



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 02:12 AM UTC

PDB ID : 5ZLT / pdb_00005zlt
Title : Crystal structure of UDP-GlcNAc 2-epimerase NeuC complexed with UDP
Authors : Ko, T.P.; Hsieh, T.J.; Yang, C.S.; Chen, Y.
Deposited on : 2018-03-29
Resolution : 2.50 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

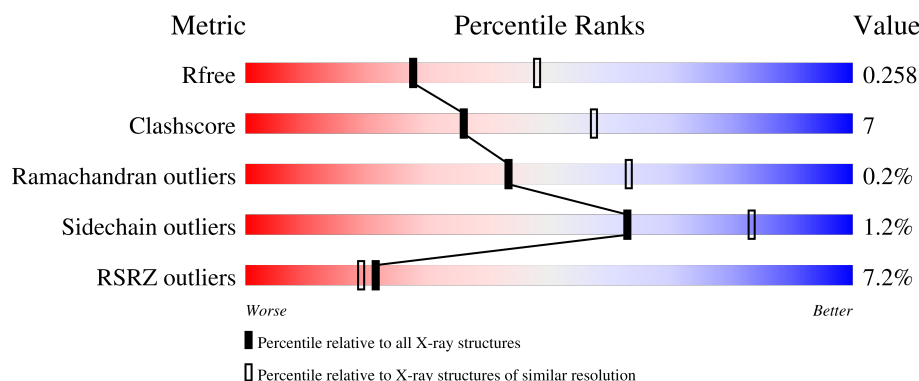
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	380	9% 79% 18% ..
1	B	380	2% 85% 11% ..
1	C	380	15% 79% 18% ..
1	D	380	2% 83% 13% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12117 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 GDP/UDP-N,N'-diacetylbaicillosamine 2-epimerase (Hydrolyzing).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2905	1860	484	550	11			
1	B	366	Total	C	N	O	S	0	0	0
			2878	1842	479	546	11			
1	C	370	Total	C	N	O	S	0	0	0
			2905	1860	484	550	11			
1	D	366	Total	C	N	O	S	0	0	0
			2879	1842	480	546	11			

There are 8 discrepancies between the modelled and reference sequences:

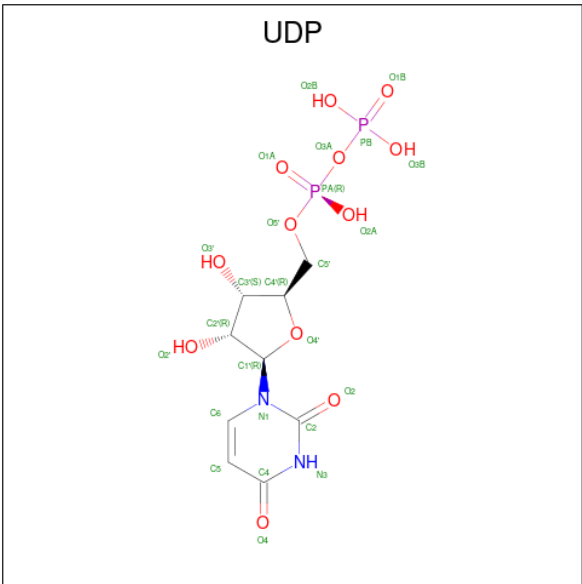
Chain	Residue	Modelled	Actual	Comment	Reference
A	379	LEU	-	expression tag	UNP A0A154EJU5
A	380	GLU	-	expression tag	UNP A0A154EJU5
B	379	LEU	-	expression tag	UNP A0A154EJU5
B	380	GLU	-	expression tag	UNP A0A154EJU5
C	379	LEU	-	expression tag	UNP A0A154EJU5
C	380	GLU	-	expression tag	UNP A0A154EJU5
D	379	LEU	-	expression tag	UNP A0A154EJU5
D	380	GLU	-	expression tag	UNP A0A154EJU5

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: C₉H₁₄N₂O₁₂P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			21	8	1	10	2		

Continued on next page...

Continued from previous page...

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

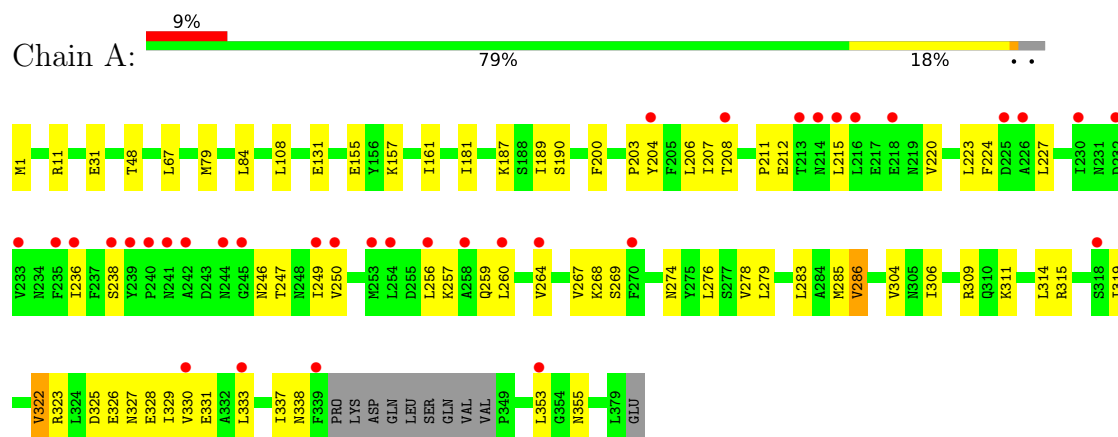
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	127	Total	O	0	0
			127	127		
4	B	103	Total	O	0	0
			103	103		
4	C	131	Total	O	0	0
			131	131		
4	D	133	Total	O	0	0
			133	133		

