



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 07:59 PM UTC

PDB ID : 5FPV / pdb_00005fpv
Title : Crystal structure of human JMJD2A in complex with compound KDOAM20A
Authors : Srikannathasan, V.; Gileadi, C.; von Delft, F.; Arrowsmith, C.H.; Bountra, C.;
Edwards, A.; Oppermann, U.
Deposited on : 2015-12-03
Resolution : 2.44 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

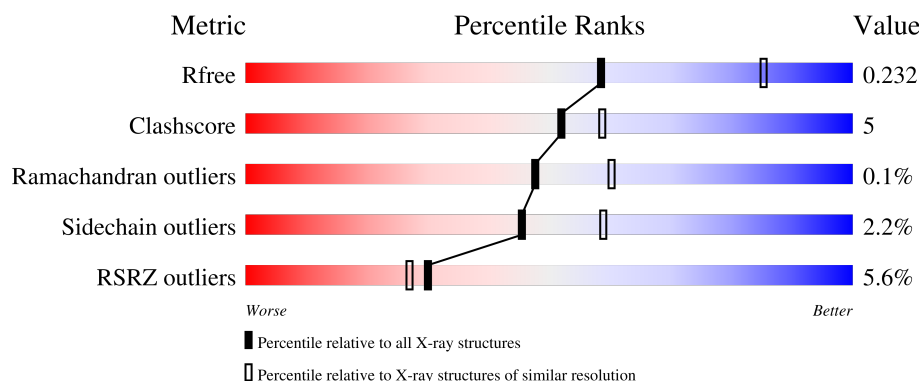
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	360	4% 86% 7% • 6%
1	B	360	7% 86% 8% • 5%
1	C	360	6% 84% 9% • 5%
1	D	360	5% 88% 5% • 5%
1	E	360	5% 87% 7% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	360	5% 82% 11% • 5%
1	G	360	7% 88% 7% • 5%
1	H	360	3% 85% 8% • 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23005 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 LYSINE-SPECIFIC DEMETHYLASE 4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2703	1761	445	482	15			
1	B	343	Total	C	N	O	S	0	1	0
			2751	1792	452	493	14			
1	C	342	Total	C	N	O	S	0	0	0
			2739	1782	450	492	15			
1	D	342	Total	C	N	O	S	0	0	0
			2744	1787	452	490	15			
1	E	341	Total	C	N	O	S	0	0	0
			2731	1778	449	489	15			
1	F	342	Total	C	N	O	S	0	0	0
			2747	1788	452	492	15			
1	G	343	Total	C	N	O	S	0	0	0
			2754	1791	455	493	15			
1	H	340	Total	C	N	O	S	0	0	0
			2738	1781	452	490	15			

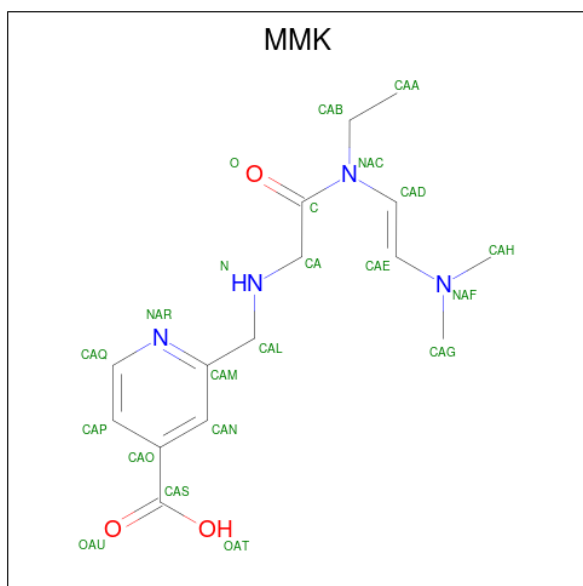
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP O75164
B	1	SER	-	expression tag	UNP O75164
C	1	SER	-	expression tag	UNP O75164
D	1	SER	-	expression tag	UNP O75164
E	1	SER	-	expression tag	UNP O75164
F	1	SER	-	expression tag	UNP O75164
G	1	SER	-	expression tag	UNP O75164
H	1	SER	-	expression tag	UNP O75164

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	E	1	Total Mn 1 1	0	0
2	F	1	Total Mn 1 1	0	0
2	G	1	Total Mn 1 1	0	0
2	H	1	Total Mn 1 1	0	0

- Molecule 3 is 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
3	A	1	Total C N O 22 15 4 3	0	0
3	B	1	Total C N O 22 15 4 3	0	0
3	C	1	Total C N O 22 15 4 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			22	15	4	3		
3	E	1	Total	C	N	O	0	0
			22	15	4	3		
3	F	1	Total	C	N	O	0	0
			22	15	4	3		
3	G	1	Total	C	N	O	0	0
			22	15	4	3		
3	H	1	Total	C	N	O	0	0
			22	15	4	3		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		
4	G	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		

- Molecule 5 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total 1	Ni 1	0	0
5	H	4	Total 4	Ni 4	0	0

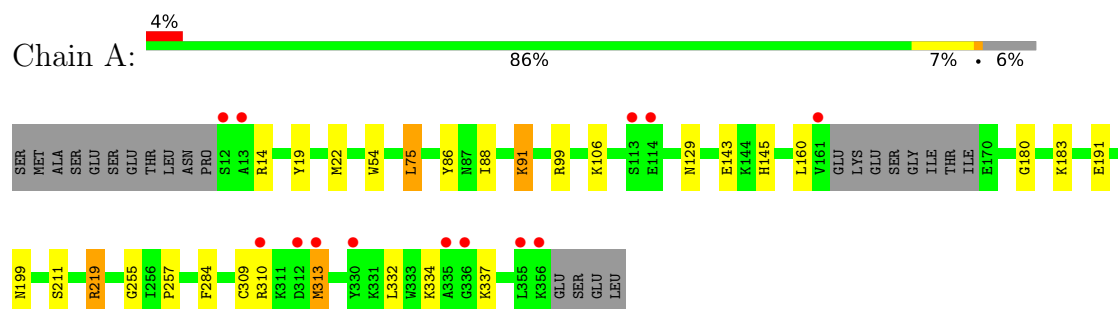
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	135	Total 135	O 135	0	0
6	B	128	Total 128	O 128	0	0
6	C	129	Total 129	O 129	0	0
6	D	121	Total 121	O 121	0	0
6	E	95	Total 95	O 95	0	0
6	F	91	Total 91	O 91	0	0
6	G	72	Total 72	O 72	0	0
6	H	120	Total 120	O 120	0	0

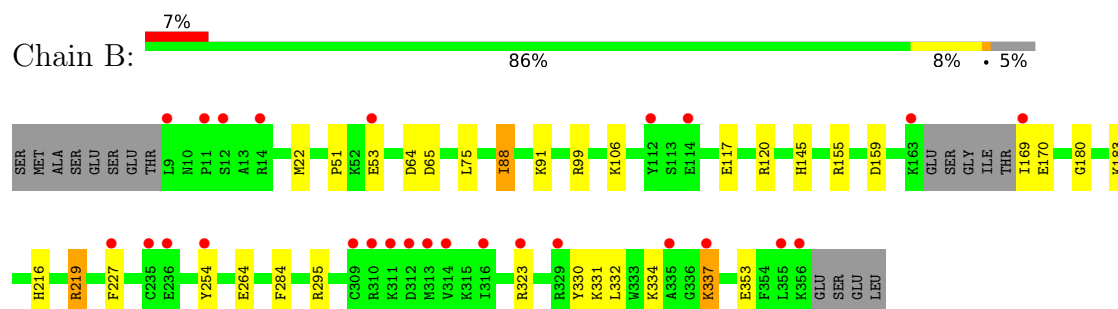
3 Residue-property plots [i](#)

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.

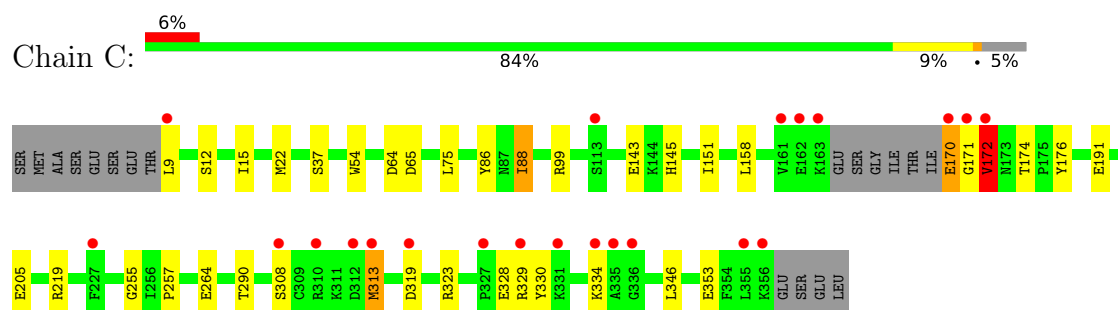
• Molecule 1: LYSINE-SPECIFIC DEMETHYLASE 4A



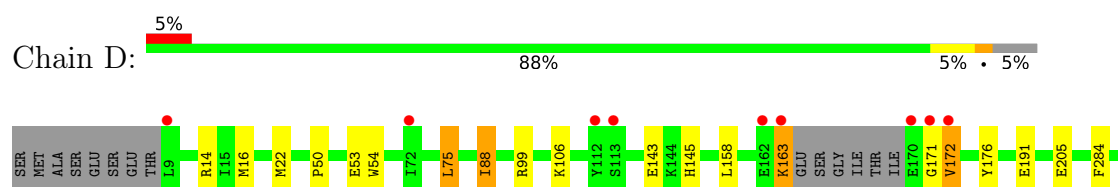
• Molecule 1: LYSINE-SPECIFIC DEMETHYLASE 4A

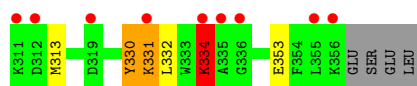


• Molecule 1: LYSINE-SPECIFIC DEMETHYLASE 4A

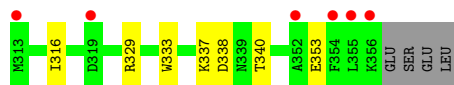
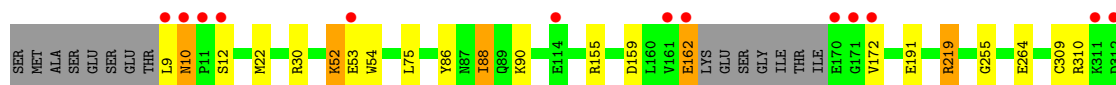
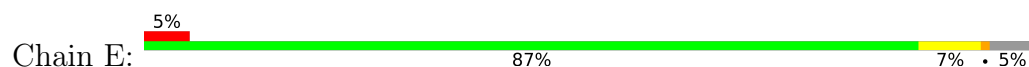


• Molecule 1: LYSINE-SPECIFIC DEMETHYLASE 4A

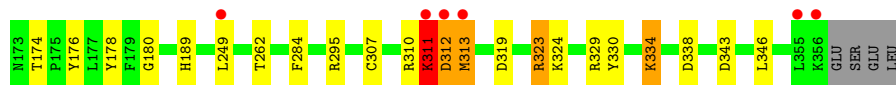
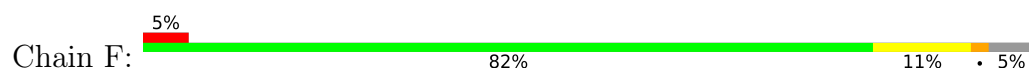




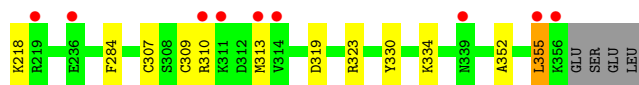
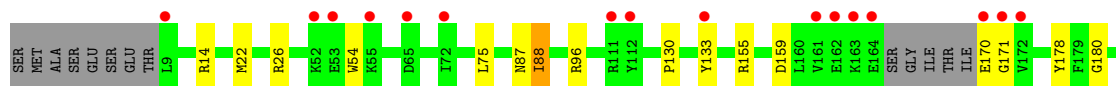
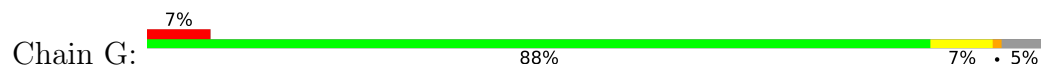
• Molecule 1: LYSINE-SPECIFIC DEMETHYLASE 4A



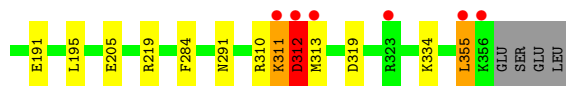
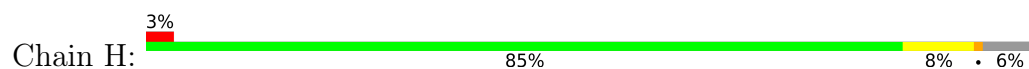
• Molecule 1: LYSINE-SPECIFIC DEMETHYLASE 4A



