



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:45 AM UTC

PDB ID : 5S87 / pdb_00005s87
Title : XChem group deposition – Crystal Structure of human ACVR1 in complex with FM010953a
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

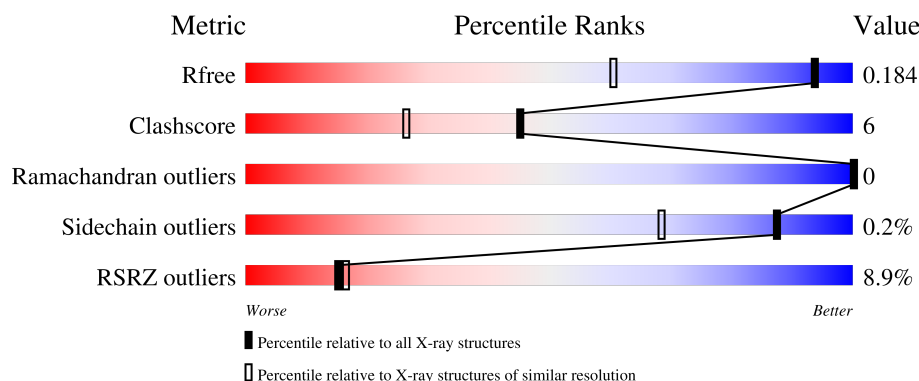
1 Overall quality at a glance

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	10% 84% 9% 6%
1	B	301	7% 91% 5% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	505	-	X	X	-
6	XKD	B	505[A]	-	-	X	-
6	XKD	B	505[B]	-	X	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5743 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.

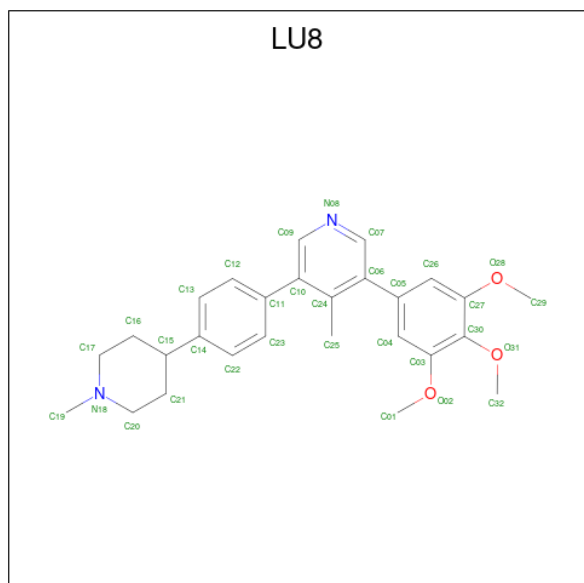
- Molecule 1 is a protein called Activin receptor type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	13	0
			2340	1498	400	427	15			
1	B	290	Total	C	N	O	S	0	8	0
			2336	1487	403	430	16			

There are 6 discrepancies between the modelled and reference sequences:

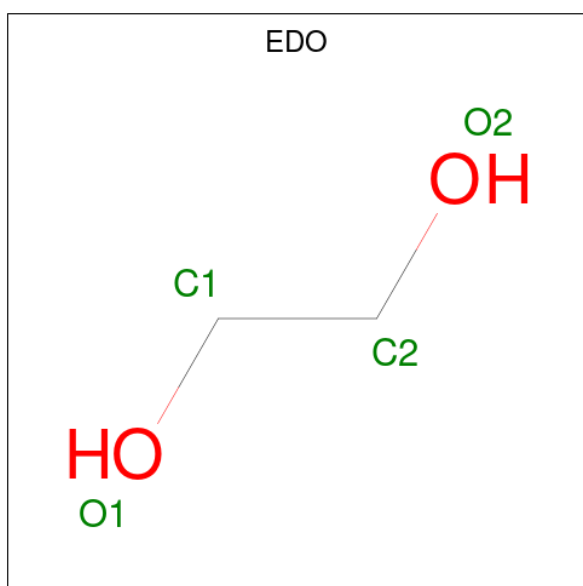
Chain	Residue	Modelled	Actual	Comment	Reference
A	199	SER	-	expression tag	UNP Q04771
A	200	MET	-	expression tag	UNP Q04771
A	207	ASP	GLN	engineered mutation	UNP Q04771
B	199	SER	-	expression tag	UNP Q04771
B	200	MET	-	expression tag	UNP Q04771
B	207	ASP	GLN	engineered mutation	UNP Q04771

- 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).



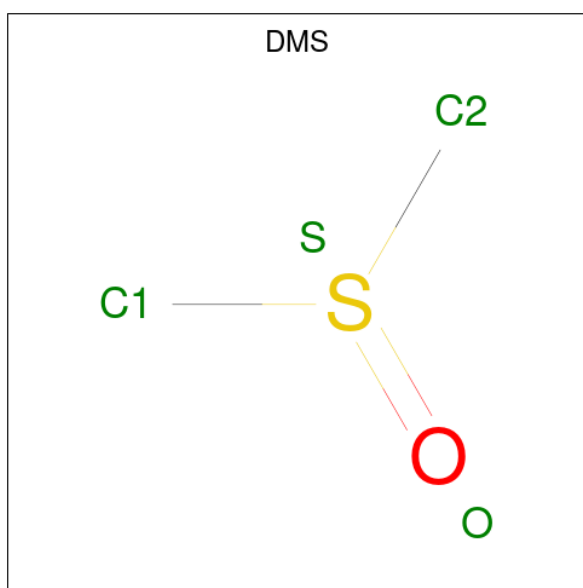
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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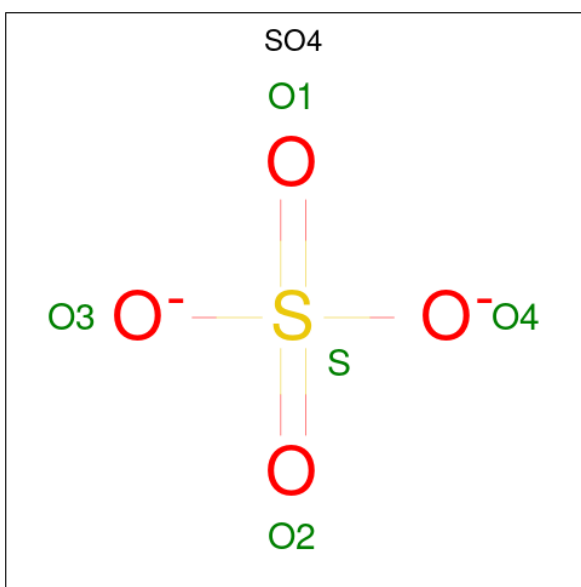
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



