



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2020 – 10:12 AM EST

PDB ID : 6VLC
Title : Crystal structure of UDP-GlcNAc 2-epimerase from *Neisseria meningitidis* bound to UDP-GlcNAc
Authors : Fisher, A.J.; Hurlburt, N.K.
Deposited on : 2020-01-23
Resolution : 2.15 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 : 2.14.6
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) : 2.14.6

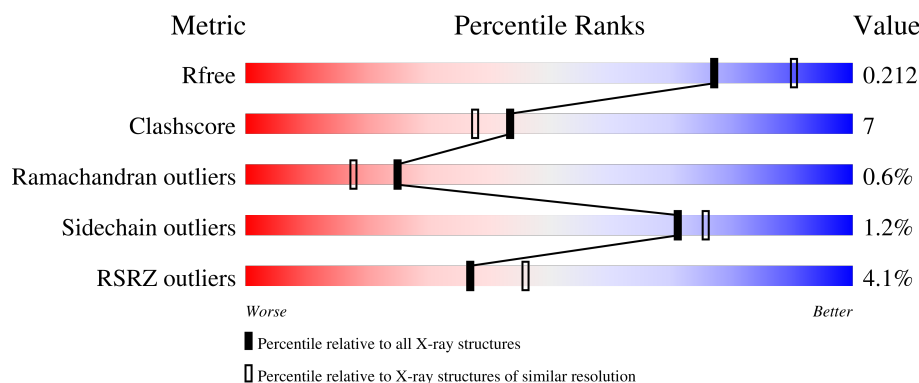
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 $\leq 5\%$. 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	380	<div> <div>4%</div> <div>81%</div> <div>13%</div> <div>...</div> </div>
1	B	380	<div> <div>3%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>
1	C	380	<div> <div>3%</div> <div>81%</div> <div>14%</div> <div>...</div> </div>
1	D	380	<div> <div>5%</div> <div>83%</div> <div>12%</div> <div>...</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12438 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 2-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2926	1874	485	557	10			
1	B	366	Total	C	N	O	S	0	0	0
			2877	1847	471	549	10			
1	C	371	Total	C	N	O	S	0	0	0
			2926	1874	485	557	10			
1	D	365	Total	C	N	O	S	0	0	0
			2873	1845	470	548	10			

There are 32 discrepancies between the modelled and reference sequences:

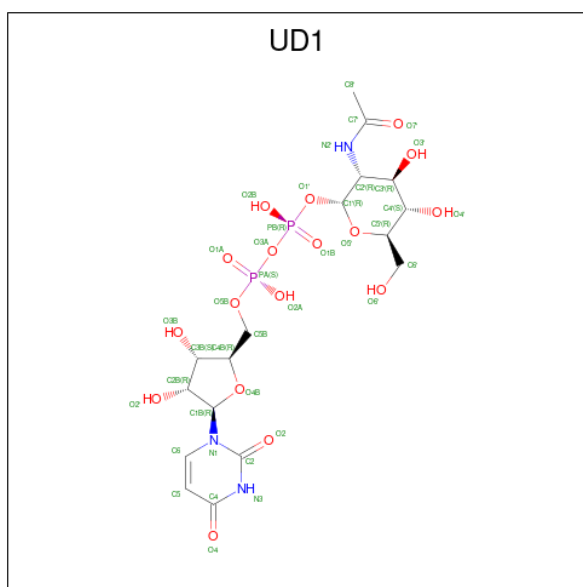
Chain	Residue	Modelled	Actual	Comment	Reference
A	373	LEU	-	expression tag	UNP A0A0U1RGY0
A	374	GLU	-	expression tag	UNP A0A0U1RGY0
A	375	HIS	-	expression tag	UNP A0A0U1RGY0
A	376	HIS	-	expression tag	UNP A0A0U1RGY0
A	377	HIS	-	expression tag	UNP A0A0U1RGY0
A	378	HIS	-	expression tag	UNP A0A0U1RGY0
A	379	HIS	-	expression tag	UNP A0A0U1RGY0
A	380	HIS	-	expression tag	UNP A0A0U1RGY0
B	373	LEU	-	expression tag	UNP A0A0U1RGY0
B	374	GLU	-	expression tag	UNP A0A0U1RGY0
B	375	HIS	-	expression tag	UNP A0A0U1RGY0
B	376	HIS	-	expression tag	UNP A0A0U1RGY0
B	377	HIS	-	expression tag	UNP A0A0U1RGY0
B	378	HIS	-	expression tag	UNP A0A0U1RGY0
B	379	HIS	-	expression tag	UNP A0A0U1RGY0
B	380	HIS	-	expression tag	UNP A0A0U1RGY0
C	373	LEU	-	expression tag	UNP A0A0U1RGY0
C	374	GLU	-	expression tag	UNP A0A0U1RGY0
C	375	HIS	-	expression tag	UNP A0A0U1RGY0
C	376	HIS	-	expression tag	UNP A0A0U1RGY0
C	377	HIS	-	expression tag	UNP A0A0U1RGY0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	378	HIS	-	expression tag	UNP A0A0U1RGY0
C	379	HIS	-	expression tag	UNP A0A0U1RGY0
C	380	HIS	-	expression tag	UNP A0A0U1RGY0
D	373	LEU	-	expression tag	UNP A0A0U1RGY0
D	374	GLU	-	expression tag	UNP A0A0U1RGY0
D	375	HIS	-	expression tag	UNP A0A0U1RGY0
D	376	HIS	-	expression tag	UNP A0A0U1RGY0
D	377	HIS	-	expression tag	UNP A0A0U1RGY0
D	378	HIS	-	expression tag	UNP A0A0U1RGY0
D	379	HIS	-	expression tag	UNP A0A0U1RGY0
D	380	HIS	-	expression tag	UNP A0A0U1RGY0

- Molecule 2 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: $C_{17}H_{27}N_3O_{17}P_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	C	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	179	Total	O	0	0
			179	179		