• Molecule 1: LYSINE-SPECIFIC DEMETHYLASE 4A



• Molecule 1: LYSINE-SPECIFIC DEMETHYLASE 4A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.35Å 103.51Å 157.10Å 90.00° 106.37° 90.00°	Depositor
Resolution (Å)	85.33 – 2.44 85.33 – 2.44	Depositor EDS
% Data completeness (in resolution range)	98.5 (85.33-2.44) 91.4 (85.33-2.44)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.45Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.196 , 0.229 0.200 , 0.232	Depositor DCC
R_{free} test set	6218 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtrriage
Anisotropy	0.462	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23005	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.60 % 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 6.3174e-05. 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MMK, NI, MN

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	0.41	0/2788	0.75	0/3786
1	B	0.44	0/2837	0.81	1/3855 (0.0%)
1	C	0.40	0/2825	0.78	1/3839 (0.0%)
1	D	0.60	4/2830 (0.1%)	0.87	8/3843 (0.2%)
1	E	0.39	0/2817	0.78	2/3828 (0.1%)
1	F	0.39	0/2833	0.80	4/3847 (0.1%)
1	G	0.37	0/2840	0.78	3/3857 (0.1%)
1	H	0.41	0/2824	0.78	2/3835 (0.1%)
All	All	0.43	4/22594 (0.0%)	0.79	21/30690 (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	E	0	1
1	F	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	331	LYS	CA-CB	12.85	1.74	1.53
1	D	334	LYS	CE-NZ	11.00	1.82	1.49
1	D	332	LEU	CA-CB	-6.43	1.43	1.53
1	D	334	LYS	CA-C	-5.63	1.45	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	330	TYR	CA-C-O	-11.99	108.23	120.82
1	H	311	LYS	N-CA-C	-10.85	96.20	110.53
1	G	171	GLY	N-CA-C	9.94	125.22	110.42
1	E	10	ASN	CA-C-N	9.18	129.37	119.28
1	E	10	ASN	C-N-CA	9.18	129.37	119.28
1	D	330	TYR	N-CA-C	-8.52	101.95	111.07
1	D	330	TYR	CA-C-N	8.32	134.82	120.68
1	D	330	TYR	C-N-CA	8.32	134.82	120.68
1	H	311	LYS	CA-C-O	-7.79	112.83	121.87
1	D	330	TYR	N-CA-CB	7.41	120.75	110.01
1	B	170	GLU	N-CA-C	-7.21	98.46	109.85
1	F	312	ASP	CB-CA-C	-7.17	102.73	109.83
1	C	172	VAL	N-CA-C	-6.62	106.39	111.62
1	F	311	LYS	CA-C-N	-6.36	116.88	126.86
1	F	311	LYS	C-N-CA	-6.36	116.88	126.86
1	G	170	GLU	CA-C-N	-5.86	111.36	120.86
1	G	170	GLU	C-N-CA	-5.86	111.36	120.86
1	D	334	LYS	CB-CA-C	-5.80	98.88	110.42
1	F	311	LYS	N-CA-C	-5.79	98.47	110.80
1	D	331	LYS	CA-C-O	5.70	126.51	119.79
1	D	334	LYS	O-C-N	5.00	129.24	122.59

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	9	LEU	Peptide
1	F	9	LEU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2703	0	2560	26	0
1	B	2751	0	2602	35	0
1	C	2739	0	2583	30	0
1	D	2744	0	2603	32	0
1	E	2731	0	2579	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2747	0	2605	36	0
1	G	2754	0	2607	23	0
1	H	2738	0	2599	32	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	22	0	21	1	0
3	B	22	0	21	1	0
3	C	22	0	21	1	0
3	D	22	0	21	1	0
3	E	22	0	21	2	0
3	F	22	0	21	1	0
3	G	22	0	21	0	0
3	H	22	0	21	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	3	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	3	0	0	0	0
5	G	1	0	0	0	0
5	H	4	0	0	0	0
6	A	135	0	0	5	0
6	B	128	0	0	14	0
6	C	129	0	0	7	0
6	D	121	0	0	5	1
6	E	95	0	0	2	0
6	F	91	0	0	2	1
6	G	72	0	0	2	0
6	H	120	0	0	4	0
All	All	23005	0	20906	219	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 5.

