



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:12 AM UTC

PDB ID : 5F38 / pdb_00005f38
Title : X-ray crystal structure of a thiolase from Escherichia coli at 1.8 Å resolution
Authors : Ithayaraja, M.; Neelanjana, J.; Wierenga, R.; Savithri, H.S.; Murthy, M.R.N.
Deposited on : 2015-12-02
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

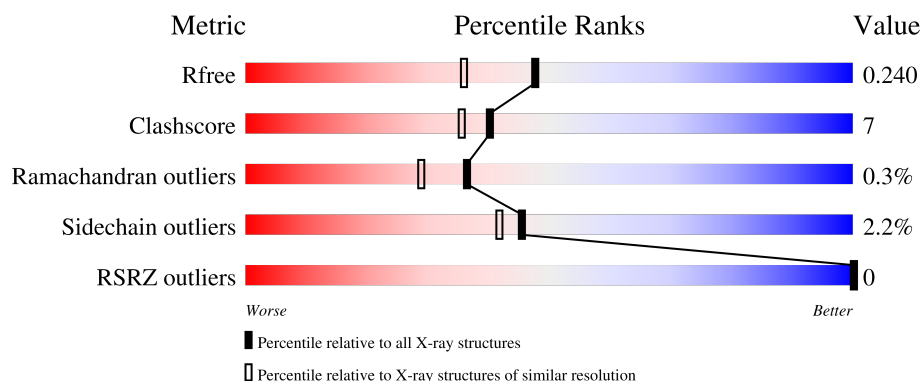
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	B	393	 92% 7% .
2	A	394	 85% 9% . 5%
3	D	394	 91% 8% .
4	C	395	 90% 9% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MLY	B	86	-	-	X	-
2	MLY	A	86	-	-	X	-
3	MLY	D	86	-	-	X	-
4	MLY	C	86	-	-	X	-
6	EDO	A	407	-	-	X	-
6	EDO	B	407	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12020 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 Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	392	Total	C	N	O	S	0	2	1
			2714	1702	471	525	16			

- Molecule 2 is a protein called Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	375	Total	C	N	O	S	0	2	4
			2503	1563	441	485	14			

- Molecule 3 is a protein called Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	394	Total	C	N	O	S	0	3	0
			2755	1734	475	529	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ALA	-	expression tag	UNP P76461
D	0	SER	-	expression tag	UNP P76461

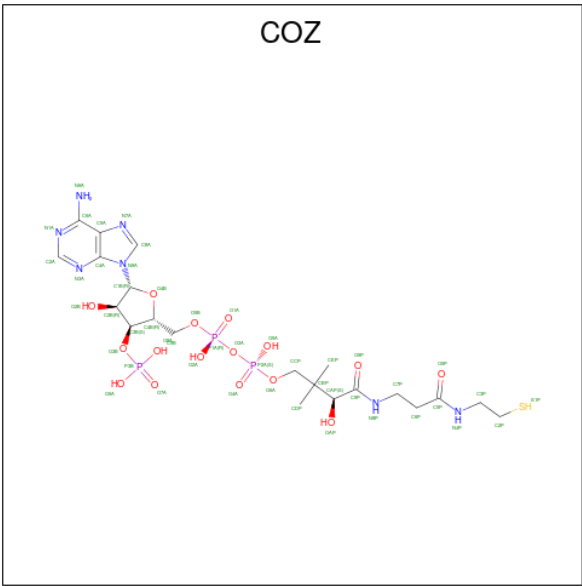
- Molecule 4 is a protein called Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	392	Total	C	N	O	S	0	4	0
			2791	1747	491	535	18			

There are 2 discrepancies between the modelled and reference sequences:

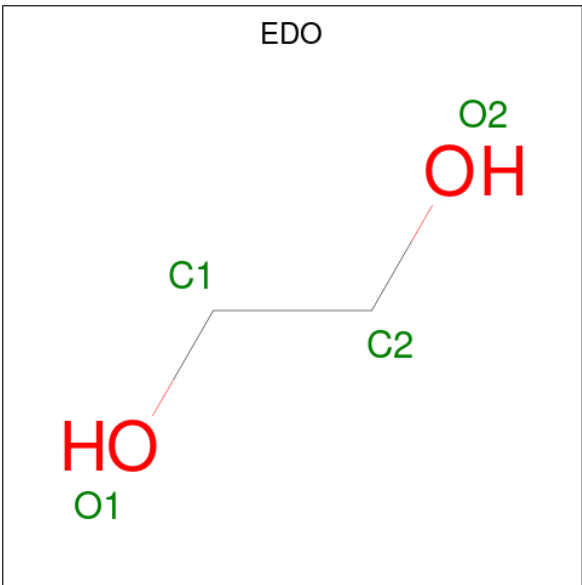
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	ALA	-	expression tag	UNP P76461
C	0	SER	-	expression tag	UNP P76461

- Molecule 5 is COENZYME A (CCD ID: COZ) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	B	1	4	2	2	0	0
6	B	1	4	2	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0

