



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:11 PM UTC

PDB ID : 1HV9 / pdb_00001hv9
Title : STRUCTURE OF E. COLI GLMU: ANALYSIS OF PYROPHOSPHORYLASE AND ACETYLTRANSFERASE ACTIVE SITES
Authors : Olsen, L.R.; Roderick, S.L.
Deposited on : 2001-01-08
Resolution : 2.10 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

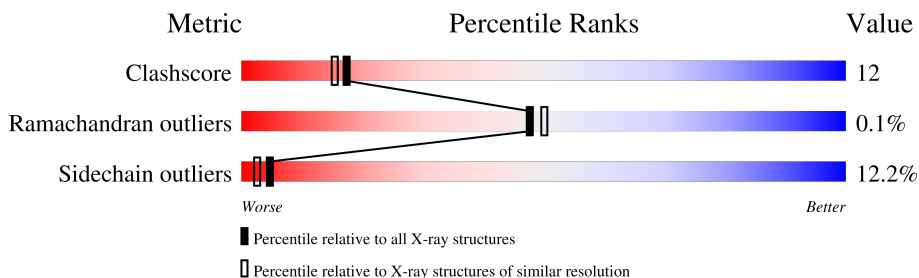
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	456	 69% 25% . .
1	B	456	 70% 23% 5% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7194 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.

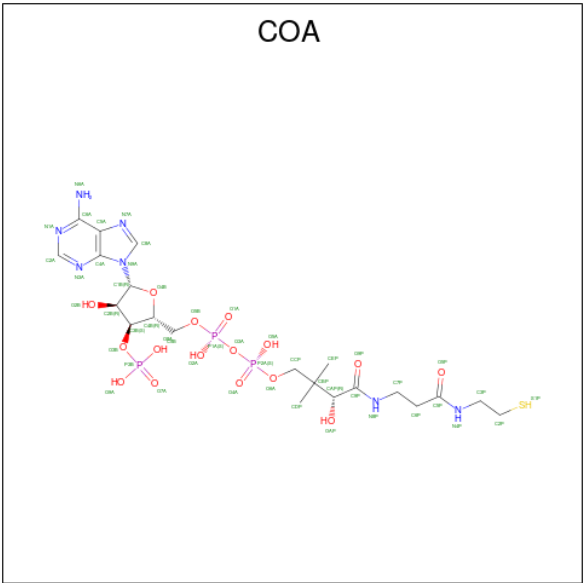
- Molecule 1 is a protein called UDP-N-ACETYLGLUCOSAMINE PYROPHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3370	2103	607	649	11			
1	B	450	Total	C	N	O	S	0	0	0
			3388	2112	612	653	11			

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

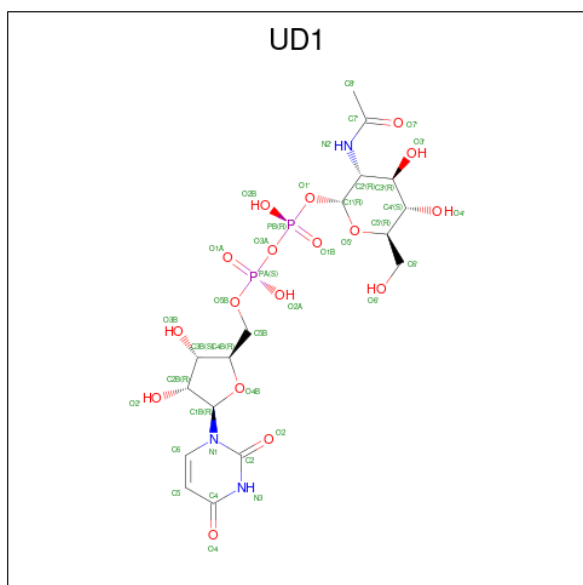
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Co	0	0
			2	2		
2	B	3	Total	Co	0	0
			3	3		

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	
			48	21	7	16	3	1	
3	B	1	Total	C	N	O	P	S	
			48	21	7	16	3	1	

- Molecule 4 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (CCD ID: UD1) (formula: $C_{17}H_{27}N_3O_{17}P_2$).



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

- Molecule 5 is water.

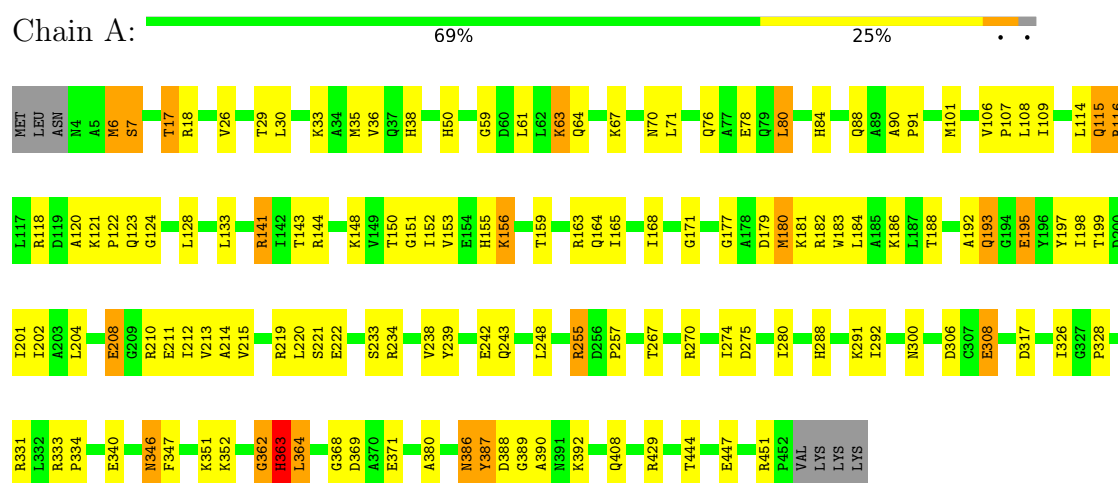
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	127	Total	O		
			127	127	0	0
5	B	130	Total	O		
			130	130	0	0

