Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:25 PM UTC

PDB ID	:	5S7L / pdb_00005s7l
Title	:	XChem group deposition – Crystal Structure of human ACVR1 in complex with FM010943a
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	:	1.36 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:

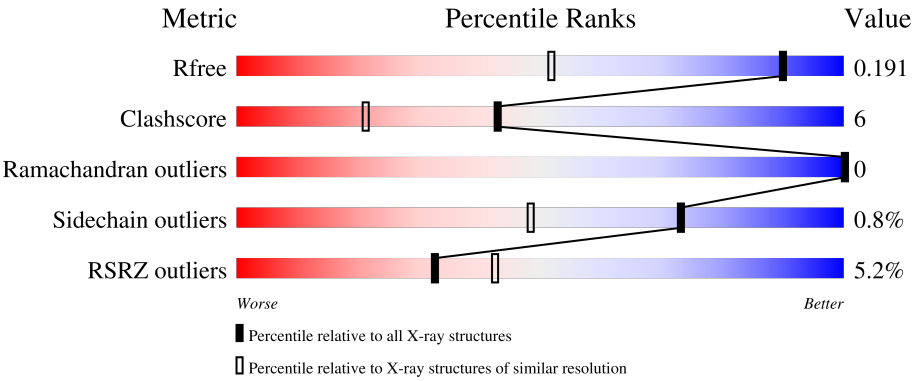
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.36 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	1216 (1.36-1.36)
Clashscore	190562	1232 (1.36-1.36)
Ramachandran outliers	187476	1220 (1.36-1.36)
Sidechain outliers	187428	1220 (1.36-1.36)
RSRZ outliers	180081	1214 (1.36-1.36)

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 <=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	6% 85% 9% • 5%
1	B	301	4% 88% 9% •

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5836 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.

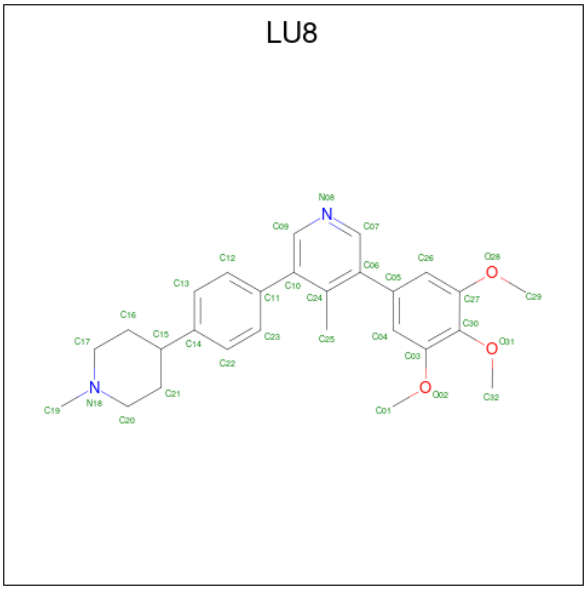
- Molecule 1 is a protein called Activin receptor type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	14	0
			2384	1525	410	433	16			
1	B	292	Total	C	N	O	S	0	11	0
			2404	1532	414	442	16			

There are 6 discrepancies between the modelled and reference sequences:

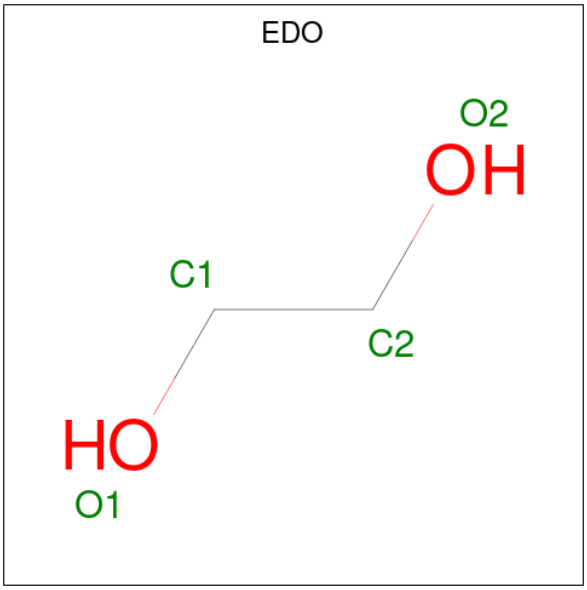
Chain	Residue	Modelled	Actual	Comment	Reference
A	199	SER	-	expression tag	UNP Q04771
A	200	MET	-	expression tag	UNP Q04771
A	207	ASP	GLN	engineered mutation	UNP Q04771
B	199	SER	-	expression tag	UNP Q04771
B	200	MET	-	expression tag	UNP Q04771
B	207	ASP	GLN	engineered mutation	UNP Q04771

- Molecule 2 is 4-methyl-3-[4-(1-methylpiperidin-4-yl)phenyl]-5-(3,4,5-trimethoxyphenyl)pyridine (CCD ID: LU8) (formula: $C_{27}H_{32}N_2O_3$).



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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



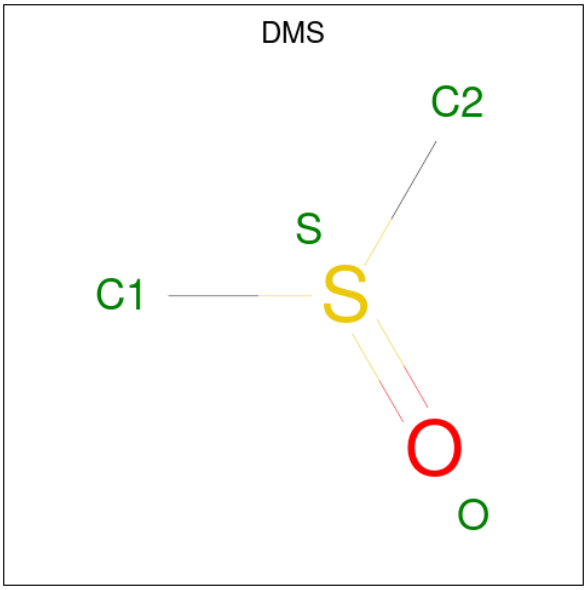
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

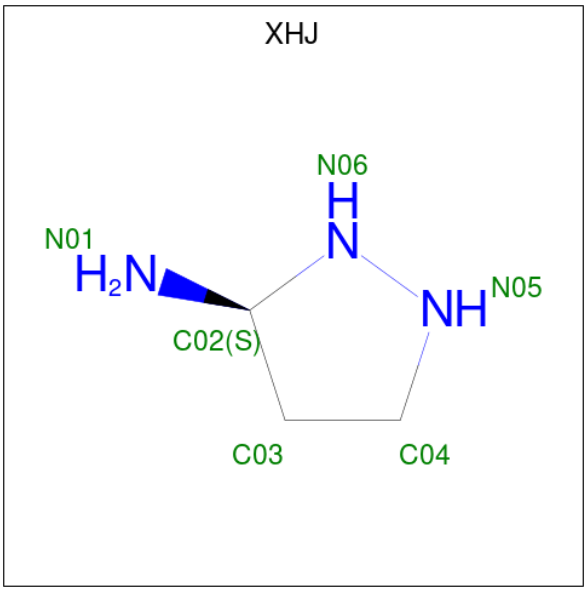
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

