



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:06 PM UTC

PDB ID : 5S75 / pdb_00005s75
Title : XChem group deposition – Crystal Structure of human ACVR1 in complex with FM010913a
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 : 1.30 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

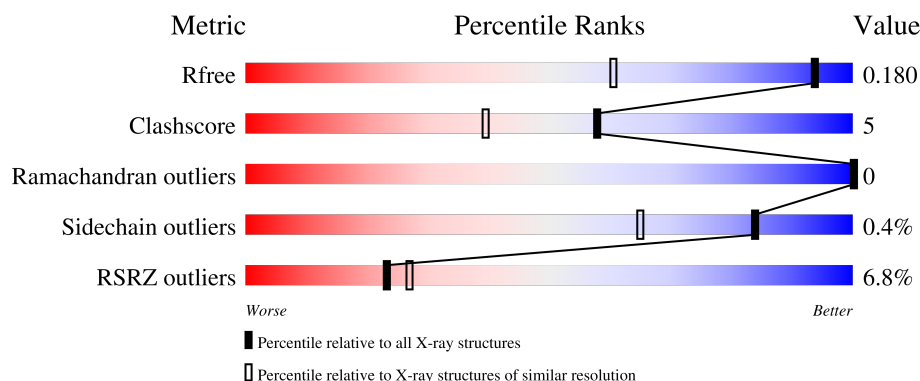
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (1.30-1.30)

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	8% 86% 8% 6%
1	B	301	5% 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
6	HUH	A	511	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5766 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	12	0
			2329	1492	398	424	15			
1	B	293	Total	C	N	O	S	0	8	1
			2381	1515	413	437	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: C₂₇H₃₂N₂O₃).



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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



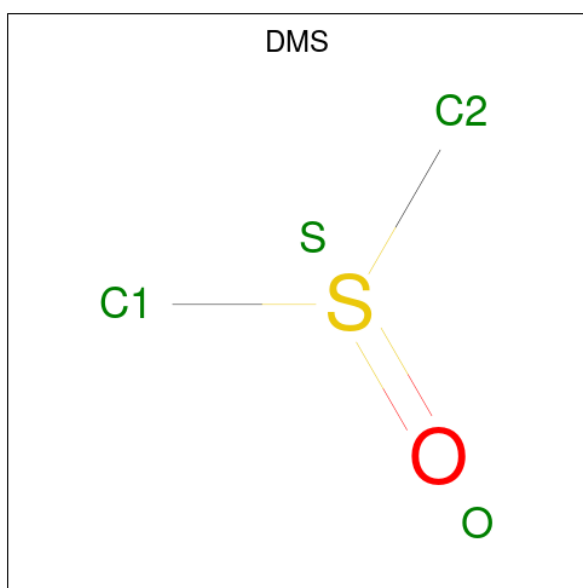
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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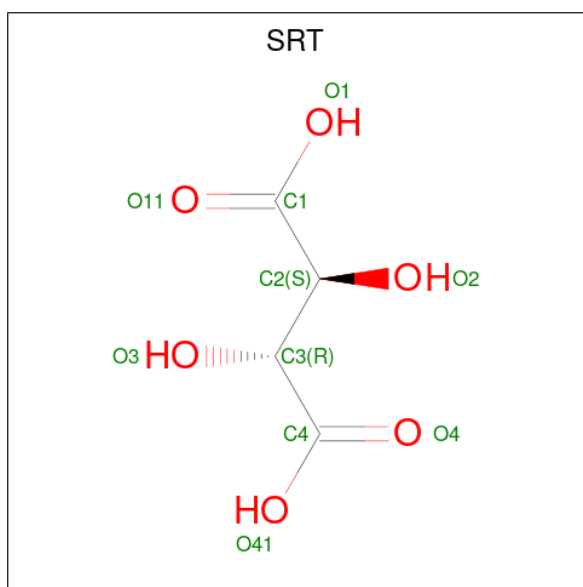
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

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



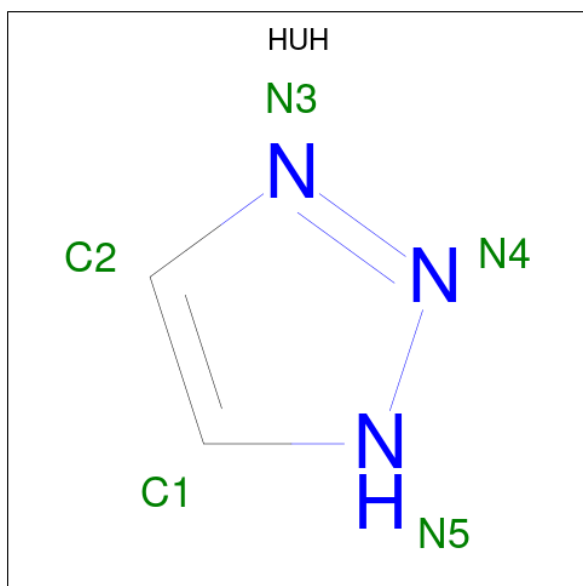
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is S,R MESO-TARTARIC ACID (CCD ID: SRT) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	4	6		

- Molecule 6 is 1 {H}-1,2,3-triazole (CCD ID: HUH) (formula: $C_2H_3N_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			5	2	3		
6	A	1	Total	C	N	0	0
			5	2	3		
6	B	1	Total	C	N	0	0
			5	2	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	N	0	0
			5	2	3		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

