



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:21 AM UTC

PDB ID : 7U98 / pdb_00007u98
Title : EGFR(T790M/V948R) in complex with a macrocyclic inhibitor
Authors : Beyett, T.S.; Eck, M.J.
Deposited on : 2022-03-10
Resolution : 3.42 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

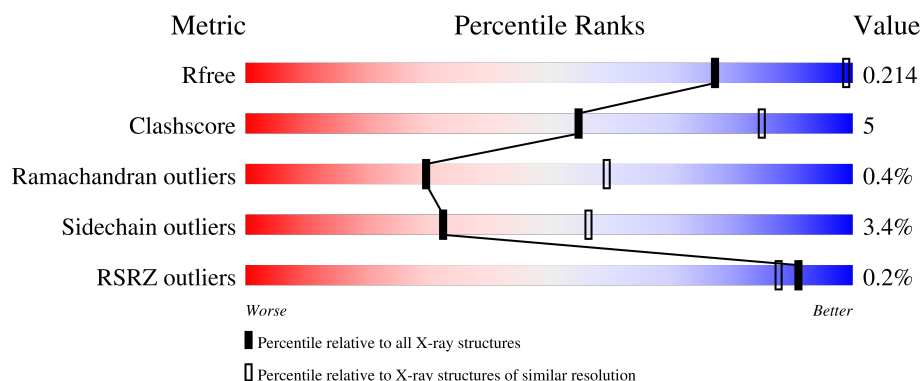
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

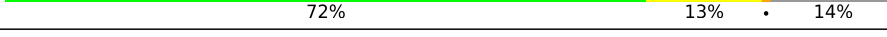
The reported resolution of this entry is 3.42 Å.

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	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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	331	
1	B	331	
1	C	331	
1	D	331	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9427 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.

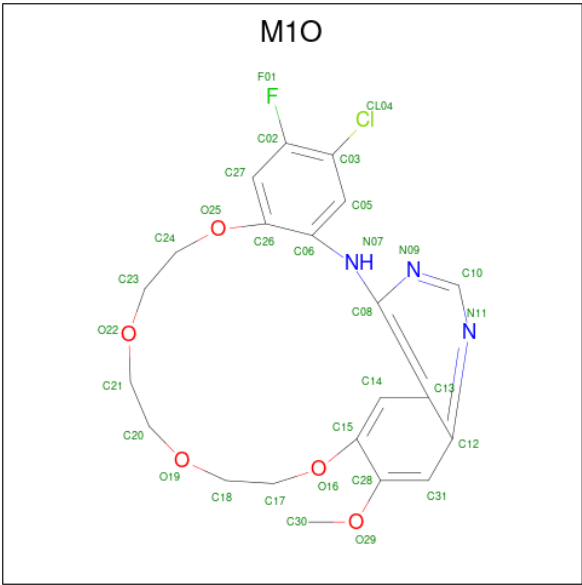
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2322	1495	395	413	19			
1	B	293	Total	C	N	O	S	0	0	0
			2365	1523	403	421	18			
1	C	286	Total	C	N	O	S	0	0	0
			2312	1489	393	411	19			
1	D	285	Total	C	N	O	S	0	0	0
			2304	1482	392	411	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	692	GLY	-	expression tag	UNP P00533
A	693	SER	-	expression tag	UNP P00533
A	694	THR	-	expression tag	UNP P00533
A	790	MET	THR	engineered mutation	UNP P00533
A	948	ARG	VAL	engineered mutation	UNP P00533
B	692	GLY	-	expression tag	UNP P00533
B	693	SER	-	expression tag	UNP P00533
B	694	THR	-	expression tag	UNP P00533
B	790	MET	THR	engineered mutation	UNP P00533
B	948	ARG	VAL	engineered mutation	UNP P00533
C	692	GLY	-	expression tag	UNP P00533
C	693	SER	-	expression tag	UNP P00533
C	694	THR	-	expression tag	UNP P00533
C	790	MET	THR	engineered mutation	UNP P00533
C	948	ARG	VAL	engineered mutation	UNP P00533
D	692	GLY	-	expression tag	UNP P00533
D	693	SER	-	expression tag	UNP P00533
D	694	THR	-	expression tag	UNP P00533
D	790	MET	THR	engineered mutation	UNP P00533
D	948	ARG	VAL	engineered mutation	UNP P00533

- Molecule 2 is 19-chloro-18-fluoro-22-methoxy-8,9,11,12,14,15-hexahydro-21H-4,6-etheno pyrimido[5,4-m][1,4,7,10,15]benzotetraoxazacycloheptadecine (CCD ID: M1O) (formula: C₂₁H₂₁ClFN₃O₅) (labeled as "Ligand of Interest" by depositor).



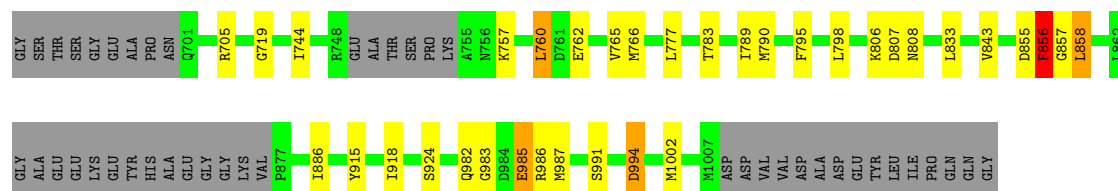
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			31	21	1	1	3	5		
2	B	1	Total	C	Cl	F	N	O	0	0
			31	21	1	1	3	5		
2	C	1	Total	C	Cl	F	N	O	0	0
			31	21	1	1	3	5		
2	D	1	Total	C	Cl	F	N	O	0	0
			31	21	1	1	3	5		

3 Residue-property plots

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.

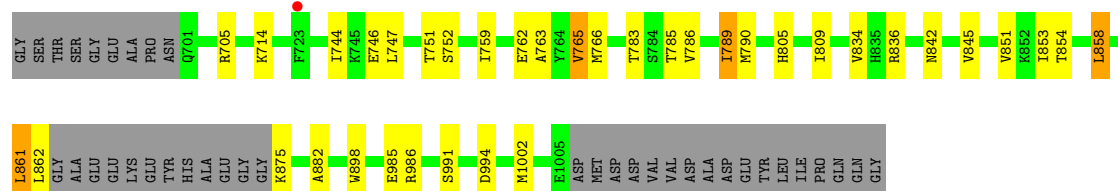
- Molecule 1: Epidermal growth factor receptor

Chain A: 



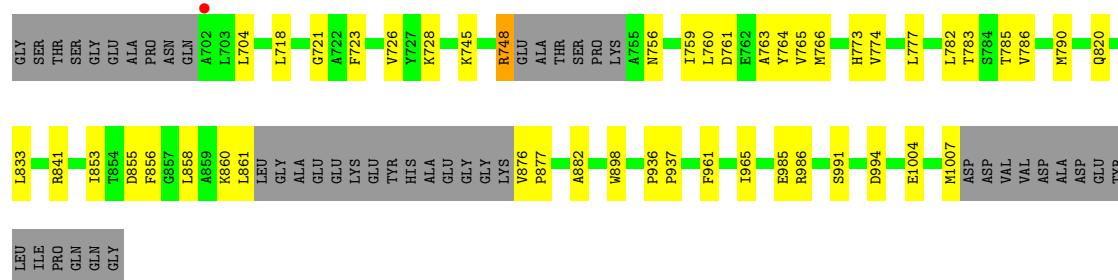
- Molecule 1: Epidermal growth factor receptor

