



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:00 PM UTC

PDB ID : 4UF0 / pdb_00004uf0
Title : Crystal structure of JmjC domain of human histone demethylase UTY in complex with epitherapeutic compound 2-(((2-((2-(dimethylamino)ethyl) (ethyl)amino)-2-oxoethyl)amino)methyl)isonicotinic acid.
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Deposited on : 2014-12-22
Resolution : 1.78 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](#) ①) 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

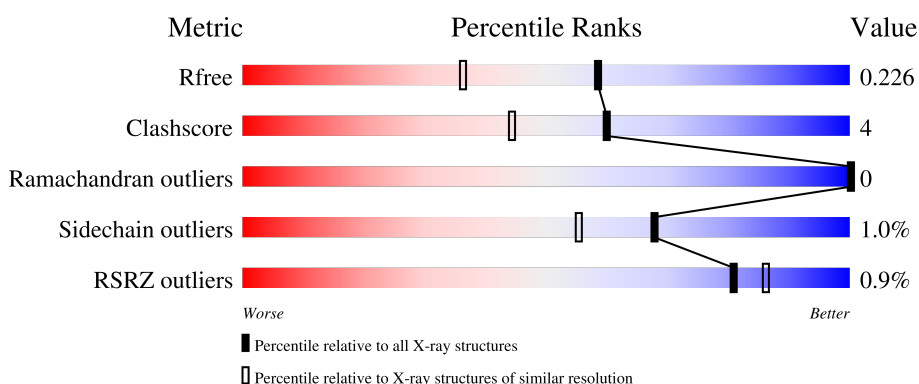
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	478	% 86% 7% 7%
2	B	478	% 83% 9% 8%

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
4	MMK	A	2268	-	X	-	-
6	EDO	B	2275	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7696 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 HISTONE DEMETHYLASE UTY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	1
			3540	2275	608	637	20			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	877	MET	-	expression tag	UNP O14607
A	1348	ALA	-	expression tag	UNP O14607
A	1349	GLU	-	expression tag	UNP O14607
A	1350	ASN	-	expression tag	UNP O14607
A	1351	LEU	-	expression tag	UNP O14607
A	1352	TYR	-	expression tag	UNP O14607
A	1353	PHE	-	expression tag	UNP O14607
A	1354	GLN	-	expression tag	UNP O14607
A	1272	GLU	ASP	conflict	UNP O14607

- Molecule 2 is a protein called HISTONE DEMETHYLASE UTY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	439	Total	C	N	O	S	0	4	1
			3540	2271	606	643	20			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	877	MET	-	expression tag	UNP O14607
B	1348	ALA	-	expression tag	UNP O14607
B	1349	GLU	-	expression tag	UNP O14607
B	1350	ASN	-	expression tag	UNP O14607
B	1351	LEU	-	expression tag	UNP O14607
B	1352	TYR	-	expression tag	UNP O14607
B	1353	PHE	-	expression tag	UNP O14607

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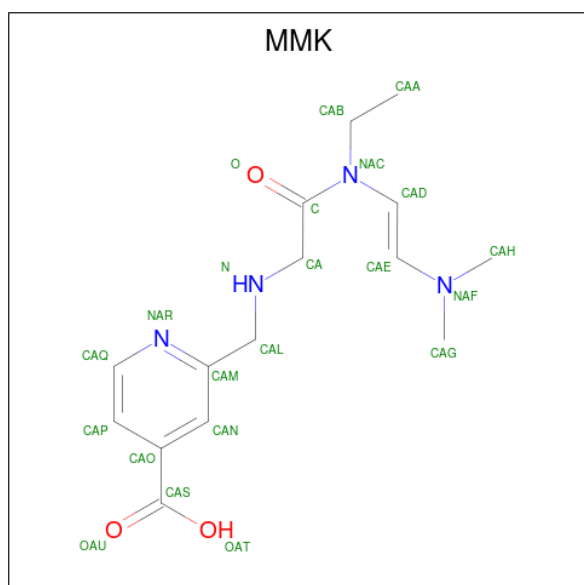
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Chain	Residue	Modelled	Actual	Comment	Reference
B	1354	GLN	-	expression tag	UNP O14607
B	1332	GLU	GLN	conflict	UNP O14607

- Molecule 3 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe 1 1	0	0
3	B	1	Total Fe 1 1	0	0

- Molecule 4 is 2-{{(2-{{(E)-2-(dimethylamino)ethenyl}}(ethyl)amino}-2-oxoethyl)amino]methyl}pyridine-4-carboxylic acid (CCD ID: MMK) (formula: C₁₅H₂₂N₄O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 22 15 4 3	4	0
4	B	1	Total C N O 22 15 4 3	4	0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