3 Residue-property plots [i](#)

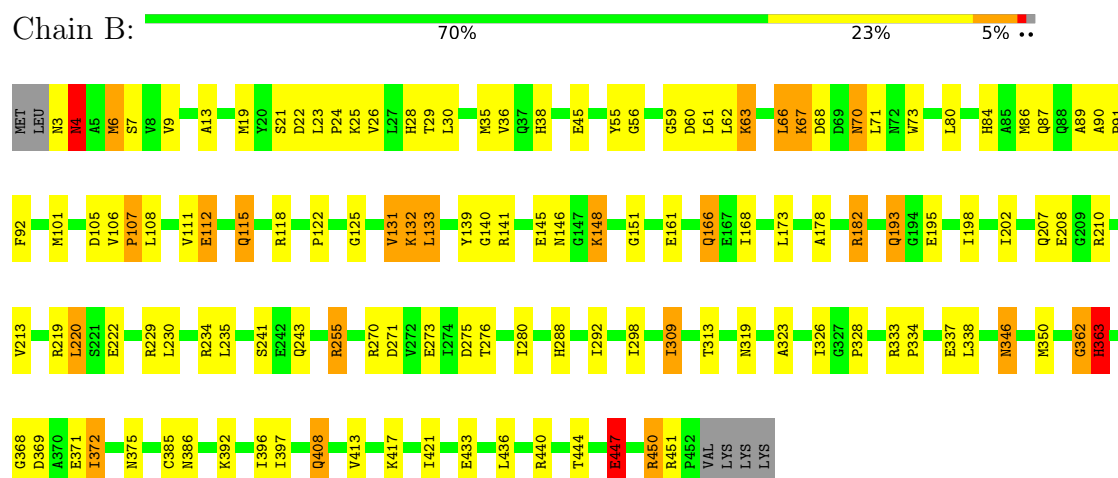
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: UDP-N-ACETYLGLUCOSAMINE PYROPHOSPHORYLASE



• Molecule 1: UDP-N-ACETYLGLUCOSAMINE PYROPHOSPHORYLASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	104.50Å 104.50Å 648.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.25 – 2.10	Depositor
% Data completeness (in resolution range)	95.3 (30.25-2.10)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.211 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7194	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO, COA, 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	0.50	0/3418	0.98	13/4638 (0.3%)
1	B	0.47	0/3436	0.95	14/4661 (0.3%)
All	All	0.49	0/6854	0.97	27/9299 (0.3%)

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	A	0	1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	ASN	N-CA-C	9.71	122.96	109.18
1	A	362	GLY	N-CA-C	9.61	125.07	112.77
1	B	447	GLU	N-CA-C	9.20	126.46	111.37
1	B	106	VAL	CA-C-N	8.26	128.21	119.05
1	B	106	VAL	C-N-CA	8.26	128.21	119.05
1	A	106	VAL	CA-C-N	7.90	127.56	119.19
1	A	106	VAL	C-N-CA	7.90	127.56	119.19
1	B	107	PRO	N-CA-C	7.22	123.56	113.53
1	B	22	ASP	N-CA-C	-6.84	104.67	113.16
1	A	29	THR	N-CA-C	6.54	119.38	110.55
1	A	107	PRO	N-CA-C	6.46	122.04	113.57
1	A	17	THR	N-CA-C	6.45	119.13	111.71
1	A	208	GLU	N-CA-C	-6.42	105.08	113.17
1	A	306	ASP	N-CA-C	6.33	120.33	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	GLU	N-CA-C	6.16	119.30	110.24
1	B	363	HIS	N-CA-C	5.99	118.25	108.55
1	A	363	HIS	N-CA-C	5.98	118.21	108.76
1	A	386	ASN	N-CA-C	5.87	119.96	113.21
1	B	323	ALA	N-CA-C	5.72	119.57	112.24
1	B	29	THR	N-CA-C	5.60	119.22	110.32
1	B	451	ARG	N-CA-C	-5.53	102.81	109.72
1	B	362	GLY	N-CA-C	5.29	125.71	113.18
1	B	140	GLY	N-CA-C	-5.12	104.58	111.54
1	B	271	ASP	N-CA-C	5.03	118.38	111.54
1	B	276	THR	N-CA-C	5.03	117.59	110.50
1	A	71	LEU	N-CA-C	5.03	116.95	108.96
1	A	267	THR	N-CA-C	-5.01	102.10	110.17

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	387	TYR	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	3370	0	3366	82	0
1	B	3388	0	3387	91	1
2	A	2	0	0	0	0
2	B	3	0	0	0	0
3	A	48	0	32	0	0
3	B	48	0	32	0	1
4	A	39	0	25	0	0
4	B	39	0	25	1	0
5	A	127	0	0	0	0
5	B	130	0	0	2	1
All	All	7194	0	6867	172	2

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 12.