Chain B: 



- Molecule 1: Epidermal growth factor receptor

Chain C: 



- Molecule 1: Epidermal growth factor receptor

Chain D: 

GLY	SER	THR	SER	GLY	GLU	ALA	PRO	ASN	Q701	F723	L747	R748	GLU	ALA	THR	SER	PRO	LYS	A755	N756	K757	L760	D761	V765	M766	V774	L782	T783	V786	M790	M793	H805	K806	D807	N808	I809	G810	S811	L833	R841	L844	I853	I854	D855	F856
G857	L858	A859	LYS	LEU	LEU	GLY	ALA	GLU	GLU	LYS	GLU	TYR	HIS	ALA	GLU	GLY	GLY	LYS	V876	P877	A882	R889	H893	V897	W898	Y944	R948	R962	S969	R970	R973	Q976	D984	N987	T993	D994	R999	M1002	D1003	E1004	M1007	ASP	ASP		
VAL	VAL	ASP	ALA	ASP	GLU	TYR	LEU	ILE	PRO	GLN	GLN	GLY																																	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.35Å 100.92Å 88.31Å 90.00° 102.17° 90.00°	Depositor
Resolution (Å)	86.32 – 3.42 86.32 – 3.42	Depositor EDS
% Data completeness (in resolution range)	98.2 (86.32-3.42) 98.5 (86.32-3.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.215 , 0.244 (Not available) , 0.214	Depositor DCC
R_{free} test set	808 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	82.8	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9427	wwPDB-VP
Average B, all atoms (Å ²)	79.0	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 33.99 % 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 7.3208e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: M1O

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	0.23	0/2372	0.52	4/3203 (0.1%)
1	B	0.11	0/2417	0.28	0/3267
1	C	0.20	0/2362	0.45	0/3191
1	D	0.23	0/2354	0.49	0/3181
All	All	0.20	0/9505	0.45	4/12842 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	856	PHE	CA-C-N	6.33	128.31	120.34
1	A	856	PHE	C-N-CA	6.33	128.31	120.34
1	A	986	ARG	CA-C-N	5.80	130.05	120.94
1	A	986	ARG	C-N-CA	5.80	130.05	120.94

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2322	0	2374	21	0
1	B	2365	0	2426	23	0
1	C	2312	0	2363	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2304	0	2347	26	0
2	A	31	0	0	0	0
2	B	31	0	0	1	0
2	C	31	0	0	0	0
2	D	31	0	0	2	0
All	All	9427	0	9510	90	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 5.

All (90) 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:B:751:THR:HG21	1:B:786:VAL:HG23	1.66	0.78
1:A:766:MET:HE2	1:A:857:GLY:HA3	1.69	0.74
1:A:705:ARG:NH1	1:B:994:ASP:OD1	2.20	0.74
1:D:766:MET:HE2	1:D:857:GLY:HA3	1.69	0.73
1:B:985:GLU:HG2	1:B:986:ARG:HD3	1.74	0.69
1:D:747:LEU:HD12	1:D:786:VAL:HB	1.75	0.68
1:D:793:MET:H	2:D:1101:M1O:C10	2.09	0.65
1:B:759:ILE:HA	1:B:861:LEU:HD21	1.77	0.65
1:D:774:VAL:HG22	1:D:853:ILE:HD11	1.82	0.62
1:A:991:SER:HB3	1:A:994:ASP:HB2	1.82	0.61
1:D:969:SER:O	1:D:973:ARG:HG3	2.00	0.61
1:B:747:LEU:O	1:B:785:THR:HB	2.02	0.60
1:D:790:MET:HG2	2:D:1101:M1O:CL04	2.38	0.60
1:A:719:GLY:HA2	1:D:962:ARG:NH1	2.18	0.58
1:C:1004:GLU:HB2	1:D:1004:GLU:HB2	1.84	0.58
1:C:985:GLU:HG2	1:C:986:ARG:HD3	1.86	0.56
1:C:991:SER:HB3	1:C:994:ASP:HB2	1.88	0.55
1:C:756:ASN:HA	1:C:759:ILE:HD12	1.87	0.54
1:D:833:LEU:HD22	1:D:856:PHE:HZ	1.72	0.53
1:B:790:MET:HG2	2:B:1101:M1O:CL04	2.45	0.52
1:A:994:ASP:OD1	1:B:705:ARG:NH1	2.42	0.52
1:C:761:ASP:O	1:C:765:VAL:HG23	2.09	0.52
1:A:985:GLU:H	1:A:985:GLU:CD	2.18	0.51
1:B:834:VAL:HG12	1:B:836:ARG:HG3	1.93	0.51
1:D:976:GLN:HG2	1:D:984:ASP:OD2	2.11	0.50
1:A:762:GLU:O	1:A:766:MET:HG3	2.12	0.49
1:C:841:ARG:HH22	1:C:877:PRO:HB3	1.78	0.49
1:C:704:LEU:HB3	1:C:764:TYR:CE1	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:721:GLY:CA	1:C:748:ARG:HH12	2.26	0.48
1:B:882:ALA:HA	1:B:898:TRP:CD2	2.49	0.48
1:A:856:PHE:CG	1:A:857:GLY:N	2.81	0.48
1:D:833:LEU:HD13	1:D:856:PHE:CZ	2.48	0.47
1:A:915:TYR:HB3	1:A:918:ILE:HD12	1.95	0.47
1:B:747:LEU:HD21	1:B:862:LEU:HD21	1.96	0.47
1:B:991:SER:HB3	1:B:994:ASP:HB2	1.97	0.47
1:D:782:LEU:HD23	1:D:786:VAL:HG13	1.97	0.47
1:A:795:PHE:HE1	1:A:1002:MET:HE1	1.80	0.47
1:D:805:HIS:O	1:D:809:ILE:HG13	2.15	0.47
1:B:714:LYS:NZ	1:B:746:GLU:OE1	2.48	0.46
1:C:718:LEU:HD11	1:C:728:LYS:HB2	1.97	0.46
1:B:861:LEU:HD23	1:B:861:LEU:HA	1.73	0.46
1:A:833:LEU:HD22	1:A:856:PHE:HZ	1.79	0.46
1:C:882:ALA:HA	1:C:898:TRP:CD2	2.50	0.46
1:C:777:LEU:HA	1:C:790:MET:HG2	1.98	0.46
1:C:726:VAL:HG22	1:C:745:LYS:HD3	1.97	0.46
1:C:773:HIS:CD2	1:C:820:GLN:HB3	2.51	0.46
1:C:726:VAL:CG2	1:C:745:LYS:HD3	2.46	0.46
1:C:782:LEU:O	1:C:783:THR:C	2.59	0.46
1:D:999:ARG:HH12	1:D:1007:MET:HG3	1.81	0.45
1:D:841:ARG:HH22	1:D:877:PRO:HB3	1.81	0.45
1:D:944:TYR:CZ	1:D:948:ARG:HD3	2.52	0.45
1:A:798:LEU:N	1:A:843:VAL:O	2.40	0.45
1:B:842:ASN:O	1:B:854:THR:HG22	2.17	0.45
1:D:994:ASP:N	1:D:994:ASP:OD1	2.50	0.44
1:A:760:LEU:HD23	1:A:760:LEU:HA	1.75	0.44
1:B:744:ILE:HG12	1:B:789:ILE:HG13	1.99	0.44
1:C:833:LEU:HD13	1:C:856:PHE:CZ	2.52	0.44
1:D:811:SER:OG	1:D:984:ASP:OD2	2.26	0.44
1:B:762:GLU:O	1:B:765:VAL:HG12	2.17	0.44
1:A:886:ILE:HG21	1:A:924:SER:HB3	2.00	0.44
1:A:833:LEU:HD13	1:A:856:PHE:CZ	2.53	0.43
1:C:858:LEU:O	1:C:858:LEU:HG	2.18	0.43
1:C:723:PHE:CD2	1:C:861:LEU:HD22	2.53	0.43
1:D:760:LEU:HD23	1:D:760:LEU:HA	1.78	0.43
1:A:806:LYS:HE3	1:A:806:LYS:HB2	1.67	0.43
1:B:862:LEU:HD13	1:B:862:LEU:HA	1.86	0.43
1:C:961:PHE:O	1:C:965:ILE:HG13	2.19	0.42
1:D:970:LYS:HB3	1:D:970:LYS:HE2	1.81	0.42
1:B:783:THR:OG1	1:B:785:THR:O	2.27	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:858:LEU:HD23	1:B:858:LEU:HA	1.84	0.42
1:B:845:VAL:HG22	1:B:851:VAL:HG12	2.02	0.42
1:D:723:PHE:O	1:D:748:ARG:HB2	2.20	0.41
1:C:721:GLY:C	1:C:748:ARG:HH12	2.28	0.41
1:C:936:PRO:HA	1:C:937:PRO:HD3	1.91	0.41
1:D:793:MET:HG3	1:D:844:LEU:HD13	2.02	0.41
1:A:808:ASN:HA	1:A:987:MET:SD	2.61	0.41
1:D:882:ALA:HA	1:D:898:TRP:CD2	2.56	0.41
1:A:777:LEU:HA	1:A:790:MET:HG2	2.02	0.41
1:C:723:PHE:HA	1:C:748:ARG:NE	2.35	0.41
1:D:757:LYS:O	1:D:760:LEU:N	2.54	0.41
1:C:774:VAL:HG22	1:C:853:ILE:HD11	2.02	0.41
1:D:761:ASP:O	1:D:765:VAL:HG23	2.21	0.41
1:A:744:ILE:HG12	1:A:789:ILE:HG13	2.03	0.41
1:A:983:GLY:O	1:A:987:MET:HG2	2.21	0.41
1:B:805:HIS:O	1:B:809:ILE:HG13	2.21	0.41
1:C:763:ALA:HA	1:C:766:MET:SD	2.61	0.41
1:D:893:HIS:O	1:D:897:VAL:HG23	2.21	0.41
1:B:985:GLU:CD	1:B:985:GLU:H	2.29	0.40
1:A:766:MET:HE2	1:A:857:GLY:CA	2.46	0.40
1:B:763:ALA:HA	1:B:766:MET:HE3	2.03	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	281/331 (85%)	270 (96%)	7 (2%)	4 (1%)	9	31
1	B	289/331 (87%)	283 (98%)	6 (2%)	0	100	100
1	C	280/331 (85%)	269 (96%)	11 (4%)	0	100	100
1	D	279/331 (84%)	268 (96%)	10 (4%)	1 (0%)	30	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1129/1324 (85%)	1090 (96%)	34 (3%)	5 (0%)	30 59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	807	ASP
1	A	858	LEU
1	A	783	THR
1	A	856	PHE
1	D	783	THR

