5,5	0.53	0
3	NAG	A	702	1	14,14,15	0.73	1 (7%)	17,19,21	1.95	3 (17%)
5	EDO	A	705	-	3,3,3	0.47	0	2,2,2	0.44	0
6	GOL	D	705	-	5,5,5	0.33	0	5,5,5	0.69	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	EDO	D	704	-	-	1/1/1/1	-
4	UDP	C	703	2	-	6/16/32/32	0/2/2/2
5	EDO	A	704	-	-	1/1/1/1	-
4	UDP	D	703	2	-	2/16/32/32	0/2/2/2
5	EDO	B	704	-	-	0/1/1/1	-
5	EDO	C	705	-	-	1/1/1/1	-
3	NAG	D	702	1	-	1/6/23/26	0/1/1/1
5	EDO	C	704	-	-	0/1/1/1	-
4	UDP	B	703	2	-	4/16/32/32	0/2/2/2
3	NAG	B	702	1	-	2/6/23/26	0/1/1/1
4	UDP	A	703	2	-	4/16/32/32	0/2/2/2
3	NAG	C	702	1	-	0/6/23/26	0/1/1/1
6	GOL	B	705	-	-	4/4/4/4	-
3	NAG	A	702	1	-	3/6/23/26	0/1/1/1
5	EDO	A	705	-	-	1/1/1/1	-
6	GOL	D	705	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	NAG	O5-C1	2.44	1.47	1.43
4	B	703	UDP	PA-O3A	2.27	1.61	1.59
4	A	703	UDP	C6-C5	2.04	1.39	1.35
4	A	703	UDP	PA-O3A	2.01	1.61	1.59

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	702	NAG	C1-O5-C5	8.59	123.70	112.19
4	C	703	UDP	C4-N3-C2	-6.19	118.92	126.61
4	B	703	UDP	C4-N3-C2	-5.81	119.40	126.61
4	D	703	UDP	C4-N3-C2	-5.60	119.67	126.61
3	A	702	NAG	C1-O5-C5	5.51	119.57	112.19
4	A	703	UDP	C4-N3-C2	-5.17	120.19	126.61
3	B	702	NAG	C1-O5-C5	4.77	118.58	112.19
4	C	703	UDP	N3-C2-N1	4.33	120.53	114.89
4	A	703	UDP	N3-C2-N1	4.33	120.52	114.89
3	A	702	NAG	C1-C2-N2	4.02	116.77	110.43
4	B	703	UDP	N3-C2-N1	3.95	120.03	114.89
4	D	703	UDP	N3-C2-N1	3.75	119.77	114.89
3	A	702	NAG	C2-N2-C7	3.40	127.45	122.90
4	C	703	UDP	C5-C4-N3	3.37	119.52	114.80
4	C	703	UDP	O2-C2-N1	-3.25	118.57	122.80
4	D	703	UDP	C5-C4-N3	3.24	119.34	114.80
4	B	703	UDP	C5-C4-N3	3.14	119.20	114.80
4	B	703	UDP	C5-C6-N1	-2.95	117.04	121.84
4	C	703	UDP	O4-C4-C5	-2.82	120.29	125.16
4	A	703	UDP	C6-N1-C2	-2.81	117.58	121.00
4	A	703	UDP	O2-C2-N1	-2.69	119.30	122.80
4	C	703	UDP	C5-C6-N1	-2.66	117.51	121.84
4	D	703	UDP	O4-C4-C5	-2.63	120.63	125.16
3	C	702	NAG	C1-O5-C5	2.57	115.64	112.19
4	D	703	UDP	C5-C6-N1	-2.56	117.68	121.84
4	B	703	UDP	O4-C4-C5	-2.44	120.96	125.16
4	A	703	UDP	C5-C4-N3	2.38	118.13	114.80
4	A	703	UDP	O2A-PA-O3A	2.23	113.30	107.27
4	A	703	UDP	C5-C6-N1	-2.22	118.23	121.84
4	B	703	UDP	O2-C2-N1	-2.21	119.92	122.80
4	A	703	UDP	C2'-C3'-C4'	2.09	106.65	102.61
3	B	702	NAG	C2-N2-C7	2.07	125.68	122.90
4	A	703	UDP	O4-C4-C5	-2.06	121.62	125.16

There are no chirality outliers.

