



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:37 AM UTC

PDB ID : 5S7B / pdb_00005s7b
Title : XChem group deposition – Crystal Structure of human ACVR1 in complex with FM000329d
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 : 1.32 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

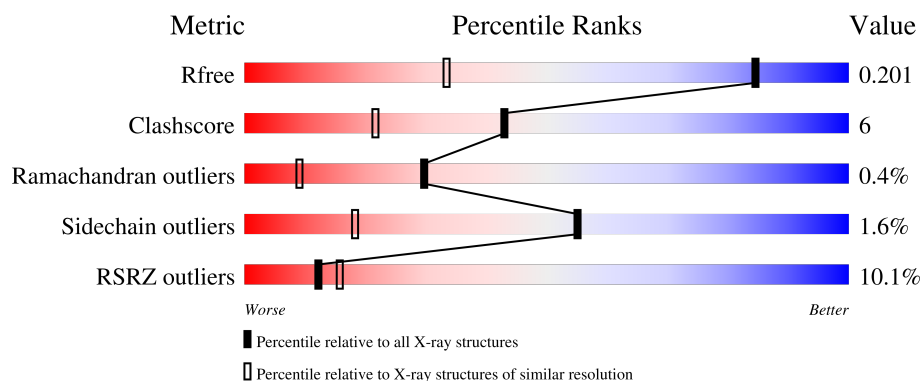
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.32 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	9% 81% 12% • 5%
1	B	301	10% 89% 7% • •

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5619 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.

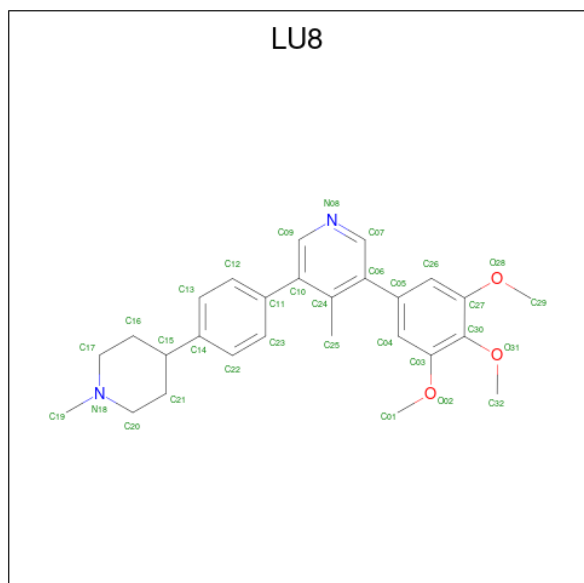
- Molecule 1 is a protein called Activin receptor type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	11	0
			2336	1494	401	426	15			
1	B	292	Total	C	N	O	S	0	5	0
			2334	1490	404	426	14			

There are 6 discrepancies between the modelled and reference sequences:

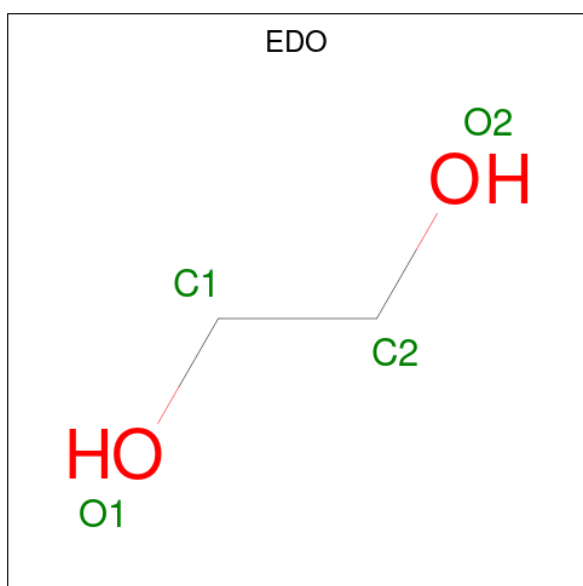
Chain	Residue	Modelled	Actual	Comment	Reference
A	199	SER	-	expression tag	UNP Q04771
A	200	MET	-	expression tag	UNP Q04771
A	207	ASP	GLN	engineered mutation	UNP Q04771
B	199	SER	-	expression tag	UNP Q04771
B	200	MET	-	expression tag	UNP Q04771
B	207	ASP	GLN	engineered mutation	UNP Q04771

- 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).



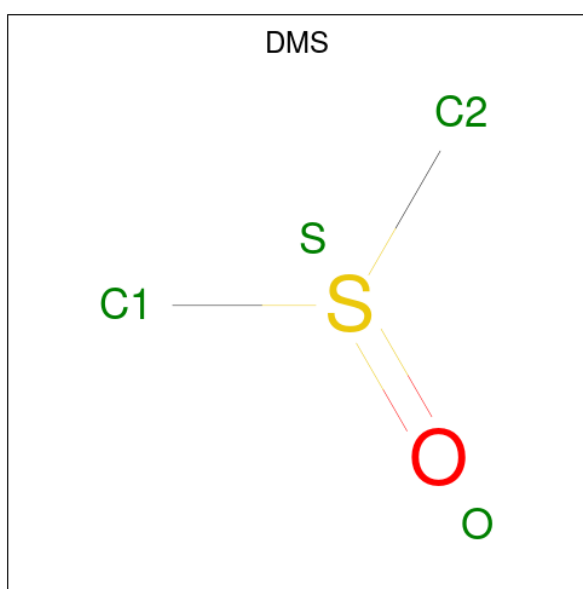
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

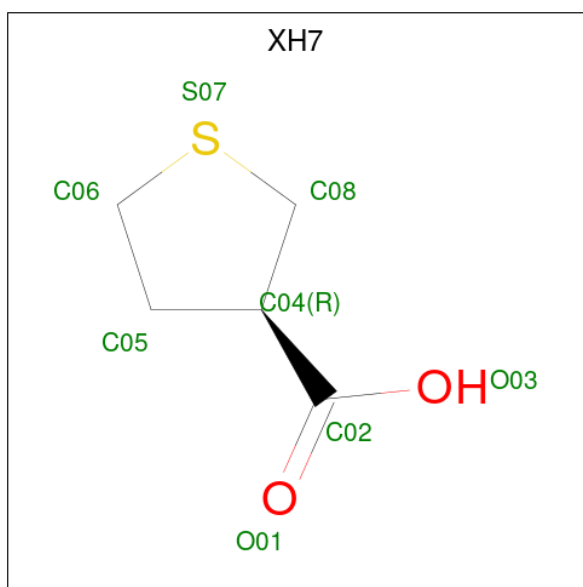
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