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	257/290 (89%)	249 (97%)	8 (3%)	35 58
1	B	262/290 (90%)	254 (97%)	8 (3%)	35 58
1	C	256/290 (88%)	248 (97%)	8 (3%)	35 58
1	D	255/290 (88%)	244 (96%)	11 (4%)	26 50
All	All	1030/1160 (89%)	995 (97%)	35 (3%)	32 56

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	757	LYS
1	A	760	LEU
1	A	765	VAL
1	A	855	ASP
1	A	858	LEU
1	A	982	GLN
1	A	985	GLU
1	A	994	ASP
1	B	752	SER
1	B	765	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	789	ILE
1	B	853	ILE
1	B	858	LEU
1	B	861	LEU
1	B	875	LYS
1	B	1002	MET
1	C	748	ARG
1	C	760	LEU
1	C	785	THR
1	C	786	VAL
1	C	855	ASP
1	C	860	LYS
1	C	876	VAL
1	C	1007	MET
1	D	748	ARG
1	D	760	LEU
1	D	807	ASP
1	D	841	ARG
1	D	855	ASP
1	D	858	LEU
1	D	889	ARG
1	D	987	MET
1	D	993	THR
1	D	994	ASP
1	D	1002	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	787	GLN
1	A	791	GLN
1	B	787	GLN
1	B	812	GLN
1	B	816	ASN
1	C	791	GLN
1	D	988	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	M1O	C	1101	-	34,34,34	1.95	10 (29%)	46,46,46	1.99	17 (36%)
2	M1O	A	1101	-	34,34,34	1.77	10 (29%)	46,46,46	1.72	15 (32%)
2	M1O	B	1101	-	34,34,34	1.87	8 (23%)	46,46,46	1.77	17 (36%)
2	M1O	D	1101	-	34,34,34	1.98	13 (38%)	46,46,46	1.70	13 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	M1O	C	1101	-	-	11/19/19/19	0/3/4/4
2	M1O	A	1101	-	-	11/19/19/19	0/3/4/4
2	M1O	B	1101	-	-	11/19/19/19	0/3/4/4
2	M1O	D	1101	-	-	10/19/19/19	0/3/4/4