- # 5UG
-
- The chemical structure of 5-uridylyl-UMP (5UG) is shown. It consists of a uracil base (labeled O4A) linked via a pyrophosphate bridge to a ribose sugar (labeled O5A). The ribose is further linked via a pyrophosphate bridge to another ribose sugar (labeled O5A), which is then linked via a pyrophosphate bridge to a uracil base (labeled O4A). The structure is labeled with various atoms and groups, including O4A, O5A, O6A, O7A, O8A, O9A, O10A, O11A, O12A, O13A, O14A, O15A, O16A, O17A, O18A, O19A, O20A, O21A, O22A, O23A, O24A, O25A, O26A, O27A, O28A, O29A, O30A, O31A, O32A, O33A, O34A, O35A, O36A, O37A, O38A, O39A, O40A, O41A, O42A, O43A, O44A, O45A, O46A, O47A, O48A, O49A, O50A, O51A, O52A, O53A, O54A, O55A, O56A, O57A, O58A, O59A, O60A, O61A, O62A, O63A, O64A, O65A, O66A, O67A, O68A, O69A, O70A, O71A, O72A, O73A, O74A, O75A, O76A, O77A, O78A, O79A, O80A, O81A, O82A, O83A, O84A, O85A, O86A, O87A, O88A, O89A, O90A, O91A, O92A, O93A, O94A, O95A, O96A, O97A, O98A, O99A, O100A, O101A, O102A, O103A, O104A, O105A, O106A, O107A, O108A, O109A, O110A, O111A, O112A, O113A, O114A, O115A, O116A, O117A, O118A, O119A, O120A, O121A, O122A, O123A, O124A, O125A, O126A, O127A, O128A, O129A, O130A, O131A, O132A, O133A, O134A, O135A, O136A, O137A, O138A, O139A, O140A, O141A, O142A, O143A, O144A, O145A, O146A, O147A, O148A, O149A, O150A, O151A, O152A, O153A, O154A, O155A, O156A, O157A, O158A, O159A, O160A, O161A, O162A, O163A, O164A, O165A, O166A, O167A, O168A, O169A, O170A, O171A, O172A, O173A, O174A, O175A, O176A, O177A, O178A, O179A, O180A, O181A, O182A, O183A, O184A, O185A, O186A, O187A, O188A, O189A, O190A, O191A, O192A, O193A, O194A, O195A, O196A, O197A, O198A, O199A, O200A, O201A, O202A, O203A, O204A, O205A, O206A, O207A, O208A, O209A, O210A, O211A, O212A, O213A, O214A, O215A, O216A, O217A, O218A, O219A, O220A, O221A, O222A, O223A, O224A, O225A, O226A, O227A, O228A, O229A, O230A, O231A, O232A, O233A, O234A, O235A, O236A, O237A, O238A, O239A, O240A, O241A, O242A, O243A, O244A, O245A, O246A, O247A, O248A, O249A, O250A, O251A, O252A, O253A, O254A, O255A, O256A, O257A, O258A, O259A, O260A, O261A, O262A, O263A, O264A, O265A, O266A, O267A, O268A, O269A, O270A, O271A, O272A, O273A, O274A, O275A, O276A, O277A, O278A, O279A, O280A, O281A, O282A, O283A, O284A, O285A, O286A, O287A, O288A, O289A, O290A, O291A, O292A, O293A, O294A, O295A, O296A, O297A, O298A, O299A, O300A, O301A, O302A, O303A, O304A, O305A, O306A, O307A, O308A, O309A, O310A, O311A, O312A, O313A, O314A, O315A, O316A, O317A, O318A, O319A, O320A, O321A, O322A, O323A, O324A, O325A, O326A, O327A, O328A, O329A, O330A, O331A, O332A, O333A, O334A, O335A, O336A, O337A, O338A, O339A, O340A, O341A, O342A, O343A, O344A, O345A, O346A, O347A, O348A, O349A, O350A, O351A, O352A, O353A, O354A, O355A, O356A, O357A, O358A, O359A, O360A, O361A, O362A, O363A, O364A, O365A, O366A, O367A, O368A, O369A, O370A, O371A, O372A, O373A, O374A, O375A, O376A, O377A, O378A, O379A, O380A, O381A, O382A, O383A, O384A, O385A, O386A, O387A, O388A, O389A, O390A, O391A, O392A, O393A, O394A, O395A, O396A, O397A, O398A, O399A, O400A, O401A, O402A, O403A, O404A, O405A, O406A, O407A, O408A, O409A, O410A, O411A, O412A, O413A, O414A, O415A, O416A, O417A, O418A, O419A, O420A, O421A, O422A, O423A, O424A, O425A, O426A, O427A, O428A, O429A, O430A, O431A, O432A, O433A, O434A, O435A, O436A, O437A, O438A, O439A, O440A, O441A, O442A, O443A, O444A, O445A, O446A, O447A, O448A, O449A, O450A, O451A, O452A, O453A, O454A, O455A, O456A, O457A, O458A, O459A, O460A, O461A, O462A, O463A, O464A, O465A, O466A, O467A, O468A, O469A, O470A, O471A, O472A, O473A, O474A, O475A, O476A, O477A, O478A, O479A, O480A, O481A, O482A, O483A, O484A, O485A, O486A, O487A, O488A, O489A, O490A, O491A, O492A, O493A, O494A, O495A, O496A, O497A, O498A, O499A, O500A, O501A, O502A, O503A, O504A, O505A, O506A, O507A, O508A, O509A, O510A, O511A, O512A, O513A, O514A, O515A, O516A, O517A, O518A, O519A, O520A, O521A, O522A, O523A, O524A, O525A, O526A, O527A, O528A, O529A, O530A, O531A, O532A, O533A, O534A, O535A, O536A, O537A, O538A, O539A, O540A, O541A, O542A, O543A, O544A, O545A, O546A, O547A, O548A, O549A, O550A, O551A, O552A, O553A, O554A, O555A, O556A, O557A, O558A, O559A, O560A, O561A, O562A, O563A, O564A, O565A, O566A, O567A, O568A, O569A, O570A, O571A, O572A, O573A, O574A, O575A, O576A, O577A, O578A, O579A, O580A, O581A, O582A, O583A, O584A, O585A, O586A, O587A, O588A, O589A, O590A, O591A, O592A, O593A, O594A, O595A, O596A, O597A, O598A, O599A, O600A, O601A, O602A, O603A, O604A, O605A, O606A, O607A, O608A, O609A, O610A, O611A, O612A, O613A, O614A, O615A, O616A, O617A, O618A, O619A, O620A, O621A, O622A, O623A, O624A, O625A, O626A, O627A, O628A, O629A, O630A, O631A, O632A, O633A, O634A, O635A, O636A, O637A, O638A, O639A, O640A, O641A, O642A, O643A, O644A, O645A, O646A, O647A, O648A, O649A, O650A, O651A, O652A, O653A, O654A, O655A, O656A, O657A, O658A, O659A, O660A, O661A, O662A, O663A, O664A, O665A, O666A, O667A, O668A, O669A, O670A, O671A, O672A, O673A, O674A, O675A, O676A, O677A, O678A, O67