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



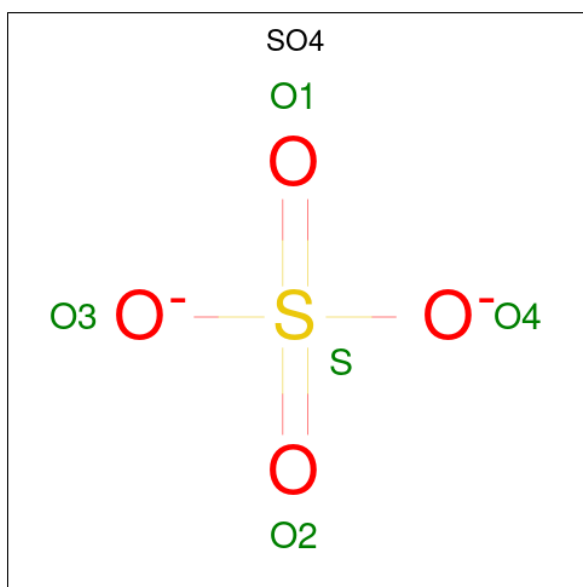
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is (3R)-thiolane-3-carboxylic acid (CCD ID: XH7) (formula: $C_5H_8O_2S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			8	5	2	1		
5	A	1	Total	C	O	S	0	0
			8	5	2	1		
5	B	1	Total	C	O	S	0	0
			8	5	2	1		

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



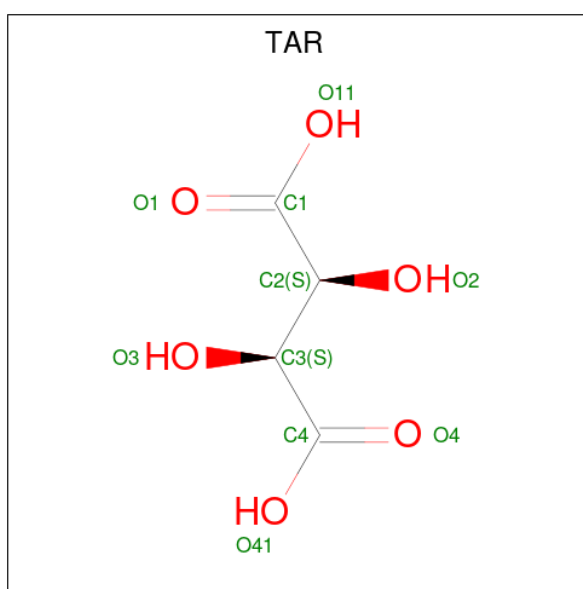
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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		
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 D(-)-TARTARIC ACID (CCD ID: TAR) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	4	6		

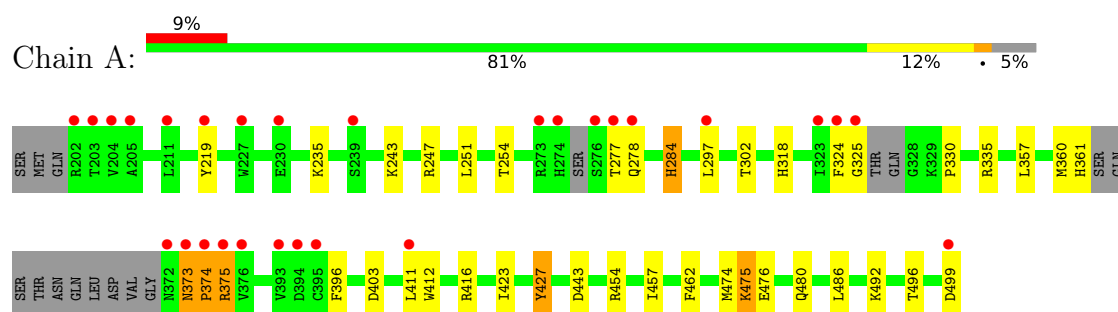
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	359	Total	O	0	1
			359	359		
8	B	347	Total	O	0	0
			347	347		

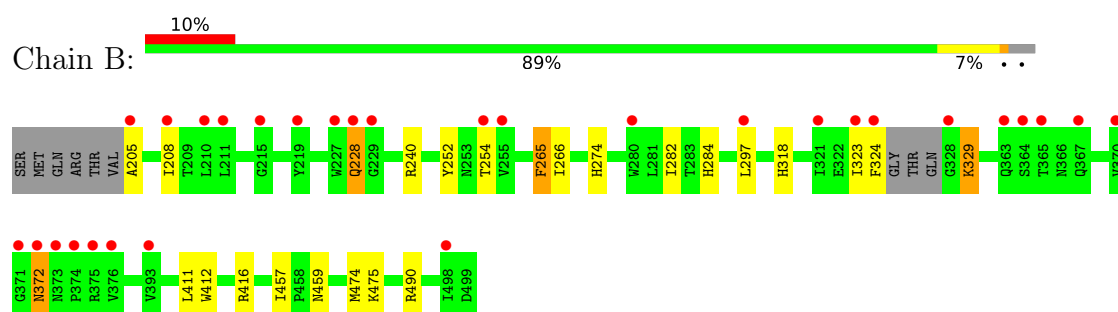
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 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	127.19Å 84.63Å 88.13Å 90.00° 131.06° 90.00°	Depositor
Resolution (Å)	66.45 – 1.32 66.45 – 1.32	Depositor EDS
% Data completeness (in resolution range)	74.9 (66.45-1.32) 74.9 (66.45-1.32)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.32Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.168 , 0.195 0.172 , 0.201	Depositor DCC
R_{free} test set	8380 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h+k-l,-l,-k 0.000 for -h-k-l,l,k 0.017 for -h-2*l,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5619	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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: XH7, DMS, EDO, LU8, TAR, SO4