All (172) 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:B:270:ARG:H	1:B:288:HIS:HD2	1.04	1.00
1:A:270:ARG:H	1:A:288:HIS:HD2	1.00	0.97
1:A:270:ARG:H	1:A:288:HIS:CD2	1.92	0.84
1:A:76:GLN:HE21	1:A:84:HIS:HD2	1.24	0.84
1:B:270:ARG:H	1:B:288:HIS:CD2	1.96	0.82
1:A:122:PRO:HG3	1:A:213:VAL:HG23	1.61	0.82
1:A:204:LEU:O	1:A:208:GLU:HG3	1.83	0.77
1:B:450:ARG:HH11	1:B:450:ARG:HA	1.48	0.76
1:A:59:GLY:O	1:A:63:LYS:HD3	1.86	0.76
1:B:447:GLU:HA	1:B:447:GLU:OE1	1.86	0.76
1:A:116:ARG:HH11	1:A:116:ARG:HG3	1.50	0.75
1:A:197:TYR:HB3	1:A:199:THR:HG22	1.68	0.74
1:A:197:TYR:HB3	1:A:199:THR:CG2	2.17	0.74
1:B:450:ARG:HA	1:B:450:ARG:NH1	2.02	0.74
1:B:4:ASN:HD22	1:B:4:ASN:N	1.86	0.73
1:A:193:GLN:HG3	1:A:197:TYR:OH	1.90	0.71
1:B:270:ARG:N	1:B:288:HIS:HD2	1.87	0.69
1:B:148:LYS:HB2	1:B:148:LYS:NZ	2.08	0.67
1:B:178:ALA:O	1:B:182:ARG:HG3	1.96	0.66
1:A:152:ILE:HB	1:A:199:THR:OG1	1.97	0.65
1:B:133:LEU:O	1:B:166:GLN:HG2	1.95	0.65
1:B:67:LYS:HD2	1:B:67:LYS:O	1.97	0.64
1:B:182:ARG:HH22	1:B:208:GLU:CD	2.05	0.64
1:B:193:GLN:HB3	1:B:195:GLU:HG3	1.79	0.64
1:B:3:ASN:HB3	1:B:4:ASN:HD22	1.63	0.63
1:A:270:ARG:N	1:A:288:HIS:HD2	1.84	0.62
1:B:292:ILE:HD13	1:B:298:ILE:CD1	2.30	0.62
1:B:122:PRO:HG2	1:B:125:GLY:HA3	1.82	0.61
1:B:68:ASP:HB2	1:B:71:LEU:HG	1.83	0.61
1:B:112:GLU:CD	1:B:112:GLU:H	2.09	0.60
1:B:386:ASN:O	1:B:392:LYS:HA	2.00	0.60
1:B:208:GLU:HB2	1:B:210:ARG:HG2	1.84	0.60
1:B:68:ASP:C	1:B:70:ASN:H	2.10	0.59
1:A:122:PRO:HG3	1:A:213:VAL:CG2	2.33	0.58
1:A:333:ARG:HB3	1:A:334:PRO:HD2	1.85	0.57
1:B:86:MET:HG3	1:B:198:ILE:HD13	1.86	0.57
1:A:141:ARG:NH2	1:A:155:HIS:ND1	2.53	0.56
1:A:219:ARG:O	1:A:222:GLU:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:MET:HE3	1:A:184:LEU:HG	1.88	0.56
1:A:177:GLY:O	1:A:181:LYS:HG3	2.05	0.56
1:A:388:ASP:OD1	1:A:388:ASP:C	2.49	0.56
1:A:212:ILE:HD12	1:A:212:ILE:N	2.20	0.56
1:B:198:ILE:O	1:B:198:ILE:HG13	2.07	0.56
1:B:313:THR:HG21	1:B:326:ILE:HD12	1.88	0.56
1:B:255:ARG:NH1	1:B:273:GLU:OE2	2.39	0.55
1:A:7:SER:OG	1:A:50:HIS:HB2	2.06	0.55
1:B:13:ALA:HB2	1:B:55:TYR:C	2.32	0.55
1:B:132:LYS:HG2	1:B:166:GLN:HB3	1.89	0.55
1:A:386:ASN:O	1:A:392:LYS:HA	2.06	0.55
1:A:116:ARG:HG3	1:A:116:ARG:NH1	2.18	0.55
1:A:133:LEU:HD12	1:A:168:ILE:HG12	1.89	0.55
1:B:148:LYS:HZ2	1:B:148:LYS:CB	2.19	0.55
1:B:19:MET:HG3	1:B:25:LYS:HG3	1.89	0.55
1:B:447:GLU:OE1	1:B:447:GLU:CA	2.52	0.55
1:A:141:ARG:HG3	1:A:165:ILE:HB	1.88	0.54
1:B:4:ASN:HD22	1:B:4:ASN:H	1.52	0.54
1:B:372:ILE:HD13	1:B:397:ILE:HD12	1.88	0.54
1:B:148:LYS:HB2	1:B:148:LYS:HZ2	1.72	0.54
1:B:151:GLY:HA2	1:B:202:ILE:CG2	2.37	0.54
1:B:70:ASN:O	1:B:71:LEU:HD23	2.07	0.54
1:B:68:ASP:C	1:B:70:ASN:N	2.62	0.53
1:A:291:LYS:HD2	1:A:308:GLU:OE2	2.09	0.53
1:A:148:LYS:O	1:A:150:THR:HG23	2.08	0.52
1:A:124:GLY:O	1:A:210:ARG:NH1	2.41	0.52
1:A:255:ARG:HB2	1:A:275:ASP:HA	1.91	0.52
1:A:182:ARG:O	1:A:186:LYS:HG3	2.09	0.52
1:A:179:ASP:HA	1:A:182:ARG:NH1	2.25	0.51
1:A:122:PRO:HG2	1:A:211:GLU:O	2.10	0.51
1:B:4:ASN:N	1:B:4:ASN:ND2	2.50	0.51
1:B:151:GLY:HA2	1:B:202:ILE:HG22	1.93	0.51
1:A:369:ASP:OD2	1:A:386:ASN:ND2	2.42	0.51
1:A:193:GLN:HB2	1:A:195:GLU:HG3	1.91	0.51
1:B:23:LEU:HD12	1:B:24:PRO:HD2	1.94	0.50
1:B:26:VAL:HB	1:B:36:VAL:HB	1.92	0.50
1:B:62:LEU:HD22	1:B:66:LEU:HD11	1.94	0.50
1:B:173:LEU:HD12	1:B:173:LEU:C	2.36	0.50
1:A:179:ASP:HB3	1:A:183:TRP:CH2	2.45	0.50
1:B:111:VAL:O	1:B:115:GLN:HG2	2.12	0.50
1:B:68:ASP:CB	1:B:71:LEU:HG	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LYS:HG3	1:A:192:ALA:HB1	1.93	0.49
1:A:363:HIS:CD2	1:A:363:HIS:N	2.81	0.49
1:B:333:ARG:HB3	1:B:334:PRO:HD2	1.93	0.49
1:A:346:ASN:HD22	1:A:346:ASN:C	2.21	0.49
1:A:26:VAL:HB	1:A:36:VAL:HB	1.95	0.49
1:B:30:LEU:O	1:B:38:HIS:HE1	1.96	0.49
