



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2025 – 10:08 AM EDT

PDB ID : 5S7Q / pdb\_00005s7q  
Title : XChem group deposition – Crystal Structure of human ACVR1 in complex with FM010944a  
Authors : Williams, E.P.; Adamson, R.J.; Smil, D.; Krojer, T.; Burgess-Brown, N.; von Delft, F.; Bountra, C.; Bullock, A.N.  
Deposited on : 2020-12-11  
Resolution : 1.53 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

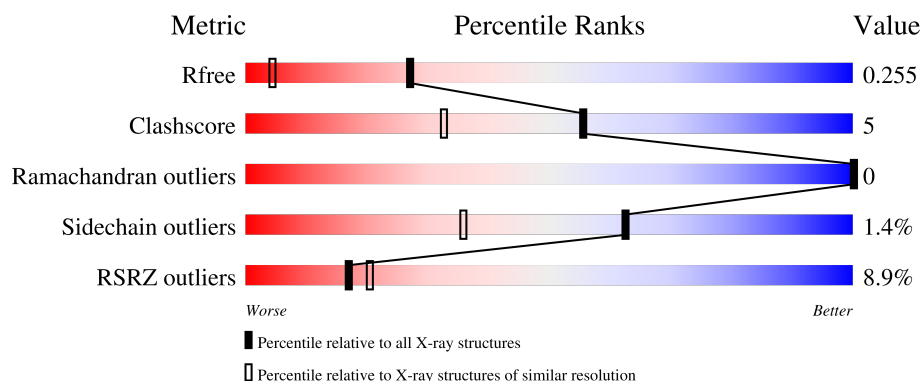
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.53 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))
$R_{free}$	164625	3511 (1.56-1.52)
Clashscore	180529	3784 (1.56-1.52)
Ramachandran outliers	177936	3720 (1.56-1.52)
Sidechain outliers	177891	3717 (1.56-1.52)
RSRZ outliers	164620	3510 (1.56-1.52)

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  $\geq 3$ , 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	301	<div> <div>9%</div> <div>84%</div> <div>9%</div> <div>6%</div> </div>
1	B	301	<div> <div>8%</div> <div>88%</div> <div>8%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5586 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.

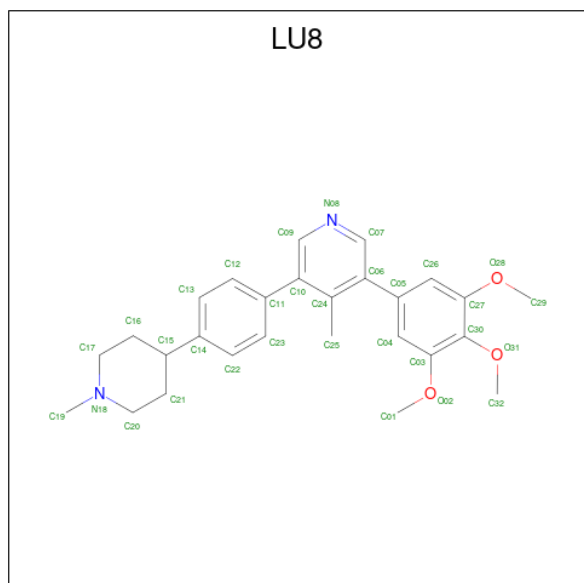
- Molecule 1 is a protein called Activin receptor type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	13	0
			2327	1488	397	427	15			
1	B	291	Total	C	N	O	S	0	7	0
			2351	1497	405	433	16			

There are 6 discrepancies between the modelled and reference sequences:

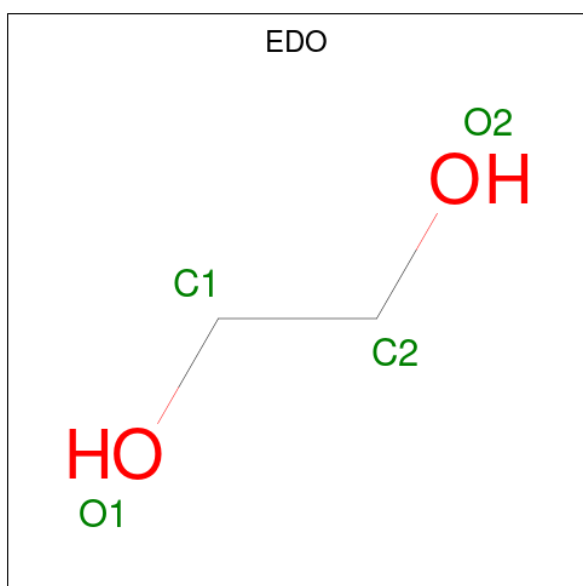
Chain	Residue	Modelled	Actual	Comment	Reference
A	199	SER	-	expression tag	UNP Q04771
A	200	MET	-	expression tag	UNP Q04771
A	207	ASP	GLN	engineered mutation	UNP Q04771
B	199	SER	-	expression tag	UNP Q04771
B	200	MET	-	expression tag	UNP Q04771
B	207	ASP	GLN	engineered mutation	UNP Q04771

- Molecule 2 is 4-methyl-3-[4-(1-methylpiperidin-4-yl)phenyl]-5-(3,4,5-trimethoxyphenyl)pyridine (CCD ID: LU8) (formula: C<sub>27</sub>H<sub>32</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	1
			64	54	4	6		
2	A	1	Total	C	N	O	0	0
			32	27	2	3		
2	A	1	Total	C	N	O	0	0
			32	27	2	3		
2	B	1	Total	C	N	O	0	0
			32	27	2	3		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



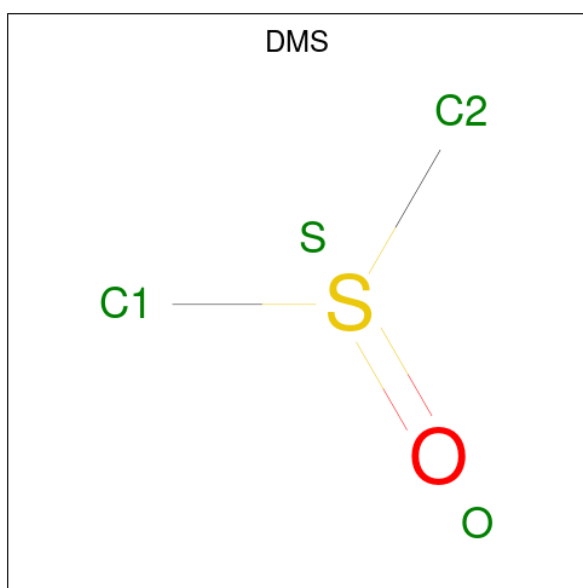
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula:  $C_2H_6OS$ ).



