



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:22 PM UTC

PDB ID : 7SEL / pdb_00007sel
Title : E. coli MsbA in complex with LPS and inhibitor G7090 (compound 3)
Authors : Payandeh, J.; Koth, C.M.; Verma, V.A.
Deposited on : 2021-09-30
Resolution : 2.98 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)
Xtrriage (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

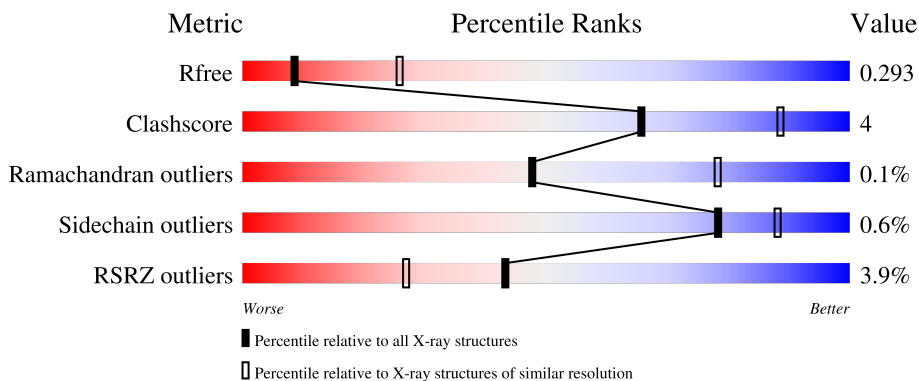
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	599	 3% 89% 7%
1	B	599	 4% 82% 11% 6%

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	KDL	B	602	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 18060 atoms, of which 9093 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 ATP-dependent lipid A-core flippase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	575	9053	2827	4588	777	834	27	0	0	0
1	B	565	8831	2764	4473	757	812	25	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

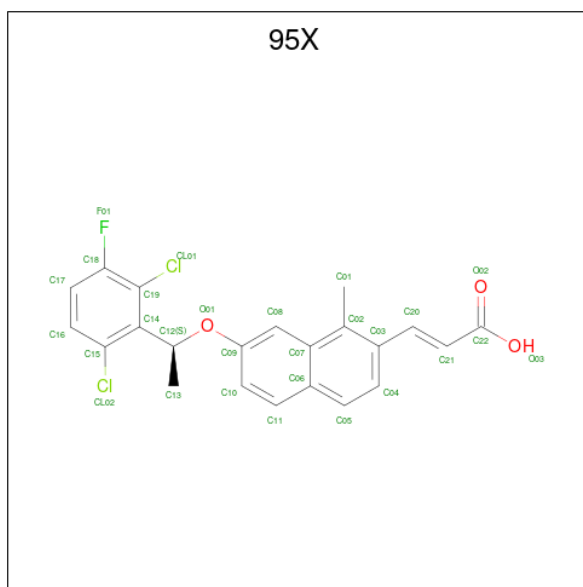
Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP A0A140NBS6
A	-15	ASP	-	expression tag	UNP A0A140NBS6
A	-14	TYR	-	expression tag	UNP A0A140NBS6
A	-13	LYS	-	expression tag	UNP A0A140NBS6
A	-12	ASP	-	expression tag	UNP A0A140NBS6
A	-11	ASP	-	expression tag	UNP A0A140NBS6
A	-10	ASP	-	expression tag	UNP A0A140NBS6
A	-9	ASP	-	expression tag	UNP A0A140NBS6
A	-8	LYS	-	expression tag	UNP A0A140NBS6
A	-7	GLY	-	expression tag	UNP A0A140NBS6
A	-6	GLU	-	expression tag	UNP A0A140NBS6
A	-5	ASN	-	expression tag	UNP A0A140NBS6
A	-4	LEU	-	expression tag	UNP A0A140NBS6
A	-3	TYR	-	expression tag	UNP A0A140NBS6
A	-2	PHE	-	expression tag	UNP A0A140NBS6
A	-1	GLN	-	expression tag	UNP A0A140NBS6
A	0	GLY	-	expression tag	UNP A0A140NBS6
A	1	SER	-	expression tag	UNP A0A140NBS6
B	-16	MET	-	initiating methionine	UNP A0A140NBS6
B	-15	ASP	-	expression tag	UNP A0A140NBS6
B	-14	TYR	-	expression tag	UNP A0A140NBS6
B	-13	LYS	-	expression tag	UNP A0A140NBS6
B	-12	ASP	-	expression tag	UNP A0A140NBS6
B	-11	ASP	-	expression tag	UNP A0A140NBS6
B	-10	ASP	-	expression tag	UNP A0A140NBS6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	ASP	-	expression tag	UNP A0A140NBS6
B	-8	LYS	-	expression tag	UNP A0A140NBS6
B	-7	GLY	-	expression tag	UNP A0A140NBS6
B	-6	GLU	-	expression tag	UNP A0A140NBS6
B	-5	ASN	-	expression tag	UNP A0A140NBS6
B	-4	LEU	-	expression tag	UNP A0A140NBS6
B	-3	TYR	-	expression tag	UNP A0A140NBS6
B	-2	PHE	-	expression tag	UNP A0A140NBS6
B	-1	GLN	-	expression tag	UNP A0A140NBS6
B	0	GLY	-	expression tag	UNP A0A140NBS6
B	1	SER	-	expression tag	UNP A0A140NBS6

