



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2021 – 06:22 PM EDT

PDB ID : 5S7X
Title : XChem group deposition – Crystal Structure of human ACVR1 in complex with FM000376d
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.20
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.20

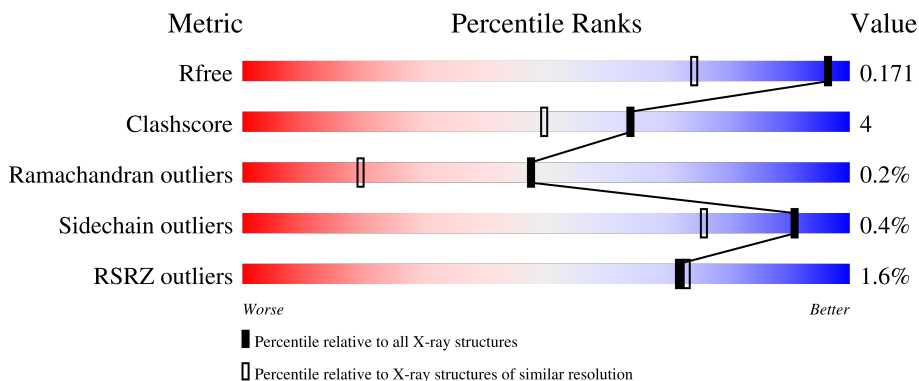
1 Overall quality at a glance

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}	130704	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (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	 85% 8% 6%
1	B	301	 89% 7% 2% 2%

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	LGA	B	505	-	X	-	-

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 5716 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.

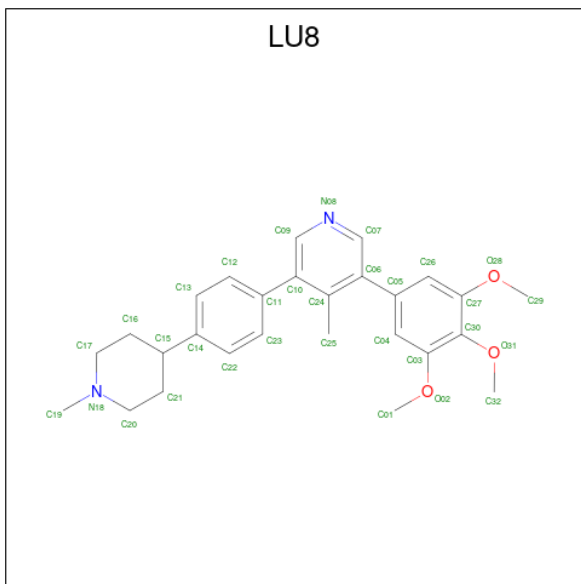
- Molecule 1 is a protein called Activin receptor type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	283	Total 2347	C 1504	N 398	O 430	S 15	0	15	0
1	B	292	Total 2361	C 1505	N 405	O 436	S 15	0	9	0

There are 6 discrepancies between the modelled and reference sequences:

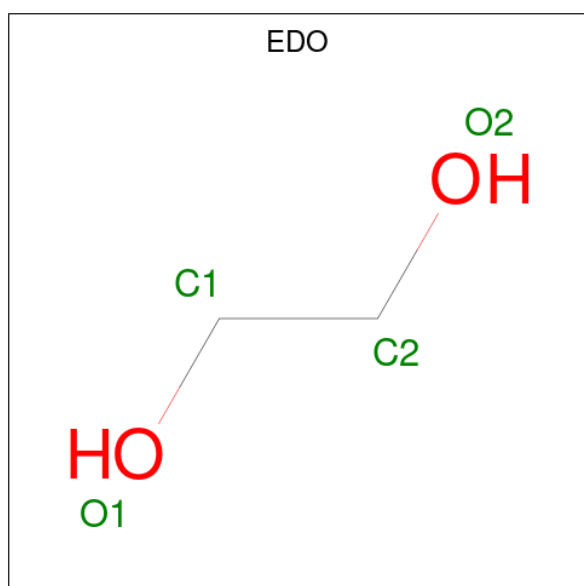
Chain	Residue	Modelled	Actual	Comment	Reference
A	199	SER	-	expression tag	UNP Q04771
A	200	MET	-	expression tag	UNP Q04771
A	207	ASP	GLN	engineered mutation	UNP Q04771
B	199	SER	-	expression tag	UNP Q04771
B	200	MET	-	expression tag	UNP Q04771
B	207	ASP	GLN	engineered mutation	UNP Q04771

- Molecule 2 is 4-methyl-3-[4-(1-methylpiperidin-4-yl)phenyl]-5-(3,4,5-trimethoxyphenyl)pyridine (three-letter code: 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 (three-letter code: EDO) (formula: C₂H₆O₂).



