



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:22 PM UTC

PDB ID : 5S86 / pdb_00005s86
Title : XChem group deposition – Crystal Structure of human ACVR1 in complex with FM010952a
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 : 1.31 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

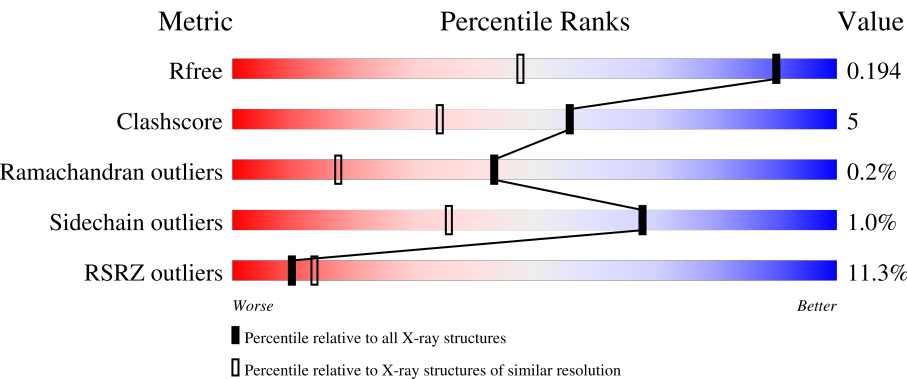
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.31 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	2531 (1.34-1.30)
Clashscore	190562	2585 (1.34-1.30)
Ramachandran outliers	187476	2528 (1.34-1.30)
Sidechain outliers	187428	2528 (1.34-1.30)
RSRZ outliers	180081	2528 (1.34-1.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	301	11% 84% 8% • 6%
1	B	301	11% 89% 7% • •

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
3	EDO	A	505	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5671 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	283	Total	C	N	O	S	0	13	0
			2336	1498	396	427	15			
1	B	292	Total	C	N	O	S	0	7	0
			2342	1493	407	427	15			

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: C₂₇H₃₂N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	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: C₂H₆O₂).



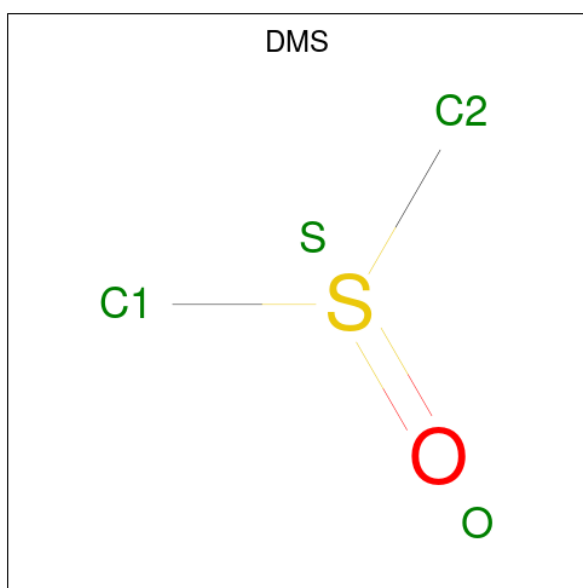
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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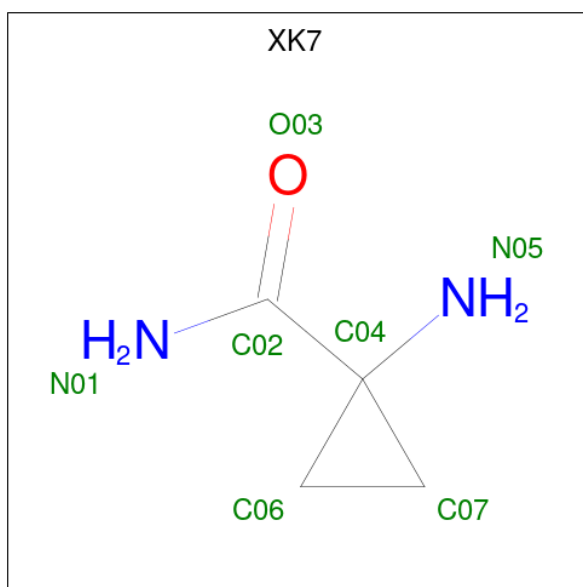
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

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



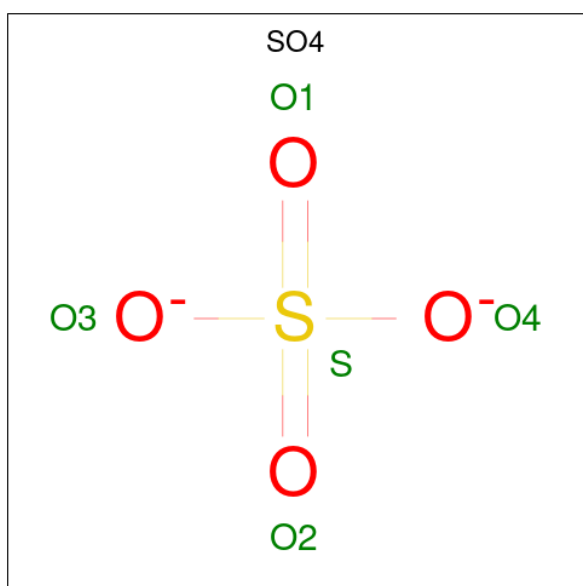
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is 1-aminocyclopropane-1-carboxamide (CCD ID: XK7) (formula: $C_4H_8N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			7	4	2	1		
5	B	1	Total	C	N	O	0	0
			7	4	2	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