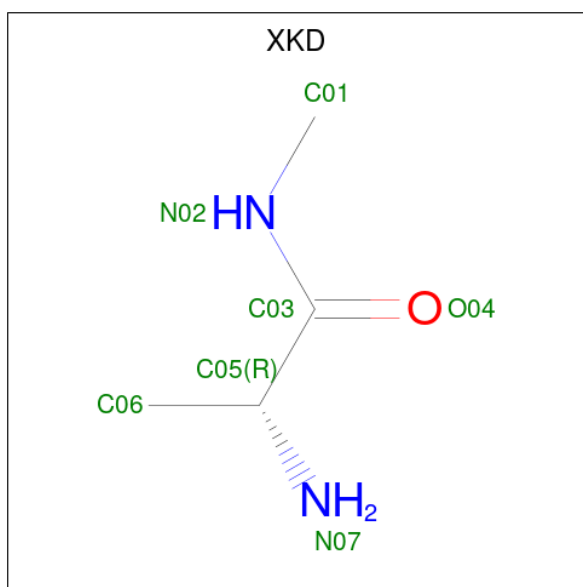
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO₄) (formula: O₄S).



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

- Molecule 6 is N-methyl-D-alaninamide (CCD ID: XKD) (formula: C₄H₁₀N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	1
			14	8	4	2		

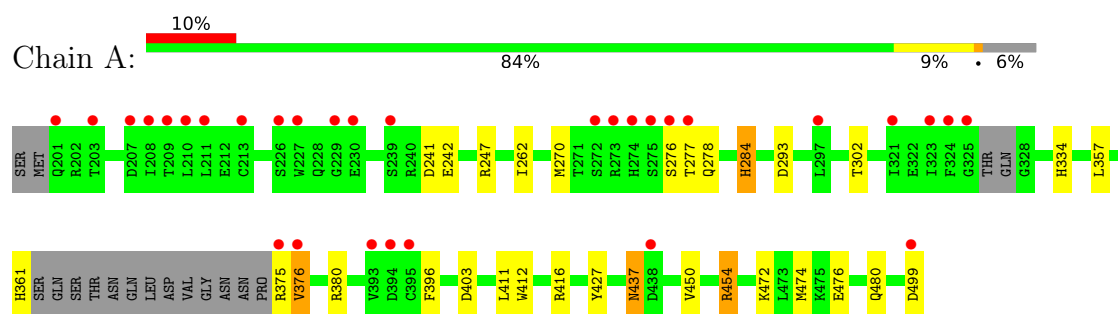
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	395	Total	O	0	1
			396	396		
7	B	407	Total	O	0	0
			407	407		

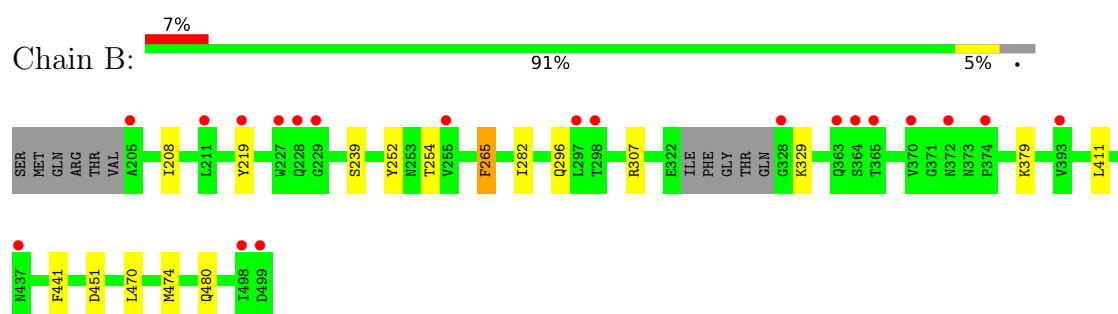
3 Residue-property plots [i](#)

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	127.17Å 84.86Å 87.94Å 90.00° 130.95° 90.00°	Depositor
Resolution (Å)	42.47 – 1.30 42.47 – 1.30	Depositor EDS
% Data completeness (in resolution range)	73.9 (42.47-1.30) 74.0 (42.47-1.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 1.31Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.160 , 0.181 0.162 , 0.184	Depositor DCC
R_{free} test set	8719 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h+k-l,-l,-k 0.000 for -h-k-l,l,k 0.014 for -h-2*l,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5743	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: SO4, LU8, XKD, DMS, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.02	1/2401 (0.0%)	1.15	5/3254 (0.2%)
1	B	1.08	0/2394	1.20	2/3251 (0.1%)
All	All	1.05	1/4795 (0.0%)	1.17	7/6505 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	334	HIS	CE1-NE2	5.31	1.37	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	451	ASP	CA-CB-CG	7.13	119.73	112.60
1	A	403	ASP	CA-CB-CG	6.08	118.68	112.60
1	A	284	HIS	CA-CB-CG	-5.98	107.82	113.80
1	A	376	VAL	CA-C-O	-5.31	116.04	121.67
1	A	454	ARG	O-C-N	-5.21	118.38	121.71
1	B	265	PHE	N-CA-CB	-5.10	102.48	109.97
1	A	437	ASN	CA-C-O	-5.04	115.19	120.63

There are no chirality outliers.

There are no planarity outliers.

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	2340	0	2309	34	0
1	B	2336	0	2279	14	0
2	A	128	0	0	0	0
2	B	32	0	0	2	0
3	A	36	0	51	8	0
3	B	16	0	23	2	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
5	A	15	0	0	1	0
5	B	15	0	0	0	0
6	B	14	0	0	9	0
7	A	396	0	0	12	0
7	B	407	0	0	7	1
All	All	5743	0	4674	57	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 6.