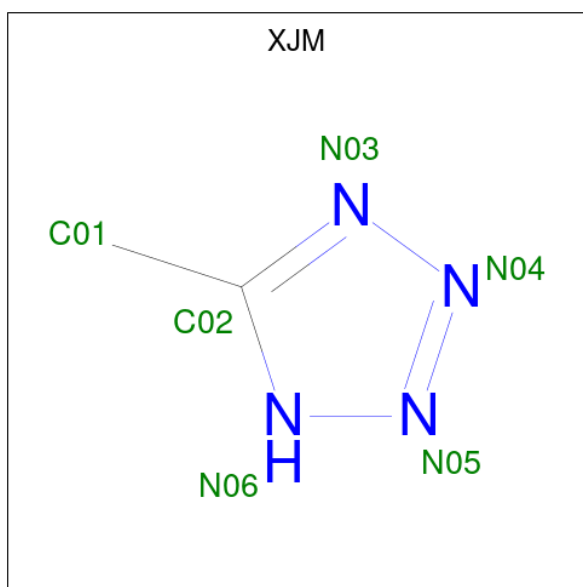
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is SULFATE ION (CCD ID:  $SO_4$ ) (formula:  $O_4S$ ).



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

- Molecule 6 is 5-methyl-1H-tetrazole (CCD ID: XJM) (formula: C<sub>2</sub>H<sub>4</sub>N<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	N	0	1
			12	4	8		
6	B	1	Total	C	N	0	0
			6	2	4		

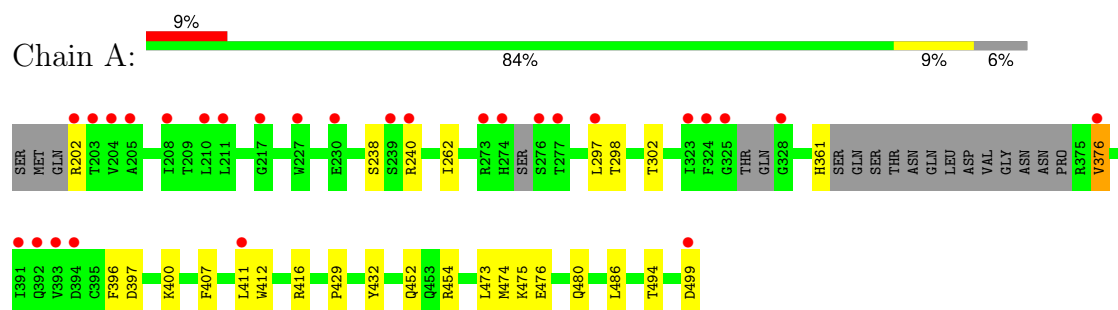
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	299	Total	O	0	0
			299	299		
7	B	341	Total	O	0	0
			341	341		

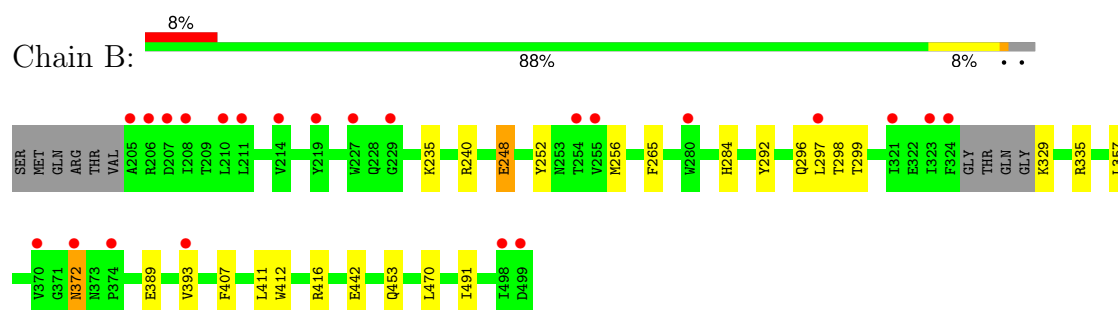
### 3 Residue-property plots [i](#)

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: Activin receptor type-1



#### • Molecule 1: Activin receptor type-1





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.60Å 84.57Å 88.45Å 90.00° 131.33° 90.00°	Depositor
Resolution (Å)	66.42 – 1.53 66.42 – 1.53	Depositor EDS
% Data completeness (in resolution range)	95.6 (66.42-1.53) 95.6 (66.42-1.53)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.01 (at 1.53Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.207 , 0.243 0.219 , 0.255	Depositor DCC
$R_{free}$ test set	5000 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.8	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h-2*1,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5586	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: LU8, EDO, SO4, DMS, XJM

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	0.68	0/2387	0.81	0/3235
1	B	0.72	1/2409 (0.0%)	0.82	0/3272
All	All	0.70	1/4796 (0.0%)	0.81	0/6507

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	248	GLU	CD-OE2	-6.37	1.18	1.25

There are no bond angle outliers.

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	2327	0	2291	23	0
1	B	2351	0	2313	19	0
2	A	128	0	0	1	0
2	B	32	0	0	1	0
3	A	36	0	54	1	0
3	B	16	0	24	3	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	15	0	0	0	0
5	B	15	0	0	0	0
6	B	18	0	0	1	0
7	A	299	0	0	3	1
7	B	341	0	0	4	1
All	All	5586	0	4694	44	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 5.