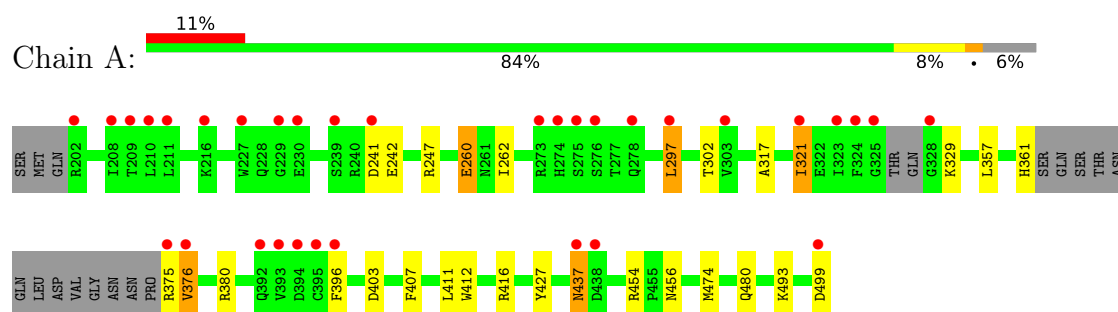
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	377	Total	O	0	1
			378	378		
7	B	383	Total	O	0	0
			383	383		

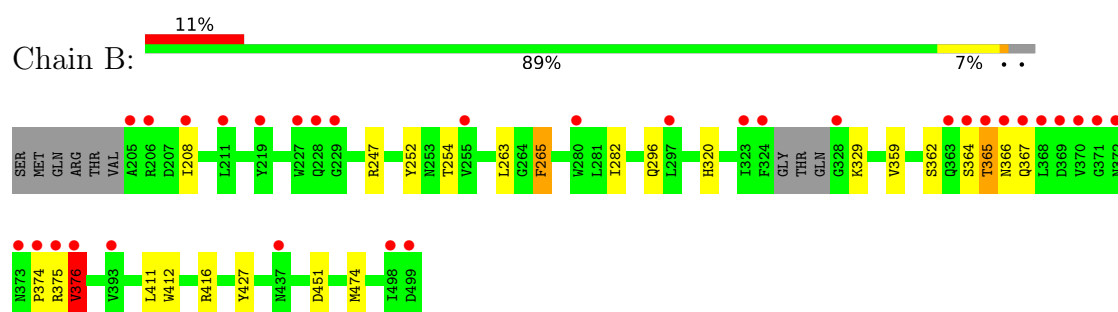
3 Residue-property plots [i](#)

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, α , β , γ	127.30Å 84.83Å 88.07Å 90.00° 131.10° 90.00°	Depositor
Resolution (Å)	66.37 – 1.31 66.37 – 1.31	Depositor EDS
% Data completeness (in resolution range)	75.4 (66.37-1.31) 75.4 (66.37-1.31)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.31Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.168 , 0.190 0.172 , 0.194	Depositor DCC
R_{free} test set	6433 reflections (3.81%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.011 for -h+k-l,-l,-k 0.000 for -h-k-l,l,k 0.016 for -h-2*l,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5671	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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: LU8, SO4, XK7, DMS, EDO

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	1.03	1/2391 (0.0%)	1.14	4/3243 (0.1%)
1	B	1.09	3/2401 (0.1%)	1.22	6/3261 (0.2%)
All	All	1.06	4/4792 (0.1%)	1.18	10/6504 (0.2%)

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	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	376	VAL	C-O	7.19	1.33	1.24
1	A	260	GLU	CD-OE1	6.19	1.37	1.25
1	B	374	PRO	C-O	5.13	1.30	1.24
1	B	320	HIS	CE1-NE2	5.07	1.37	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	265	PHE	N-CA-CB	-6.19	100.71	110.06
1	B	451	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	260	GLU	CB-CG-CD	5.79	122.44	112.60
1	B	376	VAL	CB-CA-C	5.73	119.38	111.19
1	B	375	ARG	CA-C-N	-5.71	114.22	122.45
1	B	375	ARG	C-N-CA	-5.71	114.22	122.45
1	A	403	ASP	CA-CB-CG	5.53	118.13	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	VAL	CA-C-O	-5.50	115.84	121.67
1	A	437	ASN	CA-C-O	-5.39	114.80	120.63
1	B	376	VAL	CA-CB-CG2	5.31	119.43	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	366	ASN	Peptide

