



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 02:54 AM BST

PDB ID : 2HD0
Title : Structure of the catalytic domain of hepatitis C virus NS2
Authors : Lorenz, I.C.; Rice, C.M.; Marcotrigiano, J.
Deposited on : 2006-06-19
Resolution : 2.28 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

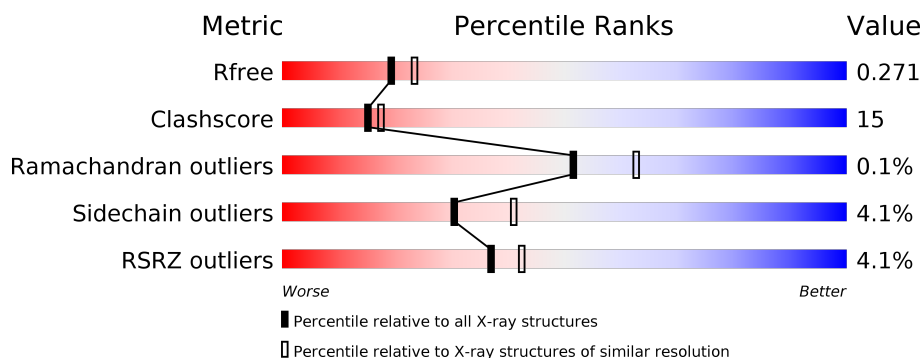
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	128	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>28%</div> <div>..</div> </div> </div>
1	B	128	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div>..</div> </div> </div>
1	C	128	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div>..</div> </div> </div>
1	D	128	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div>...</div> </div> </div>
1	E	128	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>25%</div> <div>..</div> </div> </div>
1	F	128	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>23%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	128	
1	H	128	
1	I	128	
1	J	128	
1	K	128	
1	L	128	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BOG	H	218	-	-	-	X
3	DMU	I	218	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11930 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 Protease NS2-3 (p23).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	0	0	0
			974	625	177	166	6			
1	B	127	Total	C	N	O	S	0	0	0
			958	616	170	166	6			
1	C	127	Total	C	N	O	S	0	0	0
			966	620	175	165	6			
1	D	127	Total	C	N	O	S	0	0	0
			958	618	172	162	6			
1	E	127	Total	C	N	O	S	0	0	0
			964	620	174	164	6			
1	F	127	Total	C	N	O	S	0	0	0
			950	611	168	165	6			
1	G	127	Total	C	N	O	S	0	0	0
			951	613	169	163	6			
1	H	128	Total	C	N	O	S	0	0	0
			958	617	170	165	6			
1	I	127	Total	C	N	O	S	0	0	0
			952	613	167	166	6			
1	J	127	Total	C	N	O	S	0	0	0
			970	622	176	166	6			
1	K	127	Total	C	N	O	S	0	0	0
			948	611	167	164	6			
1	L	127	Total	C	N	O	S	0	0	0
			952	614	167	165	6			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P27958
A	2	SER	-	cloning artifact	UNP P27958
A	3	HIS	-	cloning artifact	UNP P27958
A	4	MET	-	cloning artifact	UNP P27958
A	139	TYR	CYS	variant	UNP P27958