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



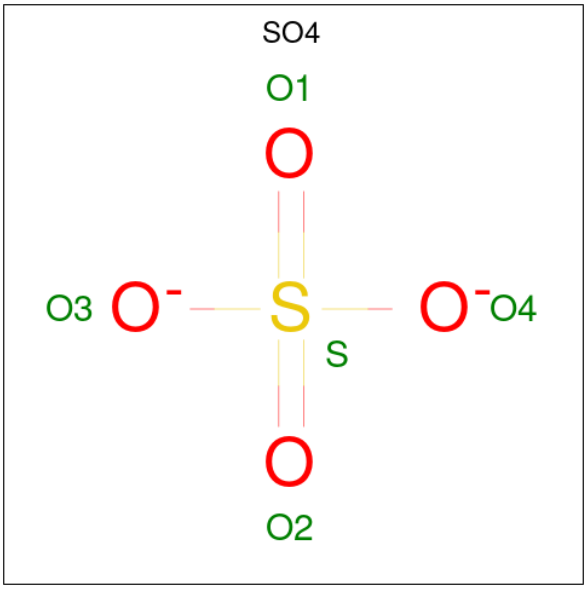
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O S 4 2 1 1	0	0
4	B	1	Total C O S 4 2 1 1	0	0

- Molecule 5 is (3S)-pyrazolidin-3-amine (CCD ID: XHJ) (formula: $C_3H_9N_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 18 9 9	0	1
5	B	1	Total C N 6 3 3	0	0
5	B	1	Total C N 6 3 3	0	0
5	B	1	Total C N 6 3 3	0	0
5	B	1	Total C N 12 6 6	0	1

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 7 is water.

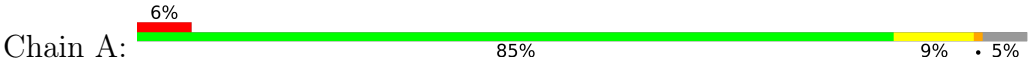
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	372	Total O 373 373	0	1
7	B	390	Total O 390 390	0	0

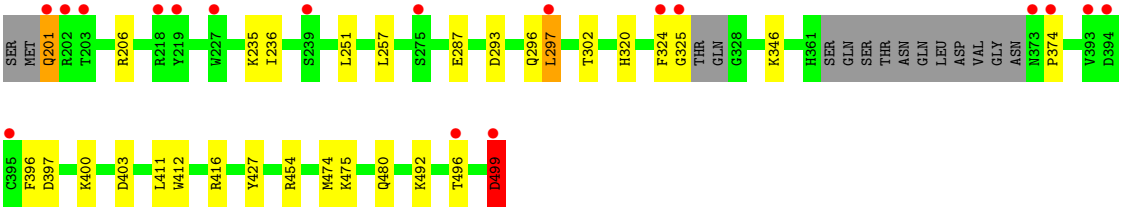
3 Residue-property plots (i)

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

• Molecule 1: Activin receptor type-1

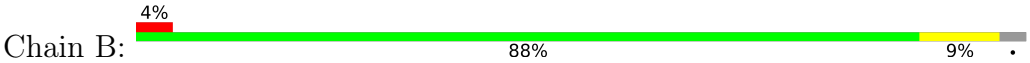
Chain A:

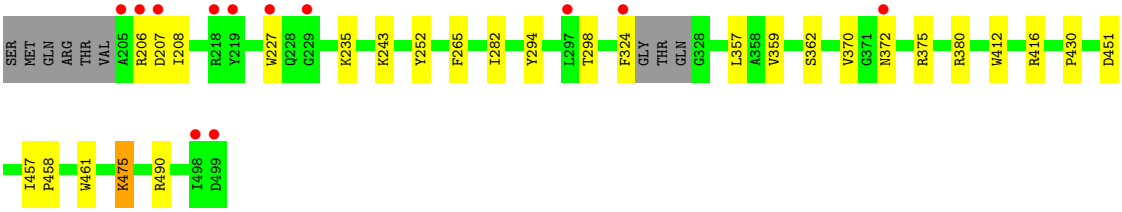




• Molecule 1: Activin receptor type-1

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	127.15Å 84.79Å 88.01Å 90.00° 131.08° 90.00°	Depositor
Resolution (Å)	47.97 – 1.36 47.97 – 1.36	Depositor EDS
% Data completeness (in resolution range)	83.0 (47.97-1.36) 83.0 (47.97-1.36)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 1.36Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.166 , 0.188 0.169 , 0.191	Depositor DCC
R_{free} test set	6246 reflections (4.14%)	wwPDB-VP
Wilson B-factor (Å^2)	16.2	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.012 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	5836	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: XHJ, DMS, SO4, EDO, LU8

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	1.01	1/2447 (0.0%)	1.15	3/3314 (0.1%)
1	B	1.05	1/2465 (0.0%)	1.12	2/3347 (0.1%)
All	All	1.03	2/4912 (0.0%)	1.14	5/6661 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	362	SER	CA-CB	-5.20	1.45	1.53
1	A	236	ILE	C-O	5.09	1.29	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	403	ASP	CA-CB-CG	6.05	118.65	112.60
1	A	499	ASP	CA-C-O	-5.58	111.32	120.80
1	A	374	PRO	CB-CA-C	-5.29	103.89	111.62
1	B	451	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	324	PHE	CA-C-O	-5.26	111.86	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	GLN	Peptide