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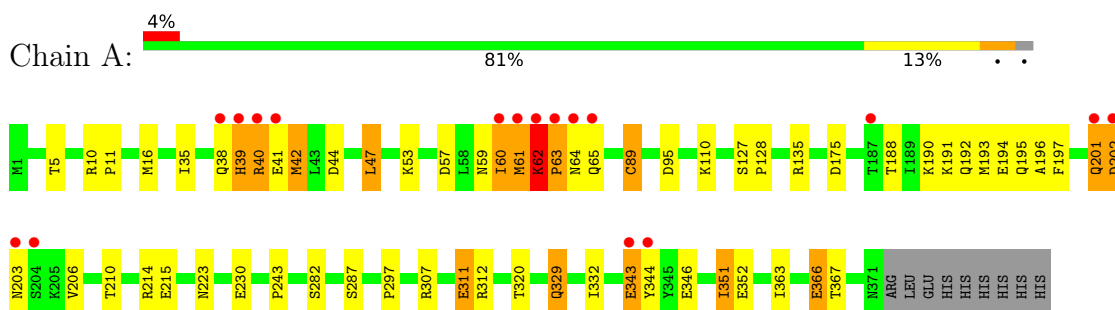
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	207	Total 207	O 207	0	0
3	C	169	Total 169	O 169	0	0
3	D	203	Total 203	O 203	0	0

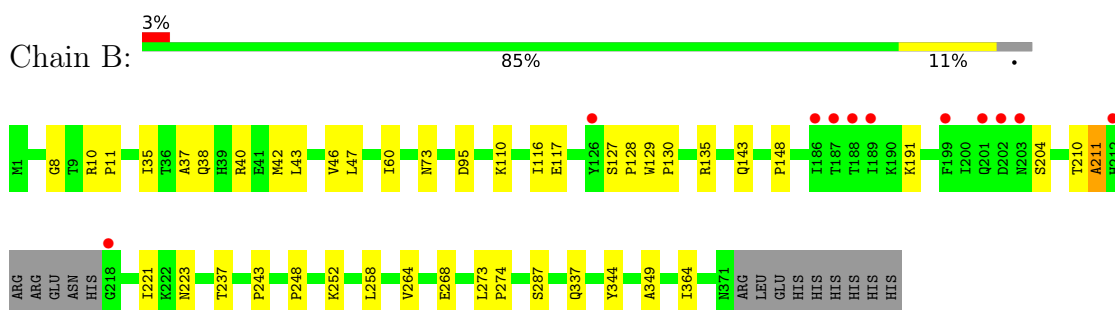
3 Residue-property plots [i](#)

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.

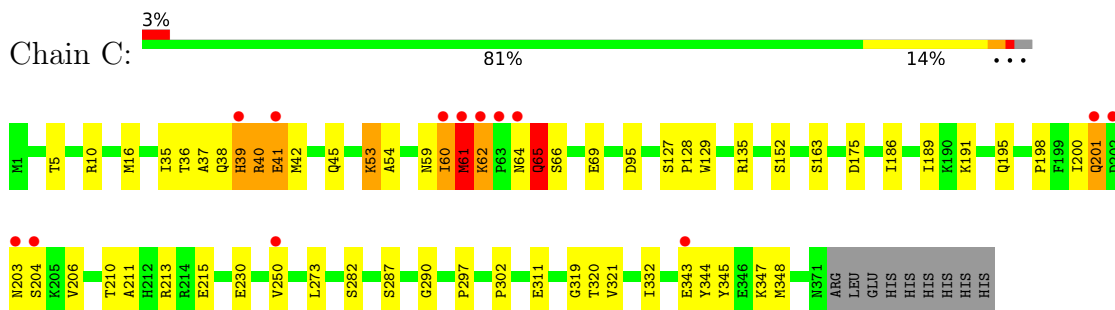
- Molecule 1: UDP-N-acetylglucosamine 2-epimerase



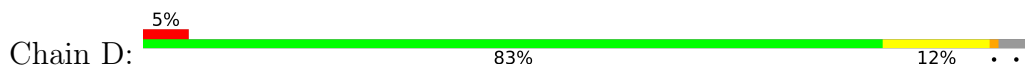
- Molecule 1: UDP-N-acetylglucosamine 2-epimerase

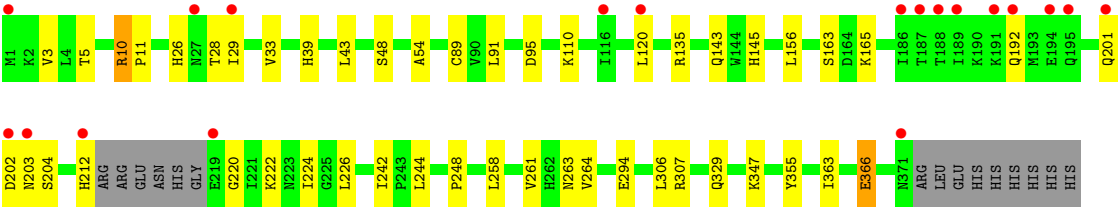


- Molecule 1: UDP-N-acetylglucosamine 2-epimerase



- Molecule 1: UDP-N-acetylglucosamine 2-epimerase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	124.88Å 129.74Å 213.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.97 – 2.15 39.64 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.9 (38.97-2.15) 98.9 (39.64-2.15)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.168 , 0.212 0.168 , 0.212	Depositor DCC
R_{free} test set	2006 reflections (2.16%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.036 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12438	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UD1

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	0.64	4/2984 (0.1%)	0.91	20/4056 (0.5%)
1	B	0.48	0/2933	0.66	2/3987 (0.1%)
1	C	0.62	3/2984 (0.1%)	0.80	7/4056 (0.2%)
1	D	0.55	2/2929 (0.1%)	0.77	9/3982 (0.2%)
All	All	0.57	9/11830 (0.1%)	0.79	38/16081 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	3
All	All	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	CYS	CB-SG	-10.35	1.64	1.82
1	A	343	GLU	CG-CD	-9.04	1.38	1.51
1	D	366	GLU	CB-CG	-8.29	1.36	1.52
1	C	53	LYS	CD-CE	7.30	1.69	1.51
1	C	53	LYS	CB-CG	-6.10	1.36	1.52
1	C	53	LYS	CE-NZ	6.10	1.64	1.49
1	D	366	GLU	CD-OE2	5.35	1.31	1.25
1	A	41	GLU	CB-CG	-5.31	1.42	1.52
1	A	343	GLU	CD-OE2	5.05	1.31	1.25