All (57) 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:B:505[A]:XKD:O04	7:B:601:HOH:O	1.79	0.97
2:B:501:LU8:C29	6:B:505[B]:XKD:C06	2.47	0.93
1:B:307:ARG:NH1	7:B:602:HOH:O	2.01	0.84
1:A:411:LEU:HG	1:A:474:MET:HE2	1.62	0.82
1:B:219:TYR:CD2	6:B:505[B]:XKD:O04	2.36	0.79
1:A:302:THR:HG21	1:A:499:ASP:OD2	1.86	0.74
1:A:241:ASP:OD2	7:A:603:HOH:O	2.06	0.72
6:B:505[A]:XKD:C06	6:B:505[A]:XKD:C01	2.70	0.69
1:A:242:GLU:OE1	7:A:604:HOH:O	2.10	0.69
1:A:247:ARG:CD	7:A:784:HOH:O	2.40	0.69
3:B:508:EDO:H12	7:B:792:HOH:O	1.92	0.68
1:B:411[B]:LEU:HG	1:B:474:MET:HE2	1.74	0.68
1:A:476[B]:GLU:OE1	7:A:605:HOH:O	2.12	0.66
1:B:252:TYR:CD1	1:B:265:PHE:HB2	2.31	0.66
1:A:293[B]:ASP:HB2	7:A:608:HOH:O	1.96	0.64
1:B:208:ILE:HD11	1:B:282:ILE:HD13	1.79	0.64
1:B:208:ILE:CD1	1:B:282:ILE:HD13	2.28	0.64
1:A:380:ARG:HH22	3:A:505:EDO:C1	2.11	0.63
6:B:505[A]:XKD:O04	7:B:603:HOH:O	2.16	0.62
1:A:357[B]:LEU:HD11	1:A:375:ARG:HG2	1.81	0.62
1:B:254[A]:THR:HG21	1:B:329:LYS:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ARG:HH22	1:A:480[B]:GLN:CD	2.10	0.59
1:A:361:HIS:HB2	1:A:396:PHE:CD1	2.41	0.56
1:A:437:ASN:HA	3:A:505:EDO:H12	1.88	0.55
1:B:219:TYR:CG	6:B:505[B]:XKD:O04	2.60	0.54
1:A:357[B]:LEU:HD21	1:A:375:ARG:HB3	1.89	0.53
1:A:277:THR:HB	7:A:604:HOH:O	2.08	0.52
1:A:437:ASN:O	5:A:511:SO4:O2	2.29	0.51
1:A:284:HIS:HE1	7:A:782:HOH:O	1.95	0.50
6:B:505[A]:XKD:C03	7:B:603:HOH:O	2.60	0.50
1:A:380:ARG:HH22	3:A:505:EDO:H12	1.78	0.47
1:A:357[B]:LEU:HD21	1:A:375:ARG:CG	2.45	0.47
1:A:450:VAL:HG22	3:A:504:EDO:H11	1.96	0.46
3:A:512:EDO:H11	7:A:752:HOH:O	2.15	0.46
1:A:472:LYS:O	1:A:476[B]:GLU:HG3	2.15	0.45
1:A:276:SER:HB2	7:A:878:HOH:O	2.16	0.45
1:A:412:TRP:CZ2	1:A:416:ARG:HD2	2.51	0.45
1:A:357[B]:LEU:HG	1:A:375:ARG:HD3	2.00	0.44
1:A:293[B]:ASP:CB	7:A:608:HOH:O	2.62	0.44
1:B:296[B]:GLN:HA	1:B:296[B]:GLN:OE1	2.19	0.43
1:B:254[A]:THR:CG2	1:B:329:LYS:HG3	2.48	0.43
1:B:480:GLN:NE2	7:B:614:HOH:O	2.51	0.43
1:A:454:ARG:NH2	1:A:480[B]:GLN:OE1	2.52	0.42
1:B:411[B]:LEU:HD11	1:B:470:LEU:HD22	2.01	0.42
1:A:270:MET:HG3	1:A:277:THR:CG2	2.48	0.42
1:A:278:GLN:HG2	7:A:610:HOH:O	2.20	0.42
1:A:302:THR:CG2	1:A:499:ASP:OD2	2.61	0.42
1:A:427:TYR:CD2	1:A:427:TYR:C	2.98	0.42
1:A:262[A]:ILE:O	3:A:502:EDO:H11	2.20	0.41
2:B:501:LU8:O28	6:B:505[B]:XKD:C01	2.68	0.41
1:A:357[B]:LEU:HD21	1:A:375:ARG:CB	2.49	0.41
1:A:376:VAL:HG21	7:A:991:HOH:O	2.19	0.41
1:A:380:ARG:NH2	3:A:505:EDO:C1	2.82	0.41
1:B:379:LYS:HD2	1:B:441:PHE:N	2.36	0.41
3:B:510:EDO:H12	7:B:721:HOH:O	2.21	0.40
1:A:380:ARG:NH2	3:A:505:EDO:H11	2.37	0.40
1:B:219:TYR:CE2	6:B:505[B]:XKD:O04	2.75	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)
7:B:916:HOH:O	7:B:916:HOH:O[2_454]	1.29	0.91

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	291/301 (97%)	287 (99%)	4 (1%)	0	100	100
1	B	294/301 (98%)	290 (99%)	4 (1%)	0	100	100
All	All	585/602 (97%)	577 (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%)	253 (100%)	0	100	100
1	B	253/270 (94%)	252 (100%)	1 (0%)	84	65
All	All	506/540 (94%)	505 (100%)	1 (0%)	87	68

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	239	SER

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

sidechains are listed below:

Mol	Chain	Res	Type
1	A	284	HIS
1	A	361	HIS
1	B	284	HIS
1	B	452	GLN
1	B	480	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