1:B:243:GLN:HG3	5:B:6354:HOH:O	2.13	0.48
1:A:182:ARG:NH2	1:A:208:GLU:OE1	2.44	0.48
1:A:197:TYR:HB3	1:A:199:THR:HG23	1.95	0.48
1:A:363:HIS:CD2	1:A:380:ALA:HB2	2.48	0.48
1:B:146:ASN:HB2	1:B:148:LYS:NZ	2.29	0.48
1:A:198:ILE:O	1:A:201:ILE:HG12	2.14	0.48
1:B:333:ARG:HB3	1:B:334:PRO:CD	2.44	0.48
1:B:230:LEU:O	1:B:234:ARG:HG3	2.14	0.48
1:B:122:PRO:HG3	1:B:213:VAL:HG23	1.95	0.48
1:A:6:MET:HG2	1:A:7:SER:N	2.29	0.47
1:B:4:ASN:H	1:B:4:ASN:ND2	2.12	0.47
1:B:92:PHE:CD1	1:B:92:PHE:N	2.82	0.47
1:A:90:ALA:HB3	1:A:91:PRO:HD3	1.95	0.47
1:B:23:LEU:HD12	1:B:24:PRO:CD	2.45	0.47
1:B:105:ASP:C	1:B:107:PRO:HD3	2.40	0.47
1:B:362:GLY:C	1:B:363:HIS:CG	2.93	0.47
1:A:128:LEU:O	1:A:214:ALA:HA	2.15	0.46
1:A:115:GLN:HA	1:A:115:GLN:OE1	2.15	0.46
1:B:89:ALA:C	1:B:91:PRO:HD2	2.40	0.46
1:B:148:LYS:NZ	1:B:148:LYS:CB	2.75	0.46
1:A:362:GLY:C	1:A:363:HIS:CG	2.93	0.46
1:A:179:ASP:HB3	1:A:183:TRP:CZ2	2.50	0.46
1:A:35:MET:O	1:A:38:HIS:HB2	2.16	0.46
1:A:144:ARG:HA	1:A:148:LYS:O	2.15	0.46
1:B:6:MET:HE2	1:B:6:MET:HB2	1.74	0.46
1:B:60:ASP:HB2	5:B:5095:HOH:O	2.16	0.46
1:B:337:GLU:C	1:B:338:LEU:HD12	2.41	0.46
1:B:21:SER:HB2	1:B:229:ARG:NH2	2.31	0.45
1:B:108:LEU:HB2	1:B:222:GLU:HA	1.97	0.45
1:B:63:LYS:HA	1:B:73:TRP:CH2	2.52	0.45
1:A:444:THR:HG21	1:B:444:THR:HG21	1.99	0.45
1:A:351:LYS:O	1:A:368:GLY:HA2	2.15	0.45
1:A:328:PRO:O	1:A:346:ASN:HA	2.16	0.45
1:B:368:GLY:O	1:B:369:ASP:C	2.60	0.45
1:A:387:TYR:CE2	1:A:389:GLY:HA2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:MET:HE2	1:A:171:GLY:O	2.16	0.45
1:B:80:LEU:HB2	1:B:84:HIS:CG	2.51	0.45
1:A:133:LEU:CD1	1:A:168:ILE:HG12	2.47	0.44
1:B:66:LEU:HD12	1:B:73:TRP:HH2	1.82	0.44
1:A:116:ARG:HH11	1:A:116:ARG:CG	2.25	0.44
1:B:90:ALA:N	1:B:91:PRO:CD	2.80	0.44
1:B:131:VAL:HG21	1:B:220:LEU:HD22	2.00	0.43
1:A:156:LYS:HD3	1:A:156:LYS:HA	1.72	0.43
1:B:90:ALA:HB3	1:B:91:PRO:HD3	2.00	0.43
1:A:64:GLN:O	1:A:67:LYS:HE3	2.18	0.43
1:A:109:ILE:HG12	1:A:114:LEU:HD21	2.00	0.43
1:A:143:THR:HG23	1:A:153:VAL:HG23	1.99	0.43
1:B:255:ARG:HB2	1:B:275:ASP:HA	2.00	0.43
1:A:159:THR:O	1:A:163:ARG:HG3	2.19	0.43
1:B:30:LEU:HB3	1:B:38:HIS:CE1	2.53	0.43
1:A:248:LEU:HD11	1:A:257:PRO:HG3	2.00	0.43
1:A:30:LEU:C	1:A:30:LEU:HD23	2.44	0.42
1:A:108:LEU:O	1:A:109:ILE:C	2.63	0.42
1:A:388:ASP:OD1	1:A:390:ALA:N	2.51	0.42
1:B:328:PRO:O	1:B:346:ASN:HA	2.19	0.42
1:B:70:ASN:HD22	1:B:70:ASN:HA	1.62	0.42
1:B:101:MET:HE2	1:B:173:LEU:HG	2.02	0.42
1:B:168:ILE:H	1:B:168:ILE:HG13	1.74	0.42
1:B:35:MET:O	1:B:38:HIS:HB2	2.20	0.42
1:B:84:HIS:O	1:B:87:GLN:HB2	2.19	0.42
1:A:274:ILE:HG12	1:A:292:ILE:HD12	2.00	0.42
1:B:6:MET:HE3	1:B:118:ARG:CD	2.49	0.42
1:A:151:GLY:HA2	1:A:202:ILE:CG2	2.50	0.42
1:B:23:LEU:HB3	1:B:28:HIS:CE1	2.55	0.42
1:A:300:ASN:O	1:A:317:ASP:HA	2.20	0.41
1:A:347:PHE:HB2	1:A:364:LEU:HD13	2.02	0.41
1:B:313:THR:HG21	1:B:326:ILE:CD1	2.49	0.41
1:B:182:ARG:NH2	1:B:208:GLU:OE2	2.53	0.41
1:B:346:ASN:HD22	1:B:346:ASN:C	2.28	0.41
1:A:193:GLN:HE21	1:A:193:GLN:HB3	1.70	0.41
1:A:363:HIS:O	1:A:364:LEU:C	2.63	0.41
1:B:122:PRO:HD3	1:B:213:VAL:CG2	2.51	0.41
1:B:139:TYR:CD2	4:B:3002:UD1:H6'2	2.55	0.41
1:A:78:GLU:HB2	1:A:80:LEU:HD13	2.01	0.41
1:A:210:ARG:HG3	1:A:210:ARG:HH11	1.86	0.41
1:A:238:VAL:O	1:A:242:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ILE:HD13	1:B:298:ILE:HD11	2.03	0.41
1:B:350:MET:HE2	1:B:350:MET:HB3	1.97	0.41
1:A:239:TYR:O	1:A:243:GLN:HG2	2.21	0.40
1:B:309:ILE:HG23	1:B:326:ILE:HD11	2.03	0.40
1:A:88:GLN:O	1:A:91:PRO:HD2	2.22	0.40
1:A:180:MET:CE	1:A:184:LEU:HG	2.51	0.40
1:B:408:GLN:H	1:B:408:GLN:HG2	1.77	0.40
1:A:120:ALA:O	1:A:121:LYS:C	2.65	0.40
1:A:143:THR:CG2	1:A:153:VAL:HG23	2.51	0.40
1:A:333:ARG:HB3	1:A:334:PRO:CD	2.50	0.40
1:B:59:GLY:O	1:B:60:ASP:C	2.64	0.40