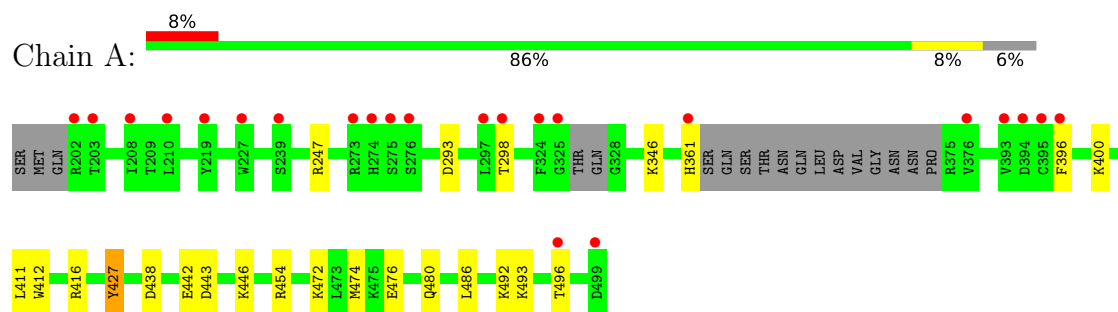
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	378	Total	O	0	1
			379	379		
8	B	397	Total	O	0	0
			397	397		

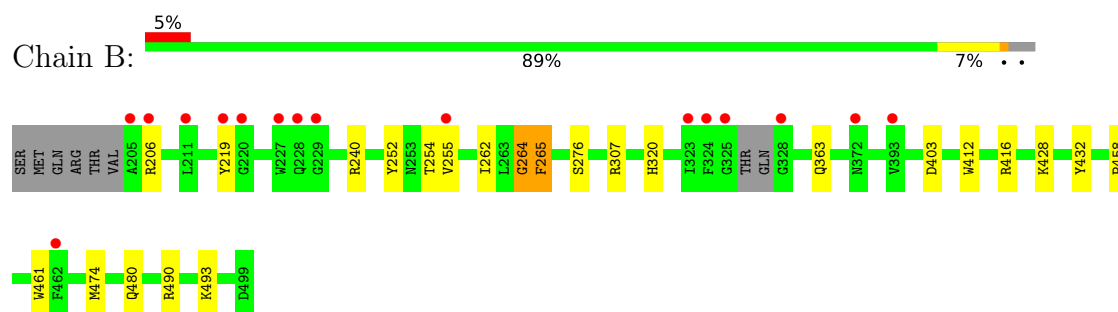
3 Residue-property plots [i](#)

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	127.49Å 84.71Å 88.08Å 90.00° 131.02° 90.00°	Depositor
Resolution (Å)	48.14 – 1.30 48.14 – 1.30	Depositor EDS
% Data completeness (in resolution range)	72.8 (48.14-1.30) 72.9 (48.14-1.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 1.31Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.155 , 0.173 0.164 , 0.180	Depositor DCC
R_{free} test set	8702 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h+k-l,-l,-k 0.000 for -h-k-l,l,k 0.012 for -h-2*l,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5766	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: DMS, SO4, EDO, HUH, LU8, SRT

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	0/2390	1.13	2/3239 (0.1%)
1	B	1.10	2/2440 (0.1%)	1.17	5/3310 (0.2%)
All	All	1.06	2/4830 (0.0%)	1.15	7/6549 (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	264	GLY	C-O	-6.18	1.17	1.24
1	B	320	HIS	CE1-NE2	5.45	1.38	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	443	ASP	CA-CB-CG	5.85	118.45	112.60
1	B	403	ASP	CA-CB-CG	5.85	118.45	112.60
1	B	254	THR	CA-CB-OG1	-5.54	101.28	109.60
1	B	255	VAL	CA-C-O	-5.38	115.36	120.95
1	B	474	MET	CB-CA-C	-5.22	102.69	110.88
1	A	438	ASP	CA-C-O	5.17	124.46	120.48
1	B	265	PHE	N-CA-CB	-5.08	102.38	110.06

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	2329	0	2306	19	0
1	B	2381	0	2348	20	0
2	A	128	0	0	1	0
2	B	32	0	0	0	0
3	A	36	0	54	2	0
3	B	16	0	24	3	0
4	A	4	0	6	0	0
4	B	4	0	6	2	0
5	A	10	0	4	0	0
6	A	10	0	0	2	0
6	B	10	0	0	0	0
7	A	15	0	0	0	0
7	B	15	0	0	0	0
8	A	379	0	0	10	0
8	B	397	0	0	12	1
All	All	5766	0	4748	44	1

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

All (44) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:511:HUH:N4	8:A:602:HOH:O	1.77	1.14
6:A:511:HUH:N5	8:A:602:HOH:O	1.99	0.91
1:B:307:ARG:NH1	8:B:601:HOH:O	2.02	0.82
1:A:396:PHE:HE2	1:A:400[B]:LYS:HE3	1.45	0.80
1:A:454:ARG:NH2	1:A:480[B]:GLN:OE1	2.20	0.75
1:A:472:LYS:HG3	8:A:760:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:PHE:CE2	1:A:400[B]:LYS:HE3	2.22	0.73
1:B:480:GLN:CG	8:B:634:HOH:O	2.37	0.72
1:B:480:GLN:HB2	8:B:634:HOH:O	1.88	0.72
1:A:454:ARG:HH22	1:A:480[B]:GLN:CD	1.97	0.71
1:B:276:SER:HB2	8:B:635:HOH:O	1.89	0.71
1:B:480:GLN:CB	8:B:634:HOH:O	2.39	0.70
1:B:428:LYS:HG3	8:B:694:HOH:O	1.96	0.66
1:B:363:GLN:NE2	8:B:603:HOH:O	2.29	0.64
1:A:293[B]:ASP:HB2	8:A:614:HOH:O	1.99	0.62
1:A:442:GLU:HG2	8:A:651:HOH:O	2.02	0.60
1:A:492:LYS:O	1:A:496:THR:HG23	2.03	0.58
1:B:490:ARG:HH22	4:B:504:DMS:H12	1.69	0.58
1:B:219:TYR:HB2	8:B:607:HOH:O	2.05	0.57
1:B:432:TYR:CE2	8:B:694:HOH:O	2.52	0.57
1:A:247:ARG:CD	8:A:871:HOH:O	2.54	0.55
1:B:480:GLN:CD	8:B:634:HOH:O	2.49	0.54
1:A:476[B]:GLU:HB3	1:A:486:LEU:HG	1.89	0.53
1:B:252:TYR:CD1	1:B:265:PHE:HB2	2.44	0.52
1:B:264:GLY:HA3	3:B:509:EDO:H22	1.93	0.51
1:B:432:TYR:CZ	8:B:694:HOH:O	2.58	0.50
1:A:411:LEU:HG	1:A:474:MET:HE2	1.92	0.50
3:A:515:EDO:H11	8:A:753:HOH:O	2.13	0.49
1:A:346:LYS:CE	8:A:874:HOH:O	2.61	0.48
1:B:262:ILE:O	3:B:509:EDO:H12	2.15	0.47
1:A:412:TRP:CZ2	1:A:416:ARG:HD2	2.50	0.46
1:A:476[A]:GLU:HB3	1:A:486:LEU:HG	1.95	0.46
2:A:501[B]:LU8:C25	2:A:501[B]:LU8:C12	2.94	0.46
1:A:396:PHE:HE2	1:A:400[B]:LYS:CE	2.24	0.45
1:B:206:ARG:NH2	8:B:610:HOH:O	2.44	0.44
1:B:412:TRP:CZ2	1:B:416:ARG:HD2	2.52	0.44
1:B:493:LYS:NZ	4:B:504:DMS:H13	2.33	0.44
1:A:442:GLU:HG3	1:A:446[B]:LYS:HE3	2.01	0.42
3:A:504:EDO:C1	8:A:616:HOH:O	2.68	0.41
1:A:361:HIS:HB2	1:A:396:PHE:CD1	2.56	0.41
1:B:264:GLY:CA	3:B:509:EDO:H22	2.50	0.41
1:A:493:LYS:NZ	8:A:622:HOH:O	2.54	0.40
1:A:427:TYR:CD2	1:A:427:TYR:C	3.00	0.40
1:B:458:PRO:HD2	1:B:461:TRP:CE2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:886:HOH:O	8:B:886:HOH:O[2_454]	2.10	0.10