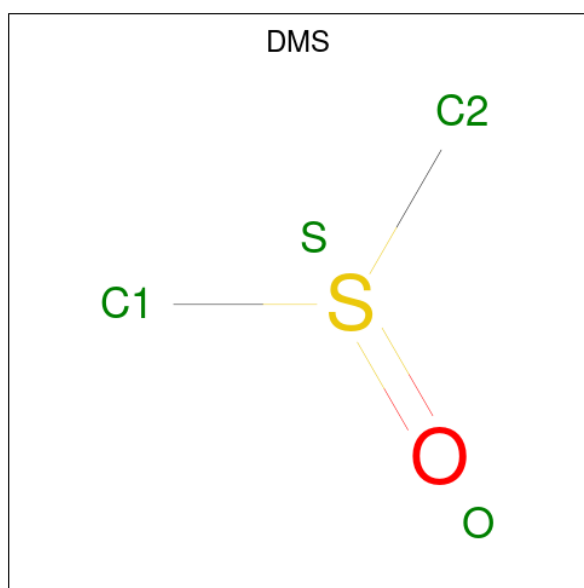
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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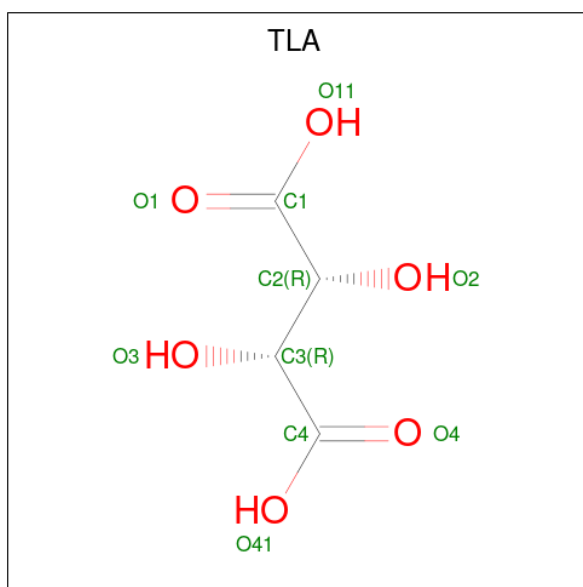
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



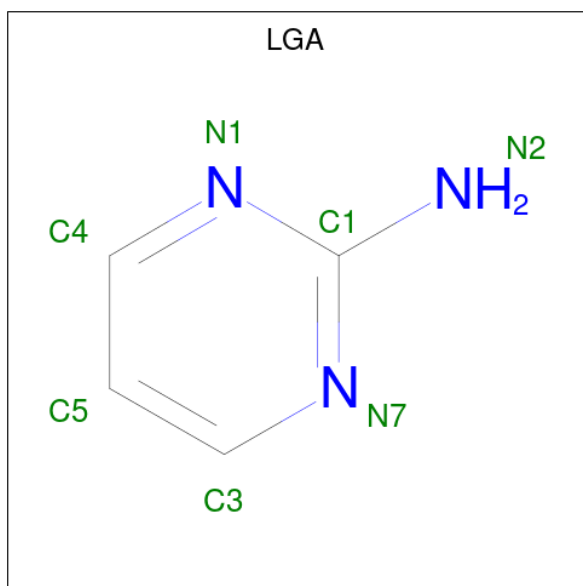
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C₄H₆O₆).



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

- Molecule 6 is PYRIMIDIN-2-AMINE (three-letter code: LGA) (formula: $C_4H_5N_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			7	4	3		
6	B	1	Total	C	N	0	0
			7	4	3		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

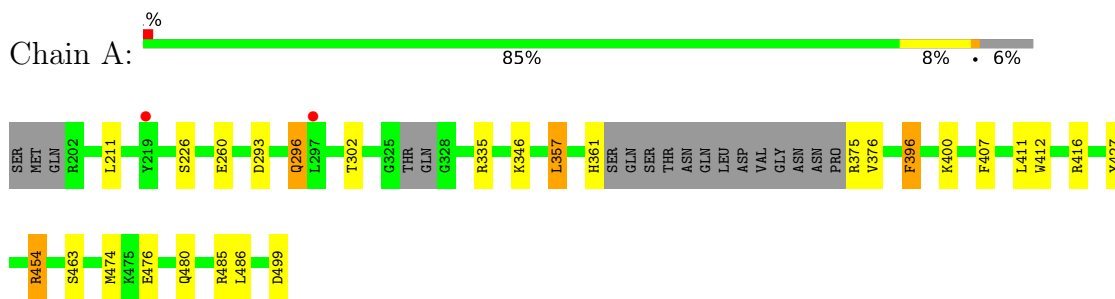
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	379	Total O 380 380	0	1
8	B	391	Total O 391 391	0	0

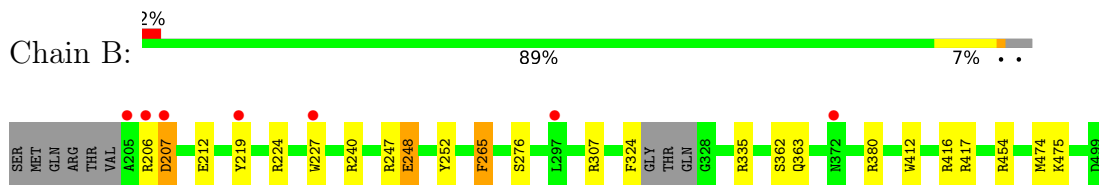
3 Residue-property plots [i](#)