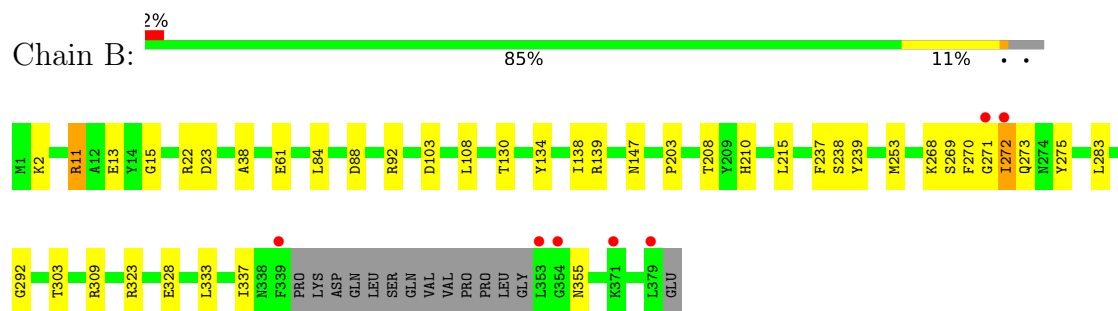
3 Residue-property plots [i](#)

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.

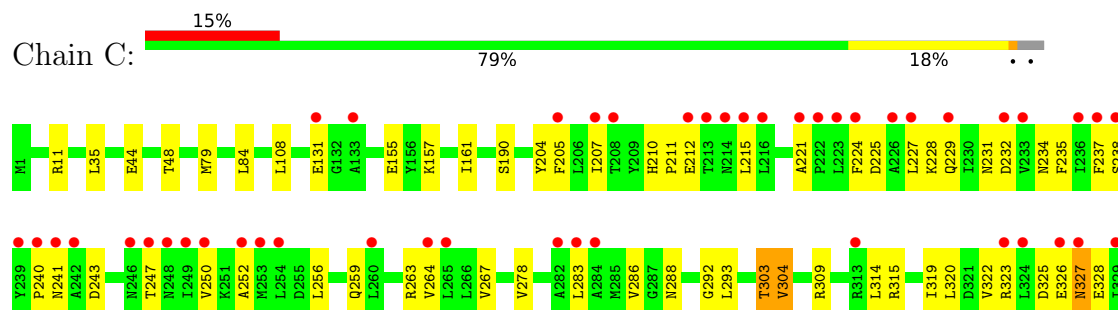
- Molecule 1: GDP/UDP-N,N'-diacetylbaucillosamine 2-epimerase (Hydrolyzing)

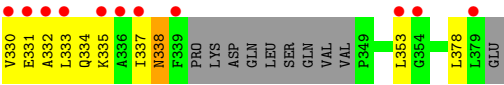


- Molecule 1: GDP/UDP-N,N'-diacetylbaucillosamine 2-epimerase (Hydrolyzing)

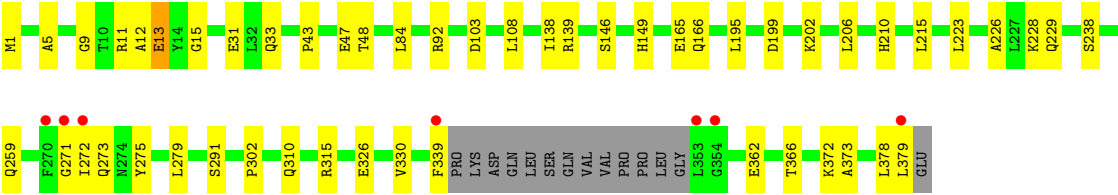
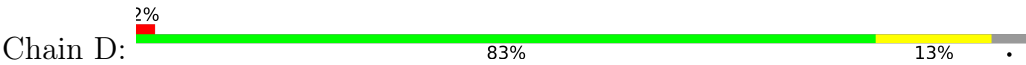


- Molecule 1: GDP/UDP-N,N'-diacetylbaucillosamine 2-epimerase (Hydrolyzing)





● Molecule 1: GDP/UDP-N,N'-diacetylba



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.59Å 126.14Å 146.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.59 – 2.50 29.59 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.59-2.50) 96.8 (29.59-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.204 , 0.257 0.206 , 0.258	Depositor DCC
R_{free} test set	2720 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12117	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4760e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: UDP, SO4

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	0.16	0/2959	0.41	0/4005
1	B	0.13	0/2930	0.35	1/3964 (0.0%)
1	C	0.20	0/2959	0.47	0/4005
1	D	0.12	0/2931	0.32	0/3966
All	All	0.16	0/11779	0.39	1/15940 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	38	ALA	CB-CA-C	-5.36	110.37	116.54

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	2905	0	2936	45	0
1	B	2878	0	2905	29	0
1	C	2905	0	2936	61	0
1	D	2879	0	2907	38	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	21	0	10	4	0
3	D	25	0	11	4	0
4	A	127	0	0	1	0
4	B	103	0	0	1	0
4	C	131	0	0	1	0
4	D	133	0	0	0	0
All	All	12117	0	11705	170	0