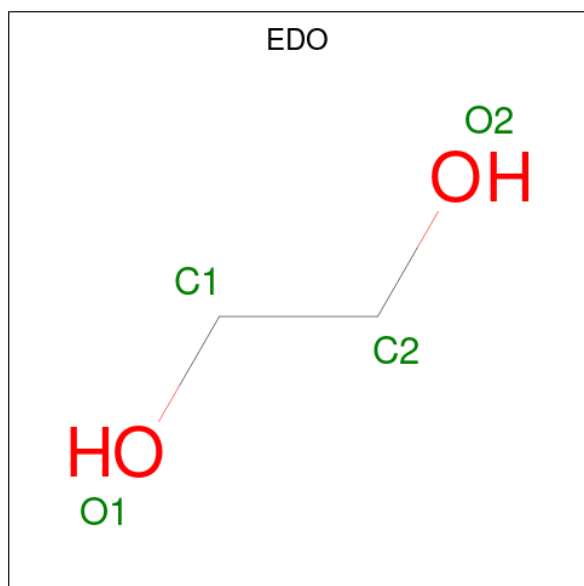
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

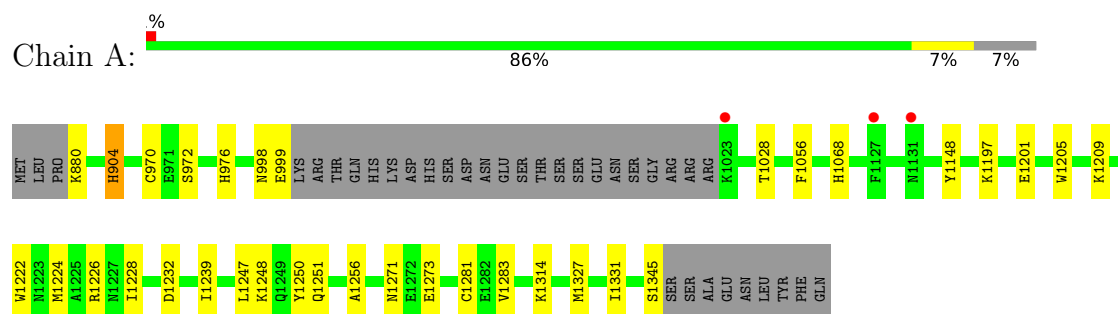
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	229	Total O 229 229	0	0
7	B	259	Total O 259 259	0	0

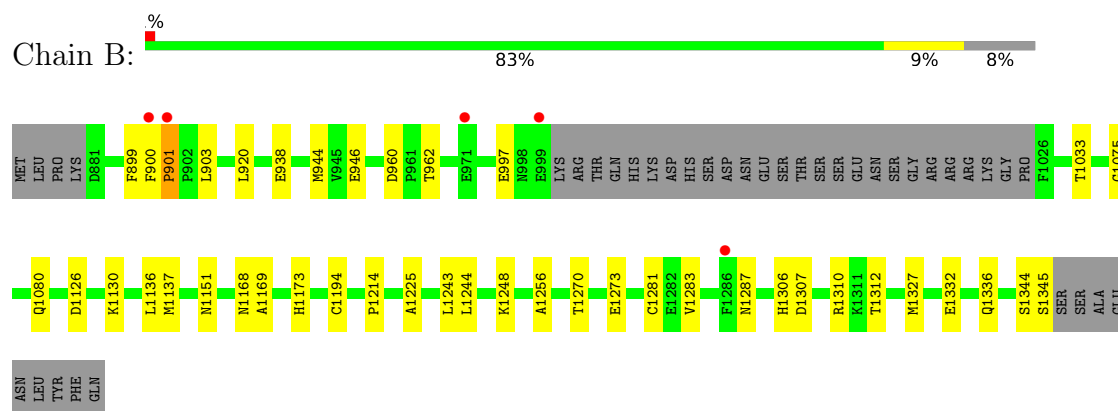
3 Residue-property plots [i](#)

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: HISTONE DEMETHYLASE UTY



• Molecule 2: HISTONE DEMETHYLASE UTY



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.49Å 110.46Å 119.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.03 – 1.78 81.03 – 1.78	Depositor EDS
% Data completeness (in resolution range)	100.0 (81.03-1.78) 100.0 (81.03-1.78)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.149 , 0.215 0.162 , 0.226	Depositor DCC
R_{free} test set	5650 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.1	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	0.97	EDS
Total number of atoms	7696	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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: FE2, EDO, ZN, MMK