All (44) 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:454:ARG:NH2	1:A:480[B]:GLN:OE1	2.11	0.83
1:B:389:GLU:OE2	6:B:1801[A]:XJM:N06	2.29	0.66
1:A:452:GLN:O	7:A:601:HOH:O	2.15	0.64
2:A:501[B]:LU8:C25	2:A:501[B]:LU8:C12	2.77	0.62
1:A:238:SER:HB2	1:A:240:ARG:HD3	1.82	0.62
1:A:240:ARG:H	1:A:240:ARG:CD	2.12	0.62
1:A:240:ARG:H	1:A:240:ARG:HD2	1.65	0.62
1:A:407:PHE:CE2	1:A:411:LEU:HD13	2.37	0.60
1:B:284:HIS:HB2	3:B:1809:EDO:H22	1.83	0.59
1:B:252:TYR:CD1	1:B:265:PHE:HB2	2.39	0.58
1:A:361:HIS:HB2	1:A:396:PHE:CD1	2.39	0.57
1:B:284:HIS:HB2	3:B:1809:EDO:C2	2.34	0.57
1:A:454:ARG:HH22	1:A:480[B]:GLN:CD	2.07	0.57
1:A:475:LYS:CB	7:A:748:HOH:O	2.53	0.57
1:B:372:ASN:H	1:B:372:ASN:HD22	1.55	0.55
1:B:412:TRP:CZ2	1:B:416:ARG:HD2	2.42	0.55
1:B:256:MET:HB2	1:B:329:LYS:HB2	1.88	0.54
1:B:298[A]:THR:HG22	1:B:299:THR:O	2.11	0.51
1:B:453:GLN:OE1	3:B:1804:EDO:H12	2.10	0.51
1:B:407:PHE:CE2	1:B:491:ILE:HG21	2.46	0.51
1:A:240:ARG:HD2	1:A:240:ARG:N	2.24	0.50
1:A:412:TRP:CZ2	1:A:416:ARG:HD2	2.46	0.50
1:A:407:PHE:CZ	1:A:411:LEU:HD13	2.46	0.50
1:A:376:VAL:HA	7:A:602:HOH:O	2.11	0.50
1:B:407:PHE:CZ	1:B:411[A]:LEU:HD21	2.47	0.49
1:B:442:GLU:OE1	7:B:1901:HOH:O	2.20	0.49
2:B:1802:LU8:C25	2:B:1802:LU8:C23	2.91	0.49
1:B:235:LYS:NZ	7:B:1902:HOH:O	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ASP:HA	1:A:400[A]:LYS:HE2	1.95	0.47
1:B:372:ASN:HD22	1:B:372:ASN:N	2.13	0.47
1:B:411[B]:LEU:HD11	1:B:470:LEU:HD22	1.97	0.46
1:B:393:VAL:HB	7:B:2198:HOH:O	2.15	0.46
1:B:248:GLU:OE1	7:B:1902:HOH:O	2.21	0.45
1:A:473:LEU:HD13	1:A:494:THR:HG21	1.97	0.45
1:A:476[A]:GLU:HB3	1:A:486:LEU:HG	1.99	0.45
1:A:262[A]:ILE:O	3:A:502:EDO:O1	2.23	0.44
1:A:476[B]:GLU:HB3	1:A:486:LEU:HG	2.00	0.44
1:A:302:THR:HG21	1:A:499:ASP:OD2	2.18	0.43
1:A:240:ARG:CD	1:A:240:ARG:N	2.80	0.42
1:A:473:LEU:HD12	1:A:473:LEU:HA	1.89	0.41
1:B:335:ARG:HD3	1:B:357:LEU:O	2.19	0.41
1:B:292:TYR:O	1:B:296[B]:GLN:HG3	2.20	0.41
1:A:411:LEU:HD23	1:A:474:MET:HB3	2.02	0.41
1:A:429:PRO:O	1:A:432:TYR:HB3	2.21	0.41

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)
7:A:881:HOH:O	7:B:2218:HOH:O[2_555]	2.07	0.13

## 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	287/301 (95%)	281 (98%)	6 (2%)	0	100	100
1	B	294/301 (98%)	291 (99%)	3 (1%)	0	100	100
All	All	581/602 (96%)	572 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	253/270 (94%)	249 (98%)	4 (2%)	58	30
1	B	259/270 (96%)	256 (99%)	3 (1%)	67	43
All	All	512/540 (95%)	505 (99%)	7 (1%)	62	36

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	ARG
1	A	297	LEU
1	A	298	THR
1	A	376	VAL
1	B	240	ARG
1	B	297	LEU
1	B	372	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	361	HIS
1	B	372	ASN

### 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](#)

29 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	LU8	A	501[A]	-	35,35,35	0.77	0	47,49,49	1.89	11 (23%)
4	DMS	A	506	-	3,3,3	0.23	0	3,3,3	0.19	0
3	EDO	A	515	-	3,3,3	0.07	0	2,2,2	0.08	0
5	SO4	B	1808	-	4,4,4	0.36	0	6,6,6	0.07	0
3	EDO	A	503	-	3,3,3	0.59	0	2,2,2	0.50	0
2	LU8	A	501[B]	-	35,35,35	0.60	0	47,49,49	1.48	9 (19%)
3	EDO	A	513	-	3,3,3	0.06	0	2,2,2	0.14	0
5	SO4	A	511	-	4,4,4	0.36	0	6,6,6	0.21	0
3	EDO	B	1811	-	3,3,3	0.14	0	2,2,2	0.31	0
3	EDO	A	502	-	3,3,3	0.43	0	2,2,2	0.50	0
6	XJM	B	1801[A]	-	4,6,6	1.67	1 (25%)	4,7,7	5.01	4 (100%)
3	EDO	A	514	-	3,3,3	0.21	0	2,2,2	0.36	0
3	EDO	A	504	-	3,3,3	0.16	0	2,2,2	0.17	0
4	DMS	B	1805	-	3,3,3	0.26	0	3,3,3	0.14	0
3	EDO	A	512	-	3,3,3	0.17	0	2,2,2	0.24	0
3	EDO	B	1810	-	3,3,3	0.13	0	2,2,2	0.02	0
3	EDO	A	505	-	3,3,3	0.74	0	2,2,2	0.97	0
6	XJM	B	1801[B]	-	4,6,6	1.77	1 (25%)	4,7,7	4.68	4 (100%)
2	LU8	A	507	-	35,35,35	0.74	0	47,49,49	1.96	12 (25%)
2	LU8	A	508	-	35,35,35	0.78	0	47,49,49	1.61	7 (14%)
5	SO4	A	509	-	4,4,4	0.34	0	6,6,6	0.27	0
6	XJM	B	1806	-	4,6,6	1.21	0	4,7,7	3.71	3 (75%)
2	LU8	B	1802	-	35,35,35	0.78	0	47,49,49	1.47	8 (17%)
5	SO4	A	510	-	4,4,4	0.46	0	6,6,6	0.18	0
5	SO4	B	1803	-	4,4,4	0.25	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	B	1807	-	4,4,4	0.33	0	6,6,6	0.10	0
3	EDO	B	1804	-	3,3,3	0.82	0	2,2,2	0.71	0
3	EDO	B	1809	-	3,3,3	0.41	0	2,2,2	0.48	0
3	EDO	A	516	-	3,3,3	0.20	0	2,2,2	0.32	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
2	LU8	A	501[A]	-	-	0/18/28/28	0/4/4/4
3	EDO	A	515	-	-	1/1/1/1	-
3	EDO	A	503	-	-	1/1/1/1	-
2	LU8	A	501[B]	-	-	0/18/28/28	0/4/4/4
3	EDO	A	513	-	-	1/1/1/1	-
3	EDO	B	1811	-	-	1/1/1/1	-
6	XJM	B	1801[A]	-	-	-	0/1/1/1
3	EDO	A	502	-	-	1/1/1/1	-
3	EDO	A	514	-	-	0/1/1/1	-
3	EDO	A	504	-	-	1/1/1/1	-
3	EDO	A	512	-	-	1/1/1/1	-
3	EDO	B	1810	-	-	1/1/1/1	-
3	EDO	A	505	-	-	1/1/1/1	-
6	XJM	B	1801[B]	-	-	-	0/1/1/1
2	LU8	A	507	-	-	1/18/28/28	0/4/4/4
2	LU8	A	508	-	-	2/18/28/28	0/4/4/4
6	XJM	B	1806	-	-	-	0/1/1/1
2	LU8	B	1802	-	-	0/18/28/28	0/4/4/4
3	EDO	B	1804	-	-	0/1/1/1	-
3	EDO	B	1809	-	-	1/1/1/1	-
3	EDO	A	516	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1801[B]	XJM	N05-N04	2.65	1.36	1.32
6	B	1801[A]	XJM	N05-N04	2.18	1.35	1.32

