



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:44 PM UTC

PDB ID : 8GIH / pdb_00008gih
Title : Structure of Hepatitis B Virus Capsid Y132A mutant in complex with Compound 24
Authors : Shaffer, P.L.
Deposited on : 2023-03-14
Resolution : 2.65 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

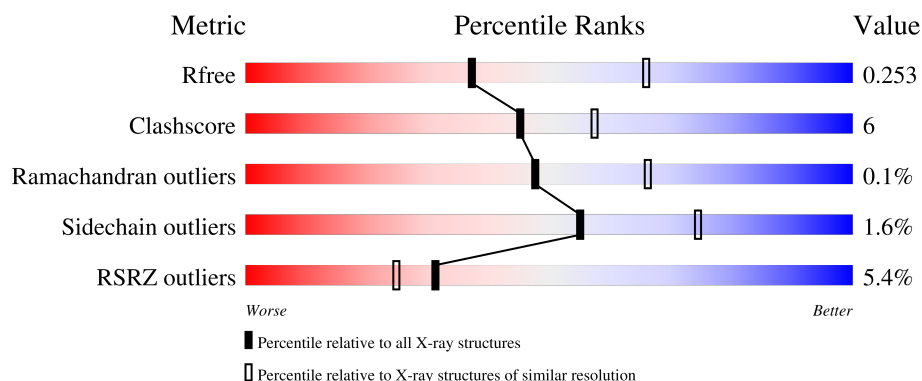
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

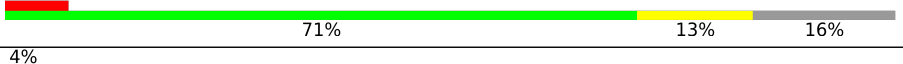
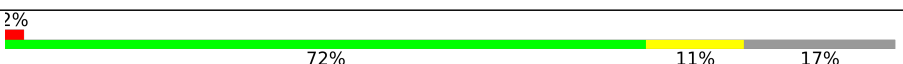
The reported resolution of this entry is 2.65 Å.

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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	160	
1	B	160	
1	C	160	
1	D	160	
1	E	160	

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Mol	Chain	Length	Quality of chain
1	F	160	3% 76% 10% 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6413 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	0	1	0
			1097	712	183	197	5			
1	B	134	Total	C	N	O	S	0	0	0
			1035	676	169	185	5			
1	C	134	Total	C	N	O	S	0	0	0
			1019	662	170	182	5			
1	D	128	Total	C	N	O	S	0	0	0
			982	640	162	175	5			
1	E	133	Total	C	N	O	S	0	0	0
			1028	672	168	183	5			
1	F	137	Total	C	N	O	S	0	0	0
			1032	672	172	183	5			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP L7R9I1
A	-1	GLY	-	expression tag	UNP L7R9I1
A	0	SER	-	expression tag	UNP L7R9I1
A	132	ALA	TYR	engineered mutation	UNP L7R9I1
A	150	LYS	-	expression tag	UNP L7R9I1
A	151	LEU	-	expression tag	UNP L7R9I1
A	152	GLU	-	expression tag	UNP L7R9I1
A	153	ASN	-	expression tag	UNP L7R9I1
A	154	LEU	-	expression tag	UNP L7R9I1
A	155	TYR	-	expression tag	UNP L7R9I1
A	156	PHE	-	expression tag	UNP L7R9I1
A	157	GLN	-	expression tag	UNP L7R9I1
B	-2	MET	-	initiating methionine	UNP L7R9I1
B	-1	GLY	-	expression tag	UNP L7R9I1
B	0	SER	-	expression tag	UNP L7R9I1
B	132	ALA	TYR	engineered mutation	UNP L7R9I1
B	150	LYS	-	expression tag	UNP L7R9I1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	151	LEU	-	expression tag	UNP L7R9I1
B	152	GLU	-	expression tag	UNP L7R9I1
B	153	ASN	-	expression tag	UNP L7R9I1
B	154	LEU	-	expression tag	UNP L7R9I1
B	155	TYR	-	expression tag	UNP L7R9I1
B	156	PHE	-	expression tag	UNP L7R9I1
B	157	GLN	-	expression tag	UNP L7R9I1
C	-2	MET	-	initiating methionine	UNP L7R9I1
C	-1	GLY	-	expression tag	UNP L7R9I1
C	0	SER	-	expression tag	UNP L7R9I1
C	132	ALA	TYR	engineered mutation	UNP L7R9I1
C	150	LYS	-	expression tag	UNP L7R9I1
C	151	LEU	-	expression tag	UNP L7R9I1
C	152	GLU	-	expression tag	UNP L7R9I1
C	153	ASN	-	expression tag	UNP L7R9I1
C	154	LEU	-	expression tag	UNP L7R9I1
C	155	TYR	-	expression tag	UNP L7R9I1
C	156	PHE	-	expression tag	UNP L7R9I1
C	157	GLN	-	expression tag	UNP L7R9I1
D	-2	MET	-	initiating methionine	UNP L7R9I1
D	-1	GLY	-	expression tag	UNP L7R9I1
D	0	SER	-	expression tag	UNP L7R9I1
D	132	ALA	TYR	engineered mutation	UNP L7R9I1
D	150	LYS	-	expression tag	UNP L7R9I1
D	151	LEU	-	expression tag	UNP L7R9I1
D	152	GLU	-	expression tag	UNP L7R9I1
D	153	ASN	-	expression tag	UNP L7R9I1
D	154	LEU	-	expression tag	UNP L7R9I1
D	155	TYR	-	expression tag	UNP L7R9I1
D	156	PHE	-	expression tag	UNP L7R9I1
D	157	GLN	-	expression tag	UNP L7R9I1
E	-2	MET	-	initiating methionine	UNP L7R9I1
E	-1	GLY	-	expression tag	UNP L7R9I1
E	0	SER	-	expression tag	UNP L7R9I1
E	132	ALA	TYR	engineered mutation	UNP L7R9I1
E	150	LYS	-	expression tag	UNP L7R9I1
E	151	LEU	-	expression tag	UNP L7R9I1
E	152	GLU	-	expression tag	UNP L7R9I1
E	153	ASN	-	expression tag	UNP L7R9I1
E	154	LEU	-	expression tag	UNP L7R9I1
E	155	TYR	-	expression tag	UNP L7R9I1
E	156	PHE	-	expression tag	UNP L7R9I1