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	1.07	2/3635 (0.1%)	1.03	2/4951 (0.0%)
2	B	1.06	2/3645 (0.1%)	1.01	4/4963 (0.1%)
All	All	1.06	4/7280 (0.1%)	1.02	6/9914 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1312	THR	CB-CG2	-6.93	1.29	1.52
2	B	1287	ASN	N-CA	6.84	1.55	1.46
1	A	1028	THR	CB-CG2	-5.58	1.34	1.52
1	A	1248	LYS	CA-C	5.26	1.59	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	PHE	CA-C-N	11.15	131.87	120.38
2	B	900	PHE	C-N-CA	11.15	131.87	120.38
2	B	901	PRO	N-CA-C	8.69	121.30	110.70
1	A	1273	GLU	CA-C-N	-5.66	114.77	120.21
1	A	1273	GLU	C-N-CA	-5.66	114.77	120.21
2	B	1173	HIS	N-CA-C	5.23	117.02	109.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	998	ASN	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	3540	0	3461	19	0
2	B	3540	0	3468	36	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	22	0	19	0	0
4	B	22	0	21	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	32	0	48	2	0
6	B	48	0	71	19	0
7	A	229	0	0	7	0
7	B	259	0	0	13	0
All	All	7696	0	7088	62	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 (62) 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)
2:B:1307:ASP:HB2	7:B:2234:HOH:O	1.74	0.86
2:B:1169:ALA:O	6:B:2275:EDO:H21	1.78	0.82
2:B:1168:ASN:HB3	6:B:2275:EDO:H12	1.67	0.76
6:B:2272:EDO:H21	7:B:2017:HOH:O	1.85	0.74
1:A:1256:ALA:HB2	6:A:2271:EDO:H12	1.68	0.73
1:A:1345:SER:N	7:A:2229:HOH:O	2.20	0.73
1:A:880:LYS:N	1:A:1148:TYR:HH	1.87	0.72
2:B:1310[A]:ARG:NH2	7:B:2234:HOH:O	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:976:HIS:HD2	7:A:2060:HOH:O	1.77	0.67
2:B:1168:ASN:HB3	6:B:2275:EDO:C1	2.29	0.63
1:A:1205:TRP:CZ2	1:A:1209:LYS:HE3	2.36	0.61
2:B:944:MET:HB3	6:B:2273:EDO:H12	1.82	0.60
1:A:999:GLU:CB	7:A:2073:HOH:O	2.49	0.60
2:B:1327:MET:HE1	7:B:2189:HOH:O	2.02	0.60
6:B:2277:EDO:H22	7:B:2209:HOH:O	2.01	0.59
2:B:1307:ASP:OD2	7:B:2235:HOH:O	2.17	0.58
1:A:1247:LEU:HD21	1:A:1331:ILE:HD13	1.85	0.58
2:B:1344:SER:OG	7:B:2257:HOH:O	2.17	0.56
1:A:904:HIS:HB2	1:A:1056:PHE:CG	2.41	0.56
2:B:1256:ALA:HB2	6:B:2280:EDO:C2	2.35	0.56
6:B:2275:EDO:H22	7:B:2136:HOH:O	2.06	0.55
2:B:1256:ALA:HB2	6:B:2280:EDO:H21	1.89	0.55
6:B:2272:EDO:C2	7:B:2017:HOH:O	2.50	0.53
7:A:2221:HOH:O	2:B:1310[A]:ARG:HD2	2.09	0.53
7:A:2221:HOH:O	2:B:1310[A]:ARG:CD	2.56	0.53
2:B:1214:PRO:O	6:B:2277:EDO:C1	2.58	0.52
1:A:1224:MET:HG2	1:A:1228:ILE:HD12	1.93	0.50
6:B:2278:EDO:C1	7:B:2259:HOH:O	2.60	0.50
2:B:899:PHE:O	2:B:901:PRO:HD3	2.12	0.49
1:A:904:HIS:HB2	1:A:1056:PHE:CD1	2.48	0.49
2:B:1126:ASP:OD2	6:B:2270:EDO:O2	2.30	0.48
2:B:1270:THR:HG23	2:B:1273:GLU:HB2	1.96	0.48
1:A:1197:LYS:NZ	1:A:1201:GLU:OE2	2.48	0.47
7:A:2221:HOH:O	2:B:1310[A]:ARG:NH1	2.24	0.47
1:A:1224:MET:HE2	1:A:1239:ILE:CD1	2.46	0.46
1:A:1251:GLN:HG2	1:A:1327:MET:CE	2.45	0.46
2:B:1194:CYS:HB3	6:B:2281:EDO:H21	1.97	0.46
2:B:920:LEU:C	2:B:920:LEU:HD13	2.41	0.46
1:A:1232:ASP:OD2	7:A:2147:HOH:O	2.21	0.46
2:B:946:GLU:O	2:B:1033:THR:HG22	2.16	0.46
2:B:946:GLU:HG3	6:B:2274:EDO:O1	2.16	0.45
2:B:1244:LEU:HD11	2:B:1248:LYS:HE3	1.99	0.45
2:B:960:ASP:OD2	2:B:962:THR:OG1	2.28	0.44
2:B:1306:HIS:CE1	2:B:1310[B]:ARG:HE	2.35	0.44
2:B:1075:GLY:HA2	2:B:1080:GLN:HG2	1.99	0.44
1:A:1281:CYS:SG	1:A:1283:VAL:HG12	2.58	0.44
2:B:1256:ALA:HB2	6:B:2280:EDO:H22	1.99	0.44
2:B:1126:ASP:O	2:B:1130:LYS:HG3	2.18	0.43
6:B:2277:EDO:C2	7:B:2209:HOH:O	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1345:SER:N	7:B:2256:HOH:O	2.51	0.42
6:B:2278:EDO:H12	7:B:2259:HOH:O	2.20	0.42
1:A:1222:TRP:O	1:A:1226:ARG:HG3	2.20	0.42
1:A:1256:ALA:HB2	6:A:2271:EDO:C1	2.44	0.42
2:B:1270:THR:CG2	2:B:1273:GLU:HB2	2.49	0.42
2:B:901:PRO:C	2:B:903:LEU:N	2.78	0.41
2:B:944:MET:HG2	6:B:2274:EDO:H22	2.03	0.41
1:A:1068:HIS:CG	1:A:1228:ILE:HD11	2.55	0.41
2:B:1225:ALA:HB2	2:B:1243:LEU:HD11	2.03	0.41
2:B:1136:LEU:HB3	2:B:1137:MET:HE2	2.02	0.40
1:A:1250:TYR:CE2	1:A:1327:MET:HE2	2.56	0.40
2:B:1332:GLU:HG3	2:B:1336:GLN:NE2	2.37	0.40
2:B:1281:CYS:SG	2:B:1283:VAL:HG12	2.62	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	439/478 (92%)	431 (98%)	8 (2%)	0	100	100
2	B	439/478 (92%)	427 (97%)	12 (3%)	0	100	100
All	All	878/956 (92%)	858 (98%)	20 (2%)	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	385/432 (89%)	380 (99%)	5 (1%)	61	46
2	B	389/432 (90%)	386 (99%)	3 (1%)	73	63
All	All	774/864 (90%)	766 (99%)	8 (1%)	68	55

