



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 12:55 PM UTC

PDB ID : 2OI5 / pdb_00002oi5
Title : E. coli GlmU- Complex with UDP-GlcNAc and Acetyl-CoA
Authors : Olsen, L.R.; Vetting, M.W.; Roderick, S.L.
Deposited on : 2007-01-10
Resolution : 2.25 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

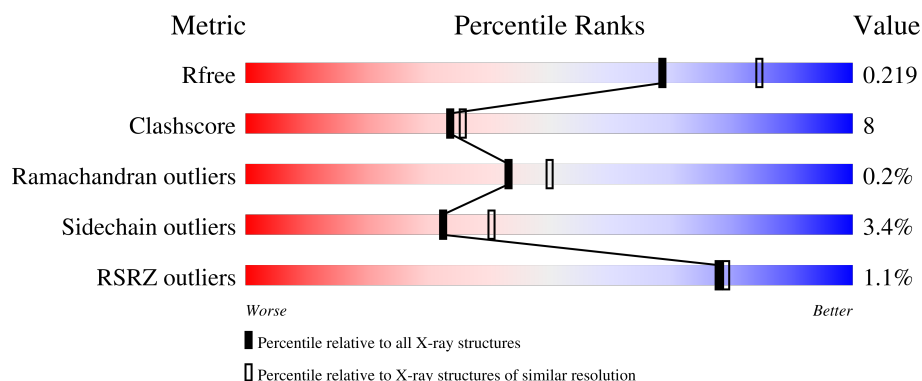
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	456	
1	B	456	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7590 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.

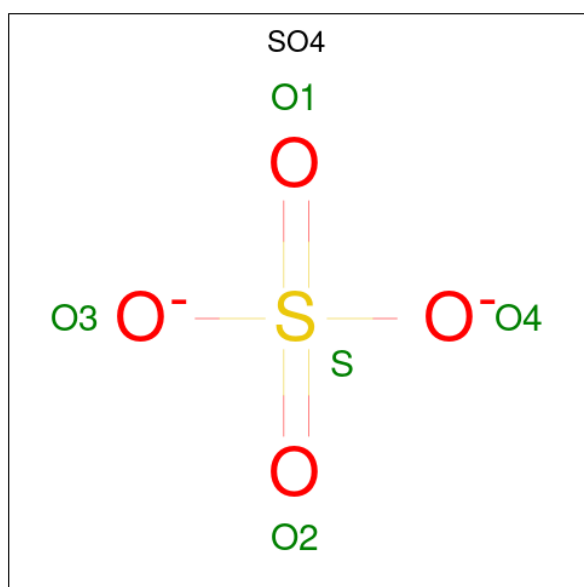
- Molecule 1 is a protein called Bifunctional protein glmU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3373	2105	607	649	12			
1	B	450	Total	C	N	O	S	0	0	0
			3388	2112	610	654	12			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

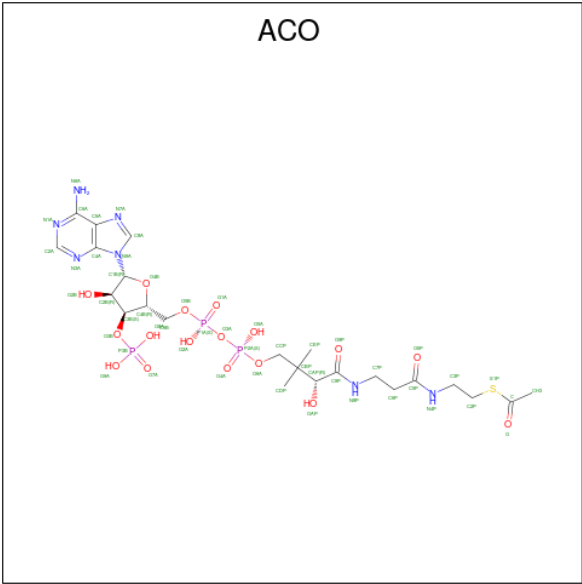
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	3	Total	Mg	0	0
			3	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



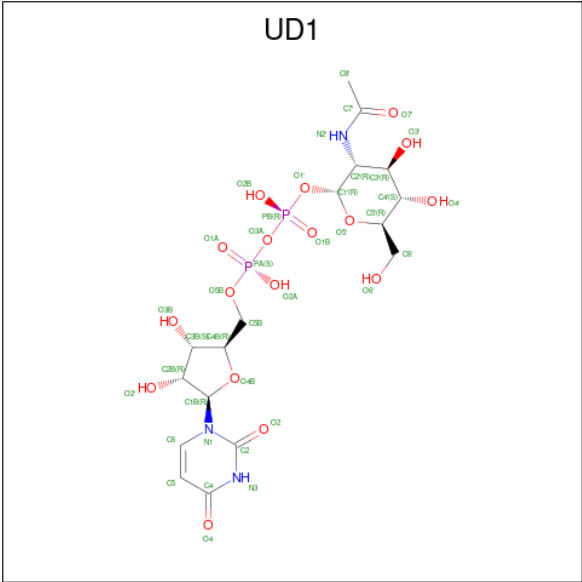
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 5 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (CCD ID: UD1) (formula: C₁₇H₂₇N₃O₁₇P₂).



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

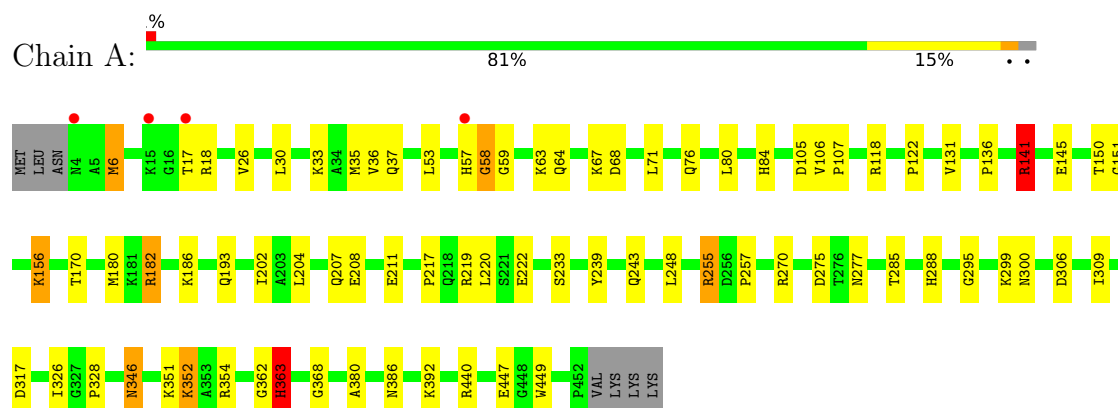
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	293	Total	O	0	0
			293	293		
6	B	336	Total	O	0	0
			336	336		