All (30) torsion outliers are listed below:

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

There are no ring outliers.

7 monomers are involved in 14 short contacts:

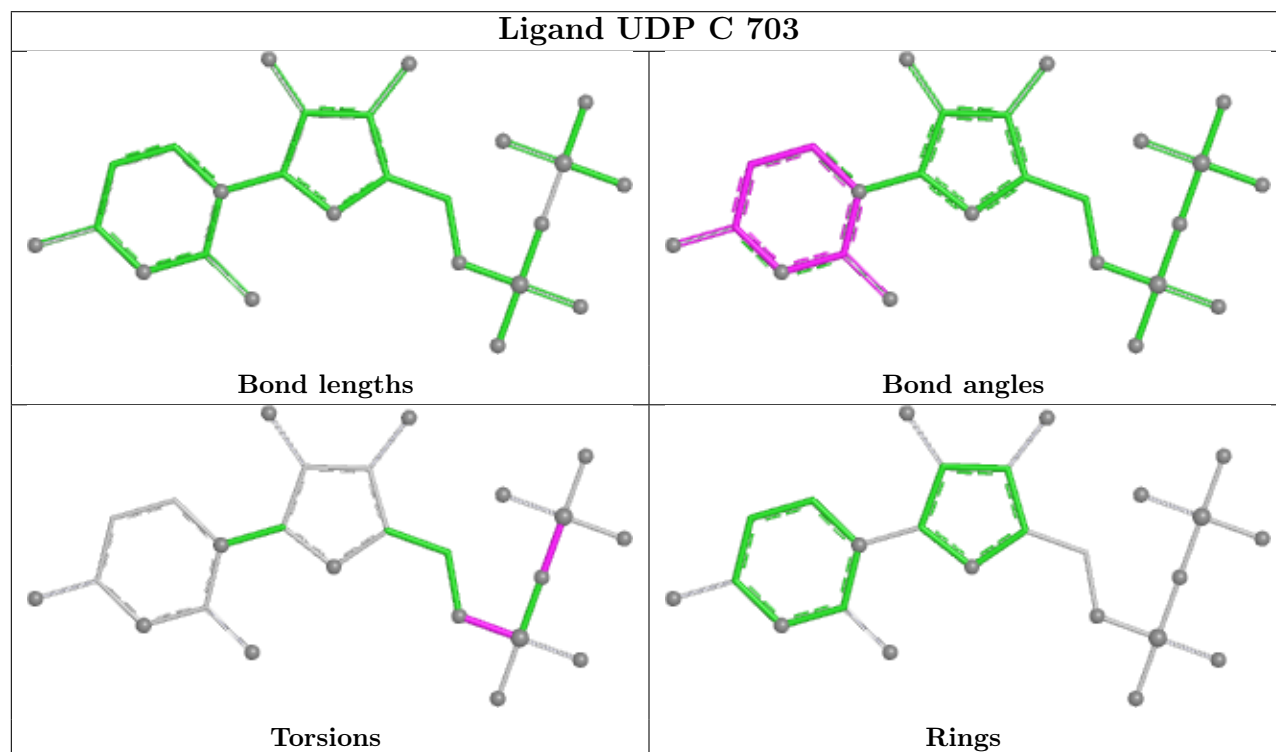
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	703	UDP	4	0
5	C	705	EDO	1	0
4	B	703	UDP	1	0
3	B	702	NAG	1	0
4	A	703	UDP	2	0
6	B	705	GOL	2	0