All (219) 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:D:334:LYS:CE	1:D:334:LYS:NZ	1.82	1.39
1:D:331:LYS:HA	1:D:334:LYS:HG3	1.37	1.05
1:D:331:LYS:HA	1:D:334:LYS:HE2	1.30	1.05
1:B:330:TYR:O	6:B:2125:HOH:O	1.81	0.98
1:H:311:LYS:O	1:H:312:ASP:HB3	1.61	0.97
1:E:10:ASN:OD1	1:E:12:SER:OG	1.83	0.96
1:F:59:SER:OG	1:F:61:ASP:OD1	1.83	0.95
1:D:331:LYS:HA	1:D:334:LYS:CE	2.01	0.90
1:A:219:ARG:HH21	1:A:257:PRO:HD3	1.36	0.90
1:D:330:TYR:HD2	1:D:334:LYS:HZ2	1.16	0.90
1:D:331:LYS:CA	1:D:334:LYS:HG3	2.02	0.90
1:H:91:LYS:HD2	1:H:91:LYS:H	1.38	0.88
1:F:311:LYS:O	1:F:312:ASP:HB2	1.74	0.87
1:B:353:GLU:OE2	1:C:145:HIS:NE2	2.11	0.84
1:B:22:MET:HE2	1:B:53:GLU:HG3	1.59	0.82
1:F:343:ASP:HB3	1:F:346:LEU:HD12	1.62	0.81
1:C:329:ARG:NH1	6:C:2127:HOH:O	2.13	0.80
1:A:219:ARG:NH2	1:A:257:PRO:HD3	1.98	0.78
1:B:323:ARG:HH11	1:B:323:ARG:HG2	1.46	0.78
1:E:30:ARG:NH2	1:E:353:GLU:OE2	2.18	0.77
1:D:330:TYR:CD2	1:D:334:LYS:NZ	2.51	0.76
1:B:88:ILE:HD12	1:G:88:ILE:HD12	1.67	0.75
1:G:96:ARG:NH1	6:G:2024:HOH:O	2.19	0.74
1:F:170:GLU:HG2	1:F:174:THR:HG21	1.71	0.73
1:D:330:TYR:O	1:D:334:LYS:HG2	1.89	0.72
1:B:51:PRO:HB2	1:B:53:GLU:CD	2.13	0.72
1:B:332:LEU:HD11	1:B:337:LYS:HG2	1.72	0.71
1:B:264:GLU:OE1	6:B:2026:HOH:O	2.09	0.71
1:D:331:LYS:HA	1:D:334:LYS:CG	2.20	0.70
1:E:172:VAL:HG21	1:E:316:ILE:HD11	1.73	0.70
1:C:15:ILE:O	6:C:2004:HOH:O	2.11	0.69
1:F:323:ARG:HD3	1:F:330:TYR:CE1	2.27	0.69
1:B:65:ASP:O	6:B:2036:HOH:O	2.11	0.69
1:B:145:HIS:NE2	1:C:353:GLU:OE2	2.23	0.69
1:B:51:PRO:HB2	1:B:53:GLU:OE2	1.93	0.68
1:G:26:ARG:HH11	1:G:26:ARG:HG2	1.60	0.67
1:H:75:LEU:HD13	1:H:88:ILE:HD13	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:295:ARG:NE	6:F:2077:HOH:O	2.27	0.67
1:G:88:ILE:HD13	1:G:88:ILE:N	2.10	0.67
1:B:88:ILE:N	1:B:88:ILE:HD13	2.10	0.67
1:F:307:CYS:HB3	1:F:313:MET:SD	2.35	0.67
1:H:91:LYS:O	6:H:2035:HOH:O	2.13	0.66
1:C:171:GLY:HA2	1:C:176:TYR:OH	1.95	0.66
1:E:162:GLU:HA	1:E:162:GLU:OE1	1.95	0.66
1:F:319:ASP:OD1	1:F:334:LYS:HE2	1.95	0.66
1:D:191:GLU:OE1	3:D:1358:MMK:HA1C	1.96	0.65
1:F:323:ARG:HD3	1:F:330:TYR:CZ	2.32	0.65
1:H:91:LYS:HD2	1:H:91:LYS:N	2.10	0.65
1:D:171:GLY:HA2	1:D:176:TYR:OH	1.96	0.64
1:F:160:LEU:HD11	1:F:324:LYS:HD3	1.79	0.64
1:E:329:ARG:NH1	1:E:340:THR:OG1	2.29	0.64
1:B:264:GLU:OE1	6:B:2025:HOH:O	2.15	0.64
1:F:310:ARG:C	1:F:311:LYS:O	2.34	0.64
1:F:133:TYR:OH	1:F:178:TYR:HB3	1.98	0.63
1:E:337:LYS:NZ	6:E:2089:HOH:O	2.31	0.63
1:G:54:TRP:O	6:G:2012:HOH:O	2.16	0.63
1:A:145:HIS:CE1	1:D:353:GLU:OE2	2.51	0.63
1:B:334:LYS:HB2	6:B:2125:HOH:O	1.98	0.63
1:A:337:LYS:O	1:A:337:LYS:HG3	1.97	0.62
1:H:162:GLU:HG3	1:H:173:ASN:ND2	2.14	0.62
1:A:199:ASN:HB2	6:A:2098:HOH:O	1.98	0.62
1:C:75:LEU:HD21	1:F:86:TYR:CD1	2.34	0.62
1:C:319:ASP:OD1	1:C:323:ARG:CZ	2.48	0.61
1:A:19:TYR:OH	6:A:2008:HOH:O	2.10	0.61
1:A:219:ARG:NH2	1:A:255:GLY:O	2.26	0.61
1:A:191:GLU:OE1	3:A:1358:MMK:HA1C	2.01	0.61
1:A:143:GLU:HB3	6:A:2078:HOH:O	2.01	0.60
1:D:50:PRO:O	6:D:2016:HOH:O	2.16	0.60
1:A:75:LEU:HD12	1:A:88:ILE:HD13	1.83	0.60
1:G:133:TYR:CE1	1:G:180:GLY:HA2	2.35	0.60
1:F:311:LYS:O	1:F:312:ASP:CB	2.45	0.60
1:A:75:LEU:HD12	1:A:88:ILE:CD1	2.32	0.60
1:B:295:ARG:NE	6:B:2119:HOH:O	2.37	0.58
1:C:22:MET:HE1	1:C:54:TRP:HB2	1.85	0.58
1:B:323:ARG:HG2	1:B:323:ARG:NH1	2.18	0.58
1:C:328:GLU:OE2	1:C:329:ARG:NH1	2.37	0.57
1:D:99:ARG:NH1	6:D:2045:HOH:O	2.38	0.57
1:D:330:TYR:HD2	1:D:334:LYS:NZ	1.95	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:LYS:N	1:E:52:LYS:HD3	2.19	0.57
1:C:313:MET:HE2	6:C:2125:HOH:O	2.04	0.56
1:F:12:SER:HB2	1:F:14:ARG:HG3	1.87	0.56
1:H:191:GLU:OE1	3:H:1358:MMK:HA1C	2.05	0.56
1:B:227:PHE:HZ	1:B:254:TYR:CZ	2.23	0.56
1:A:86:TYR:CD1	1:H:75:LEU:HD21	2.40	0.56
1:B:334:LYS:N	6:B:2125:HOH:O	2.03	0.56
1:B:88:ILE:CD1	1:G:88:ILE:HD12	2.35	0.56
1:B:99:ARG:NH1	6:B:2054:HOH:O	2.38	0.55
1:C:9:LEU:HD21	1:C:37:SER:O	2.05	0.55
1:D:331:LYS:CA	1:D:334:LYS:HE2	2.22	0.55
1:D:14:ARG:NH2	1:D:16:MET:HA	2.21	0.55
1:B:64:ASP:OD1	6:B:2029:HOH:O	2.18	0.55
1:C:319:ASP:OD1	1:C:323:ARG:NH1	2.38	0.55
1:D:22:MET:HE1	1:D:54:TRP:HB2	1.89	0.54
1:C:86:TYR:CD1	1:F:75:LEU:HD21	2.42	0.54
1:G:133:TYR:CD1	1:G:180:GLY:HA2	2.43	0.54
1:G:352:ALA:HA	1:G:355:LEU:HD12	1.90	0.54
1:B:353:GLU:CD	1:C:145:HIS:HE2	2.14	0.54
1:D:158:LEU:HD21	1:D:172:VAL:HG13	1.90	0.54
1:B:99:ARG:NH2	6:B:2035:HOH:O	2.36	0.53
1:F:133:TYR:CE1	1:F:180:GLY:HA2	2.44	0.53
1:G:180:GLY:O	1:G:284:PHE:HA	2.09	0.53
1:H:116:GLU:O	1:H:120:ARG:HG3	2.08	0.53
1:F:133:TYR:CD1	1:F:180:GLY:HA2	2.45	0.52
1:G:22:MET:HE1	1:G:54:TRP:HB2	1.91	0.52
1:E:22:MET:HE1	1:E:54:TRP:HB2	1.90	0.52
1:E:90:LYS:O	6:E:2015:HOH:O	2.19	0.52
1:A:145:HIS:HE1	1:D:353:GLU:OE2	1.90	0.52
1:A:332:LEU:HD11	1:A:337:LYS:HG2	1.91	0.52
1:G:26:ARG:HG2	1:G:26:ARG:NH1	2.24	0.52
1:B:99:ARG:NH1	6:B:2035:HOH:O	2.41	0.52
1:H:90:LYS:O	6:H:2029:HOH:O	2.19	0.51
1:A:22:MET:HE1	1:A:54:TRP:HB2	1.92	0.51
1:F:262:THR:OG1	6:F:2058:HOH:O	2.19	0.51
1:B:216:HIS:ND1	1:B:219:ARG:NH2	2.54	0.51
1:F:75:LEU:HD13	1:F:88:ILE:HD11	1.92	0.51
1:D:331:LYS:C	1:D:334:LYS:HG3	2.36	0.50
1:A:211:SER:HB2	6:A:2027:HOH:O	2.11	0.50
1:C:319:ASP:OD1	1:C:330:TYR:CE1	2.64	0.50
1:D:75:LEU:HD21	1:E:86:TYR:CD1	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:307:CYS:HB3	1:G:313:MET:HG3	1.92	0.50
1:C:205:GLU:OE2	6:C:2110:HOH:O	2.19	0.49
1:D:145:HIS:HB2	6:D:2074:HOH:O	2.13	0.49
1:B:99:ARG:HG3	1:B:284:PHE:CE2	2.48	0.49
1:D:205:GLU:OE2	6:D:2097:HOH:O	2.19	0.49
1:B:117:GLU:HG3	1:B:120:ARG:NH2	2.28	0.49
1:F:10:ASN:OD1	1:F:13:ALA:N	2.45	0.49
1:G:133:TYR:OH	1:G:178:TYR:HB3	2.12	0.49
1:D:14:ARG:NH1	1:D:16:MET:HG2	2.28	0.49
1:B:75:LEU:HD13	1:B:88:ILE:HD11	1.95	0.49
3:E:1358:MMK:HA1C	3:E:1358:MMK:HAA3	1.93	0.48
1:B:331:LYS:C	6:B:2125:HOH:O	2.55	0.48
1:C:191:GLU:OE1	3:C:1358:MMK:HA1C	2.13	0.48
1:E:75:LEU:HD12	1:E:88:ILE:HD11	1.94	0.48
1:F:329:ARG:HD3	1:F:338:ASP:OD2	2.14	0.48
1:F:160:LEU:CD1	1:F:324:LYS:HD3	2.42	0.47
1:A:106:LYS:NZ	1:A:129:ASN:OD1	2.46	0.47
1:C:219:ARG:NH2	1:C:255:GLY:O	2.46	0.47
1:H:162:GLU:CG	1:H:173:ASN:ND2	2.76	0.47
1:C:170:GLU:HA	1:C:174:THR:HG21	1.97	0.47
1:H:311:LYS:O	1:H:312:ASP:CB	2.45	0.47
1:H:22:MET:HE1	1:H:54:TRP:HB2	1.97	0.47
1:H:158:LEU:HD21	1:H:172:VAL:HG22	1.95	0.47
1:C:329:ARG:HH11	1:C:329:ARG:HG3	1.80	0.47
1:C:158:LEU:HD21	1:C:172:VAL:HG13	1.96	0.47
1:C:88:ILE:HD13	1:C:88:ILE:N	2.30	0.46
1:B:264:GLU:CD	6:B:2026:HOH:O	2.56	0.46
1:F:171:GLY:HA2	1:F:176:TYR:OH	2.15	0.46
1:H:172:VAL:HG21	1:H:195:LEU:HD13	1.98	0.46
1:C:143:GLU:HB3	6:C:2085:HOH:O	2.15	0.46
3:B:1358:MMK:HAG2	3:B:1358:MMK:HAD	1.63	0.46
1:D:99:ARG:HG3	1:D:284:PHE:CE2	2.51	0.45
1:A:91:LYS:HD2	1:A:91:LYS:HA	1.65	0.45
1:E:219:ARG:NH2	1:E:255:GLY:O	2.49	0.45
1:F:22:MET:HE1	1:F:54:TRP:HB2	1.98	0.45
1:H:319:ASP:OD2	1:H:334:LYS:HE2	2.17	0.45
1:A:309:CYS:SG	1:A:310:ARG:HG3	2.56	0.45
1:D:331:LYS:CG	1:D:334:LYS:HE2	2.46	0.45
1:H:155:ARG:HA	1:H:159:ASP:OD2	2.17	0.45
1:H:219:ARG:NH2	6:H:2087:HOH:O	2.49	0.45
1:A:332:LEU:CD1	1:A:337:LYS:HG2	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:319:ASP:OD1	1:G:323:ARG:CZ	2.65	0.45
1:H:172:VAL:HG21	1:H:195:LEU:CD1	2.48	0.44
1:D:334:LYS:HG2	1:D:334:LYS:H	1.29	0.44
1:F:189:HIS:CE1	3:F:1358:MMK:HAL2	2.52	0.44
1:F:133:TYR:CD2	1:F:135:ALA:HB2	2.53	0.44
1:G:75:LEU:HD21	1:G:130:PRO:HG3	1.99	0.43
1:C:64:ASP:CG	1:C:99:ARG:HH22	2.26	0.43
1:E:191:GLU:OE1	3:E:1358:MMK:HA1C	2.17	0.43
1:D:75:LEU:HD13	1:D:88:ILE:HD11	2.00	0.43
1:C:65:ASP:HB2	6:C:2026:HOH:O	2.17	0.43
1:A:313:MET:HE2	1:A:313:MET:HB3	1.90	0.43
1:E:309:CYS:SG	1:E:310:ARG:HG2	2.59	0.43
1:F:99:ARG:HG3	1:F:284:PHE:CE2	2.53	0.43
1:G:133:TYR:CE1	1:G:180:GLY:CA	3.02	0.43
1:G:330:TYR:CZ	1:G:334:LYS:HD2	2.53	0.43
1:H:159:ASP:O	1:H:162:GLU:HB2	2.19	0.42
1:B:75:LEU:CD1	1:B:88:ILE:HG12	2.49	0.42
1:C:151:ILE:HG23	1:C:290:THR:HG22	2.00	0.42
1:A:99:ARG:HG3	1:A:284:PHE:CE2	2.55	0.42
1:A:183:LYS:HE3	6:A:2068:HOH:O	2.19	0.42
1:C:319:ASP:OD1	1:C:330:TYR:HE1	2.01	0.42
1:F:180:GLY:O	1:F:284:PHE:HA	2.18	0.42
1:B:180:GLY:O	1:B:284:PHE:HA	2.18	0.42
1:D:330:TYR:O	1:D:334:LYS:CG	2.65	0.42
1:G:87:ASN:C	1:G:88:ILE:HD13	2.44	0.42
1:H:180:GLY:O	1:H:284:PHE:HA	2.20	0.42
1:H:312:ASP:O	1:H:312:ASP:OD1	2.38	0.42
1:F:20:PRO:HB3	1:F:31:TYR:CZ	2.55	0.42
1:F:58:ALA:N	1:F:143:GLU:OE2	2.41	0.42
1:H:172:VAL:HG22	1:H:291:ASN:HB2	2.02	0.42
1:E:155:ARG:HA	1:E:159:ASP:OD2	2.20	0.42
1:F:143:GLU:OE1	1:F:145:HIS:NE2	2.49	0.42
1:A:180:GLY:O	1:A:284:PHE:HA	2.20	0.41
1:F:323:ARG:HD3	1:F:330:TYR:CD1	2.54	0.41
1:H:37:SER:HB2	1:H:355:LEU:HD21	2.02	0.41
1:C:219:ARG:NH2	1:C:257:PRO:HD3	2.35	0.41
1:B:155:ARG:HA	1:B:159:ASP:OD2	2.21	0.41
1:C:346:LEU:O	6:C:2123:HOH:O	2.22	0.41
1:G:133:TYR:HE1	1:G:180:GLY:CA	2.34	0.41
1:B:91:LYS:HB3	1:B:91:LYS:HE3	1.74	0.41
1:A:160:LEU:CD2	1:D:163:LYS:HG2	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:LYS:HE3	6:B:2074:HOH:O	2.20	0.41
1:D:143:GLU:HB3	6:D:2074:HOH:O	2.20	0.41
1:A:86:TYR:CG	1:H:75:LEU:HD21	2.55	0.41
1:G:307:CYS:SG	1:G:313:MET:HG3	2.61	0.41
1:H:312:ASP:OD1	1:H:312:ASP:C	2.62	0.41
1:H:312:ASP:OD1	1:H:313:MET:HE2	2.21	0.41
1:F:9:LEU:N	1:F:9:LEU:HD12	2.36	0.41
1:F:88:ILE:N	1:F:88:ILE:HD13	2.35	0.41
1:H:83:PHE:CZ	1:H:126:LEU:HD21	2.56	0.41
1:H:136:ASP:HA	1:H:176:TYR:HD2	1.86	0.41
1:E:333:TRP:HA	1:E:338:ASP:HB2	2.03	0.41
1:F:62:ASP:OD1	1:F:62:ASP:N	2.54	0.41
1:H:37:SER:HB2	1:H:355:LEU:CD2	2.51	0.41
1:G:155:ARG:HA	1:G:159:ASP:OD2	2.22	0.40
1:H:205:GLU:OE2	6:H:2084:HOH:O	2.22	0.40
1:C:313:MET:HE3	1:C:313:MET:HB3	1.89	0.40
1:G:309:CYS:SG	1:G:310:ARG:HG3	2.61	0.40
1:H:310:ARG:C	1:H:311:LYS:O	2.56	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)
6:D:2102:HOH:O	6:F:2068:HOH:O[2_645]	2.10	0.10

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	333/360 (92%)	328 (98%)	5 (2%)	0	100	100
1	B	340/360 (94%)	332 (98%)	8 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	338/360 (94%)	332 (98%)	6 (2%)	0	100	100
1	D	338/360 (94%)	330 (98%)	8 (2%)	0	100	100
1	E	337/360 (94%)	331 (98%)	6 (2%)	0	100	100
1	F	338/360 (94%)	328 (97%)	9 (3%)	1 (0%)	36	44
1	G	339/360 (94%)	336 (99%)	3 (1%)	0	100	100
1	H	336/360 (93%)	329 (98%)	6 (2%)	1 (0%)	36	44
All	All	2699/2880 (94%)	2646 (98%)	51 (2%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	312	ASP
1	F	311	LYS

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	274/316 (87%)	268 (98%)	6 (2%)	45	59
1	B	279/316 (88%)	274 (98%)	5 (2%)	51	64
1	C	278/316 (88%)	270 (97%)	8 (3%)	37	49
1	D	279/316 (88%)	271 (97%)	8 (3%)	37	49
1	E	277/316 (88%)	271 (98%)	6 (2%)	45	59
1	F	280/316 (89%)	273 (98%)	7 (2%)	42	54
1	G	280/316 (89%)	276 (99%)	4 (1%)	59	70
1	H	280/316 (89%)	275 (98%)	5 (2%)	51	64
All	All	2227/2528 (88%)	2178 (98%)	49 (2%)	45	59

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	75	LEU
1	A	91	LYS
1	A	219	ARG
1	A	313	MET
1	A	334	LYS
1	B	88	ILE
1	B	106	LYS
1	B	169	ILE
1	B	219	ARG
1	B	337	LYS
1	C	12	SER
1	C	88	ILE
1	C	170	GLU
1	C	172	VAL
1	C	264	GLU
1	C	308	SER
1	C	313	MET
1	C	334	LYS
1	D	53	GLU
1	D	75	LEU
1	D	88	ILE
1	D	106	LYS
1	D	163	LYS
1	D	172	VAL
1	D	313	MET
1	D	334	LYS
1	E	52	LYS
1	E	53	GLU
1	E	88	ILE
1	E	162	GLU
1	E	219	ARG
1	E	264	GLU
1	F	75	LEU
1	F	88	ILE
1	F	162	GLU
1	F	249	LEU
1	F	313	MET
1	F	323	ARG
1	F	334	LYS
1	G	14	ARG
1	G	88	ILE
1	G	218	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	355	LEU
1	H	52	LYS
1	H	90	LYS
1	H	173	ASN
1	H	312	ASP
1	H	355	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	145	HIS
1	A	216	HIS
1	C	85	GLN
1	C	216	HIS
1	E	85	GLN
1	E	87	ASN
1	E	138	ASN
1	E	216	HIS
1	F	85	GLN
1	F	138	ASN
1	F	216	HIS
1	H	85	GLN
1	H	129	ASN

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

Of 39 ligands modelled in this entry, 31 are monoatomic - leaving 8 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
3	MMK	D	1358	2	22,22,22	3.18	6 (27%)	24,28,28	4.40	11 (45%)
3	MMK	A	1358	2	22,22,22	3.33	6 (27%)	24,28,28	3.88	10 (41%)
3	MMK	H	1358	2	22,22,22	3.27	6 (27%)	24,28,28	4.13	11 (45%)
3	MMK	G	1358	2	22,22,22	3.25	6 (27%)	24,28,28	3.11	9 (37%)
3	MMK	F	1358	2	22,22,22	3.38	6 (27%)	24,28,28	5.44	8 (33%)
3	MMK	B	1358	2	22,22,22	3.19	6 (27%)	24,28,28	3.72	14 (58%)
3	MMK	C	1358	2	22,22,22	3.30	6 (27%)	24,28,28	5.26	8 (33%)
3	MMK	E	1358	2	22,22,22	3.31	6 (27%)	24,28,28	5.05	10 (41%)

