



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2020 – 10:38 AM BST

PDB ID : 3LJZ
Title : Crystal Structure of Human MMP-13 complexed with an Amino-2-indanol compound
Authors : Shieh, H.-S.; Kiefer, J.R.
Deposited on : 2010-01-26
Resolution : 2.00 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 : 2.13
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) : 2.13

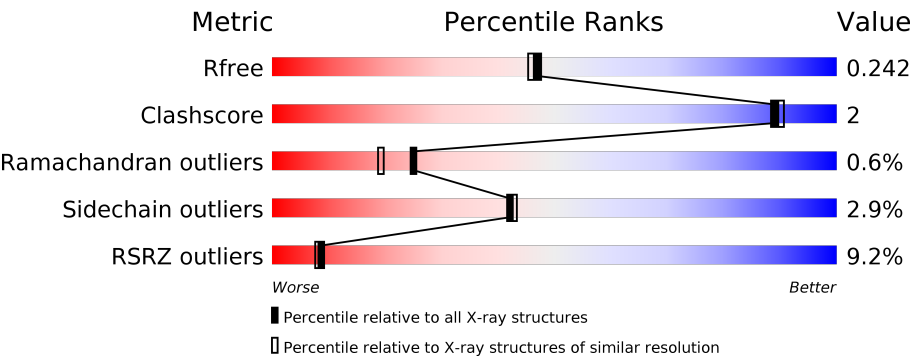
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	164	<div><div>10%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>96%</div><div><div></div><div></div></div><div>..</div></div>
1	B	164	<div><div>7%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>94%</div><div><div></div><div></div><div></div></div><div>5% ..</div></div>
1	C	164	<div><div>12%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>94%</div><div><div></div><div></div><div></div></div><div>5% .</div></div>
1	D	164	<div><div>9%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>95%</div><div><div></div><div></div><div></div></div><div>..</div></div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	D	9	-	-	-	X
6	EPE	C	1	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5778 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 Collagenase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	0	0
			1285	833	208	239	5			
1	B	164	Total	C	N	O	S	0	0	0
			1299	841	211	242	5			
1	C	164	Total	C	N	O	S	0	0	0
			1288	835	206	242	5			
1	D	164	Total	C	N	O	S	0	0	0
			1300	841	211	243	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	ALA	TYR	ENGINEERED MUTATION	UNP P45452
B	104	ALA	TYR	ENGINEERED MUTATION	UNP P45452
C	104	ALA	TYR	ENGINEERED MUTATION	UNP P45452
D	104	ALA	TYR	ENGINEERED MUTATION	UNP P45452

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		
2	D	2	Total	Ca	0	0
			2	2		
2	C	2	Total	Ca	0	0
			2	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	Zn 2	0	0
3	A	2	Total 2	Zn 2	0	0
3	D	2	Total 2	Zn 2	0	0
3	C	2	Total 2	Zn 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



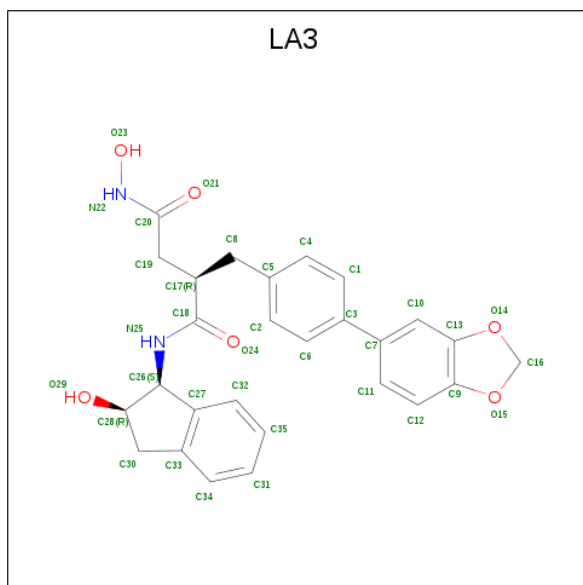
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	S 1	0	0
4	A	1	Total 5	O 4	S 1	0	0
4	B	1	Total 5	O 4	S 1	0	0
4	B	1	Total 5	O 4	S 1	0	0
4	C	1	Total 5	O 4	S 1	0	0
4	C	1	Total 5	O 4	S 1	0	0
4	D	1	Total 5	O 4	S 1	0	0
4	D	1	Total 5	O 4	S 1	0	0

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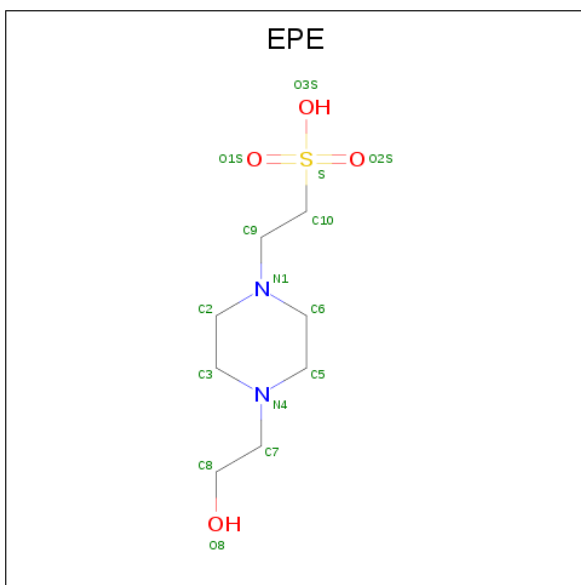
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is (2R)-2-[4-(1,3-benzodioxol-5-yl)benzyl]-N 4 -hydroxy-N 1 -[(1S,2R)-2-hydroxy-2,3-dihydro-1H-inden-1-yl]butanediamide (three-letter code: LA3) (formula: C₂₇H₂₆N₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			35	27	2	6		
5	B	1	Total	C	N	O	0	0
			35	27	2	6		
5	C	1	Total	C	N	O	0	0
			35	27	2	6		
5	D	1	Total	C	N	O	0	0
			35	27	2	6		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