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	289/301 (96%)	285 (99%)	4 (1%)	0	100	100
1	B	297/301 (99%)	293 (99%)	4 (1%)	0	100	100
All	All	586/602 (97%)	578 (99%)	8 (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	253/270 (94%)	252 (100%)	1 (0%)	84	65
1	B	263/270 (97%)	262 (100%)	1 (0%)	84	65
All	All	516/540 (96%)	514 (100%)	2 (0%)	84	65

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298	THR
1	B	240	ARG

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	B	459	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	LU8	B	501	-	35,35,35	1.23	4 (11%)	47,49,49	1.88	12 (25%)
3	EDO	B	511	-	3,3,3	0.17	0	2,2,2	0.27	0
3	EDO	A	519	-	3,3,3	0.32	0	2,2,2	0.41	0
3	EDO	A	502	-	3,3,3	0.28	0	2,2,2	0.32	0
3	EDO	A	504	-	3,3,3	0.08	0	2,2,2	0.32	0
3	EDO	B	503	-	3,3,3	1.06	0	2,2,2	0.48	0
2	LU8	A	508	-	35,35,35	1.22	3 (8%)	47,49,49	1.74	13 (27%)
7	SO4	A	513	-	4,4,4	0.38	0	6,6,6	0.31	0
6	HUH	B	505	-	5,5,5	1.40	1 (20%)	5,5,5	1.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LU8	A	501[B]	-	35,35,35	0.94	2 (5%)	47,49,49	1.09	4 (8%)
3	EDO	A	505	-	3,3,3	0.08	0	2,2,2	0.70	0
5	SRT	A	507	-	9,9,9	1.04	0	12,12,12	1.03	0
7	SO4	B	508	-	4,4,4	0.56	0	6,6,6	0.17	0
3	EDO	A	515	-	3,3,3	0.44	0	2,2,2	0.40	0
7	SO4	B	502	-	4,4,4	0.25	0	6,6,6	0.34	0
7	SO4	A	512	-	4,4,4	0.38	0	6,6,6	0.17	0
6	HUH	A	511	-	5,5,5	1.53	1 (20%)	5,5,5	1.43	1 (20%)
3	EDO	A	516	-	3,3,3	0.18	0	2,2,2	0.12	0
6	HUH	A	510	-	5,5,5	1.77	1 (20%)	5,5,5	1.08	0
3	EDO	A	517	-	3,3,3	0.46	0	2,2,2	0.28	0
3	EDO	A	503	-	3,3,3	0.70	0	2,2,2	0.48	0
6	HUH	B	506	-	5,5,5	1.61	1 (20%)	5,5,5	1.53	0
2	LU8	A	501[A]	-	35,35,35	1.19	5 (14%)	47,49,49	1.43	5 (10%)
4	DMS	B	504	-	3,3,3	0.28	0	3,3,3	0.09	0
3	EDO	A	518	-	3,3,3	0.06	0	2,2,2	0.17	0
3	EDO	B	509	-	3,3,3	0.61	0	2,2,2	1.54	1 (50%)
2	LU8	A	509	-	35,35,35	1.30	4 (11%)	47,49,49	1.76	11 (23%)
7	SO4	B	507	-	4,4,4	0.27	0	6,6,6	0.12	0
4	DMS	A	506	-	3,3,3	0.36	0	3,3,3	0.25	0
3	EDO	B	510	-	3,3,3	0.13	0	2,2,2	0.11	0
7	SO4	A	514	-	4,4,4	0.18	0	6,6,6	0.17	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LU8	B	501	-	-	0/18/28/28	0/4/4/4
3	EDO	B	511	-	-	1/1/1/1	-
3	EDO	A	519	-	-	0/1/1/1	-
3	EDO	A	502	-	-	0/1/1/1	-
3	EDO	A	504	-	-	0/1/1/1	-
3	EDO	B	503	-	-	0/1/1/1	-
2	LU8	A	508	-	-	0/18/28/28	0/4/4/4
6	HUH	B	505	-	-	-	0/1/1/1
2	LU8	A	501[B]	-	-	1/18/28/28	0/4/4/4
3	EDO	A	505	-	-	0/1/1/1	-
5	SRT	A	507	-	-	3/12/12/12	-
3	EDO	A	515	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HUH	A	511	-	-	-	0/1/1/1
3	EDO	A	516	-	-	1/1/1/1	-
6	HUH	A	510	-	-	-	0/1/1/1
3	EDO	A	517	-	-	1/1/1/1	-
3	EDO	A	503	-	-	0/1/1/1	-
6	HUH	B	506	-	-	-	0/1/1/1
2	LU8	A	501[A]	-	-	0/18/28/28	0/4/4/4
3	EDO	A	518	-	-	1/1/1/1	-
3	EDO	B	509	-	-	1/1/1/1	-
2	LU8	A	509	-	-	4/18/28/28	0/4/4/4
3	EDO	B	510	-	-	1/1/1/1	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	508	LU8	C10-C11	-3.49	1.43	1.49
6	B	506	HUH	N3-N4	3.45	1.37	1.31
6	A	510	HUH	N3-N4	3.22	1.37	1.31
2	A	508	LU8	C26-C05	3.08	1.45	1.39
2	A	508	LU8	C06-C24	-3.02	1.35	1.40
2	A	501[A]	LU8	C12-C13	2.92	1.43	1.38
2	A	509	LU8	C10-C24	2.86	1.44	1.40
2	A	509	LU8	C26-C27	-2.85	1.34	1.38
2	B	501	LU8	C27-C30	-2.63	1.35	1.41
6	A	511	HUH	N3-N4	2.49	1.36	1.31
6	B	505	HUH	N3-N4	2.41	1.36	1.31
2	A	501[A]	LU8	C10-C11	2.31	1.53	1.49
2	B	501	LU8	C09-C10	-2.25	1.35	1.39
2	A	509	LU8	C12-C11	2.24	1.43	1.39
2	A	501[B]	LU8	C23-C22	2.24	1.42	1.38
2	B	501	LU8	C07-N08	2.22	1.39	1.34
2	A	501[B]	LU8	C27-C30	-2.19	1.36	1.41
2	A	509	LU8	C03-C30	-2.19	1.36	1.41
2	A	501[A]	LU8	O02-C03	2.15	1.40	1.37
2	A	501[A]	LU8	C27-C30	-2.08	1.36	1.41
2	B	501	LU8	O02-C03	2.06	1.40	1.37
2	A	501[A]	LU8	C04-C03	2.03	1.42	1.38