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	2336	0	2304	26	0
1	B	2342	0	2279	16	0
2	A	96	0	0	0	0
2	B	32	0	0	0	0
3	A	36	0	50	7	0
3	B	16	0	24	2	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
5	A	7	0	0	2	0
5	B	7	0	0	0	0
6	A	15	0	0	1	0
6	B	15	0	0	1	0
7	A	378	0	0	5	0
7	B	383	0	0	4	0
All	All	5671	0	4669	45	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (45) 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:241:ASP:OD2	7:A:602:HOH:O	1.99	0.80
1:A:411[A]:LEU:HG	1:A:474:MET:HE2	1.70	0.71
1:B:364:SER:O	1:B:365:THR:HG22	1.91	0.70
1:B:252:TYR:CD1	1:B:265:PHE:HB2	2.26	0.70
1:A:317:ALA:O	1:A:321[B]:ILE:HD13	1.91	0.69
1:B:411[B]:LEU:HG	1:B:474:MET:HE2	1.78	0.66
3:B:508:EDO:H12	7:B:752:HOH:O	1.96	0.65
1:A:302:THR:HG21	1:A:499:ASP:OD2	1.98	0.64
5:A:509:XK7:C07	7:A:958:HOH:O	2.47	0.62
1:A:380:ARG:HH22	3:A:505:EDO:C1	2.14	0.60
1:A:456[A]:ASN:ND2	3:A:503:EDO:O1	2.37	0.58
1:A:376:VAL:HG23	5:A:509:XK7:C06	2.35	0.56
6:B:506:SO4:O1	7:B:601:HOH:O	2.16	0.56
1:A:437:ASN:HA	3:A:505:EDO:H12	1.88	0.55
1:B:364:SER:C	1:B:365:THR:HG22	2.32	0.55
1:A:357[B]:LEU:HD21	7:A:879:HOH:O	2.06	0.55
1:A:361:HIS:HB2	1:A:396:PHE:CD1	2.44	0.53
1:A:262[A]:ILE:O	3:A:502:EDO:H11	2.11	0.50
1:B:208:ILE:HD11	1:B:282:ILE:HD13	1.93	0.50
1:A:454:ARG:HH22	1:A:480:GLN:CD	2.19	0.50
1:A:247:ARG:CD	7:A:771:HOH:O	2.60	0.49
1:A:407:PHE:HE2	1:A:411[B]:LEU:HD11	1.77	0.48
1:A:329:LYS:HB3	3:A:513:EDO:H21	1.96	0.47
1:B:208:ILE:CD1	1:B:282:ILE:HD13	2.45	0.47
1:B:412:TRP:CZ2	1:B:416:ARG:HD2	2.49	0.47
1:A:407:PHE:CE2	1:A:411[B]:LEU:HD11	2.49	0.46
1:A:412:TRP:CZ2	1:A:416:ARG:HD2	2.51	0.46
1:A:321[A]:ILE:HD11	7:B:750:HOH:O	2.15	0.45
1:A:437:ASN:O	6:A:512:SO4:O2	2.34	0.45
1:B:364:SER:O	1:B:365:THR:CG2	2.63	0.45
1:B:296[B]:GLN:HA	1:B:296[B]:GLN:OE1	2.17	0.44
1:B:247:ARG:HH21	1:B:359:VAL:HA	1.82	0.44
1:A:427:TYR:CD2	1:A:427:TYR:C	2.96	0.44
1:A:297:LEU:H	1:A:297:LEU:HG	1.69	0.44
1:B:252:TYR:CE1	1:B:265:PHE:HB2	2.53	0.44
1:B:427:TYR:CD2	1:B:427:TYR:C	2.96	0.43
1:B:263:LEU:HA	3:B:508:EDO:H21	2.00	0.43
1:B:362:SER:HB2	1:B:365:THR:HG23	2.01	0.43
1:A:357[A]:LEU:HD21	1:A:375:ARG:CB	2.48	0.43
1:A:380:ARG:NH2	3:A:505:EDO:H11	2.34	0.42
1:A:380:ARG:HH22	3:A:505:EDO:H12	1.84	0.42
1:A:493:LYS:NZ	7:A:614:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:THR:HG21	1:B:329:LYS:HG3	2.03	0.41
1:A:260:GLU:H	1:A:260:GLU:CD	2.29	0.41
1:B:376:VAL:HG12	7:B:930:HOH:O	2.21	0.41

There are no symmetry-related clashes.

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	290/301 (96%)	288 (99%)	2 (1%)	0	100	100
1	B	295/301 (98%)	287 (97%)	7 (2%)	1 (0%)	36	15
All	All	585/602 (97%)	575 (98%)	9 (2%)	1 (0%)	43	17

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	365	THR

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%)	55	18
1	B	251/270 (93%)	249 (99%)	2 (1%)	73	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	504/540 (93%)	498 (99%)	6 (1%)	68 28

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	GLU
1	A	297	LEU
1	A	321[A]	ILE
1	A	321[B]	ILE
1	B	367	GLN
1	B	376	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	361	HIS
1	A	437	ASN
1	B	284	HIS
1	B	366	ASN
1	B	367	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

27 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	502	-	3,3,3	0.90	0	2,2,2	1.37	0
3	EDO	A	504	-	3,3,3	0.14	0	2,2,2	0.27	0
3	EDO	A	516	-	3,3,3	0.12	0	2,2,2	0.08	0
2	LU8	A	507	-	35,35,35	1.17	2 (5%)	47,49,49	2.09	15 (31%)
2	LU8	A	501	-	35,35,35	1.35	4 (11%)	47,49,49	1.79	11 (23%)
3	EDO	A	503	-	3,3,3	1.19	0	2,2,2	1.07	0
6	SO4	B	507	-	4,4,4	0.55	0	6,6,6	0.20	0
3	EDO	A	514	-	3,3,3	0.21	0	2,2,2	0.25	0
3	EDO	B	509	-	3,3,3	0.23	0	2,2,2	0.13	0
4	DMS	B	504	-	3,3,3	0.24	0	3,3,3	0.03	0
6	SO4	B	502	-	4,4,4	0.39	0	6,6,6	0.30	0
3	EDO	B	508	-	3,3,3	0.58	0	2,2,2	1.59	0
6	SO4	A	511	-	4,4,4	0.26	0	6,6,6	0.29	0
2	LU8	B	501	-	35,35,35	1.06	2 (5%)	47,49,49	1.51	7 (14%)
3	EDO	A	515	-	3,3,3	0.67	0	2,2,2	0.40	0
3	EDO	A	513	-	3,3,3	0.25	0	2,2,2	0.93	0
5	XK7	A	509	-	5,7,7	3.69	2 (40%)	6,11,11	3.94	4 (66%)
6	SO4	A	510	-	4,4,4	0.26	0	6,6,6	0.16	0
6	SO4	B	506	-	4,4,4	0.33	0	6,6,6	0.19	0
4	DMS	A	506	-	3,3,3	0.25	0	3,3,3	0.06	0
2	LU8	A	508	-	35,35,35	1.00	2 (5%)	47,49,49	1.48	8 (17%)
3	EDO	A	517	-	3,3,3	0.36	0	2,2,2	0.44	0
5	XK7	B	505	-	5,7,7	4.30	4 (80%)	6,11,11	3.31	2 (33%)
3	EDO	B	510	-	3,3,3	0.15	0	2,2,2	0.19	0
3	EDO	A	505	-	3,3,3	1.81	1 (33%)	2,2,2	0.83	0
6	SO4	A	512	-	4,4,4	0.37	0	6,6,6	0.13	0
3	EDO	B	503	-	3,3,3	0.94	0	2,2,2	1.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	502	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	504	-	-	1/1/1/1	-
3	EDO	A	516	-	-	1/1/1/1	-
2	LU8	A	507	-	-	0/18/28/28	0/4/4/4
2	LU8	A	501	-	-	0/18/28/28	0/4/4/4
3	EDO	A	503	-	-	1/1/1/1	-
3	EDO	A	514	-	-	1/1/1/1	-
3	EDO	B	509	-	-	1/1/1/1	-
3	EDO	B	508	-	-	0/1/1/1	-
2	LU8	B	501	-	-	0/18/28/28	0/4/4/4
3	EDO	A	515	-	-	0/1/1/1	-
3	EDO	A	513	-	-	1/1/1/1	-
5	XK7	A	509	-	-	4/4/10/10	0/1/1/1
2	LU8	A	508	-	-	4/18/28/28	0/4/4/4
3	EDO	A	517	-	-	0/1/1/1	-
5	XK7	B	505	-	-	2/4/10/10	0/1/1/1
3	EDO	B	510	-	-	1/1/1/1	-
3	EDO	A	505	-	-	1/1/1/1	-
3	EDO	B	503	-	-	0/1/1/1	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	505	XK7	C02-N01	7.75	1.47	1.32
5	A	509	XK7	C02-N01	6.61	1.45	1.32
5	B	505	XK7	O03-C02	-4.16	1.15	1.23
5	A	509	XK7	C06-C04	4.07	1.55	1.51
2	A	501	LU8	C10-C11	3.61	1.55	1.49
2	A	507	LU8	C10-C11	-3.41	1.43	1.49
2	A	501	LU8	C12-C13	3.40	1.44	1.38
2	A	507	LU8	C26-C05	2.88	1.44	1.39
3	A	505	EDO	O1-C1	-2.62	1.28	1.42
5	B	505	XK7	C07-C04	2.55	1.54	1.51
5	B	505	XK7	C06-C04	2.49	1.53	1.51
2	B	501	LU8	C10-C24	2.47	1.44	1.40
2	A	501	LU8	C07-C06	-2.30	1.35	1.39
2	A	508	LU8	C27-C30	-2.18	1.36	1.41
2	B	501	LU8	C13-C14	-2.17	1.35	1.39
2	A	508	LU8	C12-C13	-2.12	1.35	1.38
2	A	501	LU8	C03-C30	-2.08	1.36	1.41