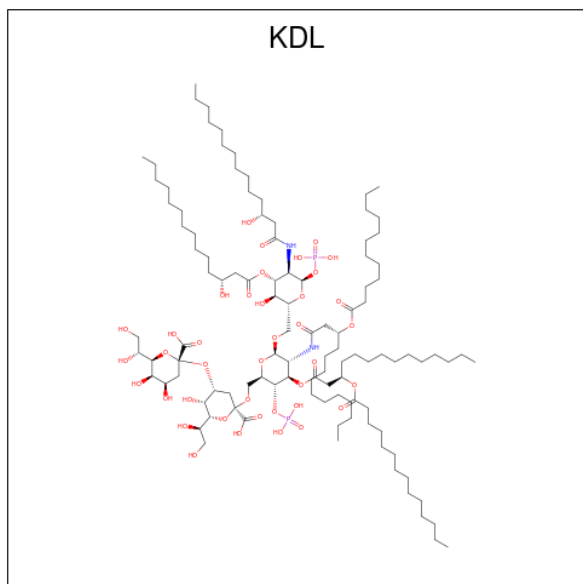
- Molecule 2 is (2E)-3-{7-[(1S)-1-(2,6-dichloro-3-fluorophenyl)ethoxy]-1-methylnaphthalen-2-yl}prop-2-enoic acid (CCD ID: 95X) (formula: C₂₂H₁₇Cl₂FO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	F	H			O
2	A	1	Total	C	Cl	F	H	O	0	0
			44	22	2	1	16	3		
2	B	1	Total	C	Cl	F	H	O	0	0
			44	22	2	1	16	3		

- Molecule 3 is (2 {R},4 {R},5 {R},6 {R})-6-[(1 {R})-1,2-bis(oxidanyl)ethyl]-2-[(2 {R},4 {R},5 {R},6 {R})-6-[(1 {R})-1,2-bis(oxidanyl)ethyl]-2-carboxy-2-[(2 {R},3 {S},4 {R},5 {R},6 {R})-5-[(3 {R})-3-dodecanoyloxytetradecanoyl]amino]-6-[(2 {R},3 {S},4 {R},5 {R},6 {R})-3-oxidanyl-5-[(3 {R})-3-oxidanyltetradecanoyl]amino]-4-[(3 {R})-3-oxidanyltetradecanoyl]oxy-6-phosphonoxy-oxan-2-yl]methoxy]-3-phosphonoxy-4-[(3 {R})-3-tetradecanoyloxytetra

adecanoyl]oxy-oxan-2-yl]methoxy]-5-oxidanyl-oxan-4-yl]oxy-4,5-bis(oxidanyl)oxane-2-carboxylic acid (CCD ID: KDL) (formula: $C_{110}H_{202}N_2O_{39}P_2$) (labeled as "Ligand of Interest" by depositor).

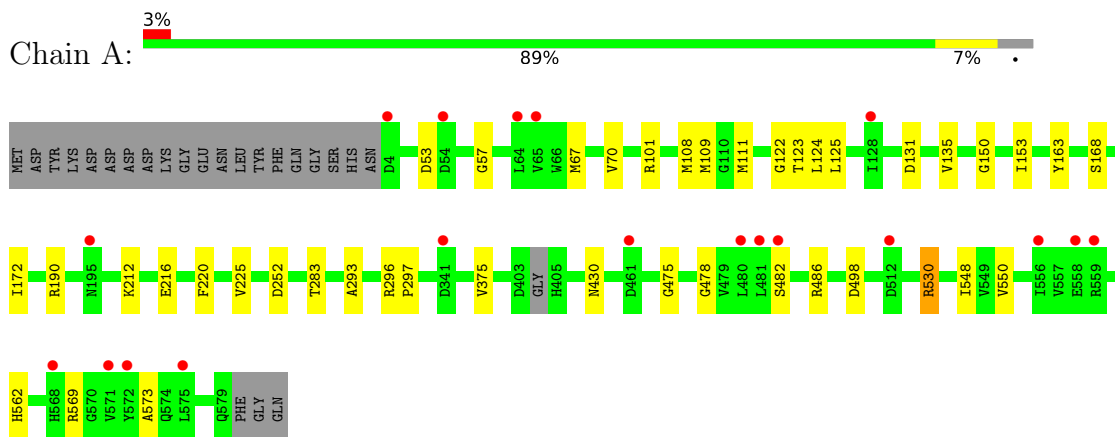


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
3	B	1	88	48	2	36	2	0	0

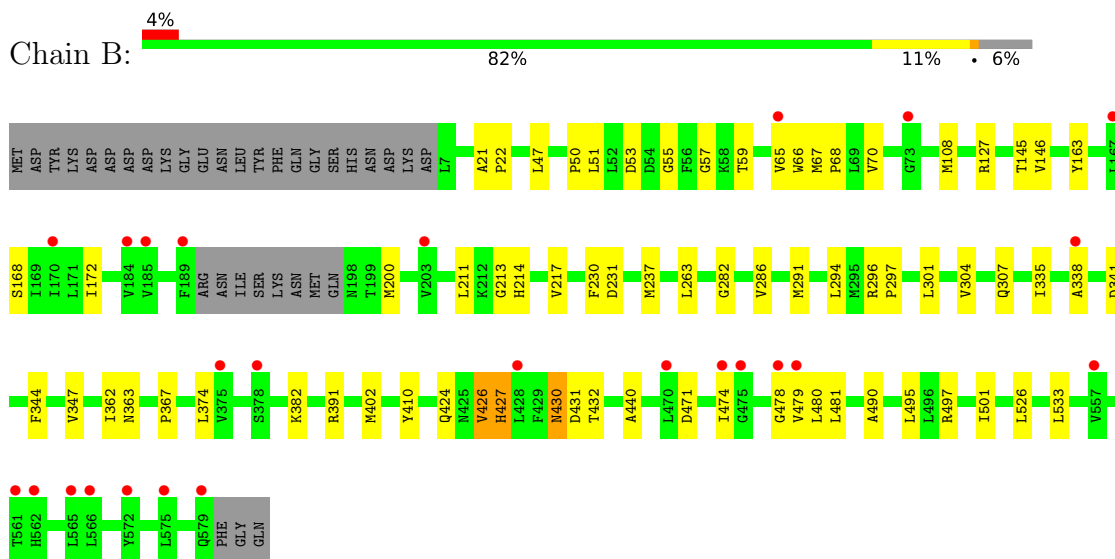
3 Residue-property plots [i](#)