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

All (170) 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:322:VAL:HG23	1:A:328:GLU:HG2	1.45	0.97
1:B:272:ILE:HA	1:B:275:TYR:HB3	1.61	0.82
1:A:268:LYS:HD3	1:A:268:LYS:H	1.54	0.71
1:C:323:ARG:NH1	1:C:325:ASP:O	2.22	0.71
1:B:11:ARG:NH2	1:B:270:PHE:H	1.90	0.70
1:C:331:GLU:O	1:C:335:LYS:HB2	1.91	0.69
1:C:325:ASP:OD1	1:C:326:GLU:N	2.25	0.69
1:C:211:PRO:HG2	1:C:243:ASP:HB2	1.76	0.68
1:C:204:TYR:OH	1:C:278:VAL:O	2.03	0.67
1:C:323:ARG:CZ	1:C:328:GLU:HB3	2.25	0.66
1:D:229:GLN:NE2	1:D:326:GLU:OE2	2.29	0.66
1:B:61:GLU:OE2	1:B:92:ARG:NH1	2.29	0.65
1:C:234:ASN:HA	1:C:263:ARG:HG2	1.78	0.65
1:A:1:MET:HE3	1:A:31:GLU:HB2	1.79	0.65
1:C:304:VAL:HG12	1:C:320:LEU:HB2	1.78	0.65
1:C:224:PHE:HB2	1:C:256:LEU:HD13	1.79	0.64
1:D:302:PRO:HB3	1:D:339:PHE:HZ	1.62	0.64
1:D:310:GLN:O	1:D:315:ARG:NH2	2.31	0.63
1:B:103:ASP:OD2	1:B:139:ARG:NH2	2.32	0.62
1:D:210:HIS:NE2	3:D:400:UDP:O2A	2.33	0.62
1:D:11:ARG:HG3	1:D:272:ILE:HD11	1.82	0.62
1:B:103:ASP:HB3	1:B:139:ARG:HB2	1.83	0.60
1:D:302:PRO:HB3	1:D:339:PHE:CZ	2.36	0.60
1:C:207:ILE:HG13	1:C:286:VAL:HG12	1.84	0.59
1:C:228:LYS:HE2	1:C:256:LEU:HD12	1.85	0.59
1:A:327:ASN:O	1:A:330:VAL:N	2.36	0.58
1:D:272:ILE:HA	1:D:275:TYR:HB3	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ARG:HH21	1:B:269:SER:HA	1.69	0.57
1:D:11:ARG:HH11	1:D:271:GLY:HA2	1.68	0.57
1:B:323:ARG:NH2	1:B:328:GLU:OE1	2.38	0.57
1:C:247:THR:HA	1:C:250:VAL:HG12	1.86	0.57
1:C:293:LEU:HG	1:C:319:ILE:HD12	1.87	0.56
1:C:323:ARG:CZ	1:C:325:ASP:HB3	2.36	0.56
1:A:207:ILE:HG13	1:A:286:VAL:HG22	1.87	0.56
1:A:315:ARG:HD2	1:A:319:ILE:HG21	1.87	0.56
1:B:84:LEU:HD13	1:D:84:LEU:HD13	1.87	0.55
1:D:362:GLU:O	1:D:366:THR:HG23	2.07	0.55
1:C:286:VAL:HG23	1:C:304:VAL:HG23	1.88	0.55
1:C:221:ALA:HA	1:C:224:PHE:CZ	2.42	0.55
1:D:379:LEU:HD12	1:D:379:LEU:H	1.72	0.55
1:C:378:LEU:HD12	1:D:378:LEU:HD12	1.88	0.54
1:D:15:GLY:HA3	1:D:272:ILE:HD13	1.89	0.54
1:A:204:TYR:OH	1:A:278:VAL:O	2.22	0.53
1:A:247:THR:O	1:A:250:VAL:HG12	2.08	0.53
1:A:322:VAL:HG22	1:A:323:ARG:O	2.09	0.53
1:C:157:LYS:O	1:C:161:ILE:HG12	2.08	0.52
1:C:207:ILE:HB	1:C:237:PHE:CD1	2.43	0.52
1:C:155:GLU:CD	1:C:314:LEU:HD21	2.35	0.52
1:C:304:VAL:CG1	1:C:332:ALA:HB1	2.40	0.52
1:D:223:LEU:O	1:D:226:ALA:HB3	2.09	0.52
1:A:189:ILE:HG23	1:A:200:PHE:HB2	1.92	0.52
1:C:304:VAL:HG12	1:C:332:ALA:HB1	1.91	0.52
1:D:11:ARG:NH1	1:D:271:GLY:HA2	2.25	0.52
1:C:303:THR:HG21	1:C:319:ILE:HD13	1.92	0.51
1:D:326:GLU:O	1:D:330:VAL:HG23	2.10	0.51
1:C:323:ARG:NH1	1:C:328:GLU:HB3	2.26	0.51
1:D:228:LYS:NZ	1:D:259:GLN:OE1	2.38	0.51
1:A:84:LEU:HD13	1:C:84:LEU:HD13	1.91	0.51
1:A:223:LEU:O	1:A:227:LEU:HD12	2.11	0.51
1:A:155:GLU:CD	1:A:314:LEU:HD21	2.36	0.51
1:A:208:THR:HG22	1:A:238:SER:OG	2.11	0.51
1:C:330:VAL:HA	1:C:333:LEU:HD13	1.93	0.51
1:A:325:ASP:O	1:A:329:ILE:HG13	2.11	0.51
1:C:288:ASN:HB2	1:C:309:ARG:HB3	1.93	0.51
1:C:303:THR:CG2	1:C:319:ILE:HD13	2.41	0.50
1:D:108:LEU:HB2	1:D:138:ILE:HG23	1.92	0.50
1:B:271:GLY:O	1:B:273:GLN:N	2.41	0.50
1:A:79:MET:HE1	1:A:108:LEU:HD23	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:ARG:HD2	1:C:319:ILE:HG21	1.94	0.50
1:A:224:PHE:HB3	1:A:256:LEU:HD13	1.93	0.50
1:C:323:ARG:NE	1:C:325:ASP:HB3	2.27	0.50
1:A:236:ILE:HD13	1:A:278:VAL:HG11	1.93	0.49
1:C:238:SER:HA	1:C:267:VAL:O	2.13	0.49
1:C:331:GLU:OE1	1:C:331:GLU:N	2.42	0.49
1:B:355:ASN:N	1:B:355:ASN:OD1	2.45	0.49
1:D:9:GLY:N	1:D:13:GLU:OE1	2.39	0.49
1:D:146:SER:O	1:D:372:LYS:NZ	2.44	0.49
1:D:11:ARG:HD3	1:D:48:THR:HB	1.94	0.49
1:D:1:MET:HE3	1:D:31:GLU:HB2	1.95	0.49
1:B:210:HIS:NE2	3:B:400:UDP:O1A	2.44	0.48
1:C:232:ASP:H	1:C:263:ARG:NH2	2.12	0.48
1:D:103:ASP:HB3	1:D:139:ARG:HB2	1.94	0.48
1:B:15:GLY:HA3	1:B:272:ILE:HD12	1.95	0.48
1:A:257:LYS:HD3	1:A:264:VAL:HB	1.95	0.48
1:B:292:GLY:O	1:B:303:THR:HG21	2.14	0.48
1:C:235:PHE:O	1:C:264:VAL:HA	2.14	0.48
1:C:228:LYS:NZ	1:C:259:GLN:HE22	2.12	0.48
1:B:11:ARG:HD3	3:B:400:UDP:H1'	1.96	0.48