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1801[A]	XJM	N06-N05-N04	-6.50	105.32	109.54
6	B	1801[A]	XJM	C02-N06-N05	5.76	110.15	104.33
2	A	501[A]	LU8	C16-C17-N18	5.71	118.56	111.20
6	B	1801[B]	XJM	N06-N05-N04	-5.62	105.89	109.54
6	B	1801[B]	XJM	C02-N06-N05	5.26	109.64	104.33
2	A	501[A]	LU8	C01-O02-C03	5.26	125.22	117.51
2	A	501[B]	LU8	C20-C21-C15	-5.12	105.01	111.00
2	A	507	LU8	C29-O28-C27	5.09	124.97	117.51
2	A	508	LU8	C01-O02-C03	5.03	124.89	117.51
6	B	1806	XJM	N06-N05-N04	-5.02	106.28	109.54
2	A	501[A]	LU8	C20-N18-C17	4.99	117.48	109.54
2	A	508	LU8	C29-O28-C27	4.97	124.81	117.51
2	A	501[A]	LU8	C29-O28-C27	4.29	123.80	117.51
6	B	1801[A]	XJM	C02-N03-N04	4.27	108.64	104.33
6	B	1806	XJM	C02-N06-N05	4.19	108.56	104.33
2	A	507	LU8	O28-C27-C30	4.07	122.12	115.14
6	B	1801[B]	XJM	C02-N03-N04	3.95	108.32	104.33
2	A	507	LU8	O02-C03-C30	3.93	121.87	115.14
2	A	507	LU8	C01-O02-C03	3.81	123.09	117.51
2	A	501[A]	LU8	C17-C16-C15	3.70	115.33	111.00
6	B	1801[B]	XJM	N03-N04-N05	-3.58	107.22	109.54
2	A	507	LU8	C26-C05-C06	-3.56	114.64	120.61
2	A	508	LU8	C06-C07-N08	-3.56	119.25	124.27
2	B	1802	LU8	C29-O28-C27	3.27	122.31	117.51
2	B	1802	LU8	C01-O02-C03	3.21	122.22	117.51
2	B	1802	LU8	C09-C10-C11	-3.18	114.96	119.56
2	A	507	LU8	C07-C06-C05	-3.12	115.05	119.56
2	A	507	LU8	C04-C05-C26	3.10	122.88	118.35
2	A	501[B]	LU8	C09-N08-C07	3.04	121.64	117.51
2	A	507	LU8	C06-C07-N08	-3.04	119.99	124.27
6	B	1806	XJM	C02-N03-N04	3.01	107.37	104.33
2	A	507	LU8	O28-C27-C26	-2.99	118.93	124.08
2	A	508	LU8	C09-N08-C07	2.99	121.57	117.51
2	A	507	LU8	O02-C03-C04	-2.83	119.20	124.08
2	A	501[B]	LU8	C10-C09-N08	-2.73	120.42	124.27
2	A	507	LU8	C23-C11-C10	-2.70	116.44	120.91
2	A	501[B]	LU8	C21-C15-C14	2.65	118.95	112.67
6	B	1801[A]	XJM	N03-N04-N05	-2.59	107.85	109.54
2	A	501[A]	LU8	C07-C06-C05	-2.52	115.91	119.56
2	A	501[A]	LU8	C09-C10-C11	-2.52	115.92	119.56
2	A	501[A]	LU8	C06-C07-N08	-2.50	120.74	124.27
2	B	1802	LU8	C20-N18-C17	2.50	113.52	109.54
2	A	508	LU8	C20-N18-C17	2.50	113.52	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1802	LU8	C10-C09-N08	-2.46	120.81	124.27
2	A	501[B]	LU8	C06-C07-N08	-2.32	121.00	124.27
2	A	501[B]	LU8	O02-C03-C30	2.32	119.11	115.14
2	B	1802	LU8	C21-C15-C14	-2.30	107.21	112.67
2	A	501[A]	LU8	C09-N08-C07	2.27	120.60	117.51
2	A	501[B]	LU8	C20-N18-C17	2.24	113.11	109.54
2	A	501[A]	LU8	C21-C15-C14	-2.24	107.38	112.67
2	B	1802	LU8	C13-C12-C11	-2.22	118.28	121.12
2	A	501[B]	LU8	C01-O02-C03	2.16	120.67	117.51
2	A	501[A]	LU8	C11-C10-C24	2.13	125.98	122.47
2	A	507	LU8	C13-C12-C11	-2.12	118.40	121.12
2	B	1802	LU8	C09-N08-C07	2.09	120.35	117.51
2	A	508	LU8	C05-C06-C24	-2.04	119.11	122.47
2	A	508	LU8	C32-O31-C30	2.01	120.20	114.74
2	A	501[B]	LU8	O28-C27-C30	2.01	118.58	115.14

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	505	EDO	O1-C1-C2-O2
3	A	502	EDO	O1-C1-C2-O2
3	A	513	EDO	O1-C1-C2-O2
3	A	504	EDO	O1-C1-C2-O2
3	A	515	EDO	O1-C1-C2-O2
3	B	1809	EDO	O1-C1-C2-O2
3	A	512	EDO	O1-C1-C2-O2
2	A	507	LU8	C30-C03-O02-C01
2	A	508	LU8	C04-C05-C06-C07
3	B	1811	EDO	O1-C1-C2-O2
2	A	508	LU8	C26-C05-C06-C07
3	B	1810	EDO	O1-C1-C2-O2
3	A	503	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 7 short contacts:

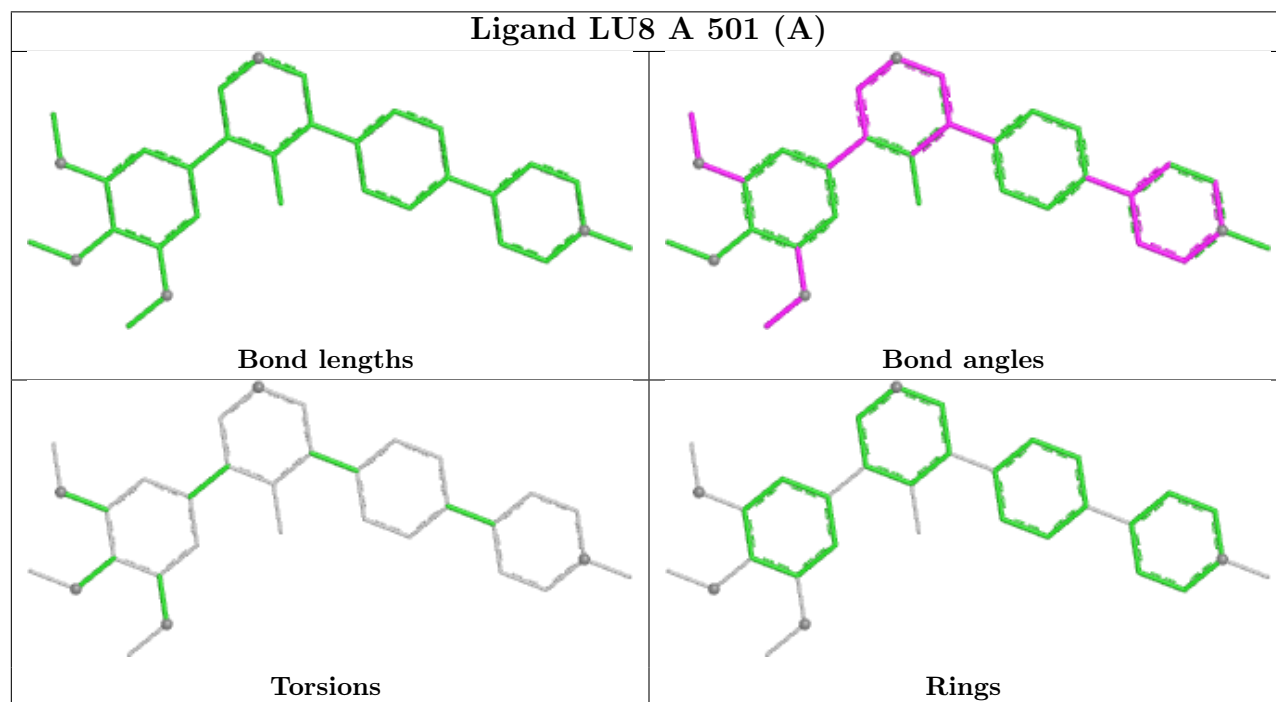
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501[B]	LU8	1	0
3	A	502	EDO	1	0
6	B	1801[A]	XJM	1	0

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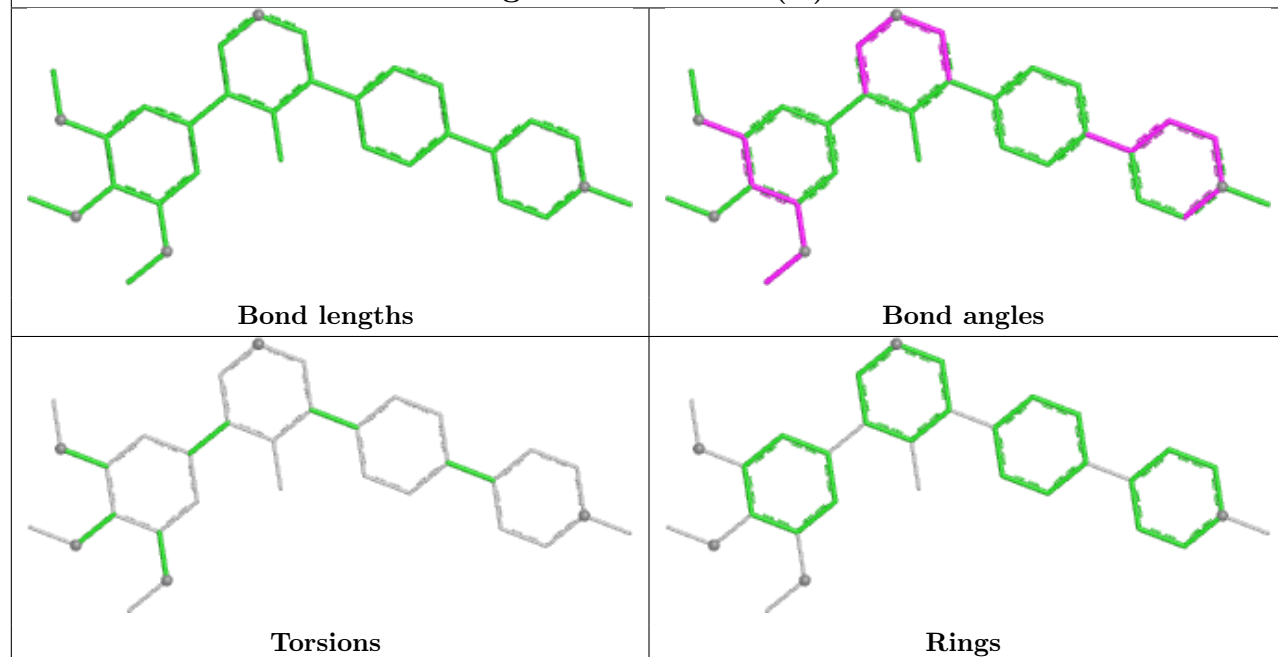
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1802	LU8	1	0
3	B	1804	EDO	1	0
3	B	1809	EDO	2	0