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



- 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	127.11Å 84.55Å 87.72Å 90.00° 130.91° 90.00°	Depositor
Resolution (Å)	66.29 – 1.30 66.30 – 1.30	Depositor EDS
% Data completeness (in resolution range)	74.5 (66.29-1.30) 74.5 (66.30-1.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.31Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.150 , 0.169 0.152 , 0.171	Depositor DCC
R_{free} test set	6359 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	14.3	Xtrriage
Anisotropy	0.030	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.011 for -h+k-l,-l,-k 0.000 for -h-k-l,l,k 0.013 for -h-2*l,-k,l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5716	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LGA, LU8, SO4, EDO, TLA, DMS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.79	1/2408 (0.0%)	0.97	7/3264 (0.2%)
1	B	0.84	2/2423 (0.1%)	1.02	9/3291 (0.3%)
All	All	0.82	3/4831 (0.1%)	1.00	16/6555 (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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	362	SER	CA-CB	-7.06	1.42	1.52
1	B	248	GLU	CD-OE2	-6.36	1.18	1.25
1	A	463	SER	CA-CB	-5.21	1.45	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	335	ARG	NE-CZ-NH1	10.26	125.43	120.30
1	B	335	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	B	454	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	B	474	MET	CG-SD-CE	7.10	111.56	100.20
1	A	474	MET	CG-SD-CE	6.48	110.57	100.20
1	A	454	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	A	454	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	B	454	ARG	NE-CZ-NH2	-6.28	117.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	GLN	C-N-CA	5.96	136.61	121.70
1	A	485	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	B	380	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	296	GLN	O-C-N	5.64	131.72	122.70
1	B	265	PHE	CB-CG-CD1	-5.44	116.99	120.80
1	B	247	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	417	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	396	PHE	CB-CG-CD2	-5.16	117.19	120.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	GLN	Peptide
1	A	427	TYR	Sidechain

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	2347	0	2318	24	0
1	B	2361	0	2309	13	0
2	A	96	0	0	0	0
2	B	32	0	0	0	0
3	A	36	0	54	4	0
3	B	16	0	23	0	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
5	A	10	0	4	0	0
6	A	7	0	5	0	0
6	B	7	0	5	0	0
7	A	15	0	0	0	0
7	B	10	0	0	0	0
8	A	380	0	0	8	1
8	B	391	0	0	7	1
All	All	5716	0	4730	41	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 4.

All (41) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ARG:HA	1:B:227:TRP:HE1	1.35	0.91
1:B:307:ARG:NH1	8:B:601:HOH:O	2.01	0.88
1:A:396:PHE:HE2	1:A:400[B]:LYS:HE3	1.42	0.85
1:A:454:ARG:NH2	1:A:480[B]:GLN:OE1	2.09	0.84
1:A:396:PHE:CE2	1:A:400[B]:LYS:HE3	2.18	0.76
1:A:476[B]:GLU:OE1	8:A:602:HOH:O	2.04	0.75
1:A:454:ARG:HH22	1:A:480[B]:GLN:CD	1.96	0.68
1:B:276[B]:SER:HB2	8:B:603:HOH:O	1.90	0.68
1:A:407:PHE:HE2	1:A:411[B]:LEU:HD11	1.59	0.67
1:B:248:GLU:OE1	8:B:602:HOH:O	2.15	0.63
1:A:346:LYS:CE	8:A:886:HOH:O	2.46	0.62
1:A:293[B]:ASP:HB2	8:A:609:HOH:O	1.99	0.62
1:A:407:PHE:CE2	1:A:411[B]:LEU:HD11	2.35	0.61
1:A:357[B]:LEU:HD21	1:A:375:ARG:HB3	1.84	0.59
1:A:302:THR:HG21	1:A:499:ASP:OD2	2.05	0.57
1:B:219:TYR:HB2	8:B:606:HOH:O	2.04	0.56
1:A:396:PHE:HE2	1:A:400[B]:LYS:CE	2.15	0.55
1:A:407:PHE:CZ	1:A:411[B]:LEU:HD21	2.41	0.55
1:B:252:TYR:CD1	1:B:265:PHE:HB2	2.41	0.55
1:A:476[B]:GLU:HB3	1:A:486:LEU:HG	1.90	0.53
1:A:361:HIS:HB2	1:A:396:PHE:CD1	2.43	0.53
1:A:260[B]:GLU:H	1:A:260[B]:GLU:CD	2.12	0.51
1:A:357[B]:LEU:HD11	1:A:375:ARG:HG2	1.92	0.50
1:A:357[B]:LEU:HD21	1:A:375:ARG:CG	2.41	0.49
1:A:335:ARG:NH1	1:A:357[A]:LEU:HD22	2.27	0.49
1:A:412:TRP:CZ2	1:A:416:ARG:HD2	2.49	0.48
1:B:324:PHE:C	8:B:911:HOH:O	2.52	0.48
3:A:514:EDO:H21	8:A:882:HOH:O	2.14	0.47
1:A:357[B]:LEU:HD21	1:A:375:ARG:CB	2.45	0.46
1:B:475:LYS:HB3	8:B:908:HOH:O	2.16	0.44
3:A:514:EDO:C1	8:A:772:HOH:O	2.65	0.44
1:B:252:TYR:CE1	1:B:265:PHE:HB2	2.54	0.43
1:B:363:GLN:CB	8:B:963:HOH:O	2.66	0.43
1:A:376:VAL:HG12	8:A:685:HOH:O	2.20	0.42
1:A:211:LEU:HD11	1:A:226:SER:HB2	2.02	0.42
1:A:357[A]:LEU:HD23	1:A:357[A]:LEU:HA	1.93	0.41
1:B:412:TRP:CZ2	1:B:416:ARG:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:514:EDO:H11	8:A:772:HOH:O	2.19	0.41
1:B:212:GLU:HG3	1:B:224:ARG:HB3	2.02	0.41
3:A:504:EDO:C1	8:A:636:HOH:O	2.68	0.40
1:B:206:ARG:O	1:B:207:ASP:HB2	2.22	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:A:915:HOH:O	8:B:665:HOH:O[3_445]	2.19	0.01

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	292/301 (97%)	289 (99%)	3 (1%)	0	100	100
1	B	297/301 (99%)	293 (99%)	3 (1%)	1 (0%)	41	17
All	All	589/602 (98%)	582 (99%)	6 (1%)	1 (0%)	47	19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	207	ASP