1:C:210:HIS:HD2	1:C:241:ASN:H	1.62	0.48
1:C:205:PHE:CE1	1:C:333:LEU:HD23	2.49	0.48
1:C:225:ASP:O	1:C:229:GLN:NE2	2.47	0.47
1:B:88:ASP:HB3	1:B:92:ARG:HH21	1.80	0.47
1:A:212:GLU:HG2	1:A:309:ARG:HB2	1.97	0.47
1:A:327:ASN:O	1:A:331:GLU:OE1	2.33	0.47
1:C:335:LYS:HA	1:C:338:ASN:OD1	2.15	0.47
1:A:325:ASP:HB3	1:A:328:GLU:HB3	1.97	0.47
1:B:203:PRO:HB3	1:B:283:LEU:HD11	1.97	0.47
1:B:333:LEU:O	1:B:337:ILE:HG13	2.15	0.46
1:D:206:LEU:HD23	1:D:279:LEU:HD13	1.97	0.46
1:C:224:PHE:CE2	1:C:252:ALA:HB1	2.50	0.46
1:C:353:LEU:HD23	1:C:353:LEU:H	1.80	0.46
1:D:291:SER:HB3	3:D:400:UDP:H5'1	1.98	0.46
1:A:211:PRO:HG3	1:A:246:ASN:HB3	1.98	0.46
1:A:325:ASP:OD1	1:A:326:GLU:N	2.49	0.46
1:C:303:THR:HG23	1:C:319:ILE:HA	1.97	0.46
1:D:11:ARG:HH21	1:D:48:THR:HG22	1.81	0.46
1:C:247:THR:O	1:C:250:VAL:HG12	2.15	0.46
1:A:203:PRO:HB3	1:A:283:LEU:HD21	1.97	0.45
1:B:237:PHE:HB3	1:B:253:MET:HE3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:GLU:OE2	4:C:501:HOH:O	2.21	0.45
1:A:11:ARG:HB2	1:A:48:THR:HG21	1.98	0.45
1:A:268:LYS:HG2	1:A:269:SER:N	2.32	0.45
1:B:208:THR:OG1	1:B:238:SER:OG	2.31	0.45
1:B:88:ASP:HB3	1:B:92:ARG:NH2	2.31	0.45
1:A:206:LEU:HD23	1:A:279:LEU:HD13	1.97	0.45
1:B:147:ASN:OD1	4:B:501:HOH:O	2.21	0.45
1:D:12:ALA:HA	3:D:400:UDP:H1'	1.99	0.45
1:C:322:VAL:HB	1:C:328:GLU:HG2	1.99	0.44
1:D:271:GLY:O	1:D:273:GLN:N	2.48	0.44
1:B:130:THR:HB	1:B:309:ARG:O	2.18	0.44
1:C:292:GLY:O	1:C:303:THR:HG21	2.17	0.44
1:A:157:LYS:O	1:A:161:ILE:HG13	2.18	0.44
1:A:238:SER:HA	1:A:267:VAL:O	2.18	0.44
1:C:225:ASP:OD1	1:C:228:LYS:HE3	2.17	0.44
1:C:334:GLN:O	1:C:337:ILE:N	2.51	0.44
1:C:221:ALA:HA	1:C:224:PHE:CE2	2.52	0.44
1:A:355:ASN:ND2	4:A:505:HOH:O	2.51	0.43
1:D:15:GLY:CA	1:D:272:ILE:HD13	2.48	0.43
1:C:131:GLU:OE2	1:C:309:ARG:HA	2.18	0.43
1:A:326:GLU:O	1:A:330:VAL:HG23	2.19	0.43
1:D:199:ASP:HB3	1:D:202:LYS:HE2	2.00	0.43
1:A:220:VAL:HG11	1:A:249:ILE:HG12	2.00	0.43
1:B:275:TYR:CE2	3:B:400:UDP:H3'	2.53	0.43
1:C:235:PHE:HD2	1:C:264:VAL:HG22	1.83	0.43
1:B:215:LEU:HD12	1:B:215:LEU:HA	1.91	0.43
1:D:103:ASP:OD2	1:D:139:ARG:NH2	2.46	0.42
1:D:5:ALA:HA	1:D:33:GLN:HB2	2.01	0.42
1:B:2:LYS:HB2	1:B:2:LYS:HE3	1.76	0.42
1:D:238:SER:HB2	3:D:400:UDP:O4	2.19	0.42
1:A:306:ILE:HA	1:A:322:VAL:O	2.19	0.42
1:C:210:HIS:CD2	1:C:240:PRO:HA	2.55	0.42
1:B:239:TYR:O	3:B:400:UDP:H5	2.03	0.42
1:C:155:GLU:OE2	1:C:314:LEU:HD21	2.19	0.41
1:A:131:GLU:HG3	1:A:311:LYS:HB3	2.02	0.41
1:A:353:LEU:H	1:A:353:LEU:HD23	1.85	0.41
1:C:323:ARG:HH22	1:C:327:ASN:N	2.17	0.41
1:A:286:VAL:HB	1:A:304:VAL:HB	2.03	0.41
1:A:322:VAL:HG21	1:A:329:ILE:HA	2.01	0.41
1:C:11:ARG:HB2	1:C:48:THR:HG21	2.01	0.41
1:C:79:MET:HE1	1:C:108:LEU:HD23	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:GLU:OE1	1:C:215:LEU:HD23	2.20	0.41
1:A:279:LEU:HD11	1:A:285:MET:HB2	2.02	0.41
1:D:166:GLN:HG3	1:D:373:ALA:HB1	2.01	0.41
1:B:22:ARG:NH2	1:B:23:ASP:OD1	2.47	0.41
1:D:43:PRO:HA	1:D:47:GLU:HG3	2.02	0.41
1:D:202:LYS:HB2	1:D:202:LYS:HE3	1.86	0.41
1:A:187:LYS:NZ	1:A:274:ASN:OD1	2.47	0.41
1:B:108:LEU:HB2	1:B:138:ILE:HG23	2.02	0.41
1:C:283:LEU:HA	1:C:283:LEU:HD23	1.81	0.41
1:C:283:LEU:HD13	1:C:337:ILE:HG13	2.03	0.41
1:A:215:LEU:HD12	1:A:215:LEU:HA	1.81	0.40
1:A:268:LYS:HG2	1:A:269:SER:H	1.86	0.40
1:A:333:LEU:O	1:A:337:ILE:HG13	2.21	0.40
1:B:239:TYR:CD1	1:B:268:LYS:HA	2.56	0.40
1:C:231:ASN:HB3	1:C:263:ARG:HH22	1.86	0.40
1:A:181:ILE:HD13	1:A:276:LEU:HD13	2.04	0.40
1:D:149:HIS:NE2	1:D:165:GLU:OE1	2.54	0.40
1:D:215:LEU:HD12	1:D:215:LEU:HA	1.94	0.40
1:A:259:GLN:HB2	1:A:260:LEU:HD12	2.02	0.40
1:C:227:LEU:HD23	1:C:333:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	366/380 (96%)	347 (95%)	18 (5%)	1 (0%)	36	55
1	B	362/380 (95%)	348 (96%)	13 (4%)	1 (0%)	36	55
1	C	366/380 (96%)	342 (93%)	23 (6%)	1 (0%)	36	55
1	D	362/380 (95%)	346 (96%)	16 (4%)	0	100	100
All	All	1456/1520 (96%)	1383 (95%)	70 (5%)	3 (0%)	43	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	338	ASN
1	C	327	ASN
1	B	272	ILE