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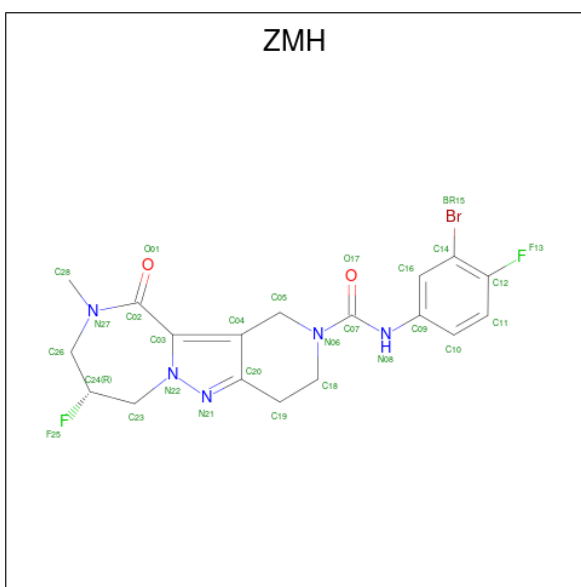
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Chain	Residue	Modelled	Actual	Comment	Reference
E	157	GLN	-	expression tag	UNP L7R9I1
F	-2	MET	-	initiating methionine	UNP L7R9I1
F	-1	GLY	-	expression tag	UNP L7R9I1
F	0	SER	-	expression tag	UNP L7R9I1
F	132	ALA	TYR	engineered mutation	UNP L7R9I1
F	150	LYS	-	expression tag	UNP L7R9I1
F	151	LEU	-	expression tag	UNP L7R9I1
F	152	GLU	-	expression tag	UNP L7R9I1
F	153	ASN	-	expression tag	UNP L7R9I1
F	154	LEU	-	expression tag	UNP L7R9I1
F	155	TYR	-	expression tag	UNP L7R9I1
F	156	PHE	-	expression tag	UNP L7R9I1
F	157	GLN	-	expression tag	UNP L7R9I1

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cl 2 2	0	0
2	B	1	Total Cl 1 1	0	0
2	C	3	Total Cl 3 3	0	0
2	D	2	Total Cl 2 2	0	0
2	E	2	Total Cl 2 2	0	0
2	F	2	Total Cl 2 2	0	0

- Molecule 3 is (6S,8R)-N-(3-bromo-4-fluorophenyl)-8-fluoro-10-methyl-11-oxo-1,3,4,7,8,9,10,11-octahydro-2H-pyrido[4',3':3,4]pyrazolo[1,5-a][1,4]diazepine-2-carboxamide (CCD ID: ZMH) (formula: C₁₈H₁₈BrF₂N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 28	Br 1	C 18	F 2	N 5	O 2	0	0
3	B	1	Total 28	Br 1	C 18	F 2	N 5	O 2	0	0
3	C	1	Total 28	Br 1	C 18	F 2	N 5	O 2	0	0
3	D	1	Total 28	Br 1	C 18	F 2	N 5	O 2	0	0
3	E	1	Total 28	Br 1	C 18	F 2	N 5	O 2	0	0
3	F	1	Total 28	Br 1	C 18	F 2	N 5	O 2	0	0

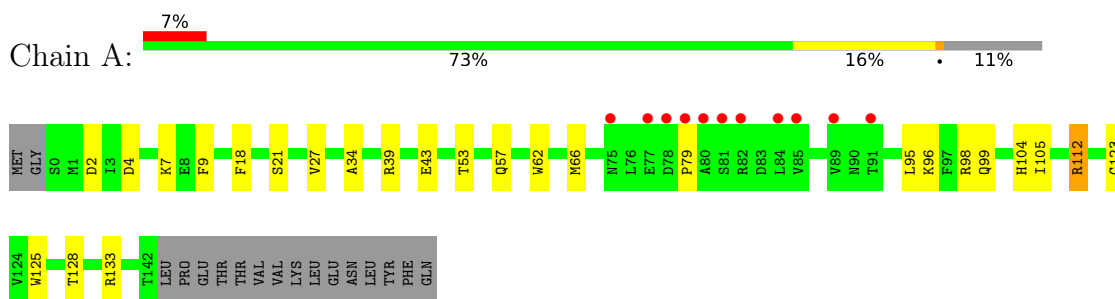
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	11	Total O 11 11	0	0
4	B	8	Total O 8 8	0	0
4	C	6	Total O 6 6	0	0
4	D	5	Total O 5 5	0	0
4	E	6	Total O 6 6	0	0
4	F	4	Total O 4 4	0	0

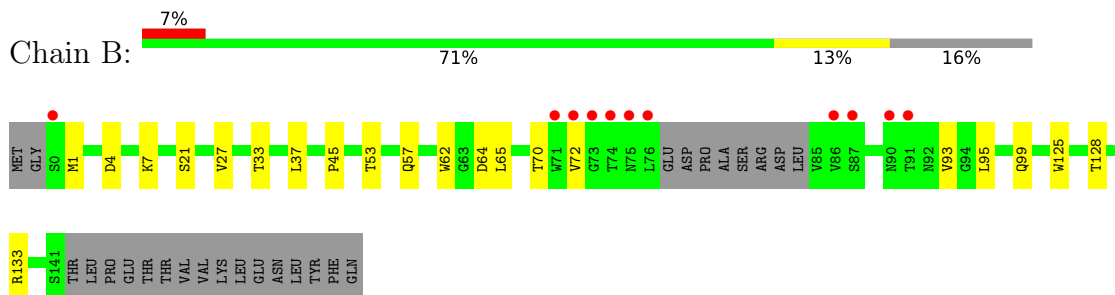
3 Residue-property plots [i](#)

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.

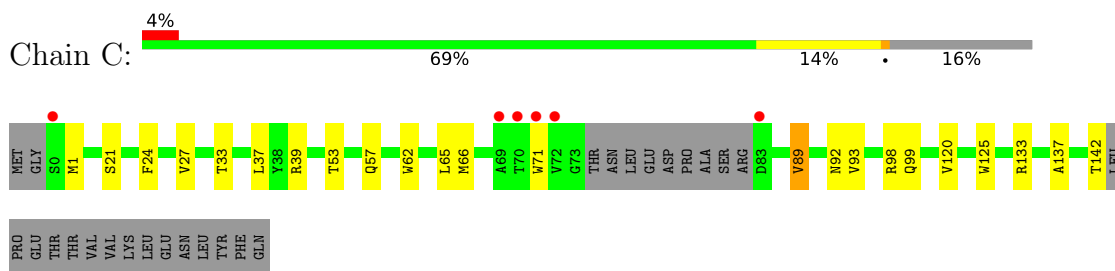
- Molecule 1: Capsid protein



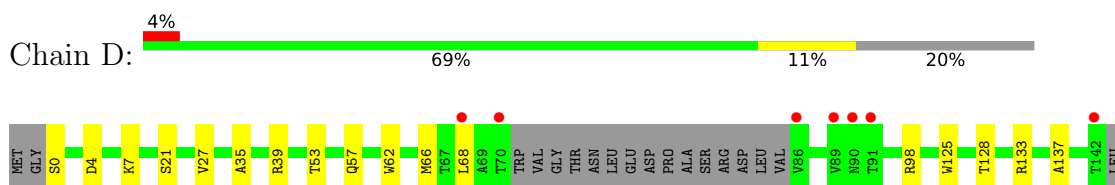
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



PRO
GLU
THR
THR
VAL
VAL
LYS
LEU
GLU
ASN
LEU
TYR
PHE
GLN

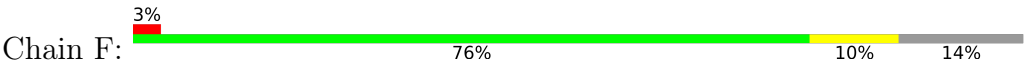
● Molecule 1: Capsid protein



MET GLY S0 D4 K7 E8 F9 S21 D22 F23 V27 R39 T53 Q57 W62 M66 T67 A69 T70 W71 VAL GLY THR ASN ASN LEU GLU ASP PRO ALA SER R82 D83 R88 H104 R112 W125 T128 R133 T142 LEU PRO GLU THR