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	LU8	C20-N18-C17	6.03	119.14	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	508	LU8	C26-C05-C06	-4.52	113.03	120.61
2	A	501[A]	LU8	C20-N18-C17	4.48	116.67	109.54
2	A	509	LU8	C20-C21-C15	-4.47	105.77	111.00
2	A	509	LU8	C09-N08-C07	4.24	123.27	117.51
2	A	509	LU8	C17-C16-C15	4.15	115.86	111.00
2	A	509	LU8	C06-C07-N08	-4.00	118.63	124.27
2	A	508	LU8	C07-C06-C05	-3.96	113.83	119.56
2	A	501[A]	LU8	C09-C10-C11	-3.95	113.84	119.56
2	A	501[A]	LU8	C20-C21-C15	-3.92	106.42	111.00
2	B	501	LU8	C22-C14-C13	3.74	122.95	118.30
2	B	501	LU8	C06-C07-N08	-3.60	119.19	124.27
2	B	501	LU8	C16-C17-N18	3.55	115.77	111.20
2	A	508	LU8	C27-C30-C03	3.54	123.01	119.56
2	A	509	LU8	C06-C24-C10	3.50	122.64	118.39
2	B	501	LU8	C17-C16-C15	3.36	114.94	111.00
2	A	501[A]	LU8	C11-C10-C24	3.29	127.89	122.47
2	B	501	LU8	C23-C22-C14	-3.17	118.02	121.18
2	A	509	LU8	C32-O31-C30	3.08	123.09	114.74
2	A	501[B]	LU8	C12-C13-C14	-2.88	118.31	121.18
2	A	501[A]	LU8	C17-C16-C15	2.78	114.26	111.00
2	A	501[B]	LU8	C19-N18-C20	-2.77	105.36	110.63
2	A	509	LU8	C22-C14-C15	-2.69	114.26	121.09
2	A	508	LU8	C04-C05-C06	2.66	125.07	120.61
2	A	508	LU8	C06-C07-N08	-2.51	120.73	124.27
2	A	509	LU8	C16-C15-C21	2.50	115.11	109.68
2	B	501	LU8	C06-C24-C10	-2.46	115.41	118.39
2	A	508	LU8	O02-C03-C30	2.41	119.27	115.14
2	A	509	LU8	C13-C14-C15	2.36	127.07	121.09
2	B	501	LU8	C21-C15-C14	-2.32	107.18	112.67
2	A	508	LU8	C10-C09-N08	-2.30	121.03	124.27
2	A	509	LU8	C21-C15-C14	2.29	118.11	112.67
2	A	508	LU8	C22-C14-C15	2.29	126.89	121.09
2	A	508	LU8	C23-C11-C10	-2.26	117.17	120.91
2	A	508	LU8	C04-C05-C26	2.25	121.64	118.35
2	B	501	LU8	C13-C14-C15	-2.23	115.42	121.09
2	A	508	LU8	O02-C03-C04	-2.22	120.25	124.08
2	A	508	LU8	C09-N08-C07	2.19	120.49	117.51
2	A	509	LU8	C11-C10-C24	2.19	126.08	122.47
2	A	501[B]	LU8	C06-C07-N08	-2.17	121.21	124.27
2	B	501	LU8	C23-C11-C12	2.13	121.49	117.68
2	A	501[B]	LU8	C22-C23-C11	-2.11	118.41	121.12
2	A	508	LU8	C12-C13-C14	2.10	123.27	121.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	LU8	C13-C12-C11	-2.08	118.45	121.12
3	B	509	EDO	O1-C1-C2	-2.07	96.66	112.39
2	B	501	LU8	C10-C09-N08	2.02	127.11	124.27
6	A	511	HUH	C1-N5-N4	-2.01	107.21	110.84