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	10	ARG	NE-CZ-NH1	-14.41	113.10	120.30
1	A	343	GLU	CA-CB-CG	-12.15	86.68	113.40
1	A	42	MET	CG-SD-CE	-11.58	81.67	100.20
1	A	41	GLU	CA-CB-CG	11.04	137.69	113.40
1	B	42	MET	CA-CB-CG	10.52	131.18	113.30
1	A	41	GLU	N-CA-CB	-10.46	91.77	110.60
1	C	347	LYS	CA-CB-CG	10.46	136.40	113.40
1	A	40	ARG	NE-CZ-NH2	-9.80	115.40	120.30
1	D	10	ARG	NE-CZ-NH2	8.73	124.67	120.30
1	C	65	GLN	CA-CB-CG	-8.71	94.24	113.40
1	C	347	LYS	CB-CG-CD	-8.53	89.42	111.60
1	A	343	GLU	CG-CD-OE1	-8.05	102.20	118.30
1	C	347	LYS	CB-CA-C	7.94	126.28	110.40
1	A	41	GLU	CB-CA-C	7.92	126.24	110.40
1	C	41	GLU	CA-CB-CG	7.86	130.68	113.40
1	D	10	ARG	CG-CD-NE	-7.60	95.83	111.80
1	C	347	LYS	CD-CE-NZ	7.55	129.07	111.70
1	B	42	MET	CG-SD-CE	7.42	112.07	100.20
1	A	343	GLU	CB-CG-CD	7.25	133.79	114.20
1	A	65	GLN	CA-CB-CG	7.04	128.89	113.40
1	A	41	GLU	CB-CG-CD	-6.84	95.72	114.20
1	A	47	LEU	CB-CG-CD1	-6.80	99.43	111.00
1	A	61	MET	CG-SD-CE	-6.77	89.37	100.20
1	D	10	ARG	CA-CB-CG	6.77	128.29	113.40
1	A	39	HIS	N-CA-CB	-6.69	98.55	110.60
1	C	201	GLN	CA-CB-CG	-6.50	99.11	113.40
1	A	329	GLN	CA-CB-CG	6.40	127.48	113.40
1	D	226	LEU	CB-CG-CD2	-6.28	100.32	111.00
1	A	329	GLN	CB-CA-C	-6.13	98.14	110.40
1	D	120	LEU	CB-CG-CD1	6.04	121.27	111.00
1	A	53	LYS	CG-CD-CE	5.94	129.72	111.90
1	D	202	ASP	C-N-CA	5.62	135.75	121.70
1	D	192	GLN	CB-CA-C	-5.58	99.25	110.40
1	A	62	LYS	CA-CB-CG	5.39	125.26	113.40
1	A	40	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	62	LYS	CG-CD-CE	-5.21	96.29	111.90
1	A	343	GLU	CB-CA-C	-5.18	100.03	110.40
1	D	10	ARG	N-CA-CB	-5.10	101.42	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	211	ALA	Peptide
1	C	40	ARG	Peptide
1	C	62	LYS	Peptide
1	C	65	GLN	Sidechain