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	509	XK7	C06-C04-C02	7.18	123.16	116.54
5	B	505	XK7	C07-C04-C02	5.63	121.73	116.54
5	B	505	XK7	C06-C04-C02	-5.59	111.38	116.54
2	A	507	LU8	C26-C05-C06	-5.53	111.34	120.61
2	A	501	LU8	C20-N18-C17	5.37	118.08	109.54
2	A	507	LU8	C07-C06-C05	-5.35	111.83	119.56
5	A	509	XK7	C07-C04-C02	-5.33	111.62	116.54
2	A	501	LU8	C16-C17-N18	4.52	117.03	111.20
2	A	507	LU8	C12-C11-C10	4.42	128.23	120.91
2	A	501	LU8	C22-C14-C13	4.29	123.63	118.30
2	A	507	LU8	C23-C11-C10	-4.25	113.87	120.91
2	B	501	LU8	C20-C21-C15	3.94	115.61	111.00
2	B	501	LU8	C17-C16-C15	3.71	115.34	111.00
2	A	501	LU8	C23-C11-C10	-3.62	114.91	120.91
2	A	508	LU8	C06-C24-C10	3.57	122.73	118.39
2	A	508	LU8	C20-C21-C15	-3.19	107.27	111.00
2	A	508	LU8	C06-C07-N08	-3.16	119.81	124.27
2	A	507	LU8	C13-C14-C15	3.13	129.01	121.09
2	A	501	LU8	C21-C15-C14	-3.07	105.41	112.67
2	A	508	LU8	C29-O28-C27	2.97	121.86	117.51
2	A	507	LU8	C04-C05-C06	2.96	125.57	120.61
2	B	501	LU8	C06-C24-C10	-2.87	114.92	118.39
2	A	507	LU8	C04-C05-C26	2.85	122.51	118.35
2	B	501	LU8	C23-C22-C14	-2.81	118.38	121.18
2	B	501	LU8	C06-C07-N08	-2.77	120.36	124.27
5	A	509	XK7	O03-C02-N01	-2.76	117.75	123.14
2	A	507	LU8	C22-C14-C15	-2.73	114.15	121.09
2	A	507	LU8	C06-C07-N08	-2.70	120.46	124.27
2	A	501	LU8	C12-C13-C14	-2.68	118.51	121.18
2	A	507	LU8	C32-O31-C30	2.60	121.81	114.74
2	A	507	LU8	C27-C30-C03	2.59	122.09	119.56
2	B	501	LU8	C13-C12-C11	-2.59	117.79	121.12
2	A	501	LU8	C23-C11-C12	2.53	122.20	117.68
2	A	508	LU8	C09-N08-C07	2.51	120.92	117.51
2	A	501	LU8	C22-C23-C11	-2.39	118.06	121.12
2	A	501	LU8	C13-C12-C11	-2.39	118.06	121.12
2	A	507	LU8	C16-C17-N18	2.38	114.26	111.20
2	A	501	LU8	C17-C16-C15	2.37	113.77	111.00
2	A	507	LU8	C19-N18-C17	-2.30	106.26	110.63
2	A	508	LU8	O31-C30-C27	2.20	123.28	120.12
2	A	507	LU8	C05-C04-C03	-2.17	117.24	120.19
2	A	507	LU8	C29-O28-C27	2.13	120.64	117.51
2	A	501	LU8	C13-C14-C15	-2.13	115.69	121.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	508	LU8	C17-C16-C15	2.12	113.48	111.00
2	A	508	LU8	C22-C14-C15	-2.11	115.72	121.09
5	A	509	XK7	C06-C07-C04	2.01	61.17	60.31
2	B	501	LU8	C19-N18-C17	-2.00	106.82	110.63

There are no chirality outliers.