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	318/328 (97%)	314 (99%)	4 (1%)	61	82
1	B	315/328 (96%)	312 (99%)	3 (1%)	68	86
1	C	318/328 (97%)	313 (98%)	5 (2%)	55	79
1	D	315/328 (96%)	312 (99%)	3 (1%)	68	86
All	All	1266/1312 (96%)	1251 (99%)	15 (1%)	63	83

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	190	SER
1	A	286	VAL
1	A	322	VAL
1	B	11	ARG
1	B	13	GLU
1	B	134	TYR
1	C	35	LEU
1	C	190	SER
1	C	303	THR
1	C	304	VAL
1	C	338	ASN
1	D	13	GLU
1	D	92	ARG
1	D	195	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	HIS
1	A	305	ASN
1	A	355	ASN
1	B	118	HIS
1	B	140	HIS
1	B	172	ASN
1	B	274	ASN
1	B	300	GLN
1	C	172	ASN
1	C	210	HIS
1	C	229	GLN
1	C	259	GLN
1	C	334	GLN
1	D	45	HIS
1	D	172	ASN
1	D	229	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	UDP	D	400	-	25,26,26	1.03	2 (8%)	38,40,40	1.55	4 (10%)
2	SO4	C	400	-	4,4,4	0.23	0	6,6,6	0.09	0
3	UDP	B	400	-	20,21,26	1.80	3 (15%)	27,31,40	0.97	1 (3%)
2	SO4	A	400	-	4,4,4	0.24	0	6,6,6	0.14	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
3	UDP	D	400	-	-	7/16/32/32	0/2/2/2
3	UDP	B	400	-	-	6/13/30/32	0/1/1/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400	UDP	C6-C5	4.81	1.39	1.32
3	B	400	UDP	C1'-N1	3.77	1.48	1.43
3	B	400	UDP	C4-C5	-2.41	1.39	1.49
3	D	400	UDP	PA-O3A	2.07	1.61	1.59
3	D	400	UDP	C5-C4	-2.03	1.39	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	400	UDP	C4-N3-C2	-5.43	119.86	126.61
3	D	400	UDP	N3-C2-N1	3.82	119.87	114.89
3	D	400	UDP	C5-C4-N3	3.75	120.05	114.80
3	D	400	UDP	O4-C4-C5	-2.97	120.03	125.16
3	B	400	UDP	C5-C6-N1	-2.27	117.03	123.80