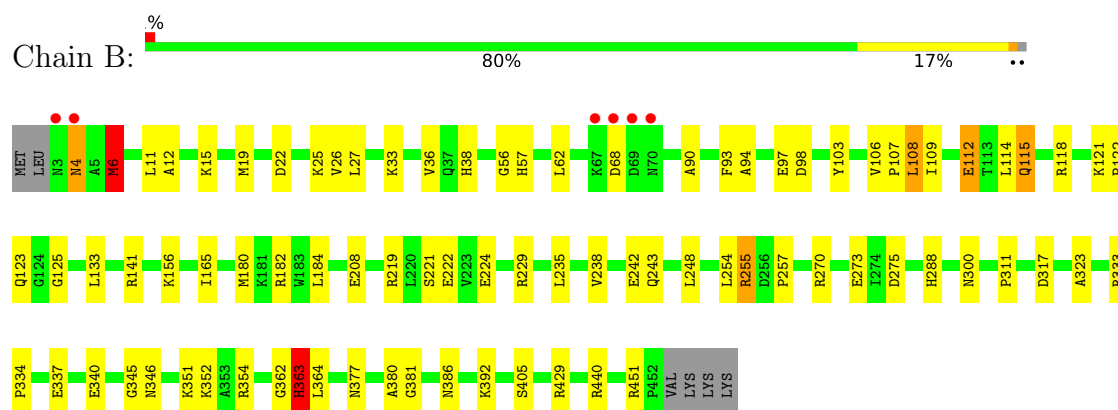
3 Residue-property plots

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: Bifunctional protein glmU



- Molecule 1: Bifunctional protein glmU



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	102.49Å 102.49Å 644.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.87 – 2.25 23.87 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.5 (23.87-2.25) 96.6 (23.87-2.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.24Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.176 , 0.219 0.177 , 0.219	Depositor DCC
R_{free} test set	3027 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7590	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.53% 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, SO4, ACO, MG

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	0.99	1/3421 (0.0%)	1.10	10/4640 (0.2%)
1	B	0.98	1/3436 (0.0%)	1.09	10/4660 (0.2%)
All	All	0.99	2/6857 (0.0%)	1.09	20/9300 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	6	MET	SD-CE	-5.28	1.66	1.79
1	A	6	MET	SD-CE	-5.21	1.66	1.79

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	PRO	N-CA-C	8.69	125.60	113.53
1	A	363	HIS	N-CA-C	7.92	120.42	108.46
1	A	107	PRO	N-CA-C	6.73	122.59	113.84
1	B	311	PRO	N-CA-C	6.64	121.68	111.11
1	B	363	HIS	N-CA-C	6.62	119.27	108.55
1	B	106	VAL	CA-C-N	6.55	126.32	119.05
1	B	106	VAL	C-N-CA	6.55	126.32	119.05
1	B	340	GLU	N-CA-C	6.10	119.33	110.42
1	A	17	THR	N-CA-C	5.77	117.24	111.07
1	B	440	ARG	N-CA-C	5.69	118.49	109.50
1	A	440	ARG	N-CA-C	5.63	118.58	109.40
1	A	106	VAL	CA-C-N	5.37	125.04	119.56
1	A	106	VAL	C-N-CA	5.37	125.04	119.56
1	A	141	ARG	NE-CZ-NH1	-5.32	116.18	121.50
1	A	58	GLY	N-CA-C	-5.31	106.91	115.08
1	A	306	ASP	N-CA-C	5.20	119.46	113.38
1	B	323	ALA	N-CA-C	5.17	119.17	112.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	22	ASP	N-CA-C	-5.12	106.73	113.17
1	A	170	THR	N-CA-C	-5.04	106.64	112.89
1	B	108	LEU	N-CA-C	5.00	119.10	113.15

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3373	0	3376	50	0
1	B	3388	0	3390	57	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
4	A	51	0	34	0	0
4	B	51	0	34	0	0
5	A	39	0	25	0	0
5	B	39	0	25	0	0
6	A	293	0	0	5	0
6	B	336	0	0	7	0
All	All	7590	0	6884	107	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 8.