28 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	A	501[B]	-	35,35,35	0.81	1 (2%)	47,49,49	1.15	5 (10%)
3	EDO	A	513	-	3,3,3	0.10	0	2,2,2	0.14	0
3	EDO	A	514	-	3,3,3	0.88	0	2,2,2	0.65	0
3	EDO	B	509	-	3,3,3	0.21	0	2,2,2	0.16	0
4	DMS	A	506	-	3,3,3	0.24	0	3,3,3	0.02	0
6	XKD	B	505[B]	-	5,6,6	4.72	2 (40%)	6,7,7	3.84	5 (83%)
6	XKD	B	505[A]	-	5,6,6	4.17	2 (40%)	6,7,7	2.44	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LU8	A	507	-	35,35,35	1.11	2 (5%)	47,49,49	2.32	18 (38%)
5	SO4	B	502	-	4,4,4	0.22	0	6,6,6	0.24	0
2	LU8	A	501[A]	-	35,35,35	0.89	1 (2%)	47,49,49	1.34	6 (12%)
3	EDO	B	510	-	3,3,3	0.12	0	2,2,2	0.20	0
3	EDO	A	502	-	3,3,3	0.88	0	2,2,2	1.22	0
3	EDO	B	508	-	3,3,3	0.88	0	2,2,2	1.90	0
3	EDO	A	504	-	3,3,3	0.23	0	2,2,2	0.32	0
3	EDO	B	503	-	3,3,3	0.91	0	2,2,2	0.81	0
5	SO4	B	506	-	4,4,4	0.27	0	6,6,6	0.14	0
3	EDO	A	515	-	3,3,3	0.17	0	2,2,2	0.10	0
5	SO4	A	510	-	4,4,4	0.23	0	6,6,6	0.39	0
2	LU8	A	508	-	35,35,35	1.22	4 (11%)	47,49,49	1.68	10 (21%)
5	SO4	A	509	-	4,4,4	0.47	0	6,6,6	0.11	0
5	SO4	B	507	-	4,4,4	0.96	0	6,6,6	0.20	0
3	EDO	A	503	-	3,3,3	1.15	0	2,2,2	0.94	0
4	DMS	B	504	-	3,3,3	0.26	0	3,3,3	0.10	0
3	EDO	A	505	-	3,3,3	2.01	1 (33%)	2,2,2	1.47	1 (50%)
5	SO4	A	511	-	4,4,4	0.31	0	6,6,6	0.18	0
3	EDO	A	512	-	3,3,3	0.31	0	2,2,2	0.76	0
2	LU8	B	501	-	35,35,35	1.04	1 (2%)	47,49,49	1.44	10 (21%)
3	EDO	A	516	-	3,3,3	0.42	0	2,2,2	0.39	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	A	501[B]	-	-	2/18/28/28	0/4/4/4
3	EDO	A	513	-	-	1/1/1/1	-
3	EDO	A	514	-	-	1/1/1/1	-
3	EDO	B	509	-	-	1/1/1/1	-
6	XKD	B	505[B]	-	-	4/6/6/6	-
6	XKD	B	505[A]	-	-	2/6/6/6	-
2	LU8	A	507	-	-	0/18/28/28	0/4/4/4
2	LU8	A	501[A]	-	-	0/18/28/28	0/4/4/4
3	EDO	B	510	-	-	1/1/1/1	-
3	EDO	A	502	-	-	0/1/1/1	-
3	EDO	B	508	-	-	1/1/1/1	-
3	EDO	A	504	-	-	1/1/1/1	-
3	EDO	B	503	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	515	-	-	1/1/1/1	-
2	LU8	A	508	-	-	4/18/28/28	0/4/4/4
3	EDO	A	503	-	-	1/1/1/1	-
3	EDO	A	505	-	-	1/1/1/1	-
3	EDO	A	512	-	-	1/1/1/1	-
2	LU8	B	501	-	-	0/18/28/28	0/4/4/4
3	EDO	A	516	-	-	1/1/1/1	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	505[B]	XKD	C03-N02	9.62	1.46	1.33
6	B	505[A]	XKD	C03-N02	8.84	1.45	1.33
6	B	505[B]	XKD	O04-C03	-3.70	1.16	1.23
3	A	505	EDO	O1-C1	-2.93	1.27	1.42
2	A	507	LU8	C10-C11	-2.92	1.44	1.49
2	B	501	LU8	C12-C13	2.72	1.43	1.38
2	A	507	LU8	C26-C05	2.68	1.44	1.39
2	A	508	LU8	C09-N08	-2.50	1.28	1.34
2	A	508	LU8	C14-C15	-2.28	1.47	1.52
6	B	505[A]	XKD	O04-C03	-2.27	1.19	1.23
2	A	508	LU8	C12-C13	-2.14	1.35	1.38
2	A	501[B]	LU8	C03-C30	-2.11	1.36	1.41
2	A	501[A]	LU8	C10-C11	2.06	1.53	1.49
2	A	508	LU8	C13-C14	2.03	1.42	1.39

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	507	LU8	C26-C05-C06	-6.04	110.48	120.61
2	A	507	LU8	C07-C06-C05	-5.83	111.13	119.56
6	B	505[B]	XKD	O04-C03-N02	-5.69	113.65	123.13
2	A	508	LU8	C20-C21-C15	-5.25	104.86	111.00
6	B	505[B]	XKD	C05-C03-N02	5.06	131.73	117.03
2	A	507	LU8	C17-C16-C15	-4.64	105.57	111.00
6	B	505[A]	XKD	O04-C03-N02	-4.28	116.00	123.13
2	A	508	LU8	C17-C16-C15	4.18	115.89	111.00
2	A	501[A]	LU8	C17-C16-C15	-4.14	106.16	111.00
2	A	501[A]	LU8	C29-O28-C27	4.09	123.51	117.51
2	A	507	LU8	C27-C30-C03	3.87	123.33	119.56
2	A	507	LU8	C20-C21-C15	3.51	115.11	111.00
2	A	507	LU8	C21-C20-N18	3.49	115.70	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	505[A]	XKD	C05-C03-N02	3.48	127.15	117.03
6	B	505[B]	XKD	C06-C05-N07	-3.47	98.31	109.98
2	A	507	LU8	C04-C05-C26	3.33	123.23	118.35
2	B	501	LU8	C20-N18-C17	3.31	114.81	109.54
2	A	508	LU8	C06-C07-N08	-3.30	119.62	124.27
2	A	508	LU8	C16-C17-N18	3.15	115.26	111.20
2	A	501[A]	LU8	C20-N18-C17	3.12	114.50	109.54
2	A	507	LU8	C04-C05-C06	3.06	125.73	120.61
6	B	505[B]	XKD	C01-N02-C03	3.03	127.48	122.21
2	A	507	LU8	C20-N18-C17	3.01	114.33	109.54
2	A	507	LU8	C06-C07-N08	-3.00	120.04	124.27
2	A	507	LU8	C16-C17-N18	2.83	114.85	111.20
2	B	501	LU8	C06-C07-N08	-2.82	120.30	124.27
2	B	501	LU8	C17-C16-C15	2.79	114.27	111.00
6	B	505[B]	XKD	O04-C03-C05	-2.70	114.61	120.56
2	B	501	LU8	C22-C14-C13	2.69	121.64	118.30
2	B	501	LU8	C23-C22-C14	-2.66	118.53	121.18
2	B	501	LU8	C23-C11-C12	2.62	122.37	117.68
2	A	508	LU8	C12-C13-C14	2.61	123.79	121.18
2	B	501	LU8	C13-C12-C11	-2.58	117.81	121.12
2	A	501[A]	LU8	C11-C10-C24	2.56	126.69	122.47
2	A	508	LU8	C09-N08-C07	2.55	120.98	117.51
2	A	507	LU8	C05-C06-C24	2.49	126.57	122.47
2	A	507	LU8	C05-C04-C03	-2.48	116.81	120.19
2	A	507	LU8	O02-C03-C04	-2.46	119.84	124.08
2	A	501[B]	LU8	C06-C07-N08	-2.44	120.84	124.27
2	A	507	LU8	O31-C30-C27	-2.44	116.63	120.12
2	A	507	LU8	O02-C03-C30	2.40	119.25	115.14
2	A	507	LU8	O28-C27-C30	2.40	119.25	115.14
2	A	501[A]	LU8	C06-C07-N08	-2.38	120.92	124.27
2	A	501[B]	LU8	C09-C10-C11	-2.37	116.13	119.56
2	A	501[B]	LU8	C01-O02-C03	-2.36	114.05	117.51
2	A	507	LU8	C26-C27-C30	-2.30	117.67	120.22
2	A	501[B]	LU8	C11-C10-C24	2.25	126.19	122.47
2	A	501[B]	LU8	C16-C17-N18	-2.24	108.30	111.20
2	B	501	LU8	C20-C21-C15	2.19	113.57	111.00
2	A	508	LU8	C11-C10-C24	2.19	126.08	122.47
2	A	508	LU8	C23-C22-C14	-2.19	119.00	121.18
2	A	508	LU8	C06-C24-C10	2.18	121.04	118.39
2	A	501[A]	LU8	C09-C10-C11	-2.16	116.44	119.56
2	A	508	LU8	C32-O31-C30	2.14	120.54	114.74
2	B	501	LU8	C13-C14-C15	-2.06	115.87	121.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	505	EDO	O2-C2-C1	-2.01	97.06	112.39
2	B	501	LU8	C21-C20-N18	2.01	113.78	111.20