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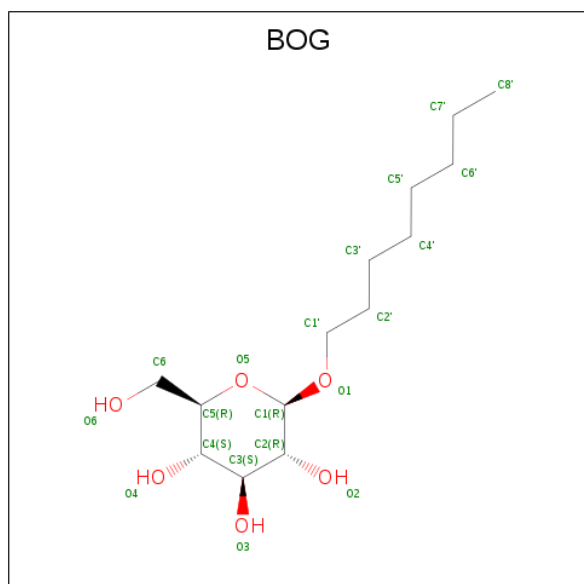
Chain	Residue	Modelled	Actual	Comment	Reference
A	145	THR	ALA	variant	UNP P27958
B	1	GLY	-	cloning artifact	UNP P27958
B	2	SER	-	cloning artifact	UNP P27958
B	3	HIS	-	cloning artifact	UNP P27958
B	4	MET	-	cloning artifact	UNP P27958
B	139	TYR	CYS	variant	UNP P27958
B	145	THR	ALA	variant	UNP P27958
C	1	GLY	-	cloning artifact	UNP P27958
C	2	SER	-	cloning artifact	UNP P27958
C	3	HIS	-	cloning artifact	UNP P27958
C	4	MET	-	cloning artifact	UNP P27958
C	139	TYR	CYS	variant	UNP P27958
C	145	THR	ALA	variant	UNP P27958
D	1	GLY	-	cloning artifact	UNP P27958
D	2	SER	-	cloning artifact	UNP P27958
D	3	HIS	-	cloning artifact	UNP P27958
D	4	MET	-	cloning artifact	UNP P27958
D	139	TYR	CYS	variant	UNP P27958
D	145	THR	ALA	variant	UNP P27958
E	1	GLY	-	cloning artifact	UNP P27958
E	2	SER	-	cloning artifact	UNP P27958
E	3	HIS	-	cloning artifact	UNP P27958
E	4	MET	-	cloning artifact	UNP P27958
E	139	TYR	CYS	variant	UNP P27958
E	145	THR	ALA	variant	UNP P27958
F	1	GLY	-	cloning artifact	UNP P27958
F	2	SER	-	cloning artifact	UNP P27958
F	3	HIS	-	cloning artifact	UNP P27958
F	4	MET	-	cloning artifact	UNP P27958
F	139	TYR	CYS	variant	UNP P27958
F	145	THR	ALA	variant	UNP P27958
G	1	GLY	-	cloning artifact	UNP P27958
G	2	SER	-	cloning artifact	UNP P27958
G	3	HIS	-	cloning artifact	UNP P27958
G	4	MET	-	cloning artifact	UNP P27958
G	139	TYR	CYS	variant	UNP P27958
G	145	THR	ALA	variant	UNP P27958
H	1	GLY	-	cloning artifact	UNP P27958
H	2	SER	-	cloning artifact	UNP P27958
H	3	HIS	-	cloning artifact	UNP P27958
H	4	MET	-	cloning artifact	UNP P27958
H	139	TYR	CYS	variant	UNP P27958