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: ATP-dependent lipid A-core flippase



- Molecule 1: ATP-dependent lipid A-core flippase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.45Å 91.99Å 110.66Å 90.00° 90.31° 90.00°	Depositor
Resolution (Å)	31.99 – 2.98 31.99 – 2.98	Depositor EDS
% Data completeness (in resolution range)	82.7 (31.99-2.98) 82.6 (31.99-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.00Å)	Xtrriage
Refinement program	PHENIX (dev_2747: ???)	Depositor
R, R_{free}	0.256 , 0.290 0.261 , 0.293	Depositor DCC
R_{free} test set	1260 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å ²)	73.7	Xtrriage
Anisotropy	0.037	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.019 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18060	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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: KDL, 95X

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	0.22	0/4529	0.40	0/6119
1	B	0.23	0/4421	0.41	0/5978
All	All	0.22	0/8950	0.40	0/12097

There are no bond length outliers.

There are no bond angle outliers.

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	4465	4588	4588	28	0
1	B	4358	4473	4473	47	0
2	A	28	16	0	0	0
2	B	28	16	0	2	0
3	B	88	0	0	1	0
All	All	8967	9093	9061	69	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (69) 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:A:190:ARG:NH1	1:A:252:ASP:OD1	2.21	0.73
1:B:53:ASP:O	1:B:57:GLY:N	2.28	0.66
1:B:291:MET:O	2:B:601:95X:F01	2.08	0.61
1:B:296:ARG:CG	1:B:297:PRO:HD3	2.36	0.55
1:B:474:ILE:HD12	1:B:481:LEU:HD13	1.89	0.55
1:B:431:ASP:OD1	1:B:432:THR:N	2.30	0.54
1:A:498:ASP:OD1	1:A:530:ARG:NH2	2.41	0.53
1:B:294:LEU:C	1:B:297:PRO:HD2	2.36	0.49
1:B:341:ASP:HB3	1:B:367:PRO:HA	1.94	0.49
1:A:430:ASN:HA	1:A:475:GLY:HA3	1.94	0.48
1:B:296:ARG:HG2	1:B:297:PRO:HD3	1.96	0.48
1:A:109:MET:O	1:B:214:HIS:NE2	2.46	0.47
1:B:230:PHE:O	1:B:231:ASP:C	2.55	0.47
1:A:131:ASP:O	1:A:135:VAL:HG23	2.15	0.47
1:B:296:ARG:HG3	1:B:297:PRO:HD3	1.97	0.47
1:B:344:PHE:O	1:B:363:ASN:HA	2.15	0.46
1:A:569:ARG:HA	1:A:573:ALA:HB2	1.96	0.46
1:B:335:ILE:HG21	1:B:338:ALA:HB2	1.97	0.46
1:A:212:LYS:HE3	1:B:427:HIS:CE1	2.51	0.46
1:A:216:GLU:HG2	1:B:426:VAL:HG22	1.99	0.45
1:A:225:VAL:HG21	1:B:440:ALA:HA	1.98	0.45
1:A:163:TYR:HB3	1:A:283:THR:HG23	1.99	0.45
1:B:282:GLY:O	1:B:286:VAL:HG12	2.17	0.45
1:A:478:GLY:HA3	1:A:486:ARG:HH11	1.82	0.44
1:B:108:MET:HE1	1:B:127:ARG:HB2	2.00	0.44
1:B:50:PRO:O	1:B:51:LEU:C	2.61	0.44
1:B:495:LEU:HG	1:B:526:LEU:HD13	1.99	0.44
1:B:145:THR:O	1:B:146:VAL:C	2.61	0.44
1:B:200:MET:HA	1:B:237:MET:SD	2.58	0.44
1:A:101:ARG:HH12	1:B:237:MET:CE	2.30	0.43
1:B:297:PRO:O	1:B:301:LEU:HG	2.18	0.43
1:A:108:MET:HE2	1:B:211:LEU:HD21	2.00	0.43
1:A:108:MET:HE1	1:A:124:LEU:HB3	2.00	0.43
1:A:296:ARG:HB3	1:A:297:PRO:HD3	2.00	0.43
1:B:21:ALA:N	1:B:22:PRO:CD	2.81	0.43
1:B:402:MET:O	1:B:410:TYR:OH	2.34	0.43
1:A:293:ALA:O	1:A:297:PRO:HD2	2.19	0.43
1:A:168:SER:O	1:A:172:ILE:HD13	2.19	0.42
1:A:122:GLY:O	1:A:123:THR:C	2.59	0.42
3:B:602:KDL:NAO	3:B:602:KDL:OHH	2.53	0.42
1:B:402:MET:HE2	1:B:501:ILE:CD1	2.49	0.42
1:B:67:MET:HB2	1:B:68:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:ILE:CG2	1:B:478:GLY:HA2	2.49	0.42
1:B:432:THR:CG2	1:B:471:ASP:HA	2.50	0.42
1:B:168:SER:O	1:B:172:ILE:HG12	2.19	0.41
1:B:213:GLY:O	1:B:217:VAL:N	2.50	0.41
1:A:482:SER:O	1:A:486:ARG:HG3	2.19	0.41
1:B:163:TYR:CD1	1:B:286:VAL:HG11	2.55	0.41
1:A:475:GLY:C	1:A:478:GLY:H	2.28	0.41
1:A:108:MET:HA	1:A:111:MET:HG2	2.02	0.41
1:A:67:MET:O	1:A:70:VAL:HG12	2.20	0.41
1:B:479:VAL:CG1	1:B:480:LEU:HD12	2.51	0.41
1:A:150:GLY:HA2	1:A:153:ILE:HG12	2.02	0.41
1:B:347:VAL:O	1:B:362:ILE:HG22	2.20	0.41
1:B:374:LEU:HD23	1:B:533:LEU:HD21	2.03	0.41
1:B:426:VAL:HG11	1:B:490:ALA:HB2	2.03	0.41
1:A:548:ILE:HD13	1:A:562:HIS:N	2.36	0.41
1:B:47:LEU:HD11	1:B:70:VAL:HG12	2.02	0.40
1:B:55:GLY:HA2	1:B:59:THR:O	2.20	0.40
1:B:263:LEU:HD11	2:B:601:95X:CL01	2.58	0.40
1:B:374:LEU:CD1	1:B:382:LYS:HB2	2.51	0.40
1:A:122:GLY:O	1:A:125:LEU:N	2.55	0.40
1:B:474:ILE:HD12	1:B:481:LEU:CD1	2.52	0.40
1:A:375:VAL:O	1:A:550:VAL:HA	2.21	0.40
1:B:474:ILE:HG22	1:B:478:GLY:HA2	2.04	0.40
1:A:53:ASP:O	1:A:57:GLY:N	2.55	0.40
1:A:220:PHE:HD1	1:B:497:ARG:NE	2.20	0.40
1:B:65:VAL:O	1:B:66:TRP:C	2.63	0.40
1:B:304:VAL:O	1:B:307:GLN:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	571/599 (95%)	548 (96%)	23 (4%)	0	100	100
1	B	561/599 (94%)	522 (93%)	38 (7%)	1 (0%)	43	73
All	All	1132/1198 (94%)	1070 (94%)	61 (5%)	1 (0%)	48	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	430	ASN