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	505[A]	XKD	O04-C03-N02-C01
6	B	505[A]	XKD	C05-C03-N02-C01
6	B	505[B]	XKD	O04-C03-N02-C01
6	B	505[B]	XKD	C05-C03-N02-C01
6	B	505[B]	XKD	N02-C03-C05-C06
6	B	505[B]	XKD	O04-C03-C05-C06
3	A	513	EDO	O1-C1-C2-O2
3	A	512	EDO	O1-C1-C2-O2
3	B	509	EDO	O1-C1-C2-O2
3	A	504	EDO	O1-C1-C2-O2
2	A	508	LU8	C04-C05-C06-C07
2	A	508	LU8	C04-C05-C06-C24
3	A	505	EDO	O1-C1-C2-O2
3	A	514	EDO	O1-C1-C2-O2
3	A	515	EDO	O1-C1-C2-O2
3	B	508	EDO	O1-C1-C2-O2
3	B	510	EDO	O1-C1-C2-O2
3	A	503	EDO	O1-C1-C2-O2
3	A	516	EDO	O1-C1-C2-O2
2	A	508	LU8	C26-C05-C06-C24
2	A	501[B]	LU8	C13-C14-C15-C21
2	A	501[B]	LU8	C22-C14-C15-C21
2	A	508	LU8	C26-C05-C06-C07

There are no ring outliers.

10 monomers are involved in 20 short contacts:

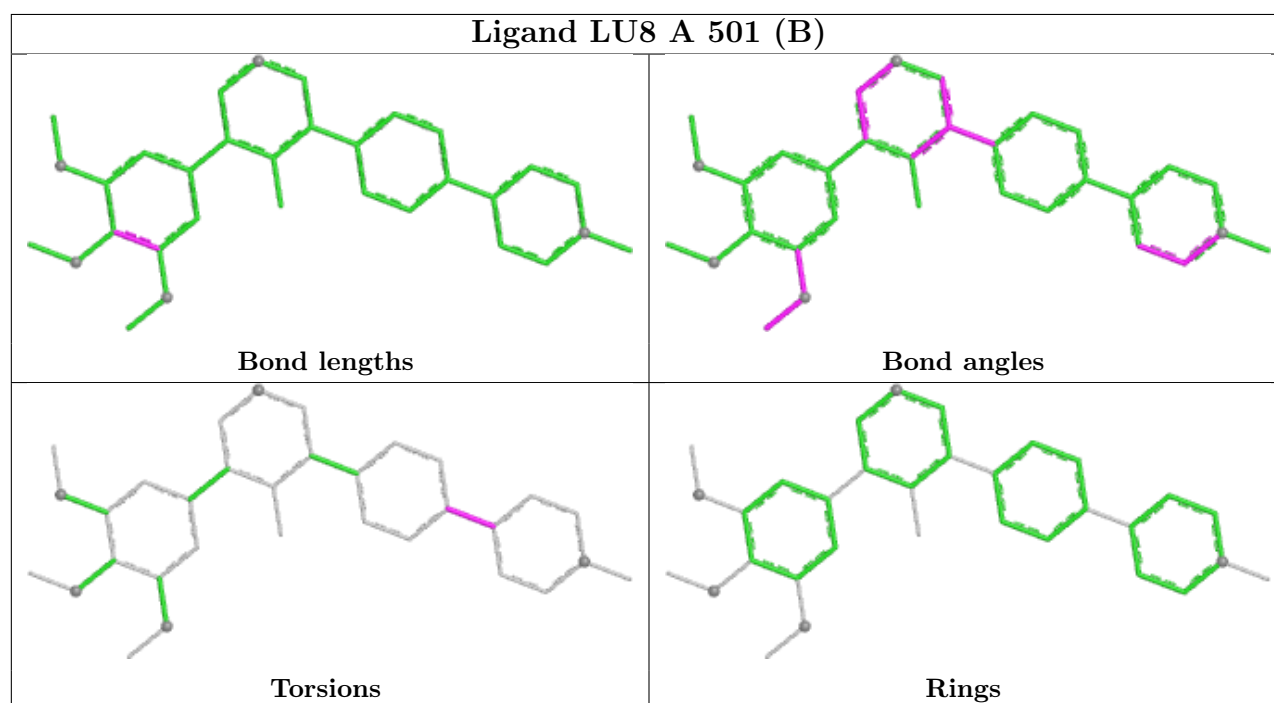
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	505[B]	XKD	5	0
6	B	505[A]	XKD	4	0
3	B	510	EDO	1	0
3	A	502	EDO	1	0
3	B	508	EDO	1	0
3	A	504	EDO	1	0