All (2) 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)
5:B:4035:HOH:O	5:B:4057:HOH:O[2_555]	1.93	0.27
1:B:385:CYS:CB	3:B:2002:COA:N4P[3_555]	2.06	0.14

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	447/456 (98%)	433 (97%)	14 (3%)	0	100	100
1	B	448/456 (98%)	430 (96%)	17 (4%)	1 (0%)	43	44
All	All	895/912 (98%)	863 (96%)	31 (4%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	348/362 (96%)	309 (89%)	39 (11%)	6	3
1	B	351/362 (97%)	305 (87%)	46 (13%)	4	2
All	All	699/724 (96%)	614 (88%)	85 (12%)	5	2

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	MET
1	A	7	SER
1	A	17	THR
1	A	18	ARG
1	A	33	LYS
1	A	61	LEU
1	A	63	LYS
1	A	70	ASN
1	A	80	LEU
1	A	115	GLN
1	A	116	ARG
1	A	118	ARG
1	A	123	GLN
1	A	141	ARG
1	A	156	LYS
1	A	164	GLN
1	A	180	MET
1	A	188	THR
1	A	193	GLN
1	A	195	GLU
1	A	215	VAL
1	A	220	LEU
1	A	221	SER
1	A	233	SER
1	A	234	ARG
1	A	255	ARG
1	A	280	ILE

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Mol	Chain	Res	Type
1	A	308	GLU
1	A	326	ILE
1	A	331	ARG
1	A	346	ASN
1	A	352	LYS
1	A	363	HIS
1	A	364	LEU
1	A	371	GLU
1	A	408	GLN
1	A	429	ARG
1	A	447	GLU
1	A	451	ARG
1	B	4	ASN
1	B	6	MET
1	B	7	SER
1	B	9	VAL
1	B	45	GLU
1	B	61	LEU
1	B	63	LYS
1	B	66	LEU
1	B	67	LYS
1	B	70	ASN
1	B	112	GLU
1	B	115	GLN
1	B	131	VAL
1	B	132	LYS
1	B	133	LEU
1	B	141	ARG
1	B	145	GLU
1	B	148	LYS
1	B	161	GLU
1	B	166	GLN
1	B	182	ARG
1	B	193	GLN
1	B	207	GLN
1	B	219	ARG
1	B	220	LEU
1	B	235	LEU
1	B	241	SER
1	B	255	ARG
1	B	280	ILE
1	B	309	ILE

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Mol	Chain	Res	Type
1	B	319	ASN
1	B	346	ASN
1	B	363	HIS
1	B	371	GLU
1	B	372	ILE
1	B	375	ASN
1	B	396	ILE
1	B	408	GLN
1	B	413	VAL
1	B	417	LYS
1	B	421	ILE
1	B	433	GLU
1	B	436	LEU
1	B	440	ARG
1	B	447	GLU
1	B	450	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	A	123	GLN
1	A	190	ASN
1	A	193	GLN
1	A	207	GLN
1	A	277	ASN
1	A	288	HIS
1	A	363	HIS
1	B	4	ASN
1	B	28	HIS
1	B	38	HIS
1	B	57	HIS
1	B	70	ASN
1	B	123	GLN
1	B	166	GLN
1	B	277	ASN
1	B	288	HIS
1	B	346	ASN
1	B	363	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 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 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$
4	UD1	A	3001	-	40,41,41	2.18	6 (15%)	59,62,62	1.07	5 (8%)
4	UD1	B	3002	2	40,41,41	2.13	7 (17%)	59,62,62	1.15	5 (8%)
3	COA	A	2001	-	47,50,50	1.11	2 (4%)	69,75,75	0.94	3 (4%)
3	COA	B	2002	-	47,50,50	1.19	2 (4%)	69,75,75	0.92	3 (4%)