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	491/511 (96%)	490 (100%)	1 (0%)	87	92
1	B	475/511 (93%)	470 (99%)	5 (1%)	65	82
All	All	966/1022 (94%)	960 (99%)	6 (1%)	78	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	530	ARG
1	B	391	ARG
1	B	424	GLN
1	B	426	VAL
1	B	427	HIS
1	B	430	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	529	ASN
1	B	240	GLN
1	B	316	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](#)

3 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	95X	A	601	-	30,30,30	0.94	0	37,43,43	1.50	6 (16%)
3	KDL	B	602	-	89,91,156	2.86	35 (39%)	123,133,201	2.29	24 (19%)
2	95X	B	601	-	30,30,30	0.96	0	37,43,43	1.36	5 (13%)

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	95X	A	601	-	-	0/13/13/13	0/3/3/3
2	95X	B	601	-	-	4/13/13/13	0/3/3/3
3	KDL	B	602	-	13/13/31/36	33/84/162/234	0/4/4/4

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	KDL	O6-CBA	11.49	1.58	1.40
3	B	602	KDL	CDO-NAO	7.62	1.50	1.34
3	B	602	KDL	C7-N2	6.10	1.54	1.34
3	B	602	KDL	C2-N2	5.97	1.55	1.45
3	B	602	KDL	OBF-CBE	5.72	1.57	1.43
3	B	602	KDL	O3-C3	5.71	1.52	1.43
3	B	602	KDL	OBH-CBG	5.63	1.52	1.44
3	B	602	KDL	OBH-CBA	5.53	1.49	1.42
3	B	602	KDL	C8-C7	5.34	1.61	1.50
3	B	602	KDL	OFZ-CGN	4.09	1.44	1.35
3	B	602	KDL	O1-C1	4.07	1.47	1.40
3	B	602	KDL	OBW-CBP	3.90	1.47	1.42
3	B	602	KDL	O1-CAV	3.67	1.50	1.43
3	B	602	KDL	CFL-CFM	3.63	1.63	1.51
3	B	602	KDL	PHG-OAM	3.55	1.65	1.59
3	B	602	KDL	CBQ-CBR	-3.52	1.47	1.53
3	B	602	KDL	CBR-CBT	-3.46	1.47	1.52
3	B	602	KDL	O5-C1	3.19	1.50	1.41
3	B	602	KDL	CFN-CFM	3.09	1.61	1.51
3	B	602	KDL	OBD-CBC	3.07	1.52	1.43
3	B	602	KDL	CGP-CGN	3.07	1.59	1.49
3	B	602	KDL	CFL-CFK	2.94	1.60	1.50
3	B	602	KDL	O6-C6	2.88	1.49	1.42
3	B	602	KDL	OAQ-CEE	2.85	1.42	1.34
3	B	602	KDL	PHC-O4	2.81	1.64	1.59
3	B	602	KDL	OAU-CAL	2.64	1.48	1.41
3	B	602	KDL	CAV-CAT	2.63	1.59	1.51
3	B	602	KDL	CAP-CAN	-2.62	1.48	1.53
3	B	602	KDL	OBW-CBV	2.57	1.47	1.44
3	B	602	KDL	CBB-CBA	2.43	1.55	1.52
3	B	602	KDL	O3-CFK	2.39	1.49	1.43
3	B	602	KDL	CAN-NAO	2.38	1.49	1.45
3	B	602	KDL	OBY-CBX	-2.23	1.38	1.43
3	B	602	KDL	CDP-CDO	2.18	1.56	1.51
3	B	602	KDL	OEC-CDO	-2.06	1.19	1.23