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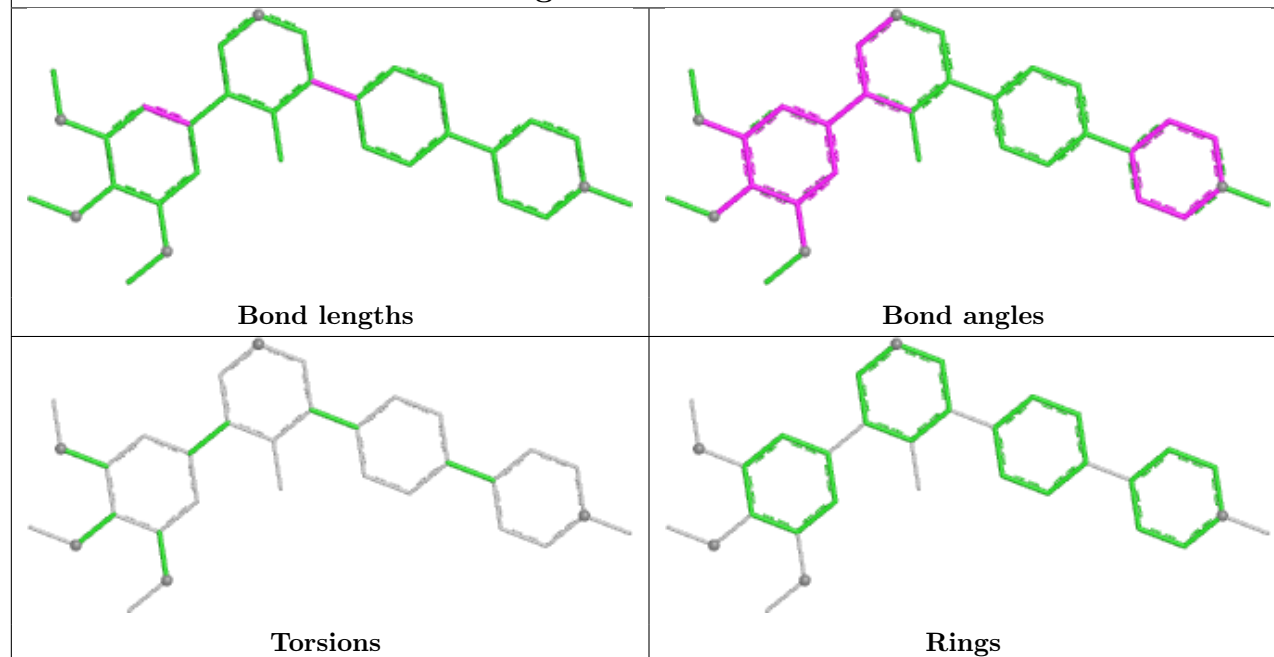
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	505	EDO	5	0
5	A	511	SO4	1	0
3	A	512	EDO	1	0
2	B	501	LU8	2	0

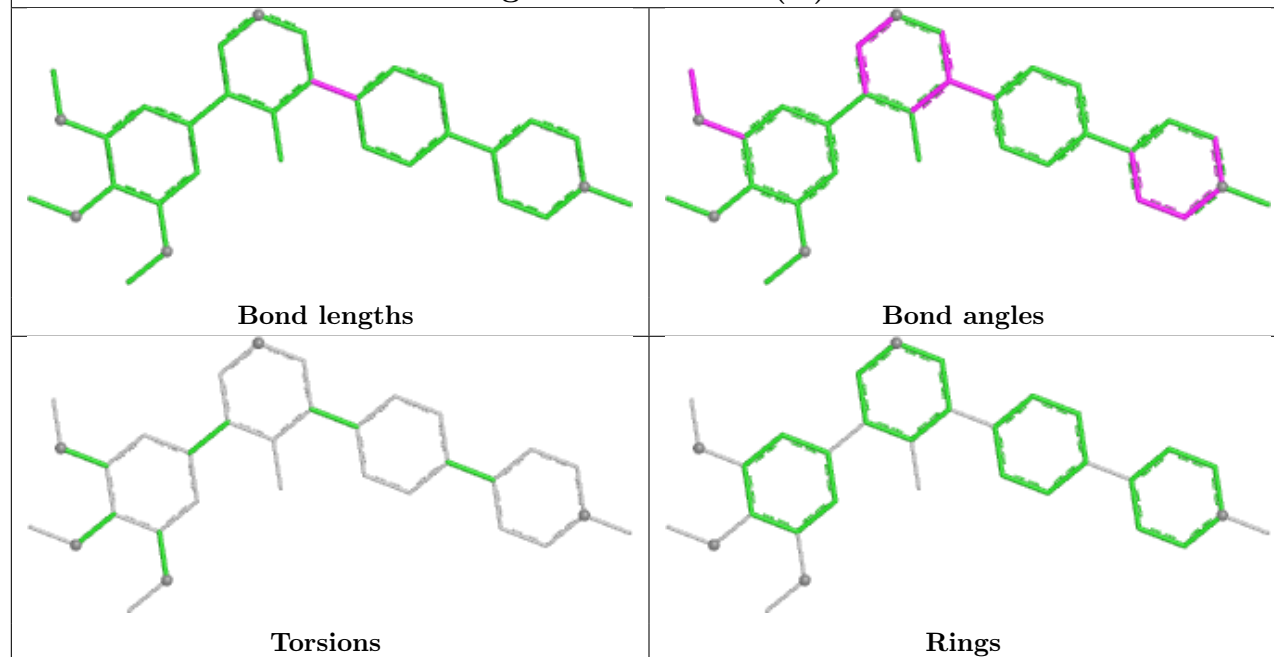
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