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	904	HIS
1	A	970	CYS
1	A	972	SER
1	A	1271	ASN
1	A	1314	LYS
2	B	938	GLU
2	B	997	GLU
2	B	1151	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	958	ASN
1	A	986	GLN
1	A	1182	ASN
1	A	1296	ASN
2	B	904	HIS
2	B	986	GLN
2	B	1182	ASN
2	B	1227	ASN
2	B	1267	HIS
2	B	1296	ASN
2	B	1304	HIS
2	B	1306	HIS
2	B	1318	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 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	$\# Z > 2$
6	EDO	B	2276	-	3,3,3	0.72	0	2,2,2	0.24	0
6	EDO	A	2272	-	3,3,3	1.07	0	2,2,2	0.65	0
6	EDO	B	2270	-	3,3,3	0.41	0	2,2,2	0.39	0
6	EDO	A	2271	-	3,3,3	0.90	0	2,2,2	1.16	0
6	EDO	B	2280	-	3,3,3	0.52	0	2,2,2	1.16	0
4	MMK	A	2268	3	22,22,22	4.57	7 (31%)	24,28,28	3.88	13 (54%)
4	MMK	B	2268	3	22,22,22	3.02	5 (22%)	24,28,28	3.55	9 (37%)
6	EDO	A	2277	-	3,3,3	0.38	0	2,2,2	0.92	0
6	EDO	B	2273	-	3,3,3	0.89	0	2,2,2	1.60	1 (50%)
6	EDO	B	2274	-	3,3,3	0.47	0	2,2,2	1.21	0
6	EDO	B	2272	-	3,3,3	0.43	0	2,2,2	0.84	0
6	EDO	A	2273	-	3,3,3	0.37	0	2,2,2	0.56	0
6	EDO	B	2275	-	3,3,3	0.40	0	2,2,2	0.46	0
6	EDO	B	2281	-	3,3,3	0.33	0	2,2,2	0.46	0
6	EDO	B	2279	-	3,3,3	0.54	0	2,2,2	0.30	0
6	EDO	A	2275	-	3,3,3	0.56	0	2,2,2	0.45	0
6	EDO	A	2270	-	3,3,3	0.53	0	2,2,2	0.58	0
6	EDO	A	2274	-	3,3,3	0.52	0	2,2,2	0.38	0
6	EDO	A	2276	-	3,3,3	0.99	0	2,2,2	0.40	0
6	EDO	B	2271	-	3,3,3	0.39	0	2,2,2	0.79	0
6	EDO	B	2278	-	3,3,3	0.17	0	2,2,2	0.30	0
6	EDO	B	2277	-	3,3,3	0.32	0	2,2,2	1.05	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
6	EDO	B	2276	-	-	1/1/1/1	-
6	EDO	A	2272	-	-	0/1/1/1	-
6	EDO	B	2270	-	-	0/1/1/1	-
6	EDO	A	2271	-	-	1/1/1/1	-
6	EDO	B	2280	-	-	1/1/1/1	-
4	MMK	A	2268	3	-	10/21/21/21	0/1/1/1
4	MMK	B	2268	3	-	9/21/21/21	0/1/1/1
6	EDO	A	2277	-	-	1/1/1/1	-
6	EDO	B	2273	-	-	0/1/1/1	-
6	EDO	B	2274	-	-	1/1/1/1	-
6	EDO	B	2272	-	-	1/1/1/1	-
6	EDO	A	2273	-	-	0/1/1/1	-
6	EDO	B	2275	-	-	1/1/1/1	-
6	EDO	B	2281	-	-	0/1/1/1	-
6	EDO	B	2279	-	-	0/1/1/1	-
6	EDO	A	2275	-	-	0/1/1/1	-
6	EDO	A	2270	-	-	0/1/1/1	-
6	EDO	A	2274	-	-	0/1/1/1	-
6	EDO	A	2276	-	-	0/1/1/1	-
6	EDO	B	2271	-	-	0/1/1/1	-
6	EDO	B	2278	-	-	0/1/1/1	-
6	EDO	B	2277	-	-	1/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2268	MMK	CAE-CAD	-16.22	0.99	1.34
4	B	2268	MMK	CAE-NAF	9.43	1.48	1.33
4	A	2268	MMK	CAE-NAF	8.86	1.47	1.33
4	B	2268	MMK	CAD-NAC	7.28	1.52	1.38
4	A	2268	MMK	CAD-NAC	7.24	1.52	1.38
4	A	2268	MMK	C-NAC	4.65	1.44	1.35
4	B	2268	MMK	CAO-CAS	-4.56	1.39	1.49
4	A	2268	MMK	CAO-CAS	-3.50	1.42	1.49
4	B	2268	MMK	CA-N	2.51	1.53	1.46
4	A	2268	MMK	CAQ-NAR	-2.29	1.29	1.34
4	A	2268	MMK	OAU-CAS	2.16	1.29	1.22
4	B	2268	MMK	C-NAC	2.13	1.39	1.35