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	400	UDP	C5'-O5'-PA-O1A
3	D	400	UDP	O4'-C4'-C5'-O5'
3	D	400	UDP	C5'-O5'-PA-O1A
3	D	400	UDP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

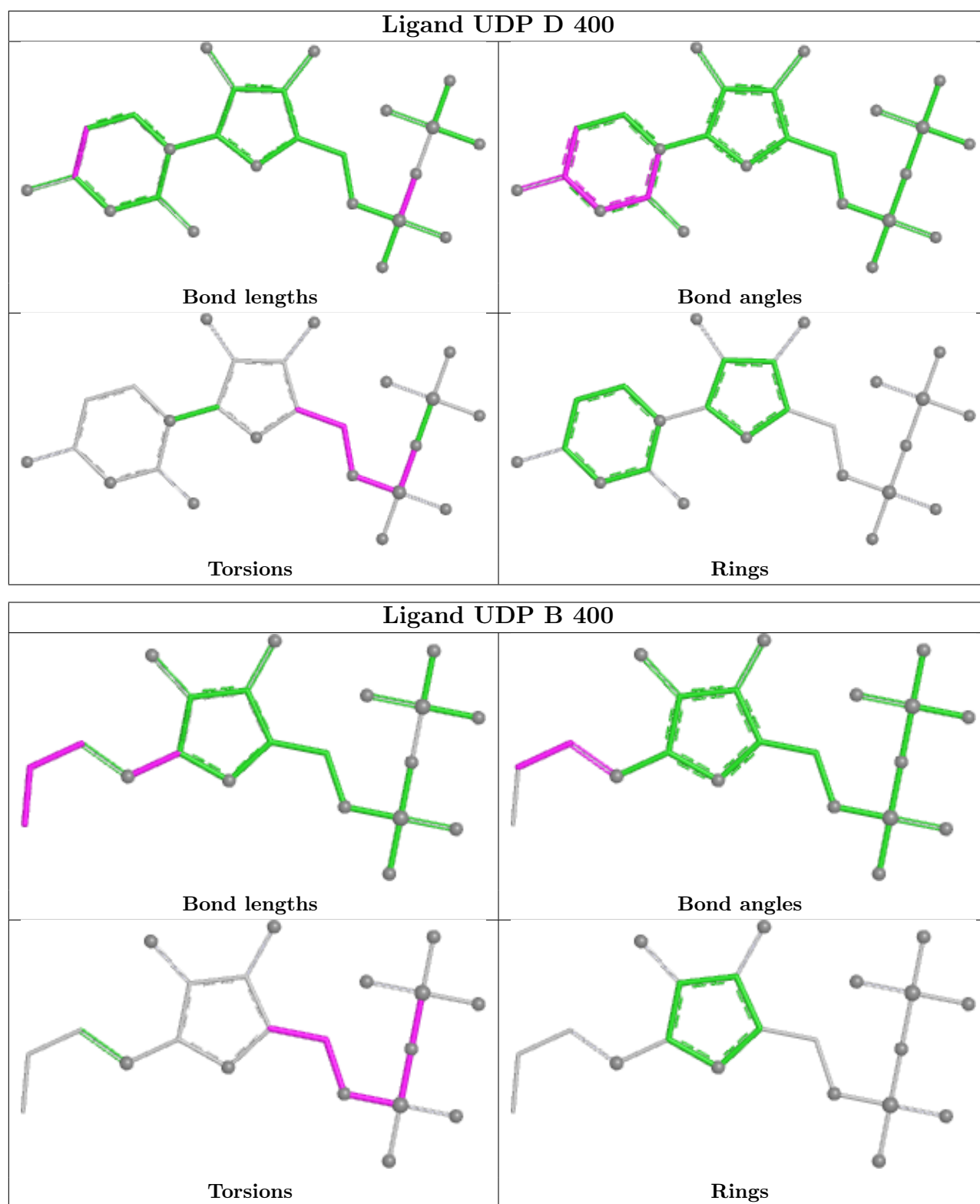
Mol	Chain	Res	Type	Atoms
3	D	400	UDP	C3'-C4'-C5'-O5'
3	B	400	UDP	C4'-C5'-O5'-PA
3	B	400	UDP	PB-O3A-PA-O1A
3	D	400	UDP	C4'-C5'-O5'-PA
3	D	400	UDP	PB-O3A-PA-O2A
3	B	400	UDP	PA-O3A-PB-O2B
3	D	400	UDP	PB-O3A-PA-O1A
3	B	400	UDP	C3'-C4'-C5'-O5'
3	B	400	UDP	PB-O3A-PA-O2A