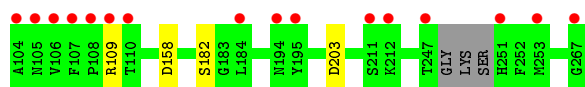
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	85	Total	O	0	0
			85	85		
7	B	97	Total	O	0	0
			97	97		
7	C	75	Total	O	0	0
			75	75		
7	D	88	Total	O	0	0
			88	88		

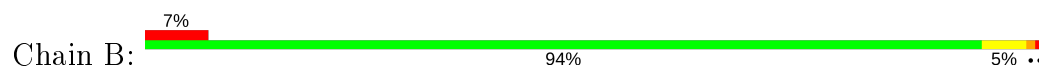
3 Residue-property plots [i](#)

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.

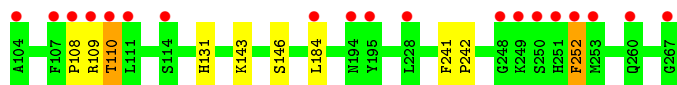
- Molecule 1: Collagenase 3



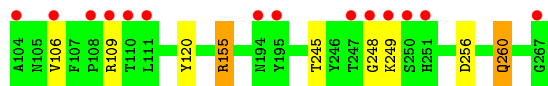
- Molecule 1: Collagenase 3



- Molecule 1: Collagenase 3



- Molecule 1: Collagenase 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.60 Å 94.93 Å 120.41 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.00 19.94 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.0 (19.94-2.00) 93.0 (19.94-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.01 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.202 , 0.228 0.216 , 0.242	Depositor DCC
R_{free} test set	2727 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	14.3	Xtriage
Anisotropy	0.939	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5778	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.20 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5799e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: LA3, ZN, EPE, CA, SO4

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	0.48	0/1330	0.56	0/1806
1	B	0.49	0/1344	0.60	2/1825 (0.1%)
1	C	0.46	0/1331	0.56	0/1807
1	D	0.51	0/1346	0.57	0/1829
All	All	0.48	0/5351	0.57	2/7267 (0.0%)

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	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	LEU	CA-CB-CG	5.12	127.09	115.30
1	B	155	ARG	NE-CZ-NH1	-5.11	117.74	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	250	SER	Peptide
1	D	248	GLY	Peptide

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	1285	0	1200	0	0
1	B	1299	0	1207	2	0
1	C	1288	0	1190	6	0
1	D	1300	0	1211	5	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	15	0	0	0	0
5	A	35	0	25	1	0
5	B	35	0	25	1	0
5	C	35	0	25	1	0
5	D	35	0	25	1	0
6	B	15	0	18	3	0
6	C	15	0	17	2	0
6	D	30	0	34	1	0
7	A	85	0	0	0	0
7	B	97	0	0	2	0
7	C	75	0	0	0	0
7	D	88	0	0	2	0
All	All	5778	0	4977	20	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 2.

All (20) 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:3:EPE:O1S	7:B:87:HOH:O	1.86	0.92
1:C:184:LEU:HD21	6:C:1:EPE:O2S	1.85	0.77
1:D:106:VAL:HG13	7:D:353:HOH:O	1.92	0.68
1:C:110:THR:HG22	1:C:110:THR:O	1.94	0.67
6:B:3:EPE:H21	7:B:277:HOH:O	2.02	0.57
1:B:249:LYS:O	1:B:250:SER:CB	2.54	0.55
1:C:184:LEU:CD2	6:C:1:EPE:O2S	2.54	0.54
1:C:108:PRO:HA	1:C:109:ARG:N	2.27	0.49
1:D:120:TYR:CE1	1:D:155:ARG:HG3	2.46	0.49
1:D:106:VAL:CG1	7:D:353:HOH:O	2.58	0.47
1:D:256:ASP:OD1	1:D:260:GLN:NE2	2.50	0.45
1:C:241:PHE:CD1	1:C:242:PRO:HD2	2.53	0.44
1:C:143:LYS:HA	1:C:146:SER:OG	2.18	0.43
1:B:176:TYR:OH	6:B:3:EPE:H22	2.19	0.43
5:C:803:LA3:H1	5:C:803:LA3:H11	1.84	0.42
6:D:4:EPE:H101	6:D:4:EPE:H21	1.93	0.40
5:D:804:LA3:H11	5:D:804:LA3:H1	1.89	0.40
5:B:802:LA3:H17	5:B:802:LA3:H4	1.91	0.40
5:A:801:LA3:H1	5:A:801:LA3:H11	1.86	0.40
1:D:120:TYR:CZ	1:D:155:ARG:HG3	2.57	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	157/164 (96%)	152 (97%)	5 (3%)	0	100	100
1	B	160/164 (98%)	153 (96%)	5 (3%)	2 (1%)	12	6
1	C	158/164 (96%)	150 (95%)	7 (4%)	1 (1%)	25	19
1	D	162/164 (99%)	155 (96%)	6 (4%)	1 (1%)	25	19
All	All	637/656 (97%)	610 (96%)	23 (4%)	4 (1%)	25	19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	249	LYS
1	B	250	SER
1	C	252	PHE
1	B	253	MET