All (107) 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:270:ARG:H	1:A:288:HIS:HD2	1.11	0.98
1:B:243:GLN:HG3	6:B:7211:HOH:O	1.66	0.92
1:B:270:ARG:H	1:B:288:HIS:HD2	1.22	0.87
1:A:76:GLN:HE21	1:A:84:HIS:HD2	1.24	0.84
1:B:115:GLN:HE21	1:B:115:GLN:HA	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ASN:HB3	6:A:7520:HOH:O	1.79	0.82
1:A:141:ARG:HG3	1:A:141:ARG:HH11	1.47	0.78
1:A:270:ARG:H	1:A:288:HIS:CD2	2.00	0.78
1:A:328:PRO:HG2	6:A:7520:HOH:O	1.84	0.77
1:A:204:LEU:O	1:A:207:GLN:HG2	1.87	0.74
1:B:270:ARG:H	1:B:288:HIS:CD2	2.05	0.73
1:A:156:LYS:HG2	1:A:193:GLN:HE21	1.54	0.72
1:B:68:ASP:HB3	6:B:7272:HOH:O	1.89	0.71
1:B:6:MET:HE3	1:B:118:ARG:HD2	1.71	0.70
1:A:59:GLY:O	1:A:63:LYS:HD3	1.93	0.69
1:B:15:LYS:HD3	1:B:57:HIS:CE1	2.28	0.69
1:B:19:MET:HG3	1:B:25:LYS:HG3	1.75	0.69
1:A:248:LEU:HD11	1:A:257:PRO:HG3	1.76	0.68
1:B:133:LEU:HD21	6:B:7289:HOH:O	1.94	0.68
1:B:4:ASN:H	1:B:4:ASN:HD22	1.42	0.66
1:A:76:GLN:HE21	1:A:84:HIS:CD2	2.12	0.65
1:B:255:ARG:NH1	1:B:273:GLU:OE2	2.30	0.63
1:B:6:MET:HG2	1:B:118:ARG:CZ	2.30	0.62
1:B:429:ARG:HD2	6:B:7482:HOH:O	2.01	0.61
1:A:156:LYS:HG2	1:A:193:GLN:NE2	2.16	0.60
1:B:4:ASN:HD22	1:B:4:ASN:N	1.97	0.59
1:B:115:GLN:HA	1:B:115:GLN:NE2	2.15	0.59
1:B:255:ARG:HB2	1:B:275:ASP:HA	1.85	0.59
1:B:112:GLU:CD	1:B:112:GLU:H	2.11	0.58
1:A:26:VAL:HB	1:A:36:VAL:HB	1.85	0.57
1:B:94:ALA:HB3	1:B:97:GLU:HG2	1.87	0.56
1:A:220:LEU:H	1:A:220:LEU:HD12	1.69	0.56
1:B:386:ASN:O	1:B:392:LYS:HA	2.05	0.56
1:B:182:ARG:NH2	1:B:208:GLU:OE2	2.38	0.56
1:A:204:LEU:O	1:A:208:GLU:HG3	2.06	0.56
1:A:300:ASN:O	1:A:317:ASP:HA	2.05	0.55
1:A:141:ARG:HG3	1:A:141:ARG:NH1	2.20	0.55
1:A:33:LYS:HD2	1:A:37:GLN:HG3	1.89	0.54
1:B:182:ARG:HH22	1:B:208:GLU:CD	2.15	0.54
1:A:141:ARG:HH11	1:A:141:ARG:CG	2.12	0.54
1:B:12:ALA:HB1	1:B:26:VAL:HG21	1.91	0.52
1:B:362:GLY:C	1:B:363:HIS:CG	2.87	0.52
1:B:122:PRO:HG2	1:B:125:GLY:HA3	1.92	0.52
1:B:26:VAL:HB	1:B:36:VAL:HB	1.91	0.52
1:A:131:VAL:HG12	1:A:217:PRO:HD2	1.93	0.51
1:B:180:MET:O	1:B:184:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ARG:HH11	1:A:182:ARG:HG3	1.76	0.50
1:A:136:PRO:HB2	1:A:141:ARG:NH1	2.27	0.50
1:B:221:SER:HA	1:B:224:GLU:HG3	1.94	0.50
1:B:90:ALA:HA	1:B:93:PHE:CD1	2.47	0.50
1:A:255:ARG:NE	1:A:255:ARG:HA	2.27	0.49
1:B:98:ASP:OD1	1:B:121:LYS:HE2	2.12	0.49
1:A:122:PRO:HG2	1:A:211:GLU:HG3	1.93	0.49
1:A:145:GLU:HB2	1:A:150:THR:HG21	1.95	0.49
1:B:333:ARG:HB3	1:B:334:PRO:CD	2.43	0.49
1:A:141:ARG:NH1	1:A:141:ARG:CG	2.72	0.48
1:B:141:ARG:HG3	1:B:165:ILE:HB	1.94	0.48
1:B:219:ARG:O	1:B:222:GLU:HG2	2.14	0.48
1:B:229:ARG:HG2	6:B:7040:HOH:O	2.13	0.47
1:B:364:LEU:O	1:B:381:GLY:HA2	2.13	0.47
1:A:219:ARG:O	1:A:222:GLU:HB2	2.14	0.47
1:B:6:MET:HE3	1:B:118:ARG:CD	2.43	0.47
1:A:33:LYS:HD2	1:A:37:GLN:CG	2.45	0.46
1:A:354:ARG:HD2	6:A:7058:HOH:O	2.14	0.46
1:B:19:MET:CG	1:B:25:LYS:HG3	2.44	0.46
1:A:277:ASN:O	1:A:295:GLY:HA2	2.16	0.46
1:B:156:LYS:HG2	6:B:7249:HOH:O	2.15	0.46
1:B:4:ASN:N	1:B:4:ASN:ND2	2.62	0.46
1:A:299:LYS:O	1:A:300:ASN:C	2.59	0.46
1:B:333:ARG:HB3	1:B:334:PRO:HD2	1.98	0.46
1:A:35:MET:HE3	1:A:105:ASP:HA	1.98	0.45
1:B:15:LYS:HB2	1:B:57:HIS:CG	2.50	0.45
1:B:363:HIS:CD2	1:B:380:ALA:HB2	2.50	0.45
1:A:255:ARG:HG2	1:A:275:ASP:HA	1.98	0.45
1:A:351:LYS:O	1:A:352:LYS:C	2.59	0.45
1:B:182:ARG:NH2	1:B:208:GLU:CD	2.75	0.45
1:A:255:ARG:HA	1:A:255:ARG:HE	1.82	0.45
1:A:362:GLY:C	1:A:363:HIS:CG	2.94	0.45
1:A:386:ASN:O	1:A:392:LYS:HA	2.18	0.44
1:A:186:LYS:NZ	6:A:7444:HOH:O	2.50	0.44
1:B:109:ILE:HG12	1:B:114:LEU:HD21	2.00	0.44
1:B:363:HIS:CD2	1:B:363:HIS:N	2.85	0.43
1:B:300:ASN:O	1:B:317:ASP:HA	2.18	0.43
1:A:182:ARG:HH11	1:A:182:ARG:CG	2.32	0.43
1:A:239:TYR:O	1:A:243:GLN:HG2	2.18	0.43
1:A:30:LEU:C	1:A:30:LEU:HD23	2.43	0.43
1:B:27:LEU:HD21	1:B:62:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:LYS:O	1:A:368:GLY:HA2	2.19	0.42
1:B:337:GLU:O	1:B:354:ARG:HA	2.20	0.42
1:A:285:THR:HG22	6:A:7548:HOH:O	2.20	0.42
1:B:248:LEU:HD11	1:B:257:PRO:HG3	2.01	0.42
1:B:351:LYS:O	1:B:352:LYS:C	2.63	0.42
1:A:6:MET:HE2	1:A:118:ARG:HD2	2.01	0.42
1:A:363:HIS:CD2	1:A:380:ALA:HB2	2.55	0.42
1:B:451:ARG:HB2	6:B:7356:HOH:O	2.18	0.42
1:A:151:GLY:HA2	1:A:202:ILE:HG22	2.02	0.42
1:A:68:ASP:HB2	1:A:71:LEU:HG	2.02	0.42
1:B:255:ARG:NH1	1:B:273:GLU:CD	2.79	0.41
1:B:11:LEU:HD12	1:B:103:TYR:CE2	2.56	0.41
1:A:64:GLN:O	1:A:67:LYS:HE3	2.21	0.41
1:B:108:LEU:HB2	1:B:222:GLU:HA	2.03	0.41
1:B:345:GLY:HA3	1:B:362:GLY:O	2.21	0.41
1:B:238:VAL:O	1:B:242:GLU:HG3	2.21	0.40
1:B:248:LEU:HD21	1:B:254:LEU:H	1.86	0.40
1:A:309:ILE:HD12	1:A:326:ILE:HD11	2.03	0.40
1:B:33:LYS:HB3	1:B:38:HIS:CE1	2.57	0.40
1:A:57:HIS:CG	1:A:58:GLY:H	2.40	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	447/456 (98%)	438 (98%)	8 (2%)	1 (0%)	43	50
1	B	448/456 (98%)	435 (97%)	12 (3%)	1 (0%)	43	50
All	All	895/912 (98%)	873 (98%)	20 (2%)	2 (0%)	43	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	B	56	GLY