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	507	SRT	O11-C1-C2-C3
5	A	507	SRT	O1-C1-C2-C3
3	B	510	EDO	O1-C1-C2-O2
3	B	511	EDO	O1-C1-C2-O2
5	A	507	SRT	O2-C2-C3-O3
2	A	509	LU8	C04-C05-C06-C07
3	A	517	EDO	O1-C1-C2-O2
2	A	509	LU8	C26-C05-C06-C07
3	B	509	EDO	O1-C1-C2-O2
2	A	509	LU8	C04-C05-C06-C24
3	A	518	EDO	O1-C1-C2-O2
3	A	516	EDO	O1-C1-C2-O2
2	A	501[B]	LU8	C13-C14-C15-C21
2	A	509	LU8	C26-C05-C06-C24

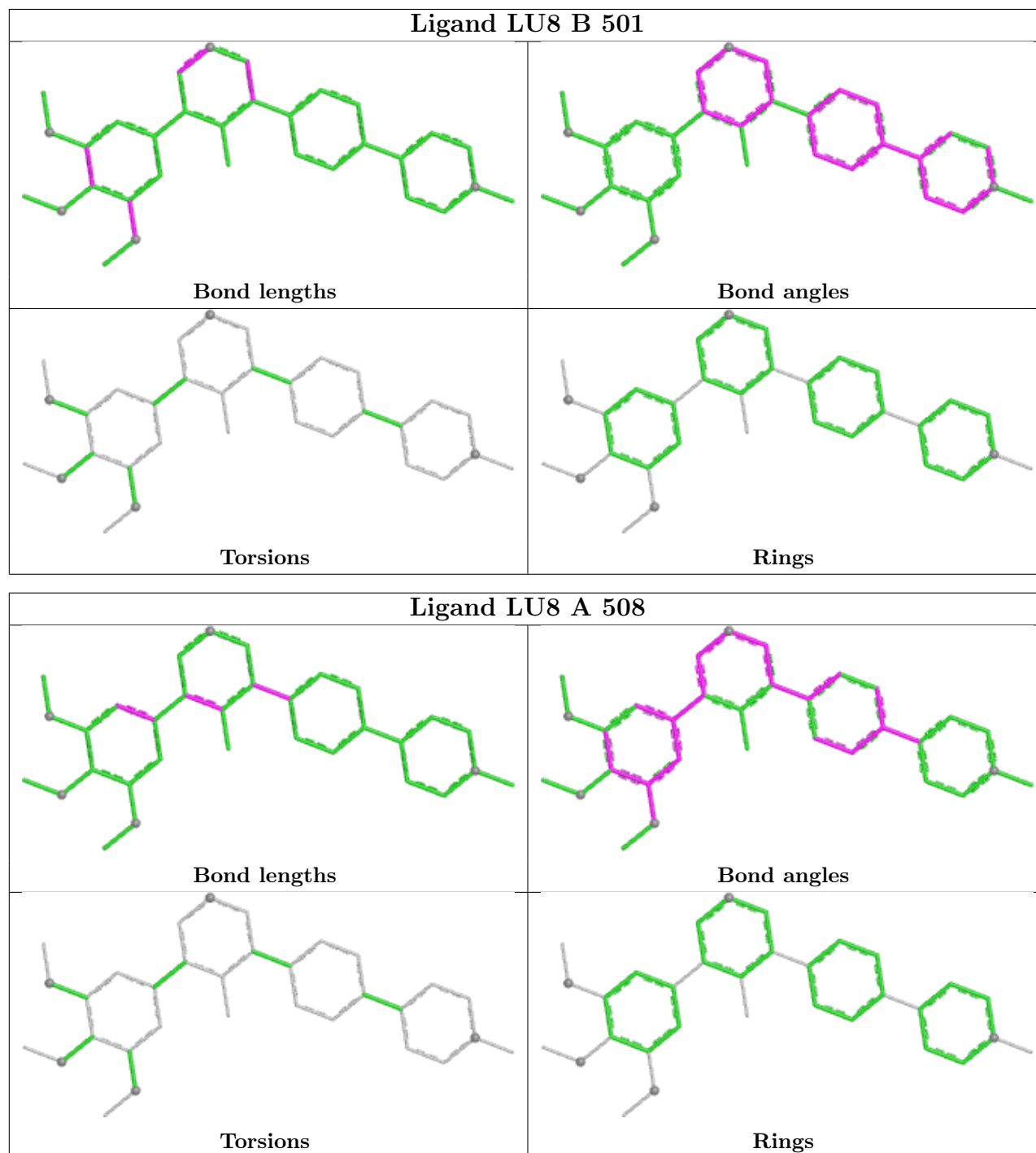
There are no ring outliers.

6 monomers are involved in 10 short contacts:

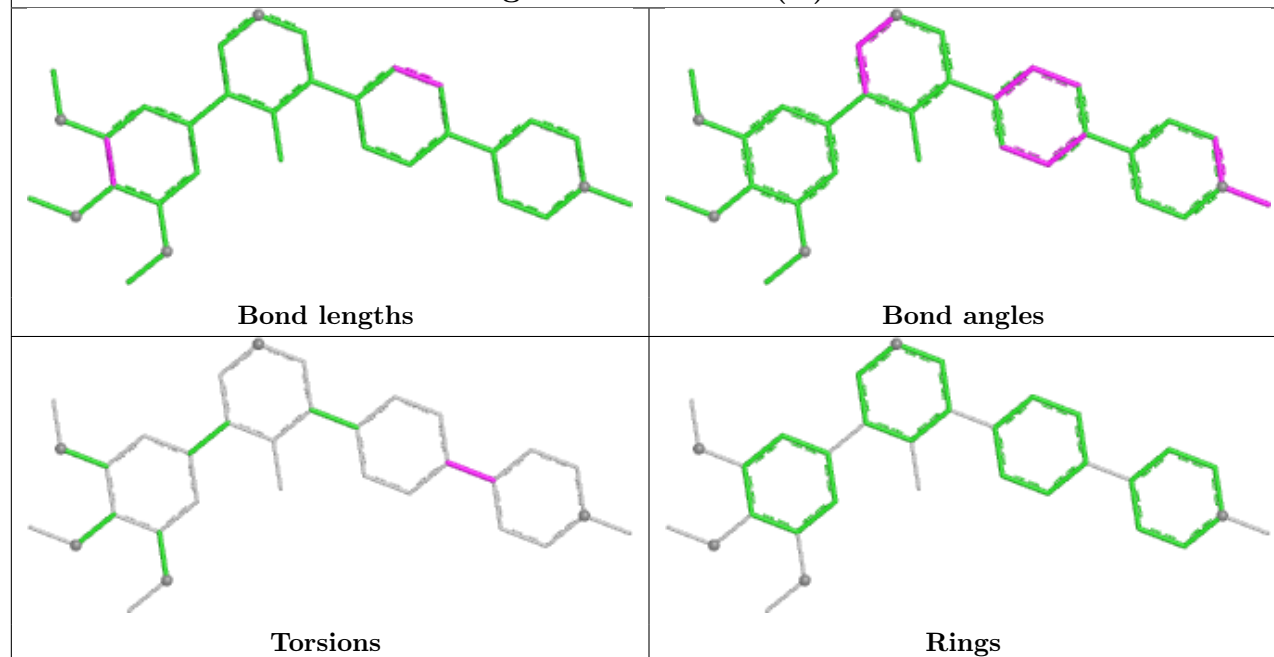
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	504	EDO	1	0
2	A	501[B]	LU8	1	0
3	A	515	EDO	1	0
6	A	511	HUH	2	0
4	B	504	DMS	2	0
3	B	509	EDO	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

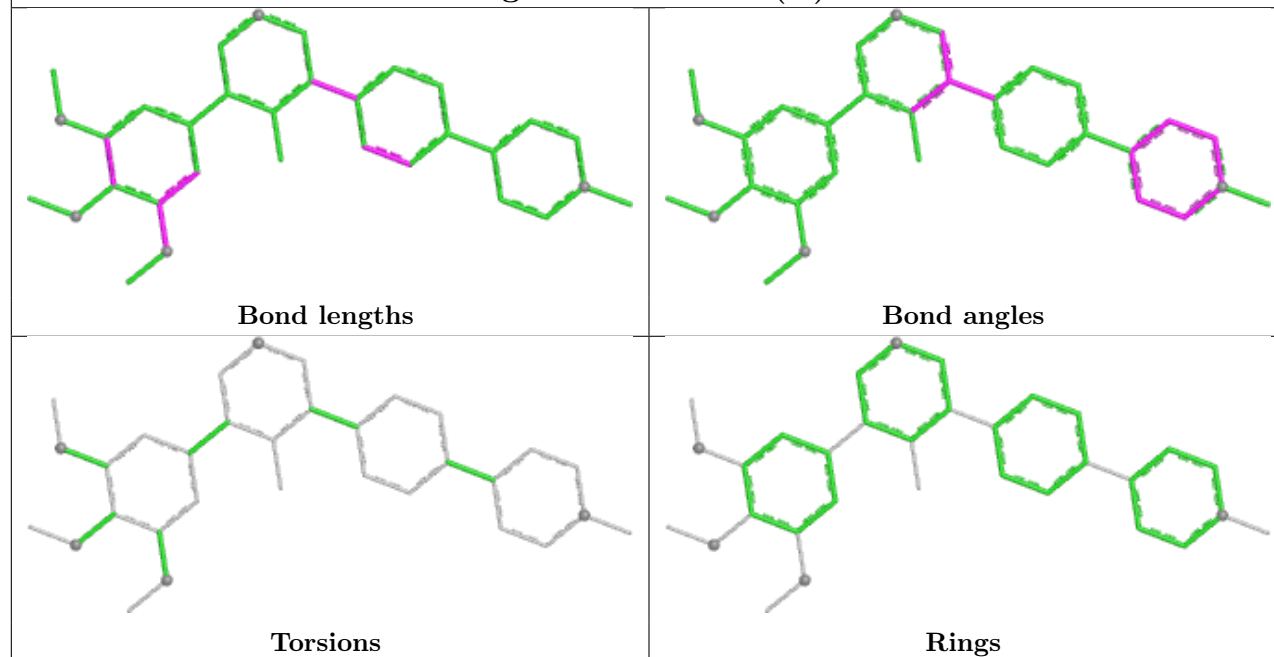
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