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	1.06	0/2395	1.16	5/3245 (0.2%)
1	B	1.08	1/2393 (0.0%)	1.23	5/3252 (0.2%)
All	All	1.07	1/4788 (0.0%)	1.20	10/6497 (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	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	274	HIS	CE1-NE2	6.67	1.39	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	HIS	CA-CB-CG	-7.07	106.73	113.80
1	B	254	THR	CA-CB-OG1	-6.65	99.63	109.60
1	A	277	THR	CA-CB-OG1	-6.28	100.19	109.60
1	B	284	HIS	CB-CA-C	6.07	120.49	109.62
1	B	265	PHE	N-CA-CB	-5.22	102.17	110.06
1	B	284	HIS	CA-CB-CG	-5.19	108.61	113.80
1	A	443	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	403	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	266	ILE	N-CA-C	-5.05	107.63	111.62
1	A	462	PHE	CA-CB-CG	-5.00	108.80	113.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	374	PRO	Peptide
1	A	427	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2336	0	2304	35	0
1	B	2334	0	2291	16	0
2	A	96	0	0	0	0
2	B	32	0	0	1	0
3	A	32	0	48	5	0
3	B	16	0	23	0	0
4	A	4	0	6	0	0
4	B	4	0	6	1	0
5	A	16	0	0	2	0
5	B	8	0	0	2	0
6	A	15	0	0	0	0
6	B	10	0	0	0	0
7	B	10	0	4	3	0
8	A	359	0	0	14	0
8	B	347	0	0	3	0
All	All	5619	0	4682	60	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 6.

All (60) 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)
5:B:506:XH7:C04	5:B:506:XH7:C05	1.82	1.40
5:A:510:XH7:C08	8:A:681:HOH:O	2.15	0.94
3:A:504:EDO:H12	8:A:850:HOH:O	1.84	0.76
1:A:247:ARG:HH12	1:A:373:ASN:HA	1.53	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:LEU:HG	1:A:474:MET:HE2	1.71	0.72
3:A:504:EDO:C1	8:A:850:HOH:O	2.41	0.68
1:A:454:ARG:HH22	1:A:480[B]:GLN:CD	2.01	0.68
1:B:324:PHE:C	8:B:867:HOH:O	2.37	0.67
1:A:475:LYS:HD2	8:A:867:HOH:O	1.95	0.67
1:A:454:ARG:NH2	1:A:480[B]:GLN:OE1	2.28	0.67
7:B:505:TAR:O11	8:B:601:HOH:O	2.13	0.66
1:B:475:LYS:NZ	8:B:602:HOH:O	2.25	0.65
1:B:490:ARG:HH22	4:B:504:DMS:H12	1.63	0.64
1:A:254:THR:HG21	1:A:360:MET:HE1	1.81	0.63
1:A:373:ASN:CB	1:A:374:PRO:HD2	2.29	0.63
1:B:372:ASN:H	1:B:372:ASN:HD22	1.48	0.60
1:A:284:HIS:HE1	8:A:643:HOH:O	1.85	0.59
1:A:457:ILE:HG13	1:A:475:LYS:HE2	1.84	0.59
1:A:492:LYS:O	1:A:496:THR:HG23	2.02	0.59
1:A:335:ARG:HH12	1:A:373:ASN:CB	2.16	0.58
1:B:318:HIS:O	1:B:329:LYS:CE	2.51	0.58
1:B:411[B]:LEU:HG	1:B:474:MET:HE2	1.86	0.57
1:A:247:ARG:HH22	1:A:373:ASN:CB	2.17	0.57
1:B:252:TYR:CD1	1:B:265:PHE:HB2	2.42	0.55
1:A:373:ASN:CB	1:A:374:PRO:CD	2.86	0.54
5:B:506:XH7:C05	5:B:506:XH7:C02	2.79	0.53
1:A:475:LYS:NZ	8:A:604:HOH:O	2.27	0.53
1:B:372:ASN:HD22	1:B:372:ASN:N	2.06	0.53
1:B:457:ILE:HG13	1:B:475:LYS:CE	2.39	0.52
1:B:318:HIS:O	1:B:329:LYS:HE3	2.11	0.49
1:A:374:PRO:HB3	8:A:658:HOH:O	2.13	0.48
1:A:247:ARG:NH1	1:A:373:ASN:HA	2.23	0.48
1:A:361:HIS:HB2	1:A:396:PHE:CD1	2.50	0.47
1:A:324:PHE:O	1:A:325:GLY:C	2.57	0.47
1:A:235:LYS:NZ	8:A:603:HOH:O	2.24	0.47
1:A:476[A]:GLU:HB3	1:A:486:LEU:HG	1.97	0.46
1:B:459:ASN:ND2	7:B:505:TAR:O1	2.36	0.45
3:A:514:EDO:H21	8:A:876:HOH:O	2.15	0.45
1:A:284:HIS:CE1	8:A:643:HOH:O	2.64	0.45
1:B:412:TRP:CZ2	1:B:416:ARG:HD2	2.51	0.45
1:A:318:HIS:ND1	5:A:510:XH7:C04	2.79	0.45
1:A:284:HIS:HE1	8:A:741:HOH:O	1.99	0.44
1:A:330:PRO:HG3	1:A:360:MET:HE3	2.00	0.43
3:A:504:EDO:H21	8:A:901:HOH:O	2.17	0.43
1:B:323:ILE:HD12	1:B:329:LYS:HG2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:TYR:CD1	1:A:235:LYS:HE3	2.54	0.43
1:B:208:ILE:HD11	1:B:282:ILE:HD13	1.99	0.43
1:A:427:TYR:CD2	1:A:427:TYR:C	2.97	0.43
1:B:205:ALA:O	1:B:228:GLN:NE2	2.52	0.43
1:A:251:LEU:C	1:A:251:LEU:HD23	2.45	0.42
1:A:357:LEU:HD21	1:A:374:PRO:HB2	2.02	0.42
1:A:423:ILE:HD12	3:A:515:EDO:O2	2.19	0.42
1:B:459:ASN:HB2	7:B:505:TAR:O1	2.19	0.42
1:A:284:HIS:CD2	8:A:897:HOH:O	2.72	0.42
1:A:335:ARG:NH1	1:A:373:ASN:CB	2.82	0.42
1:A:243:LYS:HD3	1:A:374:PRO:HA	2.02	0.42
1:A:302:THR:HG21	1:A:499:ASP:OD2	2.20	0.41
1:A:278:GLN:HG2	8:A:602:HOH:O	2.20	0.41
1:A:412:TRP:CZ2	1:A:416:ARG:HD2	2.56	0.41
2:B:501:LU8:C23	2:B:501:LU8:C25	2.99	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	288/301 (96%)	283 (98%)	3 (1%)	2 (1%)	18	3
1	B	293/301 (97%)	289 (99%)	4 (1%)	0	100	100
All	All	581/602 (96%)	572 (98%)	7 (1%)	2 (0%)	30	15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	375	ARG
1	A	373	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	254/270 (94%)	251 (99%)	3 (1%)	63	28
1	B	254/270 (94%)	249 (98%)	5 (2%)	48	12
All	All	508/540 (94%)	500 (98%)	8 (2%)	55	18