5.3.2 Protein sidechains ⓘ

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	137/139 (99%)	133 (97%)	4 (3%)	42	43
1	B	137/139 (99%)	132 (96%)	5 (4%)	35	34
1	C	135/139 (97%)	132 (98%)	3 (2%)	52	55
1	D	138/139 (99%)	134 (97%)	4 (3%)	42	43
All	All	547/556 (98%)	531 (97%)	16 (3%)	42	43

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	ARG
1	A	158	ASP
1	A	182	SER
1	A	203	ASP
1	B	112	LYS
1	B	184	LEU
1	B	203	ASP
1	B	247	THR
1	B	252	PHE
1	C	110	THR
1	C	131	HIS
1	C	252	PHE
1	D	109	ARG
1	D	155	ARG
1	D	245	THR
1	D	260	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	HIS
1	B	105	ASN
1	B	187	HIS
1	D	260	GLN
1	D	263	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 33 ligands modelled in this entry, 16 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	C	7	-	4,4,4	0.18	0	6,6,6	0.12	0
4	SO4	B	2	-	4,4,4	0.15	0	6,6,6	0.21	0
5	LA3	D	804	3	39,39,39	1.18	3 (7%)	52,55,55	1.89	9 (17%)
6	EPE	C	1	-	15,15,15	0.88	1 (6%)	18,20,20	1.10	1 (5%)
6	EPE	B	3	-	15,15,15	0.84	1 (6%)	18,20,20	1.28	2 (11%)
6	EPE	D	2	-	15,15,15	0.88	1 (6%)	18,20,20	1.19	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	D	8	-	4,4,4	0.20	0	6,6,6	0.24	0
5	LA3	A	801	3	39,39,39	1.22	2 (5%)	52,55,55	2.00	13 (25%)
4	SO4	D	9	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	A	5	-	4,4,4	0.21	0	6,6,6	0.28	0
6	EPE	D	4	-	15,15,15	1.00	1 (6%)	18,20,20	1.78	4 (22%)
4	SO4	A	1	-	4,4,4	0.13	0	6,6,6	0.32	0
5	LA3	B	802	3	39,39,39	1.24	3 (7%)	52,55,55	1.88	13 (25%)
4	SO4	D	268	-	4,4,4	0.11	0	6,6,6	0.31	0
4	SO4	B	6	-	4,4,4	0.18	0	6,6,6	0.37	0
5	LA3	C	803	3	39,39,39	1.05	2 (5%)	52,55,55	1.82	11 (21%)
4	SO4	C	3	-	4,4,4	0.14	0	6,6,6	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LA3	D	804	3	-	4/22/40/40	0/5/5/5
6	EPE	C	1	-	-	4/9/19/19	0/1/1/1
6	EPE	B	3	-	-	4/9/19/19	0/1/1/1
5	LA3	A	801	3	-	5/22/40/40	0/5/5/5
6	EPE	D	4	-	-	7/9/19/19	0/1/1/1
6	EPE	D	2	-	-	4/9/19/19	0/1/1/1
5	LA3	B	802	3	-	6/22/40/40	0/5/5/5
5	LA3	C	803	3	-	4/22/40/40	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	804	LA3	C20-N22	5.26	1.38	1.32
5	A	801	LA3	C20-N22	5.11	1.37	1.32
5	C	803	LA3	C20-N22	4.69	1.37	1.32
5	B	802	LA3	C20-N22	4.52	1.37	1.32
6	D	4	EPE	C10-S	3.23	1.82	1.77
6	C	1	EPE	C10-S	3.06	1.81	1.77
5	B	802	LA3	C28-C26	-3.04	1.52	1.55
6	D	2	EPE	C10-S	3.02	1.81	1.77
5	A	801	LA3	C28-C26	-3.01	1.52	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	802	LA3	C27-C26	-3.00	1.48	1.51
6	B	3	EPE	C10-S	2.78	1.81	1.77
5	D	804	LA3	C27-C26	-2.50	1.49	1.51
5	C	803	LA3	C18-N25	2.40	1.39	1.34
5	D	804	LA3	C28-C26	-2.22	1.52	1.55