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	D	1	Total 26	C 11	N 2	O 10	P 2	S 1	0	0
7	C	1	Total 26	C 11	N 2	O 10	P 2	S 1	0	0

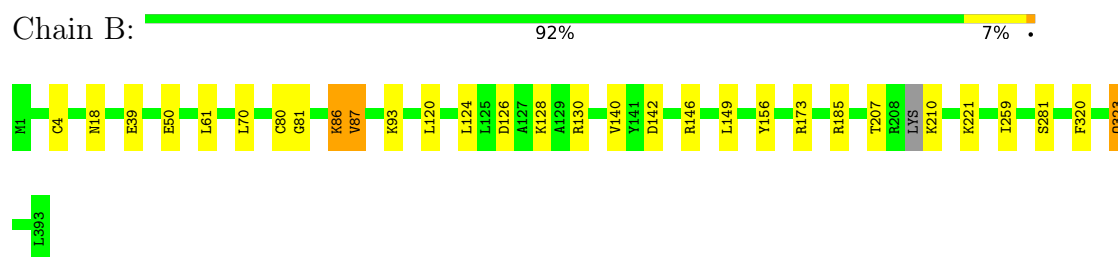
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	247	Total 247	O 247	0	0
8	A	175	Total 175	O 175	0	0
8	D	320	Total 320	O 320	0	0
8	C	291	Total 291	O 291	0	0

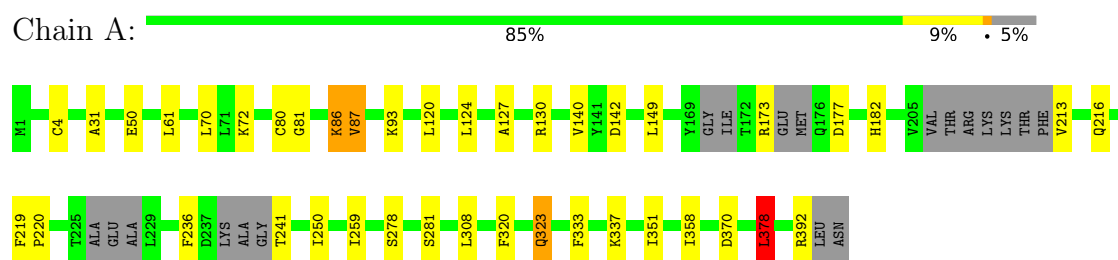
3 Residue-property plots [i](#)

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.

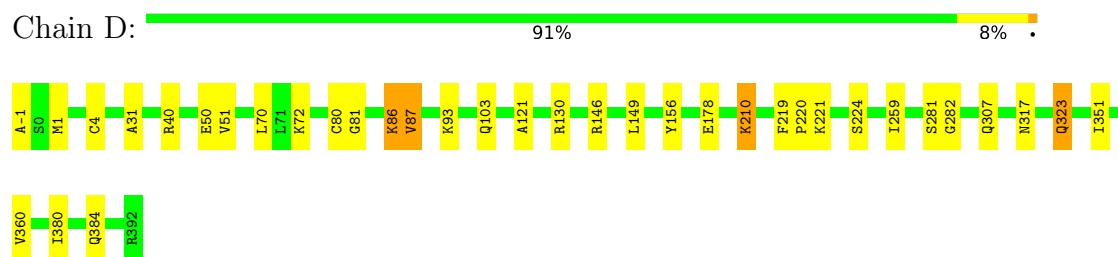
- Molecule 1: Acetyl-CoA acetyltransferase



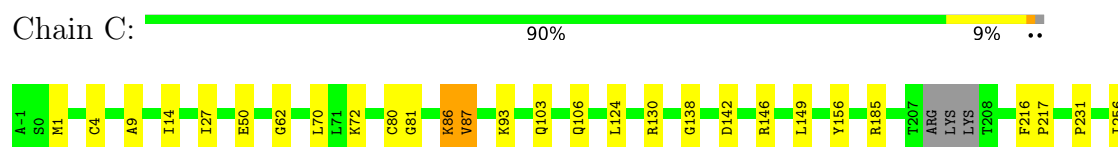
- Molecule 2: Acetyl-CoA acetyltransferase



- Molecule 3: Acetyl-CoA acetyltransferase



- Molecule 4: Acetyl-CoA acetyltransferase



P269	L270	S278	V281	Q320	R354	I355	H361	R389	L390
------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.79Å 76.25Å 266.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.80 – 1.90 36.80 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (36.80-1.90) 90.6 (36.80-1.90)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.03 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.197 , 0.235 0.203 , 0.240	Depositor DCC
R_{free} test set	5910 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.861	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.089 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12020	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: MLY, CSX, EDO, COZ, 5UG

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	B	1.03	0/2732	0.99	0/3701
2	A	0.94	0/2511	0.95	2/3384 (0.1%)
3	D	1.13	3/2777 (0.1%)	1.01	4/3760 (0.1%)
4	C	1.11	2/2811 (0.1%)	1.00	5/3802 (0.1%)
All	All	1.06	5/10831 (0.0%)	0.99	11/14647 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	360	VAL	N-CA	5.70	1.53	1.46
4	C	106	GLN	C-O	-5.48	1.16	1.24
4	C	355	ILE	C-O	-5.43	1.17	1.24
3	D	51	VAL	CA-CB	-5.02	1.48	1.54
3	D	282	GLY	N-CA	5.00	1.50	1.45

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	389	ARG	CA-C-N	6.13	132.73	121.70
4	C	389	ARG	C-N-CA	6.13	132.73	121.70
3	D	323	GLN	CA-CB-CG	6.10	126.29	114.10
4	C	389	ARG	O-C-N	-6.09	115.83	123.01
3	D	210	LYS	N-CA-C	5.87	118.03	108.76

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	B	2714	0	2672	46	0
2	A	2503	0	2380	54	0
3	D	2755	0	2752	35	0
4	C	2791	0	2814	37	0
5	B	48	0	32	3	0
6	A	40	0	60	16	0
6	B	28	0	42	7	0
6	C	16	0	24	4	0
6	D	40	0	60	2	0
7	C	26	0	0	0	0
7	D	26	0	0	0	0
8	A	175	0	0	3	0
8	B	247	0	0	9	1
8	C	291	0	0	6	1
8	D	320	0	0	9	0
All	All	12020	0	10836	143	1

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.