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	2926	0	2993	59	0
1	B	2877	0	2947	26	0
1	C	2926	0	2993	43	0
1	D	2873	0	2944	30	0
2	A	39	0	24	3	0
2	C	39	0	25	4	0
3	A	179	0	0	7	3
3	B	207	0	0	5	3
3	C	169	0	0	4	1
3	D	203	0	0	8	1
All	All	12438	0	11926	157	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (157) 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:A:343:GLU:HG3	1:A:344:TYR:N	1.72	1.03
1:C:297:PRO:HG3	1:C:320:THR:HG21	1.39	1.01
1:A:38:GLN:HG2	1:A:61:MET:HE2	1.44	0.98
1:A:346:GLU:OE2	3:A:501:HOH:O	1.82	0.96
1:D:28:THR:HG22	3:D:420:HOH:O	1.69	0.90
1:A:223:ASN:OD1	3:A:502:HOH:O	1.91	0.88
1:A:191:LYS:NZ	1:A:194:GLU:OE1	2.08	0.86
2:C:400:UD1:N2'	3:C:501:HOH:O	2.11	0.83
1:A:35:ILE:HG12	1:A:40:ARG:NH1	1.95	0.81
1:D:143:GLN:O	3:D:401:HOH:O	1.97	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLU:HG3	1:A:344:TYR:H	1.45	0.81
1:A:60:ILE:O	1:A:64:ASN:ND2	2.14	0.81
1:C:200:ILE:C	1:C:201:GLN:HG2	2.01	0.81
1:A:188:THR:O	1:A:192:GLN:HG3	1.82	0.80
1:C:53:LYS:NZ	1:C:54:ALA:O	2.11	0.79
1:D:242:ILE:HG22	1:D:244:LEU:HD13	1.66	0.76
1:D:95:ASP:HB3	1:D:135:ARG:HB3	1.68	0.76
1:A:215:GLU:OE1	3:A:503:HOH:O	2.03	0.75
1:A:214:ARG:HH21	1:B:110:LYS:NZ	1.85	0.74
1:D:307:ARG:NH1	3:D:405:HOH:O	2.23	0.72
1:C:320:THR:HG23	1:C:321:VAL:HG13	1.71	0.71
1:D:203:ASN:OD1	1:D:204:SER:N	2.23	0.71
1:B:95:ASP:HB3	1:B:135:ARG:HB3	1.73	0.69
1:D:329:GLN:NE2	3:D:404:HOH:O	2.18	0.68
1:A:201:GLN:O	1:A:203:ASN:N	2.27	0.67
1:A:38:GLN:HG2	1:A:61:MET:CE	2.23	0.67
1:A:40:ARG:NH2	1:A:47:LEU:HD12	2.10	0.66
1:A:343:GLU:CG	1:A:344:TYR:N	2.53	0.66
1:C:343:GLU:HG2	1:C:344:TYR:N	2.10	0.65
1:A:40:ARG:HH22	1:A:47:LEU:HD12	1.60	0.65
1:B:268:GLU:OE2	3:B:401:HOH:O	2.14	0.65
1:A:40:ARG:NE	1:A:44:ASP:OD1	2.30	0.64
1:B:204:SER:OG	1:B:237:THR:O	2.12	0.64
1:A:297:PRO:HG3	1:A:320:THR:HG21	1.79	0.64
1:A:214:ARG:HH21	1:B:110:LYS:HZ3	1.46	0.63
1:D:242:ILE:HG22	1:D:244:LEU:CD1	2.28	0.62
1:D:212:HIS:NE2	3:D:408:HOH:O	2.31	0.62
1:C:198:PRO:O	1:C:201:GLN:NE2	2.33	0.62
1:A:35:ILE:HD11	1:A:57:ASP:OD1	2.00	0.61
1:B:148:PRO:HG2	3:B:445:HOH:O	2.00	0.60
1:C:35:ILE:HG22	1:C:37:ALA:H	1.66	0.60
2:C:400:UD1:H6'2	3:C:573:HOH:O	2.01	0.60
1:B:60:ILE:HD12	1:B:73:ASN:HB3	1.84	0.59
1:C:59:ASN:OD1	1:C:61:MET:HB2	2.02	0.59
1:A:62:LYS:HB3	1:A:63:PRO:HD2	1.84	0.59
1:A:243:PRO:O	3:A:504:HOH:O	2.16	0.59
1:A:5:THR:HG23	1:A:16:MET:CE	2.32	0.59
1:A:5:THR:HG23	1:A:16:MET:HE2	1.84	0.59
1:C:297:PRO:CG	1:C:320:THR:HG21	2.25	0.59
1:D:5:THR:HG22	1:D:91:LEU:HB2	1.84	0.58
1:A:307:ARG:NH1	3:A:509:HOH:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ARG:HH22	1:A:47:LEU:CD1	2.17	0.57
1:D:163:SER:OG	3:D:403:HOH:O	2.11	0.57
1:A:59:ASN:O	1:A:61:MET:N	2.38	0.57
1:B:10:ARG:HG3	1:B:46:VAL:HG21	1.86	0.56
1:A:38:GLN:HB3	1:A:39:HIS:HD2	1.69	0.56
1:C:60:ILE:HG22	1:C:60:ILE:O	2.06	0.56
1:C:38:GLN:HG2	1:C:60:ILE:C	2.26	0.56
1:A:40:ARG:NH2	1:A:44:ASP:OD1	2.39	0.55
1:C:230:GLU:HG2	1:C:332:ILE:HD13	1.88	0.55
1:C:61:MET:HG3	1:C:62:LYS:H	1.72	0.54
1:C:186:ILE:HB	1:C:189:ILE:HD12	1.90	0.53
1:A:190:LYS:HE3	1:A:194:GLU:OE2	2.08	0.53
1:B:349:ALA:O	3:B:403:HOH:O	2.19	0.53
1:A:62:LYS:HB3	1:A:63:PRO:CD	2.38	0.53
1:C:59:ASN:C	1:C:61:MET:H	2.13	0.52
1:C:206:VAL:HB	1:C:282:SER:HA	1.91	0.52
1:C:211:ALA:O	1:C:250:VAL:HG11	2.10	0.52
1:A:38:GLN:HE21	1:A:64:ASN:ND2	2.08	0.51
1:C:290:GLY:HA3	2:C:400:UD1:H8'3	1.92	0.51
1:A:343:GLU:CG	1:A:344:TYR:H	2.19	0.51
1:D:248:PRO:N	3:D:411:HOH:O	2.43	0.51
1:A:195:GLN:O	1:A:196:ALA:HB3	2.12	0.50
1:C:60:ILE:O	1:C:61:MET:O	2.29	0.50
1:C:203:ASN:OD1	1:C:204:SER:N	2.45	0.50
1:C:5:THR:HG23	1:C:16:MET:CE	2.41	0.49
1:C:191:LYS:O	1:C:195:GLN:HG3	2.13	0.49