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
3	MMK	D	1358	2	-	7/21/21/21	0/1/1/1
3	MMK	A	1358	2	-	7/21/21/21	0/1/1/1
3	MMK	H	1358	2	-	6/21/21/21	0/1/1/1
3	MMK	G	1358	2	-	4/21/21/21	0/1/1/1
3	MMK	F	1358	2	-	8/21/21/21	0/1/1/1
3	MMK	B	1358	2	-	7/21/21/21	0/1/1/1
3	MMK	C	1358	2	-	4/21/21/21	0/1/1/1
3	MMK	E	1358	2	-	6/21/21/21	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1358	MMK	CAE-CAD	9.86	1.55	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1358	MMK	CAE-CAD	9.68	1.54	1.34
3	A	1358	MMK	CAE-NAF	9.41	1.48	1.33
3	B	1358	MMK	CAE-NAF	9.38	1.48	1.33
3	E	1358	MMK	CAE-CAD	9.30	1.53	1.34
3	G	1358	MMK	CAE-CAD	9.03	1.53	1.34
3	D	1358	MMK	CAE-NAF	8.96	1.47	1.33
3	A	1358	MMK	CAE-CAD	8.94	1.53	1.34
3	H	1358	MMK	CAE-CAD	8.83	1.52	1.34
3	H	1358	MMK	CAE-NAF	8.71	1.47	1.33
3	G	1358	MMK	CAE-NAF	8.49	1.46	1.33
3	E	1358	MMK	CAE-NAF	8.37	1.46	1.33
3	D	1358	MMK	CAE-CAD	8.32	1.51	1.34
3	F	1358	MMK	CAE-NAF	8.25	1.46	1.33
3	C	1358	MMK	CAE-NAF	8.19	1.46	1.33
3	B	1358	MMK	CAE-CAD	8.07	1.51	1.34
3	F	1358	MMK	CAL-CAM	-5.61	1.38	1.50
3	H	1358	MMK	CAL-CAM	-5.38	1.39	1.50
3	E	1358	MMK	CAL-CAM	-5.27	1.39	1.50
3	D	1358	MMK	CAL-CAM	-5.19	1.39	1.50
3	F	1358	MMK	CAD-NAC	4.89	1.48	1.38
3	B	1358	MMK	CAL-CAM	-4.86	1.40	1.50
3	G	1358	MMK	CAD-NAC	4.82	1.48	1.38
3	E	1358	MMK	CAD-NAC	4.81	1.47	1.38
3	C	1358	MMK	CAL-CAM	-4.80	1.40	1.50
3	G	1358	MMK	CAL-CAM	-4.74	1.40	1.50
3	A	1358	MMK	CAD-NAC	4.73	1.47	1.38
3	F	1358	MMK	CAO-CAS	-4.72	1.39	1.49
3	A	1358	MMK	CAL-CAM	-4.59	1.41	1.50
3	H	1358	MMK	CAO-CAS	-4.51	1.39	1.49
3	H	1358	MMK	CAD-NAC	4.49	1.47	1.38
3	E	1358	MMK	CAO-CAS	-4.45	1.40	1.49
3	G	1358	MMK	CAO-CAS	-4.41	1.40	1.49
3	B	1358	MMK	CAO-CAS	-4.38	1.40	1.49
3	C	1358	MMK	CAO-CAS	-4.34	1.40	1.49
3	C	1358	MMK	CAD-NAC	4.30	1.47	1.38
3	A	1358	MMK	CAO-CAS	-4.30	1.40	1.49
3	D	1358	MMK	CAD-NAC	4.10	1.46	1.38
3	D	1358	MMK	CAO-CAS	-3.95	1.41	1.49
3	B	1358	MMK	CAD-NAC	3.64	1.45	1.38
3	D	1358	MMK	CAQ-NAR	2.73	1.40	1.34
3	G	1358	MMK	CAQ-NAR	2.72	1.40	1.34
3	C	1358	MMK	CAQ-NAR	2.68	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1358	MMK	CAQ-NAR	2.63	1.40	1.34
3	F	1358	MMK	CAQ-NAR	2.53	1.39	1.34
3	B	1358	MMK	CAQ-NAR	2.48	1.39	1.34
3	A	1358	MMK	CAQ-NAR	2.39	1.39	1.34
3	H	1358	MMK	CAQ-NAR	2.20	1.39	1.34

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1358	MMK	CAH-NAF-CAE	-21.95	98.12	121.47
3	C	1358	MMK	CAG-NAF-CAE	-20.98	99.15	121.47
3	E	1358	MMK	CAH-NAF-CAE	-19.65	100.57	121.47
3	D	1358	MMK	CAG-NAF-CAE	-16.83	103.57	121.47
3	H	1358	MMK	CAH-NAF-CAE	-16.24	104.19	121.47
3	A	1358	MMK	CAH-NAF-CAE	-13.18	107.45	121.47
3	C	1358	MMK	CAH-NAF-CAE	-13.03	107.61	121.47
3	F	1358	MMK	CAG-NAF-CAE	-12.30	108.39	121.47
3	G	1358	MMK	CAG-NAF-CAE	-11.97	108.74	121.47
3	B	1358	MMK	CAH-NAF-CAE	-11.70	109.03	121.47
3	E	1358	MMK	CAG-NAF-CAE	-10.78	110.00	121.47
3	A	1358	MMK	CAG-NAF-CAE	-7.69	113.29	121.47
3	D	1358	MMK	CAH-NAF-CAE	-7.33	113.68	121.47
3	A	1358	MMK	CAL-N-CA	6.65	120.46	112.72
3	B	1358	MMK	CAB-NAC-C	6.61	128.23	119.24
3	D	1358	MMK	CAL-N-CA	6.42	120.20	112.72
3	H	1358	MMK	CAG-NAF-CAE	-6.41	114.65	121.47
3	B	1358	MMK	CAG-NAF-CAE	-5.47	115.66	121.47
3	H	1358	MMK	CAL-N-CA	5.33	118.93	112.72
3	D	1358	MMK	CAB-NAC-C	5.05	126.11	119.24
3	E	1358	MMK	CAL-N-CA	4.98	118.52	112.72
3	E	1358	MMK	CAB-NAC-C	4.62	125.53	119.24
3	B	1358	MMK	CA-C-NAC	4.50	122.33	116.61
3	B	1358	MMK	CAP-CAQ-NAR	-4.45	118.52	123.97
3	F	1358	MMK	C-CA-N	-4.44	103.11	112.81
3	G	1358	MMK	CAH-NAF-CAE	-4.28	116.92	121.47
3	B	1358	MMK	CAM-CAL-N	-3.99	105.83	113.29
3	A	1358	MMK	CAB-NAC-C	3.95	124.61	119.24
3	H	1358	MMK	CAB-NAC-C	3.88	124.52	119.24
3	F	1358	MMK	CAG-NAF-CAH	-3.86	98.24	117.35
3	C	1358	MMK	CAP-CAQ-NAR	-3.75	119.38	123.97
3	H	1358	MMK	CAP-CAQ-NAR	-3.71	119.42	123.97
3	A	1358	MMK	CAP-CAQ-NAR	-3.68	119.46	123.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1358	MMK	CAP-CAQ-NAR	-3.55	119.62	123.97
3	D	1358	MMK	CA-C-NAC	3.55	121.13	116.61
3	E	1358	MMK	CA-C-NAC	3.49	121.06	116.61
3	G	1358	MMK	CAM-CAL-N	-3.46	106.83	113.29
3	D	1358	MMK	CAP-CAQ-NAR	-3.43	119.76	123.97
3	F	1358	MMK	CAP-CAQ-NAR	-3.34	119.88	123.97
3	G	1358	MMK	CAP-CAQ-NAR	-3.34	119.89	123.97
3	B	1358	MMK	CAQ-NAR-CAM	3.26	121.98	117.41
3	A	1358	MMK	CA-C-NAC	3.17	120.64	116.61
3	B	1358	MMK	CAL-N-CA	3.09	116.32	112.72
3	E	1358	MMK	CAG-NAF-CAH	-3.01	102.44	117.35
3	B	1358	MMK	C-CA-N	-2.97	106.33	112.81
3	A	1358	MMK	C-CA-N	-2.96	106.33	112.81
3	C	1358	MMK	CAQ-NAR-CAM	2.88	121.45	117.41
3	F	1358	MMK	CA-C-NAC	2.87	120.26	116.61
3	A	1358	MMK	OAT-CAS-CAO	2.86	122.18	114.84
3	G	1358	MMK	CAQ-NAR-CAM	2.81	121.36	117.41
3	H	1358	MMK	CAQ-NAR-CAM	2.79	121.32	117.41
3	H	1358	MMK	C-CA-N	-2.77	106.76	112.81
3	B	1358	MMK	O-C-NAC	-2.64	117.98	121.66
3	A	1358	MMK	OAT-CAS-OAU	-2.63	117.71	123.35
3	H	1358	MMK	CA-C-NAC	2.59	119.91	116.61
3	G	1358	MMK	CAB-NAC-C	2.52	122.67	119.24
3	G	1358	MMK	CAL-N-CA	2.50	115.64	112.72
3	E	1358	MMK	OAT-CAS-CAO	2.49	121.24	114.84
3	D	1358	MMK	CAQ-NAR-CAM	2.49	120.91	117.41
3	B	1358	MMK	OAT-CAS-CAO	2.48	121.20	114.84
3	E	1358	MMK	CAQ-NAR-CAM	2.46	120.87	117.41
3	C	1358	MMK	OAT-CAS-CAO	2.42	121.04	114.84
3	B	1358	MMK	CAL-CAM-CAN	2.41	124.69	120.45
3	F	1358	MMK	OAT-CAS-CAO	2.36	120.90	114.84
3	A	1358	MMK	CAQ-NAR-CAM	2.34	120.69	117.41
3	G	1358	MMK	OAT-CAS-CAO	2.34	120.84	114.84
3	D	1358	MMK	OAT-CAS-OAU	-2.34	118.33	123.35
3	D	1358	MMK	OAT-CAS-CAO	2.32	120.80	114.84
3	H	1358	MMK	OAT-CAS-CAO	2.29	120.71	114.84
3	H	1358	MMK	OAT-CAS-OAU	-2.28	118.44	123.35
3	C	1358	MMK	CAL-N-CA	2.28	115.38	112.72
3	D	1358	MMK	CAG-NAF-CAH	-2.27	106.10	117.35
3	E	1358	MMK	OAT-CAS-OAU	-2.27	118.48	123.35
3	D	1358	MMK	C-CA-N	-2.26	107.88	112.81
3	F	1358	MMK	CAQ-NAR-CAM	2.16	120.45	117.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1358	MMK	CAG-NAF-CAH	-2.12	106.86	117.35
3	C	1358	MMK	OAT-CAS-OAU	-2.06	118.92	123.35
3	B	1358	MMK	CAG-NAF-CAH	-2.03	107.32	117.35
3	G	1358	MMK	OAT-CAS-OAU	-2.03	119.00	123.35
3	B	1358	MMK	OAT-CAS-OAU	-2.01	119.03	123.35
3	H	1358	MMK	CAA-CAB-NAC	-2.01	104.98	111.74

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1358	MMK	CAE-CAD-NAC-C
3	A	1358	MMK	CAD-CAE-NAF-CAH
3	A	1358	MMK	CAD-CAE-NAF-CAG
3	B	1358	MMK	CA-C-NAC-CAB
3	B	1358	MMK	CAE-CAD-NAC-CAB
3	B	1358	MMK	CAD-CAE-NAF-CAG
3	C	1358	MMK	CA-C-NAC-CAB
3	C	1358	MMK	NAC-CAD-CAE-NAF
3	C	1358	MMK	CAD-CAE-NAF-CAG
3	D	1358	MMK	CA-C-NAC-CAB
3	D	1358	MMK	CAD-CAE-NAF-CAH
3	D	1358	MMK	CAD-CAE-NAF-CAG
3	E	1358	MMK	CAE-CAD-NAC-C
3	E	1358	MMK	CAD-CAE-NAF-CAH
3	F	1358	MMK	CA-C-NAC-CAB
3	F	1358	MMK	NAC-CAD-CAE-NAF
3	F	1358	MMK	CAD-CAE-NAF-CAH
3	G	1358	MMK	CA-C-NAC-CAB
3	G	1358	MMK	CAD-CAE-NAF-CAH
3	H	1358	MMK	CA-C-NAC-CAB
3	H	1358	MMK	CAE-CAD-NAC-C
3	H	1358	MMK	CAD-CAE-NAF-CAH
3	H	1358	MMK	CAD-CAE-NAF-CAG
3	F	1358	MMK	CAD-CAE-NAF-CAG
3	D	1358	MMK	CAE-CAD-NAC-CAB
3	H	1358	MMK	CAE-CAD-NAC-CAB
3	A	1358	MMK	CA-C-NAC-CAB
3	E	1358	MMK	CA-C-NAC-CAB
3	B	1358	MMK	CAE-CAD-NAC-C
3	B	1358	MMK	NAC-CAD-CAE-NAF
3	B	1358	MMK	CAD-CAE-NAF-CAH