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	2384	0	2365	26	0
1	B	2404	0	2357	24	0
2	A	128	0	0	2	0
2	B	32	0	0	0	0
3	A	32	0	46	3	0
3	B	12	0	18	2	0
4	A	4	0	6	0	0
4	B	4	0	6	2	0
5	A	18	0	0	0	0
5	B	30	0	0	7	0
6	A	15	0	0	0	0
6	B	10	0	0	1	0
7	A	373	0	0	5	0
7	B	390	0	0	11	0
All	All	5836	0	4798	61	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 (61) 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:508[B]:XHJ:N05	7:B:601:HOH:O	1.74	1.16
5:B:508[A]:XHJ:C03	7:B:601:HOH:O	1.98	1.09
1:B:207[B]:ASP:O	1:B:227[B]:TRP:CD1	2.13	1.01
5:B:508[B]:XHJ:N01	7:B:603:HOH:O	1.95	0.99
5:B:505:XHJ:N01	7:B:602:HOH:O	1.94	0.99
5:B:508[B]:XHJ:C04	7:B:607:HOH:O	2.11	0.97
1:A:396:PHE:HE2	1:A:400[B]:LYS:HE3	1.34	0.92
1:A:396:PHE:CE2	1:A:400[B]:LYS:HE3	2.09	0.85
6:B:509:SO4:O3	7:B:604:HOH:O	2.00	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ARG:NH2	1:A:480[B]:GLN:OE1	2.22	0.73
1:B:206:ARG:C	1:B:227[B]:TRP:HE1	1.99	0.70
1:A:293[A]:ASP:OD2	7:A:601[A]:HOH:O	2.10	0.69
1:A:454:ARG:HH22	1:A:480[B]:GLN:CD	2.01	0.68
1:A:257:LEU:HA	3:A:513:EDO:C2	2.26	0.66
1:B:206:ARG:C	1:B:227[B]:TRP:NE1	2.52	0.66
1:A:257:LEU:HA	3:A:513:EDO:H22	1.79	0.65
1:A:396:PHE:HE2	1:A:400[B]:LYS:CE	2.09	0.62
3:B:511:EDO:H12	7:B:831:HOH:O	2.05	0.57
1:A:302:THR:HG21	1:A:499:ASP:OD2	2.06	0.56
1:A:492:LYS:O	1:A:496:THR:HG23	2.05	0.56
1:A:287:GLU:CD	1:A:346:LYS:CE	2.79	0.54
1:B:235:LYS:NZ	7:B:606:HOH:O	2.39	0.54
1:A:325:GLY:C	7:A:629:HOH:O	2.51	0.53
2:A:501[B]:LU8:C26	2:A:501[B]:LU8:C25	2.86	0.53
1:B:490:ARG:HH22	4:B:504:DMS:H12	1.74	0.53
1:B:206:ARG:O	1:B:227[B]:TRP:CE2	2.62	0.52
1:B:206:ARG:HA	1:B:227[B]:TRP:HZ2	1.74	0.51
1:B:412:TRP:CZ2	1:B:416:ARG:HD2	2.45	0.51
1:B:294:TYR:CZ	1:B:298:THR:HG21	2.47	0.50
1:B:206:ARG:HA	1:B:227[B]:TRP:CZ2	2.47	0.50
1:A:287:GLU:OE2	1:A:346:LYS:CE	2.60	0.50
1:B:357[B]:LEU:HD21	1:B:375:ARG:CG	2.43	0.49
1:B:252:TYR:CD1	1:B:265:PHE:HB2	2.48	0.49
1:A:427:TYR:CD2	1:A:427:TYR:C	2.92	0.48
1:B:206:ARG:O	1:B:227[B]:TRP:CZ2	2.66	0.48
1:A:411:LEU:HG	1:A:474:MET:HE2	1.95	0.47
1:B:243:LYS:HD3	1:B:372:ASN:O	2.15	0.46
1:A:296:GLN:HB2	1:A:297:LEU:HD23	1.97	0.46
1:A:412:TRP:CZ2	1:A:416:ARG:HD2	2.50	0.46
1:B:207[B]:ASP:O	1:B:227[B]:TRP:HD1	1.84	0.46
1:B:457:ILE:CG1	1:B:475:LYS:HE2	2.47	0.44
1:A:480[A]:GLN:NE2	7:A:608:HOH:O	2.39	0.44
5:B:508[A]:XHJ:C02	7:B:607:HOH:O	2.65	0.44
3:B:511:EDO:C1	7:B:831:HOH:O	2.65	0.43
1:A:320:HIS:O	1:A:400[B]:LYS:HE2	2.18	0.43
1:A:251:LEU:C	1:A:251:LEU:HD23	2.44	0.42
1:A:257:LEU:HD23	3:A:513:EDO:H22	2.00	0.42
1:A:235:LYS:NZ	7:A:603:HOH:O	2.31	0.42
1:A:324[B]:PHE:CD1	1:A:325:GLY:N	2.88	0.42
1:B:380:ARG:HD3	1:B:430:PRO:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:LYS:N	1:B:475:LYS:HD3	2.35	0.41
1:B:208:ILE:HD11	1:B:282:ILE:HD13	2.01	0.41
1:A:397:ASP:OD1	1:A:400[A]:LYS:CE	2.69	0.41
1:B:359:VAL:HG22	1:B:370:VAL:HA	2.03	0.41
1:A:475:LYS:HB2	7:A:840:HOH:O	2.21	0.41
1:B:490:ARG:HH22	4:B:504:DMS:H23	1.86	0.41
1:B:208:ILE:CD1	1:B:282:ILE:HD13	2.50	0.41
1:B:357[A]:LEU:HD12	1:B:357[A]:LEU:HA	1.91	0.40
1:B:458:PRO:HD2	1:B:461:TRP:CE2	2.56	0.40
1:A:206:ARG:HG2	2:A:507:LU8:C27	2.51	0.40
5:B:508[A]:XHJ:C02	7:B:601:HOH:O	2.49	0.40

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	294/301 (98%)	291 (99%)	3 (1%)	0	100	100
1	B	299/301 (99%)	296 (99%)	3 (1%)	0	100	100
All	All	593/602 (98%)	587 (99%)	6 (1%)	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	261/270 (97%)	258 (99%)	3 (1%)	65 35
1	B	265/270 (98%)	264 (100%)	1 (0%)	84 69
All	All	526/540 (97%)	522 (99%)	4 (1%)	73 48

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	GLN
1	A	297	LEU
1	A	499	ASP
1	B	475	LYS

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

Mol	Chain	Res	Type
1	A	361	HIS
1	A	373	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