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	297	LEU
1	A	375	ARG
1	A	475	LYS
1	B	228	GLN
1	B	240	ARG
1	B	297	LEU
1	B	329	LYS
1	B	372	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	GLN
1	A	274	HIS
1	A	284	HIS
1	A	453	GLN
1	B	228	GLN
1	B	372	ASN
1	B	452	GLN

5.3.3 RNA ⓘ

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$
6	SO4	A	513	-	4,4,4	0.41	0	6,6,6	0.22	0
3	EDO	A	517	-	3,3,3	0.16	0	2,2,2	0.29	0
5	XH7	A	509	-	7,8,8	3.89	2 (28%)	5,10,10	1.94	3 (60%)
3	EDO	B	503	-	3,3,3	0.91	0	2,2,2	0.62	0
6	SO4	B	502	-	4,4,4	0.24	0	6,6,6	0.45	0
2	LU8	A	508	-	35,35,35	1.01	3 (8%)	47,49,49	1.49	11 (23%)
5	XH7	A	510	-	7,8,8	4.00	2 (28%)	5,10,10	0.64	0
3	EDO	A	505	-	3,3,3	0.15	0	2,2,2	0.91	0
3	EDO	A	503	-	3,3,3	0.56	0	2,2,2	0.44	0
6	SO4	B	507	-	4,4,4	0.35	0	6,6,6	0.08	0
3	EDO	B	509	-	3,3,3	0.22	0	2,2,2	0.18	0
3	EDO	A	515	-	3,3,3	0.38	0	2,2,2	0.08	0
3	EDO	B	510	-	3,3,3	0.14	0	2,2,2	0.20	0
3	EDO	A	504	-	3,3,3	0.19	0	2,2,2	0.51	0
4	DMS	A	506	-	3,3,3	0.22	0	3,3,3	0.16	0
2	LU8	B	501	-	35,35,35	1.06	4 (11%)	47,49,49	1.59	8 (17%)
4	DMS	B	504	-	3,3,3	0.27	0	3,3,3	0.12	0
3	EDO	A	514	-	3,3,3	0.17	0	2,2,2	0.40	0
5	XH7	B	506	-	7,8,8	4.01	1 (14%)	5,10,10	1.56	2 (40%)
6	SO4	A	512	-	4,4,4	0.48	0	6,6,6	0.32	0
2	LU8	A	501	-	35,35,35	1.08	2 (5%)	47,49,49	1.46	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	TAR	B	505	-	9,9,9	0.95	0	12,12,12	1.40	2 (16%)
3	EDO	B	508	-	3,3,3	1.10	0	2,2,2	0.69	0
3	EDO	A	502	-	3,3,3	0.26	0	2,2,2	0.18	0
2	LU8	A	507	-	35,35,35	0.91	1 (2%)	47,49,49	1.68	11 (23%)
3	EDO	A	516	-	3,3,3	0.09	0	2,2,2	0.06	0
6	SO4	A	511	-	4,4,4	0.33	0	6,6,6	0.25	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	517	-	-	0/1/1/1	-
5	XH7	A	509	-	-	2/4/11/11	0/1/1/1
3	EDO	B	503	-	-	0/1/1/1	-
2	LU8	A	508	-	-	3/18/28/28	0/4/4/4
5	XH7	A	510	-	-	0/4/11/11	0/1/1/1
3	EDO	A	505	-	-	0/1/1/1	-
3	EDO	A	503	-	-	0/1/1/1	-
3	EDO	B	509	-	-	1/1/1/1	-
3	EDO	A	515	-	-	1/1/1/1	-
3	EDO	B	510	-	-	1/1/1/1	-
3	EDO	A	504	-	-	1/1/1/1	-
2	LU8	B	501	-	-	0/18/28/28	0/4/4/4
3	EDO	A	514	-	-	1/1/1/1	-
5	XH7	B	506	-	-	0/4/11/11	0/1/1/1
2	LU8	A	501	-	-	0/18/28/28	0/4/4/4
7	TAR	B	505	-	-	8/12/12/12	-
3	EDO	B	508	-	-	1/1/1/1	-
3	EDO	A	502	-	-	0/1/1/1	-
2	LU8	A	507	-	-	0/18/28/28	0/4/4/4
3	EDO	A	516	-	-	1/1/1/1	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	506	XH7	C05-C04	10.15	1.82	1.54
5	A	510	XH7	C05-C04	9.67	1.81	1.54
5	A	509	XH7	C05-C04	9.63	1.81	1.54
5	A	510	XH7	C08-S07	-2.99	1.71	1.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	LU8	C23-C22	2.78	1.43	1.38
2	A	501	LU8	C10-C11	2.56	1.54	1.49
2	A	508	LU8	C12-C11	2.26	1.43	1.39
2	B	501	LU8	C26-C05	2.24	1.43	1.39
2	B	501	LU8	O02-C03	2.23	1.40	1.37
5	A	509	XH7	C08-S07	-2.16	1.74	1.81
2	A	508	LU8	C26-C05	2.13	1.43	1.39
2	A	507	LU8	C26-C05	2.13	1.43	1.39
2	B	501	LU8	C10-C24	2.10	1.43	1.40
2	A	508	LU8	C04-C05	-2.02	1.36	1.39
2	B	501	LU8	C07-N08	2.01	1.38	1.34