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	KDL	O6-CBA-CAX	-9.20	86.50	109.86
3	B	602	KDL	OBH-CBA-CBB	9.18	123.69	111.35
3	B	602	KDL	O6-CBA-OBH	-9.10	84.87	109.97
3	B	602	KDL	O6-CBA-CBB	-8.84	85.16	107.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	KDL	O3-CFK-CFL	5.66	120.66	108.77
3	B	602	KDL	OFZ-CGN-CGP	5.13	120.23	111.09
3	B	602	KDL	CAL-CAN-CAP	5.10	119.15	109.92
3	B	602	KDL	OAQ-CEE-CEF	4.73	119.91	111.43
3	B	602	KDL	OBW-CBV-CBT	4.47	114.75	108.50
3	B	602	KDL	C4-C3-C2	3.83	117.69	110.55
2	A	601	95X	C14-C15-CL02	3.81	125.08	120.54
3	B	602	KDL	C1-O5-C5	-3.55	106.79	113.72
2	B	601	95X	C03-C20-C21	-3.44	120.17	126.91
3	B	602	KDL	C1-C2-C3	3.34	115.98	109.92
2	A	601	95X	C03-C20-C21	-2.99	121.04	126.91
2	B	601	95X	C14-C15-CL02	2.91	124.01	120.54
3	B	602	KDL	OBH-CBG-CBE	2.80	112.41	108.50
2	A	601	95X	C16-C15-CL02	-2.80	112.92	118.42
3	B	602	KDL	CBB-CBA-CAX	2.68	117.45	111.39
3	B	602	KDL	C8-C7-N2	2.61	120.45	116.12
3	B	602	KDL	C1-C2-N2	-2.58	106.59	110.92
3	B	602	KDL	OBH-CBA-CAX	2.55	117.02	107.06
2	A	601	95X	C14-C19-CL01	2.51	123.31	120.37
2	A	601	95X	O03-C22-O02	2.49	127.77	122.70
2	B	601	95X	O03-C22-O02	2.42	127.62	122.70
3	B	602	KDL	OAU-CAL-CAN	2.40	115.12	110.59
3	B	602	KDL	C3-C4-C5	2.38	115.44	110.58
3	B	602	KDL	CAP-CAN-NAO	-2.26	107.30	110.91
2	A	601	95X	C13-C12-C14	-2.18	110.03	113.20
3	B	602	KDL	CFM-OFZ-CGN	-2.13	114.08	117.85
2	B	601	95X	C16-C15-CL02	-2.13	114.23	118.42
2	B	601	95X	C09-C08-C07	2.11	122.77	120.09
3	B	602	KDL	OCA-CBZ-CBX	-2.08	106.78	111.16
3	B	602	KDL	OES-CEE-CEF	-2.07	119.84	124.65
3	B	602	KDL	CDP-CDO-NAO	2.00	118.99	116.25

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	602	KDL	CAP
3	B	602	KDL	C2
3	B	602	KDL	C4
3	B	602	KDL	CAN
3	B	602	KDL	CAT
3	B	602	KDL	CBI
3	B	602	KDL	CEG

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Mol	Chain	Res	Type	Atom
3	B	602	KDL	CBR
3	B	602	KDL	CBX
3	B	602	KDL	C3
3	B	602	KDL	CBV
3	B	602	KDL	C1
3	B	602	KDL	C5

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	KDL	C1-C2-N2-C7
3	B	602	KDL	C2-C3-O3-CFK
3	B	602	KDL	OAU-CAL-OAM-PHG
3	B	602	KDL	OAZ-CAX-CBA-CBB
3	B	602	KDL	CBB-CBC-OB-DBP
3	B	602	KDL	CBE-CBC-OB-DBP
3	B	602	KDL	OBH-CBG-CBI-OB
3	B	602	KDL	CBG-CBI-CBK-OBL
3	B	602	KDL	OBJ-CBI-CBK-OBL
3	B	602	KDL	CBT-CBV-CBX-OB
3	B	602	KDL	OBW-CBV-CBX-CB
3	B	602	KDL	OBW-CBV-CBX-OB
3	B	602	KDL	CEF-CEE-OAQ-CAP
3	B	602	KDL	CFL-CFK-O3-C3
3	B	602	KDL	OFZ-CFM-CFN-CFO
3	B	602	KDL	OES-CEE-OAQ-CAP
3	B	602	KDL	CGP-CGN-OFZ-CFM
3	B	602	KDL	O5-C1-O1-CAV
3	B	602	KDL	C8-C7-N2-C2
3	B	602	KDL	O7-C7-N2-C2
3	B	602	KDL	OGO-CGN-OFZ-CFM
3	B	602	KDL	CFL-CFM-CFN-CFO
3	B	602	KDL	CEG-CEH-CEI-CEJ
3	B	602	KDL	CAP-CAN-NAO-CDO
3	B	602	KDL	CBT-CBV-CBX-CB
2	B	601	95X	C20-C21-C22-O02
3	B	602	KDL	CFM-CFN-CFO-CFP
3	B	602	KDL	C3-C2-N2-C7
3	B	602	KDL	CDO-CDP-CDQ-CDR
2	B	601	95X	C20-C21-C22-O03
2	B	601	95X	C04-C03-C20-C21
2	B	601	95X	C02-C03-C20-C21