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2268	MMK	CAG-NAF-CAE	-12.27	108.42	121.47
4	A	2268	MMK	CAG-NAF-CAE	-11.44	109.31	121.47
4	A	2268	MMK	CAH-NAF-CAE	-11.37	109.37	121.47
4	B	2268	MMK	CAH-NAF-CAE	-8.83	112.08	121.47
4	B	2268	MMK	CAB-NAC-C	3.82	124.43	119.24
4	B	2268	MMK	OAT-CAS-CAO	3.69	124.31	114.84
4	A	2268	MMK	CAQ-NAR-CAM	3.63	122.50	117.41
4	A	2268	MMK	CAB-NAC-C	3.39	123.85	119.24
4	A	2268	MMK	CAP-CAO-CAN	-3.22	115.52	119.25
4	A	2268	MMK	CAP-CAQ-NAR	-3.01	120.29	123.97
4	A	2268	MMK	OAT-CAS-CAO	2.87	122.19	114.84
4	A	2268	MMK	OAT-CAS-OAU	-2.78	117.38	123.35
4	A	2268	MMK	CAN-CAM-NAR	-2.61	118.16	122.01
4	A	2268	MMK	CAN-CAO-CAS	2.59	124.60	119.96
4	B	2268	MMK	CAO-CAN-CAM	2.55	122.47	119.93
4	B	2268	MMK	CAN-CAM-NAR	-2.46	118.39	122.01
4	A	2268	MMK	CAQ-CAP-CAO	2.23	121.48	119.05
4	B	2268	MMK	OAT-CAS-OAU	-2.21	118.61	123.35
4	B	2268	MMK	CAP-CAO-CAN	-2.20	116.71	119.25
4	A	2268	MMK	CA-C-NAC	2.18	119.38	116.61
6	B	2273	EDO	O2-C2-C1	-2.16	95.95	112.39
4	B	2268	MMK	CAN-CAO-CAS	2.10	123.72	119.96
4	A	2268	MMK	CAO-CAN-CAM	2.03	121.95	119.93

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2268	MMK	CA-C-NAC-CAB
4	A	2268	MMK	CAE-CAD-NAC-CAB
4	A	2268	MMK	NAC-CAD-CAE-NAF
4	A	2268	MMK	CAD-CAE-NAF-CAG
4	B	2268	MMK	CA-C-NAC-CAB
4	B	2268	MMK	CAE-CAD-NAC-C
4	B	2268	MMK	CAD-CAE-NAF-CAH
4	B	2268	MMK	CAD-CAE-NAF-CAG
4	A	2268	MMK	CAP-CAO-CAS-OAU
4	B	2268	MMK	CAP-CAO-CAS-OAU
4	A	2268	MMK	CAN-CAO-CAS-OAU
4	B	2268	MMK	CAN-CAO-CAS-OAU
4	B	2268	MMK	CAN-CAO-CAS-OAT