The worst 5 of 143 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:124:LEU:CD2	2:A:124:LEU:HD23	1.74	1.16
1:B:124:LEU:HD23	2:A:124:LEU:CD2	1.72	1.16
2:A:213:VAL:N	6:A:408:EDO:HO2	1.44	1.16
1:B:124:LEU:CD2	2:A:124:LEU:CD2	2.25	1.14
3:D:50:GLU:OE2	4:C:86:MLY:HH21	1.56	1.04

All (1) 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)
8:B:723:HOH:O	8:C:719:HOH:O[1_445]	2.17	0.03

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	B	388/393 (99%)	379 (98%)	8 (2%)	1 (0%)	36	29
2	A	359/394 (91%)	346 (96%)	12 (3%)	1 (0%)	36	29
3	D	393/394 (100%)	381 (97%)	11 (3%)	1 (0%)	36	29
4	C	390/395 (99%)	380 (97%)	9 (2%)	1 (0%)	36	29
All	All	1530/1576 (97%)	1486 (97%)	40 (3%)	4 (0%)	36	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	87	VAL
1	B	87	VAL
2	A	87	VAL
3	D	87	VAL

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	B	253/280 (90%)	247 (98%)	6 (2%)	43	38
2	A	218/281 (78%)	211 (97%)	7 (3%)	34	27
3	D	260/280 (93%)	255 (98%)	5 (2%)	50	47
4	C	269/281 (96%)	263 (98%)	6 (2%)	45	42
All	All	1000/1122 (89%)	976 (98%)	24 (2%)	45	38

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	87	VAL
3	D	323	GLN
3	D	156	TYR
4	C	70	LEU
2	A	70	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	364	HIS
4	C	103	GLN
4	C	361	HIS
2	A	176	GLN
1	B	364	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](#)

8 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSX	B	88	1	3,6,7	0.61	0	1,6,8	0.96	0
3	MLY	D	86	3	9,10,11	1.22	0	6,11,13	2.18	2 (33%)
4	MLY	C	86	4	9,10,11	1.90	2 (22%)	6,11,13	1.89	2 (33%)
2	MLY	A	86	2	9,10,11	1.66	2 (22%)	6,11,13	2.14	2 (33%)
3	CSX	D	88	3	3,6,7	1.10	0	1,6,8	0.89	0
4	CSX	C	88	4	3,6,7	1.22	0	1,6,8	0.61	0
1	MLY	B	86	1	9,10,11	1.31	0	6,11,13	1.93	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CSX	A	88	2	3,6,7	0.63	0	1,6,8	1.43	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
1	CSX	B	88	1	-	0/2/5/7	-
3	MLY	D	86	3	-	2/8/9/11	-
4	MLY	C	86	4	-	2/8/9/11	-
2	MLY	A	86	2	-	2/8/9/11	-
3	CSX	D	88	3	-	0/2/5/7	-
4	CSX	C	88	4	-	0/2/5/7	-
1	MLY	B	86	1	-	2/8/9/11	-
2	CSX	A	88	2	-	0/2/5/7	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	86	MLY	CD-CE	3.95	1.67	1.51
2	A	86	MLY	CB-CA	3.00	1.58	1.53
4	C	86	MLY	CH1-NZ	-2.81	1.37	1.46
2	A	86	MLY	CD-CE	2.68	1.62	1.51

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	86	MLY	CH2-NZ-CE	4.25	127.60	110.75
2	A	86	MLY	CH2-NZ-CE	4.18	127.34	110.75
1	B	86	MLY	CH2-NZ-CE	3.61	125.05	110.75
4	C	86	MLY	CD-CG-CB	3.53	126.94	113.62
3	D	86	MLY	CD-CG-CB	2.90	124.55	113.62

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	86	MLY	CG-CD-CE-NZ
4	C	86	MLY	CG-CD-CE-NZ

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	86	MLY	CG-CD-CE-NZ
3	D	86	MLY	CG-CD-CE-NZ
4	C	86	MLY	CE-CD-CG-CB

There are no ring outliers.

4 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	86	MLY	9	0
4	C	86	MLY	10	0
2	A	86	MLY	9	0
1	B	86	MLY	11	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