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	400	UDP	4	0
3	B	400	UDP	4	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	370/380 (97%)	0.35	35 (9%) 14 12	20, 43, 128, 176	0
1	B	366/380 (96%)	-0.06	7 (1%) 66 62	17, 39, 70, 104	0
1	C	370/380 (97%)	0.55	57 (15%) 5 4	18, 43, 157, 200	0
1	D	366/380 (96%)	-0.14	7 (1%) 66 62	22, 38, 65, 95	0
All	All	1472/1520 (96%)	0.18	106 (7%) 21 19	17, 39, 125, 200	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	253	MET	6.0
1	C	250	VAL	5.2
1	C	216	LEU	4.8
1	C	208	THR	4.6
1	B	272	ILE	4.5
1	A	264	VAL	4.4
1	C	332	ALA	4.3
1	C	249	ILE	4.3
1	C	336	ALA	4.3
1	C	212	GLU	4.0
1	C	252	ALA	3.9
1	B	339	PHE	3.9
1	C	339	PHE	3.9
1	A	258	ALA	3.8
1	C	223	LEU	3.8
1	D	339	PHE	3.8
1	C	224	PHE	3.8
1	C	324	LEU	3.6
1	C	333	LEU	3.6
1	C	215	LEU	3.6
1	A	239	TYR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	353	LEU	3.5
1	C	264	VAL	3.4
1	C	330	VAL	3.4
1	A	216	LEU	3.4
1	C	265	LEU	3.4
1	D	353	LEU	3.4
1	A	230	ILE	3.4
1	C	239	TYR	3.4
1	C	240	PRO	3.4
1	A	253	MET	3.4
1	C	337	ILE	3.4
1	C	238	SER	3.4
1	C	233	VAL	3.3
1	D	379	LEU	3.3
1	D	272	ILE	3.3
1	B	271	GLY	3.3
1	C	242	ALA	3.2
1	C	227	LEU	3.2
1	A	249	ILE	3.2
1	A	339	PHE	3.1
1	A	260	LEU	3.1
1	A	226	ALA	3.1
1	A	242	ALA	3.1
1	A	240	PRO	3.1
1	A	250	VAL	3.1
1	C	221	ALA	3.0
1	A	245	GLY	3.0
1	B	379	LEU	2.9
1	D	271	GLY	2.9
1	C	229	GLN	2.9
1	C	226	ALA	2.9
1	C	354	GLY	2.9
1	C	284	ALA	2.8
1	C	131	GLU	2.8
1	C	326	GLU	2.8
1	C	247	THR	2.8
1	C	329	ILE	2.8
1	A	215	LEU	2.8
1	A	333	LEU	2.8
1	C	254	LEU	2.7
1	B	354	GLY	2.7
1	C	237	PHE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	327	ASN	2.7
1	C	282	ALA	2.7
1	C	283	LEU	2.6
1	C	379	LEU	2.6
1	A	270	PHE	2.6
1	C	236	ILE	2.5
1	C	260	LEU	2.5
1	A	256	LEU	2.5
1	A	244	ASN	2.5
1	A	318	SER	2.5
1	C	353	LEU	2.5
1	C	213	THR	2.5
1	A	213	THR	2.5
1	A	236	ILE	2.4
1	A	214	ASN	2.4
1	A	330	VAL	2.4
1	C	207	ILE	2.4
1	A	225	ASP	2.4
1	C	133	ALA	2.4
1	A	218	GLU	2.4
1	A	238	SER	2.3
1	C	323	ARG	2.3
1	A	254	LEU	2.3
1	A	233	VAL	2.3
1	A	232	ASP	2.3
1	A	208	THR	2.3
1	C	205	PHE	2.2
1	C	335	LYS	2.2
1	C	241	ASN	2.2
1	A	204	TYR	2.2
1	B	371	LYS	2.2
1	A	353	LEU	2.1
1	C	313	ARG	2.1
1	C	232	ASP	2.1
1	C	222	PRO	2.1
1	A	235	PHE	2.1
1	D	270	PHE	2.1
1	D	354	GLY	2.1
1	C	248	ASN	2.1
1	C	331	GLU	2.1
1	A	241	ASN	2.0
1	C	214	ASN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	246	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

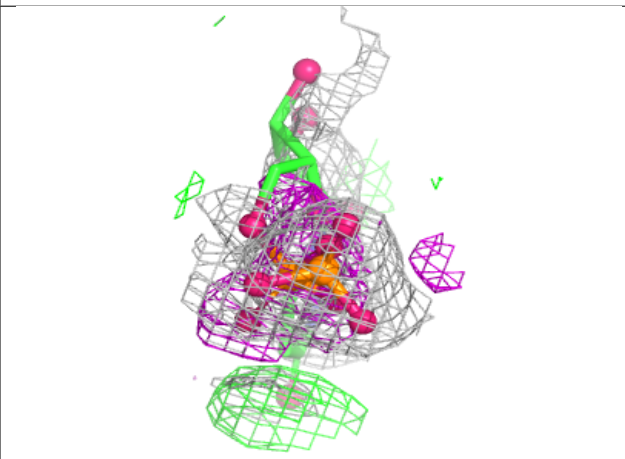
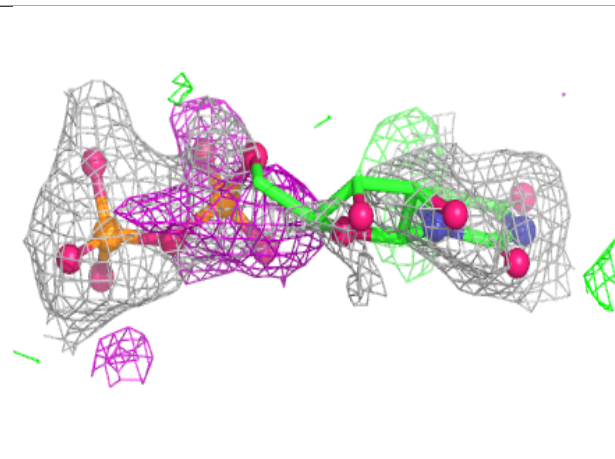
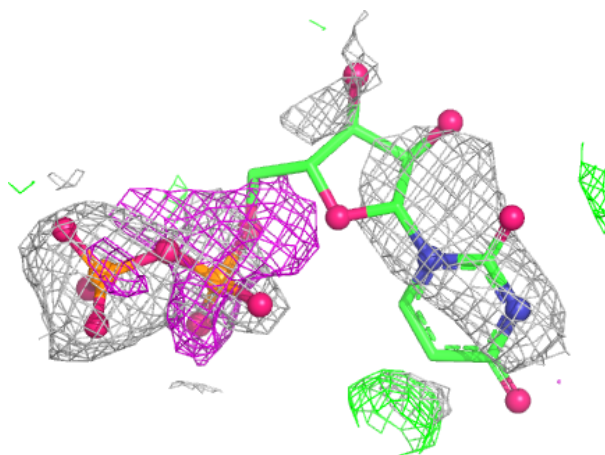
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