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	349/362 (96%)	336 (96%)	13 (4%)	30	37
1	B	352/362 (97%)	341 (97%)	11 (3%)	35	44
All	All	701/724 (97%)	677 (97%)	24 (3%)	32	40

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LEU
1	A	80	LEU
1	A	141	ARG
1	A	156	LYS
1	A	180	MET
1	A	182	ARG
1	A	233	SER
1	A	255	ARG
1	A	346	ASN
1	A	352	LYS
1	A	363	HIS
1	A	447	GLU
1	A	449	TRP
1	B	4	ASN
1	B	6	MET
1	B	112	GLU
1	B	115	GLN
1	B	123	GLN
1	B	235	LEU
1	B	255	ARG
1	B	346	ASN
1	B	363	HIS

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Mol	Chain	Res	Type
1	B	377	ASN
1	B	405	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	84	HIS
1	A	166	GLN
1	A	193	GLN
1	A	207	GLN
1	A	288	HIS
1	A	434	ASN
1	B	4	ASN
1	B	38	HIS
1	B	72	ASN
1	B	115	GLN
1	B	190	ASN
1	B	218	GLN
1	B	288	HIS

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](#)

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 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	UD1	B	4001	2	40,41,41	2.18	8 (20%)	59,62,62	1.18	5 (8%)
3	SO4	B	6002	-	4,4,4	0.54	0	6,6,6	0.71	0
4	ACO	B	2001	-	51,53,53	1.42	7 (13%)	73,79,79	1.31	8 (10%)
5	UD1	A	4000	-	40,41,41	2.25	5 (12%)	59,62,62	1.01	3 (5%)
4	ACO	A	2000	-	51,53,53	1.64	9 (17%)	73,79,79	1.34	11 (15%)
3	SO4	A	6000	-	4,4,4	0.63	0	6,6,6	0.50	0
3	SO4	B	6001	-	4,4,4	0.21	0	6,6,6	0.33	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
4	ACO	A	2000	-	-	14/51/67/67	0/3/3/3
4	ACO	B	2001	-	-	10/51/67/67	0/3/3/3
5	UD1	B	4001	2	-	0/26/63/63	0/3/3/3
5	UD1	A	4000	-	-	0/26/63/63	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	4000	UD1	PA-O3A	-10.79	1.47	1.59
5	B	4001	UD1	PA-O3A	-8.26	1.50	1.59
5	B	4001	UD1	PB-O3A	-5.90	1.53	1.59
5	A	4000	UD1	PB-O3A	-5.50	1.53	1.59
4	A	2000	ACO	C6P-C5P	4.83	1.61	1.51
5	B	4001	UD1	C6-N1	4.53	1.48	1.38
5	A	4000	UD1	C6-N1	4.41	1.48	1.38
4	B	2001	ACO	P2A-O3A	3.91	1.63	1.59
4	A	2000	ACO	C3P-N4P	3.71	1.54	1.46
4	A	2000	ACO	P2A-O3A	3.65	1.63	1.59
4	A	2000	ACO	C4A-N3A	3.45	1.40	1.34
4	A	2000	ACO	C8A-N7A	3.43	1.38	1.31
4	B	2001	ACO	C4A-N3A	3.43	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	4001	UD1	PA-O2A	-3.09	1.41	1.55
4	B	2001	ACO	C8A-N7A	3.00	1.37	1.31
4	B	2001	ACO	C2A-N1A	2.97	1.39	1.33
4	A	2000	ACO	C2A-N1A	2.93	1.39	1.33
5	B	4001	UD1	C1'-C2'	2.75	1.57	1.53
5	A	4000	UD1	C5-C4	2.62	1.49	1.43
4	B	2001	ACO	C3P-N4P	2.56	1.51	1.46
4	A	2000	ACO	C5A-N7A	2.50	1.43	1.39
5	A	4000	UD1	C4'-C5'	2.49	1.58	1.53
5	B	4001	UD1	C5-C4	2.32	1.48	1.43
4	A	2000	ACO	C5A-C6A	2.30	1.47	1.41
5	B	4001	UD1	C2'-N2'	2.26	1.49	1.45
4	B	2001	ACO	C5A-N7A	2.22	1.43	1.39
4	A	2000	ACO	O-C	2.18	1.32	1.21
5	B	4001	UD1	C2-N3	-2.14	1.34	1.38
4	B	2001	ACO	P3B-O3B	2.01	1.63	1.59