All (19) torsion outliers are listed below:

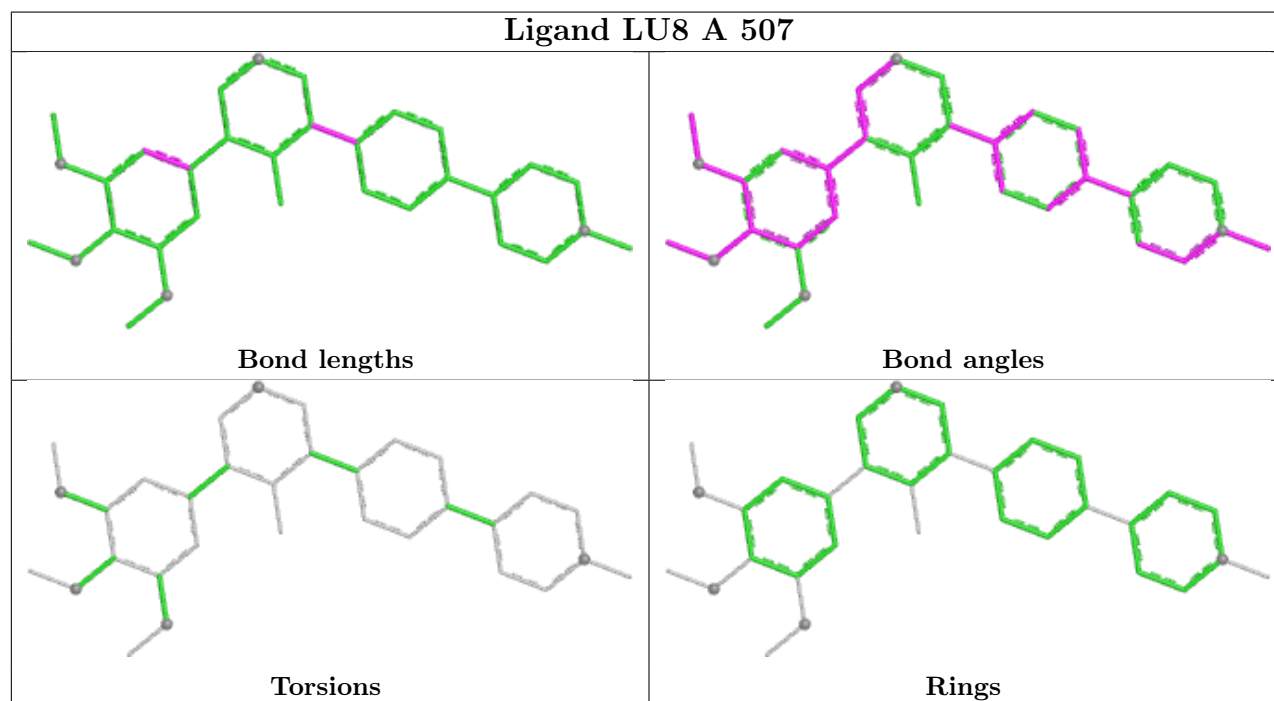
Mol	Chain	Res	Type	Atoms
5	A	509	XK7	N01-C02-C04-C07
5	A	509	XK7	O03-C02-C04-C07
5	B	505	XK7	N01-C02-C04-C07
5	B	505	XK7	O03-C02-C04-C07
5	A	509	XK7	N01-C02-C04-C06
5	A	509	XK7	O03-C02-C04-C06
3	A	502	EDO	O1-C1-C2-O2
3	A	503	EDO	O1-C1-C2-O2
3	A	514	EDO	O1-C1-C2-O2
3	A	513	EDO	O1-C1-C2-O2
3	B	509	EDO	O1-C1-C2-O2
2	A	508	LU8	C04-C05-C06-C07
3	A	516	EDO	O1-C1-C2-O2
3	B	510	EDO	O1-C1-C2-O2
2	A	508	LU8	C26-C05-C06-C07
2	A	508	LU8	C04-C05-C06-C24
3	A	504	EDO	O1-C1-C2-O2
3	A	505	EDO	O1-C1-C2-O2
2	A	508	LU8	C26-C05-C06-C24

There are no ring outliers.

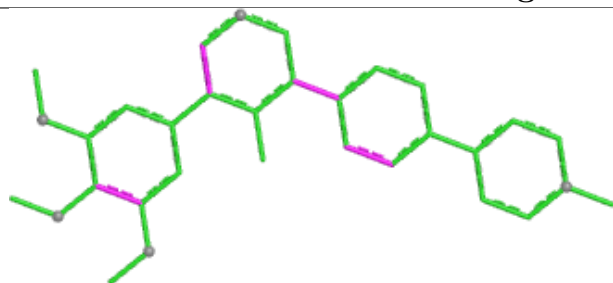
8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	EDO	1	0
3	A	503	EDO	1	0
3	B	508	EDO	2	0
3	A	513	EDO	1	0
5	A	509	XK7	2	0
6	B	506	SO4	1	0
3	A	505	EDO	4	0
6	A	512	SO4	1	0

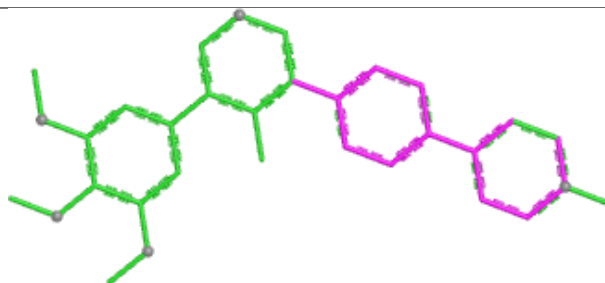
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