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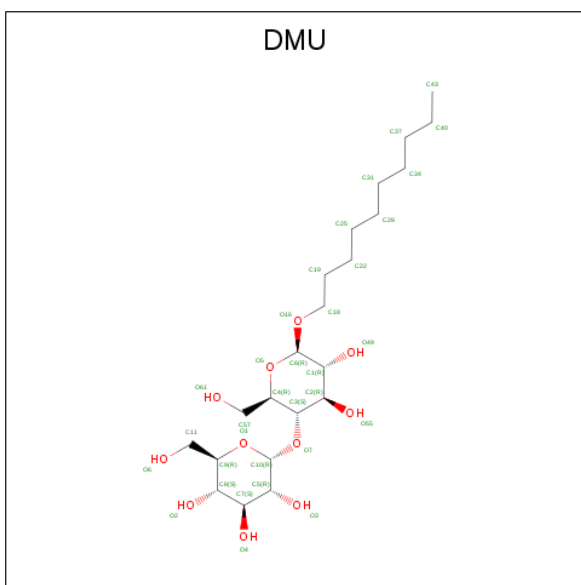
Chain	Residue	Modelled	Actual	Comment	Reference
H	145	THR	ALA	variant	UNP P27958
I	1	GLY	-	cloning artifact	UNP P27958
I	2	SER	-	cloning artifact	UNP P27958
I	3	HIS	-	cloning artifact	UNP P27958
I	4	MET	-	cloning artifact	UNP P27958
I	139	TYR	CYS	variant	UNP P27958
I	145	THR	ALA	variant	UNP P27958
J	1	GLY	-	cloning artifact	UNP P27958
J	2	SER	-	cloning artifact	UNP P27958
J	3	HIS	-	cloning artifact	UNP P27958
J	4	MET	-	cloning artifact	UNP P27958
J	139	TYR	CYS	variant	UNP P27958
J	145	THR	ALA	variant	UNP P27958
K	1	GLY	-	cloning artifact	UNP P27958
K	2	SER	-	cloning artifact	UNP P27958
K	3	HIS	-	cloning artifact	UNP P27958
K	4	MET	-	cloning artifact	UNP P27958
K	139	TYR	CYS	variant	UNP P27958
K	145	THR	ALA	variant	UNP P27958
L	1	GLY	-	cloning artifact	UNP P27958
L	2	SER	-	cloning artifact	UNP P27958
L	3	HIS	-	cloning artifact	UNP P27958
L	4	MET	-	cloning artifact	UNP P27958
L	139	TYR	CYS	variant	UNP P27958
L	145	THR	ALA	variant	UNP P27958

- Molecule 2 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 20	C 14	O 6	0	0
2	A	1	Total 20	C 14	O 6	0	0
2	A	1	Total 20	C 14	O 6	0	0
2	B	1	Total 20	C 14	O 6	0	0
2	C	1	Total 20	C 14	O 6	0	0
2	F	1	Total 20	C 14	O 6	0	0
2	F	1	Total 20	C 14	O 6	0	0
2	H	1	Total 20	C 14	O 6	0	0
2	I	1	Total 20	C 14	O 6	0	0
2	J	1	Total 20	C 14	O 6	0	0
2	K	1	Total 20	C 14	O 6	0	0

- Molecule 3 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	I	1	Total	C	O	0	0
			33	22	11		

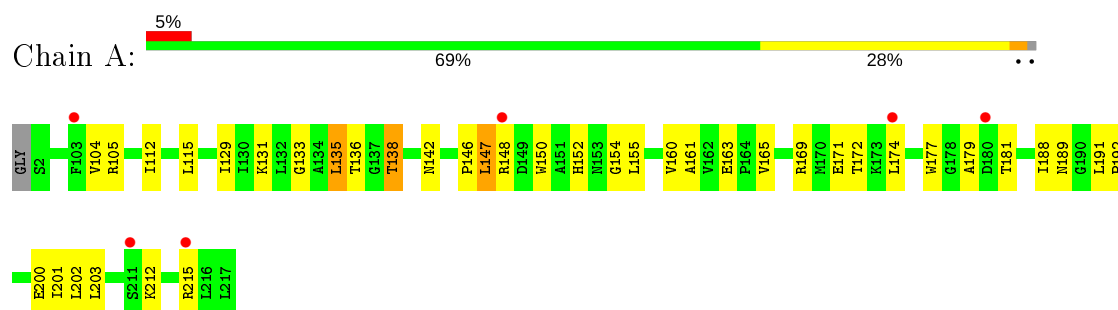
- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	16	Total	O		0	0
			16	16			
4	B	10	Total	O		0	0
			10	10			
4	C	24	Total	O		0	0
			24	24			
4	D	14	Total	O		0	0
			14	14			
4	E	29	Total	O		0	0
			29	29			
4	F	13	Total	O		0	0
			13	13			
4	G	15	Total	O		0	0
			15	15			
4	H	13	Total	O		0	0
			13	13			
4	I	14	Total	O		0	0
			14	14			
4	J	8	Total	O		0	0
			8	8			
4	K	13	Total	O		0	0
			13	13			
4	L	7	Total	O		0	0
			7	7			