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2000	ACO	C4A-N9A-C1B	-3.99	117.30	126.63
4	B	2001	ACO	C4A-N9A-C8A	3.81	109.74	105.74
4	A	2000	ACO	C4A-N9A-C8A	3.77	109.69	105.74
4	B	2001	ACO	C4A-N9A-C1B	-3.54	118.36	126.63
5	B	4001	UD1	O2A-PA-O3A	3.17	115.85	107.27
4	B	2001	ACO	N9A-C8A-N7A	-2.79	109.98	113.94
4	A	2000	ACO	O2A-P1A-O3A	2.78	114.79	107.27
4	A	2000	ACO	N9A-C8A-N7A	-2.73	110.07	113.94
4	A	2000	ACO	C6P-C5P-N4P	-2.71	111.41	116.34
5	A	4000	UD1	O4-C4-C5	-2.69	120.52	125.16
5	B	4001	UD1	O2-C2-N3	-2.66	116.57	121.49
4	A	2000	ACO	C1B-N9A-C8A	2.65	132.98	127.09
5	B	4001	UD1	C5-C4-N3	2.61	118.45	114.80
4	A	2000	ACO	CEP-CBP-CCP	2.56	112.44	108.22
5	B	4001	UD1	N3-C2-N1	2.50	118.14	114.89
5	A	4000	UD1	N3-C2-N1	2.49	118.13	114.89
4	B	2001	ACO	C6P-C7P-N8P	2.43	117.17	112.00
5	B	4001	UD1	O4-C4-C5	-2.42	120.98	125.16
4	B	2001	ACO	O2A-P1A-O3A	2.19	113.19	107.27
4	A	2000	ACO	C6P-C7P-N8P	2.19	116.66	112.00
4	B	2001	ACO	C1B-N9A-C8A	2.15	131.88	127.09
4	B	2001	ACO	CEP-CBP-CCP	2.12	111.73	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2000	ACO	C6A-C5A-C4A	-2.12	114.29	117.18
4	B	2001	ACO	C6A-C5A-C4A	-2.11	114.30	117.18
4	A	2000	ACO	O4B-C1B-N9A	2.10	112.11	108.09
4	A	2000	ACO	O6A-P2A-O4A	2.03	116.99	108.94
5	A	4000	UD1	O7'-C7'-N2'	2.02	125.56	121.98

There are no chirality outliers.

All (24) torsion outliers are listed below:

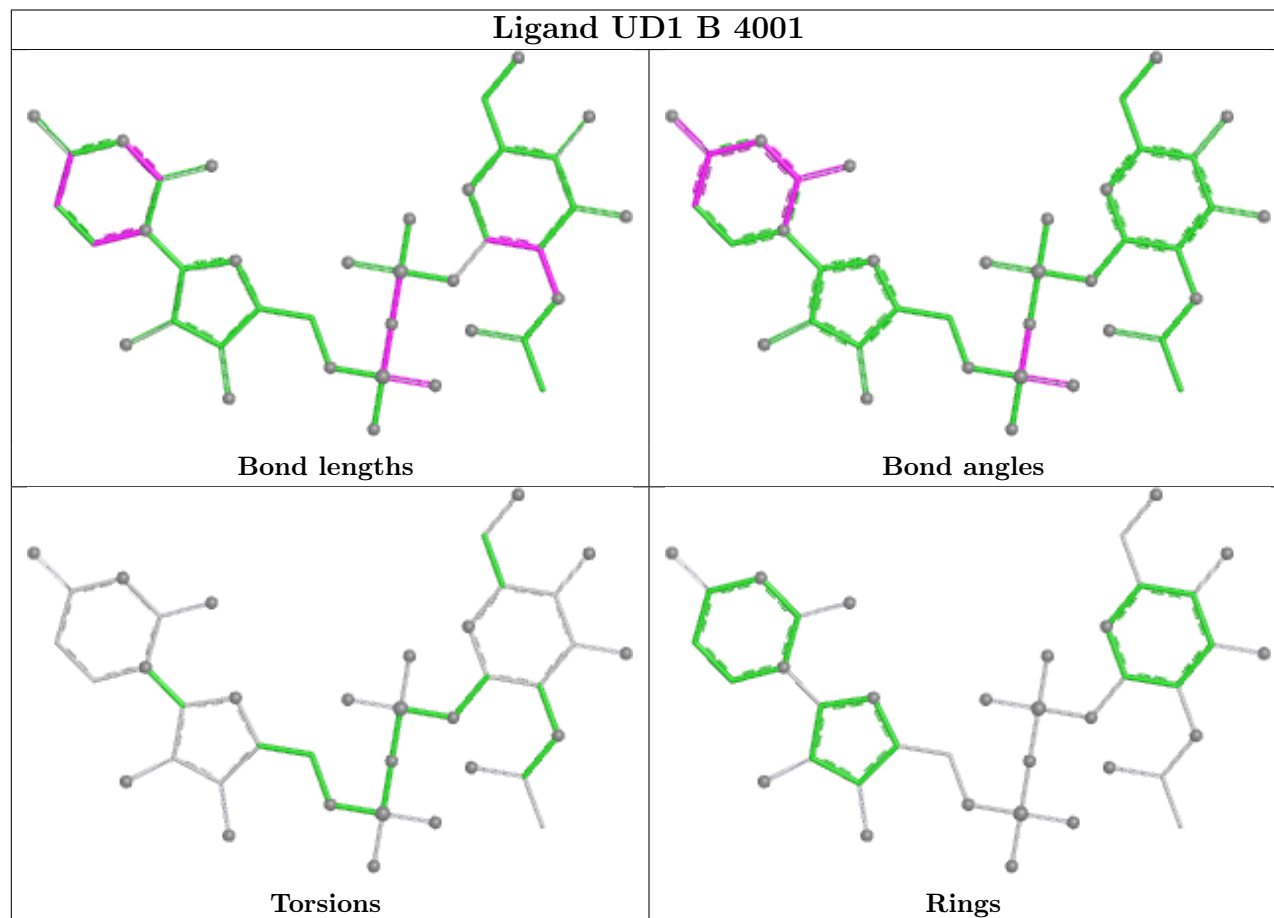
Mol	Chain	Res	Type	Atoms
4	A	2000	ACO	C5B-O5B-P1A-O1A
4	A	2000	ACO	C5B-O5B-P1A-O3A
4	A	2000	ACO	CDP-CBP-CCP-O6A
4	A	2000	ACO	CEP-CBP-CCP-O6A
4	A	2000	ACO	CAP-CBP-CCP-O6A
4	B	2001	ACO	C5B-O5B-P1A-O1A
4	B	2001	ACO	C5B-O5B-P1A-O3A
4	B	2001	ACO	CDP-CBP-CCP-O6A
4	B	2001	ACO	CEP-CBP-CCP-O6A
4	B	2001	ACO	CAP-CBP-CCP-O6A
4	B	2001	ACO	C3B-C4B-C5B-O5B
4	A	2000	ACO	C3B-C4B-C5B-O5B
4	B	2001	ACO	O4B-C4B-C5B-O5B
4	A	2000	ACO	C4B-C3B-O3B-P3B
4	A	2000	ACO	C2B-C3B-O3B-P3B
4	B	2001	ACO	C4B-C3B-O3B-P3B
4	A	2000	ACO	P1A-O3A-P2A-O4A
4	A	2000	ACO	C3B-O3B-P3B-O9A
4	A	2000	ACO	C3B-O3B-P3B-O7A
4	A	2000	ACO	N8P-C9P-CAP-OAP
4	B	2001	ACO	N8P-C9P-CAP-OAP
4	A	2000	ACO	C4B-C5B-O5B-P1A
4	A	2000	ACO	P1A-O3A-P2A-O5A
4	B	2001	ACO	P1A-O3A-P2A-O5A