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	803	LA3	O23-N22-C20	-6.90	109.60	119.79
5	D	804	LA3	O23-N22-C20	-6.80	109.74	119.79
5	A	801	LA3	O23-N22-C20	-6.13	110.73	119.79
5	D	804	LA3	C30-C28-C26	5.76	108.70	103.78
5	B	802	LA3	O23-N22-C20	-5.03	112.36	119.79
5	B	802	LA3	C19-C17-C18	-4.91	102.66	109.77
5	A	801	LA3	C30-C28-C26	4.10	107.28	103.78
5	D	804	LA3	C19-C17-C18	-3.98	104.01	109.77
5	A	801	LA3	C33-C30-C28	-3.96	99.69	103.50
5	A	801	LA3	C16-O15-C9	-3.86	100.33	105.34
5	B	802	LA3	C33-C30-C28	-3.84	99.81	103.50
5	A	801	LA3	C27-C26-C28	-3.81	99.87	102.58
5	C	803	LA3	C16-O15-C9	-3.76	100.45	105.34
5	A	801	LA3	C16-O14-C13	-3.70	100.54	105.34
6	D	4	EPE	O2S-S-C10	3.66	111.32	106.92
5	D	804	LA3	C16-O14-C13	-3.64	100.61	105.34
5	C	803	LA3	C16-O14-C13	-3.59	100.68	105.34
5	B	802	LA3	C16-O14-C13	-3.59	100.68	105.34
5	A	801	LA3	O15-C16-O14	3.57	113.78	108.08
5	D	804	LA3	C16-O15-C9	-3.56	100.71	105.34
5	B	802	LA3	C16-O15-C9	-3.56	100.72	105.34
6	D	2	EPE	O3S-S-C10	3.46	111.37	105.77
5	C	803	LA3	O15-C16-O14	3.46	113.60	108.08
5	C	803	LA3	C30-C28-C26	3.30	106.60	103.78
5	B	802	LA3	O15-C16-O14	3.27	113.30	108.08
5	B	802	LA3	C35-C32-C27	-3.18	116.97	121.01
5	A	801	LA3	C19-C17-C18	-3.17	105.18	109.77
5	B	802	LA3	O15-C9-C13	3.03	113.24	109.78
6	D	4	EPE	C2-C3-N4	3.03	116.86	110.64
5	D	804	LA3	O15-C16-O14	2.97	112.83	108.08
5	A	801	LA3	O15-C9-C13	2.93	113.11	109.78
6	C	1	EPE	O3S-S-C10	2.92	110.50	105.77
5	B	802	LA3	C27-C26-C28	-2.87	100.54	102.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	4	EPE	C9-N1-C2	2.83	118.48	111.23
6	D	4	EPE	O3S-S-C10	2.83	110.34	105.77
5	A	801	LA3	O29-C28-C30	-2.80	104.00	110.74
5	C	803	LA3	O15-C9-C13	2.73	112.89	109.78
5	A	801	LA3	C35-C32-C27	-2.58	117.73	121.01
5	C	803	LA3	C17-C18-N25	-2.56	111.77	116.21
5	C	803	LA3	C19-C20-N22	-2.45	111.44	115.14
5	D	804	LA3	O15-C9-C13	2.36	112.47	109.78
5	B	802	LA3	C31-C34-C33	-2.33	117.42	120.89
5	D	804	LA3	C19-C20-N22	-2.32	111.63	115.14
5	B	802	LA3	C19-C20-N22	-2.24	111.74	115.14
5	B	802	LA3	O21-C20-N22	2.24	126.02	123.27
6	B	3	EPE	O1S-S-C10	2.23	109.60	106.92
5	D	804	LA3	C27-C26-N25	2.16	118.07	114.61
5	A	801	LA3	C17-C18-N25	-2.15	112.50	116.21
5	C	803	LA3	C19-C17-C18	-2.13	106.68	109.77
5	A	801	LA3	O14-C13-C9	2.13	112.21	109.78
5	C	803	LA3	O21-C20-C19	2.12	124.61	121.50
5	B	802	LA3	C30-C28-C26	2.04	105.52	103.78
5	C	803	LA3	C11-C12-C9	-2.02	116.20	120.06
6	B	3	EPE	O3S-S-C10	2.01	109.02	105.77

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	804	LA3	C18-C17-C8-C5
5	C	803	LA3	C18-C17-C8-C5
6	D	4	EPE	C10-C9-N1-C2
6	D	4	EPE	C8-C7-N4-C5
6	D	4	EPE	S-C10-C9-N1
6	D	4	EPE	C9-C10-S-O2S
6	D	2	EPE	C9-C10-S-O1S
6	D	2	EPE	C9-C10-S-O2S
6	D	2	EPE	C9-C10-S-O3S
6	C	1	EPE	C9-C10-S-O1S
6	C	1	EPE	C9-C10-S-O2S
6	C	1	EPE	C9-C10-S-O3S
5	B	802	LA3	C18-C17-C8-C5
5	B	802	LA3	C19-C20-N22-O23
5	B	802	LA3	O21-C20-N22-O23
5	A	801	LA3	C19-C20-N22-O23

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Mol	Chain	Res	Type	Atoms
5	A	801	LA3	O21-C20-N22-O23
6	D	4	EPE	C9-C10-S-O3S
6	B	3	EPE	C9-C10-S-O3S
6	C	1	EPE	N4-C7-C8-O8
6	B	3	EPE	N4-C7-C8-O8
5	B	802	LA3	C4-C5-C8-C17
5	A	801	LA3	C4-C5-C8-C17
5	B	802	LA3	C2-C5-C8-C17
5	A	801	LA3	C2-C5-C8-C17
5	D	804	LA3	C4-C5-C8-C17
5	C	803	LA3	C4-C5-C8-C17
5	D	804	LA3	C2-C5-C8-C17
5	C	803	LA3	C2-C5-C8-C17
5	C	803	LA3	C19-C17-C8-C5
6	D	4	EPE	C9-C10-S-O1S
6	B	3	EPE	C9-C10-S-O1S
6	B	3	EPE	C9-C10-S-O2S
5	A	801	LA3	C18-C17-C8-C5
6	D	4	EPE	C10-C9-N1-C6
5	D	804	LA3	C19-C17-C8-C5
5	B	802	LA3	C19-C17-C8-C5
6	D	2	EPE	N4-C7-C8-O8