THR
VAL
VAL
LYS
LEU
GLU
ASN
LEU
TYR
PHE
GLN

● Molecule 1: Capsid protein



MET GLY M1 D4 K7 V27 T33 L37 S49 H52 T53 Q57 L60 G61 W62 T70 L76 GLU ASP PRO ALA SER ARG D83 V86 N90 W125 T128 R133 T142 LEU PRO GLU THR THR VAL VAL LYS LEU ASN LEU

TYR
PHE
GLN

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.78Å 87.57Å 103.26Å 90.00° 103.48° 90.00°	Depositor
Resolution (Å)	36.90 – 2.65 36.90 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.1 (36.90-2.65) 99.3 (36.90-2.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.65Å)	Xtriage
Refinement program	PHENIX DEV_2463	Depositor
R, R_{free}	0.205 , 0.253 0.206 , 0.253	Depositor DCC
R_{free} test set	2060 reflections (5.37%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	1.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6413	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.21	0/1133	0.43	0/1554
1	B	0.22	0/1067	0.42	0/1464
1	C	0.23	0/1050	0.46	0/1441
1	D	0.22	0/1011	0.45	0/1384
1	E	0.22	0/1060	0.41	0/1453
1	F	0.22	0/1063	0.45	0/1458
All	All	0.22	0/6384	0.44	0/8754

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	1097	0	1038	17	0
1	B	1035	0	989	14	0
1	C	1019	0	959	15	0
1	D	982	0	942	14	0
1	E	1028	0	982	12	0
1	F	1032	0	968	11	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	3	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	28	0	0	0	0
3	B	28	0	0	0	0
3	C	28	0	0	0	0
3	D	28	0	0	0	0
3	E	28	0	0	0	0
3	F	28	0	0	0	0
4	A	11	0	0	0	0
4	B	8	0	0	0	0
4	C	6	0	0	0	0
4	D	5	0	0	0	0
4	E	6	0	0	0	0
4	F	4	0	0	0	0
All	All	6413	0	5878	72	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 6.

All (72) 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:E:39:ARG:NH2	1:F:0:SER:O	2.30	0.65
1:B:37:LEU:HD21	1:C:120:VAL:HG11	1.83	0.60
1:A:21:SER:O	1:A:98:ARG:NH2	2.34	0.59
1:D:128:THR:HB	1:D:133:ARG:HB3	1.84	0.59
1:A:9:PHE:O	1:A:112:ARG:HD3	2.03	0.59
1:B:95:LEU:HG	1:B:99:GLN:HE21	1.68	0.58
1:A:125:TRP:CE2	1:A:133:ARG:HD2	2.40	0.56
1:B:125:TRP:CE2	1:B:133:ARG:HD2	2.41	0.56
1:C:125:TRP:CE2	1:C:133:ARG:HD2	2.43	0.54
1:A:4:ASP:HB3	1:A:7:LYS:HB2	1.89	0.53
1:A:128:THR:HB	1:A:133:ARG:HB3	1.89	0.53
1:E:66:MET:HA	1:E:66:MET:HE2	1.91	0.53
1:D:4:ASP:HB3	1:D:7:LYS:HB2	1.89	0.53
1:A:39[A]:ARG:HG3	1:B:1:MET:HG2	1.91	0.53
1:C:1:MET:HE2	1:D:35:ALA:HB2	1.91	0.53
1:E:4:ASP:HB3	1:E:7:LYS:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LYS:HE2	1:B:45:PRO:HG3	1.90	0.52
1:F:33:THR:HG22	1:F:37:LEU:HD12	1.92	0.52
1:D:125:TRP:CE2	1:D:133:ARG:HD2	2.44	0.52
1:E:27:VAL:HG11	1:E:62:TRP:CE2	2.44	0.52
1:B:53:THR:O	1:B:57:GLN:HG2	2.09	0.52
1:E:39:ARG:HG3	1:F:1:MET:HG2	1.91	0.51
1:F:125:TRP:CE2	1:F:133:ARG:HD2	2.45	0.51
1:C:24:PHE:CZ	1:C:99:GLN:HG2	2.44	0.51
1:C:33:THR:HG22	1:C:37:LEU:HD12	1.92	0.51
1:B:33:THR:HG22	1:B:37:LEU:HD12	1.93	0.50
1:D:62:TRP:CZ2	1:D:66:MET:HE3	2.45	0.50
1:B:128:THR:HB	1:B:133:ARG:HB3	1.94	0.50
1:E:27:VAL:HG22	1:E:98:ARG:HG3	1.93	0.50
1:C:53:THR:O	1:C:57:GLN:HG2	2.12	0.50
1:A:53:THR:O	1:A:57:GLN:HG2	2.12	0.49
1:A:27:VAL:HG11	1:A:62:TRP:CE2	2.48	0.49
1:F:4:ASP:HB3	1:F:7:LYS:HB2	1.92	0.49
1:C:1:MET:HG2	1:D:39:ARG:HG3	1.94	0.49
1:D:53:THR:O	1:D:57:GLN:HG2	2.13	0.48
1:B:27:VAL:HG11	1:B:62:TRP:CE2	2.48	0.48
1:E:128:THR:O	1:E:133:ARG:NH1	2.46	0.48
1:F:128:THR:O	1:F:133:ARG:NH1	2.46	0.48
1:D:128:THR:O	1:D:133:ARG:NH1	2.46	0.48
1:B:4:ASP:HB3	1:B:7:LYS:HB2	1.96	0.47
1:A:95:LEU:O	1:A:99:GLN:HG3	2.14	0.47
1:D:66:MET:HA	1:D:66:MET:HE2	1.96	0.47
1:F:128:THR:HB	1:F:133:ARG:HB3	1.96	0.47
1:A:96:LYS:NZ	1:B:64:ASP:OD2	2.46	0.47
1:A:62:TRP:CZ2	1:A:66:MET:HE3	2.50	0.46
1:F:53:THR:O	1:F:57:GLN:HG2	2.15	0.46
1:C:65:LEU:HD13	1:C:93:VAL:HG11	1.98	0.45
1:B:65:LEU:HD13	1:B:93:VAL:HG11	1.99	0.45
1:C:39:ARG:NH1	1:D:0:SER:O	2.49	0.45
1:D:21:SER:O	1:D:98:ARG:NH2	2.50	0.45
1:A:43:GLU:O	1:B:7:LYS:NZ	2.35	0.44
1:E:125:TRP:CE2	1:E:133:ARG:HD2	2.52	0.44
1:F:27:VAL:HG11	1:F:62:TRP:CE2	2.53	0.44
1:C:66:MET:HA	1:C:66:MET:HE2	1.99	0.44
1:A:128:THR:O	1:A:133:ARG:NH1	2.51	0.44
1:C:21:SER:O	1:C:98:ARG:NH2	2.48	0.43
1:C:125:TRP:CH2	1:C:137:ALA:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:SER:O	1:E:98:ARG:NH2	2.51	0.43
1:A:18:PHE:CE2	1:A:123:GLY:HA3	2.54	0.43
1:E:53:THR:O	1:E:57:GLN:HG2	2.19	0.42
1:A:9:PHE:CE2	1:A:104:HIS:HE1	2.37	0.42
1:C:24:PHE:CE2	1:C:99:GLN:HG2	2.55	0.42
1:C:27:VAL:HG11	1:C:62:TRP:CE2	2.55	0.42
1:F:49:SER:OG	1:F:52:HIS:ND1	2.38	0.41
1:D:27:VAL:HG11	1:D:62:TRP:CE2	2.56	0.41
1:C:89:VAL:HG22	1:D:68:LEU:HD11	2.01	0.41
1:A:34:ALA:HB2	1:A:105:ILE:HD11	2.02	0.41
1:D:125:TRP:CH2	1:D:137:ALA:HB2	2.56	0.41
1:E:23:PHE:CD1	1:E:23:PHE:C	2.99	0.41
1:B:128:THR:O	1:B:133:ARG:NH1	2.54	0.41
1:E:9:PHE:CE2	1:E:104:HIS:HE1	2.40	0.40
1:F:60:LEU:HD23	1:F:60:LEU:HA	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	142/160 (89%)	138 (97%)	3 (2%)	1 (1%)	18	30
1	B	130/160 (81%)	128 (98%)	2 (2%)	0	100	100
1	C	130/160 (81%)	128 (98%)	2 (2%)	0	100	100
1	D	124/160 (78%)	122 (98%)	2 (2%)	0	100	100
1	E	129/160 (81%)	126 (98%)	3 (2%)	0	100	100
1	F	133/160 (83%)	130 (98%)	3 (2%)	0	100	100
All	All	788/960 (82%)	772 (98%)	15 (2%)	1 (0%)	48	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	PRO