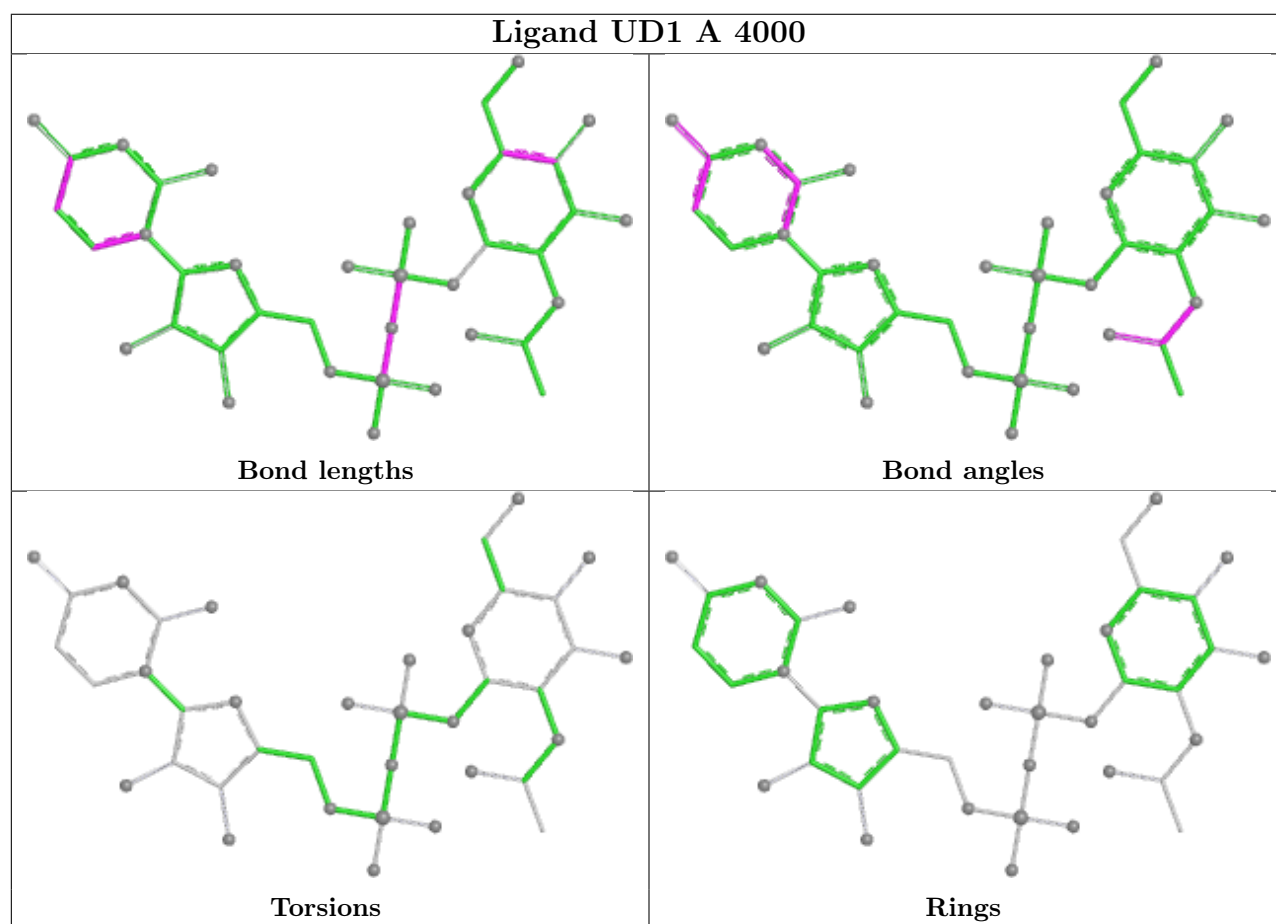
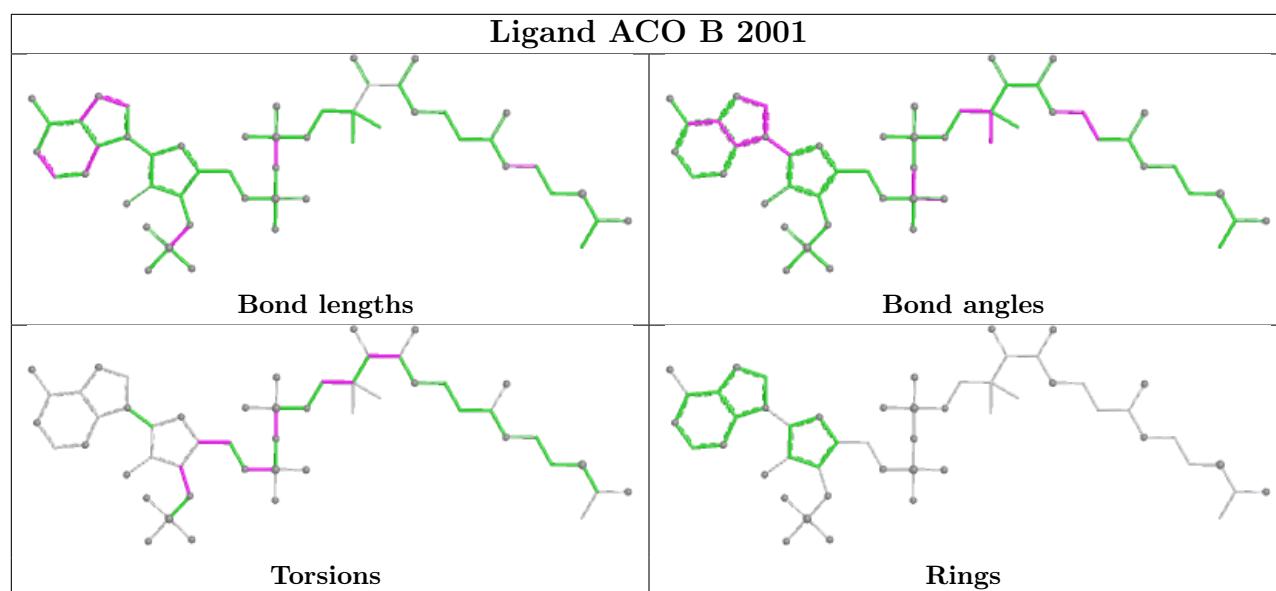
There are no ring outliers.