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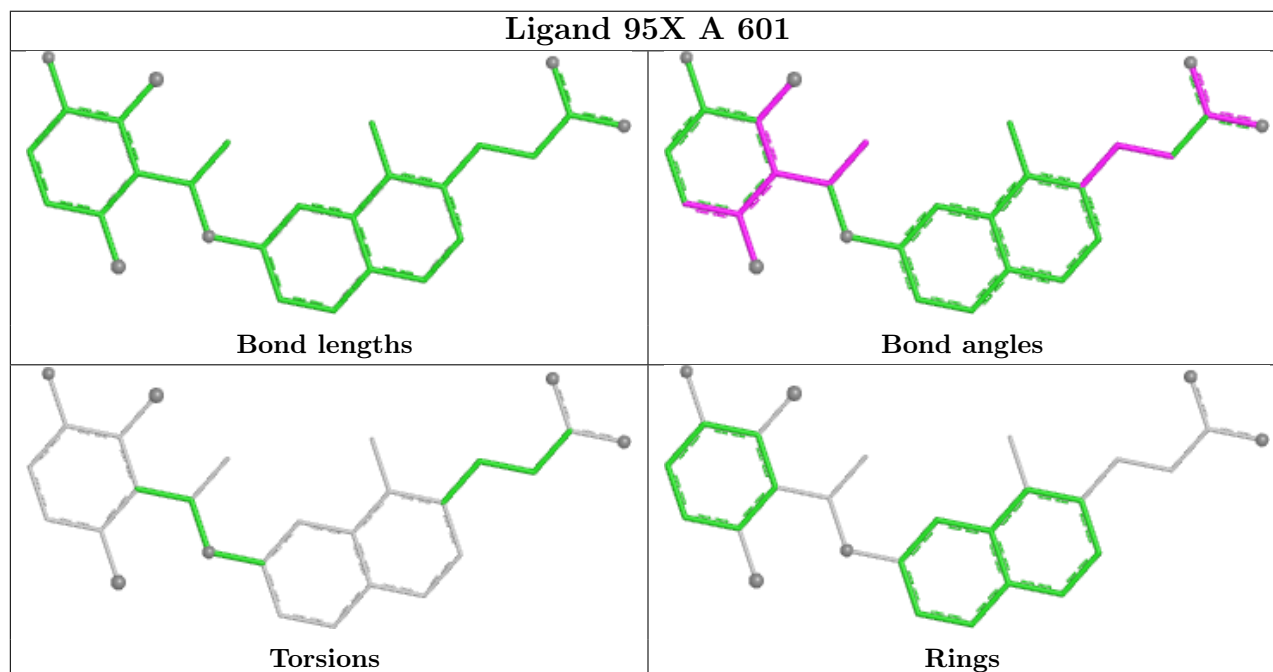
Mol	Chain	Res	Type	Atoms
3	B	602	KDL	OAY-CAX-CBA-O6
3	B	602	KDL	CBE-CBG-CBI-OBJ
3	B	602	KDL	CAN-CAP-OAQ-CEE
3	B	602	KDL	C5-C6-O6-CBA
3	B	602	KDL	C3-C4-O4-PHC

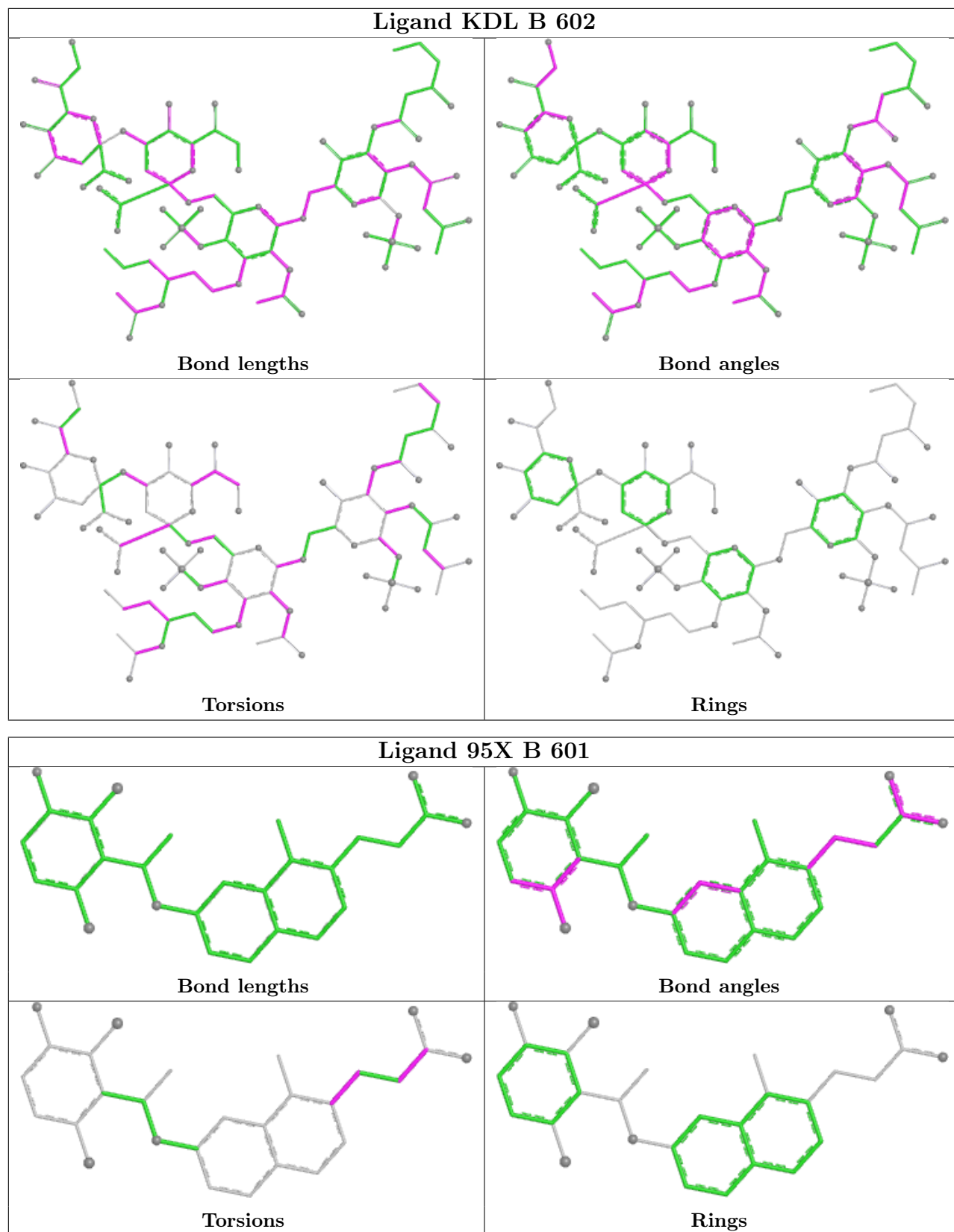
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	KDL	1	0
2	B	601	95X	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.