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	112/141 (79%)	110 (98%)	2 (2%)	51	72
1	B	108/141 (77%)	105 (97%)	3 (3%)	38	60
1	C	104/141 (74%)	100 (96%)	4 (4%)	29	49
1	D	102/141 (72%)	102 (100%)	0	100	100
1	E	107/141 (76%)	106 (99%)	1 (1%)	70	82
1	F	103/141 (73%)	103 (100%)	0	100	100
All	All	636/846 (75%)	626 (98%)	10 (2%)	55	74

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	112	ARG
1	B	21	SER
1	B	70	THR
1	B	72	VAL
1	C	71	TRP
1	C	89	VAL
1	C	92	ASN
1	C	142	THR
1	E	68	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	ZMH	A	303	-	27,31,31	0.76	1 (3%)	29,46,46	1.84	5 (17%)
3	ZMH	E	303	-	27,31,31	0.80	2 (7%)	29,46,46	2.05	4 (13%)
3	ZMH	C	204	-	27,31,31	0.77	1 (3%)	29,46,46	1.66	5 (17%)
3	ZMH	F	303	-	27,31,31	0.88	1 (3%)	29,46,46	1.66	4 (13%)
3	ZMH	D	303	-	27,31,31	0.89	1 (3%)	29,46,46	1.68	5 (17%)
3	ZMH	B	302	-	27,31,31	0.70	0	29,46,46	1.86	5 (17%)

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	ZMH	A	303	-	-	2/8/33/33	0/3/4/4
3	ZMH	E	303	-	-	2/8/33/33	0/3/4/4
3	ZMH	C	204	-	-	2/8/33/33	0/3/4/4
3	ZMH	F	303	-	-	2/8/33/33	0/3/4/4
3	ZMH	D	303	-	-	2/8/33/33	0/3/4/4
3	ZMH	B	302	-	-	2/8/33/33	0/3/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	303	ZMH	C02-N27	3.02	1.38	1.35
3	D	303	ZMH	C02-N27	2.76	1.38	1.35
3	A	303	ZMH	C02-N27	2.44	1.38	1.35
3	E	303	ZMH	C02-N27	2.28	1.38	1.35
3	C	204	ZMH	C03-C04	-2.21	1.36	1.43
3	E	303	ZMH	C03-C04	-2.18	1.36	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	303	ZMH	C04-C05-N06	-8.52	102.01	109.62
3	B	302	ZMH	C04-C05-N06	-5.75	104.48	109.62
3	C	204	ZMH	C04-C05-N06	-5.60	104.62	109.62
3	D	303	ZMH	C04-C05-N06	-5.44	104.76	109.62
3	F	303	ZMH	C04-C05-N06	-5.29	104.90	109.62
3	A	303	ZMH	C04-C05-N06	-5.20	104.98	109.62
3	A	303	ZMH	O01-C02-N27	-4.44	116.44	122.30
3	B	302	ZMH	O01-C02-N27	-4.27	116.66	122.30
3	B	302	ZMH	C28-N27-C02	-4.20	113.76	119.36
3	A	303	ZMH	C28-N27-C02	-3.87	114.20	119.36
3	A	303	ZMH	C19-C18-N06	-3.52	104.92	110.67
3	C	204	ZMH	C28-N27-C02	-3.46	114.74	119.36
3	F	303	ZMH	O01-C02-N27	-3.41	117.80	122.30
3	E	303	ZMH	O01-C02-N27	-3.29	117.96	122.30
3	D	303	ZMH	O01-C02-N27	-3.14	118.15	122.30
3	D	303	ZMH	C19-C18-N06	-3.03	105.74	110.67
3	F	303	ZMH	C28-N27-C02	-2.99	115.37	119.36
3	C	204	ZMH	C19-C18-N06	-2.86	106.00	110.67
3	E	303	ZMH	C28-N27-C02	-2.66	115.81	119.36
3	F	303	ZMH	C19-C18-N06	-2.61	106.41	110.67
3	E	303	ZMH	C19-C18-N06	-2.39	106.78	110.67
3	C	204	ZMH	C09-N08-C07	2.11	130.31	126.04
3	B	302	ZMH	C19-C18-N06	-2.09	107.26	110.67
3	B	302	ZMH	C09-C16-C14	2.07	121.07	118.75
3	D	303	ZMH	C28-N27-C02	-2.06	116.61	119.36
3	C	204	ZMH	O01-C02-N27	-2.02	119.63	122.30
3	D	303	ZMH	F13-C12-C14	2.01	123.37	119.05
3	A	303	ZMH	C16-C09-N08	2.01	126.67	120.13

There are no chirality outliers.