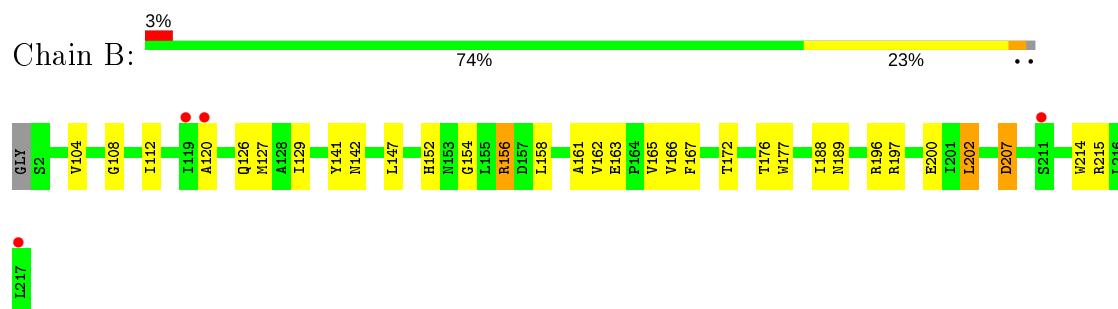
3 Residue-property plots [i](#)

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.

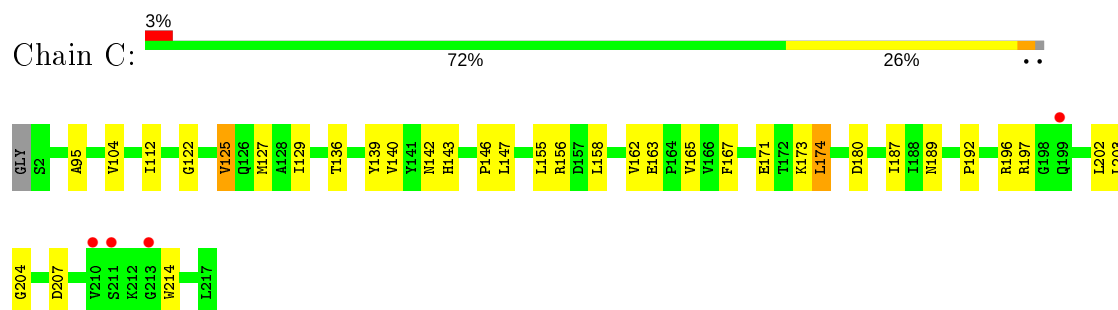
- Molecule 1: Protease NS2-3 (p23)



- Molecule 1: Protease NS2-3 (p23)

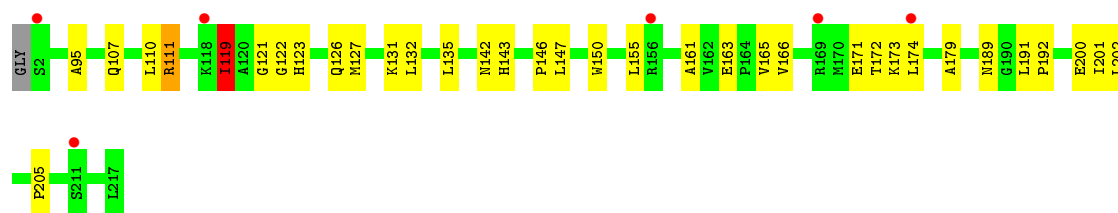


- Molecule 1: Protease NS2-3 (p23)



- Molecule 1: Protease NS2-3 (p23)