34 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	$\# Z > 2$
6	EDO	D	411	-	3,3,3	0.34	0	2,2,2	1.00	0
6	EDO	A	401	-	3,3,3	0.44	0	2,2,2	0.58	0
6	EDO	A	409	-	3,3,3	0.47	0	2,2,2	0.41	0
6	EDO	D	405	-	3,3,3	0.51	0	2,2,2	0.27	0
6	EDO	C	405	-	3,3,3	0.48	0	2,2,2	0.29	0
6	EDO	D	410	-	3,3,3	0.92	0	2,2,2	0.40	0
6	EDO	B	404	-	3,3,3	0.65	0	2,2,2	0.13	0
7	5UG	D	401	-	21,25,25	1.50	2 (9%)	31,36,36	1.67	9 (29%)
7	5UG	C	401	-	21,25,25	1.29	2 (9%)	31,36,36	1.99	8 (25%)
6	EDO	C	402	-	3,3,3	0.62	0	2,2,2	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	D	409	-	3,3,3	0.42	0	2,2,2	0.38	0
6	EDO	A	408	-	3,3,3	0.51	0	2,2,2	0.47	0
6	EDO	A	404	-	3,3,3	0.48	0	2,2,2	0.32	0
6	EDO	B	406	-	3,3,3	0.31	0	2,2,2	0.53	0
6	EDO	A	406	-	3,3,3	0.60	0	2,2,2	0.45	0
6	EDO	B	402	-	3,3,3	0.56	0	2,2,2	0.43	0
6	EDO	B	405	-	3,3,3	0.43	0	2,2,2	0.22	0
6	EDO	D	404	-	3,3,3	0.58	0	2,2,2	0.37	0
6	EDO	D	408	-	3,3,3	0.39	0	2,2,2	0.20	0
6	EDO	A	407	-	3,3,3	0.21	0	2,2,2	0.50	0
6	EDO	B	403	-	3,3,3	0.21	0	2,2,2	0.70	0
5	COZ	B	401	-	47,50,50	1.62	6 (12%)	69,75,75	2.16	19 (27%)
6	EDO	D	407	-	3,3,3	0.44	0	2,2,2	0.39	0
6	EDO	A	403	-	3,3,3	0.47	0	2,2,2	0.53	0
6	EDO	D	406	-	3,3,3	0.35	0	2,2,2	0.45	0
6	EDO	A	402	-	3,3,3	0.50	0	2,2,2	0.54	0
6	EDO	C	404	-	3,3,3	0.44	0	2,2,2	0.59	0
6	EDO	B	408	-	3,3,3	0.52	0	2,2,2	0.47	0
6	EDO	B	407	-	3,3,3	0.61	0	2,2,2	0.20	0
6	EDO	A	410	-	3,3,3	0.57	0	2,2,2	0.14	0
6	EDO	D	403	-	3,3,3	0.61	0	2,2,2	0.17	0
6	EDO	A	405	-	3,3,3	0.51	0	2,2,2	0.25	0
6	EDO	C	403	-	3,3,3	0.55	0	2,2,2	0.37	0
6	EDO	D	402	-	3,3,3	0.39	0	2,2,2	0.75	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
6	EDO	D	411	-	-	1/1/1/1	-
6	EDO	A	401	-	-	1/1/1/1	-
6	EDO	A	409	-	-	0/1/1/1	-
6	EDO	D	405	-	-	1/1/1/1	-
6	EDO	C	405	-	-	0/1/1/1	-
6	EDO	D	410	-	-	0/1/1/1	-
6	EDO	B	404	-	-	1/1/1/1	-
7	5UG	D	401	-	-	4/33/33/33	-
7	5UG	C	401	-	-	8/33/33/33	-
6	EDO	C	402	-	-	1/1/1/1	-
6	EDO	D	409	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	408	-	-	0/1/1/1	-
6	EDO	A	404	-	-	1/1/1/1	-
6	EDO	B	406	-	-	1/1/1/1	-
6	EDO	A	406	-	-	0/1/1/1	-
6	EDO	B	402	-	-	1/1/1/1	-
6	EDO	B	405	-	-	1/1/1/1	-
6	EDO	D	404	-	-	0/1/1/1	-
6	EDO	D	408	-	-	1/1/1/1	-
6	EDO	A	407	-	-	0/1/1/1	-
6	EDO	B	403	-	-	0/1/1/1	-
5	COZ	B	401	-	-	10/48/64/64	0/3/3/3
6	EDO	D	407	-	-	1/1/1/1	-
6	EDO	A	403	-	-	1/1/1/1	-
6	EDO	D	406	-	-	1/1/1/1	-
6	EDO	A	402	-	-	0/1/1/1	-
6	EDO	C	404	-	-	1/1/1/1	-
6	EDO	B	408	-	-	1/1/1/1	-
6	EDO	B	407	-	-	0/1/1/1	-
6	EDO	A	410	-	-	0/1/1/1	-
6	EDO	D	403	-	-	1/1/1/1	-
6	EDO	A	405	-	-	1/1/1/1	-
6	EDO	C	403	-	-	1/1/1/1	-
6	EDO	D	402	-	-	1/1/1/1	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	401	COZ	P1A-O3A	5.07	1.65	1.59
5	B	401	COZ	C5A-C4A	4.82	1.47	1.39
5	B	401	COZ	P2A-O3A	4.70	1.64	1.59
7	D	401	5UG	P2A-O3A	4.61	1.64	1.59
7	D	401	5UG	P1A-O5B	4.02	1.63	1.50

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	401	COZ	CEP-CBP-CAP	7.47	121.50	108.77
5	B	401	COZ	C5A-C4A-N3A	-6.44	117.84	126.72
7	C	401	5UG	CEP-CBP-CAP	5.97	118.95	108.77
5	B	401	COZ	N3A-C4A-N9A	5.01	135.69	127.17
5	B	401	COZ	CDP-CBP-CAP	-4.85	100.50	108.77

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	401	COZ	OAP-CAP-CBP-CCP
5	B	401	COZ	OAP-CAP-CBP-CDP
5	B	401	COZ	OAP-CAP-CBP-CEP
5	B	401	COZ	O9P-C9P-CAP-OAP
7	D	401	5UG	OAP-CAP-CBP-CEP