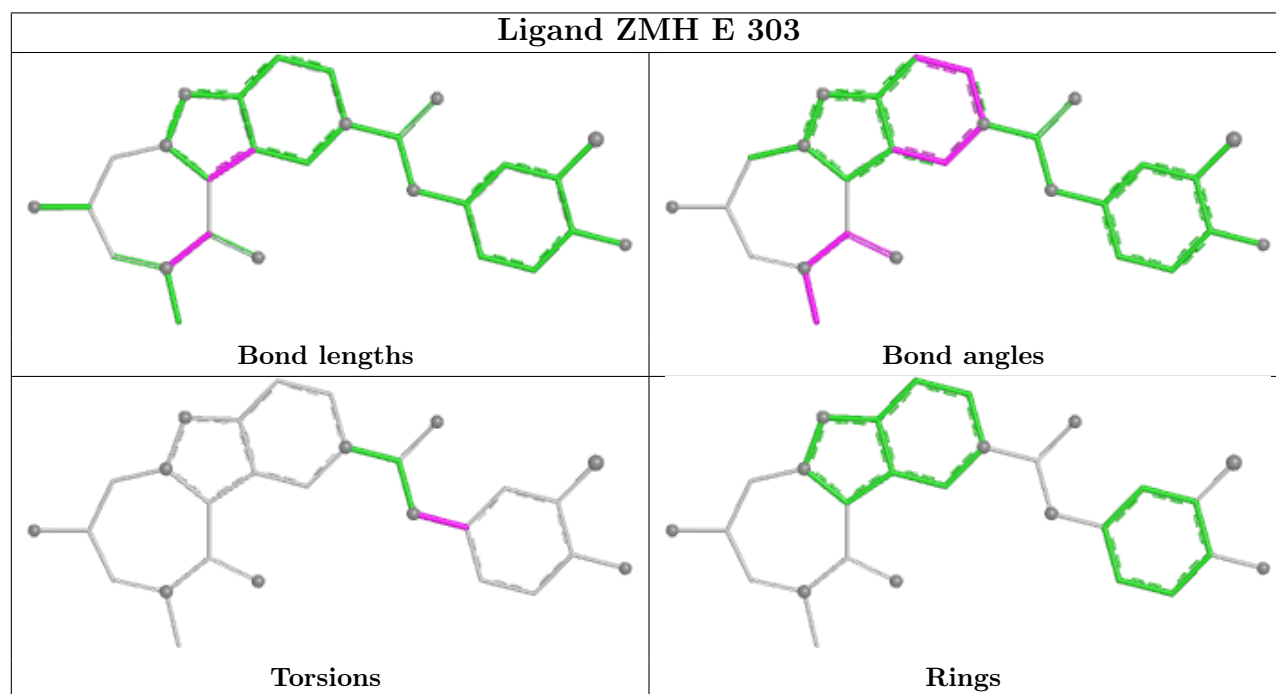
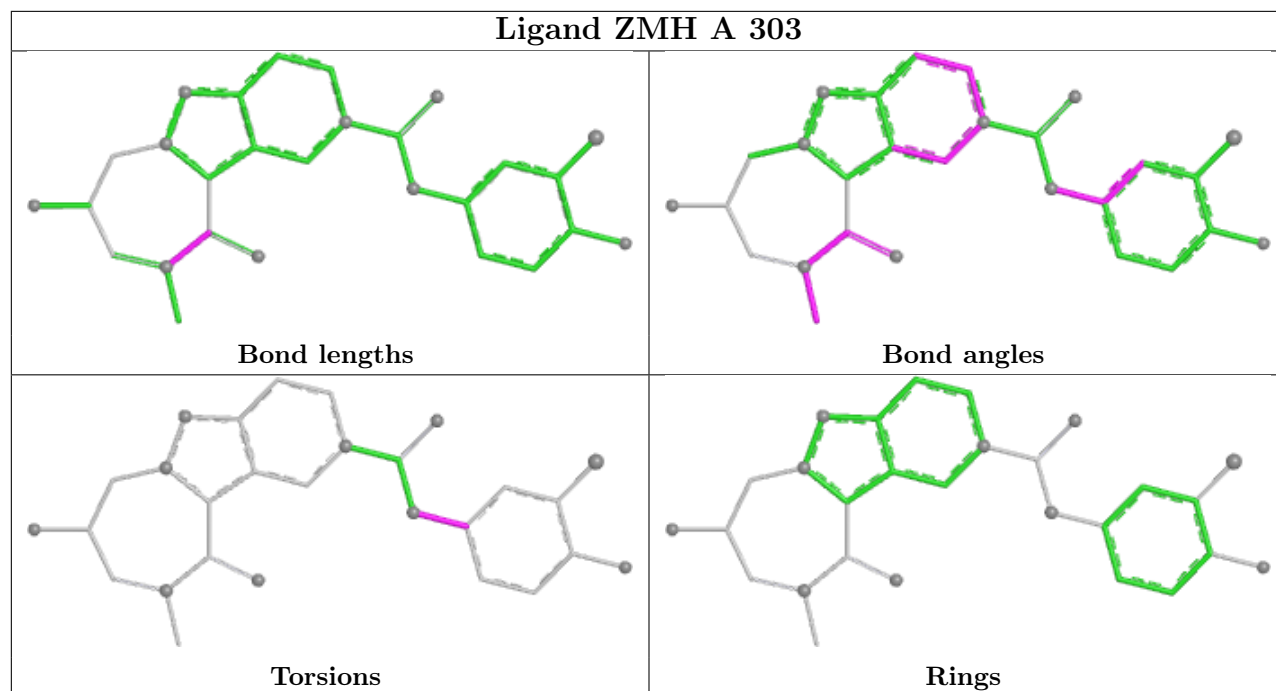
All (12) torsion outliers are listed below:

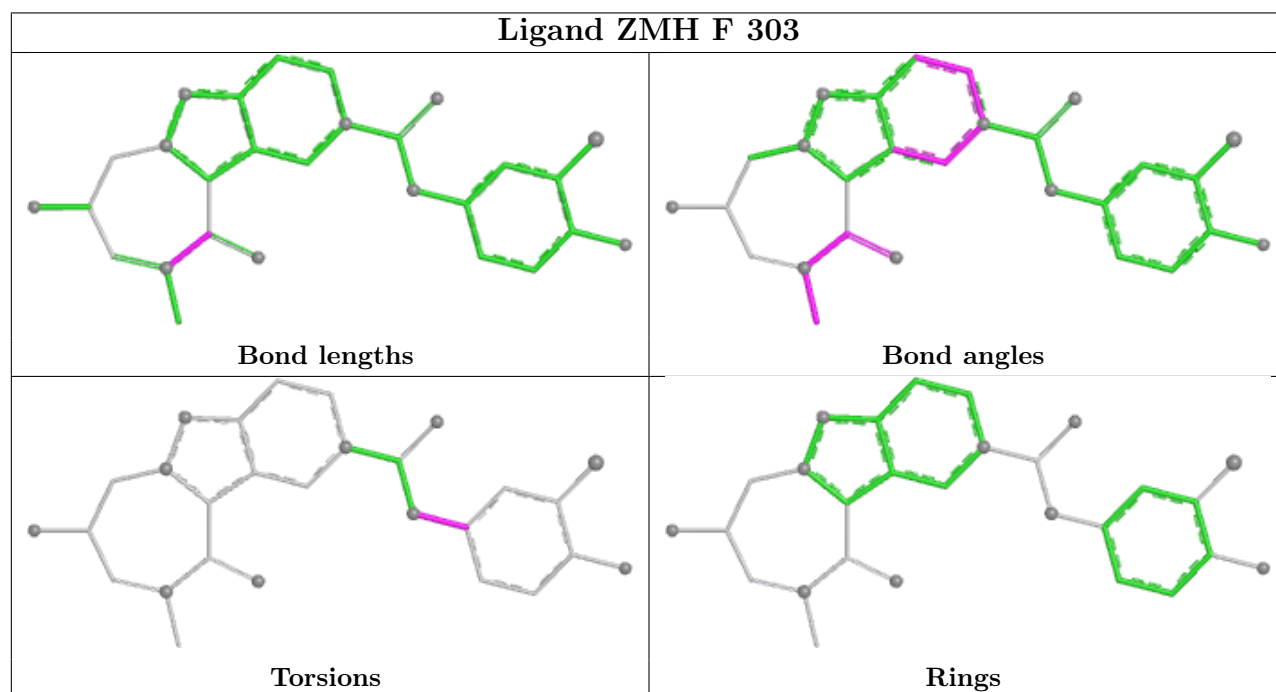
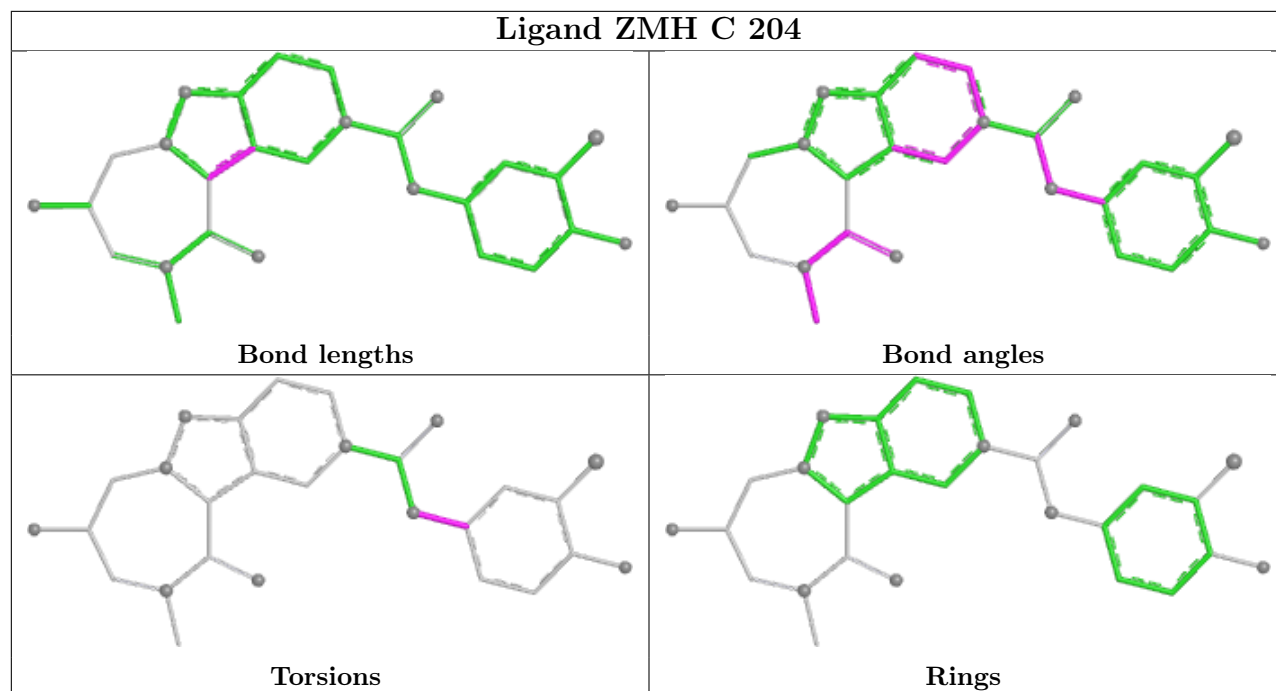
Mol	Chain	Res	Type	Atoms
3	C	204	ZMH	C10-C09-N08-C07
3	E	303	ZMH	C16-C09-N08-C07
3	C	204	ZMH	C16-C09-N08-C07
3	F	303	ZMH	C10-C09-N08-C07
3	E	303	ZMH	C10-C09-N08-C07
3	D	303	ZMH	C10-C09-N08-C07
3	F	303	ZMH	C16-C09-N08-C07
3	D	303	ZMH	C16-C09-N08-C07
3	A	303	ZMH	C16-C09-N08-C07
3	A	303	ZMH	C10-C09-N08-C07
3	B	302	ZMH	C16-C09-N08-C07
3	B	302	ZMH	C10-C09-N08-C07

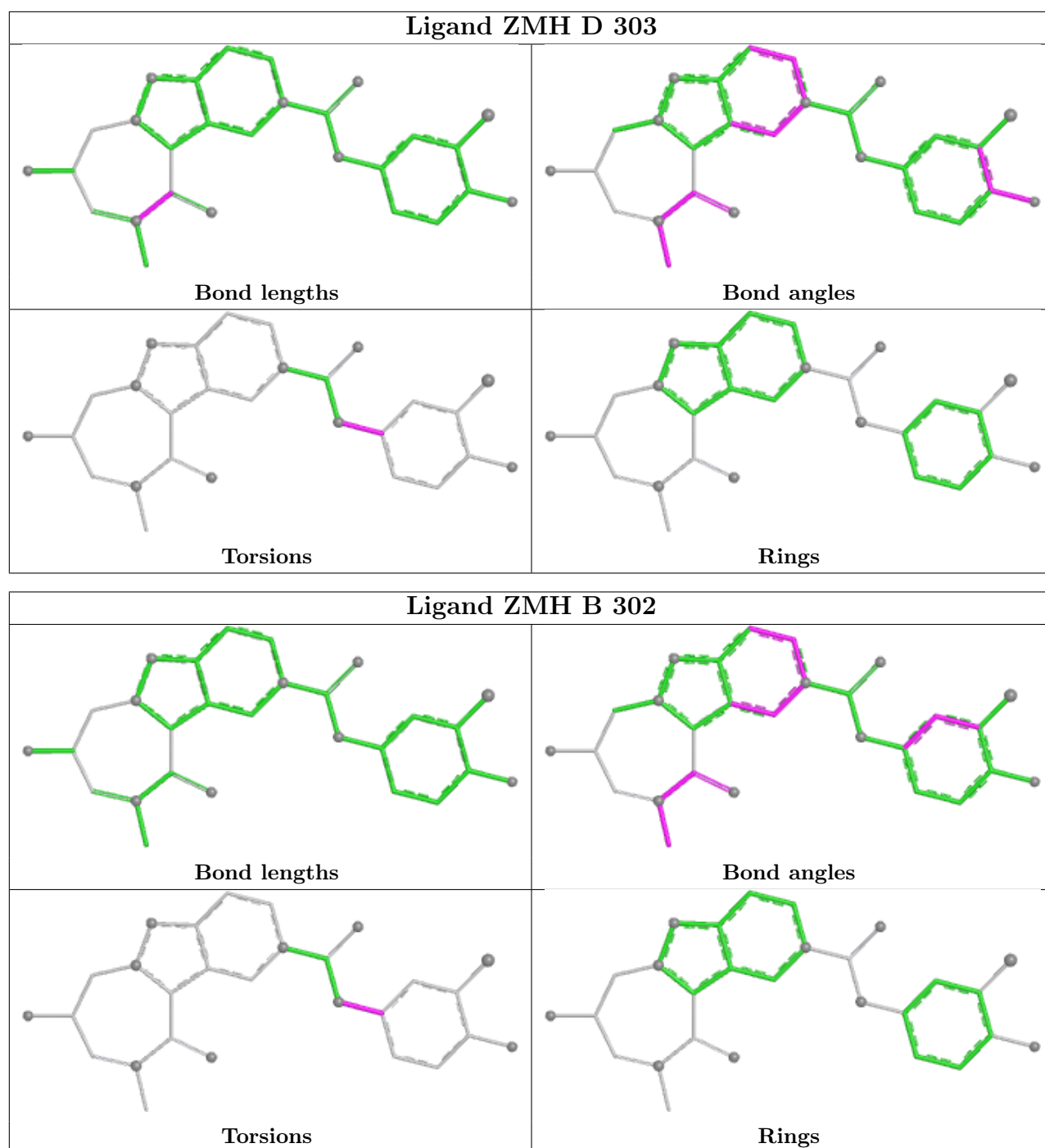
There are no ring outliers.

No monomer is involved in short contacts.