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	M1O	C08-N07	5.17	1.44	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	M1O	C08-N07	5.04	1.43	1.36
2	C	1101	M1O	C08-N07	4.71	1.43	1.36
2	A	1101	M1O	C08-N07	4.31	1.42	1.36
2	D	1101	M1O	C31-C12	4.09	1.48	1.41
2	B	1101	M1O	C08-C13	4.06	1.49	1.44
2	A	1101	M1O	C08-C13	3.97	1.49	1.44
2	C	1101	M1O	C10-N09	3.71	1.40	1.33
2	C	1101	M1O	C31-C12	3.61	1.47	1.41
2	D	1101	M1O	C08-C13	3.61	1.49	1.44
2	C	1101	M1O	C06-C26	3.54	1.47	1.40
2	D	1101	M1O	C10-N09	3.26	1.39	1.33
2	C	1101	M1O	C28-C15	3.22	1.47	1.40
2	B	1101	M1O	C10-N09	3.21	1.39	1.33
2	C	1101	M1O	C08-C13	3.08	1.48	1.44
2	A	1101	M1O	C06-C26	3.01	1.46	1.40
2	B	1101	M1O	C31-C12	2.99	1.46	1.41
2	A	1101	M1O	C10-N09	2.96	1.39	1.33
2	A	1101	M1O	C31-C12	2.94	1.46	1.41
2	B	1101	M1O	C06-C26	2.84	1.46	1.40
2	B	1101	M1O	C28-C15	2.82	1.46	1.40
2	C	1101	M1O	C12-N11	2.68	1.41	1.37
2	D	1101	M1O	C28-C15	2.61	1.46	1.40
2	D	1101	M1O	C31-C28	2.46	1.41	1.36
2	B	1101	M1O	C12-N11	2.40	1.41	1.37
2	C	1101	M1O	O29-C28	2.39	1.41	1.37
2	D	1101	M1O	C12-N11	2.31	1.41	1.37
2	A	1101	M1O	C28-C15	2.31	1.45	1.40
2	A	1101	M1O	C05-C06	2.30	1.43	1.39
2	C	1101	M1O	C31-C28	2.30	1.40	1.36
2	D	1101	M1O	O29-C28	2.27	1.40	1.37
2	C	1101	M1O	C24-C23	2.25	1.60	1.49
2	A	1101	M1O	C21-C20	2.24	1.60	1.49
2	D	1101	M1O	C03-CL04	2.20	1.78	1.73
2	A	1101	M1O	C12-N11	2.18	1.41	1.37
2	D	1101	M1O	C18-C17	2.17	1.59	1.49
2	D	1101	M1O	C06-N07	2.16	1.45	1.39
2	D	1101	M1O	C05-C06	2.10	1.42	1.39
2	D	1101	M1O	C06-C26	2.07	1.44	1.40
2	A	1101	M1O	C24-C23	2.05	1.59	1.49
2	B	1101	M1O	C24-C23	2.01	1.59	1.49

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	M1O	C08-C13-C12	4.65	118.60	115.86
2	A	1101	M1O	C13-C08-N07	4.30	124.11	119.77
2	C	1101	M1O	C08-C13-C12	4.25	118.37	115.86
2	C	1101	M1O	O25-C26-C06	3.86	121.25	114.95
2	B	1101	M1O	C13-C08-N07	3.69	123.50	119.77
2	A	1101	M1O	O25-C26-C06	3.64	120.88	114.95
2	C	1101	M1O	O16-C15-C14	-3.59	119.31	125.20
2	B	1101	M1O	O25-C26-C06	3.43	120.54	114.95
2	A	1101	M1O	C10-N09-C08	3.38	119.22	116.60
2	C	1101	M1O	O29-C28-C15	3.31	119.90	115.40
2	C	1101	M1O	O16-C15-C28	3.21	122.38	115.75
2	C	1101	M1O	C15-C14-C13	3.12	125.96	120.59
2	C	1101	M1O	C31-C28-C15	-3.08	117.14	120.06
2	D	1101	M1O	C13-C12-N11	-3.00	119.64	122.82
2	C	1101	M1O	C13-C08-N09	-3.00	119.13	121.35
2	B	1101	M1O	C10-N09-C08	2.98	118.91	116.60
2	C	1101	M1O	O16-C17-C18	2.94	118.55	108.71
2	D	1101	M1O	C15-C14-C13	2.93	125.63	120.59
2	D	1101	M1O	O25-C26-C06	2.88	119.64	114.95
2	C	1101	M1O	C10-N09-C08	2.85	118.81	116.60
2	B	1101	M1O	O29-C28-C15	2.80	119.20	115.40
2	B	1101	M1O	C08-C13-C12	2.75	117.48	115.86
2	D	1101	M1O	O16-C15-C14	-2.70	120.76	125.20
2	C	1101	M1O	C30-O29-C28	2.64	121.38	117.51
2	B	1101	M1O	O16-C15-C14	-2.63	120.89	125.20
2	D	1101	M1O	C31-C12-N11	2.59	120.98	118.01
2	B	1101	M1O	C15-C14-C13	2.55	124.97	120.59
2	D	1101	M1O	C13-C08-N07	2.53	122.32	119.77
2	D	1101	M1O	C31-C28-C15	-2.52	117.67	120.06
2	A	1101	M1O	C13-C08-N09	-2.50	119.50	121.35
2	C	1101	M1O	O25-C26-C27	-2.49	118.12	123.49
2	B	1101	M1O	C13-C08-N09	-2.47	119.52	121.35
2	C	1101	M1O	C31-C12-N11	2.44	120.81	118.01
2	B	1101	M1O	C31-C28-C15	-2.44	117.75	120.06
2	A	1101	M1O	N11-C10-N09	-2.42	125.39	128.67
2	A	1101	M1O	C10-N11-C12	2.39	118.14	115.43
2	C	1101	M1O	C13-C12-N11	-2.39	120.29	122.82
2	B	1101	M1O	C26-C06-N07	2.37	123.39	118.10
2	A	1101	M1O	O25-C26-C27	-2.37	118.38	123.49
2	B	1101	M1O	O16-C15-C28	2.33	120.56	115.75
2	A	1101	M1O	C05-C06-C26	-2.30	116.24	118.95
2	D	1101	M1O	O16-C15-C28	2.30	120.50	115.75
2	C	1101	M1O	N11-C10-N09	-2.30	125.56	128.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	M1O	N07-C08-N09	-2.30	116.13	118.71
2	C	1101	M1O	C28-C31-C12	2.29	122.94	120.11
2	D	1101	M1O	C13-C08-N09	-2.26	119.67	121.35
2	C	1101	M1O	C05-C06-C26	-2.21	116.35	118.95
2	B	1101	M1O	C05-C06-C26	-2.21	116.36	118.95
2	A	1101	M1O	C15-C14-C13	2.19	124.36	120.59
2	B	1101	M1O	N11-C10-N09	-2.18	125.72	128.67
2	B	1101	M1O	C28-C31-C12	2.15	122.77	120.11
2	B	1101	M1O	C13-C12-N11	-2.13	120.56	122.82
2	B	1101	M1O	C14-C13-C12	-2.13	116.49	118.99
2	B	1101	M1O	C10-N11-C12	2.09	117.81	115.43
2	A	1101	M1O	C13-C12-N11	-2.09	120.61	122.82
2	A	1101	M1O	O29-C28-C15	2.05	118.18	115.40
2	A	1101	M1O	O16-C15-C14	-2.04	121.85	125.20
2	D	1101	M1O	C05-C06-C26	-2.02	116.57	118.95
2	A	1101	M1O	C08-C13-C12	2.02	117.05	115.86
2	A	1101	M1O	C14-C13-C12	-2.02	116.62	118.99
2	D	1101	M1O	O25-C24-C23	2.01	115.45	108.71
2	D	1101	M1O	C14-C13-C12	-2.01	116.62	118.99