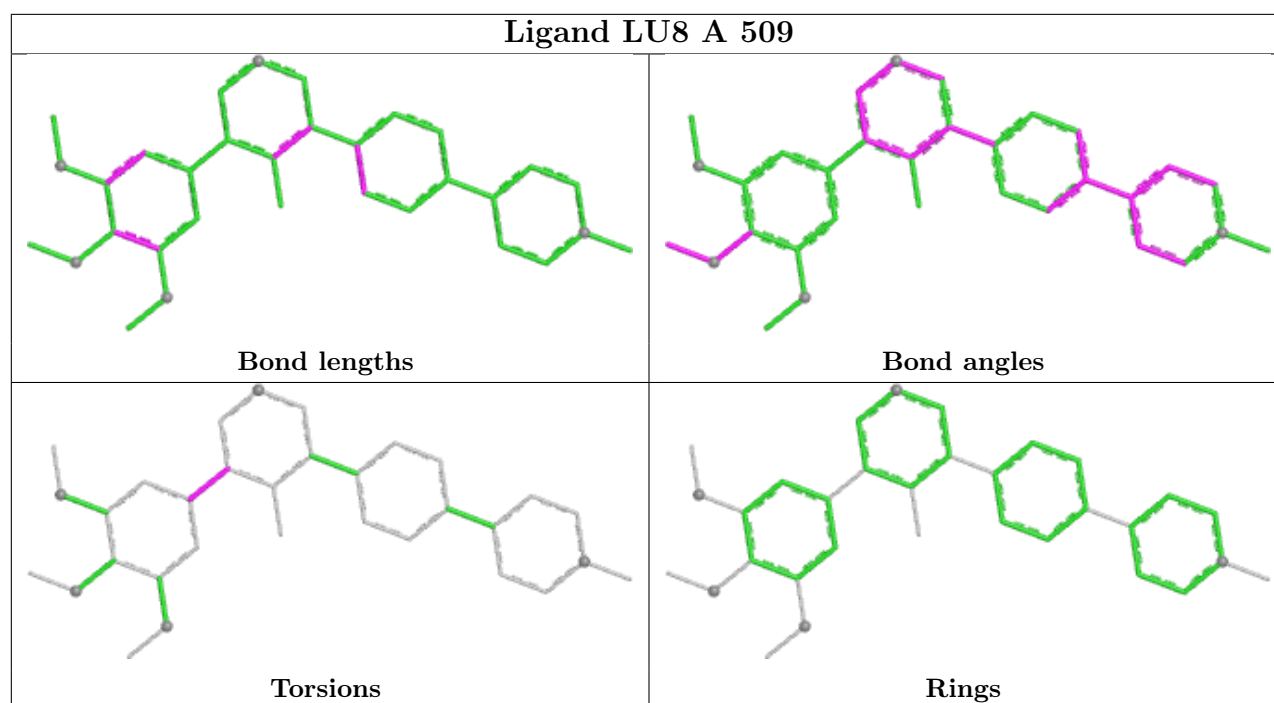


Ligand LU8 A 501 (B)



Ligand LU8 A 501 (A)





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%)	0.29	23 (8%)	18 20	5, 15, 34, 55	12 (4%)
1	B	293/301 (97%)	0.34	16 (5%)	30 35	6, 15, 33, 44	8 (2%)
All	All	576/602 (95%)	0.31	39 (6%)	23 27	5, 15, 34, 55	20 (3%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	325	GLY	5.4
1	B	205	ALA	5.0
1	B	227	TRP	4.9
1	A	297	LEU	4.8
1	B	219	TYR	4.4
1	A	275	SER	4.0
1	B	324	PHE	4.0
1	A	239	SER	3.9
1	A	499	ASP	3.8
1	B	229	GLY	3.7
1	A	324	PHE	3.7
1	A	393	VAL	3.7
1	B	372	ASN	3.6
1	A	325	GLY	3.6
1	A	394	ASP	3.5
1	A	395	CYS	3.4
1	B	255	VAL	3.4
1	A	219	TYR	3.3
1	B	206	ARG	3.2
1	A	496	THR	3.2
1	B	211	LEU	2.9
1	A	276	SER	2.7
1	B	323	ILE	2.7
1	A	274	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	227	TRP	2.6
1	A	202	ARG	2.5
1	A	273	ARG	2.5
1	B	328	GLY	2.5
1	A	396	PHE	2.5
1	A	203	THR	2.4
1	A	298	THR	2.4
1	A	376	VAL	2.4
1	B	228	GLN	2.4
1	A	361	HIS	2.1
1	B	393	VAL	2.1
1	B	220	GLY	2.1
1	A	210	LEU	2.0
1	B	462	PHE	2.0
1	A	208	ILE	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(Å ²)	Q<0.9
5	SRT	A	507	10/10	0.64	0.16	69,73,76,77	0
3	EDO	A	519	4/4	0.69	0.19	45,48,50,51	0
3	EDO	A	504	4/4	0.70	0.15	38,39,43,44	0
3	EDO	A	516	4/4	0.72	0.23	61,63,65,65	0
6	HUH	A	511	5/5	0.74	0.31	21,22,22,23	5
4	DMS	A	506	4/4	0.76	0.20	35,42,43,48	0
3	EDO	B	511	4/4	0.79	0.19	45,46,48,49	0
7	SO4	B	507	5/5	0.80	0.12	49,50,57,62	5

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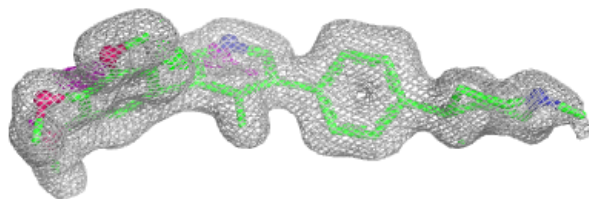
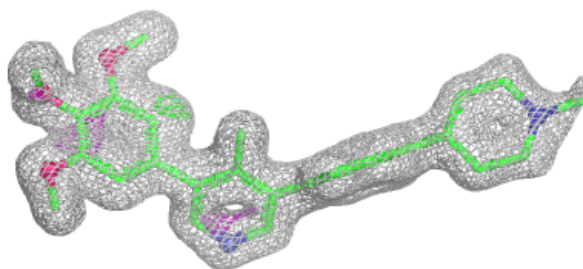
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	518	4/4	0.81	0.18	48,50,53,56	0
3	EDO	B	509	4/4	0.85	0.19	16,25,26,30	0
3	EDO	B	510	4/4	0.85	0.15	30,35,40,41	0
6	HUH	B	505	5/5	0.85	0.22	25,26,27,27	5
4	DMS	B	504	4/4	0.85	0.17	57,59,62,62	0
6	HUH	A	510	5/5	0.87	0.22	18,18,19,19	5
6	HUH	B	506	5/5	0.88	0.31	14,15,15,16	5
3	EDO	B	503	4/4	0.90	0.11	21,22,22,29	0
3	EDO	A	517	4/4	0.90	0.12	29,30,34,40	0
7	SO4	B	508	5/5	0.90	0.13	19,23,31,31	5
2	LU8	A	508	32/32	0.92	0.09	17,20,32,38	0
3	EDO	A	515	4/4	0.94	0.12	17,28,34,39	0
2	LU8	A	509	32/32	0.94	0.10	15,17,39,47	0
2	LU8	A	501[B]	32/32	0.95	0.10	12,15,25,27	32
3	EDO	A	503	4/4	0.95	0.08	17,18,19,22	0
2	LU8	A	501[A]	32/32	0.95	0.10	10,13,31,37	32
2	LU8	B	501	32/32	0.96	0.08	12,15,36,41	0
3	EDO	A	502	4/4	0.96	0.08	13,18,18,24	0
7	SO4	B	502	5/5	0.97	0.06	21,22,24,26	0
3	EDO	A	505	4/4	0.97	0.07	13,18,21,23	0
7	SO4	A	513	5/5	0.97	0.07	16,19,31,32	0
7	SO4	A	514	5/5	0.99	0.05	11,14,15,15	5
7	SO4	A	512	5/5	0.99	0.05	16,18,20,21	0