31 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	$\#\|Z\| > 2$
4	DMS	A	506	-	3,3,3	0.26	0	3,3,3	0.09	0
5	XHJ	A	509[C]	-	3,6,6	10.37	1 (33%)	0,7,7	-	-
5	XHJ	B	505	-	3,6,6	11.23	1 (33%)	0,7,7	-	-
5	XHJ	B	508[B]	-	3,6,6	12.53	1 (33%)	0,7,7	-	-
4	DMS	B	504	-	3,3,3	0.22	0	3,3,3	0.05	0
3	EDO	A	503	-	3,3,3	0.94	0	2,2,2	0.55	0
5	XHJ	B	508[A]	-	3,6,6	11.56	2 (66%)	0,7,7	-	-
3	EDO	A	505	-	3,3,3	0.57	0	2,2,2	0.88	0
3	EDO	A	515	-	3,3,3	0.15	0	2,2,2	0.20	0
3	EDO	B	510	-	3,3,3	0.55	0	2,2,2	0.53	0
6	SO4	A	512	-	4,4,4	0.32	0	6,6,6	0.25	0
5	XHJ	B	507	-	3,6,6	10.67	1 (33%)	0,7,7	-	-
3	EDO	A	504	-	3,3,3	0.19	0	2,2,2	0.23	0
2	LU8	A	501[B]	-	35,35,35	0.74	0	47,49,49	1.54	8 (17%)
5	XHJ	A	509[B]	-	3,6,6	9.99	1 (33%)	0,7,7	-	-
6	SO4	A	511	-	4,4,4	0.35	0	6,6,6	0.18	0
6	SO4	A	510	-	4,4,4	0.66	0	6,6,6	0.27	0
3	EDO	A	502	-	3,3,3	1.25	0	2,2,2	1.54	1 (50%)
2	LU8	A	508	-	35,35,35	1.25	4 (11%)	47,49,49	1.89	13 (27%)
2	LU8	A	501[A]	-	35,35,35	0.98	1 (2%)	47,49,49	1.33	7 (14%)
2	LU8	A	507	-	35,35,35	1.15	2 (5%)	47,49,49	1.78	12 (25%)
5	XHJ	A	509[A]	-	3,6,6	11.16	1 (33%)	0,7,7	-	-
3	EDO	B	511	-	3,3,3	0.28	0	2,2,2	0.30	0
6	SO4	B	509	-	4,4,4	0.31	0	6,6,6	0.13	0
3	EDO	A	516	-	3,3,3	0.36	0	2,2,2	0.40	0
3	EDO	A	513	-	3,3,3	0.20	0	2,2,2	0.94	0
2	LU8	B	501	-	35,35,35	1.08	4 (11%)	47,49,49	1.58	10 (21%)
3	EDO	A	514	-	3,3,3	0.21	0	2,2,2	0.22	0
6	SO4	B	502	-	4,4,4	0.53	0	6,6,6	0.47	0
5	XHJ	B	506	-	3,6,6	11.91	1 (33%)	0,7,7	-	-
3	EDO	B	503	-	3,3,3	1.04	0	2,2,2	0.58	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
5	XHJ	A	509[C]	-	-	-	0/1/1/1
5	XHJ	B	505	-	-	-	0/1/1/1
5	XHJ	B	508[B]	-	-	-	0/1/1/1
3	EDO	A	503	-	-	1/1/1/1	-
5	XHJ	B	508[A]	-	-	-	0/1/1/1
3	EDO	A	505	-	-	1/1/1/1	-
3	EDO	A	515	-	-	1/1/1/1	-
3	EDO	B	510	-	-	0/1/1/1	-
5	XHJ	B	507	-	-	-	0/1/1/1
3	EDO	A	504	-	-	1/1/1/1	-
2	LU8	A	501[B]	-	-	0/18/28/28	0/4/4/4
5	XHJ	A	509[B]	-	-	-	0/1/1/1
3	EDO	A	502	-	-	1/1/1/1	-
2	LU8	A	508	-	-	4/18/28/28	0/4/4/4
2	LU8	A	501[A]	-	-	0/18/28/28	0/4/4/4
2	LU8	A	507	-	-	0/18/28/28	0/4/4/4
5	XHJ	A	509[A]	-	-	-	0/1/1/1
3	EDO	B	511	-	-	1/1/1/1	-
3	EDO	A	516	-	-	1/1/1/1	-
3	EDO	A	513	-	-	0/1/1/1	-
2	LU8	B	501	-	-	0/18/28/28	0/4/4/4
3	EDO	A	514	-	-	1/1/1/1	-
5	XHJ	B	506	-	-	-	0/1/1/1
3	EDO	B	503	-	-	0/1/1/1	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	508[B]	XHJ	C03-C02	-21.66	1.27	1.52
5	B	506	XHJ	C03-C02	-20.57	1.28	1.52
5	B	508[A]	XHJ	C03-C02	-19.84	1.29	1.52
5	B	505	XHJ	C03-C02	-19.38	1.30	1.52
5	A	509[A]	XHJ	C03-C02	-19.29	1.30	1.52
5	B	507	XHJ	C03-C02	-18.45	1.31	1.52
5	A	509[C]	XHJ	C03-C02	-17.85	1.31	1.52
5	A	509[B]	XHJ	C03-C02	-17.18	1.32	1.52
2	A	507	LU8	C26-C05	3.26	1.45	1.39
2	A	508	LU8	C26-C27	-2.96	1.33	1.38
2	A	508	LU8	C12-C11	2.82	1.45	1.39
5	B	508[A]	XHJ	C03-C04	-2.57	1.49	1.53
2	A	507	LU8	C10-C11	-2.54	1.44	1.49
2	B	501	LU8	O02-C03	2.40	1.41	1.37
2	A	501[A]	LU8	C27-C30	-2.27	1.36	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	LU8	C27-C30	-2.20	1.36	1.41
2	A	508	LU8	C27-C30	-2.11	1.36	1.41
2	B	501	LU8	C09-C10	-2.10	1.36	1.39
2	B	501	LU8	C06-C24	2.05	1.43	1.40
2	A	508	LU8	C13-C14	2.01	1.42	1.39