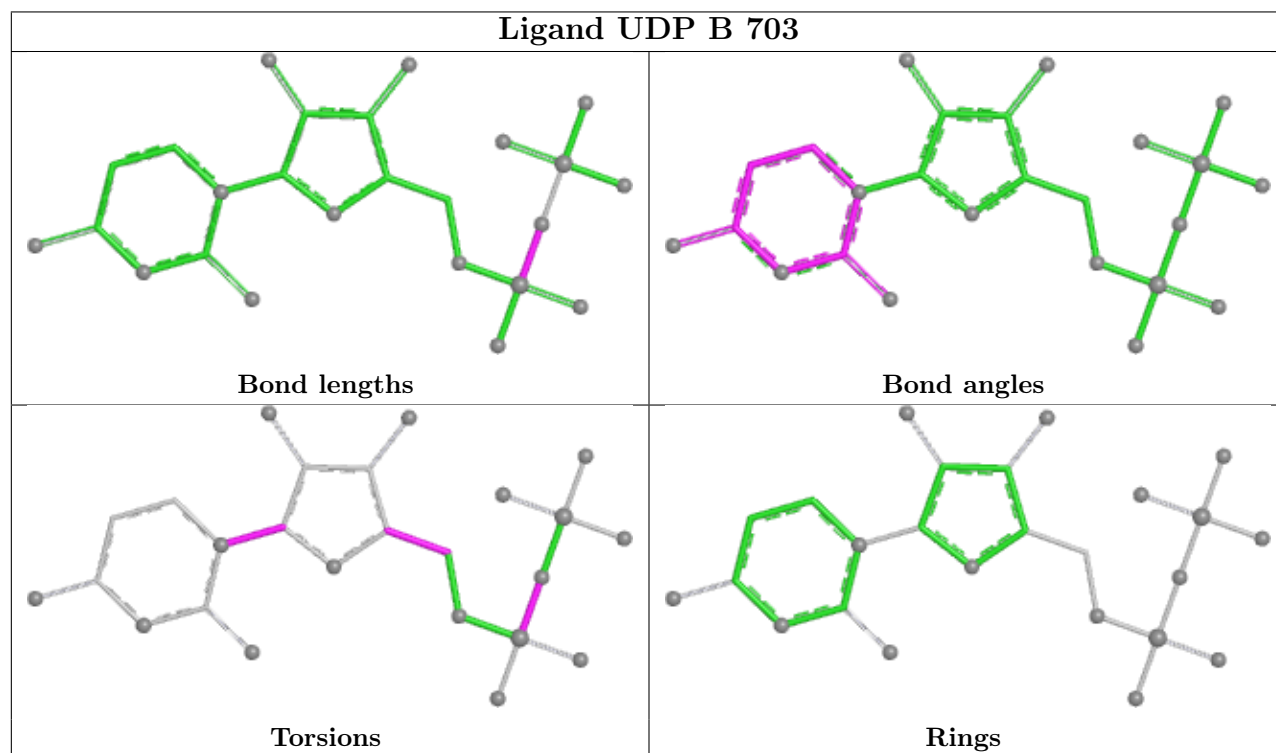
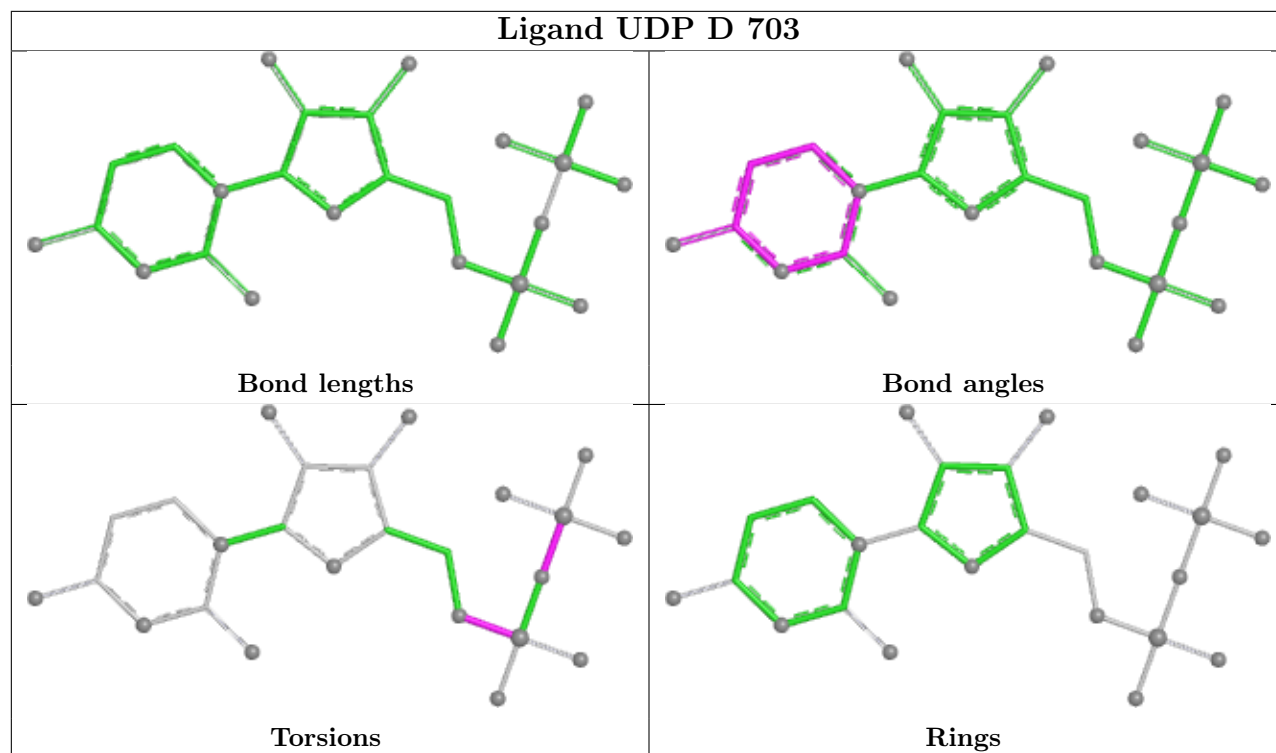
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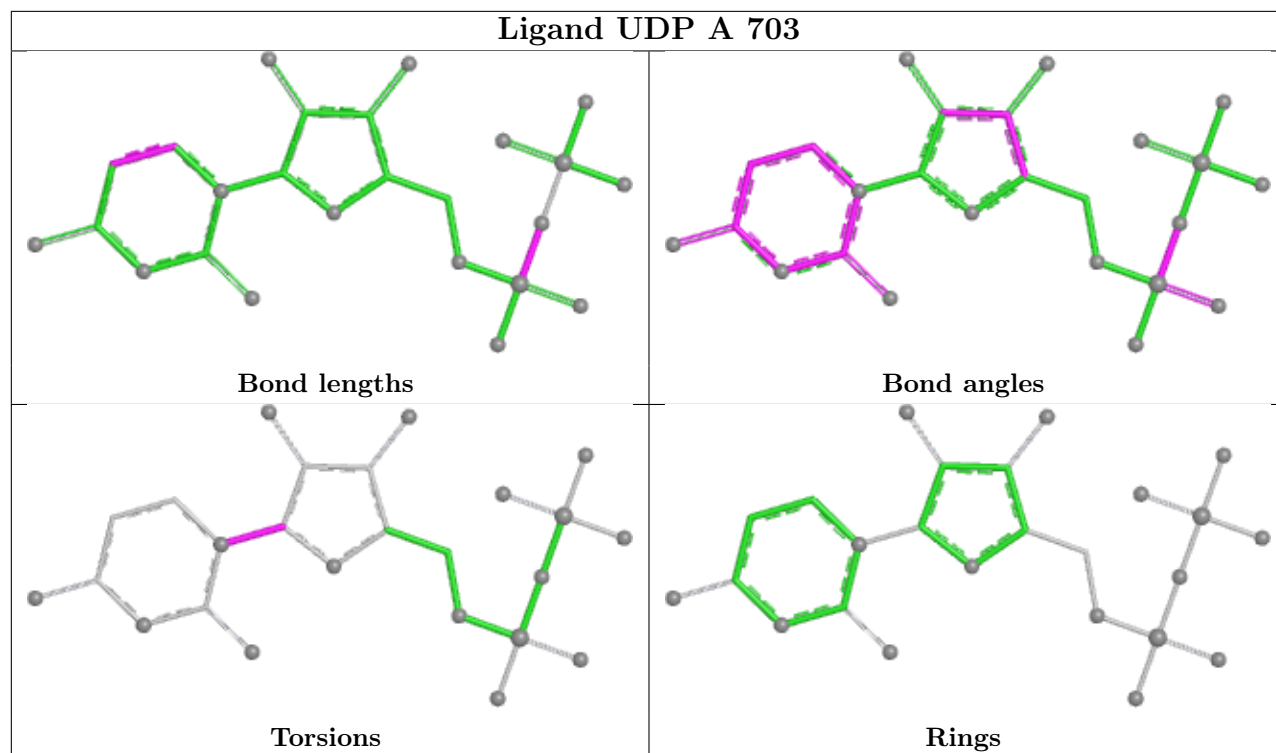
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	705	GOL	3	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	505/510 (99%)	-0.35	3 (0%) 85 80	31, 48, 77, 142	0
1	B	503/510 (98%)	-0.33	2 (0%) 88 84	25, 50, 81, 109	2 (0%)
1	C	503/510 (98%)	-0.30	5 (0%) 79 72	20, 50, 81, 143	2 (0%)
1	D	502/510 (98%)	-0.20	7 (1%) 73 64	35, 53, 85, 139	0
All	All	2013/2040 (98%)	-0.30	17 (0%) 82 75	20, 50, 82, 143	4 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	409	TRP	3.7
1	C	540	ALA	3.0
1	C	544	HIS	3.0
1	D	545	GLN	2.7
1	C	446	LYS	2.7
1	D	540	ALA	2.7
1	B	409	TRP	2.7
1	D	588	PHE	2.6
1	C	409	TRP	2.5
1	A	541	GLY	2.5
1	A	447	TRP	2.4
1	D	544	HIS	2.3
1	D	408	ILE	2.2
1	A	443	SER	2.2
1	C	452	ASN	2.1
1	B	541	GLY	2.1
1	D	445	TYR	2.1