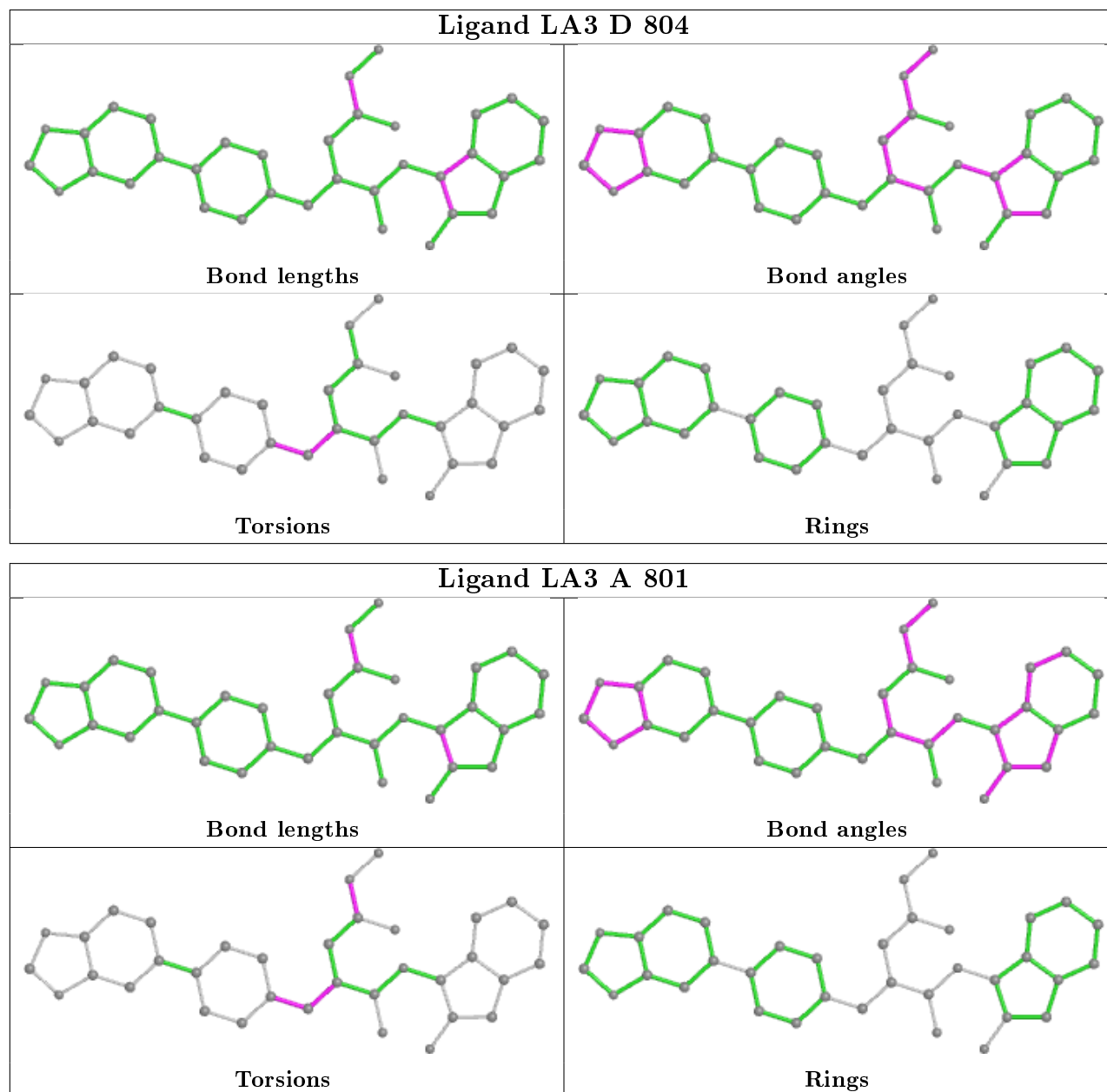
There are no ring outliers.