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	507	LU8	C26-C05-C06	-4.57	112.94	120.61
2	A	507	LU8	C07-C06-C05	-4.57	112.96	119.56
2	B	501	LU8	C20-N18-C17	4.13	116.11	109.54
2	B	501	LU8	C06-C07-N08	-3.96	118.69	124.27
2	A	501	LU8	C22-C14-C13	3.59	122.76	118.30
2	A	508	LU8	C06-C07-N08	-3.47	119.38	124.27
2	A	501	LU8	C12-C13-C14	-3.47	117.72	121.18
2	A	508	LU8	C06-C24-C10	3.34	122.44	118.39
2	A	508	LU8	C09-N08-C07	3.30	121.99	117.51
2	A	501	LU8	C17-C16-C15	3.28	114.84	111.00
2	A	507	LU8	C06-C07-N08	-3.11	119.89	124.27
2	B	501	LU8	C25-C24-C06	3.06	126.32	120.78
2	A	501	LU8	C22-C14-C15	-2.90	113.72	121.09
2	A	501	LU8	C22-C23-C11	-2.90	117.41	121.12
2	B	501	LU8	C23-C22-C14	-2.83	118.36	121.18
2	B	501	LU8	C06-C24-C10	-2.79	115.00	118.39
2	A	507	LU8	C04-C05-C06	2.76	125.24	120.61
2	A	501	LU8	C06-C07-N08	-2.75	120.39	124.27
5	A	509	XH7	O03-C02-C04	2.62	120.94	114.16
7	B	505	TAR	C3-C2-C1	2.53	115.44	109.82
2	A	507	LU8	O02-C03-C30	2.52	119.46	115.14
2	B	501	LU8	C22-C14-C13	2.48	121.38	118.30
2	A	507	LU8	C32-O31-C30	2.46	121.43	114.74
2	A	507	LU8	O02-C03-C04	-2.44	119.87	124.08
5	A	509	XH7	C05-C04-C02	-2.43	106.29	112.88
7	B	505	TAR	C2-C3-C4	-2.37	104.56	109.82
2	B	501	LU8	C10-C09-N08	2.36	127.59	124.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	506	XH7	O03-C02-C04	2.35	120.25	114.16
5	A	509	XH7	O01-C02-C04	-2.35	116.63	122.86
2	A	508	LU8	C20-C21-C15	-2.33	108.27	111.00
2	A	508	LU8	C29-O28-C27	2.33	120.93	117.51
2	A	507	LU8	C23-C11-C10	-2.32	117.06	120.91
2	A	507	LU8	C23-C22-C14	-2.32	118.87	121.18
2	B	501	LU8	C05-C06-C24	-2.26	118.74	122.47
5	B	506	XH7	O03-C02-O01	-2.24	118.99	124.08
2	A	507	LU8	C04-C05-C26	2.24	121.62	118.35
2	A	508	LU8	C32-O31-C30	2.15	120.58	114.74
2	A	507	LU8	O28-C27-C30	2.14	118.80	115.14
2	A	508	LU8	C04-C05-C06	2.07	124.08	120.61
2	A	508	LU8	C17-C16-C15	2.07	113.42	111.00
2	A	501	LU8	C21-C20-N18	-2.06	108.54	111.20
2	A	508	LU8	C25-C24-C10	-2.06	117.05	120.78
2	A	501	LU8	C23-C11-C12	2.05	121.35	117.68
2	A	508	LU8	C13-C14-C15	2.05	126.28	121.09
2	A	508	LU8	C22-C14-C15	-2.04	115.92	121.09

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	505	TAR	O1-C1-C2-O2
7	B	505	TAR	O11-C1-C2-O2
7	B	505	TAR	O3-C3-C4-O4
7	B	505	TAR	O3-C3-C4-O41
7	B	505	TAR	O11-C1-C2-C3
7	B	505	TAR	O1-C1-C2-C3
3	A	514	EDO	O1-C1-C2-O2
3	B	508	EDO	O1-C1-C2-O2
3	A	516	EDO	O1-C1-C2-O2
7	B	505	TAR	C1-C2-C3-O3
2	A	508	LU8	C04-C05-C06-C07
2	A	508	LU8	C26-C05-C06-C07
3	A	504	EDO	O1-C1-C2-O2
3	B	510	EDO	O1-C1-C2-O2
5	A	509	XH7	O01-C02-C04-C08
5	A	509	XH7	O03-C02-C04-C08
3	B	509	EDO	O1-C1-C2-O2
7	B	505	TAR	C1-C2-C3-C4
2	A	508	LU8	C04-C05-C06-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	515	EDO	O1-C1-C2-O2

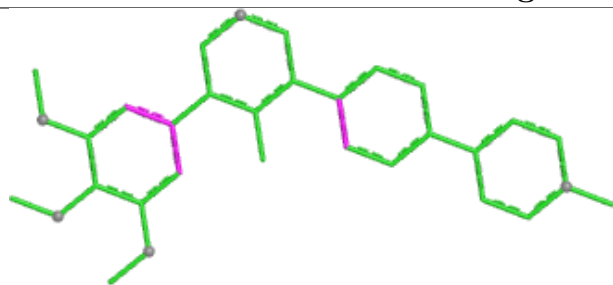
There are no ring outliers.