1:B:43:LEU:O	1:B:47:LEU:HG	2.13	0.49
1:D:294:GLU:HG2	1:D:355:TYR:CG	2.48	0.49
1:C:66:SER:OG	1:C:69:GLU:HG3	2.12	0.49
1:C:201:GLN:HB2	1:C:203:ASN:OD1	2.13	0.48
1:C:10:ARG:HD3	1:C:42:MET:HB3	1.95	0.47
1:C:36:THR:O	1:C:60:ILE:HG12	2.14	0.47
1:D:26:HIS:HB2	1:D:29:ILE:HD12	1.96	0.47
1:B:211:ALA:HB3	1:B:221:ILE:HG12	1.95	0.47
1:B:110:LYS:HA	3:B:481:HOH:O	2.15	0.47
1:D:363:ILE:HA	1:D:366:GLU:OE2	2.13	0.47
1:B:223:ASN:HA	3:B:404:HOH:O	2.14	0.47
1:C:10:ARG:HD2	3:C:634:HOH:O	2.15	0.47
1:A:95:ASP:HB3	1:A:135:ARG:HB3	1.96	0.46
1:D:258:LEU:HD13	1:D:264:VAL:HG11	1.96	0.46
1:A:312:ARG:HH12	2:A:400:UD1:H8'3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:THR:HG22	1:B:243:PRO:HG2	1.97	0.46
1:A:363:ILE:HA	1:A:366:GLU:HG2	1.97	0.46
1:C:42:MET:HA	1:C:45:GLN:NE2	2.31	0.46
1:A:38:GLN:HB3	1:A:61:MET:HE1	1.97	0.46
1:C:302:PRO:HG2	1:C:345:TYR:CE1	2.51	0.46
1:B:35:ILE:HD11	1:B:40:ARG:NH1	2.30	0.46
1:A:40:ARG:HG3	1:A:44:ASP:OD2	2.16	0.45
1:A:11:PRO:HB2	2:A:400:UD1:H6'2	1.97	0.45
1:B:116:ILE:HG12	1:B:364:ILE:HD13	1.97	0.45
1:C:129:TRP:CH2	1:D:110:LYS:HE3	2.51	0.45
1:C:5:THR:HG23	1:C:16:MET:HE2	1.99	0.45
1:B:8:GLY:O	1:B:37:ALA:HB2	2.17	0.45
1:D:163:SER:CB	3:D:403:HOH:O	2.65	0.45
1:A:230:GLU:HG2	1:A:332:ILE:HD13	1.99	0.44
1:D:10:ARG:HB3	1:D:11:PRO:HD3	1.99	0.44
1:A:366:GLU:HG3	1:A:367:THR:N	2.32	0.44
1:A:10:ARG:HD2	3:A:555:HOH:O	2.18	0.44
1:C:39:HIS:CE1	1:C:41:GLU:OE1	2.70	0.44
1:A:40:ARG:CZ	1:A:44:ASP:OD1	2.66	0.44
1:C:213:ARG:HB3	1:C:215:GLU:OE1	2.17	0.44
1:B:10:ARG:HB3	1:B:11:PRO:HD3	1.99	0.44
1:D:261:VAL:HG22	1:D:263:ASN:OD1	2.17	0.44
1:C:127:SER:HA	1:C:128:PRO:HA	1.88	0.43
1:A:60:ILE:HB	1:A:64:ASN:HD21	1.83	0.43
1:A:127:SER:HA	1:A:128:PRO:HA	1.90	0.43
1:A:35:ILE:CG1	1:A:40:ARG:NH1	2.76	0.43
1:C:38:GLN:HG2	1:C:60:ILE:O	2.19	0.43
1:C:38:GLN:HG3	1:C:38:GLN:H	1.67	0.43
1:D:347:LYS:HB3	1:D:347:LYS:HE2	1.84	0.42
1:D:201:GLN:C	1:D:203:ASN:H	2.22	0.42
1:A:195:GLN:O	1:A:197:PHE:N	2.50	0.42
1:A:311:GLU:CD	1:A:311:GLU:H	2.23	0.42
1:A:352:GLU:N	1:A:352:GLU:OE1	2.53	0.42
1:D:145:HIS:HB3	1:D:156:LEU:HD13	2.02	0.42
1:D:33:VAL:CG2	1:D:54:ALA:HA	2.50	0.42
1:A:191:LYS:HD3	1:A:191:LYS:HA	1.73	0.42
1:C:40:ARG:HB2	1:C:41:GLU:CA	2.50	0.42
1:C:273:LEU:HB2	3:C:586:HOH:O	2.20	0.42
1:A:42:MET:CE	1:D:39:HIS:CE1	3.03	0.42
1:B:248:PRO:O	1:B:252:LYS:HB3	2.20	0.42
1:D:43:LEU:HA	1:D:43:LEU:HD23	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:GLN:HG2	1:B:344:TYR:CD2	2.54	0.42
1:C:319:GLY:O	1:C:348:MET:HG2	2.20	0.42
1:B:258:LEU:HD13	1:B:264:VAL:HG11	2.02	0.42
1:C:64:ASN:C	1:C:65:GLN:HG3	2.35	0.42
1:B:210:THR:O	1:B:287:SER:HA	2.20	0.41
1:C:95:ASP:HB3	1:C:135:ARG:HB3	2.00	0.41
1:C:95:ASP:OD1	2:C:400:UD1:H4'	2.20	0.41
1:B:129:TRP:HA	1:B:130:PRO:HA	1.86	0.41
1:A:210:THR:O	1:A:287:SER:HA	2.20	0.41
1:C:210:THR:O	1:C:287:SER:HA	2.20	0.41
1:A:193:MET:O	1:A:195:GLN:O	2.38	0.41
1:A:351:ILE:H	1:A:351:ILE:HG13	1.71	0.41
2:A:400:UD1:H5'2	2:A:400:UD1:O1B	2.21	0.41
1:A:110:LYS:HA	3:A:621:HOH:O	2.21	0.41
1:A:35:ILE:HG12	1:A:40:ARG:HH12	1.77	0.41
1:B:273:LEU:HB3	1:B:274:PRO:HD3	2.02	0.41
1:D:222:LYS:HE2	1:D:222:LYS:HB3	1.85	0.41
1:B:127:SER:HA	1:B:128:PRO:HA	1.89	0.41
1:D:165:LYS:HD3	1:D:165:LYS:HA	1.91	0.41
1:A:62:LYS:HG2	1:A:62:LYS:HZ3	1.63	0.41
1:D:3:VAL:HG22	1:D:89:CYS:SG	2.61	0.41
1:B:117:GLU:HA	1:B:148:PRO:HD3	2.03	0.40
1:A:206:VAL:HB	1:A:282:SER:HA	2.03	0.40
1:D:224:ILE:HD13	1:D:306:LEU:HD13	2.02	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:632:HOH:O	3:B:574:HOH:O[4_565]	1.97	0.23
3:A:593:HOH:O	3:B:476:HOH:O[4_565]	2.04	0.16
3:C:659:HOH:O	3:D:586:HOH:O[3_554]	2.11	0.09
3:A:502:HOH:O	3:B:447:HOH:O[5_455]	2.19	0.01