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	255/270 (94%)	253 (99%)	2 (1%)	81	58
1	B	258/270 (96%)	257 (100%)	1 (0%)	91	76
All	All	513/540 (95%)	510 (99%)	3 (1%)	91	65

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	357[A]	LEU
1	A	357[B]	LEU
1	B	240	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

27 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	B	503	-	3,3,3	1.17	0	2,2,2	0.49	0
3	EDO	A	515	-	3,3,3	0.07	0	2,2,2	0.17	0
3	EDO	A	504	-	3,3,3	0.22	0	2,2,2	0.41	0
3	EDO	A	516	-	3,3,3	0.34	0	2,2,2	0.43	0
3	EDO	B	507	-	3,3,3	1.43	1 (33%)	2,2,2	1.73	1 (50%)
3	EDO	B	509	-	3,3,3	0.21	0	2,2,2	0.11	0
4	DMS	A	506	-	3,3,3	0.41	0	3,3,3	0.23	0
7	SO4	A	512	-	4,4,4	0.56	0	6,6,6	0.39	0
2	LU8	A	508	-	35,35,35	1.09	2 (5%)	46,49,49	1.69	9 (19%)
4	DMS	B	504	-	3,3,3	0.26	0	3,3,3	0.06	0
7	SO4	B	502	-	4,4,4	0.34	0	6,6,6	0.27	0
7	SO4	A	511	-	4,4,4	0.56	0	6,6,6	0.27	0
6	LGA	A	510	-	7,7,7	2.32	2 (28%)	8,8,8	2.17	4 (50%)
3	EDO	A	505	-	3,3,3	0.21	0	2,2,2	0.62	0
2	LU8	B	501	-	35,35,35	1.16	3 (8%)	46,49,49	1.67	9 (19%)
3	EDO	A	514	-	3,3,3	0.31	0	2,2,2	0.58	0
2	LU8	A	501	-	35,35,35	1.33	4 (11%)	46,49,49	1.81	13 (28%)
6	LGA	B	505	-	7,7,7	2.27	1 (14%)	8,8,8	2.63	6 (75%)
3	EDO	A	503	-	3,3,3	1.12	0	2,2,2	0.45	0
7	SO4	B	506	-	4,4,4	0.63	0	6,6,6	0.17	0
2	LU8	A	509	-	35,35,35	1.25	4 (11%)	46,49,49	1.62	11 (23%)
3	EDO	A	518	-	3,3,3	0.29	0	2,2,2	0.43	0
3	EDO	A	517	-	3,3,3	0.15	0	2,2,2	0.13	0
7	SO4	A	513	-	4,4,4	0.23	0	6,6,6	0.28	0
3	EDO	A	502	-	3,3,3	0.52	0	2,2,2	0.48	0
5	TLA	A	507	-	3,9,9	0.36	0	6,12,12	0.66	0
3	EDO	B	508	-	3,3,3	0.16	0	2,2,2	0.15	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	503	-	-	0/1/1/1	-
3	EDO	A	515	-	-	0/1/1/1	-
3	EDO	A	504	-	-	1/1/1/1	-
3	EDO	A	516	-	-	1/1/1/1	-
3	EDO	B	507	-	-	0/1/1/1	-
3	EDO	B	509	-	-	1/1/1/1	-
2	LU8	A	508	-	-	0/18/28/28	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LGA	A	510	-	-	-	0/1/1/1
3	EDO	A	505	-	-	0/1/1/1	-
2	LU8	B	501	-	-	0/18/28/28	0/4/4/4
3	EDO	A	514	-	-	1/1/1/1	-
2	LU8	A	501	-	-	0/18/28/28	0/4/4/4
6	LGA	B	505	-	-	-	0/1/1/1
3	EDO	A	503	-	-	0/1/1/1	-
2	LU8	A	509	-	-	3/18/28/28	0/4/4/4
3	EDO	A	518	-	-	0/1/1/1	-
3	EDO	A	517	-	-	1/1/1/1	-
3	EDO	A	502	-	-	0/1/1/1	-
5	TLA	A	507	-	-	4/4/12/12	-
3	EDO	B	508	-	-	1/1/1/1	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	505	LGA	C1-N2	5.40	1.44	1.33
6	A	510	LGA	C1-N2	5.37	1.44	1.33
2	A	501	LU8	C10-C11	3.21	1.55	1.49
2	A	501	LU8	C12-C13	3.15	1.44	1.38
2	B	501	LU8	C06-C05	2.90	1.54	1.49
2	B	501	LU8	C27-C30	-2.86	1.34	1.41
2	A	509	LU8	C26-C27	-2.69	1.33	1.38
2	A	508	LU8	C10-C11	-2.65	1.44	1.49
2	A	501	LU8	C13-C14	-2.58	1.34	1.39
6	A	510	LGA	C1-N7	-2.27	1.32	1.35
2	A	508	LU8	C06-C24	-2.26	1.36	1.40
2	A	509	LU8	C12-C11	2.21	1.44	1.39
2	A	509	LU8	C13-C14	2.20	1.42	1.39
2	B	501	LU8	C10-C24	2.16	1.43	1.40
2	A	509	LU8	C27-C30	-2.09	1.36	1.41
3	B	507	EDO	O2-C2	-2.04	1.31	1.42
2	A	501	LU8	O02-C03	2.04	1.40	1.37