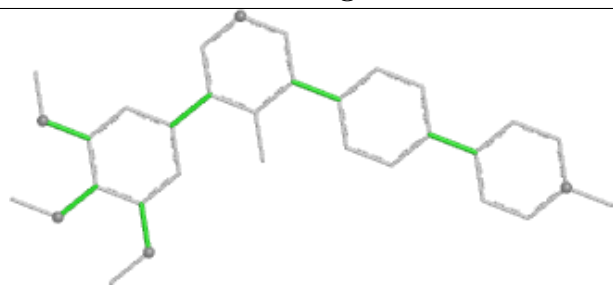
Ligand LU8 A 501



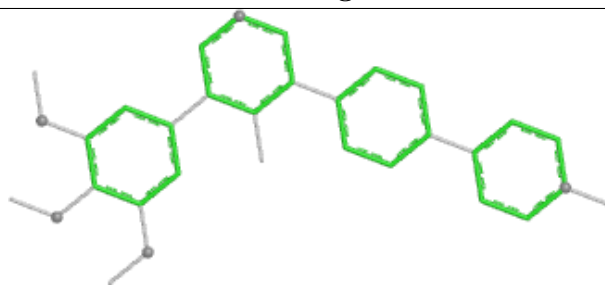
Bond lengths



Bond angles

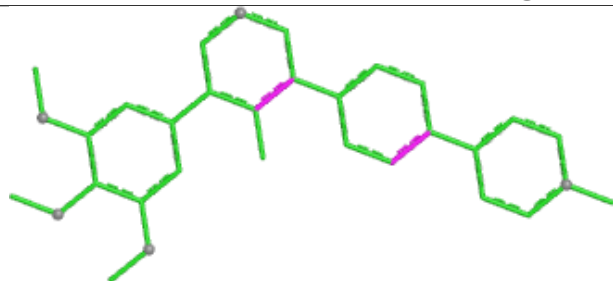


Torsions

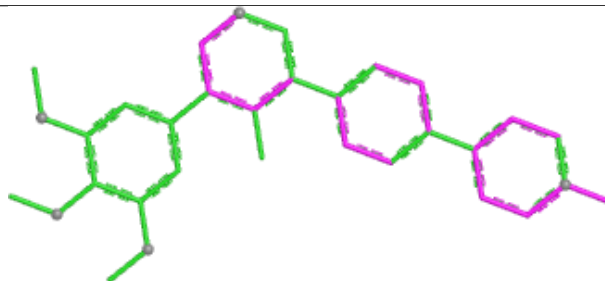


Rings

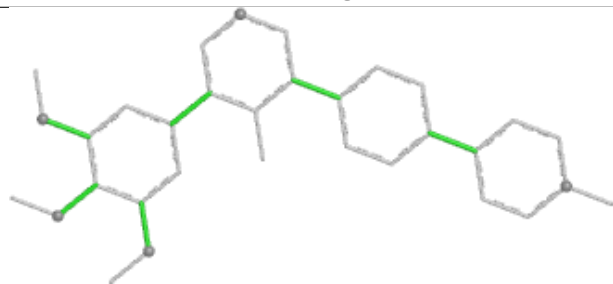
Ligand LU8 B 501



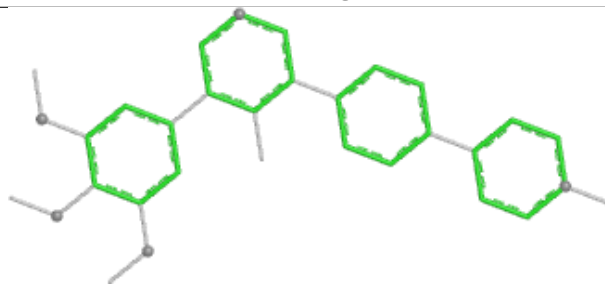
Bond lengths



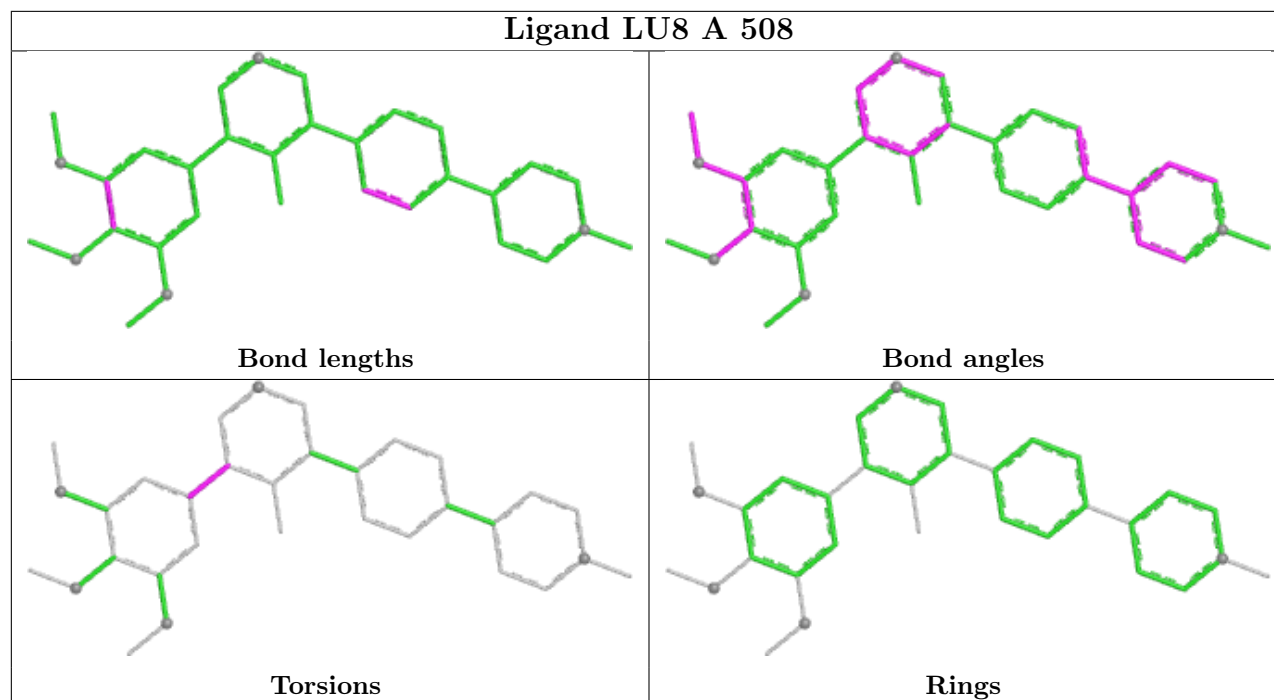
Bond angles



Torsions



Rings



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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	283/301 (94%)	0.41	33 (11%) 9 13	6, 17, 39, 56	13 (4%)
1	B	292/301 (97%)	0.58	32 (10%) 10 14	6, 19, 43, 73	7 (2%)
All	All	575/602 (95%)	0.50	65 (11%) 10 13	6, 18, 41, 73	20 (3%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	376	VAL	7.2
1	B	205	ALA	6.6
1	B	368	LEU	6.3
1	B	374	PRO	5.7
1	B	370	VAL	5.7
1	A	297	LEU	5.4
1	B	366	ASN	5.1
1	B	365	THR	5.0
1	B	255	VAL	4.5
1	A	395	CYS	4.4
1	B	499	ASP	4.3
1	B	324	PHE	4.3
1	B	367	GLN	4.2
1	B	369	ASP	4.2
1	A	324	PHE	4.2
1	B	372	ASN	4.2
1	B	323	ILE	4.1
1	A	275	SER	4.0
1	A	325	GLY	3.9
1	B	297	LEU	3.9
1	B	229	GLY	3.8
1	B	373	ASN	3.7
1	B	227	TRP	3.6
1	A	394	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	376	VAL	3.6
1	B	393	VAL	3.6
1	A	393	VAL	3.5
1	B	498	ILE	3.5
1	A	227	TRP	3.4
1	B	328	GLY	3.1
1	B	364	SER	3.1
1	A	208	ILE	3.0
1	A	375	ARG	2.8
1	B	371	GLY	2.8
1	B	211	LEU	2.8
1	B	375	ARG	2.8
1	A	211	LEU	2.8
1	B	208	ILE	2.8
1	A	209	THR	2.7
1	A	273	ARG	2.7
1	A	239	SER	2.7
1	A	499	ASP	2.7
1	B	437	ASN	2.5
1	A	278	GLN	2.5
1	A	230	GLU	2.5
1	B	228	GLN	2.5
1	A	210	LEU	2.5
1	A	323	ILE	2.4
1	A	202	ARG	2.4
1	A	438	ASP	2.4