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	UD1	A	3001	-	-	1/26/63/63	0/3/3/3
4	UD1	B	3002	2	-	1/26/63/63	0/3/3/3
3	COA	A	2001	-	-	10/48/64/64	0/3/3/3
3	COA	B	2002	-	-	12/48/64/64	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3001	UD1	PA-O3A	-10.07	1.48	1.59
4	B	3002	UD1	PA-O3A	-9.62	1.49	1.59
3	B	2002	COA	P1A-O3A	5.25	1.65	1.59
4	A	3001	UD1	C6-N1	5.14	1.50	1.38
4	B	3002	UD1	C6-N1	5.13	1.50	1.38
3	A	2001	COA	P1A-O3A	4.66	1.64	1.59
4	A	3001	UD1	PB-O3A	-4.10	1.55	1.59
4	B	3002	UD1	PB-O3A	-3.73	1.55	1.59
3	B	2002	COA	P2A-O3A	2.79	1.62	1.59
4	B	3002	UD1	C2-N3	-2.54	1.33	1.38
4	B	3002	UD1	C4-N3	-2.35	1.34	1.38
4	A	3001	UD1	C4-N3	-2.30	1.34	1.38
3	A	2001	COA	P2A-O3A	2.29	1.62	1.59
4	A	3001	UD1	C4'-C5'	2.25	1.57	1.53
4	B	3002	UD1	C1'-C2'	2.18	1.56	1.53
4	A	3001	UD1	C5-C4	2.13	1.48	1.43
4	B	3002	UD1	C5-C4	2.03	1.48	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3002	UD1	C5-C4-N3	3.11	119.16	114.80
3	A	2001	COA	C3B-C2B-C1B	2.81	106.06	99.89
4	B	3002	UD1	O2-C2-N1	2.73	126.35	122.80
4	A	3001	UD1	C5-C4-N3	2.69	118.57	114.80
4	B	3002	UD1	O2-C2-N3	-2.67	116.56	121.49
4	B	3002	UD1	O4-C4-C5	-2.66	120.58	125.16
3	B	2002	COA	C3B-C2B-C1B	2.50	105.40	99.89
4	A	3001	UD1	O2-C2-N3	-2.44	117.00	121.49
4	A	3001	UD1	O4-C4-C5	-2.33	121.14	125.16
3	B	2002	COA	P3B-O3B-C3B	2.28	129.53	123.43
3	A	2001	COA	P3B-O3B-C3B	2.28	129.51	123.43
3	B	2002	COA	O6A-CCP-CBP	2.27	114.19	110.55
4	A	3001	UD1	O2-C2-N1	2.19	125.64	122.80
3	A	2001	COA	O3B-C3B-C2B	2.16	119.41	111.68
4	A	3001	UD1	O5'-C1'-O1'	-2.09	108.63	111.36
4	B	3002	UD1	O2A-PA-O3A	2.02	112.73	107.27

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2002	COA	CCP-O6A-P2A-O5A
3	B	2002	COA	O9P-C9P-CAP-OAP
3	B	2002	COA	S1P-C2P-C3P-N4P
4	B	3002	UD1	C1'-O1'-PB-O3A
3	A	2001	COA	C2B-C3B-O3B-P3B
3	B	2002	COA	C2B-C3B-O3B-P3B
3	A	2001	COA	C3B-C4B-C5B-O5B
3	A	2001	COA	O4B-C4B-C5B-O5B
3	A	2001	COA	C4B-C3B-O3B-P3B
3	B	2002	COA	C4B-C3B-O3B-P3B
3	B	2002	COA	O4B-C4B-C5B-O5B
3	B	2002	COA	C3B-C4B-C5B-O5B
3	B	2002	COA	P2A-O3A-P1A-O2A
3	A	2001	COA	C5B-O5B-P1A-O3A
3	A	2001	COA	CCP-O6A-P2A-O3A
3	B	2002	COA	CCP-O6A-P2A-O3A
3	B	2002	COA	CCP-O6A-P2A-O4A
3	A	2001	COA	P2A-O3A-P1A-O1A
3	A	2001	COA	P2A-O3A-P1A-O2A
3	A	2001	COA	C2P-C3P-N4P-C5P
3	B	2002	COA	N8P-C9P-CAP-OAP
4	A	3001	UD1	PB-O3A-PA-O2A
3	A	2001	COA	N8P-C9P-CAP-OAP
3	B	2002	COA	P2A-O3A-P1A-O1A