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	LU8	C20-N18-C17	5.17	116.75	109.52
2	B	501	LU8	C20-N18-C17	4.07	115.21	109.52
2	A	501	LU8	C23-C11-C10	-4.04	114.37	120.91
2	B	501	LU8	C19-N18-C20	-4.02	104.64	110.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	508	LU8	C26-C05-C06	-3.99	114.00	120.61
2	A	508	LU8	C07-C06-C05	-3.99	113.55	119.52
2	A	501	LU8	C22-C14-C13	3.79	123.02	118.29
2	A	509	LU8	C21-C15-C14	3.79	121.68	112.79
6	A	510	LGA	C5-C3-N7	-3.52	117.69	123.43
2	A	509	LU8	C06-C07-N08	-3.48	118.90	124.16
2	A	501	LU8	C23-C11-C12	3.44	124.45	117.59
2	A	508	LU8	O02-C03-C30	3.44	121.20	115.16
6	B	505	LGA	C5-C4-N1	-3.43	117.82	123.43
2	A	508	LU8	C27-C30-C03	3.43	123.09	119.57
2	A	508	LU8	O02-C03-C04	-3.42	118.23	124.12
2	B	501	LU8	C06-C07-N08	-3.18	119.35	124.16
2	A	509	LU8	C09-N08-C07	3.12	121.74	117.48
6	B	505	LGA	C5-C3-N7	-3.11	118.35	123.43
6	B	505	LGA	C3-N7-C1	3.09	119.40	116.24
2	A	509	LU8	C21-C20-N18	3.04	115.31	111.22
2	B	501	LU8	C12-C11-C10	-3.03	116.01	120.91
2	A	508	LU8	C04-C05-C06	3.02	125.62	120.61
6	B	505	LGA	C4-N1-C1	2.99	119.30	116.24
6	B	505	LGA	C3-C5-C4	2.96	120.91	116.67
6	A	510	LGA	C3-N7-C1	2.88	119.19	116.24
2	A	501	LU8	C13-C12-C11	-2.85	117.03	121.13
2	A	501	LU8	C27-C30-C03	-2.79	116.71	119.57
2	A	501	LU8	C22-C23-C11	-2.77	117.15	121.13
2	A	509	LU8	C22-C14-C15	-2.76	113.94	121.11
2	A	508	LU8	C26-C27-C30	-2.75	117.11	120.22
2	B	501	LU8	C10-C09-N08	2.74	128.30	124.16
6	A	510	LGA	C3-C5-C4	2.69	120.52	116.67
2	A	509	LU8	C32-O31-C30	2.59	121.88	114.78
2	A	509	LU8	C13-C14-C15	2.57	127.78	121.11
2	A	509	LU8	C01-O02-C03	-2.55	113.69	117.53
2	A	501	LU8	C04-C03-C30	2.51	123.07	120.22
2	B	501	LU8	C21-C15-C14	-2.49	106.95	112.79
2	A	508	LU8	C06-C07-N08	-2.41	120.52	124.16
6	A	510	LGA	C5-C4-N1	-2.40	119.50	123.43
3	B	507	EDO	O2-C2-C1	2.39	129.10	111.91
2	B	501	LU8	C20-C21-C15	2.37	113.84	111.04
2	A	501	LU8	C17-C16-C15	2.36	113.83	111.04
2	A	501	LU8	C11-C10-C24	2.35	126.65	122.42
2	B	501	LU8	C13-C14-C15	-2.32	115.08	121.11
2	A	501	LU8	C13-C14-C15	-2.28	115.18	121.11
2	A	509	LU8	C22-C23-C11	2.28	124.41	121.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	509	LU8	C23-C22-C14	-2.27	118.92	121.20
2	A	509	LU8	C12-C13-C14	2.24	123.45	121.20
6	B	505	LGA	N2-C1-N1	2.19	119.66	117.44
2	B	501	LU8	C22-C14-C13	2.18	121.02	118.29
2	A	501	LU8	C12-C13-C14	-2.16	119.02	121.20
2	A	508	LU8	C05-C06-C24	2.13	126.26	122.42
2	A	501	LU8	C05-C26-C27	2.00	122.83	120.13

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	507	TLA	C1-C2-C3-O3
5	A	507	TLA	O2-C2-C3-O3
5	A	507	TLA	O2-C2-C3-C4
3	A	504	EDO	O1-C1-C2-O2
3	A	514	EDO	O1-C1-C2-O2
3	A	516	EDO	O1-C1-C2-O2
5	A	507	TLA	C1-C2-C3-C4
3	B	509	EDO	O1-C1-C2-O2
3	A	517	EDO	O1-C1-C2-O2
2	A	509	LU8	C04-C05-C06-C07
2	A	509	LU8	C26-C05-C06-C07
2	A	509	LU8	C04-C05-C06-C24
3	B	508	EDO	O1-C1-C2-O2