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501[B]	LU8	C21-C20-N18	-5.30	104.35	111.20
2	A	507	LU8	C07-C06-C05	-4.83	112.58	119.56
2	A	508	LU8	C32-O31-C30	4.47	126.86	114.74
2	A	508	LU8	C17-C16-C15	3.94	115.62	111.00
2	B	501	LU8	C20-C21-C15	3.93	115.60	111.00
2	A	507	LU8	C26-C05-C06	-3.92	114.03	120.61
2	A	508	LU8	C20-C21-C15	-3.71	106.66	111.00
2	A	508	LU8	C13-C12-C11	-3.66	116.42	121.12
2	A	501[B]	LU8	C06-C07-N08	-3.60	119.20	124.27
2	A	507	LU8	C27-C30-C03	3.53	123.00	119.56
2	A	501[B]	LU8	C20-C21-C15	-3.48	106.93	111.00
2	A	508	LU8	C22-C14-C15	-3.25	112.84	121.09
2	A	508	LU8	C12-C13-C14	3.24	124.42	121.18
2	A	501[A]	LU8	C06-C07-N08	-3.20	119.76	124.27
2	A	507	LU8	C17-C16-C15	-3.20	107.25	111.00
2	A	507	LU8	C12-C11-C10	3.13	126.09	120.91
2	A	501[A]	LU8	C29-O28-C27	3.07	122.01	117.51
2	A	508	LU8	C09-N08-C07	3.03	121.63	117.51
2	A	508	LU8	C13-C14-C15	3.02	128.76	121.09
2	A	508	LU8	C21-C15-C14	2.98	119.73	112.67
2	B	501	LU8	C19-N18-C20	-2.91	105.08	110.63
2	A	501[A]	LU8	C01-O02-C03	2.91	121.79	117.51
2	B	501	LU8	C22-C14-C13	2.88	121.88	118.30
2	A	501[A]	LU8	C07-C06-C05	-2.83	115.47	119.56
2	B	501	LU8	C06-C07-N08	-2.70	120.46	124.27
2	A	501[B]	LU8	O28-C27-C30	2.69	119.74	115.14
2	A	508	LU8	C06-C24-C10	2.68	121.64	118.39
2	B	501	LU8	C17-C16-C15	2.67	114.12	111.00
2	B	501	LU8	C06-C24-C10	-2.66	115.17	118.39
2	A	507	LU8	C21-C20-N18	-2.59	107.86	111.20
2	B	501	LU8	C27-C30-C03	2.58	122.07	119.56
2	A	501[B]	LU8	O28-C27-C26	-2.54	119.70	124.08
2	A	507	LU8	C29-O28-C27	-2.53	113.80	117.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501[B]	LU8	C23-C11-C10	-2.46	116.84	120.91
2	A	507	LU8	C06-C07-N08	-2.46	120.81	124.27
2	A	507	LU8	C23-C11-C10	-2.44	116.86	120.91
2	A	507	LU8	C04-C05-C06	2.43	124.69	120.61
2	A	508	LU8	C16-C17-N18	2.42	114.32	111.20
2	A	508	LU8	C06-C07-N08	-2.39	120.91	124.27
2	A	501[A]	LU8	C11-C10-C24	2.35	126.35	122.47
2	B	501	LU8	O02-C03-C30	2.31	119.09	115.14
2	B	501	LU8	C10-C09-N08	2.28	127.48	124.27
2	A	507	LU8	C05-C06-C24	2.27	126.22	122.47
2	A	501[B]	LU8	C12-C11-C10	2.27	124.67	120.91
2	A	508	LU8	C29-O28-C27	-2.25	114.21	117.51
2	B	501	LU8	C07-C06-C05	-2.21	116.37	119.56
2	A	507	LU8	C01-O02-C03	2.19	120.73	117.51
3	A	502	EDO	O1-C1-C2	-2.14	96.06	112.39
2	A	501[B]	LU8	C05-C06-C24	-2.02	119.14	122.47
2	A	501[A]	LU8	C09-C10-C11	-2.02	116.64	119.56
2	A	501[A]	LU8	C16-C15-C21	2.01	114.04	109.68

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	504	EDO	O1-C1-C2-O2
3	A	514	EDO	O1-C1-C2-O2
3	A	515	EDO	O1-C1-C2-O2
3	B	511	EDO	O1-C1-C2-O2
3	A	502	EDO	O1-C1-C2-O2
2	A	508	LU8	C04-C05-C06-C07
2	A	508	LU8	C26-C05-C06-C07
2	A	508	LU8	C04-C05-C06-C24
3	A	505	EDO	O1-C1-C2-O2
2	A	508	LU8	C26-C05-C06-C24
3	A	503	EDO	O1-C1-C2-O2
3	A	516	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	505	XHJ	1	0

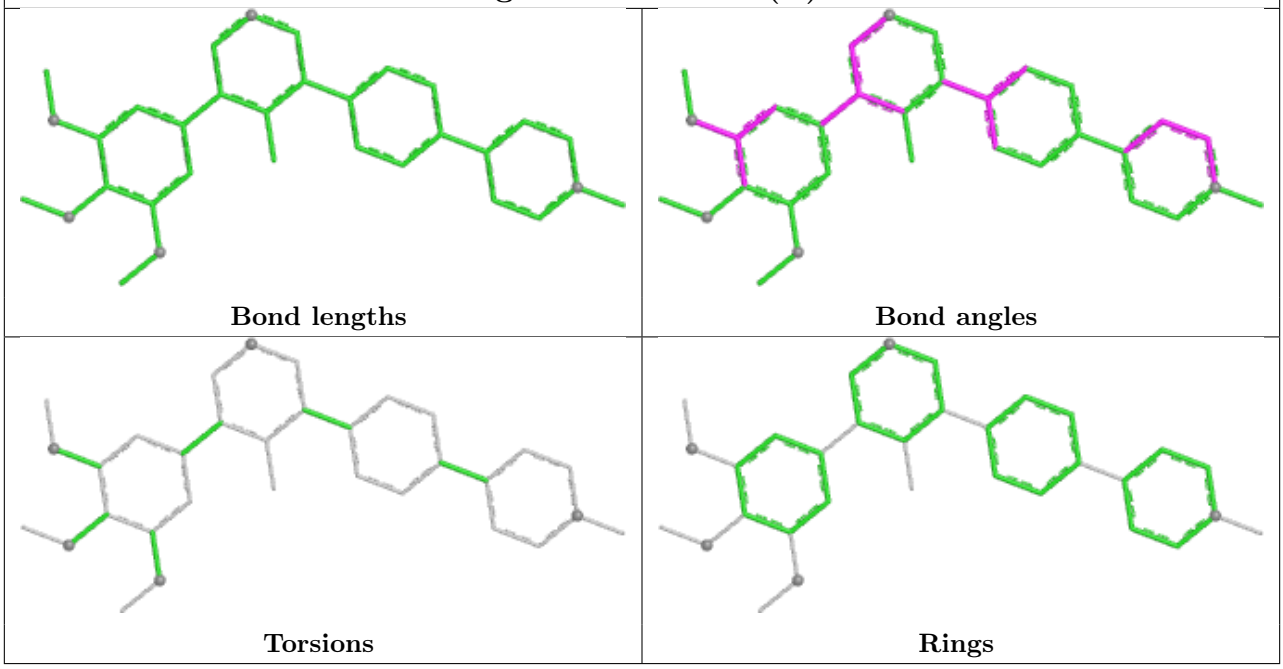
Continued on next page...

Continued from previous page...

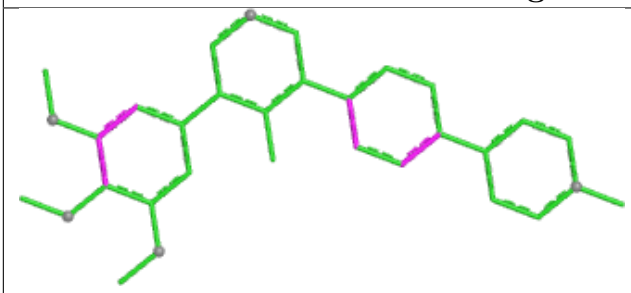
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	508[B]	XHJ	3	0
4	B	504	DMS	2	0
5	B	508[A]	XHJ	3	0
2	A	501[B]	LU8	1	0
2	A	507	LU8	1	0
3	B	511	EDO	2	0
6	B	509	SO4	1	0
3	A	513	EDO	3	0