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1101	M1O	C13-C08-N07-C06
2	D	1101	M1O	N09-C08-N07-C06
2	C	1101	M1O	C21-C20-O19-C18
2	C	1101	M1O	C20-C21-O22-C23
2	A	1101	M1O	C20-C21-O22-C23
2	C	1101	M1O	C31-C28-O29-C30
2	B	1101	M1O	O16-C17-C18-O19
2	C	1101	M1O	O19-C20-C21-O22
2	C	1101	M1O	C15-C28-O29-C30
2	B	1101	M1O	C06-C26-O25-C24
2	B	1101	M1O	C31-C28-O29-C30
2	D	1101	M1O	C31-C28-O29-C30
2	A	1101	M1O	C06-C26-O25-C24
2	A	1101	M1O	O22-C23-C24-O25
2	C	1101	M1O	O22-C23-C24-O25
2	D	1101	M1O	C21-C20-O19-C18
2	B	1101	M1O	C15-C28-O29-C30
2	A	1101	M1O	C28-C15-O16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	1101	M1O	C28-C15-O16-C17
2	D	1101	M1O	C15-C28-O29-C30
2	A	1101	M1O	C14-C15-O16-C17
2	D	1101	M1O	C28-C15-O16-C17
2	A	1101	M1O	N09-C08-N07-C06
2	D	1101	M1O	C20-C21-O22-C23
2	D	1101	M1O	O16-C17-C18-O19
2	B	1101	M1O	C14-C15-O16-C17
2	B	1101	M1O	O22-C23-C24-O25
2	A	1101	M1O	C18-C17-O16-C15
2	A	1101	M1O	O16-C17-C18-O19
2	D	1101	M1O	C14-C15-O16-C17
2	B	1101	M1O	C27-C26-O25-C24
2	A	1101	M1O	C21-C20-O19-C18
2	C	1101	M1O	C24-C23-O22-C21
2	A	1101	M1O	C27-C26-O25-C24
2	B	1101	M1O	C23-C24-O25-C26
2	C	1101	M1O	C06-C26-O25-C24
2	B	1101	M1O	C21-C20-O19-C18
2	C	1101	M1O	C27-C26-O25-C24
2	D	1101	M1O	C17-C18-O19-C20
2	C	1101	M1O	O16-C17-C18-O19
2	C	1101	M1O	C18-C17-O16-C15
2	A	1101	M1O	O19-C20-C21-O22
2	B	1101	M1O	C18-C17-O16-C15

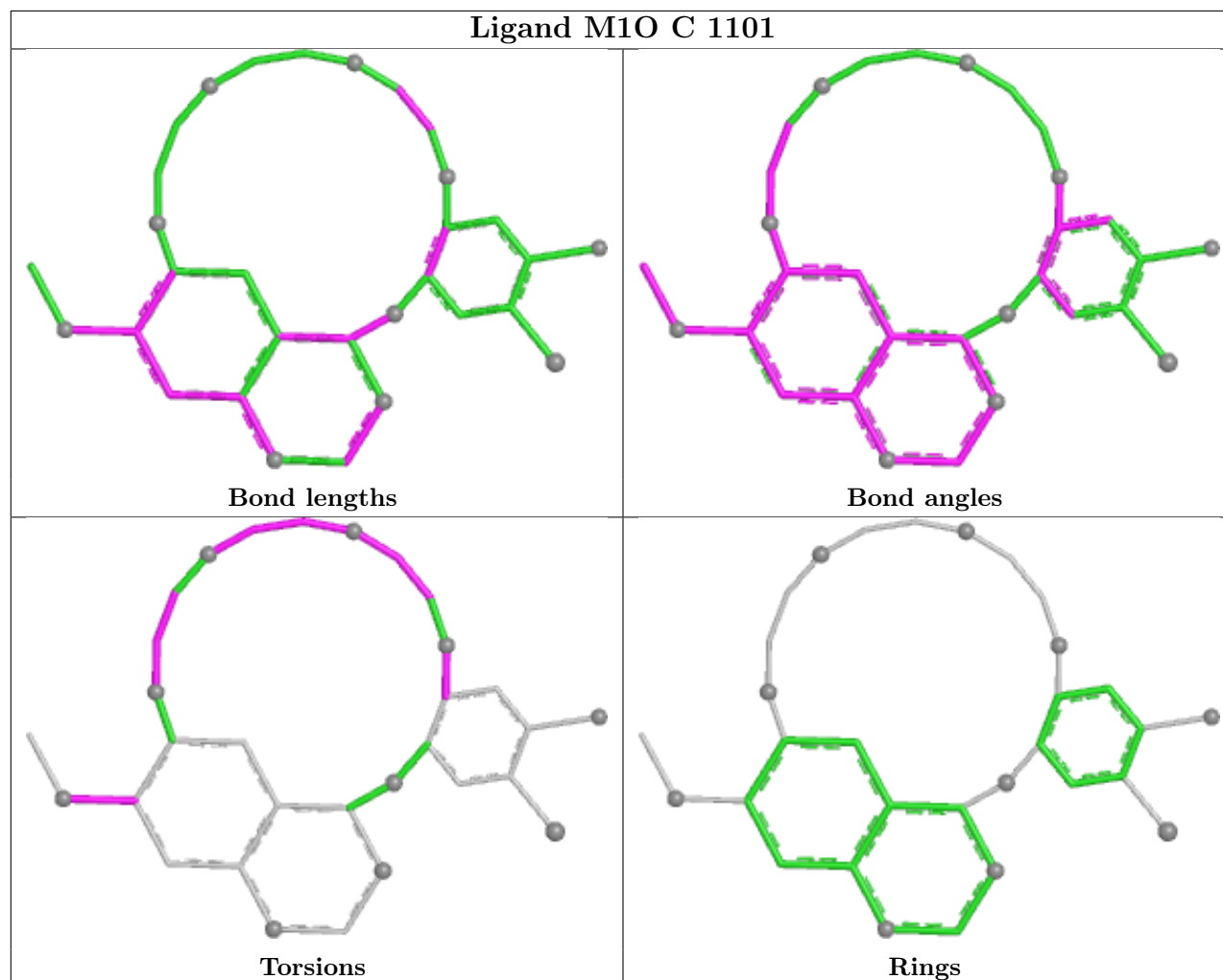
There are no ring outliers.