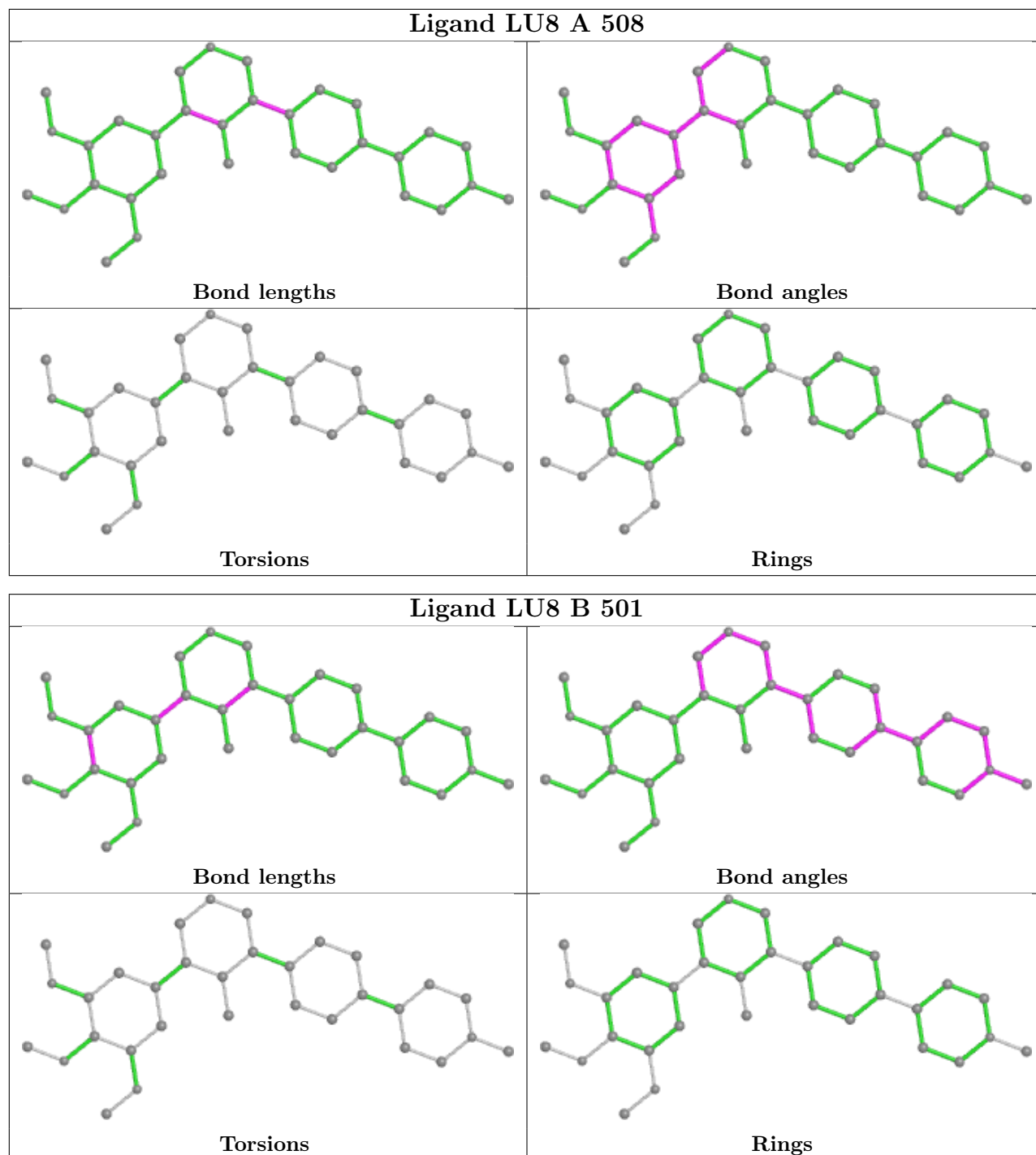
There are no ring outliers.

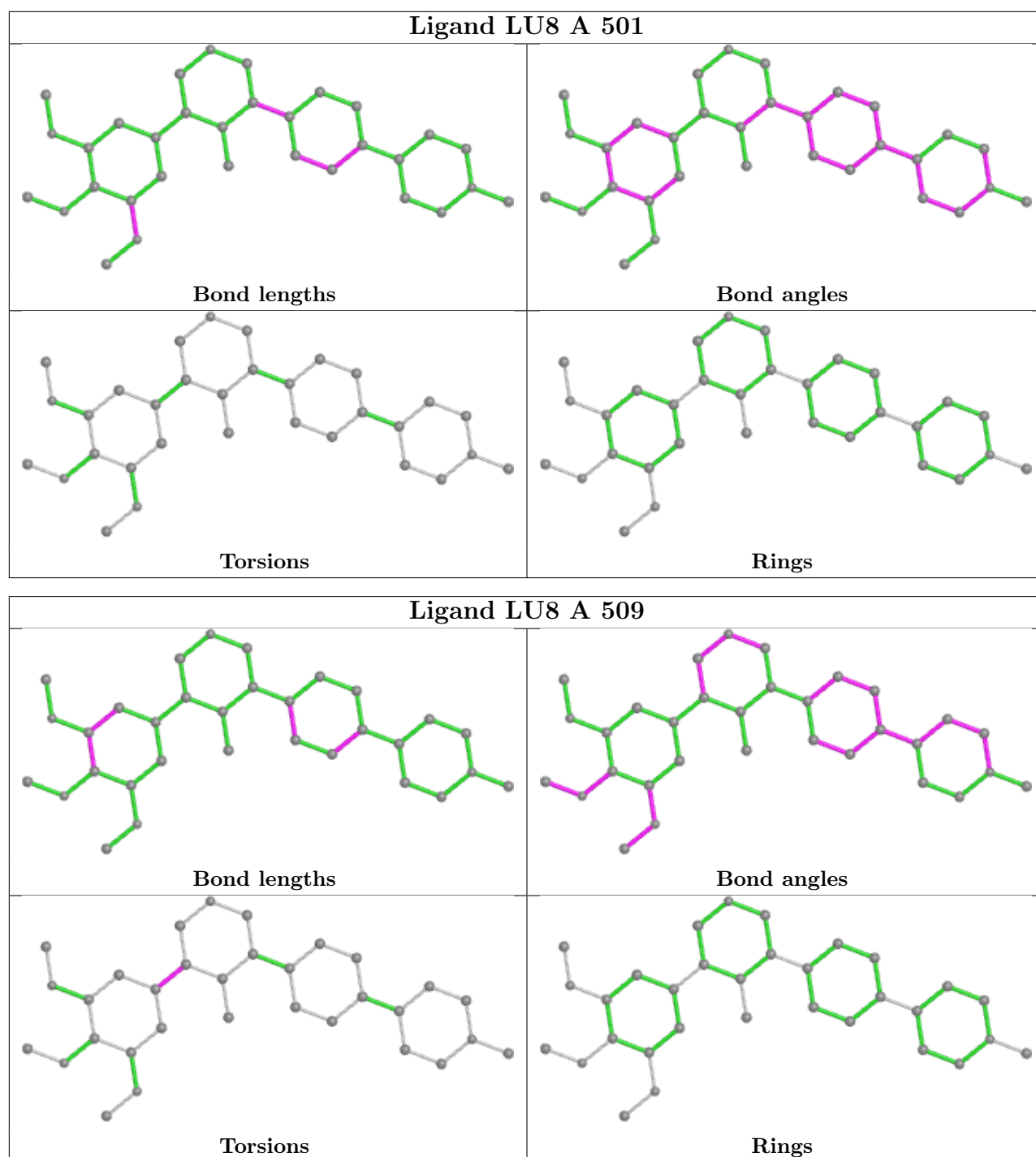
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	504	EDO	1	0
3	A	514	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.