8 monomers are involved in 14 short contacts:

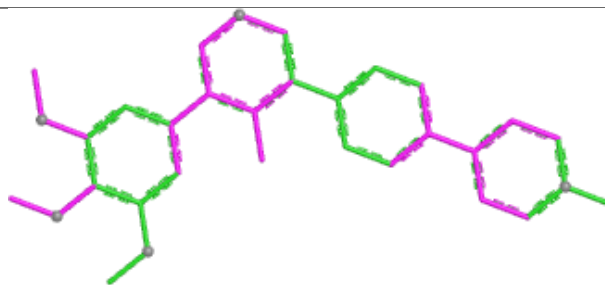
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	510	XH7	2	0
3	A	515	EDO	1	0
3	A	504	EDO	3	0
2	B	501	LU8	1	0
4	B	504	DMS	1	0
3	A	514	EDO	1	0
5	B	506	XH7	2	0
7	B	505	TAR	3	0

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.

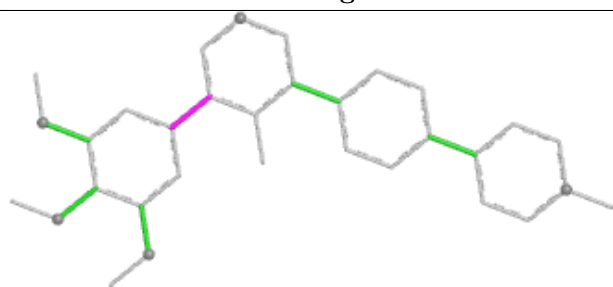
Ligand LU8 A 508



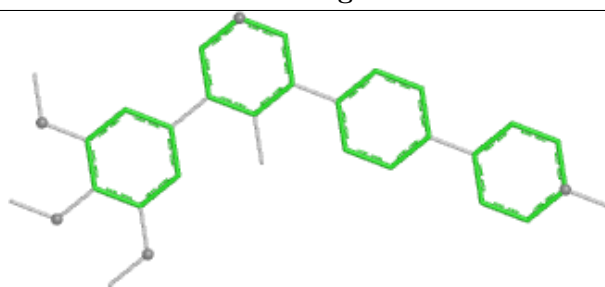
Bond lengths



Bond angles

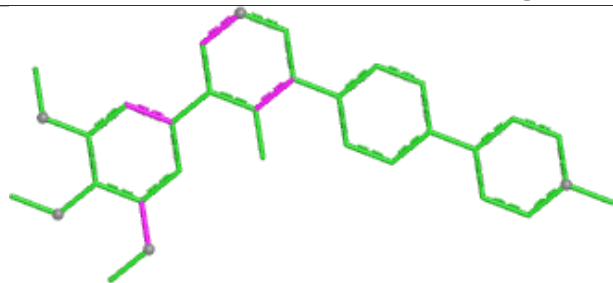


Torsions

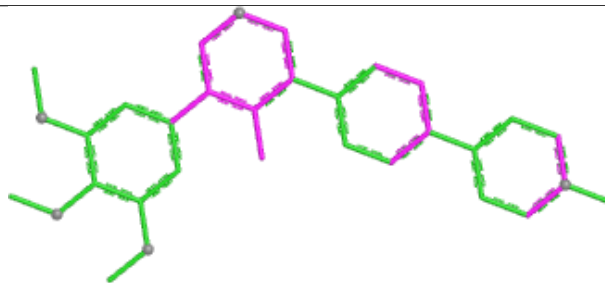


Rings

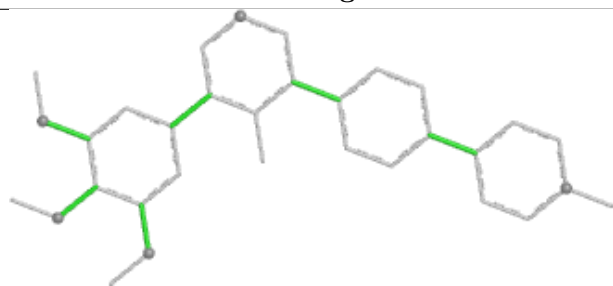
Ligand LU8 B 501



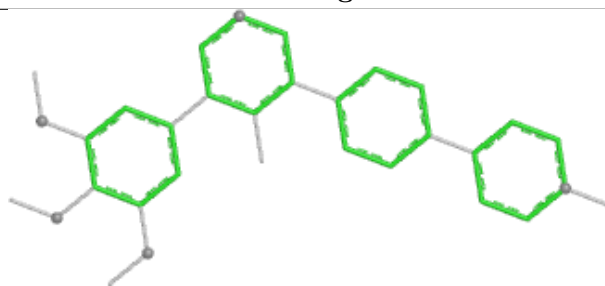
Bond lengths



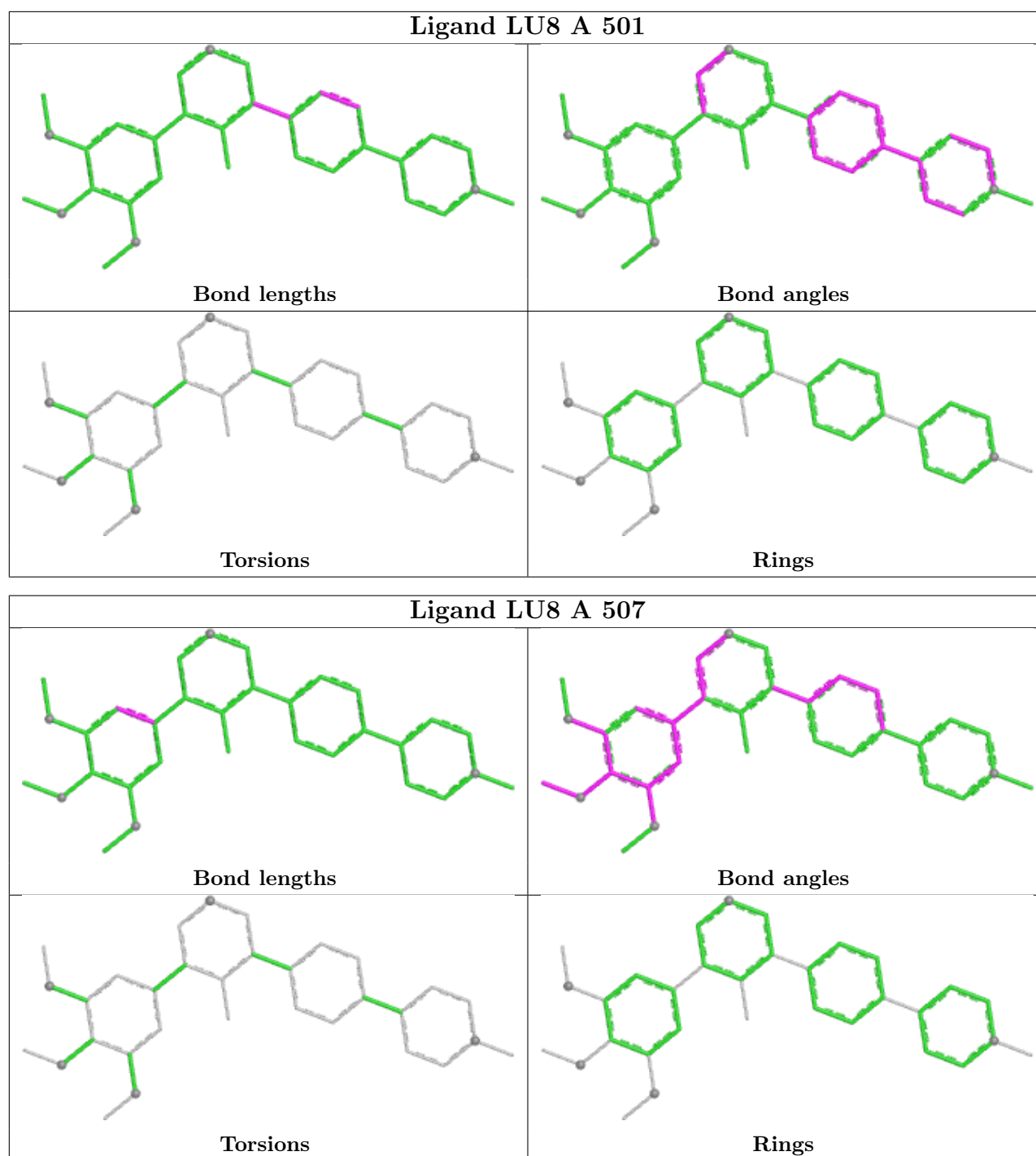
Bond angles



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	285/301 (94%)	0.45	28 (9%) 13 17	7, 18, 42, 71	11 (3%)
1	B	292/301 (97%)	0.64	30 (10%) 12 15	7, 21, 42, 56	5 (1%)
All	All	577/602 (95%)	0.54	58 (10%) 12 16	7, 20, 43, 71	16 (2%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	372	ASN	7.2