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

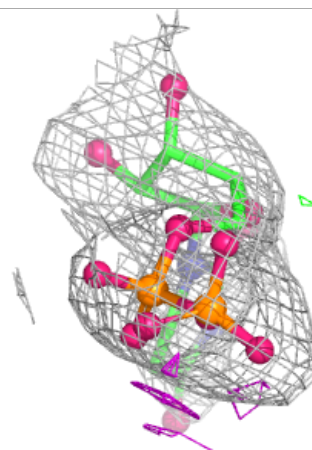
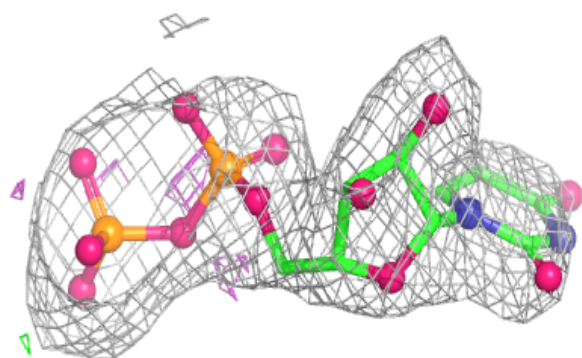
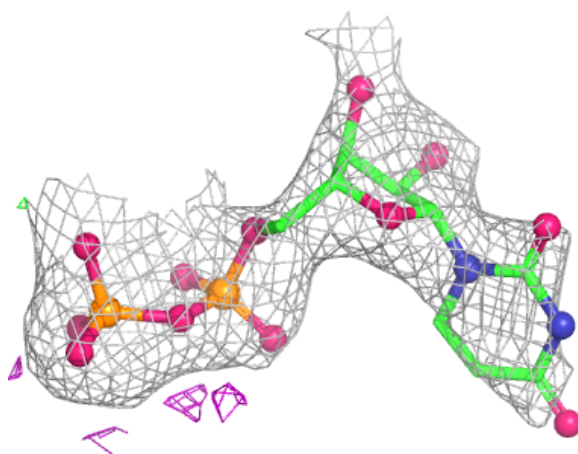
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	EDO	D	704	4/4	0.84	0.14	54,54,60,63	0
5	EDO	C	704	4/4	0.86	0.12	62,68,70,71	0
5	EDO	A	705	4/4	0.87	0.12	45,56,61,62	0
6	GOL	D	705	6/6	0.87	0.17	52,52,57,58	0
5	EDO	A	704	4/4	0.89	0.12	43,50,58,62	0
3	NAG	A	702	14/15	0.91	0.10	37,56,73,77	0
5	EDO	C	705	4/4	0.92	0.08	55,55,56,56	0
5	EDO	B	704	4/4	0.92	0.09	36,42,43,48	0
6	GOL	B	705	6/6	0.92	0.10	52,64,67,68	0
3	NAG	B	702	14/15	0.92	0.10	39,51,73,79	0
3	NAG	C	702	14/15	0.93	0.09	28,49,58,59	0
3	NAG	D	702	14/15	0.93	0.09	46,64,73,77	0
4	UDP	B	703	25/25	0.94	0.09	41,78,97,98	0
4	UDP	C	703	25/25	0.94	0.09	53,82,87,88	0
4	UDP	A	703	25/25	0.95	0.08	35,68,96,97	0
4	UDP	D	703	25/25	0.95	0.09	43,80,103,104	0
2	MN	A	701	1/1	0.99	0.06	46,46,46,46	0
2	MN	B	701	1/1	0.99	0.02	55,55,55,55	0
2	MN	C	701	1/1	0.99	0.02	54,54,54,54	0
2	MN	D	701	1/1	0.99	0.02	51,51,51,51	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.

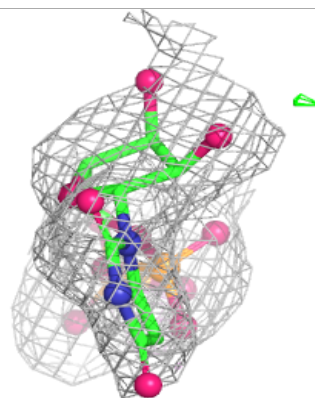
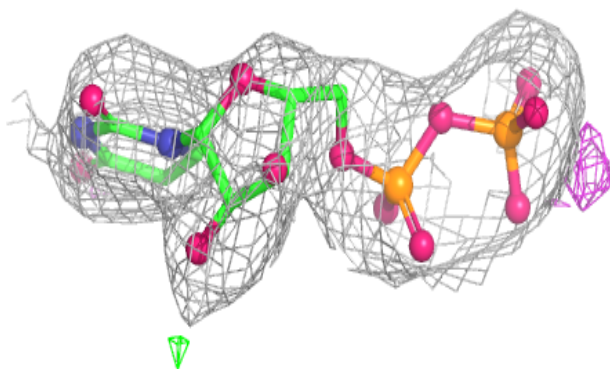
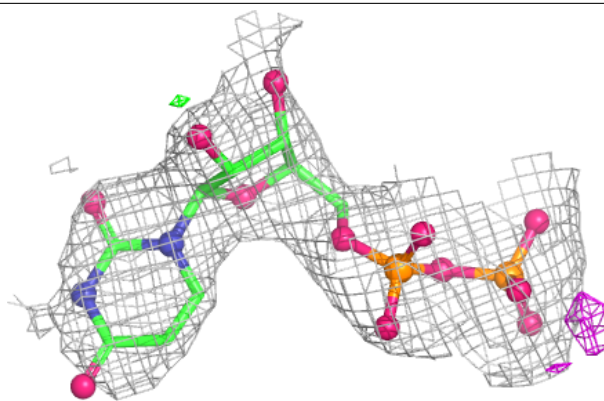
Electron density around UDP B 703:

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



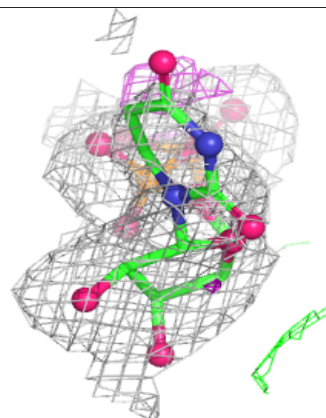
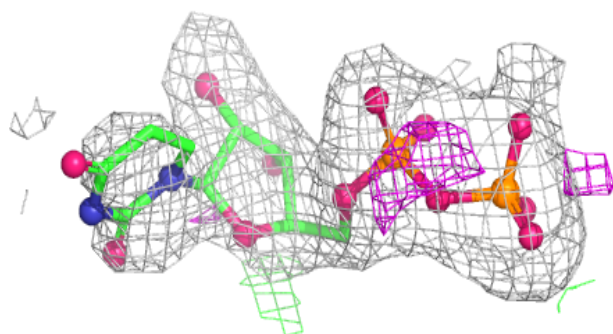
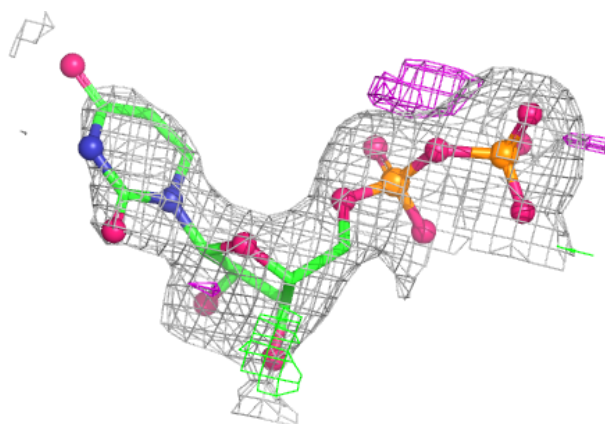
Electron density around UDP C 703:

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



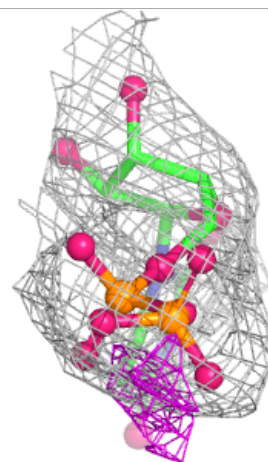
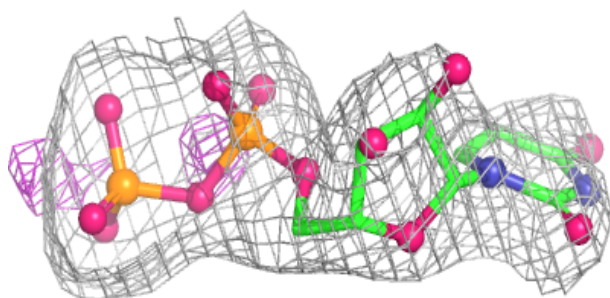
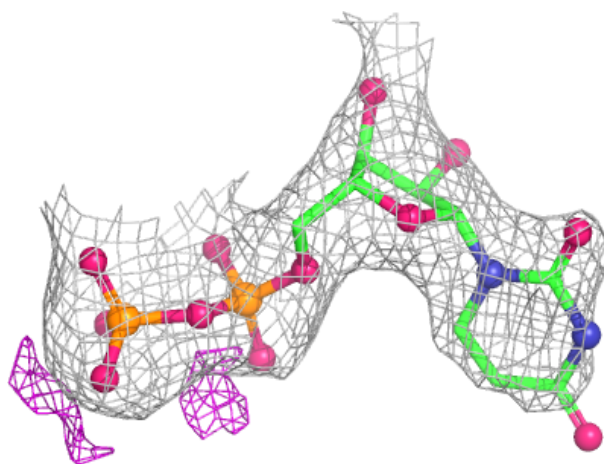
Electron density around UDP A 703:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.