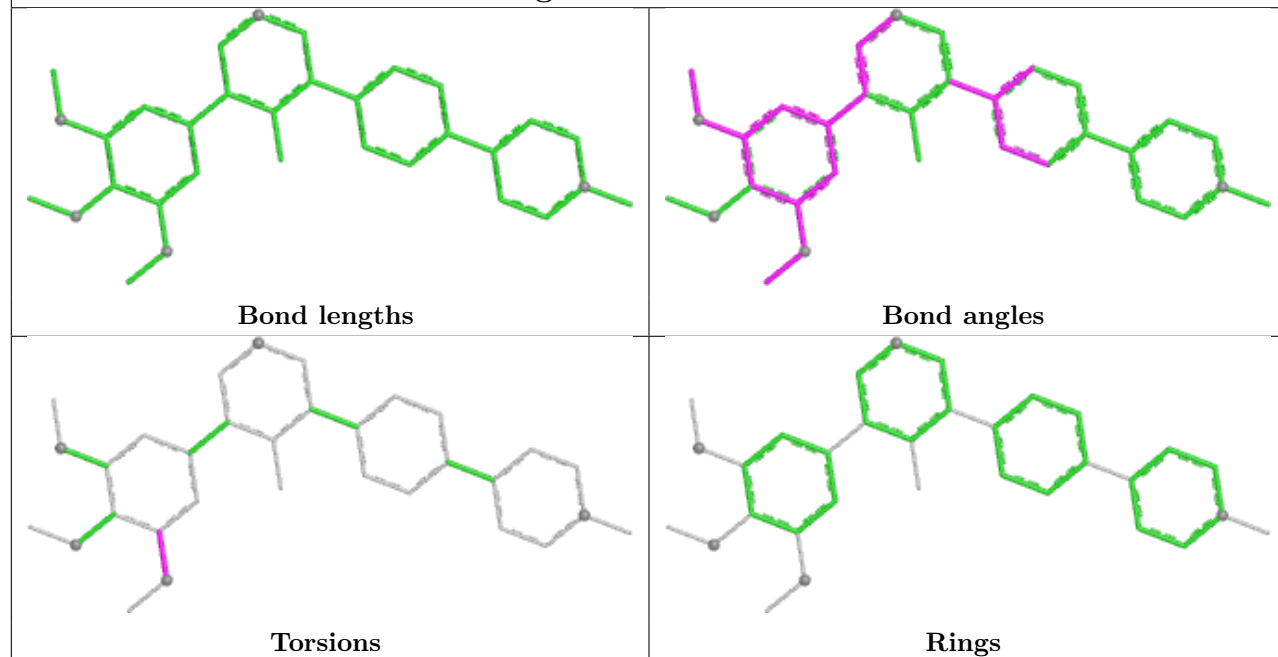
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