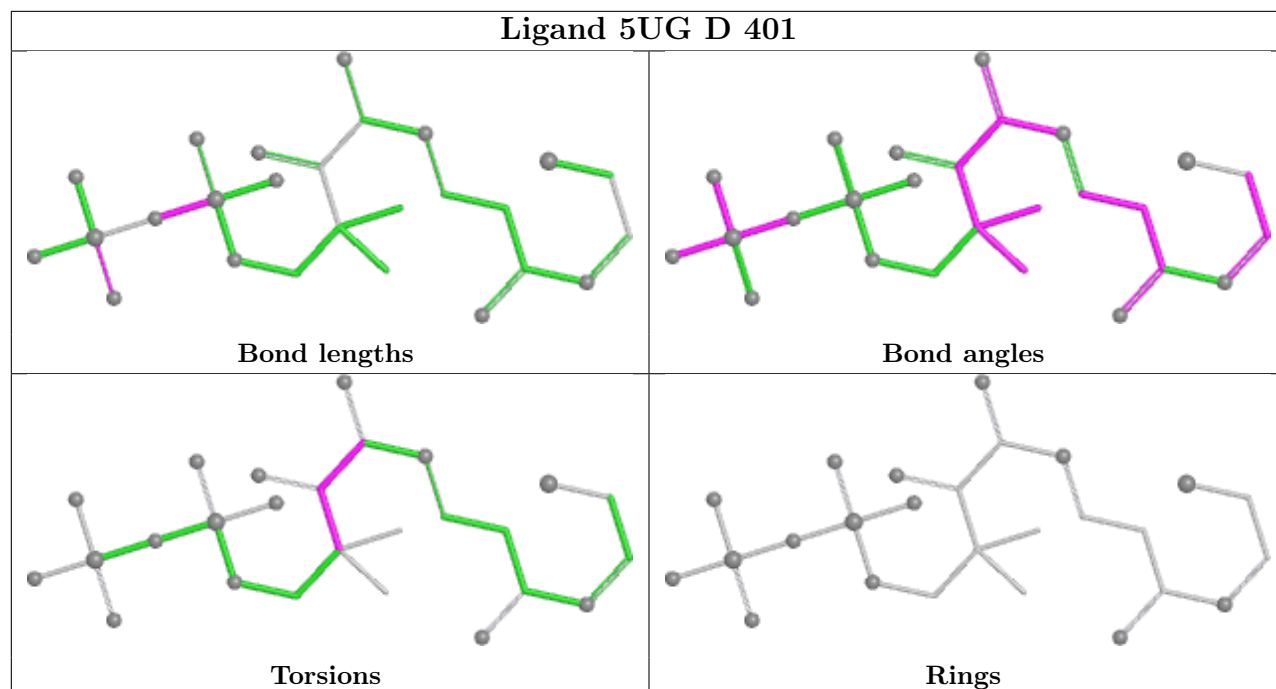
There are no ring outliers.

17 monomers are involved in 32 short contacts:

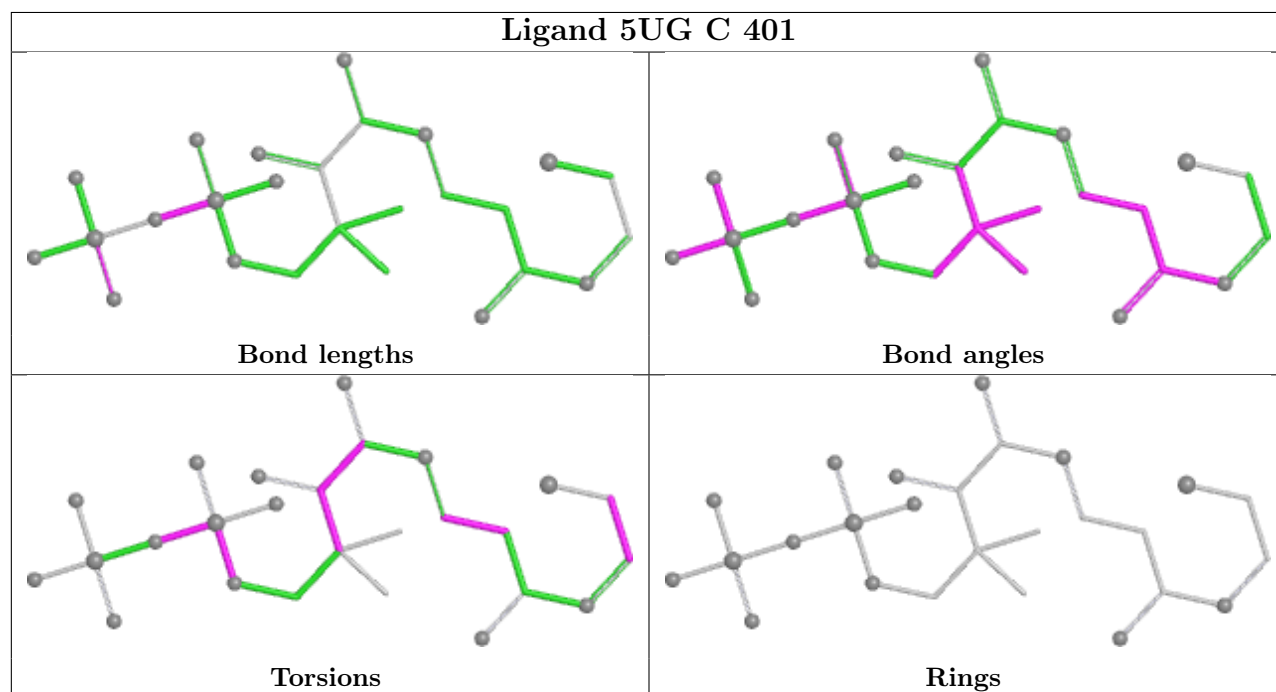
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	401	EDO	1	0
6	D	405	EDO	1	0
6	C	402	EDO	1	0
6	A	408	EDO	2	0
6	A	404	EDO	2	0
6	B	406	EDO	1	0
6	A	406	EDO	1	0
6	B	402	EDO	1	0
6	A	407	EDO	5	0
5	B	401	COZ	3	0
6	A	403	EDO	2	0
6	D	406	EDO	1	0
6	A	402	EDO	2	0
6	B	408	EDO	1	0
6	B	407	EDO	5	0
6	A	410	EDO	1	0
6	C	403	EDO	3	0