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

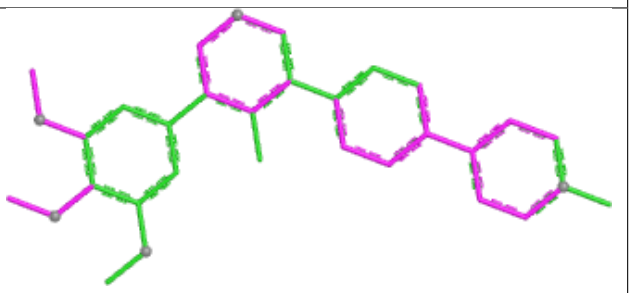
Ligand LU8 A 501 (B)



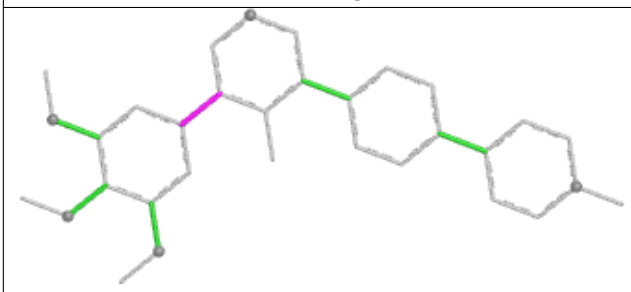
Ligand LU8 A 508



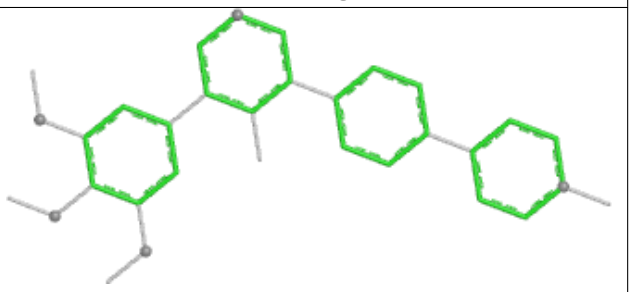
Bond lengths



Bond angles

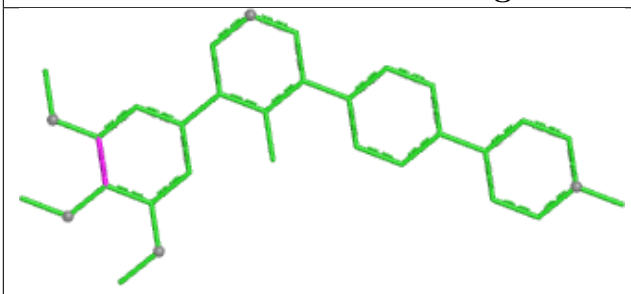


Torsions

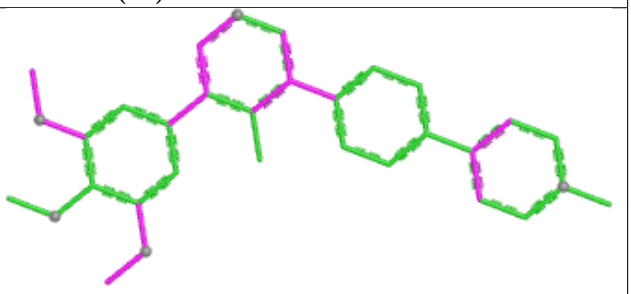


Rings

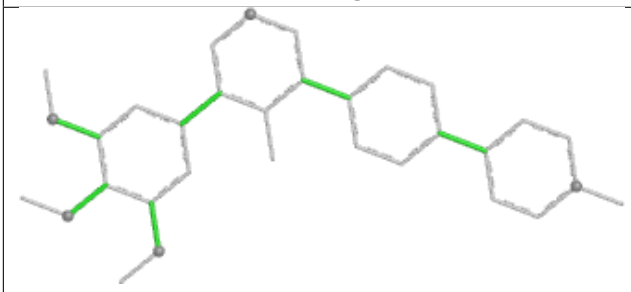
Ligand LU8 A 501 (A)