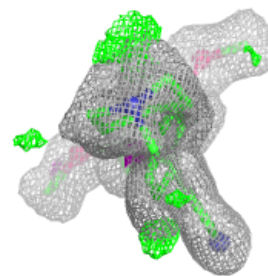
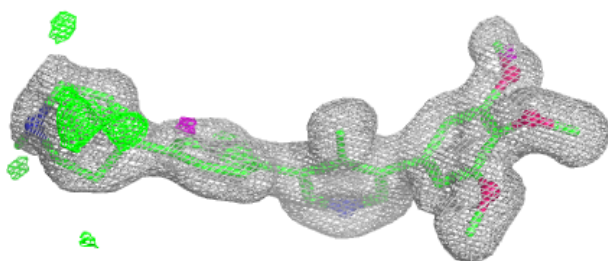
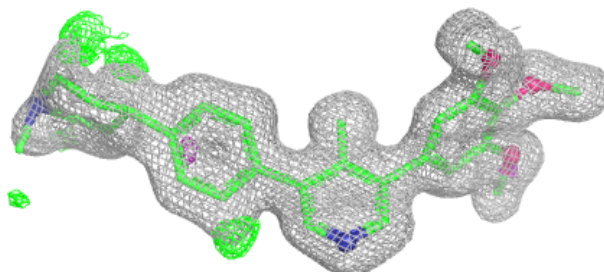
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LU8 A 508:

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

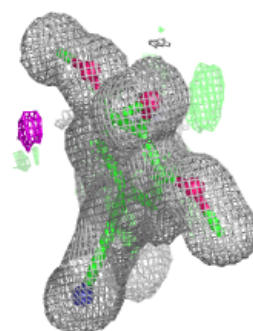
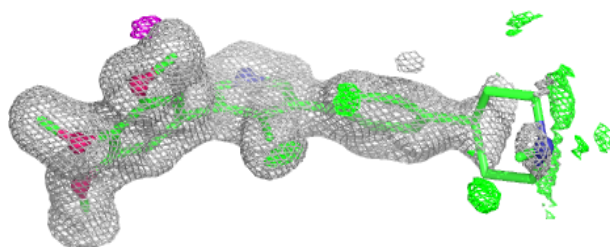
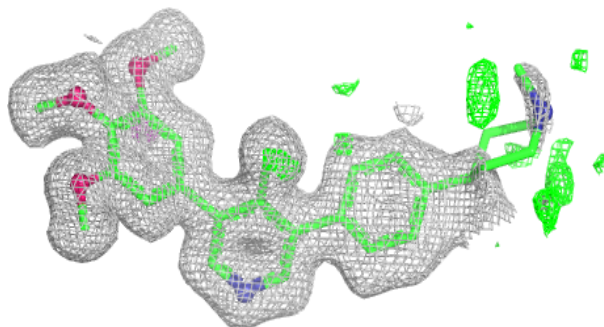
**Electron density around LU8 A 509:**

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

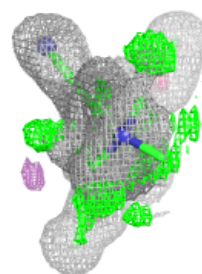
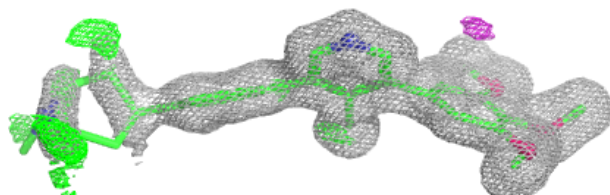
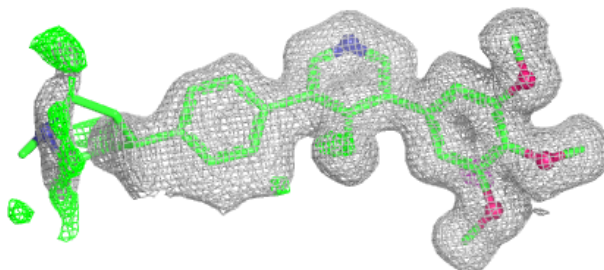


Electron density around LU8 A 501 (B):

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

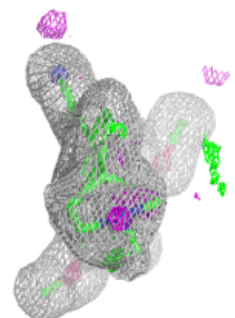
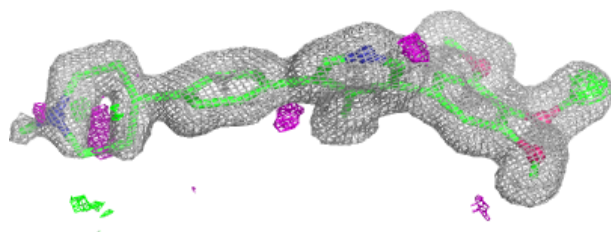
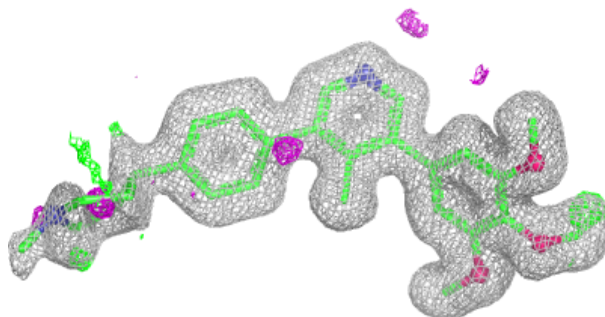
**Electron density around LU8 A 501 (A):**

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



Electron density around LU8 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.