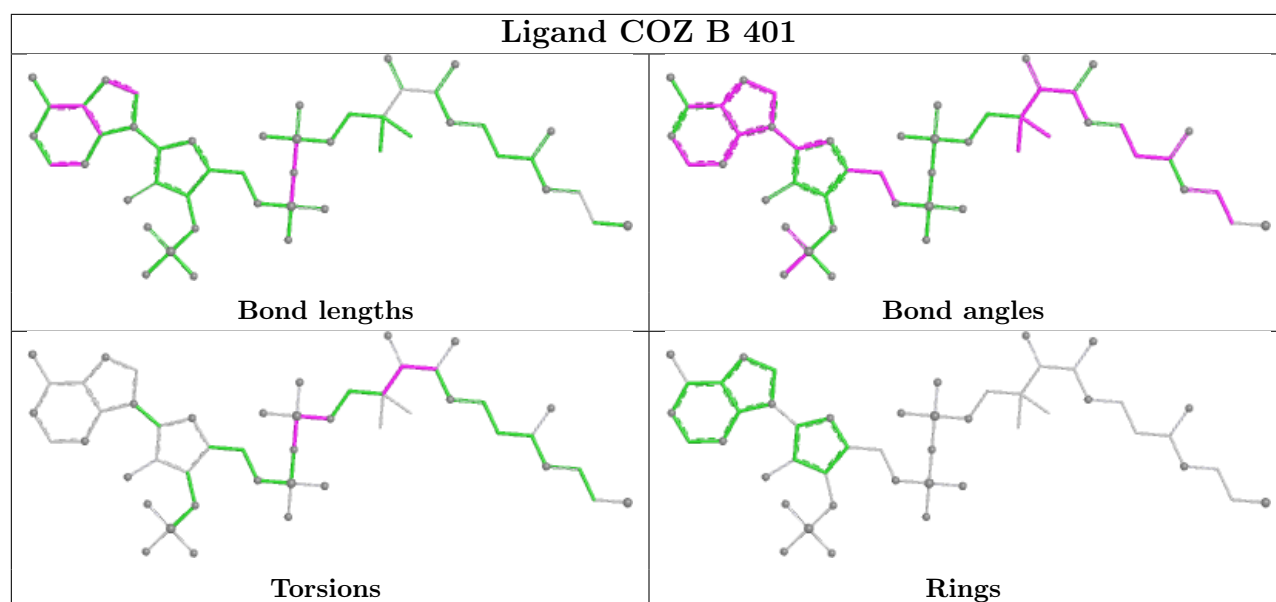
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand 5UG D 401



Ligand 5UG C 401





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	B	390/393 (99%)	-1.09	0 100 100	13, 29, 51, 66	2 (0%)
2	A	373/394 (94%)	-0.85	0 100 100	16, 37, 65, 82	2 (0%)
3	D	392/394 (99%)	-1.29	0 100 100	9, 21, 44, 61	3 (0%)
4	C	390/395 (98%)	-1.25	0 100 100	9, 23, 45, 54	4 (1%)
All	All	1545/1576 (98%)	-1.12	0 100 100	9, 27, 51, 82	11 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	MLY	A	86	11/12	0.98	0.04	17,18,19,19	0
1	CSX	B	88	7/8	0.99	0.03	18,19,30,34	0
1	MLY	B	86	11/12	0.99	0.03	15,17,17,18	0
2	CSX	A	88	7/8	0.99	0.04	23,24,32,33	0
3	MLY	D	86	11/12	0.99	0.03	11,12,14,15	0
3	CSX	D	88	7/8	0.99	0.04	16,17,29,30	0
4	MLY	C	86	11/12	0.99	0.03	10,11,13,13	0
4	CSX	C	88	7/8	1.00	0.03	15,17,24,29	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