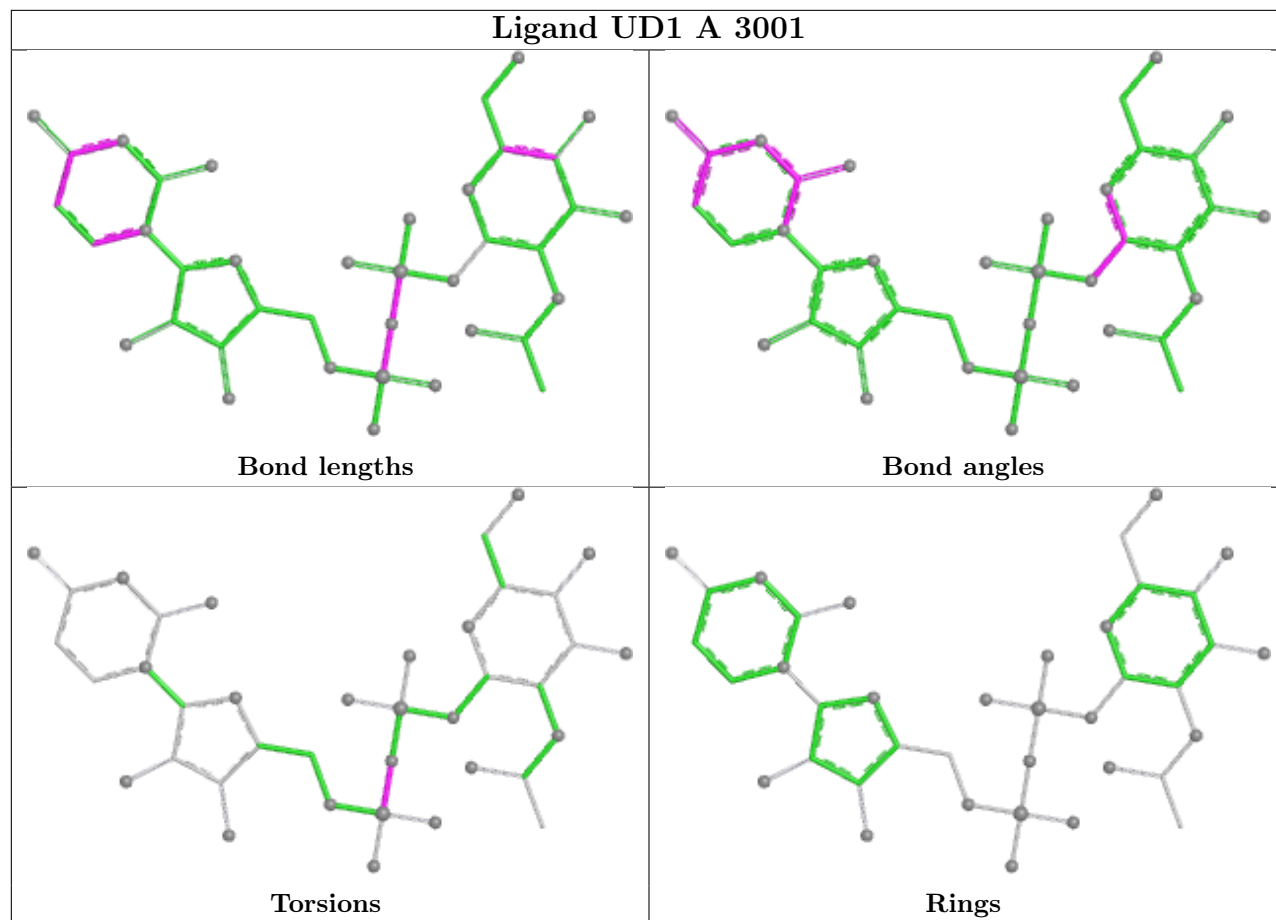
There are no ring outliers.