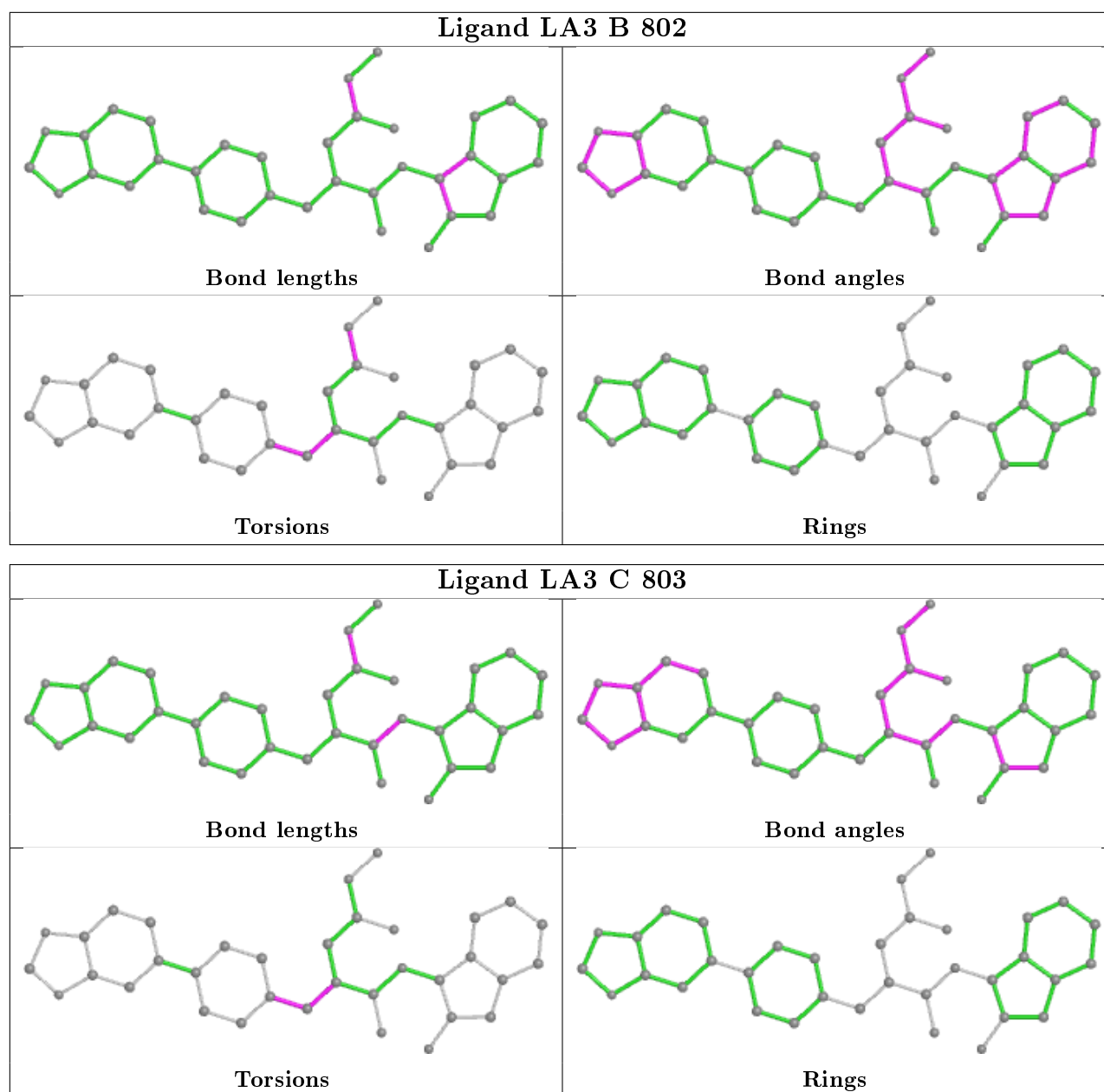
7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	804	LA3	1	0
6	C	1	EPE	2	0
6	B	3	EPE	3	0
5	A	801	LA3	1	0
6	D	4	EPE	1	0
5	B	802	LA3	1	0
5	C	803	LA3	1	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	248:GLY	C	249:LYS	N	3.16
1	C	108:PRO	C	109:ARG	N	2.83
1	C	248:GLY	C	249:LYS	N	2.78