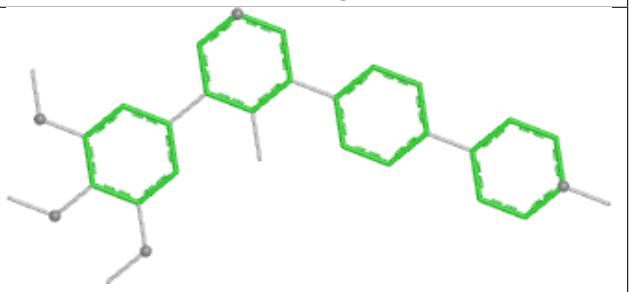
Bond lengths



Bond angles

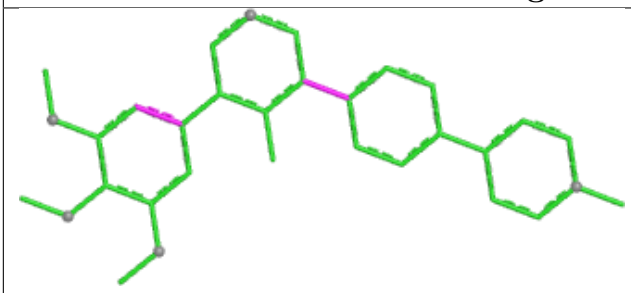


Torsions

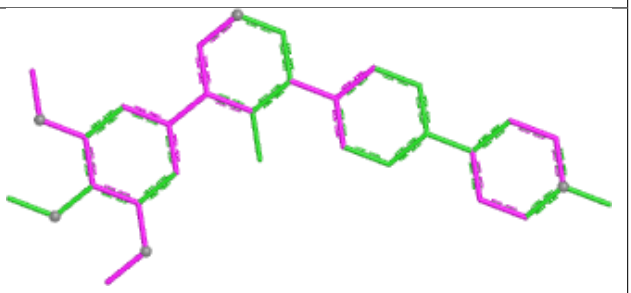


Rings

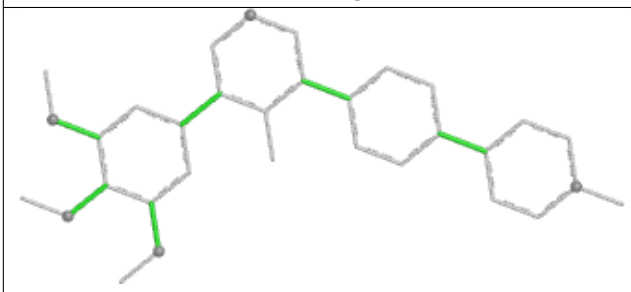
Ligand LU8 A 507



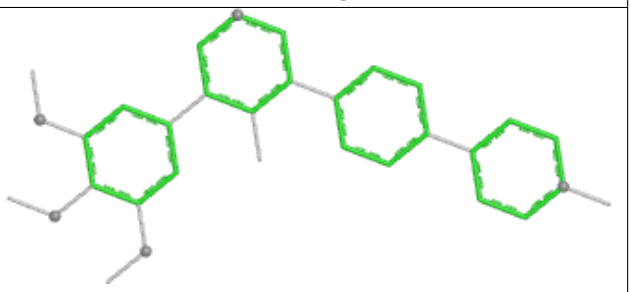
Bond lengths



Bond angles

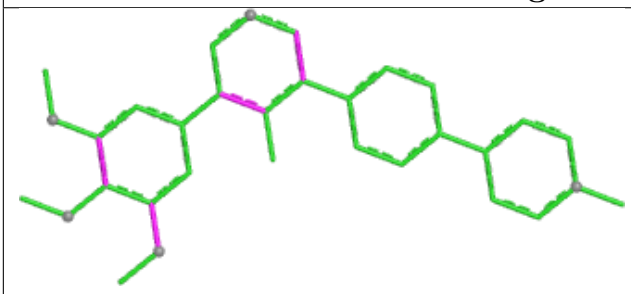


Torsions

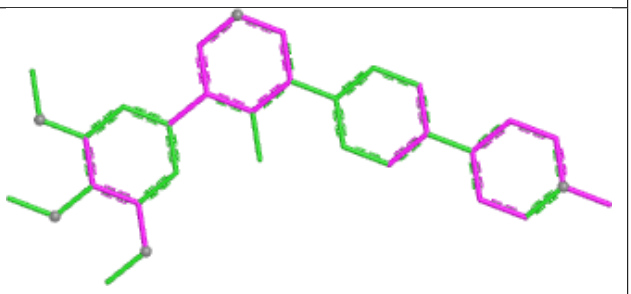


Rings

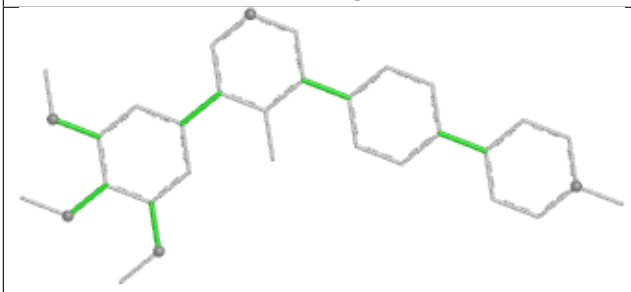
Ligand LU8 B 501



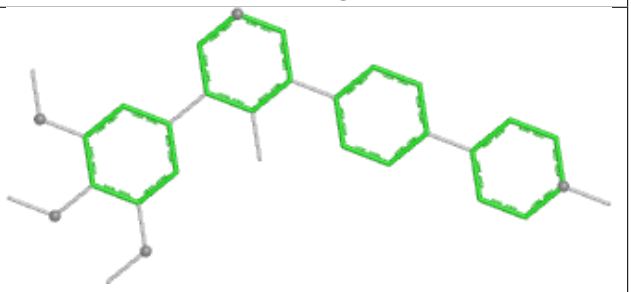
Bond lengths



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, 95^{th} 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	286/301 (95%)	0.19	18 (6%)	26	34	6, 16, 35, 63	14 (4%)
1	B	292/301 (97%)	0.14	12 (4%)	41	52	6, 17, 33, 56	11 (3%)
All	All	578/602 (96%)	0.17	30 (5%)	33	42	6, 17, 35, 63	25 (4%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	324[A]	PHE	6.3
1	A	297	LEU	5.4
1	B	219	TYR	5.0
1	A	374	PRO	4.8
1	B	205	ALA	4.7
1	B	227[A]	TRP	4.7
1	B	297	LEU	3.8
1	B	206	ARG	3.6
1	A	202	ARG	3.5
1	B	207[A]	ASP	3.4
1	A	219	TYR	3.3
1	A	325	GLY	2.8
1	A	499	ASP	2.7
1	B	498	ILE	2.5
1	B	218	ARG	2.5
1	A	239	SER	2.5
1	B	324	PHE	2.5
1	A	373	ASN	2.4
1	A	394	ASP	2.4
1	A	227	TRP	2.4
1	A	395	CYS	2.4
1	B	372	ASN	2.3
1	A	218	ARG	2.3
1	A	275	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	201	GLN	2.1
1	A	393	VAL	2.1
1	B	499	ASP	2.1
1	B	229	GLY	2.1
1	A	496	THR	2.1
1	A	203	THR	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, 95^{th} 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	XHJ	A	509[A]	6/6	0.23	0.23	15,16,16,17	6
5	XHJ	A	509[B]	6/6	0.23	0.23	9,10,11,11	6
5	XHJ	A	509[C]	6/6	0.23	0.23	22,28,31,34	6
4	DMS	A	506	4/4	0.65	0.32	86,87,88,97	0
3	EDO	A	504	4/4	0.66	0.23	49,60,61,62	0
5	XHJ	B	508[A]	6/6	0.69	0.14	17,17,19,19	6
5	XHJ	B	508[B]	6/6	0.69	0.14	23,28,30,31	6
3	EDO	A	516	4/4	0.72	0.18	43,48,50,52	0
5	XHJ	B	505	6/6	0.74	0.38	22,23,24,24	6
6	SO4	B	509	5/5	0.75	0.18	61,66,75,88	0
3	EDO	A	515	4/4	0.76	0.21	55,55,58,60	0
3	EDO	B	511	4/4	0.76	0.20	39,41,45,45	0
5	XHJ	B	506	6/6	0.78	0.27	24,25,25,26	6
5	XHJ	B	507	6/6	0.85	0.17	15,16,16,17	6
4	DMS	B	504	4/4	0.86	0.16	58,59,63,66	0
3	EDO	A	514	4/4	0.88	0.12	33,38,39,51	0
3	EDO	B	503	4/4	0.88	0.12	24,25,26,33	0

Continued on next page...

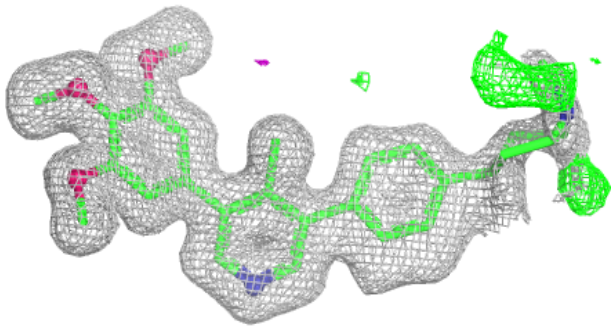
Continued from previous page...