1	A	374	PRO	6.3
1	A	324	PHE	5.8
1	A	297	LEU	5.4
1	A	373	ASN	5.3
1	B	297	LEU	5.0
1	B	205	ALA	5.0
1	A	274	HIS	4.7
1	B	324	PHE	4.4
1	B	255	VAL	4.3
1	B	323	ILE	4.2
1	A	375	ARG	4.0
1	B	211	LEU	4.0
1	B	219	TYR	4.0
1	B	374	PRO	3.8
1	A	325	GLY	3.7
1	B	227	TRP	3.7
1	B	229	GLY	3.6
1	A	376	VAL	3.6
1	A	393	VAL	3.5
1	B	370	VAL	3.5
1	B	328	GLY	3.4
1	A	202	ARG	3.2
1	B	393	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	395	CYS	3.1
1	A	499	ASP	3.1
1	B	208	ILE	3.1
1	A	394	ASP	3.0
1	B	376	VAL	2.9
1	A	277	THR	2.9
1	B	498	ILE	2.8
1	B	364	SER	2.8
1	A	227	TRP	2.8
1	A	323	ILE	2.8
1	A	219	TYR	2.7
1	B	372	ASN	2.6
1	A	273	ARG	2.6
1	A	205	ALA	2.6
1	A	239	SER	2.5
1	A	211	LEU	2.5
1	B	254	THR	2.4
1	B	210	LEU	2.4
1	A	203	THR	2.4
1	B	228	GLN	2.4
1	B	365	THR	2.3
1	B	280	TRP	2.3
1	B	367	GLN	2.3
1	B	373	ASN	2.3
1	A	230	GLU	2.3
1	B	321	ILE	2.2
1	B	371	GLY	2.2
1	B	215	GLY	2.2
1	B	375	ARG	2.1
1	A	276	SER	2.1
1	A	278	GLN	2.1
1	A	204	VAL	2.1
1	B	363	GLN	2.0
1	A	411	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