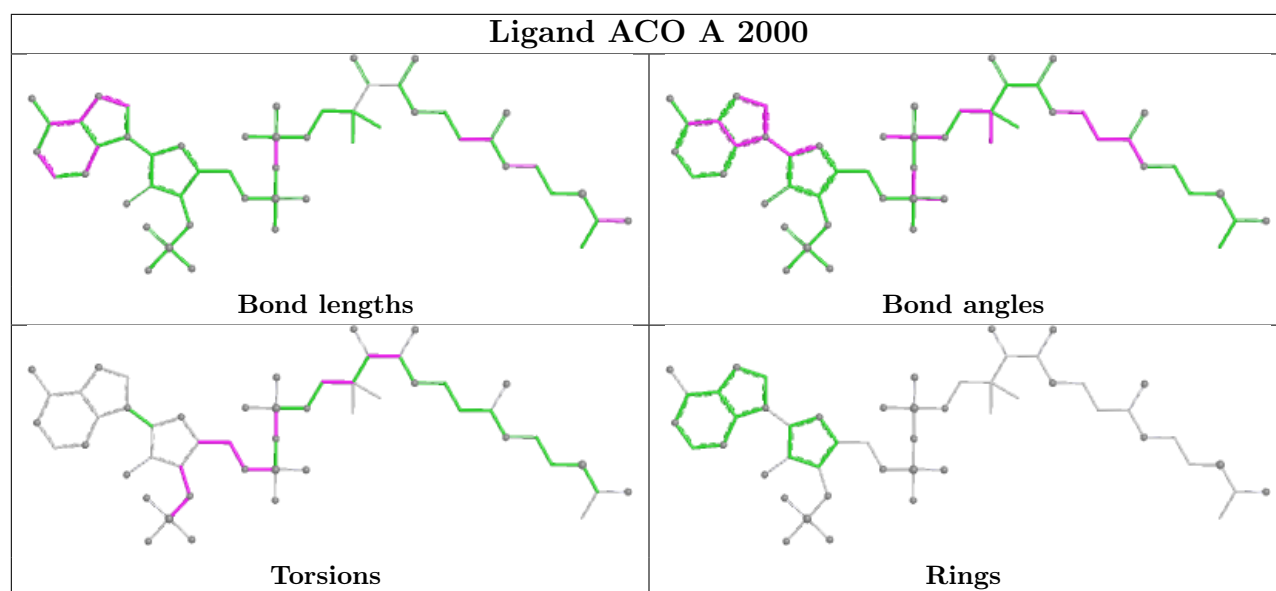
No monomer is involved in short contacts.

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	449/456 (98%)	-0.66	4 (0%) 81 82	12, 23, 42, 58	0
1	B	450/456 (98%)	-0.68	6 (1%) 75 76	12, 22, 41, 77	0
All	All	899/912 (98%)	-0.67	10 (1%) 78 79	12, 22, 42, 77	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	ASN	3.8
1	A	57	HIS	3.5
1	B	69	ASP	3.3
1	B	3	ASN	3.0
1	A	4	ASN	2.8
1	B	70	ASN	2.4
1	A	15	LYS	2.4
1	A	17	THR	2.4
1	B	67	LYS	2.2
1	B	68	ASP	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

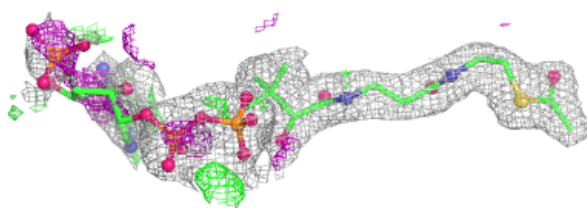
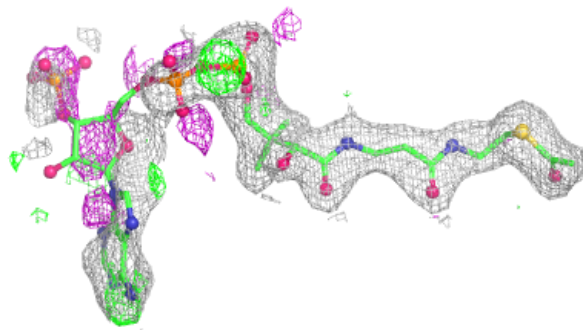
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	MG	A	5004	1/1	0.64	0.14	25,25,25,25	1
2	MG	B	5001	1/1	0.75	0.13	21,21,21,21	1
2	MG	B	5002	1/1	0.91	0.22	33,33,33,33	1
4	ACO	B	2001	51/51	0.91	0.15	14,70,97,100	0
4	ACO	A	2000	51/51	0.92	0.14	12,63,96,100	0
2	MG	B	5000	1/1	0.94	0.12	27,27,27,27	0
2	MG	A	5003	1/1	0.97	0.11	16,16,16,16	1
5	UD1	A	4000	39/39	0.97	0.05	15,24,35,40	0
3	SO4	B	6002	5/5	0.98	0.08	27,29,36,38	0
3	SO4	A	6000	5/5	0.99	0.05	22,25,28,33	0
3	SO4	B	6001	5/5	0.99	0.04	22,24,26,28	0
5	UD1	B	4001	39/39	0.99	0.04	13,19,24,28	0