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	161/164 (98%)	0.49	16 (9%) 7 6	12, 23, 46, 94	0
1	B	164/164 (100%)	0.33	11 (6%) 17 17	10, 20, 46, 70	0
1	C	164/164 (100%)	0.59	19 (11%) 4 4	12, 25, 58, 103	0
1	D	164/164 (100%)	0.34	14 (8%) 10 10	10, 20, 52, 81	0
All	All	653/656 (99%)	0.44	60 (9%) 9 8	10, 22, 52, 103	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	110	THR	11.5
1	C	250	SER	9.6
1	C	109	ARG	8.8
1	A	251	HIS	8.1
1	B	251	HIS	8.0
1	D	110	THR	6.6
1	B	248	GLY	6.1
1	D	250	SER	5.9
1	C	251	HIS	5.7
1	C	267	GLY	5.4
1	B	250	SER	5.4
1	C	108	PRO	5.3
1	A	104	ALA	5.2
1	D	249	LYS	5.1
1	D	109	ARG	4.8
1	A	108	PRO	4.7
1	D	248	GLY	4.6
1	A	107	PHE	4.6
1	B	267	GLY	4.5
1	D	251	HIS	4.2
1	B	249	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	267	GLY	3.9
1	A	267	GLY	3.6
1	C	104	ALA	3.5
1	A	105	ASN	3.4
1	A	184	LEU	3.3
1	B	108	PRO	3.2
1	D	195	TYR	3.1
1	C	107	PHE	3.1
1	A	109	ARG	3.1
1	D	108	PRO	3.1
1	A	247	THR	3.0
1	B	253	MET	2.9
1	A	253	MET	2.9
1	C	249	LYS	2.9
1	A	211	SER	2.9
1	C	194	ASN	2.8
1	A	212	LYS	2.7
1	C	260	GLN	2.7
1	C	111	LEU	2.7
1	D	247	THR	2.7
1	C	253	MET	2.6
1	C	252	PHE	2.6
1	A	195	TYR	2.6
1	B	109	ARG	2.6
1	A	110	THR	2.6
1	C	184	LEU	2.4
1	D	104	ALA	2.4
1	D	111	LEU	2.4
1	C	228	LEU	2.4
1	D	194	ASN	2.3
1	A	106	VAL	2.3
1	A	194	ASN	2.2
1	B	252	PHE	2.2
1	C	248	GLY	2.1
1	C	114	SER	2.1
1	B	228	LEU	2.0
1	D	106	VAL	2.0
1	C	195	TYR	2.0
1	B	225	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
6	EPE	C	1	15/15	0.37	0.42	78,78,80,80	0
6	EPE	D	2	15/15	0.49	0.40	76,78,80,80	0
6	EPE	D	4	15/15	0.52	0.33	30,44,60,60	0
6	EPE	B	3	15/15	0.55	0.37	58,59,64,64	0
4	SO4	D	9	5/5	0.74	0.54	97,97,97,98	0
5	LA3	D	804	35/35	0.83	0.16	18,24,35,35	0
2	CA	C	996	1/1	0.85	0.27	60,60,60,60	0
4	SO4	A	1	5/5	0.86	0.27	43,45,46,46	0
5	LA3	C	803	35/35	0.88	0.15	24,29,33,34	0
5	LA3	A	801	35/35	0.90	0.15	20,29,40,40	0
4	SO4	C	7	5/5	0.92	0.24	58,58,59,59	0
4	SO4	A	5	5/5	0.93	0.36	47,47,47,48	0
5	LA3	B	802	35/35	0.93	0.12	15,21,28,31	0
2	CA	D	996	1/1	0.94	0.36	52,52,52,52	0
4	SO4	C	3	5/5	0.95	0.18	44,45,46,47	0
4	SO4	B	6	5/5	0.96	0.24	32,32,35,37	0
4	SO4	B	2	5/5	0.96	0.23	45,45,46,47	0
2	CA	C	997	1/1	0.96	0.07	24,24,24,24	0
4	SO4	D	8	5/5	0.96	0.26	50,51,51,51	0
2	CA	A	997	1/1	0.97	0.05	27,27,27,27	0
4	SO4	D	268	5/5	0.97	0.18	40,40,41,41	0
2	CA	A	996	1/1	0.98	0.33	53,53,53,53	0
2	CA	B	996	1/1	0.98	0.19	42,42,42,42	0
3	ZN	D	999	1/1	0.99	0.07	16,16,16,16	0
3	ZN	C	998	1/1	0.99	0.06	15,15,15,15	0
2	CA	B	997	1/1	0.99	0.05	15,15,15,15	0
3	ZN	C	999	1/1	0.99	0.05	23,23,23,23	0

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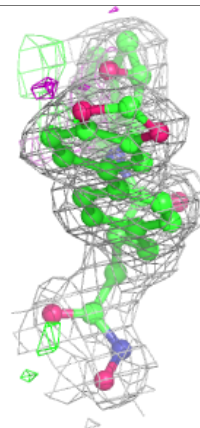
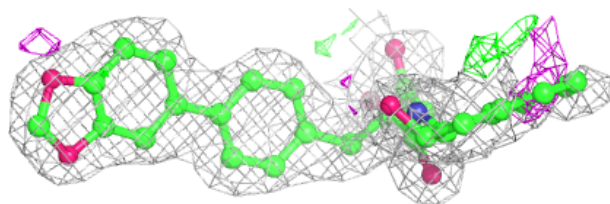
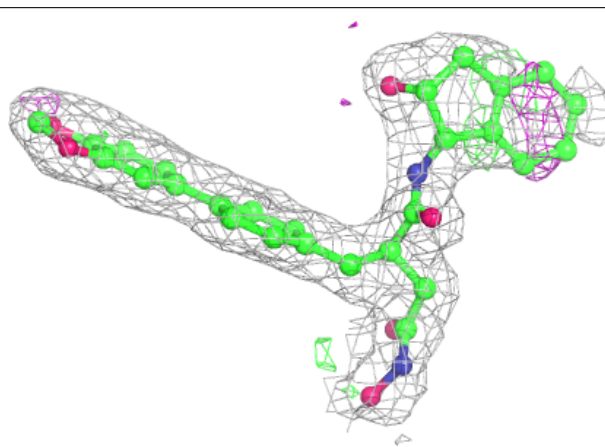
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CA	D	997	1/1	1.00	0.06	13,13,13,13	0
3	ZN	A	999	1/1	1.00	0.06	20,20,20,20	0
3	ZN	A	998	1/1	1.00	0.07	14,14,14,14	0
3	ZN	B	999	1/1	1.00	0.06	14,14,14,14	0
3	ZN	B	998	1/1	1.00	0.07	12,12,12,12	0
3	ZN	D	998	1/1	1.00	0.07	12,12,12,12	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.