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Mol	Chain	Res	Type	Atoms
4	A	2268	MMK	CAN-CAO-CAS-OAT
4	A	2268	MMK	CAP-CAO-CAS-OAT
4	B	2268	MMK	CAP-CAO-CAS-OAT
6	A	2277	EDO	O1-C1-C2-O2
6	B	2275	EDO	O1-C1-C2-O2
4	B	2268	MMK	CAE-CAD-NAC-CAB
6	B	2274	EDO	O1-C1-C2-O2
6	B	2280	EDO	O1-C1-C2-O2
4	A	2268	MMK	CAE-CAD-NAC-C
6	B	2272	EDO	O1-C1-C2-O2
6	A	2271	EDO	O1-C1-C2-O2
6	B	2276	EDO	O1-C1-C2-O2
6	B	2277	EDO	O1-C1-C2-O2
4	A	2268	MMK	O-C-NAC-CAB

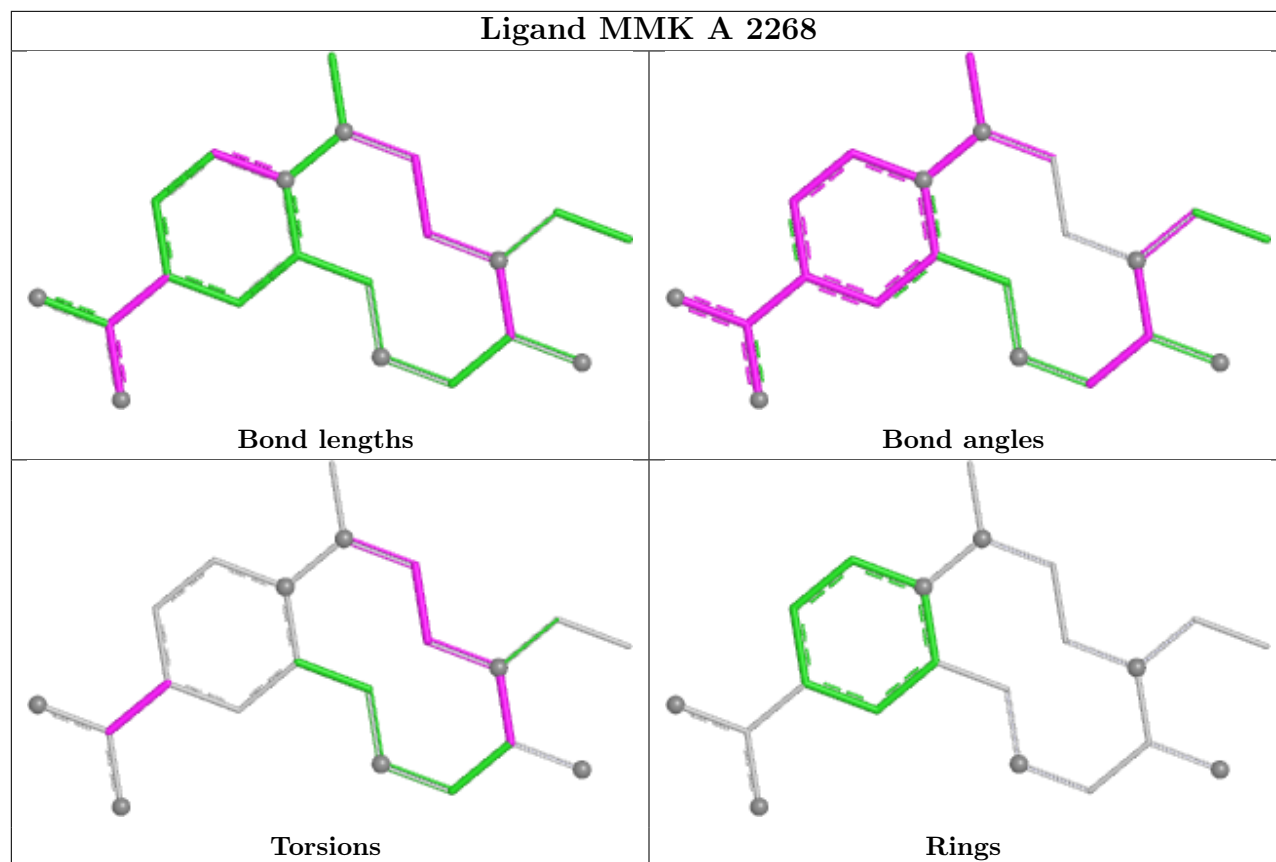
There are no ring outliers.