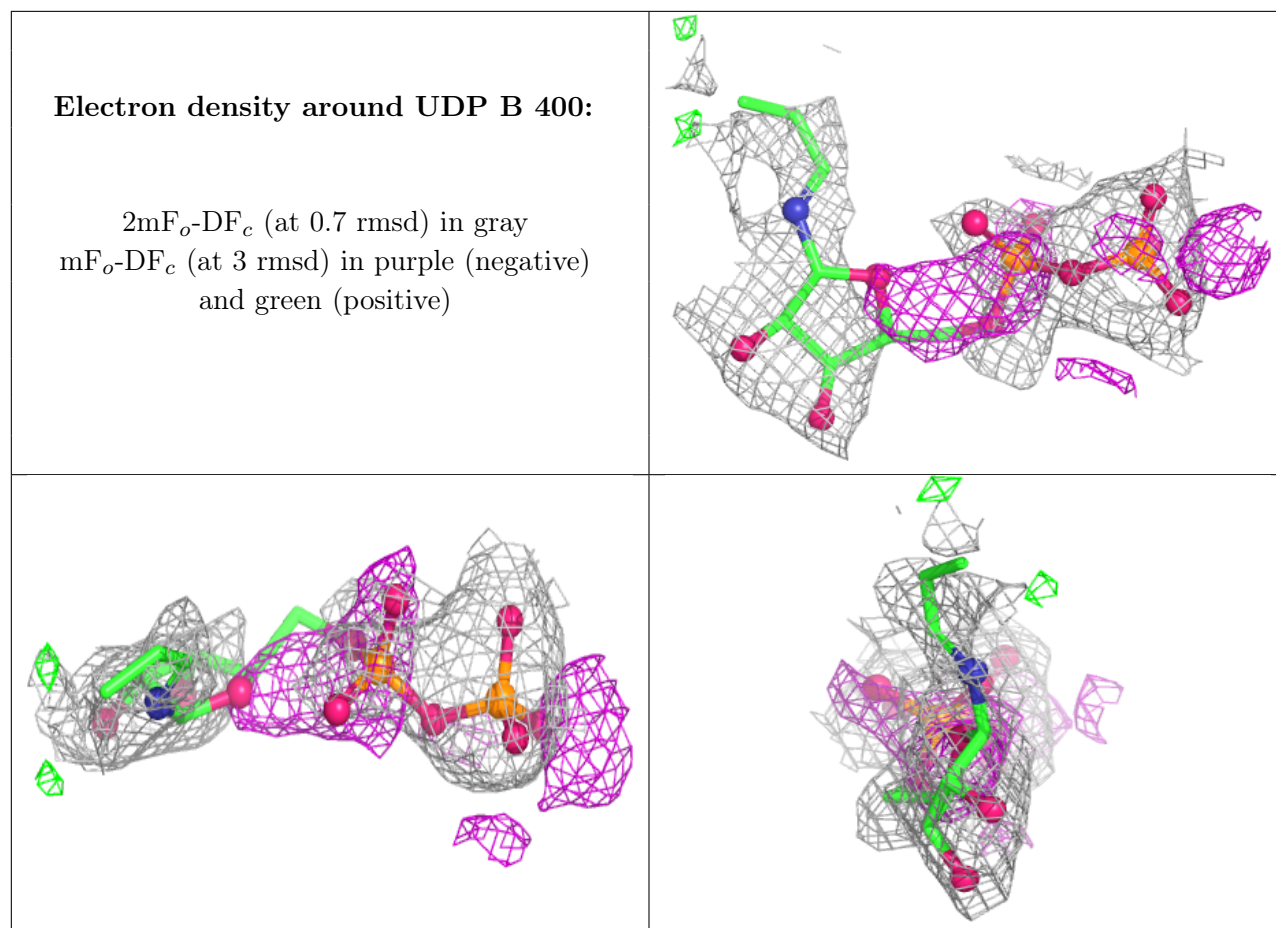
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	UDP	D	400	25/25	0.79	0.23	44,121,122,124	0
3	UDP	B	400	21/25	0.83	0.19	46,96,100,103	0
2	SO4	C	400	5/5	0.83	0.13	71,74,74,79	0
2	SO4	A	400	5/5	0.89	0.09	72,72,73,74	0

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 D 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 ⓘ

There are no such residues in this entry.