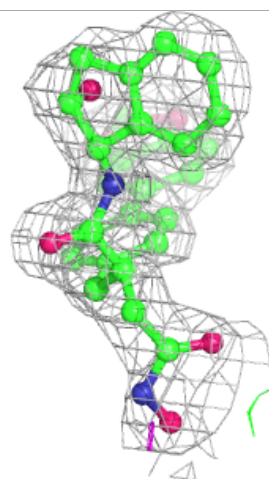
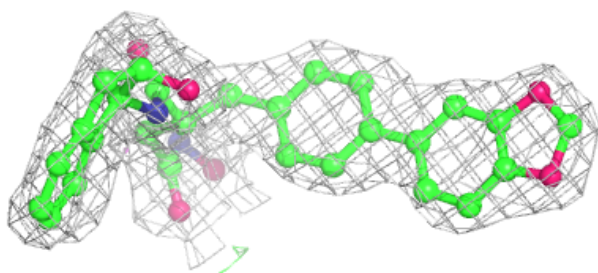
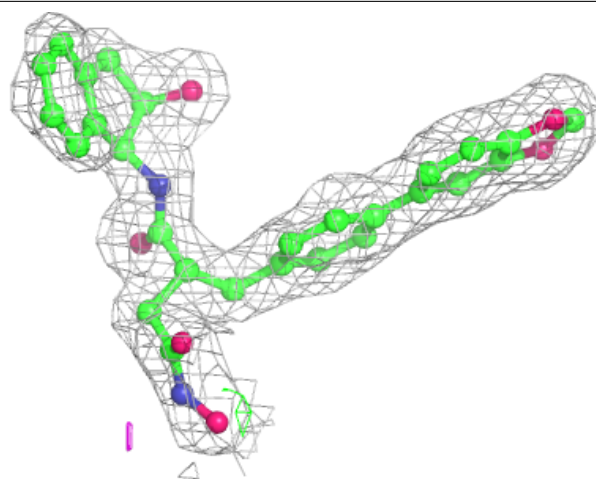
Electron density around LA3 D 804:

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



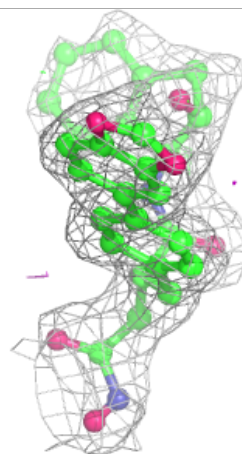
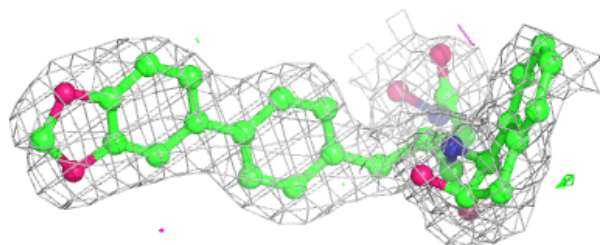
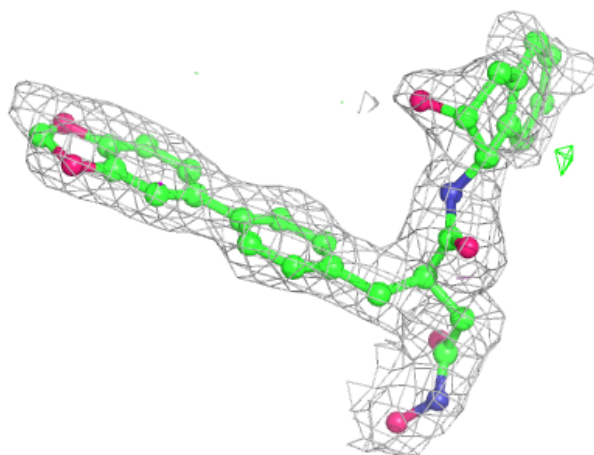
Electron density around LA3 C 803:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



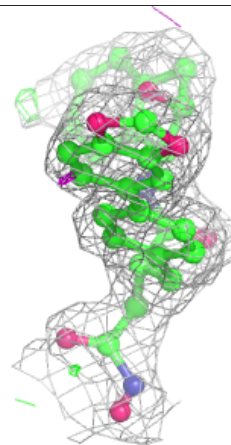
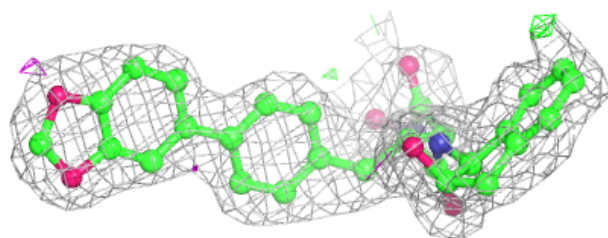
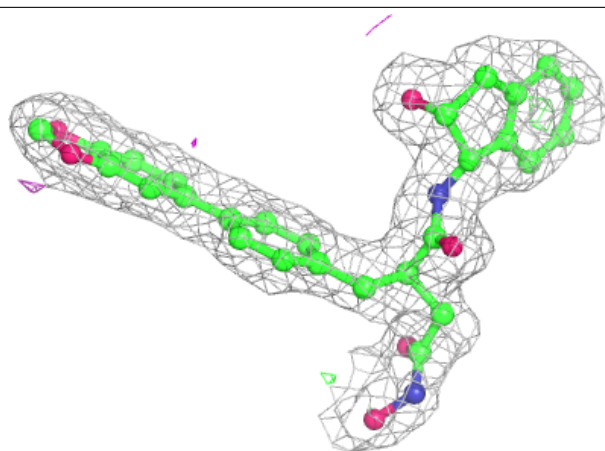
Electron density around LA3 A 801:

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



Electron density around LA3 B 802:

$2mF_o-DF_c$ (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.