10 monomers are involved in 21 short contacts:

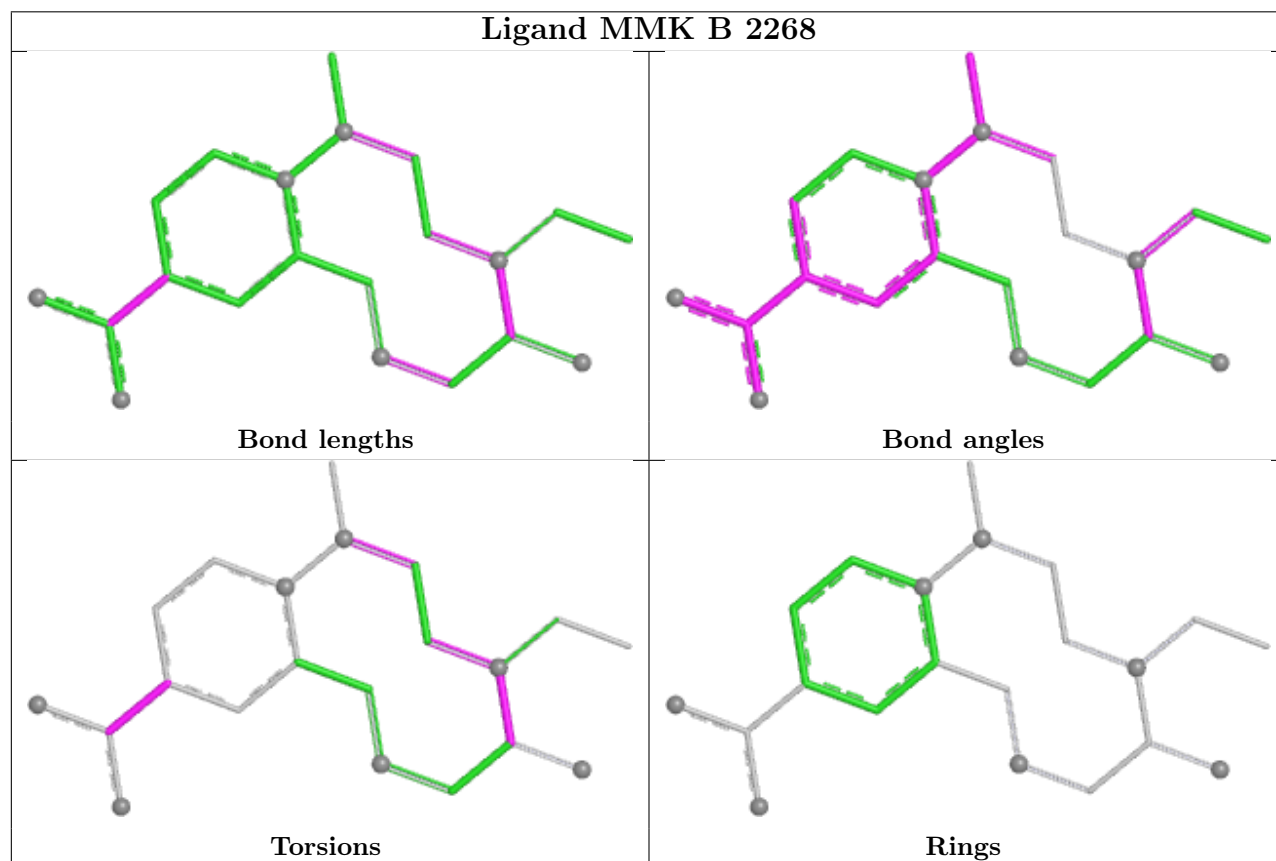
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	2270	EDO	1	0
6	A	2271	EDO	2	0
6	B	2280	EDO	3	0
6	B	2273	EDO	1	0
6	B	2274	EDO	2	0
6	B	2272	EDO	2	0
6	B	2275	EDO	4	0
6	B	2281	EDO	1	0
6	B	2278	EDO	2	0
6	B	2277	EDO	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand MMK A 2268



Ligand MMK B 2268



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	443/478 (92%)	-0.12	3 (0%) 84 88	22, 34, 57, 83	0
2	B	439/478 (91%)	-0.09	5 (1%) 78 84	19, 34, 57, 89	4 (0%)
All	All	882/956 (92%)	-0.10	8 (0%) 81 86	19, 34, 57, 89	4 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	900	PHE	4.6
2	B	901	PRO	3.8
1	A	1023	LYS	3.5
2	B	999	GLU	3.4
1	A	1131	ASN	2.7
2	B	1286	PHE	2.3
1	A	1127	PHE	2.2
2	B	971	GLU	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,