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.18	2 (0%) 87 87	9, 14, 34, 55	0
1	B	292/301 (97%)	-0.11	7 (2%) 59 58	9, 15, 30, 90	0
All	All	575/602 (95%)	-0.14	9 (1%) 72 73	9, 15, 33, 90	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	205	ALA	10.0
1	B	206	ARG	9.2
1	B	219	TYR	4.9
1	B	227	TRP	4.0
1	A	297	LEU	3.4
1	B	297	LEU	2.9
1	B	207	ASP	2.6
1	A	219	TYR	2.3
1	B	372	ASN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

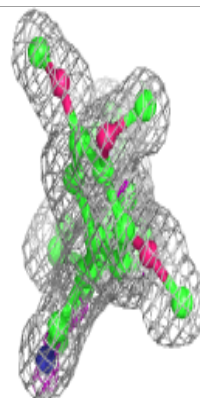
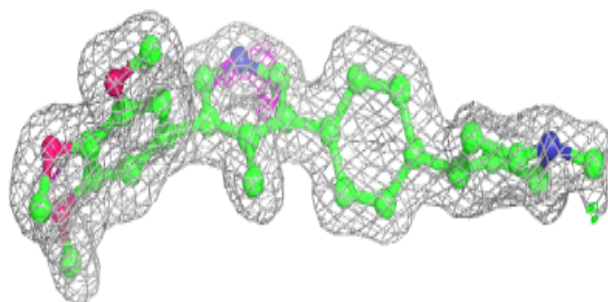
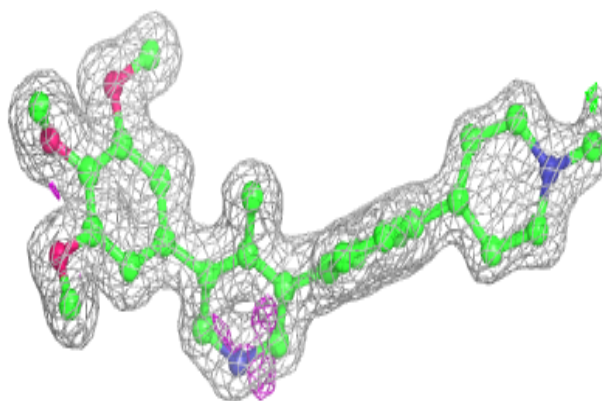
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	TLA	A	507	10/10	0.59	0.24	71,76,79,87	0
3	EDO	A	504	4/4	0.66	0.18	45,48,49,50	0
3	EDO	B	508	4/4	0.73	0.14	30,39,41,44	0
3	EDO	B	509	4/4	0.74	0.15	45,46,50,51	0
3	EDO	A	515	4/4	0.80	0.17	56,56,60,62	0
3	EDO	A	518	4/4	0.81	0.15	43,44,45,47	0
4	DMS	B	504	4/4	0.82	0.13	56,60,62,65	0
3	EDO	B	503	4/4	0.82	0.21	21,21,21,29	0
3	EDO	A	517	4/4	0.86	0.08	47,49,54,54	0
6	LGA	B	505	7/7	0.89	0.18	37,39,41,46	0
4	DMS	A	506	4/4	0.90	0.21	35,40,43,48	0
3	EDO	A	503	4/4	0.92	0.09	18,19,20,23	0
3	EDO	B	507	4/4	0.92	0.12	18,20,22,25	0
7	SO4	B	506	5/5	0.92	0.20	31,42,56,60	0
2	LU8	A	508	32/32	0.93	0.10	16,20,30,36	0
6	LGA	A	510	7/7	0.93	0.13	27,29,31,33	0
3	EDO	A	516	4/4	0.94	0.17	26,32,33,44	0
2	LU8	A	509	32/32	0.95	0.08	14,16,35,41	0
3	EDO	A	514	4/4	0.95	0.15	15,28,32,42	0
3	EDO	A	502	4/4	0.96	0.09	13,17,17,22	0
2	LU8	A	501	32/32	0.96	0.09	10,13,45,54	0
2	LU8	B	501	32/32	0.96	0.08	11,13,32,37	0
3	EDO	A	505	4/4	0.97	0.08	12,17,19,24	0
7	SO4	A	512	5/5	0.99	0.05	14,18,30,30	0
7	SO4	A	513	5/5	0.99	0.05	12,13,15,15	5
7	SO4	B	502	5/5	0.99	0.06	20,20,23,24	0
7	SO4	A	511	5/5	0.99	0.06	16,17,20,22	0