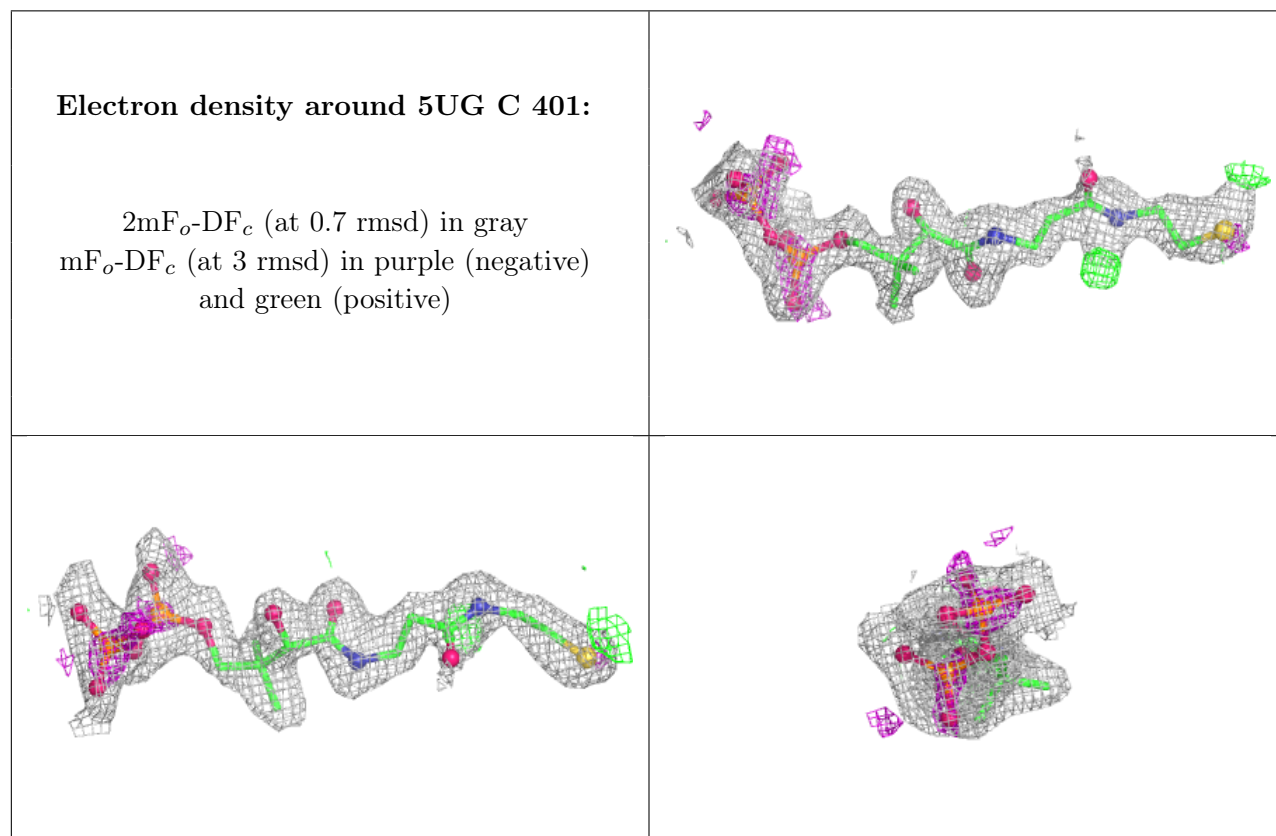
6.4 Ligands ⓘ

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(Å ²)	Q<0.9
6	EDO	D	402	4/4	0.95	0.10	42,43,43,44	0
6	EDO	D	405	4/4	0.95	0.06	47,49,51,52	0
6	EDO	D	404	4/4	0.96	0.07	48,49,51,52	0
6	EDO	A	408	4/4	0.96	0.05	48,48,50,51	0
6	EDO	C	404	4/4	0.96	0.07	46,48,49,52	0
6	EDO	A	404	4/4	0.97	0.06	34,40,42,44	0
6	EDO	A	406	4/4	0.97	0.06	38,40,41,43	0
6	EDO	B	402	4/4	0.97	0.08	34,37,38,38	0
6	EDO	A	409	4/4	0.97	0.06	51,51,51,52	0
6	EDO	B	405	4/4	0.97	0.06	44,46,47,49	0
6	EDO	B	408	4/4	0.97	0.07	30,40,43,57	0
6	EDO	A	401	4/4	0.97	0.07	47,48,49,49	0
6	EDO	D	406	4/4	0.97	0.06	54,55,56,57	0
6	EDO	A	403	4/4	0.97	0.04	37,38,41,45	0
7	5UG	C	401	26/26	0.97	0.05	26,30,40,41	0
6	EDO	A	405	4/4	0.98	0.07	42,43,43,44	0
6	EDO	D	403	4/4	0.98	0.05	39,42,44,53	0
5	COZ	B	401	48/48	0.98	0.05	24,39,83,89	0
6	EDO	A	407	4/4	0.98	0.05	33,33,34,35	0
6	EDO	B	406	4/4	0.98	0.07	45,50,52,53	0
6	EDO	D	407	4/4	0.98	0.04	33,35,36,36	0
6	EDO	D	408	4/4	0.98	0.05	32,39,39,46	0
6	EDO	D	409	4/4	0.98	0.04	49,50,51,56	0
6	EDO	D	411	4/4	0.98	0.05	33,38,39,40	0
6	EDO	C	402	4/4	0.98	0.06	35,42,42,48	0
6	EDO	C	403	4/4	0.98	0.09	28,31,33,39	0
6	EDO	B	404	4/4	0.98	0.05	40,43,45,45	0
6	EDO	C	405	4/4	0.98	0.05	44,47,47,52	0
7	5UG	D	401	26/26	0.98	0.04	14,19,39,47	0
6	EDO	A	410	4/4	0.98	0.06	46,47,48,49	0
6	EDO	D	410	4/4	0.99	0.04	25,26,31,33	0
6	EDO	B	407	4/4	0.99	0.07	19,20,20,25	0
6	EDO	A	402	4/4	0.99	0.10	20,23,24,26	0
6	EDO	B	403	4/4	0.99	0.05	37,39,43,47	0

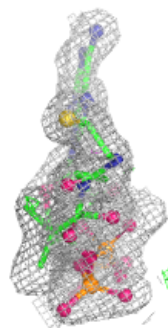
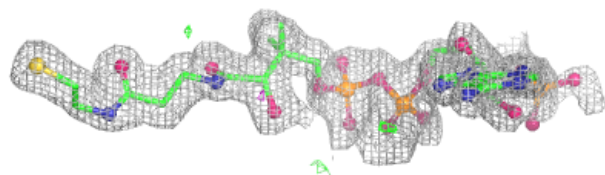
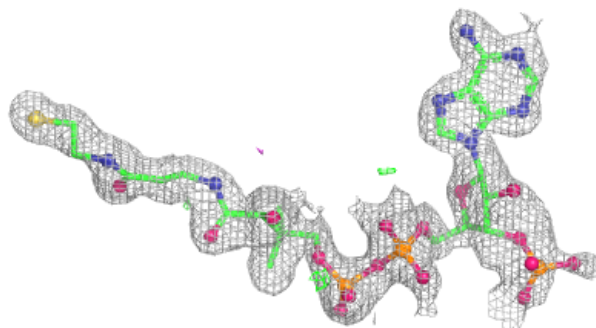
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

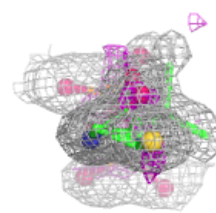
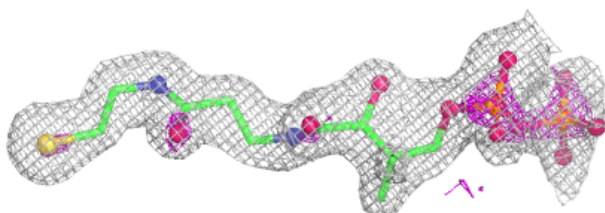
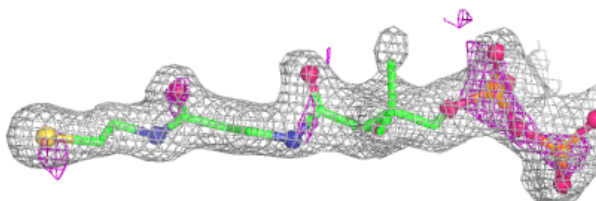


Electron density around COZ B 401:

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

**Electron density around 5UG D 401:**

$2mF_o-DF_c$ (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.