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	369/380 (97%)	350 (95%)	14 (4%)	5 (1%)	11	5
1	B	362/380 (95%)	354 (98%)	8 (2%)	0	100	100
1	C	369/380 (97%)	351 (95%)	15 (4%)	3 (1%)	19	12
1	D	361/380 (95%)	355 (98%)	5 (1%)	1 (0%)	41	37
All	All	1461/1520 (96%)	1410 (96%)	42 (3%)	9 (1%)	25	18

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	ASP
1	A	351	ILE
1	C	39	HIS
1	C	60	ILE
1	C	61	MET
1	A	62	LYS
1	D	220	GLY
1	A	60	ILE
1	A	63	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	335/344 (97%)	328 (98%)	7 (2%)	53	57
1	B	330/344 (96%)	327 (99%)	3 (1%)	78	83
1	C	335/344 (97%)	330 (98%)	5 (2%)	65	69
1	D	330/344 (96%)	329 (100%)	1 (0%)	92	95
All	All	1330/1376 (97%)	1314 (99%)	16 (1%)	71	76

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	CYS
1	A	175	ASP
1	A	201	GLN
1	A	202	ASP
1	A	311	GLU
1	A	329	GLN
1	A	366	GLU
1	B	38	GLN
1	B	143	GLN
1	B	191	LYS
1	C	61	MET
1	C	152	SER
1	C	163	SER
1	C	175	ASP
1	C	311	GLU
1	D	48	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	39	HIS
1	B	38	GLN
1	B	329	GLN
1	C	143	GLN
1	D	39	HIS
1	D	143	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

2 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
2	UD1	C	400	-	34,41,41	0.81	1 (2%)	45,62,62	2.25	9 (20%)
2	UD1	A	400	-	34,41,41	0.84	1 (2%)	45,62,62	2.44	10 (22%)

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
2	UD1	C	400	-	-	8/24/63/63	0/3/3/3
2	UD1	A	400	-	-	8/24/63/63	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	UD1	C4-N3	3.19	1.38	1.33
2	C	400	UD1	C4-N3	2.96	1.38	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	UD1	C1'-C2'-N2'	7.89	124.60	111.00
2	A	400	UD1	O5'-C1'-O1'	-6.94	102.29	111.36
2	C	400	UD1	O5'-C1'-O1'	-6.94	102.30	111.36
2	C	400	UD1	C1'-C2'-N2'	6.25	121.77	111.00
2	A	400	UD1	PB-O1'-C1'	5.25	140.03	119.74
2	C	400	UD1	C2'-N2'-C7'	5.11	135.62	123.18
2	C	400	UD1	PB-O1'-C1'	4.86	138.52	119.74
2	A	400	UD1	O3A-PB-O1'	4.62	111.81	102.48
2	A	400	UD1	O5'-C1'-C2'	-4.60	101.60	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	UD1	C3'-C2'-N2'	4.52	119.15	110.62
2	A	400	UD1	C2'-N2'-C7'	4.52	134.16	123.18
2	A	400	UD1	C3'-C2'-N2'	4.03	118.23	110.62
2	C	400	UD1	C5-C4-N3	-4.00	114.52	123.31
2	A	400	UD1	C5-C4-N3	-3.87	114.80	123.31
2	A	400	UD1	C4'-C3'-C2'	-3.87	104.68	110.34
2	C	400	UD1	O5'-C1'-C2'	-3.82	103.12	110.58
2	C	400	UD1	O3A-PB-O1'	3.78	110.11	102.48
2	C	400	UD1	O1'-C1'-C2'	2.67	113.24	108.40
2	A	400	UD1	O1'-C1'-C2'	2.21	112.39	108.40

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	400	UD1	O5'-C1'-O1'-PB
2	C	400	UD1	C3'-C2'-N2'-C7'
2	C	400	UD1	C8'-C7'-N2'-C2'
2	C	400	UD1	O7'-C7'-N2'-C2'
2	C	400	UD1	C2B-C1B-N1-C6
2	C	400	UD1	O4B-C1B-N1-C6
2	A	400	UD1	O5'-C1'-O1'-PB
2	A	400	UD1	C3'-C2'-N2'-C7'
2	A	400	UD1	C8'-C7'-N2'-C2'
2	A	400	UD1	O7'-C7'-N2'-C2'
2	A	400	UD1	C2B-C1B-N1-C6
2	A	400	UD1	O4B-C1B-N1-C6
2	C	400	UD1	O5'-C5'-C6'-O6'
2	C	400	UD1	C4'-C5'-C6'-O6'
2	A	400	UD1	O5'-C5'-C6'-O6'
2	A	400	UD1	C4'-C5'-C6'-O6'

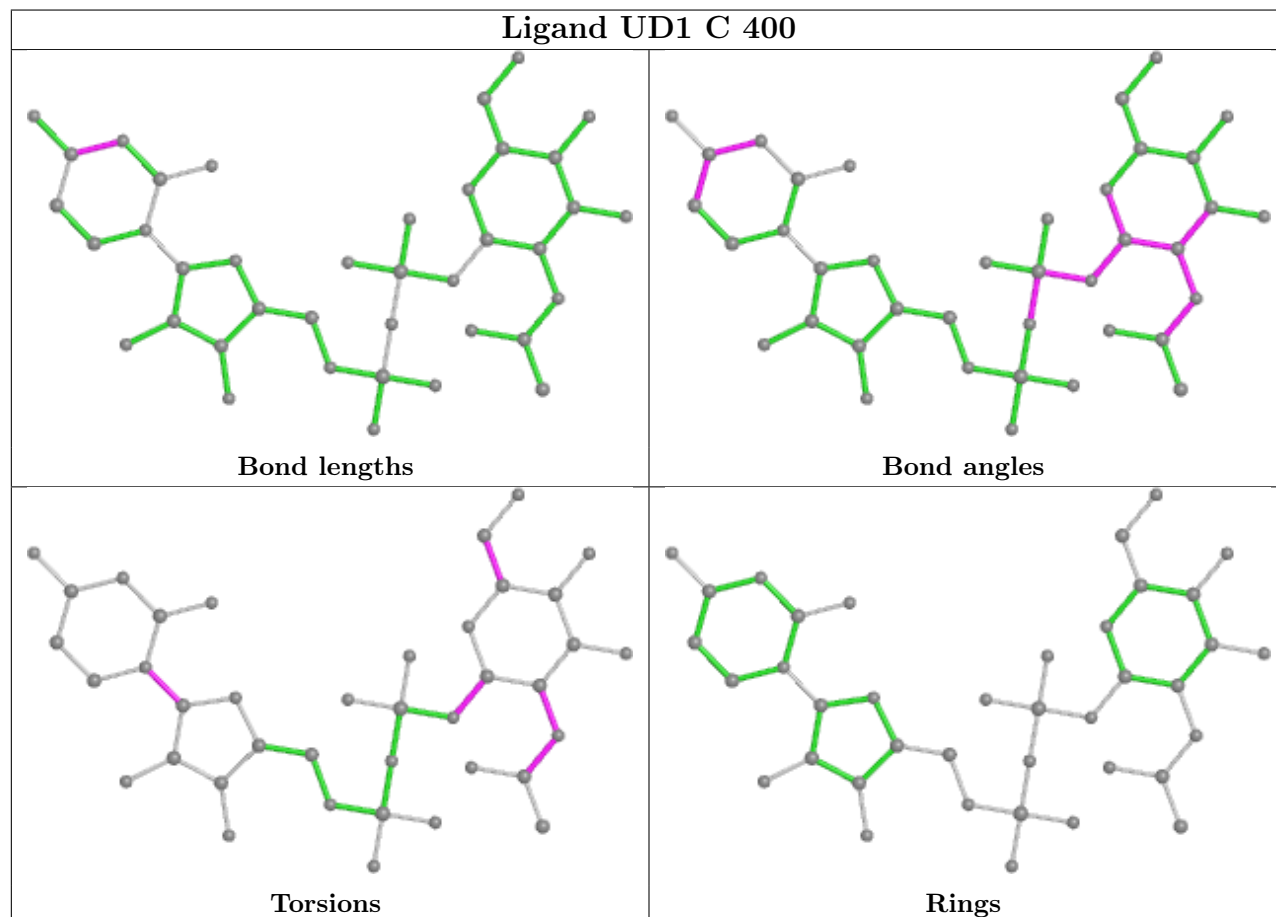
There are no ring outliers.