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1358	MMK	CAN-CAO-CAS-OAU
3	F	1358	MMK	C-CA-N-CAL
3	A	1358	MMK	CAE-CAD-NAC-CAB
3	E	1358	MMK	CAE-CAD-NAC-CAB
3	E	1358	MMK	CAN-CAO-CAS-OAU
3	D	1358	MMK	CAN-CAO-CAS-OAU
3	A	1358	MMK	O-C-NAC-CAB
3	B	1358	MMK	O-C-NAC-CAB
3	C	1358	MMK	O-C-NAC-CAB
3	D	1358	MMK	O-C-NAC-CAB
3	E	1358	MMK	O-C-NAC-CAB
3	F	1358	MMK	O-C-NAC-CAB
3	G	1358	MMK	O-C-NAC-CAB
3	H	1358	MMK	O-C-NAC-CAB
3	D	1358	MMK	CAE-CAD-NAC-C
3	F	1358	MMK	CAE-CAD-NAC-C
3	F	1358	MMK	CAE-CAD-NAC-CAB
3	G	1358	MMK	CAE-CAD-NAC-CAB

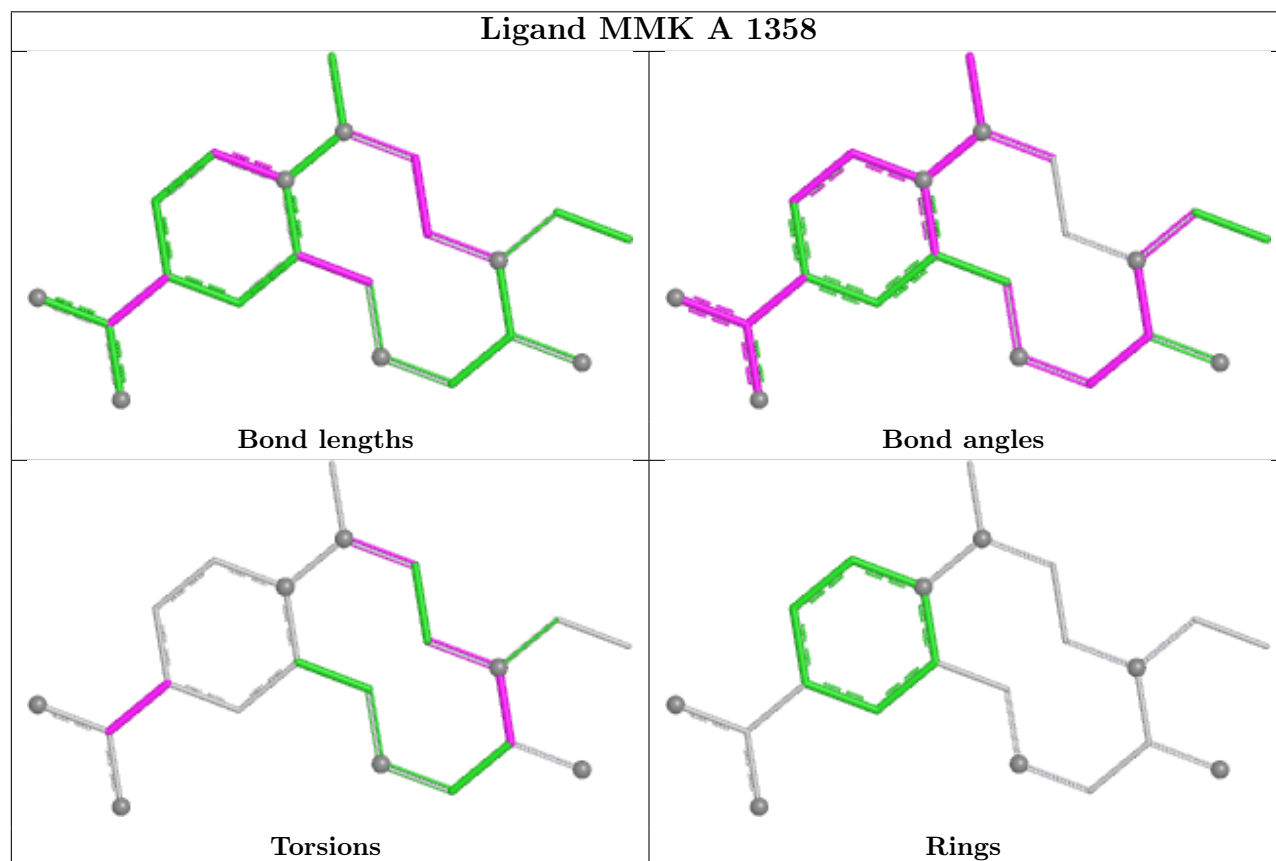
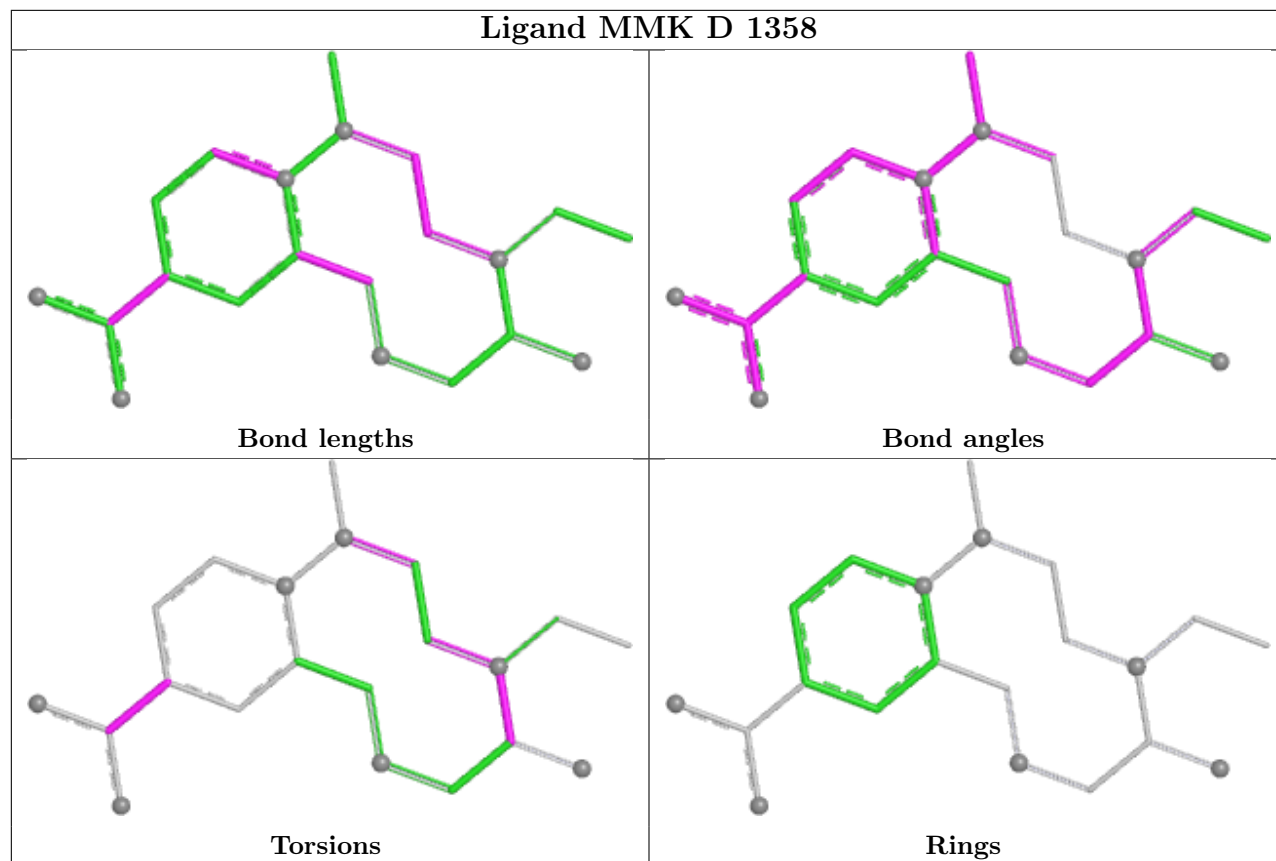
There are no ring outliers.

7 monomers are involved in 8 short contacts:

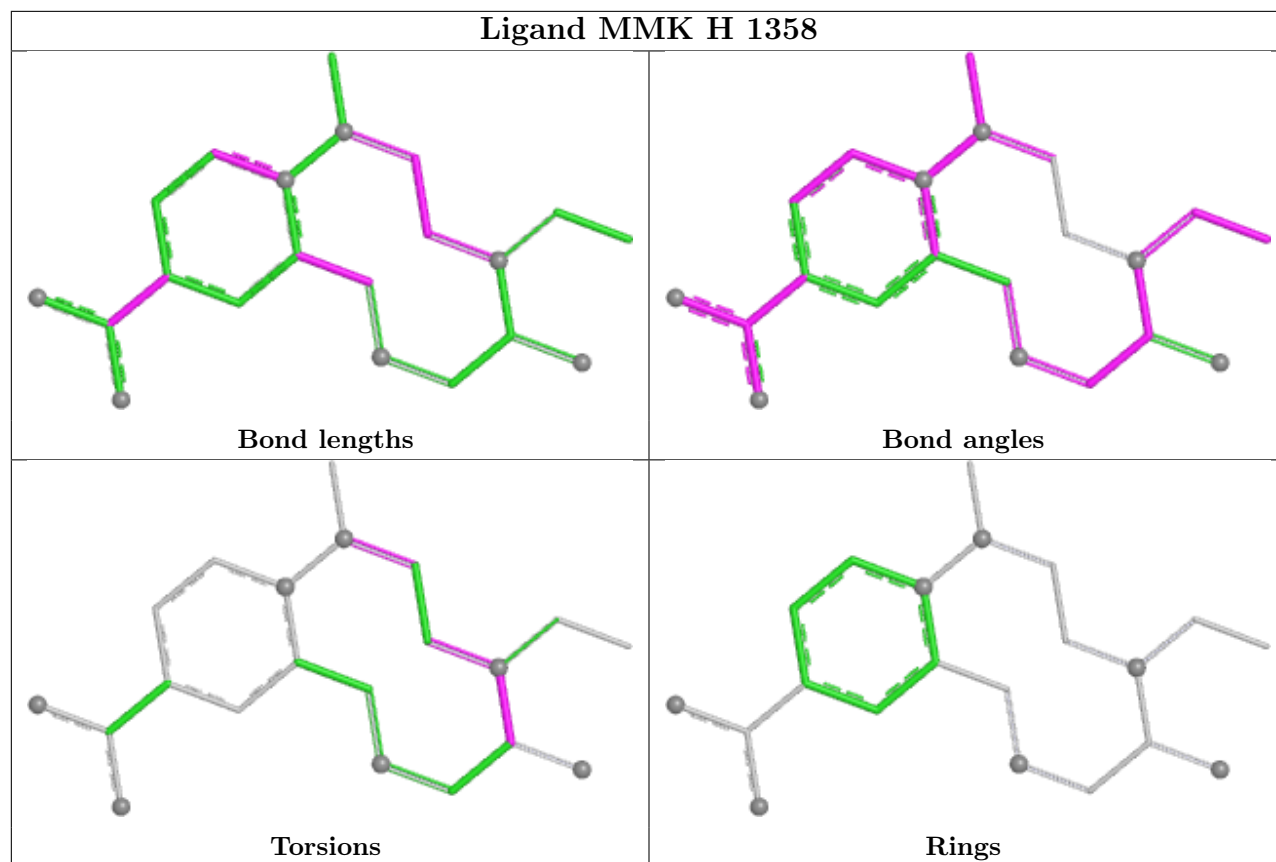
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1358	MMK	1	0
3	A	1358	MMK	1	0
3	H	1358	MMK	1	0
3	F	1358	MMK	1	0
3	B	1358	MMK	1	0
3	C	1358	MMK	1	0
3	E	1358	MMK	2	0

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

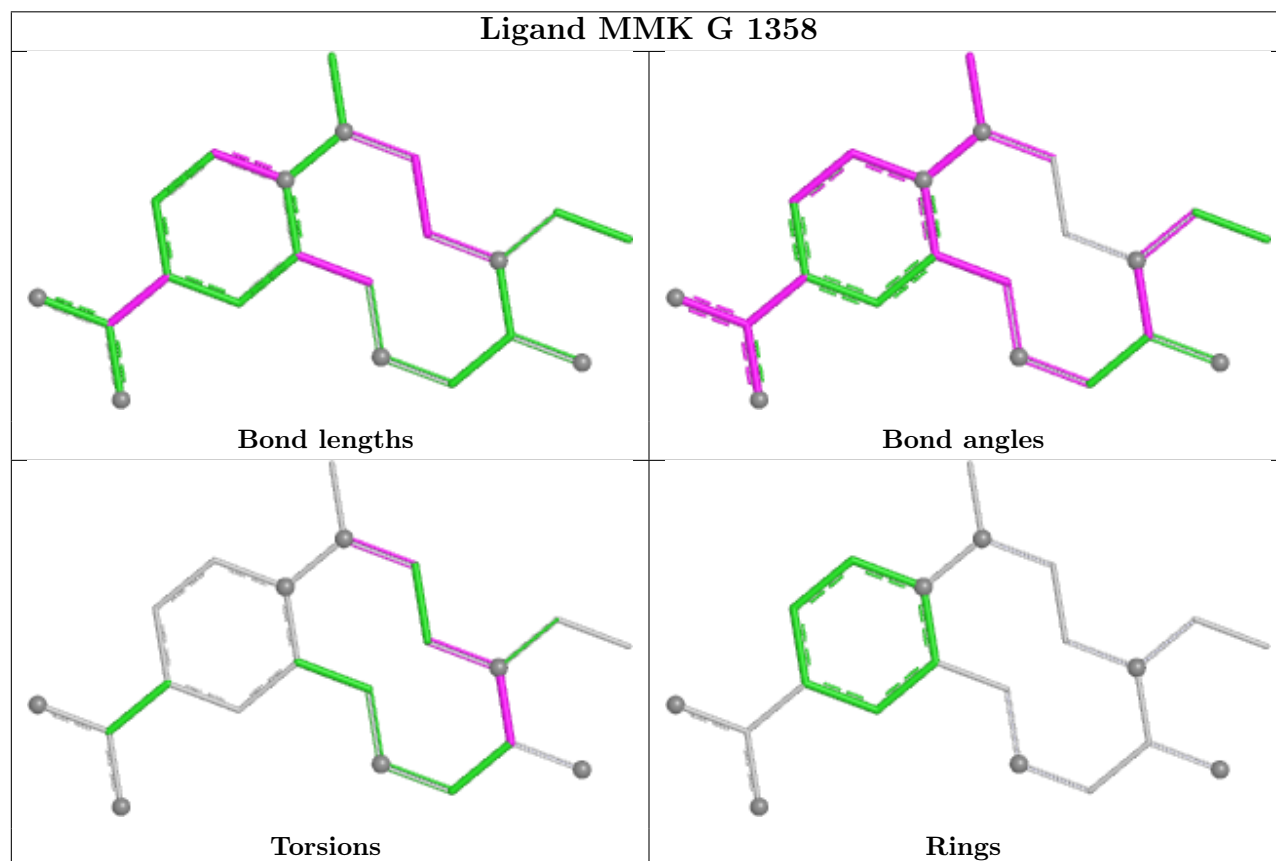
equivalents in the CSD to analyse the geometry.