1	A	274	HIS	2.3
1	A	276	SER	2.3
1	A	437	ASN	2.3
1	A	216	LYS	2.3
1	A	241	ASP	2.3
1	A	229	GLY	2.3
1	A	321[A]	ILE	2.2
1	A	328	GLY	2.2
1	A	396	PHE	2.1
1	B	280	TRP	2.1
1	B	219	TYR	2.1
1	A	303	VAL	2.1
1	B	363	GLN	2.0
1	B	206	ARG	2.0
1	A	392	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

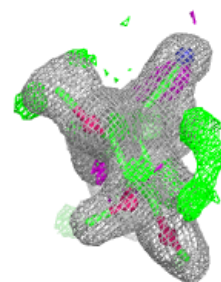
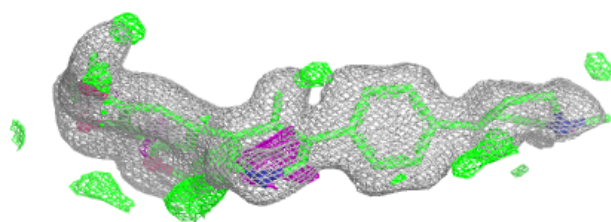
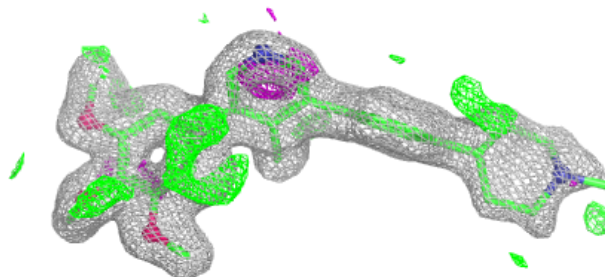
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	B	510	4/4	0.66	0.20	45,48,49,49	0
5	XK7	A	509	7/7	0.66	0.30	42,44,45,47	7
4	DMS	A	506	4/4	0.67	0.32	87,94,96,96	0
3	EDO	A	517	4/4	0.71	0.19	49,56,58,59	0
4	DMS	B	504	4/4	0.73	0.23	86,89,89,93	0
3	EDO	A	516	4/4	0.75	0.19	53,54,57,62	0
3	EDO	A	504	4/4	0.78	0.19	45,49,50,55	0
3	EDO	A	514	4/4	0.78	0.20	44,48,51,57	0
5	XK7	B	505	7/7	0.81	0.18	18,20,23,24	7
3	EDO	B	509	4/4	0.82	0.17	32,39,41,43	0
6	SO4	A	512	5/5	0.82	0.14	31,36,42,42	5
6	SO4	B	507	5/5	0.84	0.13	35,44,53,57	0
3	EDO	A	503	4/4	0.86	0.16	23,29,31,35	0
2	LU8	A	507	32/32	0.89	0.12	18,25,43,48	0
6	SO4	B	506	5/5	0.89	0.10	44,46,51,53	5
3	EDO	B	503	4/4	0.89	0.11	22,23,24,29	0
3	EDO	A	515	4/4	0.91	0.13	17,22,29,36	0
3	EDO	B	508	4/4	0.94	0.12	14,25,25,25	0
3	EDO	A	505	4/4	0.94	0.10	22,29,30,33	0
3	EDO	A	513	4/4	0.95	0.11	16,29,32,41	0
2	LU8	A	508	32/32	0.96	0.08	15,17,39,48	0
3	EDO	A	502	4/4	0.96	0.12	12,25,25,27	0
2	LU8	A	501	32/32	0.96	0.09	13,15,45,53	0
2	LU8	B	501	32/32	0.97	0.08	14,16,41,44	0
6	SO4	A	511	5/5	0.98	0.06	17,21,26,27	0
6	SO4	B	502	5/5	0.98	0.05	24,24,27,27	0
6	SO4	A	510	5/5	0.99	0.04	19,20,24,24	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.