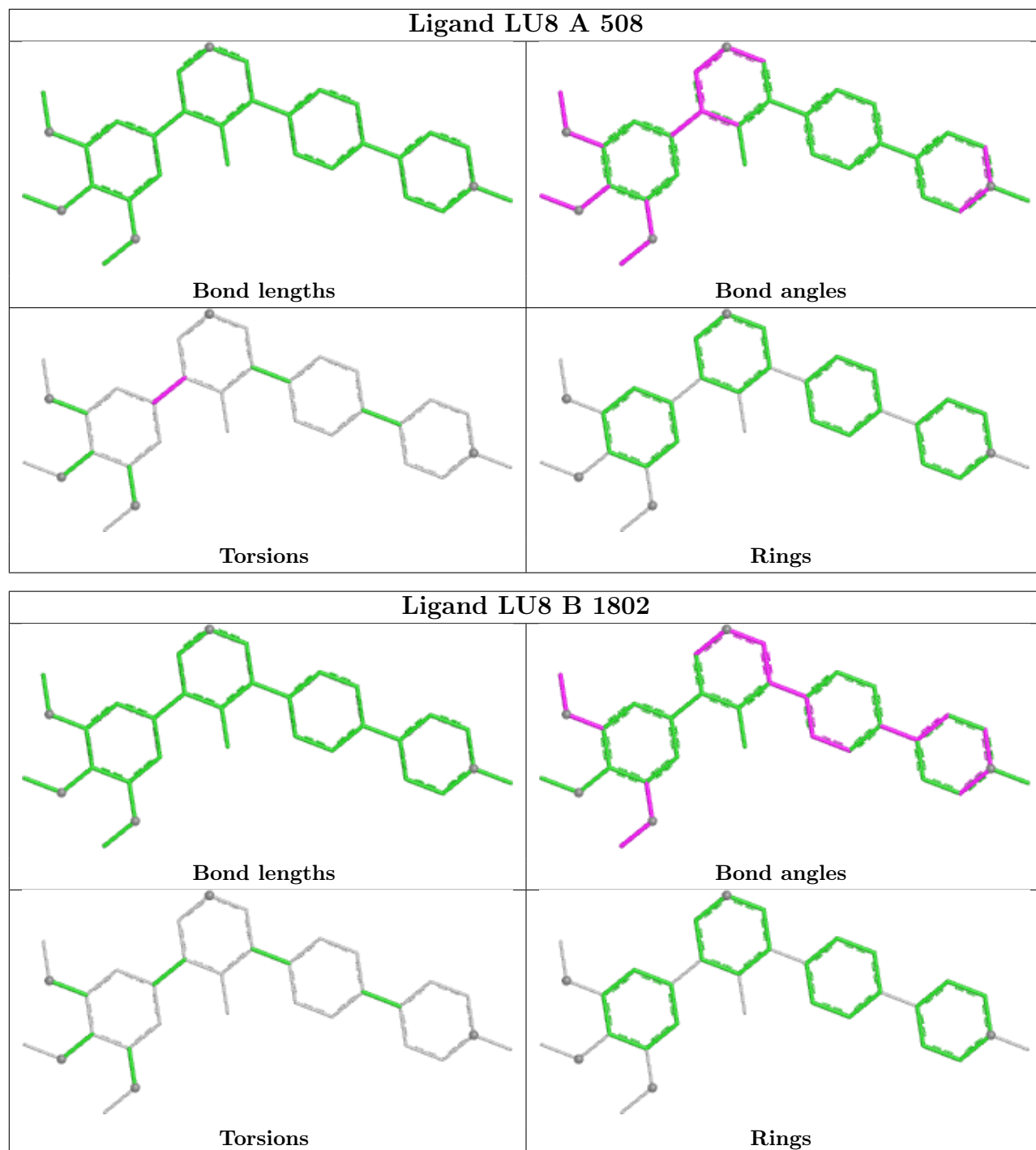


## Ligand LU8 A 501 (B)



## Ligand LU8 A 507





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	282/301 (93%)	0.70	28 (9%)	14 18	10, 26, 56, 71	13 (4%)
1	B	291/301 (96%)	0.62	23 (7%)	20 24	9, 26, 49, 81	7 (2%)
All	All	573/602 (95%)	0.65	51 (8%)	17 20	9, 26, 54, 81	20 (3%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	255	VAL	6.0
1	B	324	PHE	5.9
1	A	274	HIS	5.7
1	B	227	TRP	5.2
1	A	324	PHE	4.4
1	A	376	VAL	4.3
1	A	393	VAL	4.2
1	A	297	LEU	4.2
1	A	227	TRP	4.1
1	B	205	ALA	4.0
1	B	297	LEU	3.9
1	A	205	ALA	3.8
1	B	280	TRP	3.7
1	A	204	VAL	3.5
1	B	498	ILE	3.4
1	A	328	GLY	3.4
1	B	393	VAL	3.3
1	A	202	ARG	3.3
1	B	207	ASP	3.3
1	A	239	SER	3.3
1	A	203	THR	3.2
1	B	374	PRO	3.1
1	A	277	THR	3.1
1	B	219	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	394	ASP	2.9
1	B	214	VAL	2.8
1	B	254	THR	2.8
1	A	210	LEU	2.8
1	B	208	ILE	2.8
1	B	229	GLY	2.7
1	A	499	ASP	2.7
1	B	211	LEU	2.7
1	B	206	ARG	2.7
1	A	392	GLN	2.6
1	B	210	LEU	2.6
1	A	323	ILE	2.6
1	A	325	GLY	2.5
1	A	273	ARG	2.5
1	B	372	ASN	2.4
1	A	230	GLU	2.4
1	A	211	LEU	2.4
1	B	321	ILE	2.4
1	B	323	ILE	2.4
1	A	208	ILE	2.3
1	B	370	VAL	2.3
1	B	499	ASP	2.3
1	A	391	ILE	2.3
1	A	217	GLY	2.2
1	A	240	ARG	2.2
1	A	276	SER	2.1
1	A	411	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

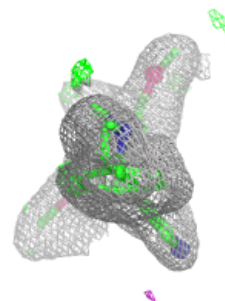
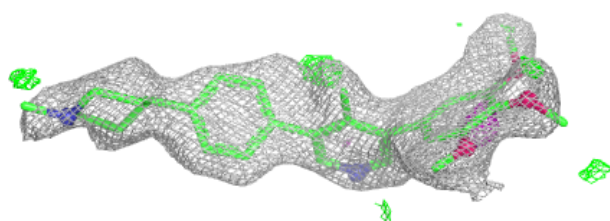
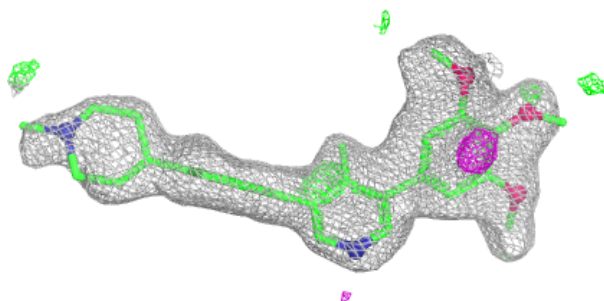
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	SO4	B	1807	5/5	0.61	0.15	86,88,93,100	5
3	EDO	A	512	4/4	0.64	0.25	47,49,51,53	0
3	EDO	A	504	4/4	0.65	0.25	64,70,70,72	0
3	EDO	B	1804	4/4	0.74	0.21	36,40,43,45	0
3	EDO	A	516	4/4	0.74	0.17	55,58,58,58	0
3	EDO	A	514	4/4	0.76	0.25	66,70,71,75	0
4	DMS	A	506	4/4	0.77	0.25	76,78,78,80	0
3	EDO	A	515	4/4	0.78	0.17	59,60,61,64	0
4	DMS	B	1805	4/4	0.79	0.18	71,73,76,79	0
3	EDO	B	1811	4/4	0.80	0.20	65,66,68,69	0
3	EDO	A	513	4/4	0.80	0.23	71,71,72,76	0
2	LU8	A	507	32/32	0.81	0.17	36,46,63,64	0
3	EDO	B	1809	4/4	0.81	0.22	33,45,52,54	0
3	EDO	B	1810	4/4	0.82	0.15	45,51,52,53	0
6	XJM	B	1801[A]	6/6	0.82	0.16	40,40,41,41	6
6	XJM	B	1801[B]	6/6	0.82	0.16	28,29,29,30	6
3	EDO	A	503	4/4	0.87	0.12	31,32,34,37	0
3	EDO	A	502	4/4	0.87	0.15	24,33,35,42	0
3	EDO	A	505	4/4	0.88	0.15	25,32,34,39	0
5	SO4	B	1808	5/5	0.89	0.10	60,62,70,74	0
2	LU8	A	508	32/32	0.90	0.13	28,33,58,63	0
6	XJM	B	1806	6/6	0.91	0.10	34,37,38,38	0
2	LU8	A	501[A]	32/32	0.92	0.12	19,22,40,42	32
2	LU8	A	501[B]	32/32	0.92	0.12	26,30,38,39	32
2	LU8	B	1802	32/32	0.95	0.09	22,26,52,55	0
5	SO4	A	510	5/5	0.96	0.08	26,33,40,40	0
5	SO4	A	511	5/5	0.97	0.05	23,25,27,28	5
5	SO4	B	1803	5/5	0.98	0.05	27,28,30,31	0
5	SO4	A	509	5/5	0.98	0.05	27,30,32,34	0

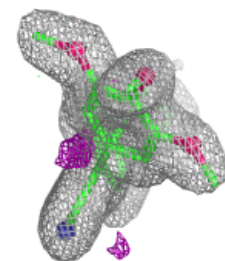
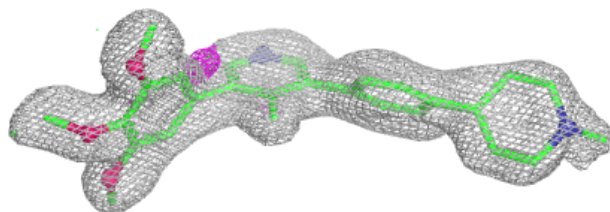
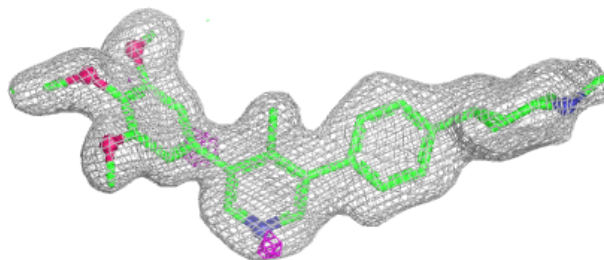
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around LU8 A 507:**