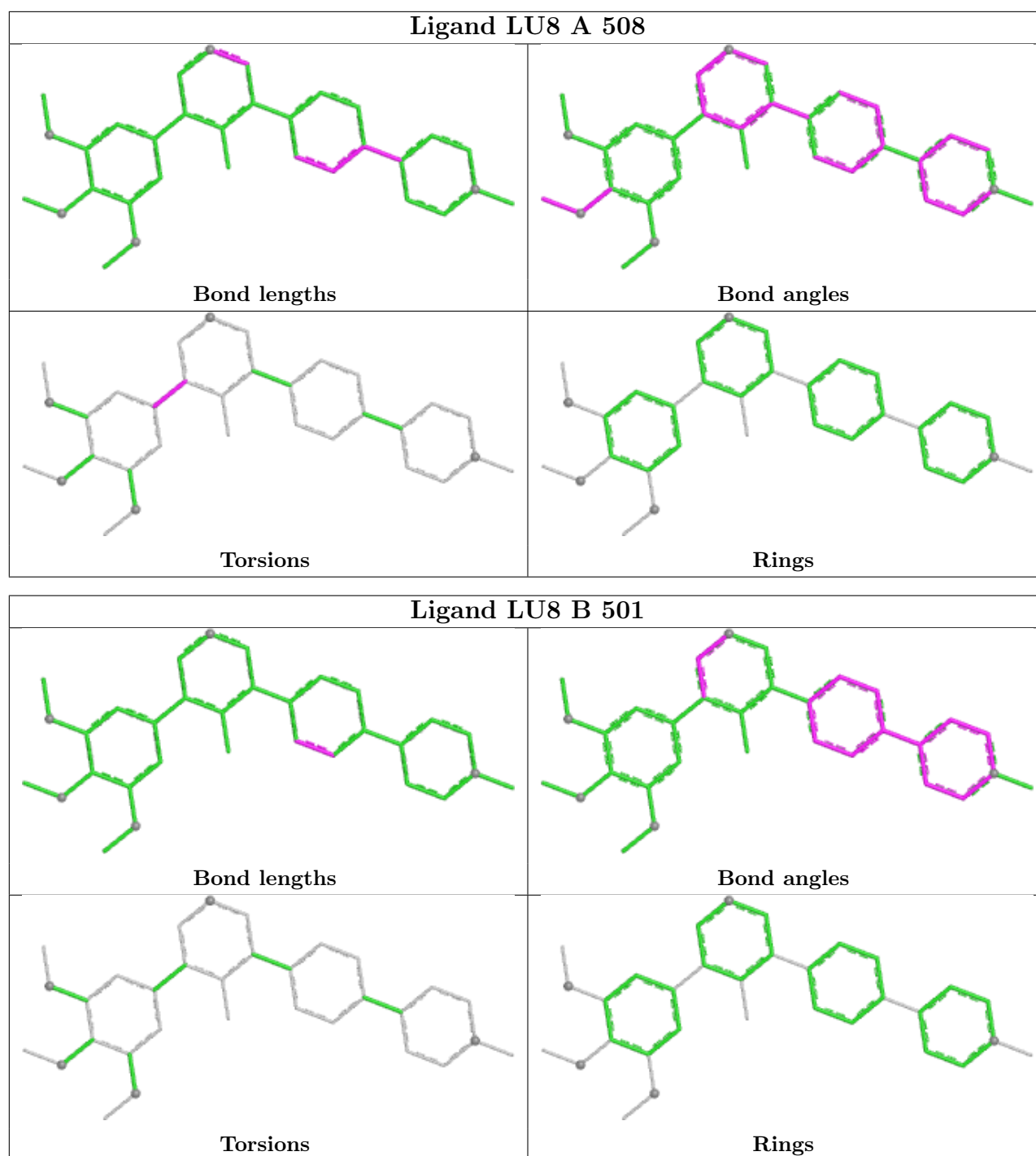


Ligand LU8 A 507



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	284/301 (94%)	0.33	31 (10%)	10 12	5, 15, 34, 59	13 (4%)
1	B	290/301 (96%)	0.27	20 (6%)	23 26	5, 15, 30, 40	8 (2%)
All	All	574/602 (95%)	0.30	51 (8%)	15 16	5, 15, 32, 59	21 (3%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	255	VAL	7.7
1	A	297	LEU	6.2
1	B	205	ALA	5.0
1	A	275	SER	4.8
1	B	297	LEU	4.5
1	B	372	ASN	4.5
1	A	324	PHE	4.0
1	B	328	GLY	3.9
1	A	273	ARG	3.8
1	A	325	GLY	3.6
1	A	393	VAL	3.6
1	A	201	GLN	3.5
1	A	395	CYS	3.4
1	B	229	GLY	3.4
1	B	370	VAL	3.3
1	B	393	VAL	3.2
1	A	227	TRP	3.2
1	B	227	TRP	3.2
1	A	277	THR	3.1
1	B	374	PRO	3.1
1	B	498	ILE	3.0
1	A	239	SER	3.0
1	A	376	VAL	2.9
1	A	499	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	394	ASP	2.8
1	A	210	LEU	2.8
1	A	208	ILE	2.8
1	A	209	THR	2.7
1	A	276	SER	2.5
1	A	211	LEU	2.5
1	A	203	THR	2.4
1	B	219	TYR	2.4
1	A	230	GLU	2.4
1	B	437	ASN	2.4
1	A	375	ARG	2.3
1	B	228	GLN	2.3
1	A	438	ASP	2.3
1	A	274	HIS	2.3
1	B	211	LEU	2.3
1	A	207	ASP	2.3
1	B	499	ASP	2.3
1	B	363	GLN	2.2
1	A	323	ILE	2.2
1	A	213	CYS	2.1
1	A	229	GLY	2.1
1	A	272	SER	2.0
1	B	364	SER	2.0
1	A	226	SER	2.0
1	A	321	ILE	2.0
1	B	298	THR	2.0
1	B	365	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,

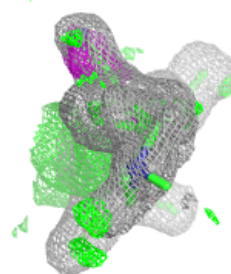
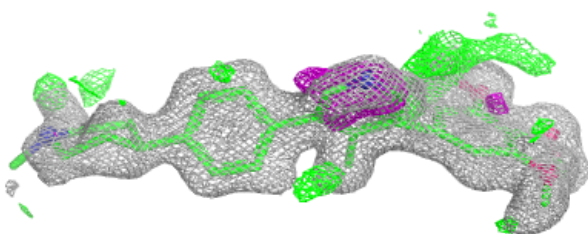
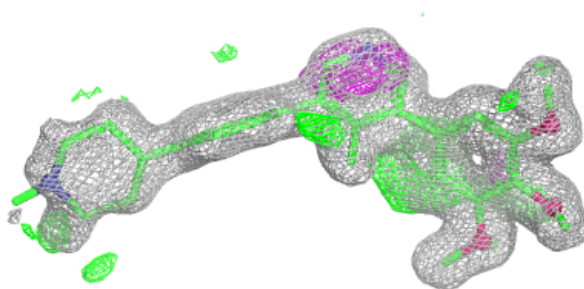
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	DMS	A	506	4/4	0.60	0.33	95,101,101,102	0
3	EDO	A	516	4/4	0.67	0.21	44,50,51,54	0
3	EDO	B	510	4/4	0.69	0.22	42,49,49,49	0
3	EDO	A	504	4/4	0.70	0.23	40,43,43,49	0
6	XKD	B	505[A]	7/7	0.71	0.16	16,21,22,23	7
6	XKD	B	505[B]	7/7	0.71	0.16	27,36,40,41	7
4	DMS	B	504	4/4	0.74	0.24	78,81,83,85	0
3	EDO	A	515	4/4	0.76	0.17	43,47,48,51	0
3	EDO	A	513	4/4	0.81	0.17	38,43,45,50	0
3	EDO	B	509	4/4	0.84	0.16	31,34,38,40	0
5	SO4	A	511	5/5	0.84	0.13	25,31,36,37	5
5	SO4	B	507	5/5	0.87	0.13	23,35,45,45	0
3	EDO	A	503	4/4	0.88	0.14	20,23,24,28	0
2	LU8	A	507	32/32	0.89	0.12	17,22,42,50	0
5	SO4	B	506	5/5	0.90	0.11	36,40,45,48	5
3	EDO	A	514	4/4	0.92	0.12	16,20,28,32	0
3	EDO	B	503	4/4	0.93	0.09	18,19,20,23	0
3	EDO	A	505	4/4	0.93	0.10	18,26,27,31	0
2	LU8	A	501[A]	32/32	0.94	0.10	11,12,27,29	32
2	LU8	A	501[B]	32/32	0.94	0.10	9,11,22,27	32
3	EDO	A	512	4/4	0.95	0.11	15,26,29,37	0
3	EDO	A	502	4/4	0.95	0.14	11,21,23,39	0
2	LU8	A	508	32/32	0.95	0.08	13,15,33,43	0
3	EDO	B	508	4/4	0.96	0.10	12,21,23,23	0
2	LU8	B	501	32/32	0.96	0.09	12,14,39,43	0
5	SO4	A	509	5/5	0.98	0.05	17,18,22,23	0
5	SO4	B	502	5/5	0.98	0.06	20,21,25,25	0
5	SO4	A	510	5/5	0.98	0.06	15,18,24,25	0