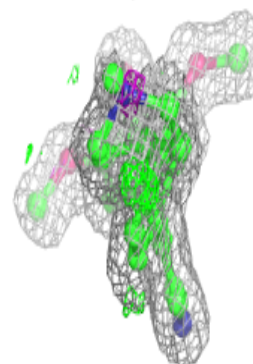
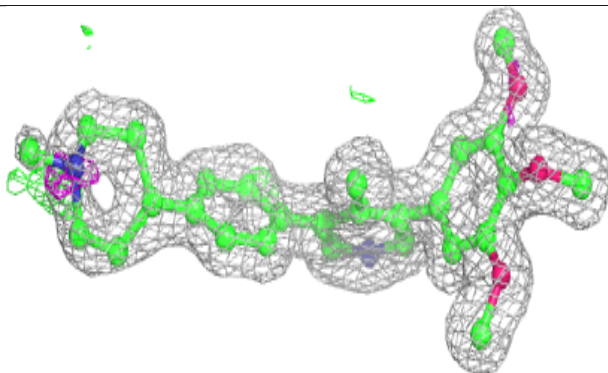
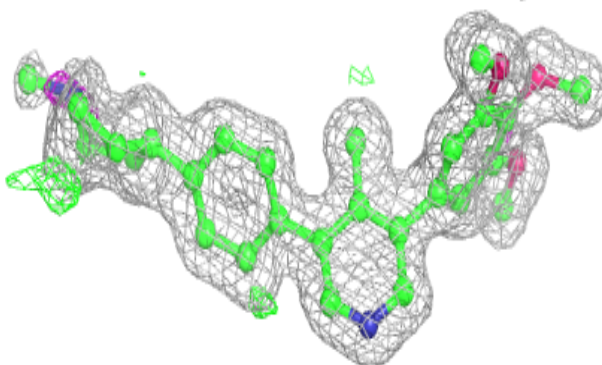
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

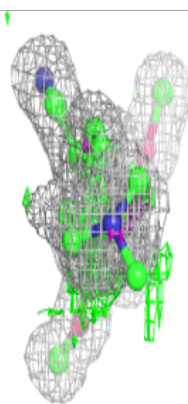
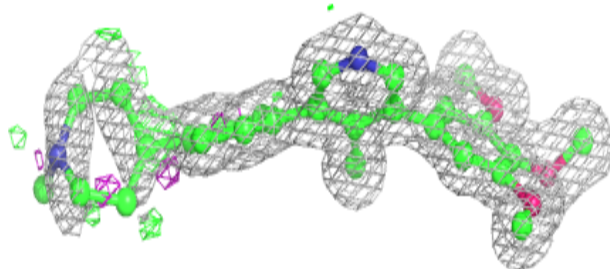
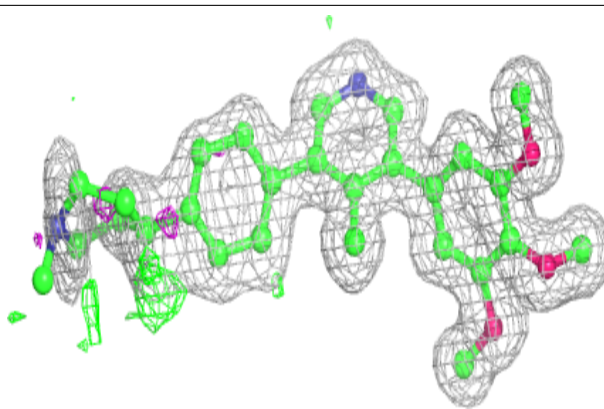
**Electron density around LU8 A 509:**

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

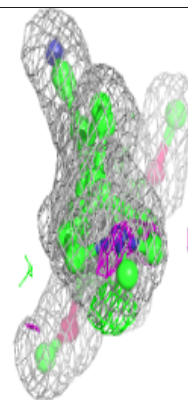
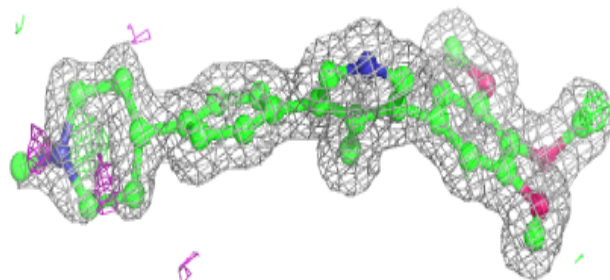
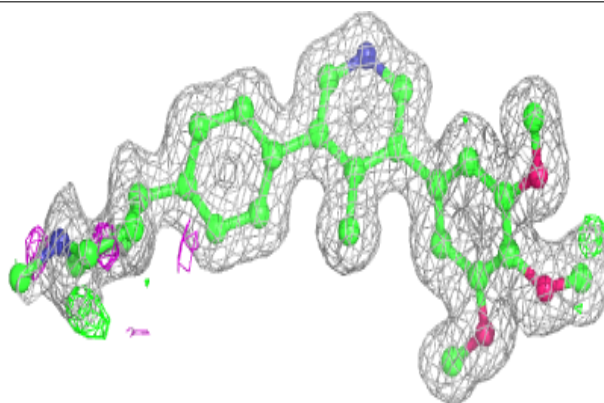


Electron density around LU8 A 501:

$2mF_o-DF_c$ (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.