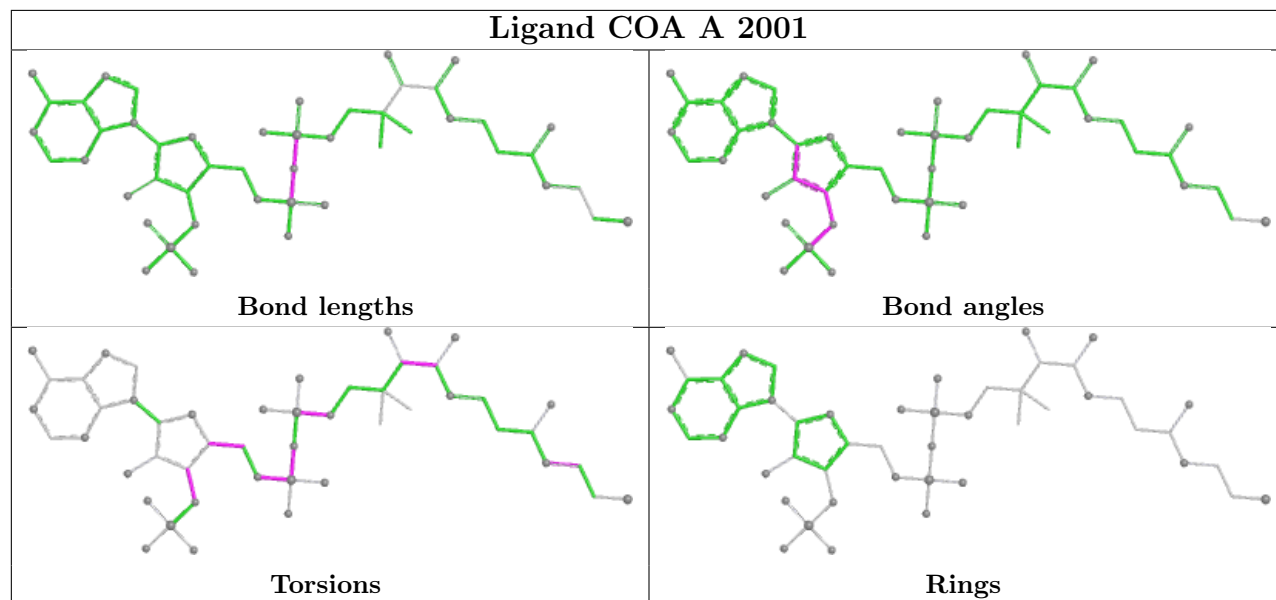
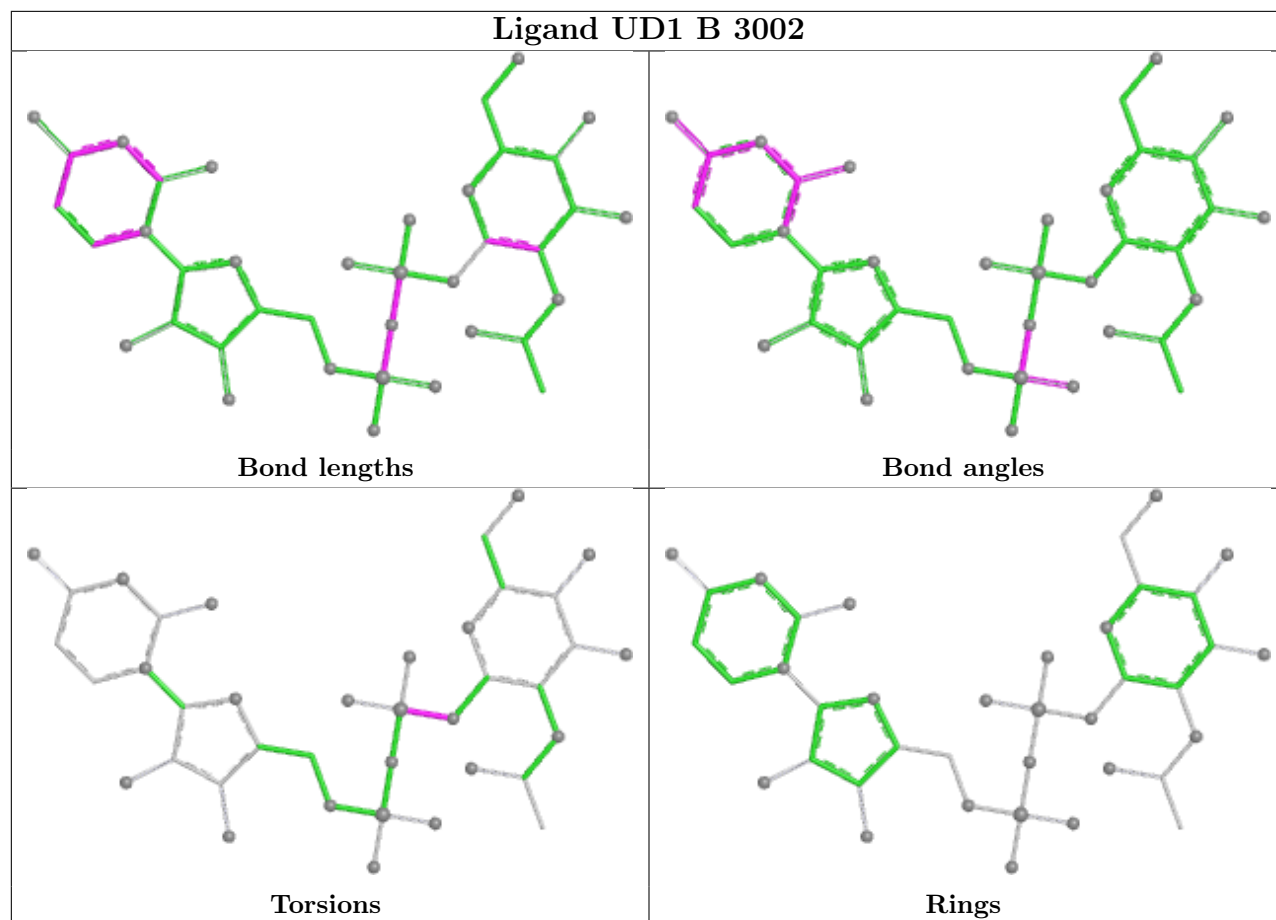
2 monomers are involved in 2 short contacts:

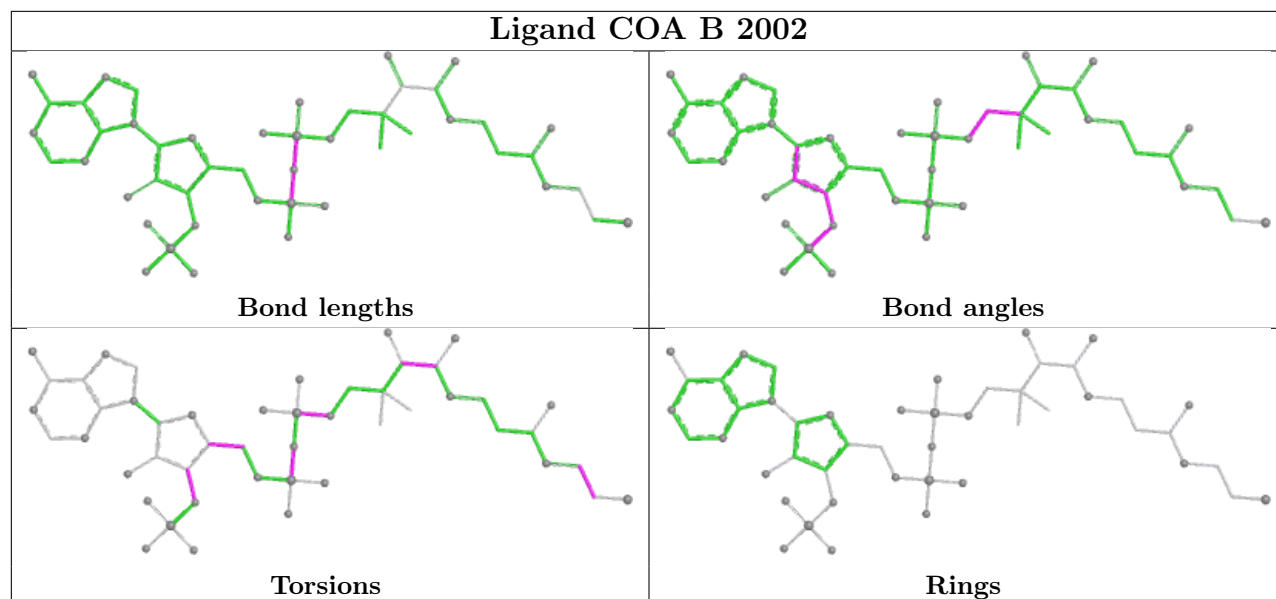
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	3002	UD1	1	0
3	B	2002	COA	0	1

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.