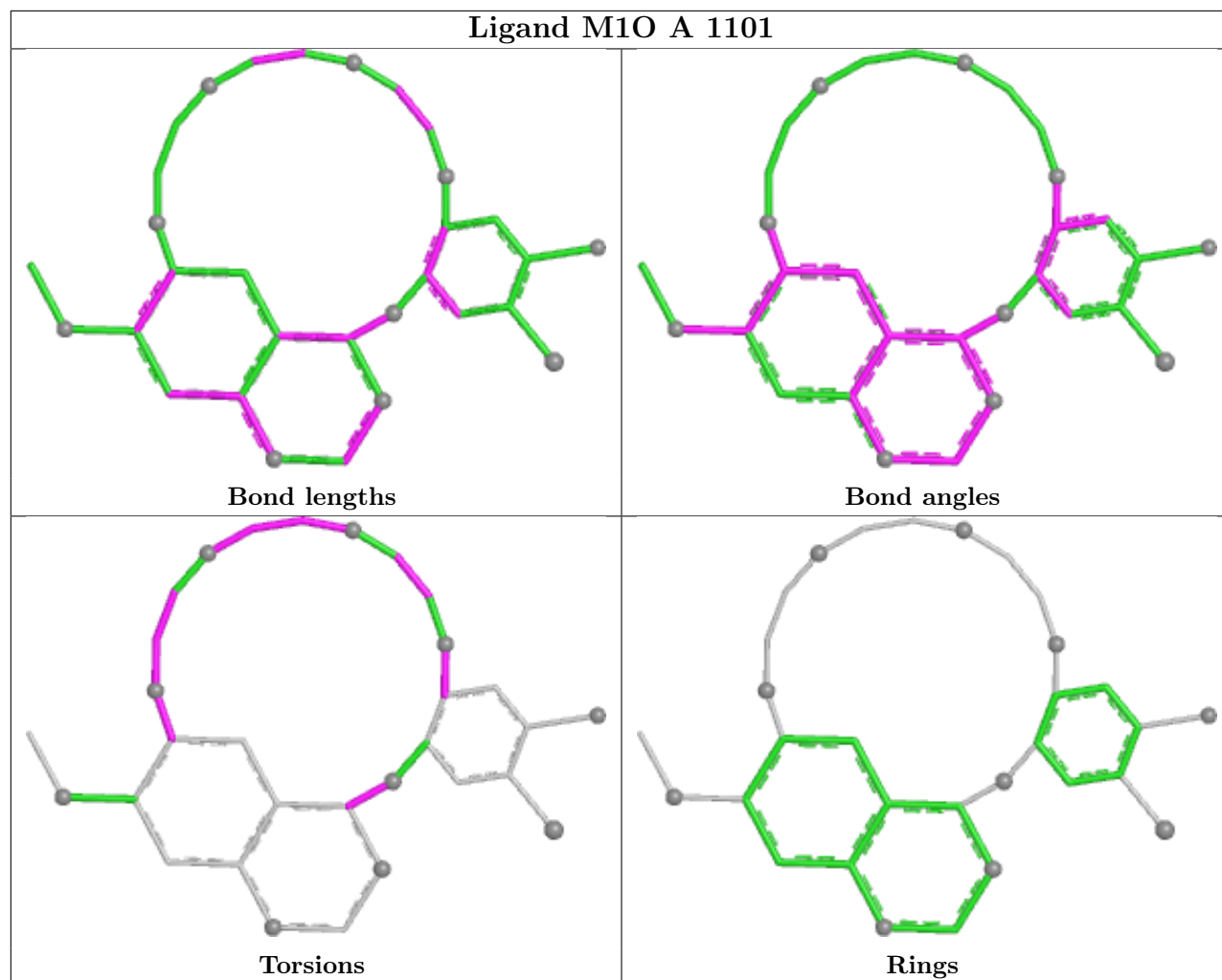
2 monomers are involved in 3 short contacts:

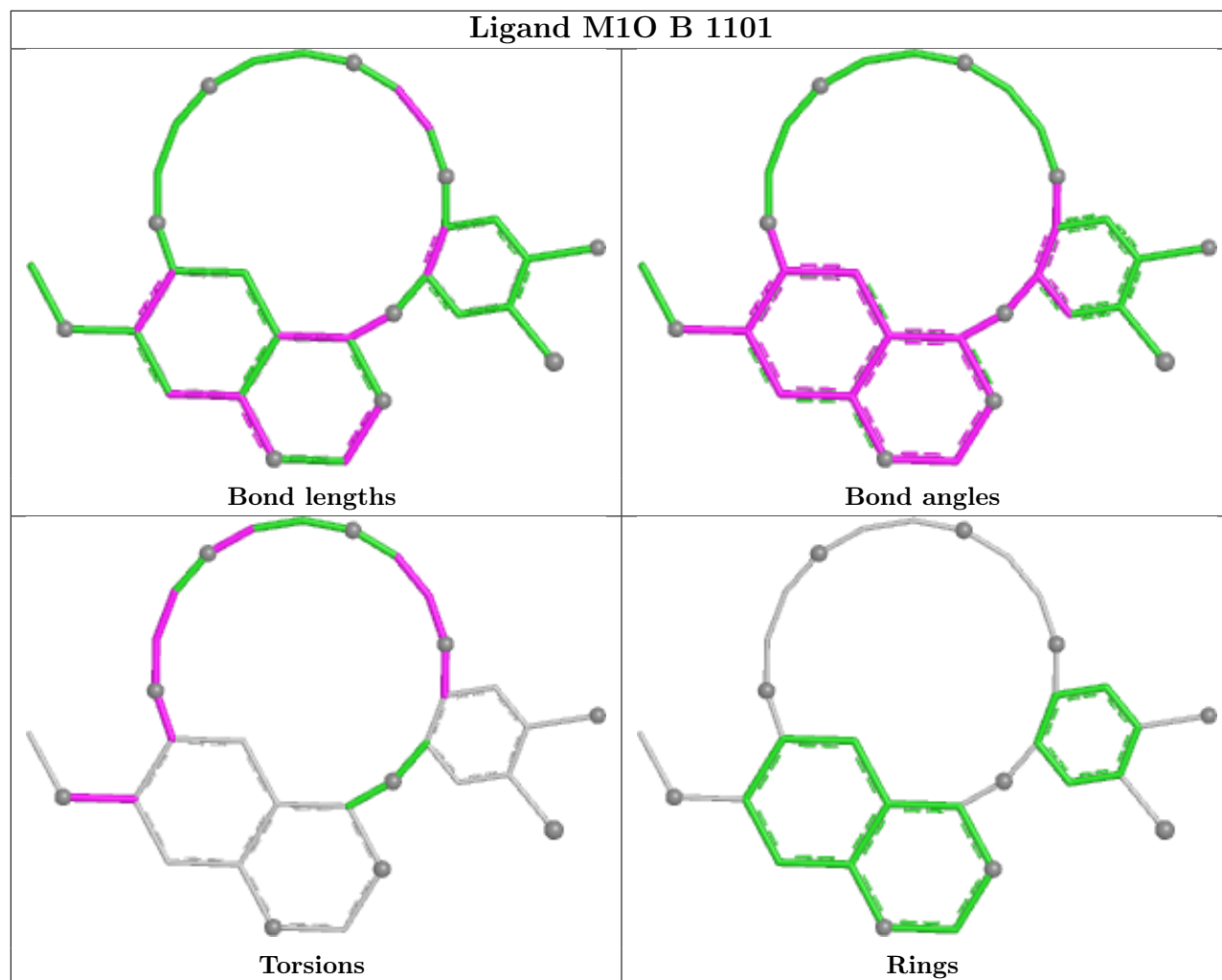
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	M1O	1	0
2	D	1101	M1O	2	0