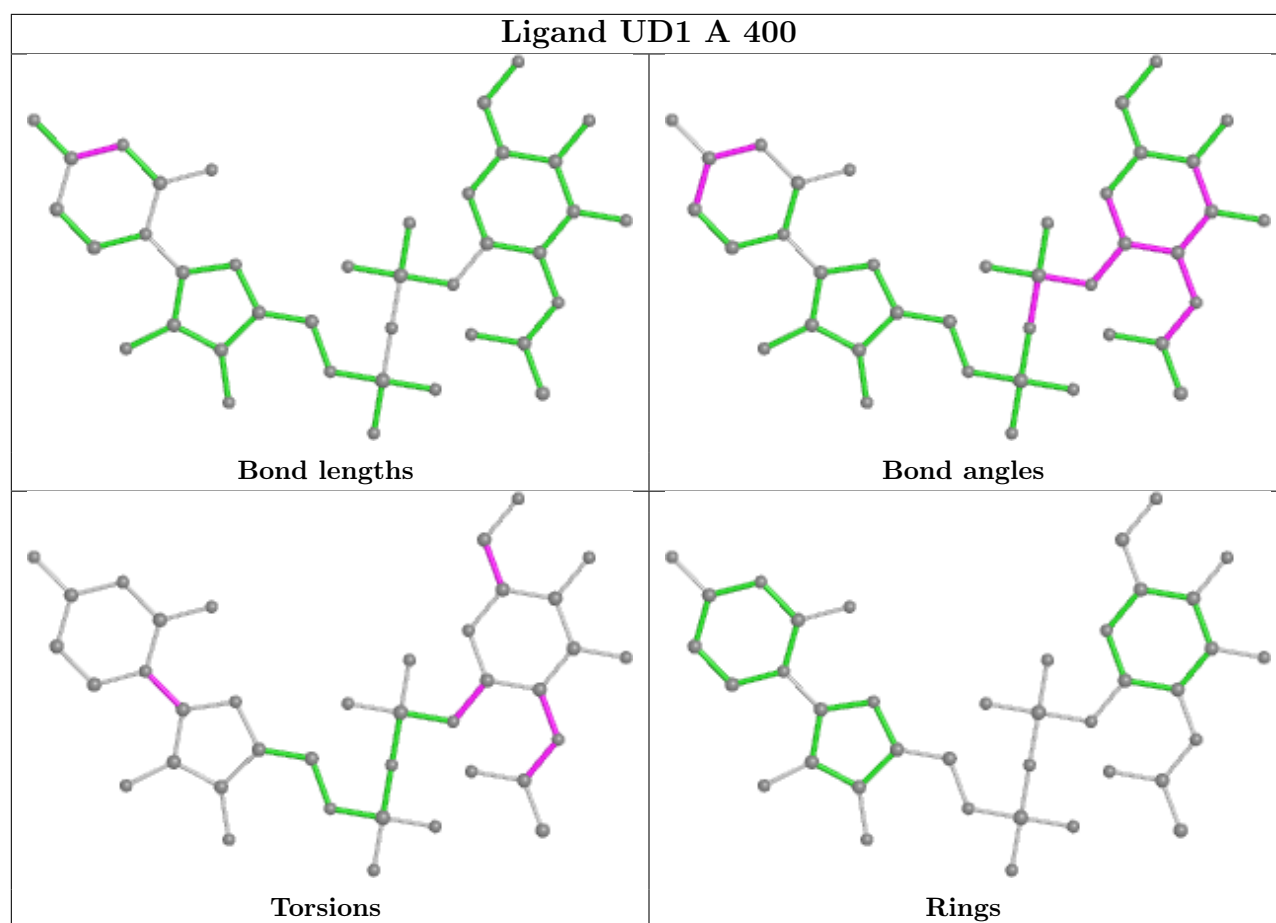
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	400	UD1	4	0
2	A	400	UD1	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