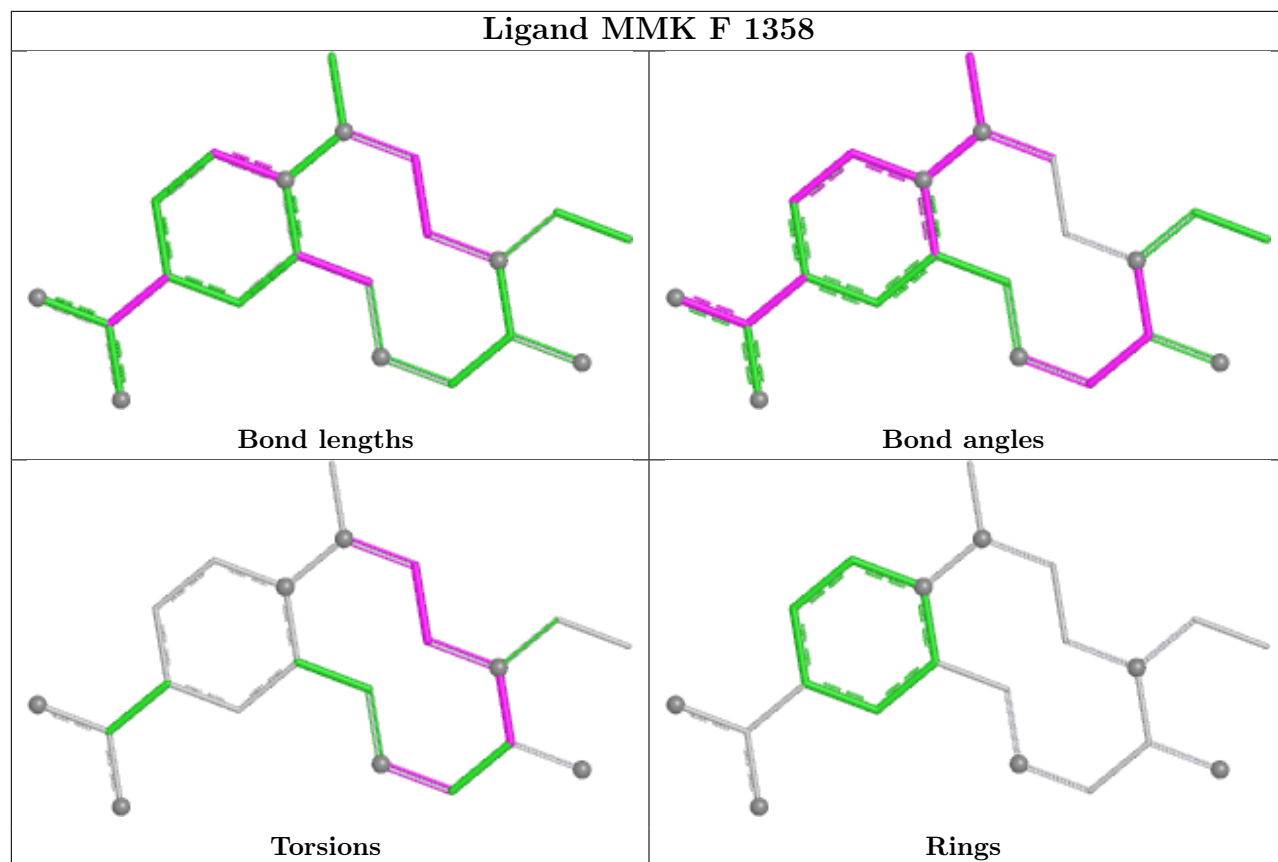
Ligand MMK H 1358



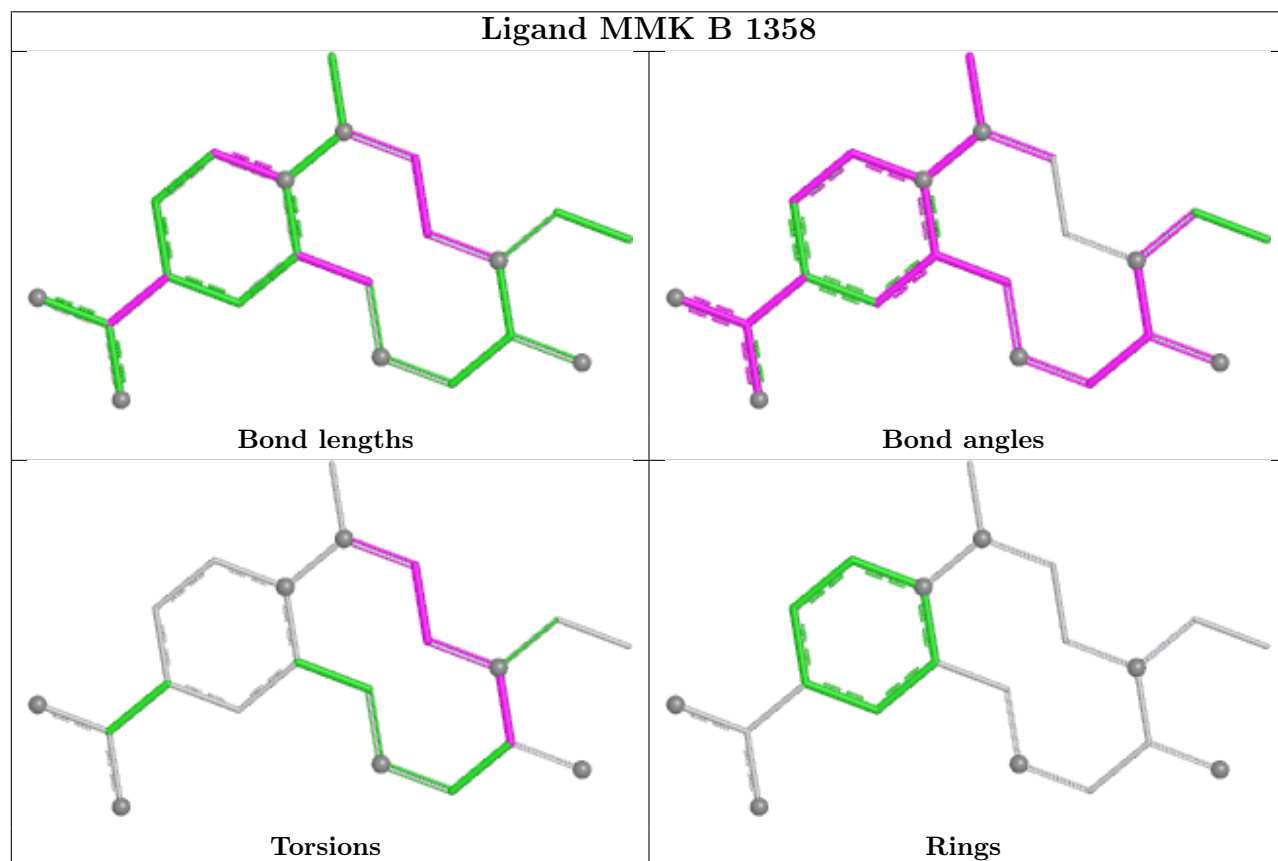
Ligand MMK G 1358



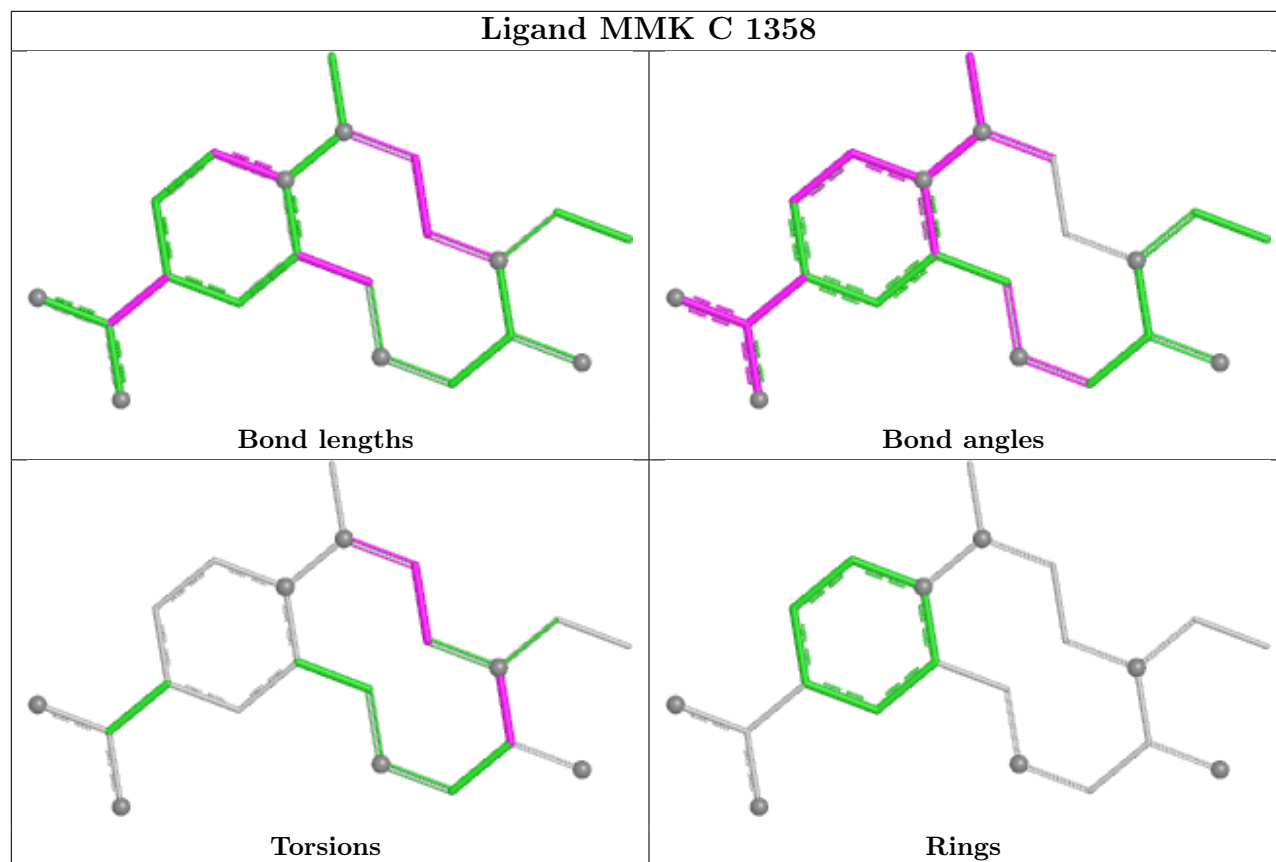
Ligand MMK F 1358



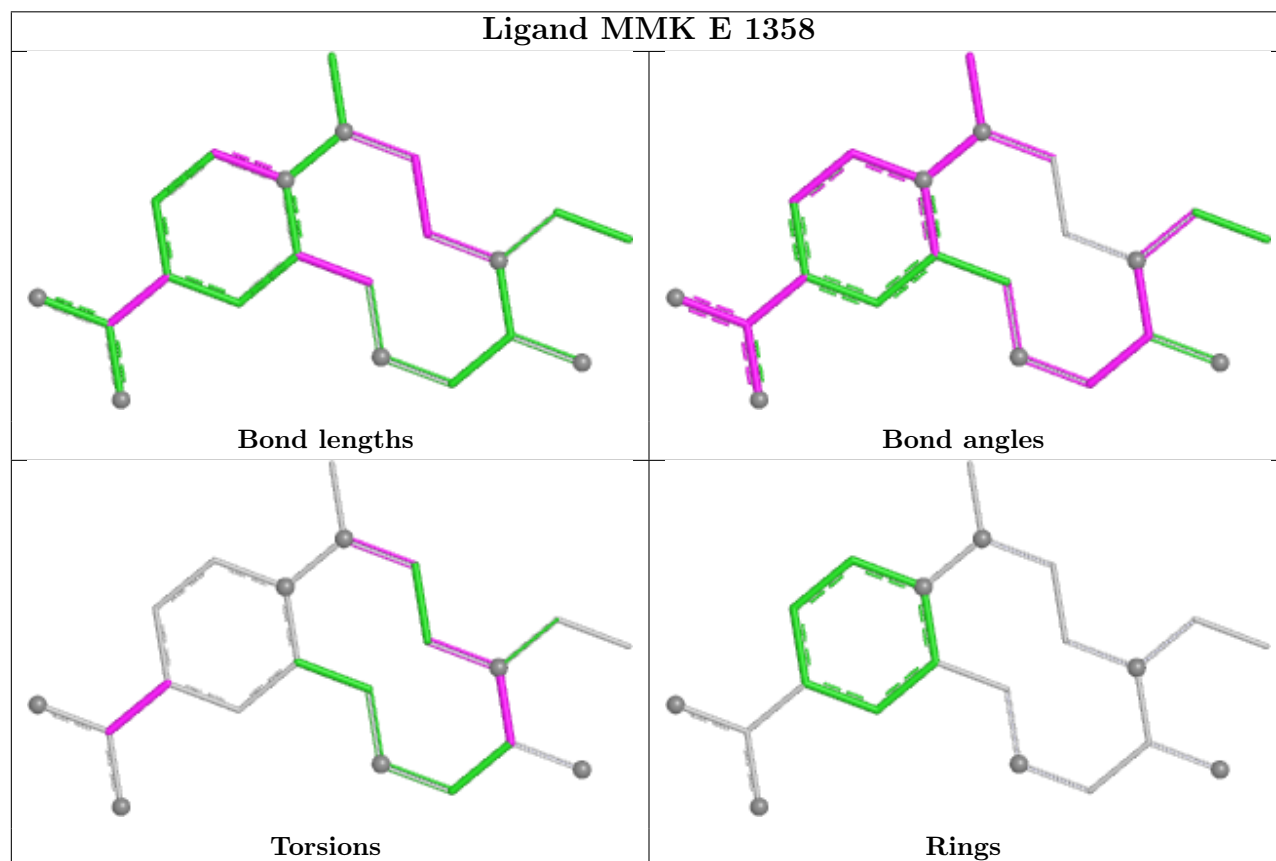
Ligand MMK B 1358



Ligand MMK C 1358



Ligand MMK E 1358



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	337/360 (93%)	0.01	13 (3%)	43	40	19, 31, 66, 97	0
1	B	343/360 (95%)	0.11	26 (7%)	20	17	12, 31, 69, 123	1 (0%)
1	C	342/360 (95%)	0.14	22 (6%)	25	22	21, 32, 71, 120	0
1	D	342/360 (95%)	-0.04	18 (5%)	32	29	21, 31, 64, 106	0
1	E	341/360 (94%)	0.23	19 (5%)	30	27	25, 39, 66, 125	0
1	F	342/360 (95%)	0.33	18 (5%)	32	29	25, 41, 68, 125	0
1	G	343/360 (95%)	0.36	25 (7%)	21	18	24, 40, 66, 115	0
1	H	340/360 (94%)	0.01	11 (3%)	50	49	19, 31, 54, 116	0
All	All	2730/2880 (94%)	0.14	152 (5%)	30	27	12, 35, 67, 125	1 (0%)

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	171	GLY	8.6
1	F	171	GLY	6.8
1	H	155	ARG	6.5
1	E	171	GLY	6.4
1	F	172	VAL	6.2
1	D	171	GLY	6.1
1	F	9	LEU	5.9
1	F	12	SER	5.7
1	G	164	GLU	5.4
1	H	356	LYS	5.3
1	B	169	ILE	5.2
1	C	9	LEU	5.0
1	D	356	LYS	4.9
1	E	10	ASN	4.8
1	E	9	LEU	4.8
1	C	356	LYS	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	12	SER	4.7
1	B	356	LYS	4.7
1	G	356	LYS	4.7
1	A	12	SER	4.6
1	D	163	LYS	4.6
1	B	53	GLU	4.5
1	F	356	LYS	4.5
1	C	313	MET	4.4
1	F	10	ASN	4.4
1	E	172	VAL	4.4
1	B	313	MET	4.3
1	B	309	CYS	4.3
1	E	170	GLU	4.2
1	C	172	VAL	4.2
1	B	163	LYS	4.1
1	A	312	ASP	4.1
1	C	170	GLU	4.1
1	F	163	LYS	4.1
1	F	114	GLU	4.0
1	C	312	ASP	4.0
1	D	336	GLY	4.0
1	B	310	ARG	4.0
1	E	161	VAL	3.9
1	E	162	GLU	3.9
1	B	312	ASP	3.8
1	G	163	LYS	3.7
1	B	9	LEU	3.7
1	H	355	LEU	3.7
1	H	162	GLU	3.6
1	H	311	LYS	3.6
1	D	9	LEU	3.5
1	A	356	LYS	3.5
1	C	163	LYS	3.5
1	C	319	ASP	3.5
1	E	312	ASP	3.5
1	G	313	MET	3.4
1	B	335	ALA	3.4
1	F	313	MET	3.3
1	A	335	ALA	3.3
1	E	114	GLU	3.3
1	A	313	MET	3.3
1	F	11	PRO	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	335	ALA	3.3
1	D	355	LEU	3.3
1	F	170	GLU	3.2
1	G	171	GLY	3.1
1	G	53	GLU	3.1
1	G	311	LYS	3.1
1	G	355	LEU	3.1
1	F	133	TYR	3.1
1	D	334	LYS	3.1
1	E	356	LYS	3.1
1	F	312	ASP	3.1
1	C	327	PRO	3.0
1	D	311	LYS	3.0
1	H	312	ASP	2.9
1	C	355	LEU	2.9
1	G	9	LEU	2.9
1	H	313	MET	2.9
1	G	133	TYR	2.9
1	A	114	GLU	2.8
1	A	336	GLY	2.8
1	A	13	ALA	2.8
1	G	65	ASP	2.8
1	F	311	LYS	2.8
1	G	170	GLU	2.8
1	A	113	SER	2.8
1	B	114	GLU	2.8
1	F	162	GLU	2.7
1	B	311	LYS	2.6
1	C	113	SER	2.6
1	B	254	TYR	2.6
1	D	172	VAL	2.6
1	D	162	GLU	2.6
1	C	336	GLY	2.6
1	B	355	LEU	2.6
1	C	308	SER	2.6
1	G	236	GLU	2.5
1	H	154	LEU	2.5
1	D	72	ILE	2.5
1	B	12	SER	2.5
1	E	11	PRO	2.5
1	B	236	GLU	2.5
1	A	355	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	52	LYS	2.5
1	C	161	VAL	2.5
1	A	310	ARG	2.5