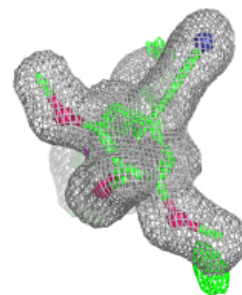
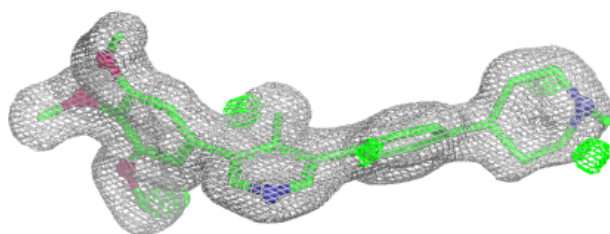
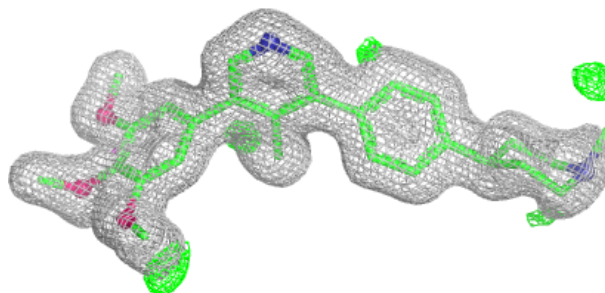
Electron density around LU8 A 507:

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

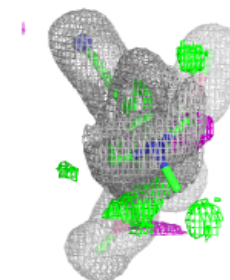
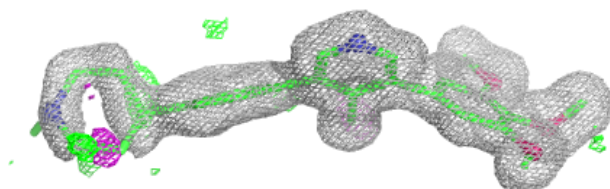
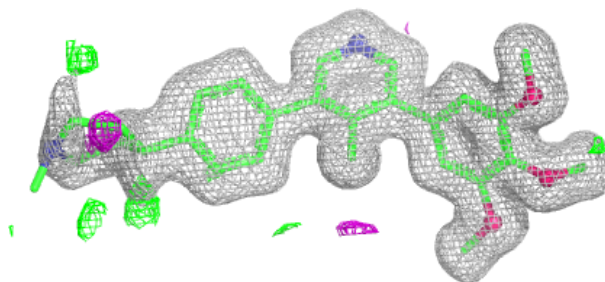


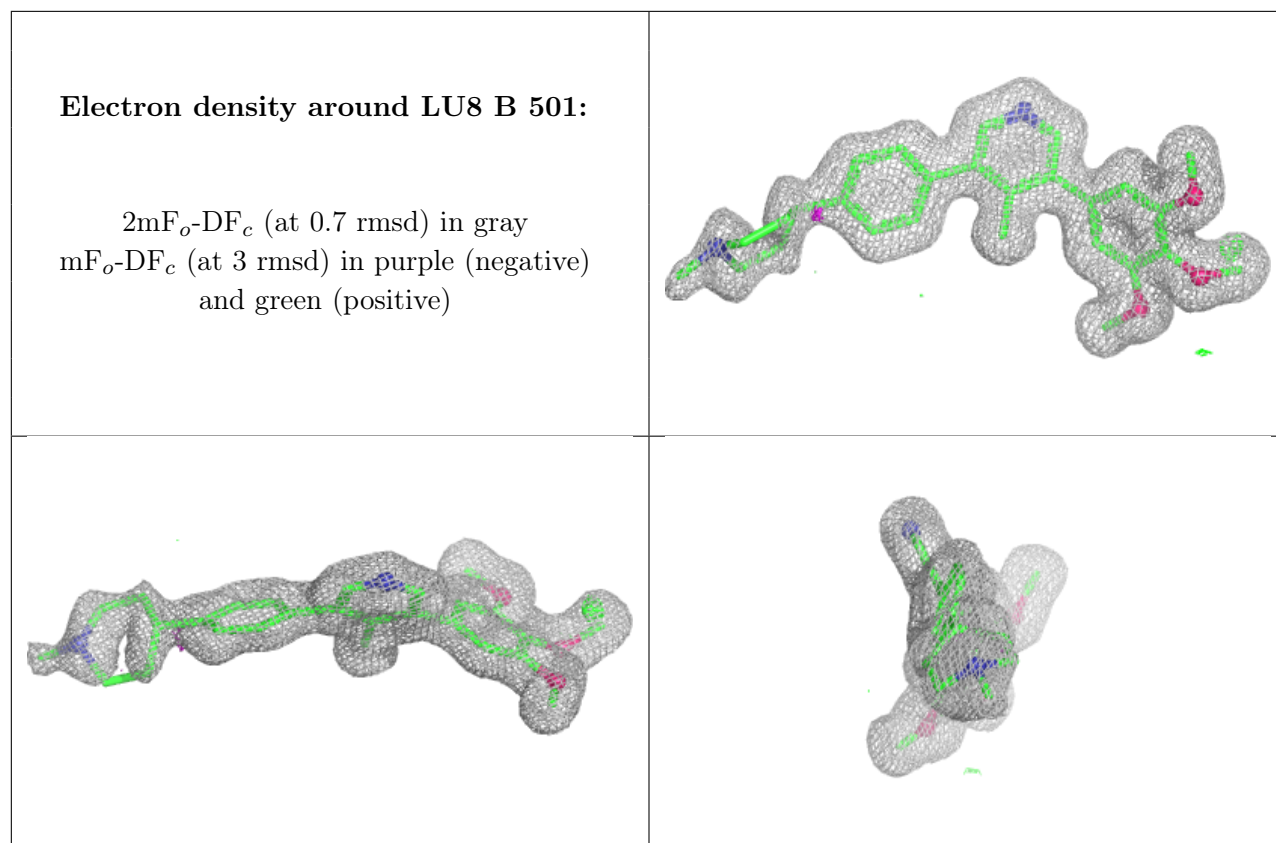
Electron density around LU8 A 508:

$2mF_o-DF_c$ (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:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.