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

**Electron density around LU8 A 508:**

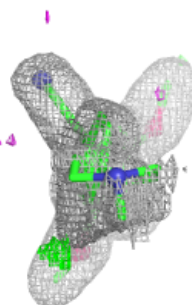
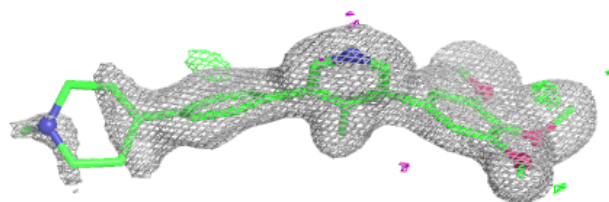
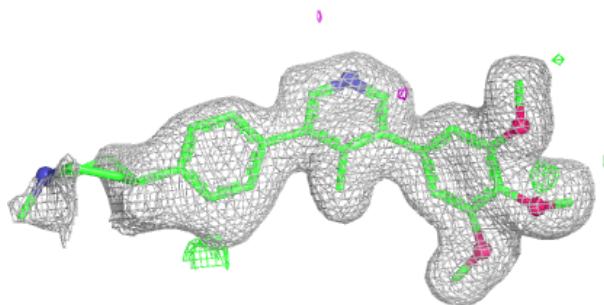
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



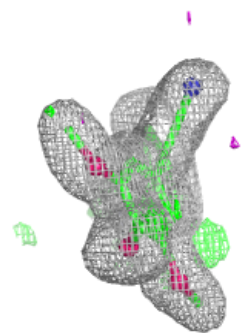
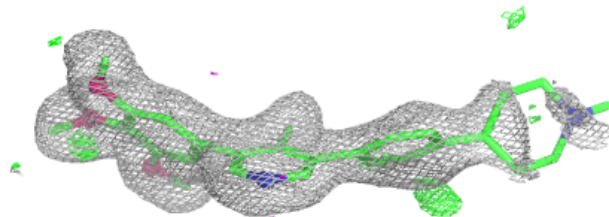
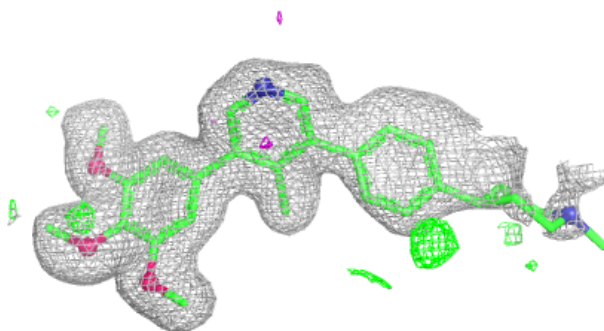


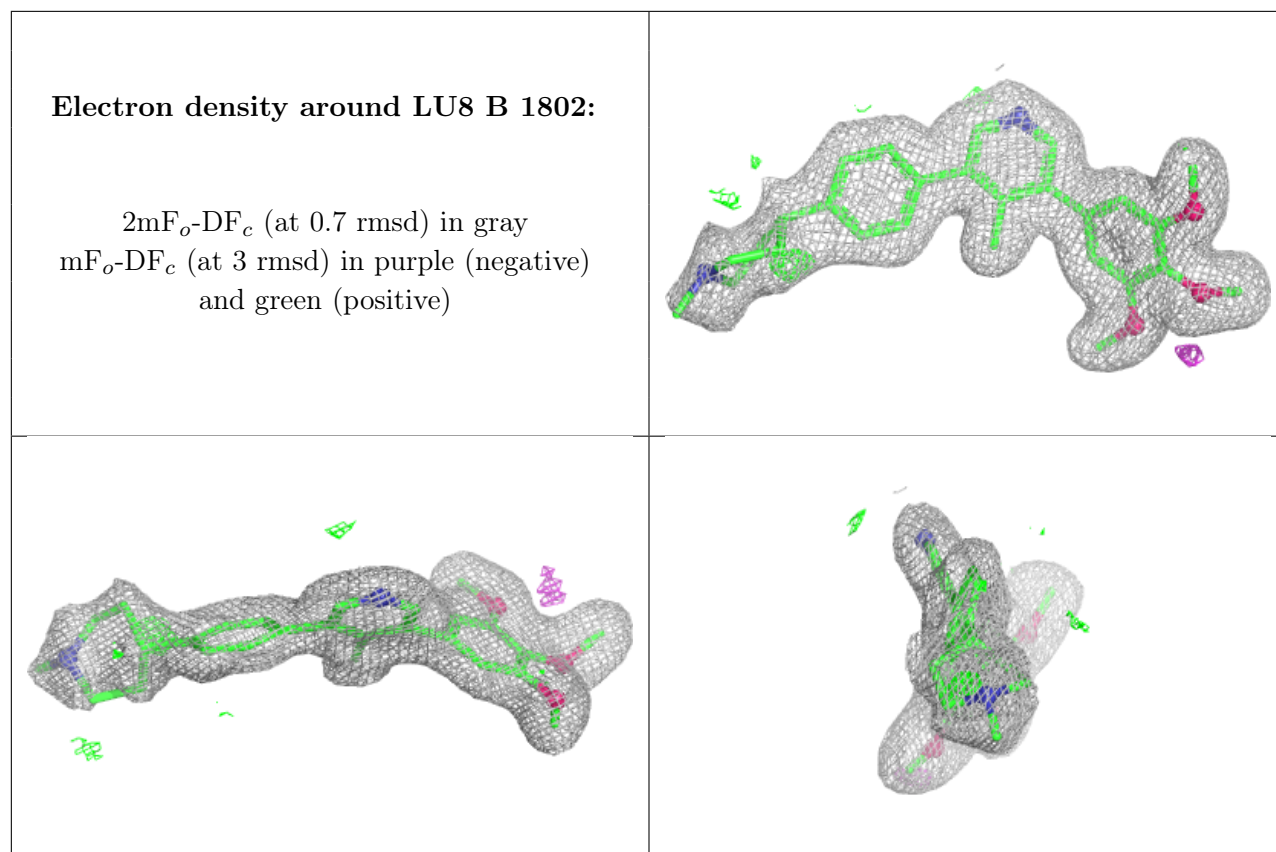
**Electron density around LU8 A 501 (A):**

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

**Electron density around LU8 A 501 (B):**

$2mF_o-DF_c$  (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.