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	143/160 (89%)	0.32	11 (7%) 19 14	38, 53, 107, 133	1 (0%)
1	B	134/160 (83%)	0.19	11 (8%) 17 13	36, 54, 115, 141	0
1	C	134/160 (83%)	0.14	6 (4%) 38 31	33, 52, 92, 119	0
1	D	128/160 (80%)	0.17	7 (5%) 30 24	41, 56, 92, 119	0
1	E	133/160 (83%)	0.09	4 (3%) 52 45	39, 54, 92, 112	0
1	F	137/160 (85%)	0.21	5 (3%) 46 38	39, 51, 104, 123	0
All	All	809/960 (84%)	0.19	44 (5%) 31 25	33, 53, 104, 141	1 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	90	ASN	4.9
1	B	86	VAL	3.7
1	A	77	GLU	3.7
1	B	91	THR	3.6
1	F	83	ASP	3.6
1	A	75	ASN	3.5
1	A	78	ASP	3.5
1	D	89	VAL	3.4
1	A	84	LEU	3.3
1	D	68	LEU	3.3
1	B	76	LEU	3.2
1	A	80	ALA	3.2
1	C	83	ASP	3.1
1	A	91	THR	2.9
1	D	91	THR	2.9
1	A	79	PRO	2.8
1	C	71	TRP	2.8
1	D	142	THR	2.7
1	B	73	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	83	ASP	2.7
1	A	81	SER	2.7
1	D	70	THR	2.7
1	B	0	SER	2.6
1	B	75	ASN	2.6
1	C	70	THR	2.6
1	C	69	ALA	2.6
1	A	85	VAL	2.5
1	E	142	THR	2.5
1	D	90	ASN	2.5
1	A	82	ARG	2.5
1	E	112	ARG	2.4
1	C	72	VAL	2.3
1	A	89	VAL	2.3
1	F	86	VAL	2.3
1	B	87	SER	2.2
1	C	0	SER	2.2
1	F	90	ASN	2.2
1	B	72	VAL	2.2
1	F	0	SER	2.2
1	E	70	THR	2.1
1	D	86	VAL	2.1
1	B	71	TRP	2.1
1	B	74	THR	2.1
1	F	70	THR	2.1

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

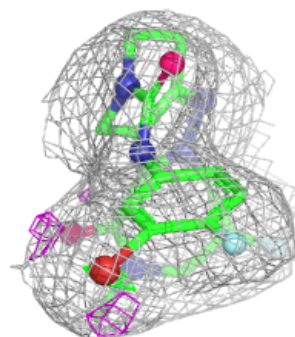
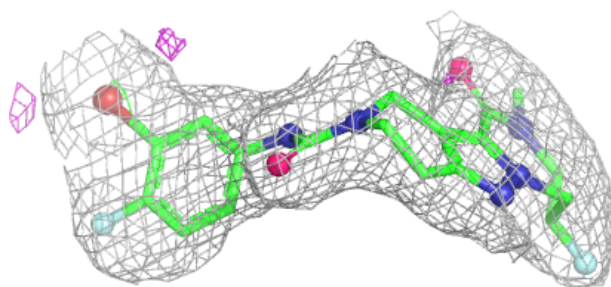
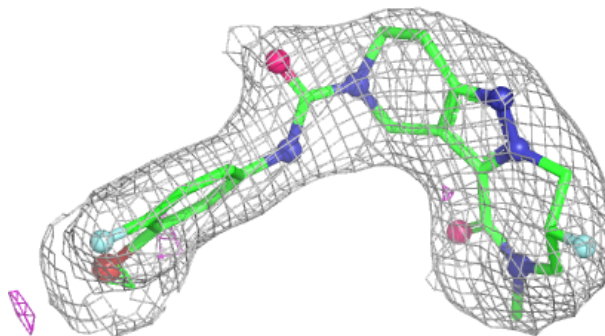
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	A	301	1/1	0.91	0.11	77,77,77,77	0
2	CL	B	301	1/1	0.91	0.17	81,81,81,81	0
2	CL	D	301	1/1	0.92	0.16	79,79,79,79	0
2	CL	C	201	1/1	0.93	0.09	60,60,60,60	0
2	CL	E	302	1/1	0.93	0.12	67,67,67,67	0
2	CL	F	301	1/1	0.93	0.15	88,88,88,88	0
2	CL	F	302	1/1	0.93	0.10	54,54,54,54	0
2	CL	C	203	1/1	0.94	0.09	52,52,52,52	0
2	CL	C	202	1/1	0.95	0.15	88,88,88,88	0
2	CL	D	302	1/1	0.95	0.09	56,56,56,56	0
2	CL	E	301	1/1	0.95	0.10	80,80,80,80	0
3	ZMH	A	303	28/28	0.95	0.09	34,49,69,82	0
3	ZMH	B	302	28/28	0.95	0.09	33,41,59,77	0
3	ZMH	C	204	28/28	0.95	0.09	38,52,71,84	0
3	ZMH	D	303	28/28	0.95	0.09	35,52,64,75	0
3	ZMH	E	303	28/28	0.95	0.10	33,57,63,73	0
3	ZMH	F	303	28/28	0.95	0.10	20,48,64,70	0
2	CL	A	302	1/1	0.96	0.06	53,53,53,53	0

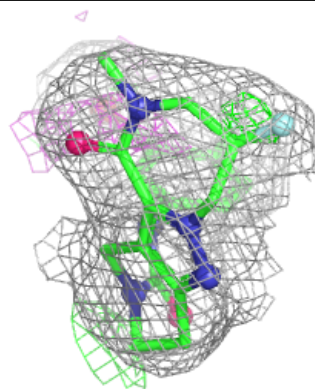
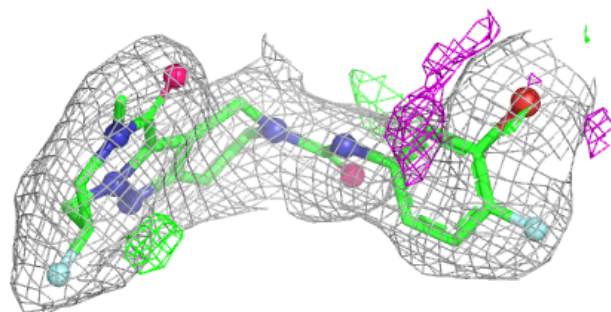
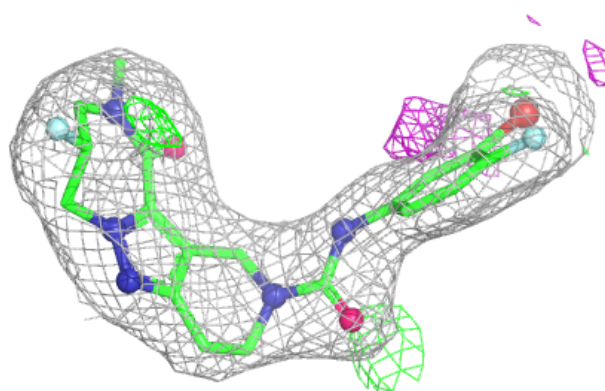
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZMH A 303:

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

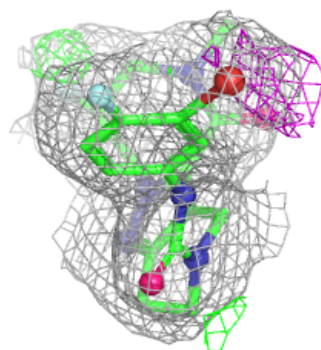
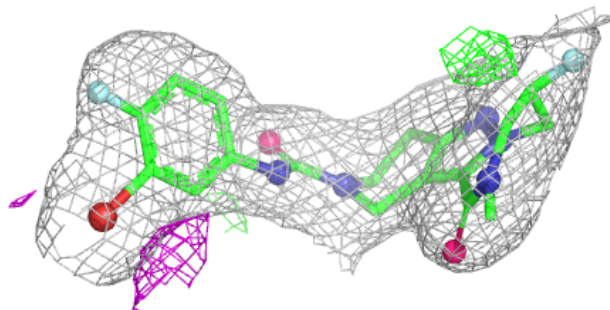
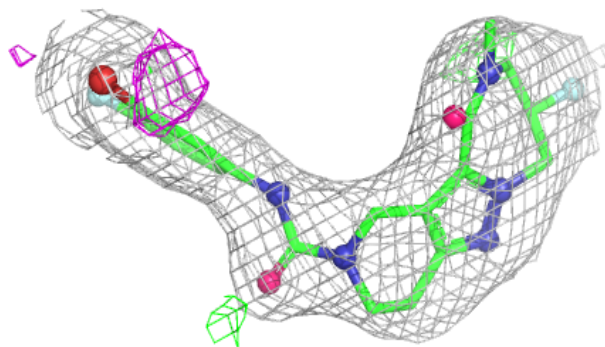
**Electron density around ZMH B 302:**

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

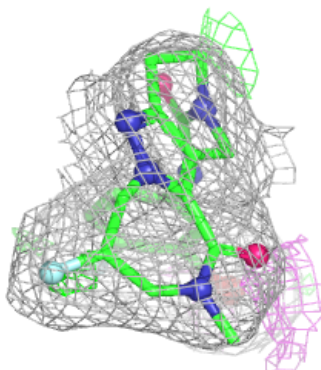
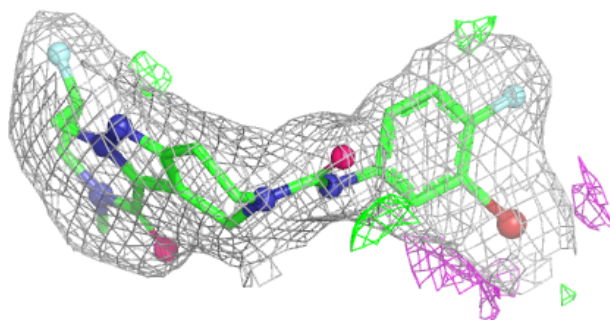
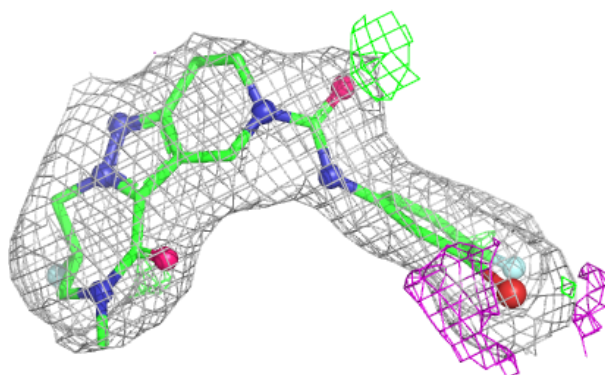


Electron density around ZMH C 204:

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

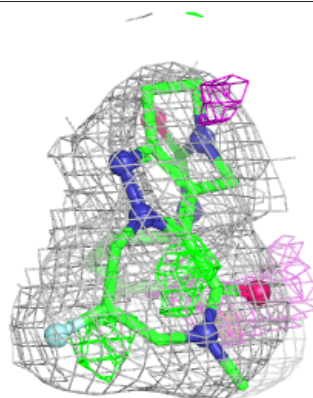
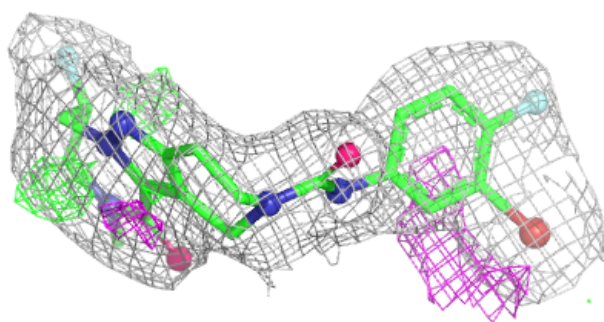
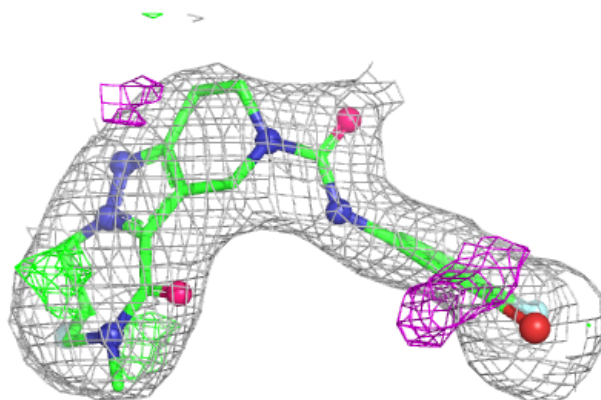
**Electron density around ZMH D 303:**

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

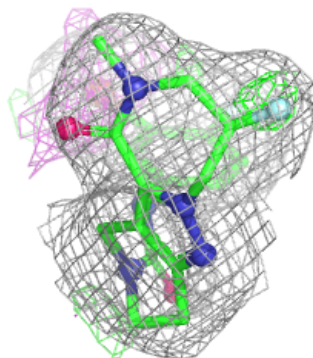
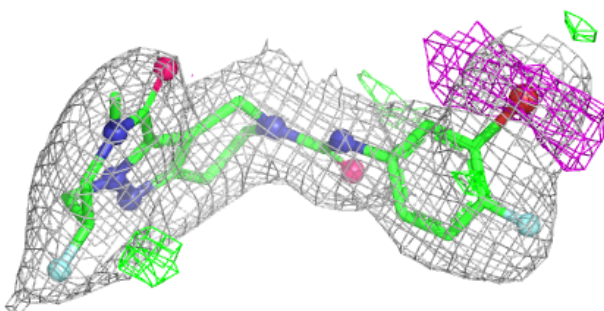
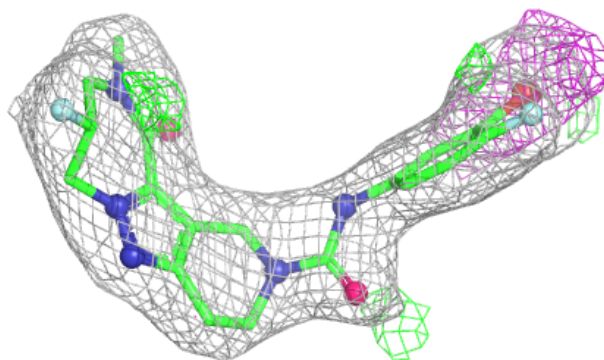


Electron density around ZMH E 303:

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

**Electron density around ZMH F 303:**

$2mF_o-DF_c$ (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.