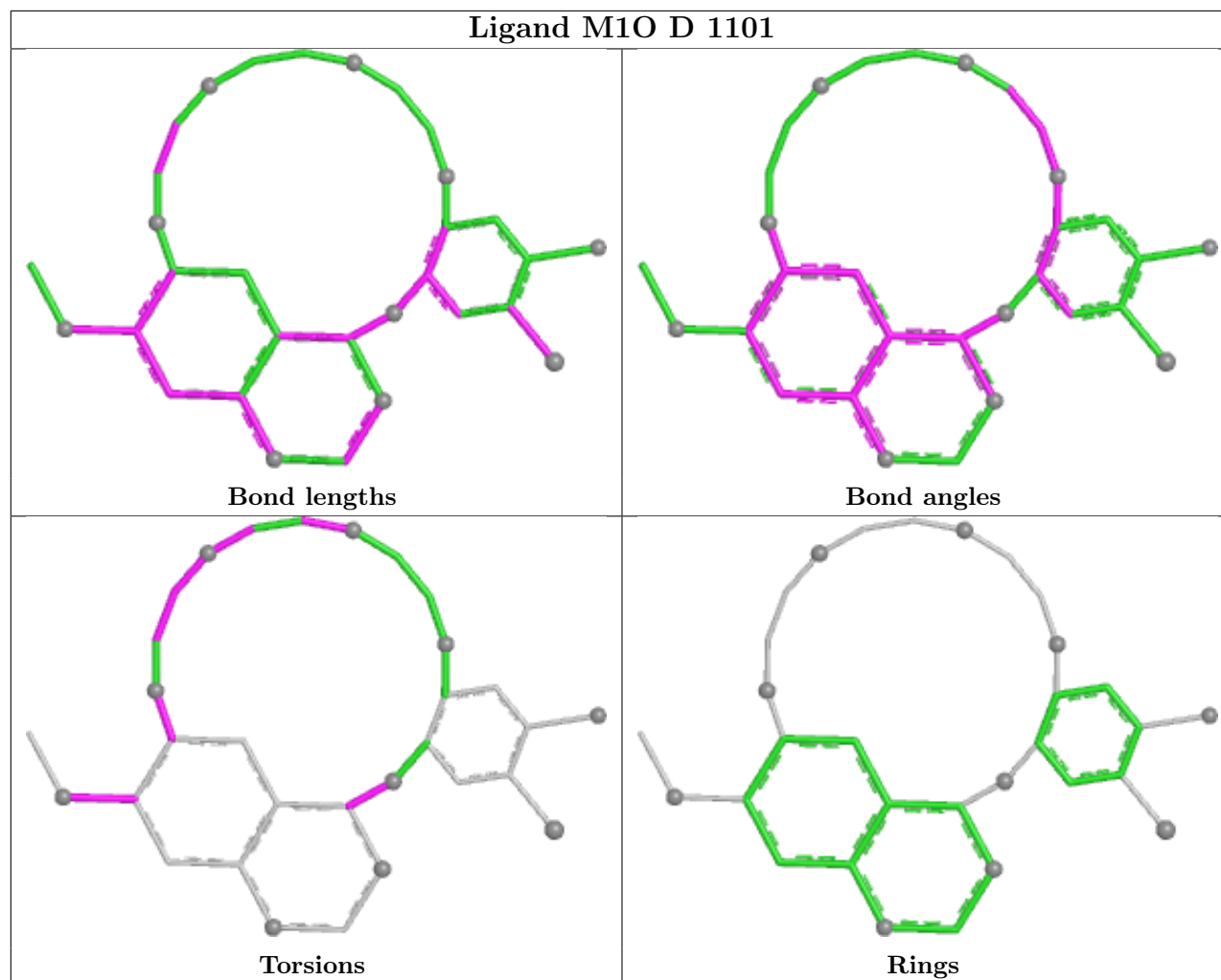
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	287/331 (86%)	-0.29	0 100 100	42, 71, 101, 121	0
1	B	293/331 (88%)	-0.30	1 (0%) 90 84	47, 77, 111, 142	0
1	C	286/331 (86%)	-0.18	1 (0%) 90 84	45, 79, 118, 152	0
1	D	285/331 (86%)	-0.20	0 100 100	48, 82, 125, 154	0
All	All	1151/1324 (86%)	-0.24	2 (0%) 91 88	42, 78, 114, 154	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	723	PHE	2.3
1	C	702	ALA	2.2

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](#)

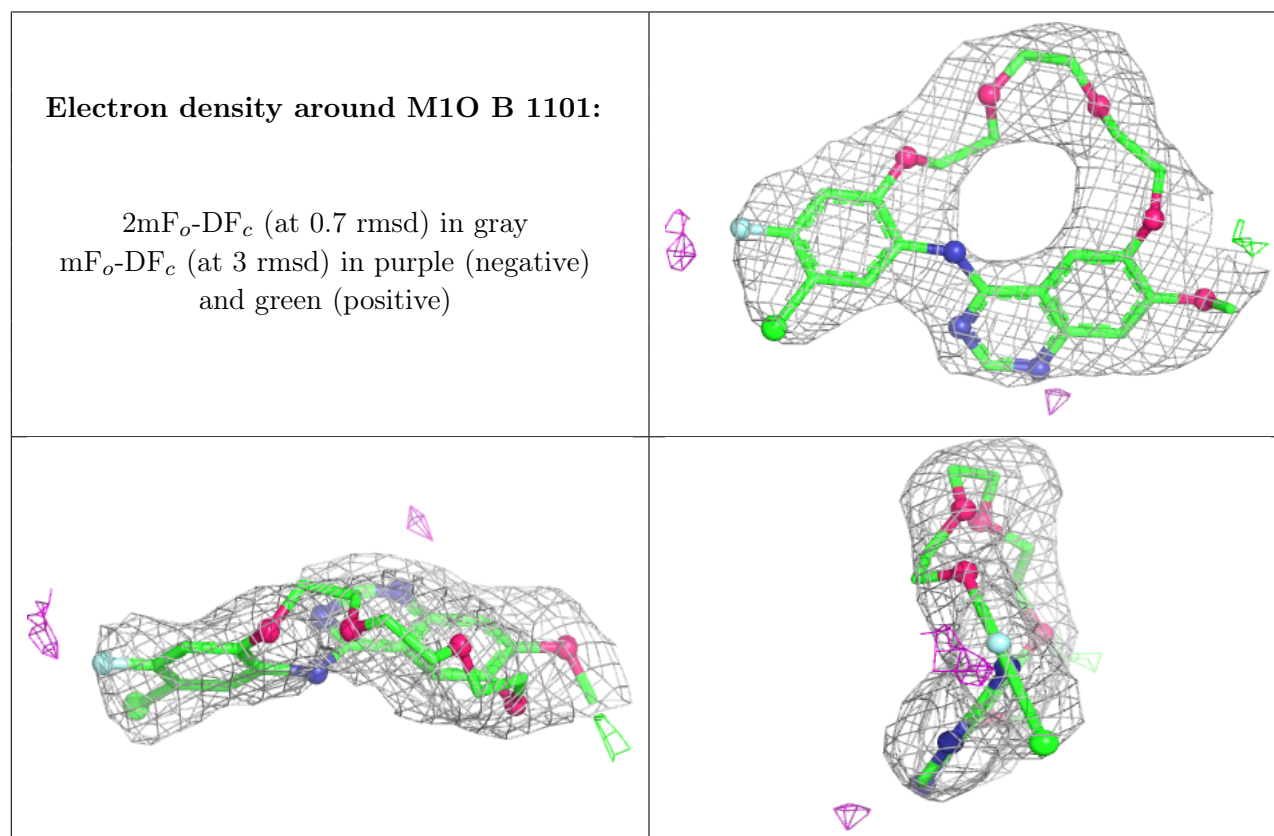
There are no oligosaccharides in this entry.