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	575/599 (95%)	0.27	19 (3%) 49 32	36, 68, 120, 147	0
1	B	565/599 (94%)	0.35	25 (4%) 39 24	37, 77, 117, 164	0
All	All	1140/1198 (95%)	0.31	44 (3%) 43 27	36, 73, 120, 164	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	575	LEU	5.8
1	B	561	THR	4.7
1	B	474	ILE	4.5
1	B	478	GLY	4.4
1	B	579	GLN	3.8
1	B	65	VAL	3.5
1	A	480	LEU	3.3
1	A	341	ASP	3.1
1	B	185	VAL	3.0
1	A	65	VAL	3.0
1	A	482	SER	3.0
1	B	562	HIS	3.0
1	A	512	ASP	2.9
1	B	184	VAL	2.8
1	B	428	LEU	2.8
1	A	556	ILE	2.8
1	B	479	VAL	2.7
1	B	475	GLY	2.7
1	B	557	VAL	2.6
1	B	470	LEU	2.5
1	A	4	ASP	2.5
1	A	575	LEU	2.5
1	B	378	SER	2.5
1	B	565	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	338	ALA	2.4
1	A	128	ILE	2.4
1	A	571	VAL	2.4
1	A	568	HIS	2.4
1	A	64	LEU	2.3
1	B	73	GLY	2.3
1	B	189	PHE	2.2
1	A	559	ARG	2.2
1	A	54	ASP	2.2
1	B	375	VAL	2.1
1	A	461	ASP	2.1
1	B	566	LEU	2.1
1	A	572	TYR	2.1
1	A	195	ASN	2.1
1	A	481	LEU	2.1
1	B	170	ILE	2.1
1	B	203	VAL	2.0
1	B	167	LEU	2.0
1	A	558	GLU	2.0
1	B	572	TYR	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](#)