1	G	339	ASN	2.5
1	G	111	ARG	2.4
1	B	227	PHE	2.4
1	C	329	ARG	2.4
1	B	329	ARG	2.4
1	C	310	ARG	2.4
1	B	323	ARG	2.4
1	E	354	PHE	2.4
1	D	335	ALA	2.4
1	B	11	PRO	2.3
1	A	161	VAL	2.3
1	C	331	LYS	2.3
1	H	160	LEU	2.3
1	A	330	TYR	2.3
1	D	170	GLU	2.3
1	F	249	LEU	2.3
1	F	61	ASP	2.3
1	E	311	LYS	2.3
1	G	72	ILE	2.3
1	E	319	ASP	2.3
1	G	172	VAL	2.3
1	C	334	LYS	2.2
1	G	161	VAL	2.2
1	H	63	ILE	2.2
1	G	314	VAL	2.2
1	E	352	ALA	2.2
1	G	55	LYS	2.2
1	B	337	LYS	2.2
1	D	331	LYS	2.2
1	E	355	LEU	2.1
1	F	355	LEU	2.1
1	B	235	CYS	2.1
1	E	53	GLU	2.1
1	E	313	MET	2.1
1	B	112	TYR	2.1
1	G	310	ARG	2.1
1	D	113	SER	2.1
1	D	319	ASP	2.1
1	B	316	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	112	TYR	2.1
1	H	323	ARG	2.1
1	C	162	GLU	2.1
1	D	312	ASP	2.1
1	B	314	VAL	2.0
1	G	162	GLU	2.0
1	D	112	TYR	2.0
1	B	14	ARG	2.0
1	C	227	PHE	2.0
1	G	219	ARG	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
5	NI	H	1363	1/1	0.75	0.20	119,119,119,119	0
5	NI	D	1362	1/1	0.78	0.18	103,103,103,103	0
4	ZN	B	1359	1/1	0.78	0.28	82,82,82,82	0
5	NI	H	1362	1/1	0.82	0.18	103,103,103,103	0
5	NI	C	1360	1/1	0.83	0.18	90,90,90,90	0
5	NI	H	1361	1/1	0.85	0.15	120,120,120,120	0
3	MMK	F	1358	22/22	0.90	0.14	36,40,52,53	0
3	MMK	E	1358	22/22	0.91	0.13	36,38,54,57	0
3	MMK	D	1358	22/22	0.91	0.13	20,29,47,49	0
3	MMK	C	1358	22/22	0.92	0.12	18,33,44,47	0
3	MMK	H	1358	22/22	0.92	0.12	21,28,40,45	0
5	NI	B	1360	1/1	0.94	0.10	73,73,73,73	0
3	MMK	G	1358	22/22	0.94	0.10	26,34,47,49	0

Continued on next page...

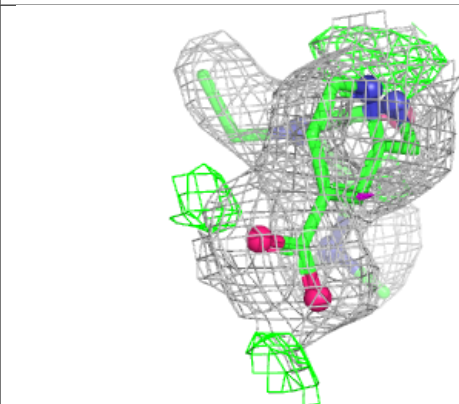
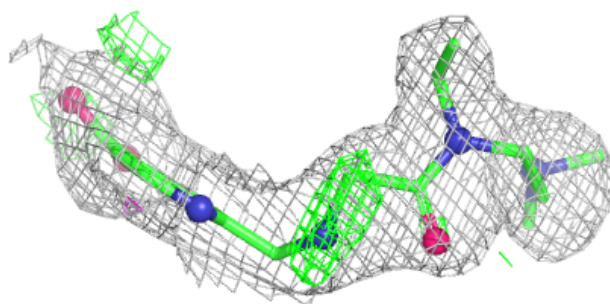
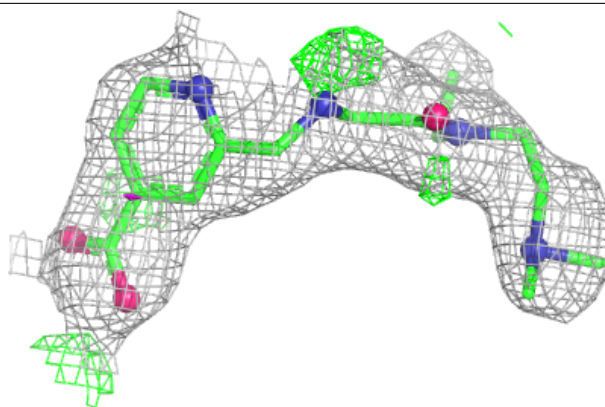
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MMK	A	1358	22/22	0.95	0.10	16,21,43,43	0
5	NI	D	1361	1/1	0.95	0.08	80,80,80,80	0
5	NI	A	1360	1/1	0.95	0.10	65,65,65,65	0
5	NI	A	1361	1/1	0.95	0.09	87,87,87,87	0
5	NI	A	1362	1/1	0.95	0.07	85,85,85,85	0
3	MMK	B	1358	22/22	0.95	0.09	17,24,38,39	0
5	NI	B	1361	1/1	0.96	0.09	69,69,69,69	0
5	NI	C	1361	1/1	0.97	0.05	62,62,62,62	0
5	NI	D	1360	1/1	0.97	0.10	64,64,64,64	0
5	NI	H	1360	1/1	0.97	0.10	57,57,57,57	0
5	NI	G	1360	1/1	0.98	0.11	65,65,65,65	0
4	ZN	A	1359	1/1	0.99	0.02	38,38,38,38	0
2	MN	F	1357	1/1	0.99	0.04	27,27,27,27	0
4	ZN	D	1359	1/1	0.99	0.02	39,39,39,39	0
4	ZN	E	1359	1/1	0.99	0.02	38,38,38,38	0
4	ZN	F	1359	1/1	0.99	0.03	38,38,38,38	0
2	MN	E	1357	1/1	1.00	0.04	26,26,26,26	0
2	MN	A	1357	1/1	1.00	0.02	20,20,20,20	0
2	MN	G	1357	1/1	1.00	0.01	23,23,23,23	0
4	ZN	G	1359	1/1	1.00	0.01	41,41,41,41	0
4	ZN	H	1359	1/1	1.00	0.01	35,35,35,35	0
2	MN	H	1357	1/1	1.00	0.02	17,17,17,17	0
2	MN	B	1357	1/1	1.00	0.01	17,17,17,17	0
2	MN	C	1357	1/1	1.00	0.01	23,23,23,23	0
2	MN	D	1357	1/1	1.00	0.01	18,18,18,18	0
4	ZN	C	1359	1/1	1.00	0.03	46,46,46,46	0