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.

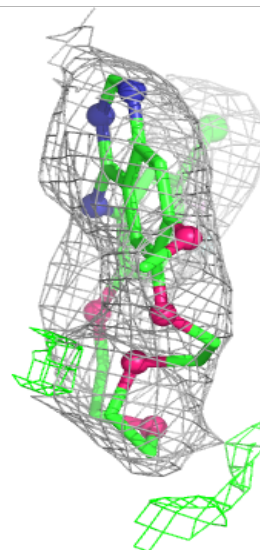
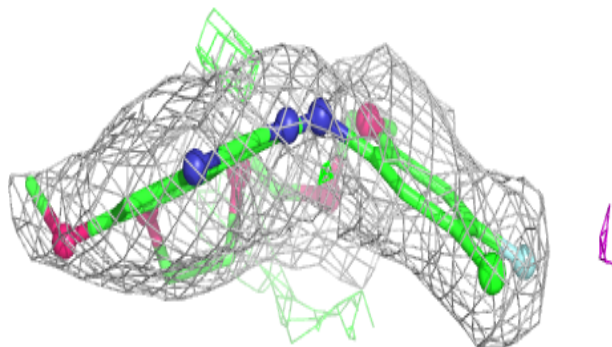
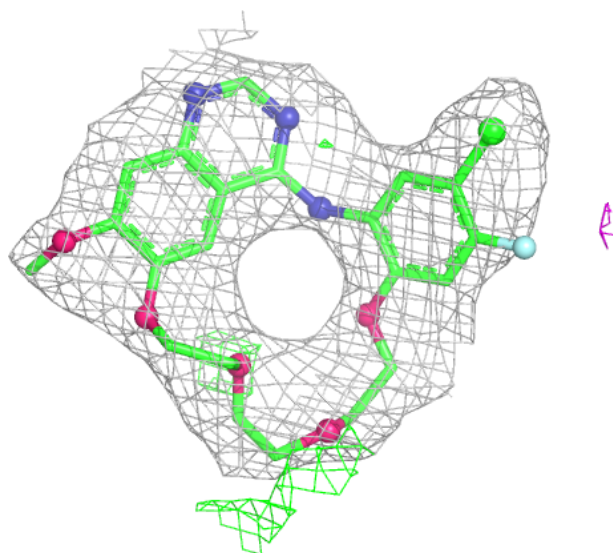
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	M1O	B	1101	31/31	0.84	0.13	72,82,98,105	0
2	M1O	D	1101	31/31	0.86	0.12	56,76,91,109	0
2	M1O	C	1101	31/31	0.87	0.10	52,66,84,94	0
2	M1O	A	1101	31/31	0.87	0.10	37,59,74,77	0

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.



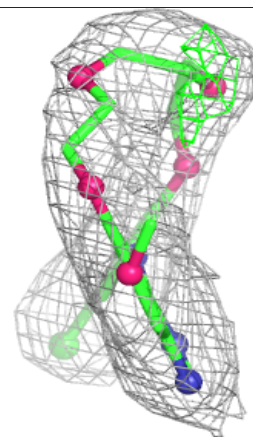
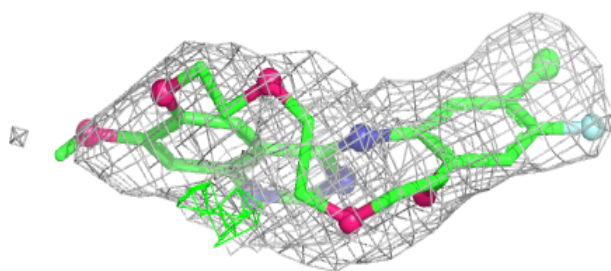
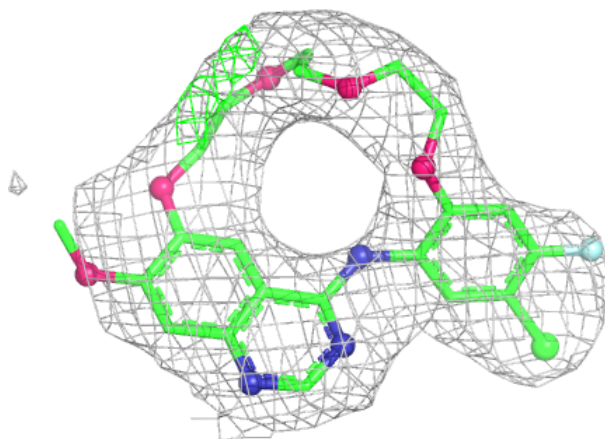
Electron density around M1O D 1101:

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



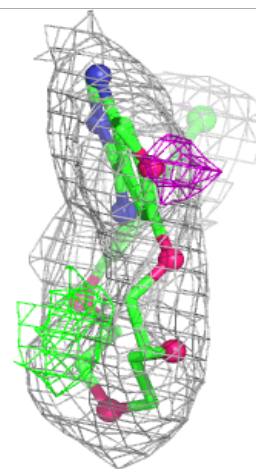
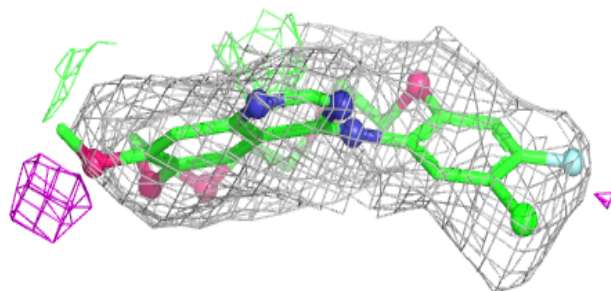
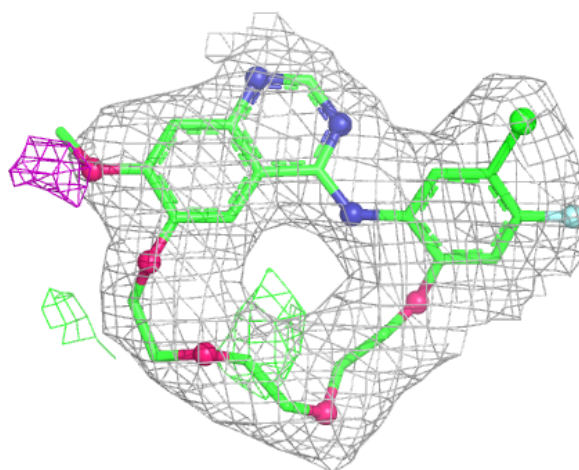
Electron density around M1O C 1101:

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



Electron density around M1O A 1101:

$2mF_o-DF_c$ (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.