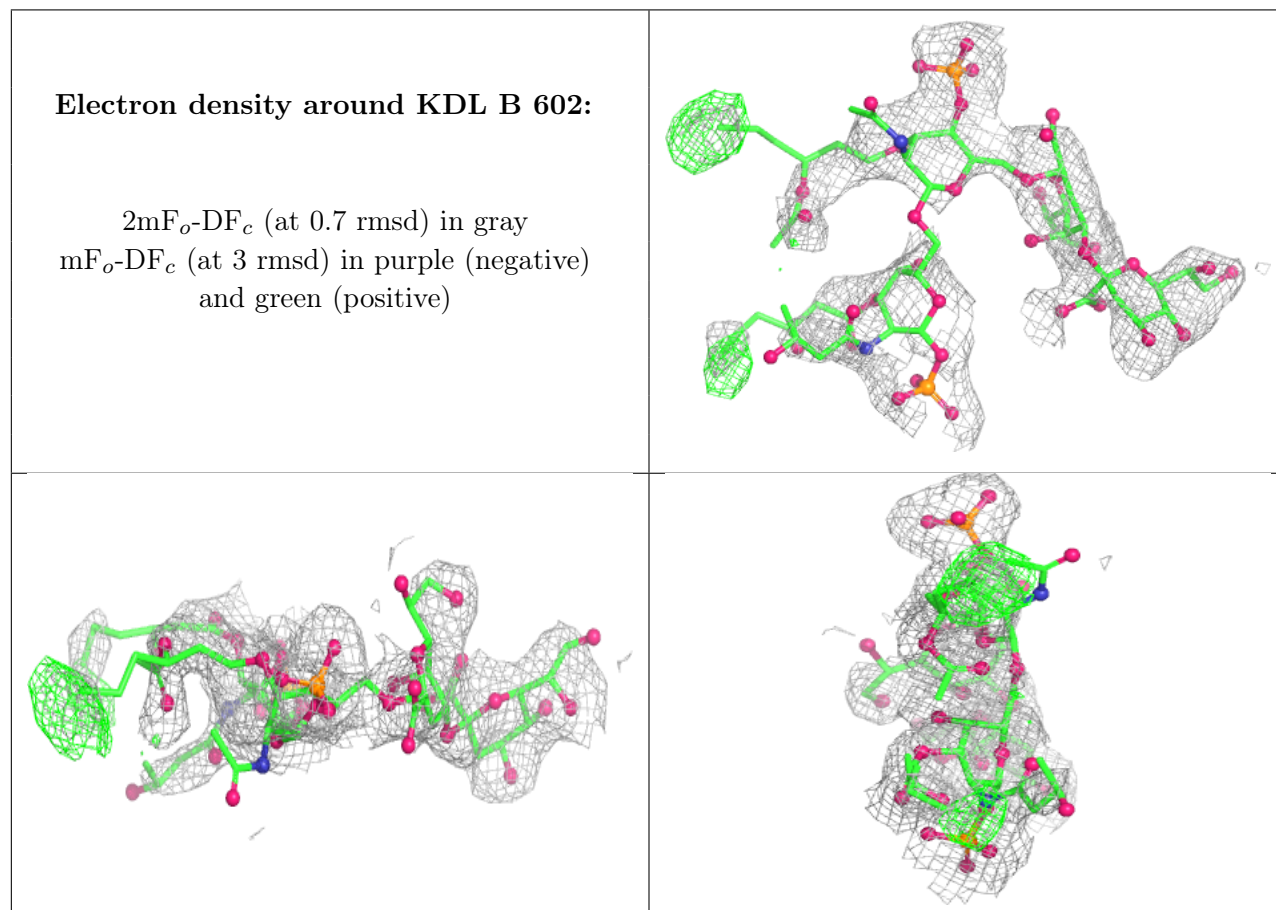
There are no oligosaccharides in this entry.

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.

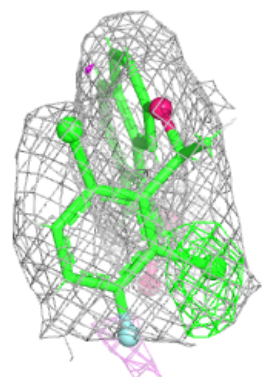
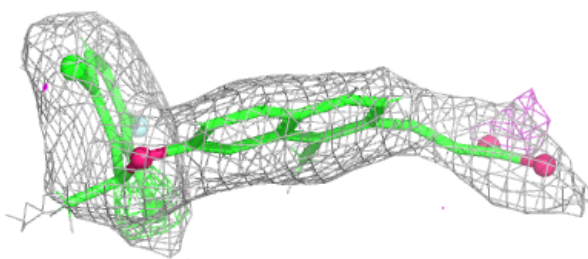
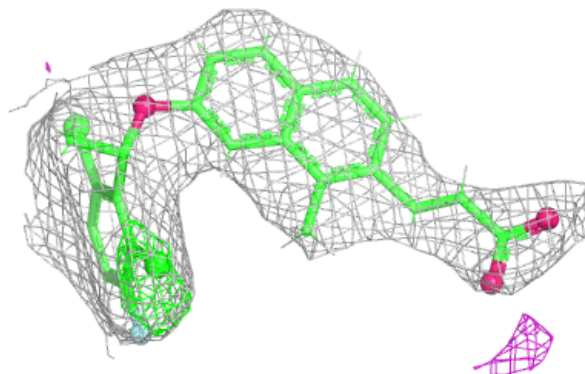
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	KDL	B	602	88/153	0.62	0.18	63,119,141,148	0
2	95X	A	601	28/28	0.84	0.14	33,49,75,169	0
2	95X	B	601	28/28	0.88	0.14	50,69,91,96	0

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.

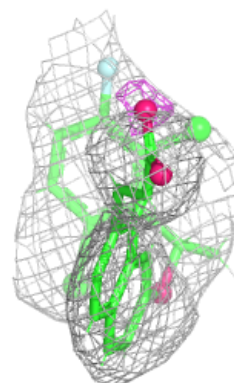
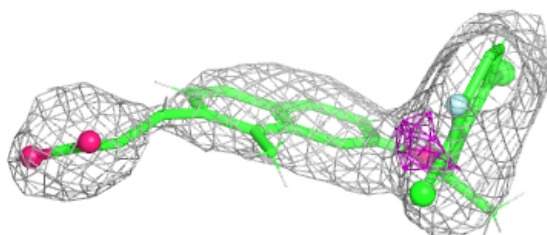
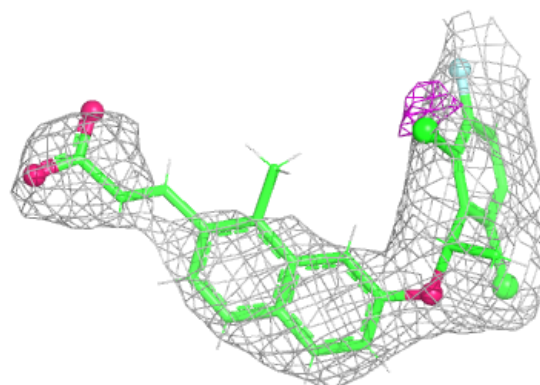


Electron density around 95X A 601:

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

**Electron density around 95X B 601:**

$2mF_o-DF_c$ (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.