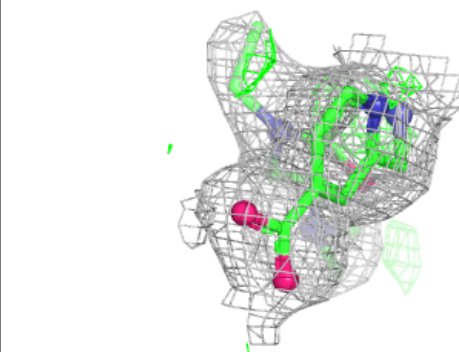
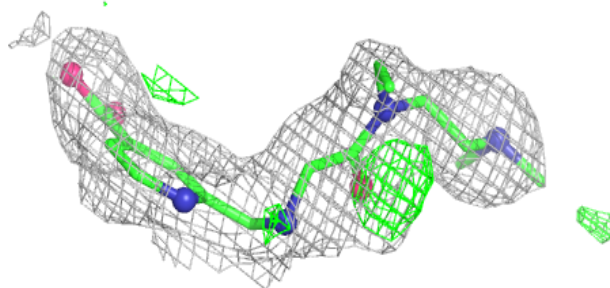
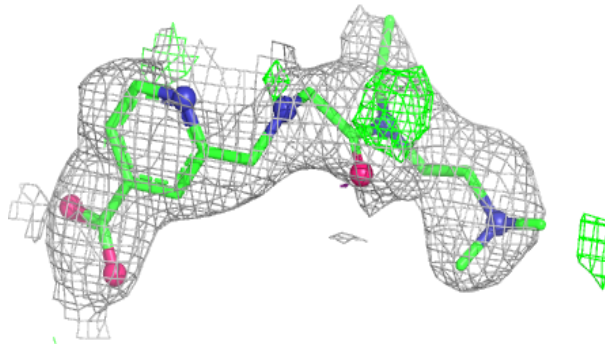
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MMK F 1358:

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

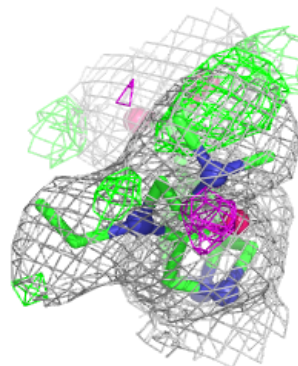
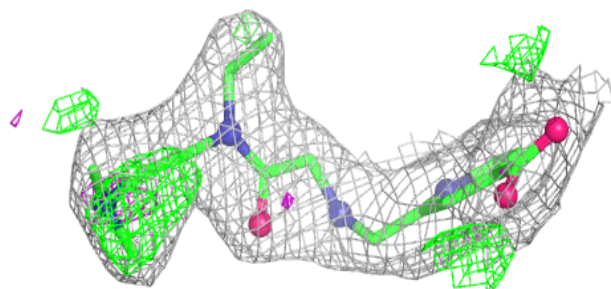
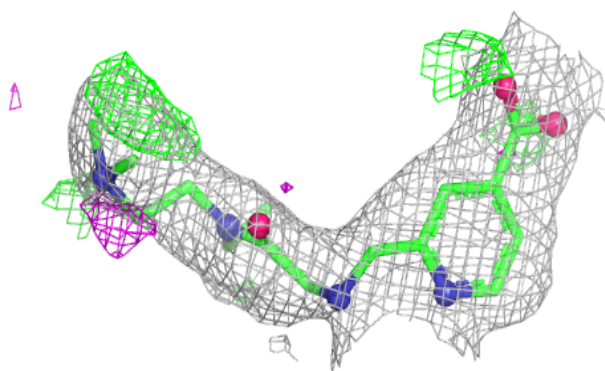
**Electron density around MMK E 1358:**

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

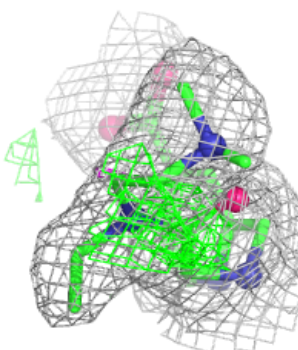
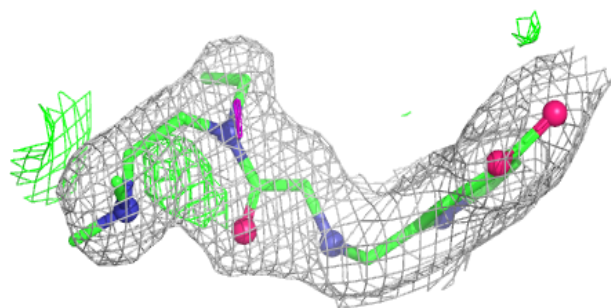
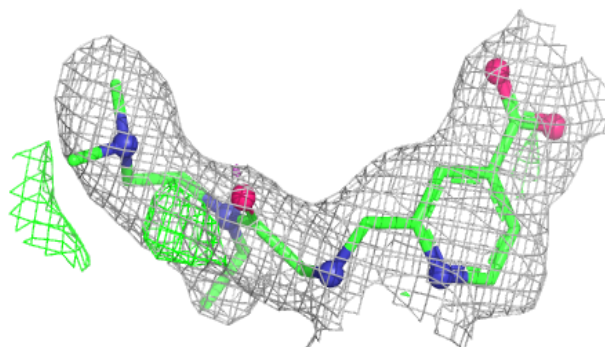


Electron density around MMK D 1358:

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

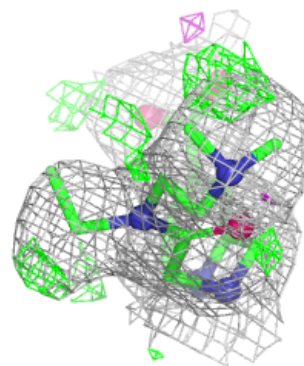
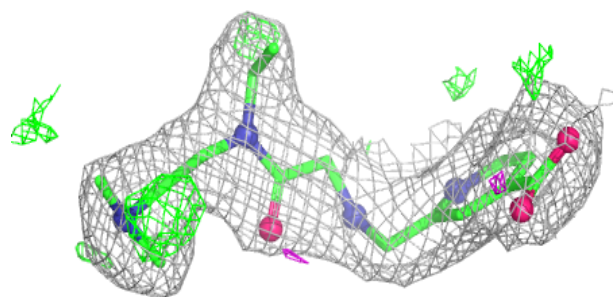
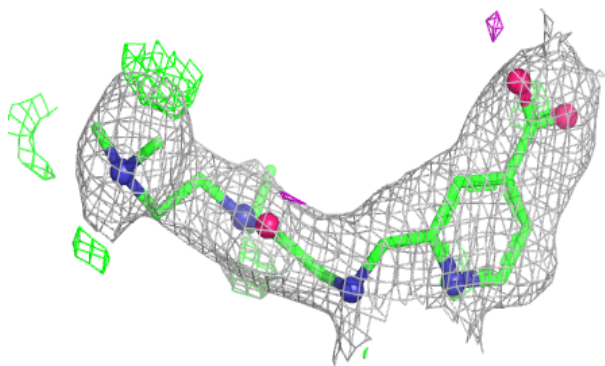
**Electron density around MMK C 1358:**

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

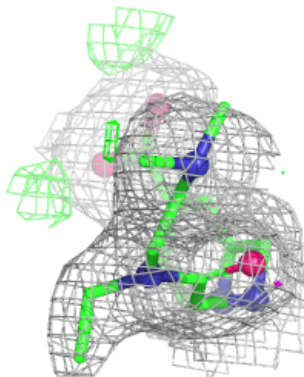
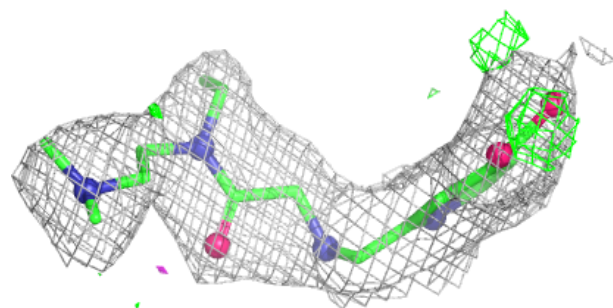
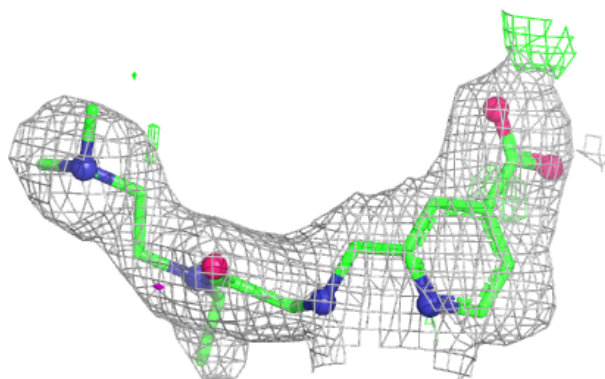


Electron density around MMK H 1358:

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

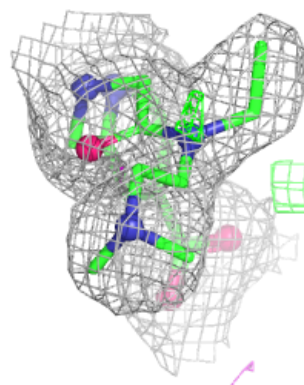
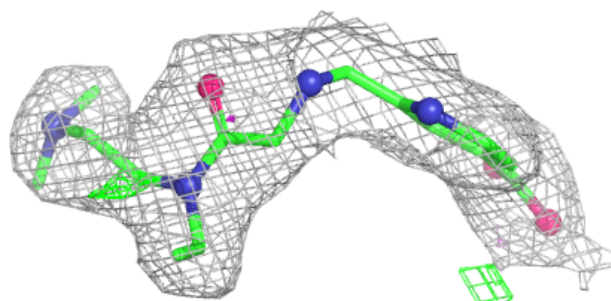
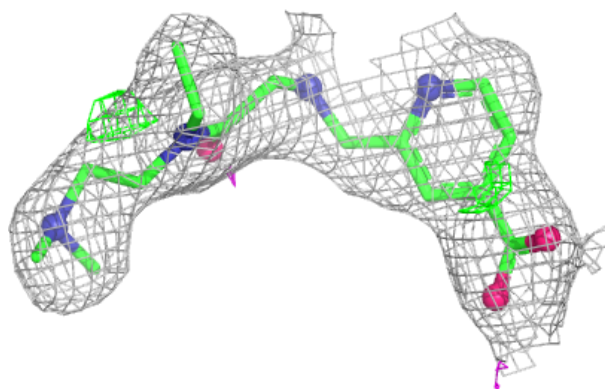
**Electron density around MMK G 1358:**

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

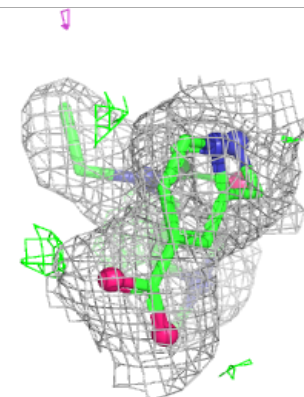
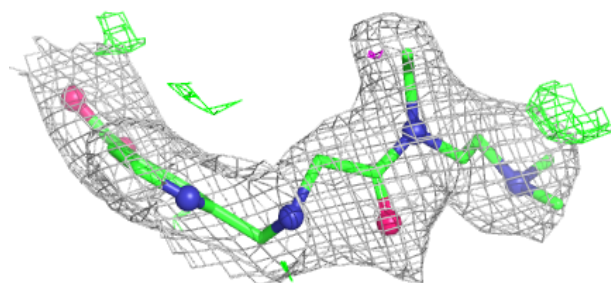
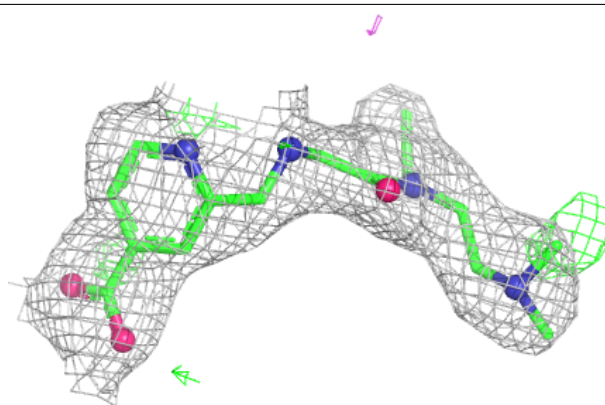


Electron density around MMK A 1358:

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

**Electron density around MMK B 1358:**

$2mF_o-DF_c$ (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.