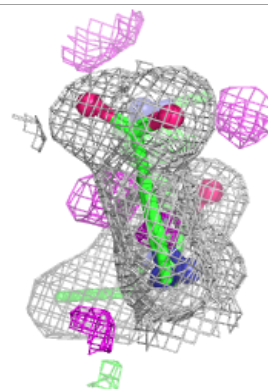
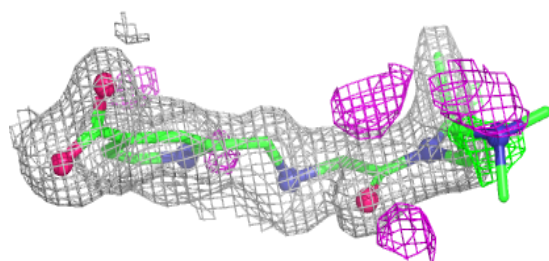
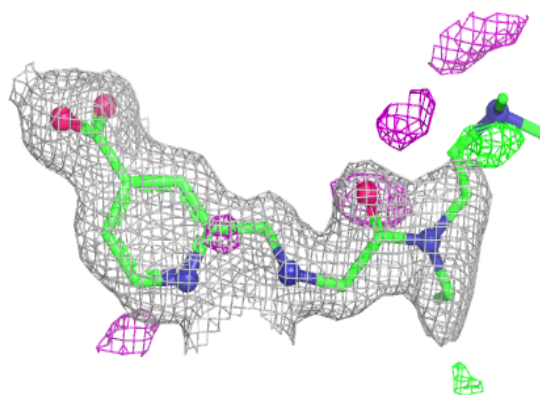
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	A	2275	4/4	0.88	0.15	49,51,56,57	0
6	EDO	A	2276	4/4	0.89	0.12	36,52,53,53	0
6	EDO	B	2271	4/4	0.89	0.17	54,59,67,73	0
6	EDO	A	2277	4/4	0.91	0.12	46,48,51,52	0
6	EDO	A	2270	4/4	0.91	0.12	44,48,51,56	0
6	EDO	B	2272	4/4	0.92	0.11	35,48,53,60	0
6	EDO	B	2276	4/4	0.92	0.13	44,44,56,64	0
4	MMK	B	2268	22/22	0.93	0.11	24,37,82,84	4
6	EDO	A	2271	4/4	0.93	0.10	39,64,64,66	0
6	EDO	B	2277	4/4	0.93	0.11	41,42,49,71	0
6	EDO	B	2275	4/4	0.94	0.21	38,39,54,54	0
6	EDO	A	2274	4/4	0.94	0.08	44,51,56,66	0
6	EDO	B	2273	4/4	0.94	0.11	33,46,47,64	0
6	EDO	B	2280	4/4	0.94	0.10	41,46,61,65	0
6	EDO	B	2270	4/4	0.95	0.09	58,61,64,68	0
6	EDO	A	2272	4/4	0.95	0.13	28,42,46,46	0
6	EDO	A	2273	4/4	0.95	0.08	44,48,51,54	0
4	MMK	A	2268	22/22	0.95	0.08	24,34,70,83	4
6	EDO	B	2279	4/4	0.96	0.09	47,48,58,60	0
6	EDO	B	2281	4/4	0.96	0.11	49,54,56,70	0
6	EDO	B	2278	4/4	0.97	0.07	40,40,41,50	0
6	EDO	B	2274	4/4	0.97	0.09	31,49,57,63	0
3	FE2	A	2267	1/1	1.00	0.01	27,27,27,27	0
3	FE2	B	2267	1/1	1.00	0.02	27,27,27,27	0
5	ZN	A	2269	1/1	1.00	0.01	33,33,33,33	0
5	ZN	B	2269	1/1	1.00	0.01	34,34,34,34	0

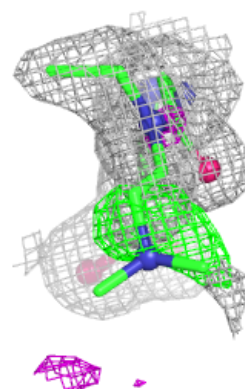
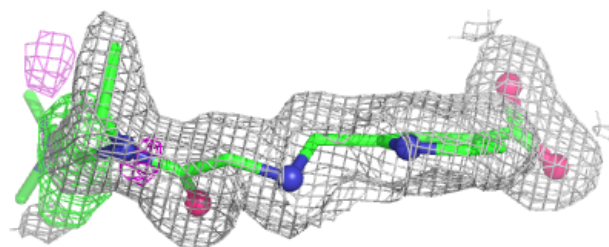
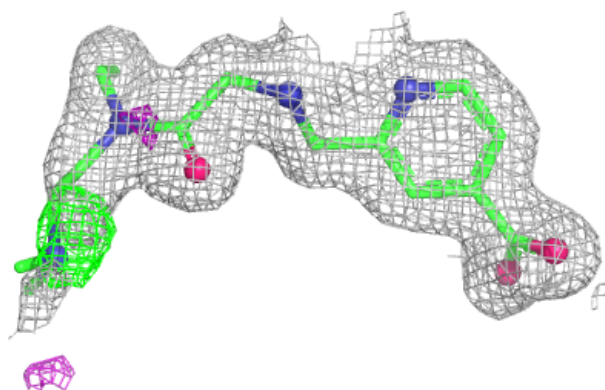
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MMK B 2268:

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

**Electron density around MMK A 2268:**

$2mF_o-DF_c$ (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.