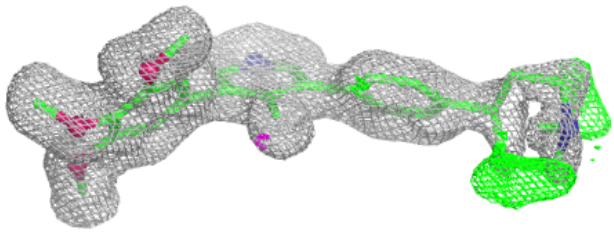
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	A	503	4/4	0.92	0.10	21,22,23,30	0
3	EDO	A	513	4/4	0.92	0.13	17,26,30,41	0
2	LU8	A	501[B]	32/32	0.93	0.09	11,14,22,24	32
3	EDO	A	502	4/4	0.93	0.13	14,24,25,36	0
2	LU8	A	501[A]	32/32	0.93	0.09	11,15,28,30	32
2	LU8	A	508	32/32	0.94	0.10	17,20,44,55	0
3	EDO	B	510	4/4	0.94	0.11	17,26,31,34	0
2	LU8	A	507	32/32	0.95	0.08	18,21,37,42	0
2	LU8	B	501	32/32	0.96	0.07	14,16,31,32	0
6	SO4	A	512	5/5	0.96	0.08	18,29,30,31	0
3	EDO	A	505	4/4	0.96	0.07	15,21,22,27	0
6	SO4	B	502	5/5	0.97	0.14	13,14,17,17	5
6	SO4	A	510	5/5	0.97	0.10	13,17,26,28	5
6	SO4	A	511	5/5	0.99	0.05	11,13,14,14	5

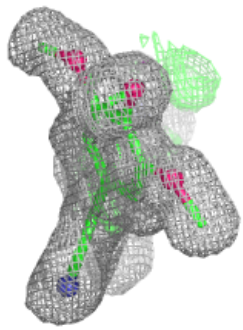
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LU8 A 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)

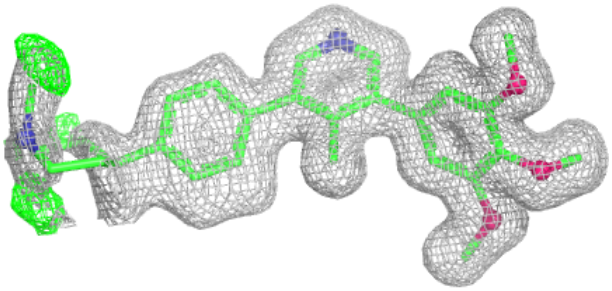


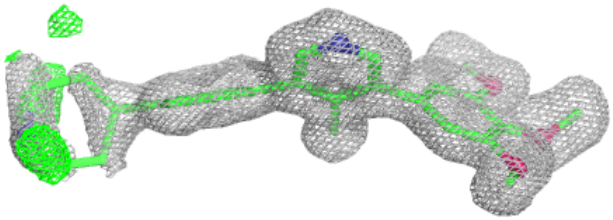


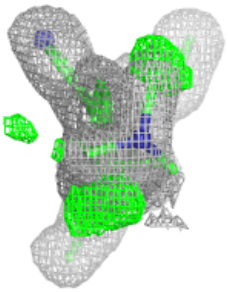


Electron density around LU8 A 501 (A):

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

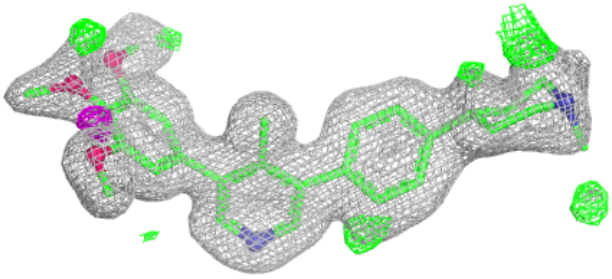


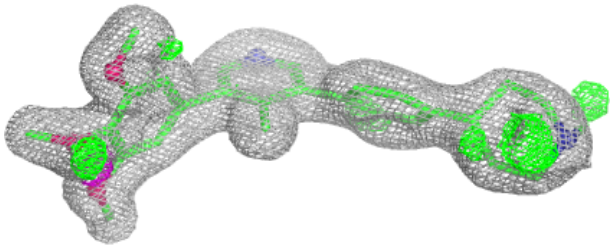


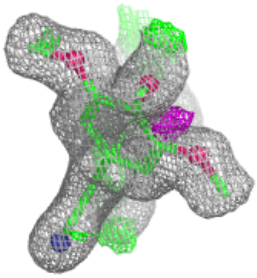


Electron density around LU8 A 508:

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

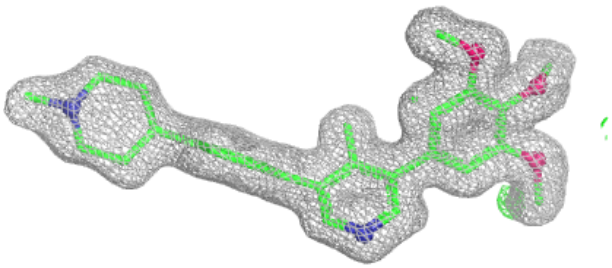


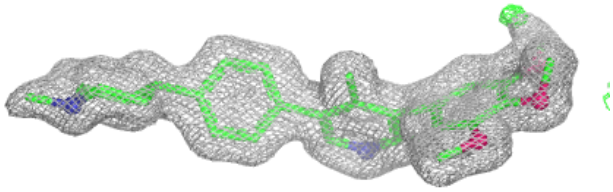


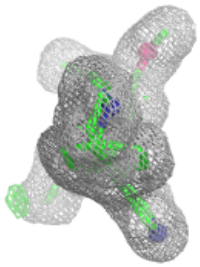


Electron density around LU8 A 507:

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

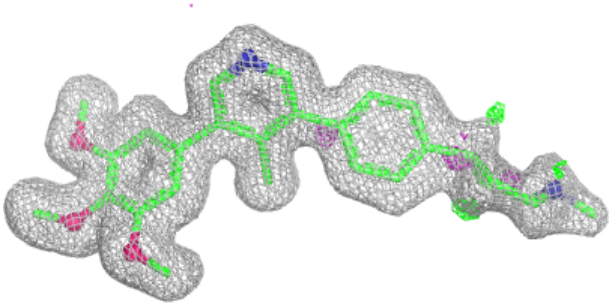


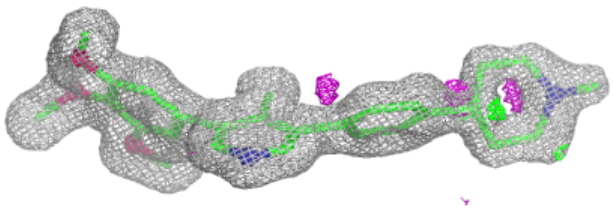


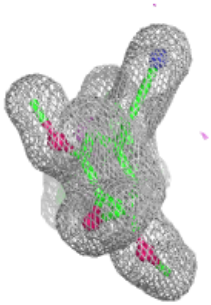


Electron density around LU8 B 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.