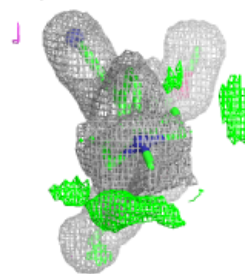
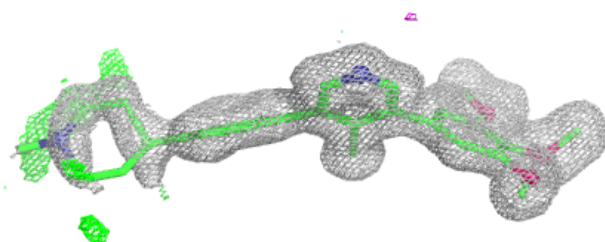
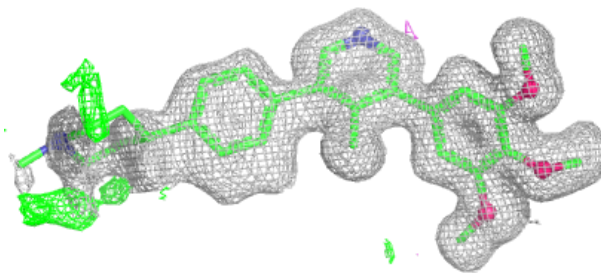
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LU8 A 507:

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

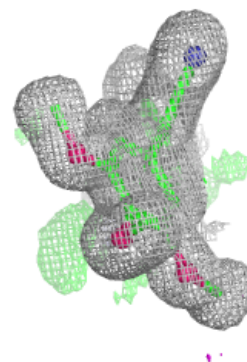
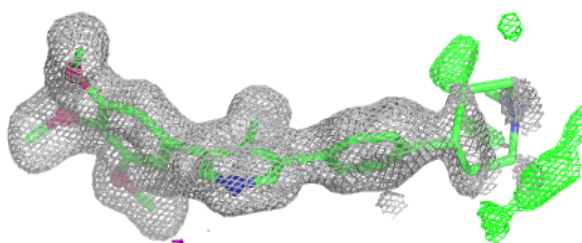
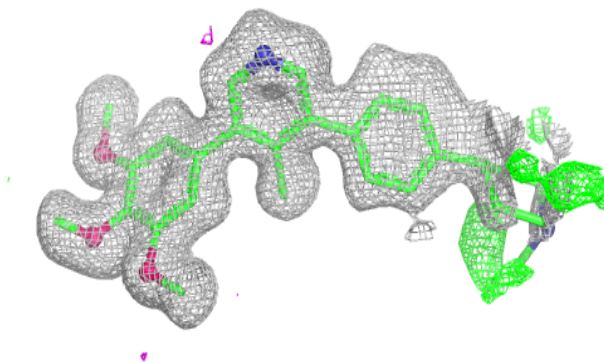
**Electron density around LU8 A 501 (A):**

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

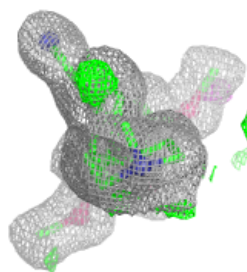
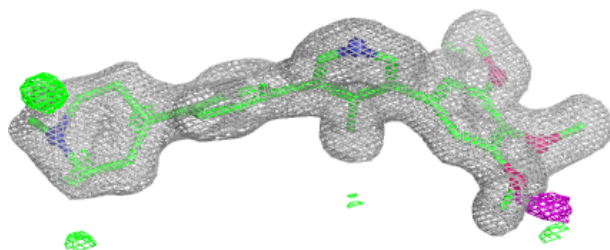
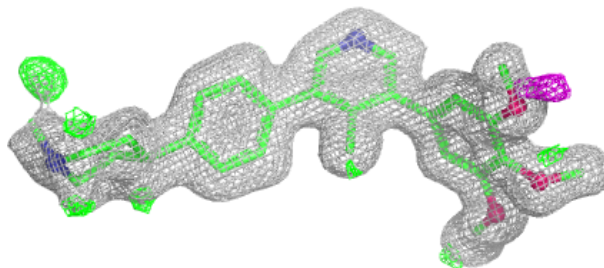


Electron density around LU8 A 501 (B):

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

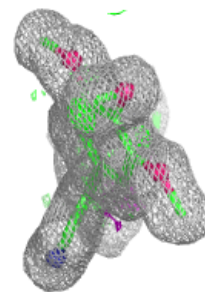
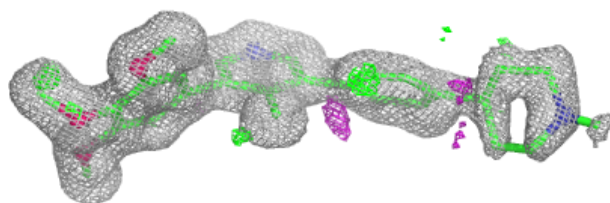
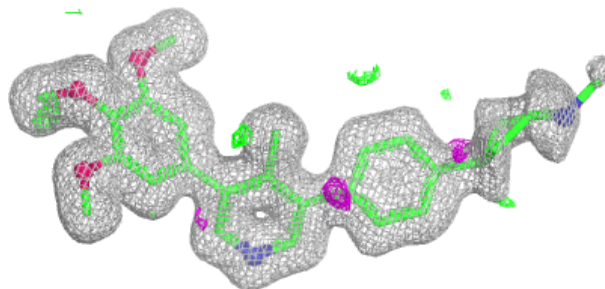
**Electron density around LU8 A 508:**

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



Electron density around LU8 B 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.