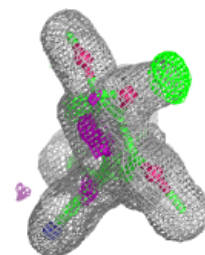
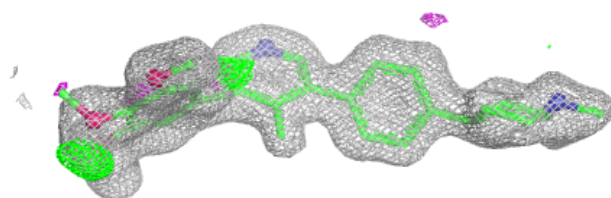
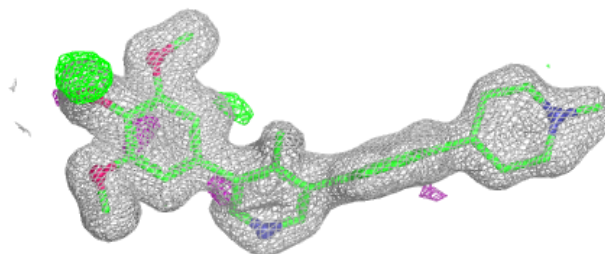
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	XH7	B	506	8/8	0.71	0.21	68,74,79,84	0
3	EDO	A	504	4/4	0.72	0.18	41,48,51,52	0
5	XH7	A	509	8/8	0.74	0.27	36,38,39,42	8
5	XH7	A	510	8/8	0.74	0.38	25,28,30,36	8
3	EDO	A	517	4/4	0.74	0.19	39,48,49,56	0
6	SO4	B	507	5/5	0.75	0.12	77,78,84,90	5
3	EDO	B	508	4/4	0.80	0.19	25,27,31,31	0
4	DMS	A	506	4/4	0.80	0.21	43,51,51,54	0
3	EDO	B	509	4/4	0.81	0.17	37,45,47,48	0
3	EDO	A	516	4/4	0.82	0.17	53,55,58,65	0
3	EDO	B	510	4/4	0.83	0.16	49,50,50,51	0
3	EDO	B	503	4/4	0.86	0.14	25,27,28,33	0
7	TAR	B	505	10/10	0.86	0.21	17,27,42,49	10
4	DMS	B	504	4/4	0.87	0.14	65,65,66,70	0
2	LU8	A	507	32/32	0.88	0.12	23,28,43,44	0
3	EDO	A	515	4/4	0.89	0.13	36,39,44,51	0
3	EDO	A	502	4/4	0.93	0.11	16,29,30,41	0
2	LU8	A	508	32/32	0.94	0.10	19,24,51,63	0
3	EDO	A	514	4/4	0.95	0.09	23,31,38,45	0
2	LU8	B	501	32/32	0.96	0.08	15,19,47,51	0
3	EDO	A	503	4/4	0.96	0.07	19,22,23,26	0
6	SO4	B	502	5/5	0.97	0.06	27,27,30,30	0
3	EDO	A	505	4/4	0.97	0.06	15,22,24,26	0
2	LU8	A	501	32/32	0.97	0.08	14,16,46,52	0
6	SO4	A	512	5/5	0.98	0.06	17,22,35,35	0
6	SO4	A	511	5/5	0.98	0.05	19,21,24,26	0
6	SO4	A	513	5/5	0.99	0.04	13,15,19,19	5

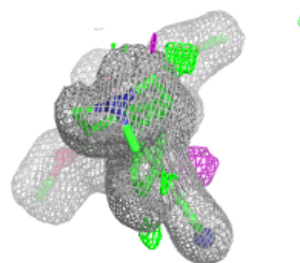
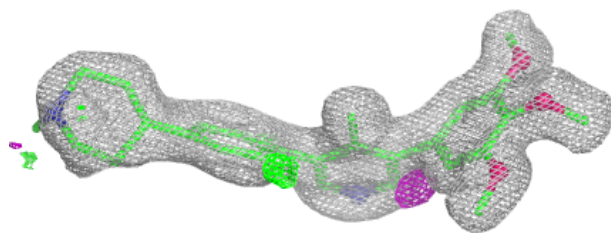
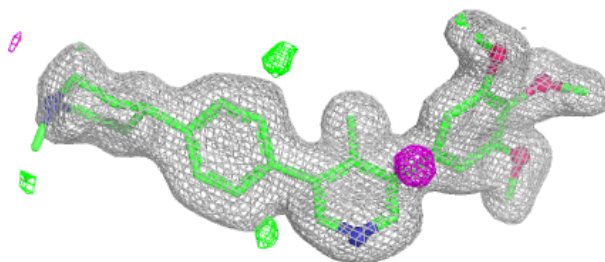
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

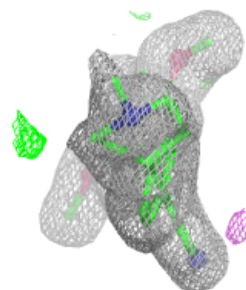
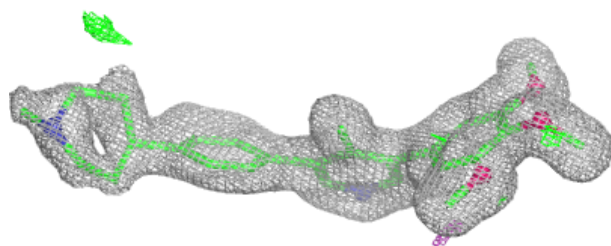
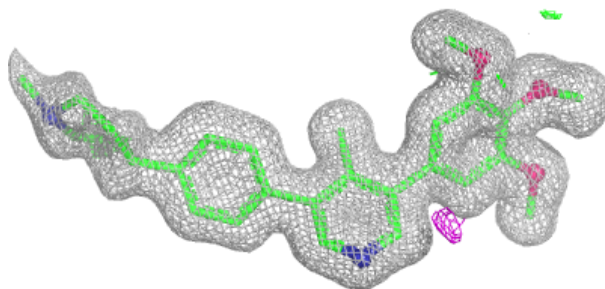
**Electron density around LU8 A 508:**

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

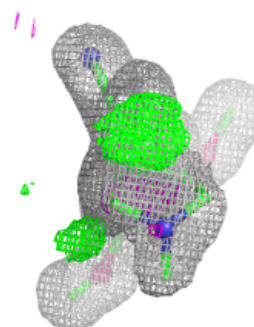
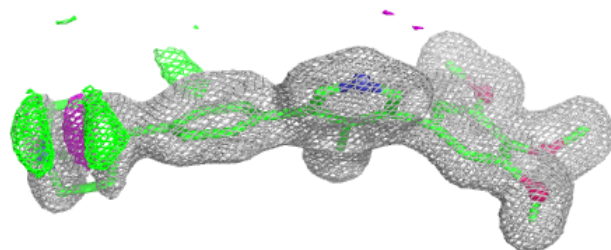
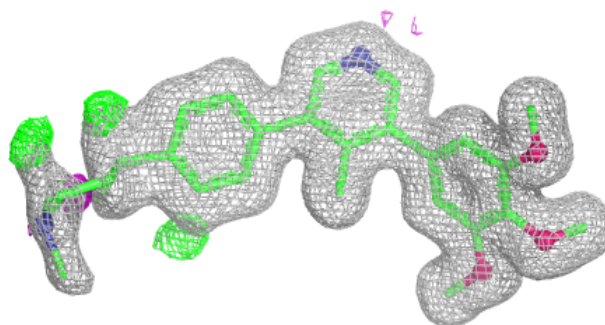


Electron density around LU8 B 501:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.