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	371/380 (97%)	-0.07	17 (4%)	32 42	21, 37, 76, 122	0
1	B	366/380 (96%)	-0.21	11 (3%)	50 59	24, 37, 70, 105	0
1	C	371/380 (97%)	-0.17	13 (3%)	44 52	20, 36, 80, 132	0
1	D	365/380 (96%)	0.04	19 (5%)	27 35	23, 41, 74, 105	0
All	All	1473/1520 (96%)	-0.10	60 (4%)	37 46	20, 38, 76, 132	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	63	PRO	12.8
1	C	63	PRO	11.2
1	A	61	MET	9.5
1	C	64	ASN	8.2
1	A	39	HIS	8.0
1	A	202	ASP	7.7
1	A	64	ASN	7.4
1	A	62	LYS	7.2
1	C	61	MET	6.1
1	A	203	ASN	5.8
1	A	40	ARG	5.6
1	A	60	ILE	5.6
1	D	219	GLU	5.4
1	D	187	THR	5.3
1	D	186	ILE	5.2
1	C	62	LYS	5.1
1	B	202	ASP	4.8
1	D	371	ASN	4.6
1	B	212	HIS	4.6
1	C	343	GLU	4.5
1	D	189	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	39	HIS	4.3
1	D	192	GLN	4.2
1	C	60	ILE	4.1
1	B	187	THR	4.1
1	D	188	THR	4.1
1	C	201	GLN	4.1
1	C	203	ASN	3.9
1	B	189	ILE	3.9
1	C	202	ASP	3.8
1	D	212	HIS	3.8
1	B	126	TYR	3.7
1	D	27	ASN	3.3
1	A	38	GLN	3.3
1	A	201	GLN	3.2
1	B	188	THR	3.1
1	A	204	SER	3.1
1	D	191	LYS	3.0
1	D	201	GLN	2.9
1	D	29	ILE	2.8
1	B	203	ASN	2.8
1	B	186	ILE	2.6
1	C	204	SER	2.6
1	A	65	GLN	2.5
1	D	202	ASP	2.5
1	A	187	THR	2.5
1	B	201	GLN	2.5
1	C	41	GLU	2.4
1	B	218	GLY	2.4
1	D	120	LEU	2.2
1	D	1	MET	2.1
1	A	343	GLU	2.1
1	A	41	GLU	2.1
1	D	195	GLN	2.1
1	C	250	VAL	2.1
1	A	344	TYR	2.1
1	D	203	ASN	2.0
1	B	199	PHE	2.0
1	D	116	ILE	2.0
1	D	194	GLU	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](#)

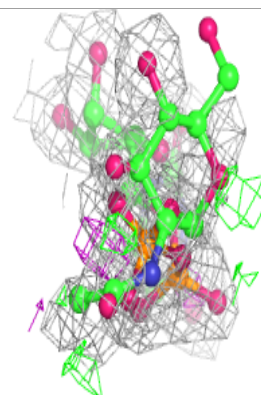
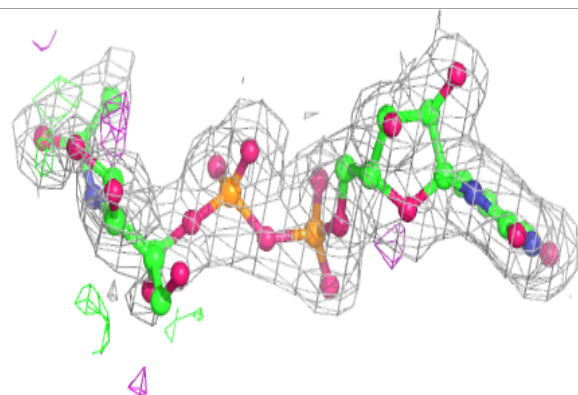
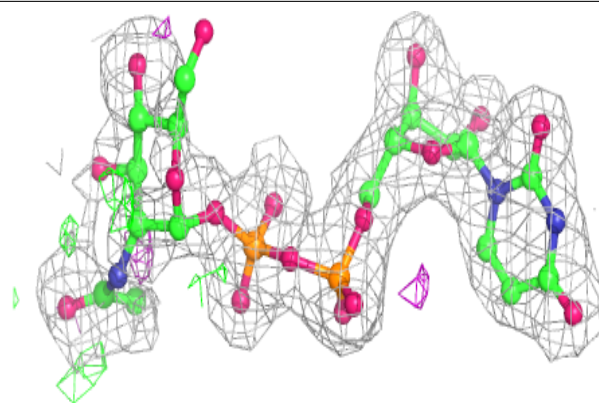
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	UD1	C	400	39/39	0.98	0.11	11,30,54,56	9
2	UD1	A	400	39/39	0.98	0.11	18,29,48,49	10

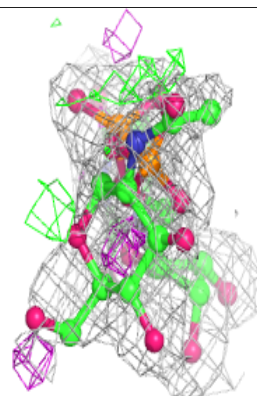
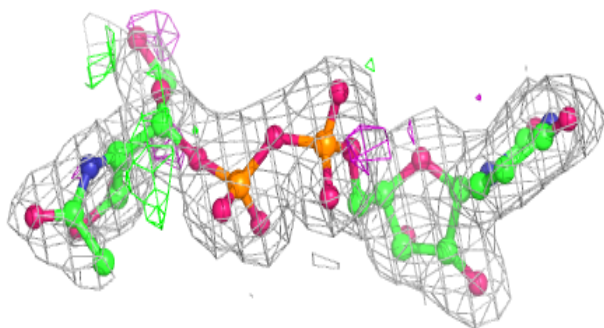
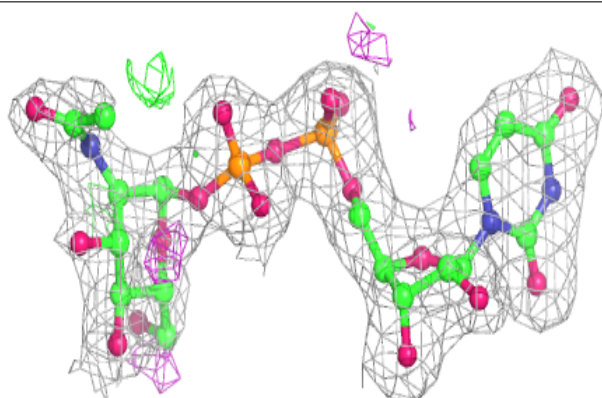
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UD1 C 400:

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

**Electron density around UD1 A 400:**

$2mF_o-DF_c$ (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.