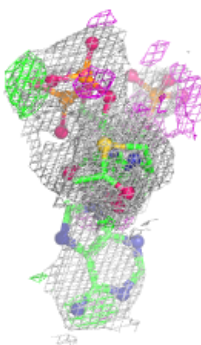
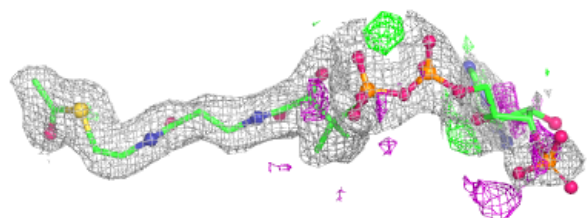
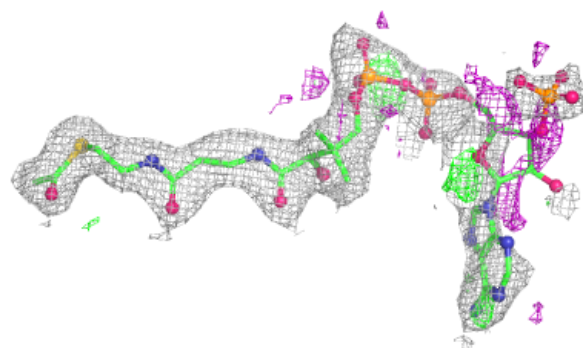
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACO B 2001:

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

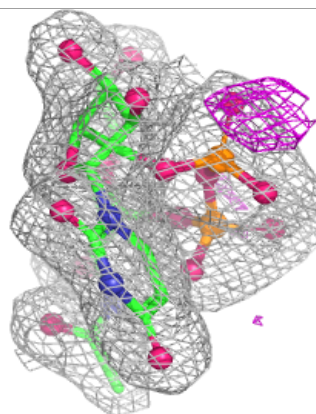
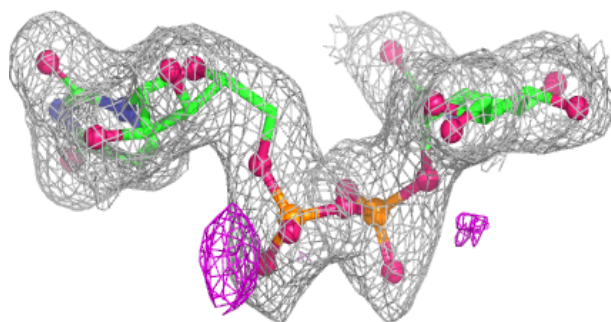
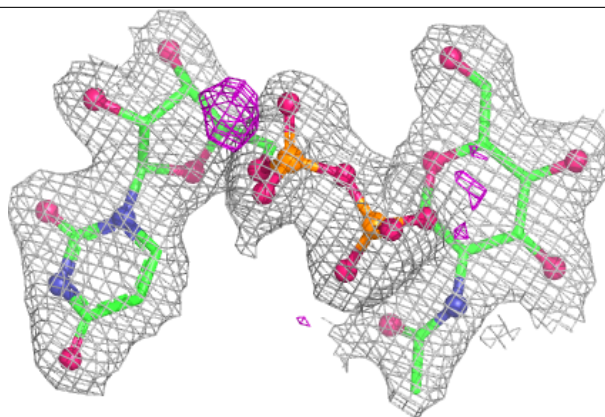
**Electron density around ACO A 2000:**

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

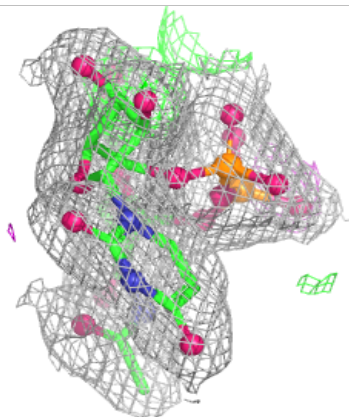
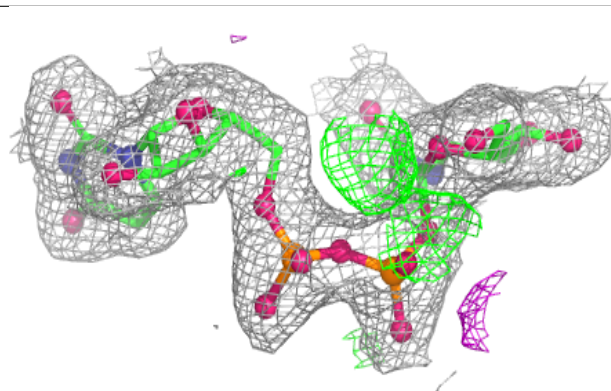
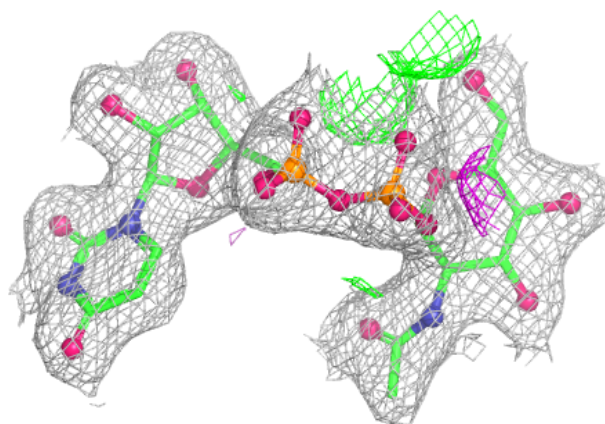


Electron density around UD1 A 4000:

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

**Electron density around UD1 B 4001:**

$2mF_o-DF_c$ (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.