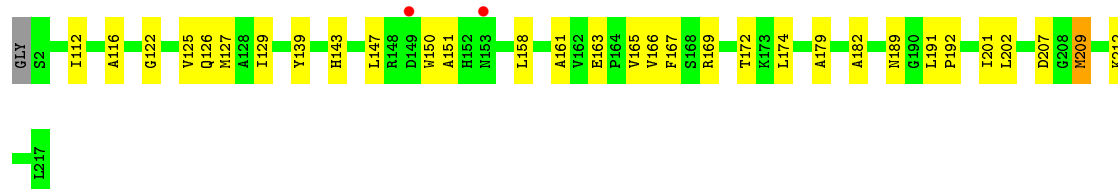
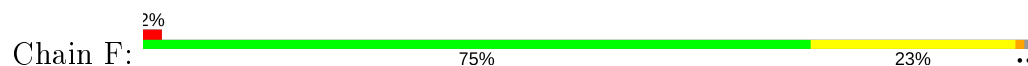




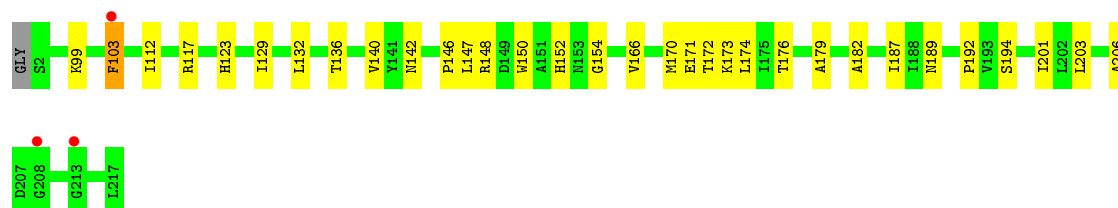
- Molecule 1: Protease NS2-3 (p23)



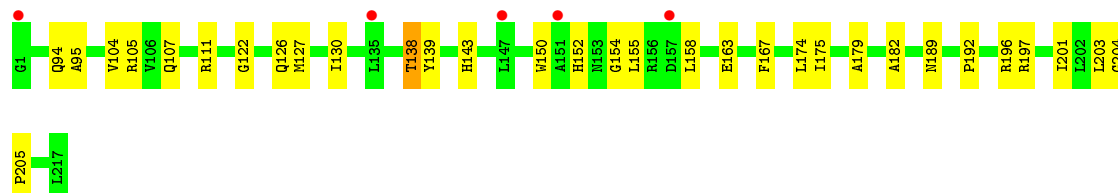
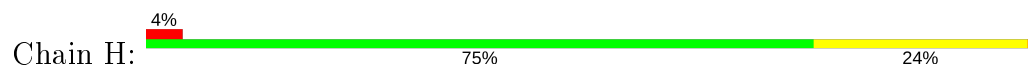
- Molecule 1: Protease NS2-3 (p23)



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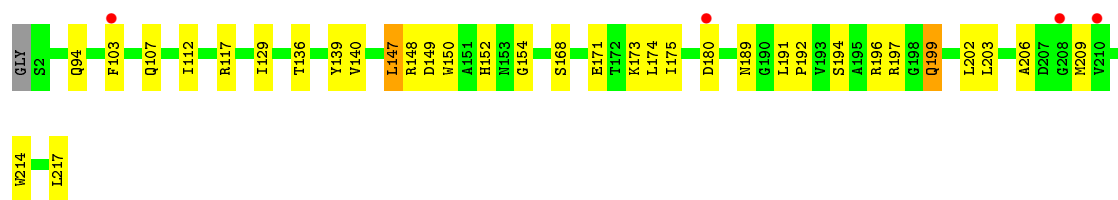


- Molecule 1: Protease NS2-3 (p23)

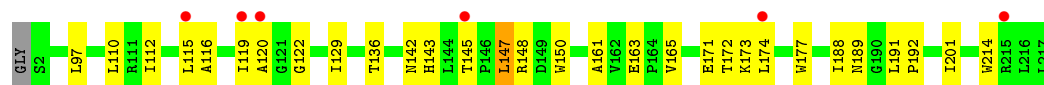


- Molecule 1: Protease NS2-3 (p23)

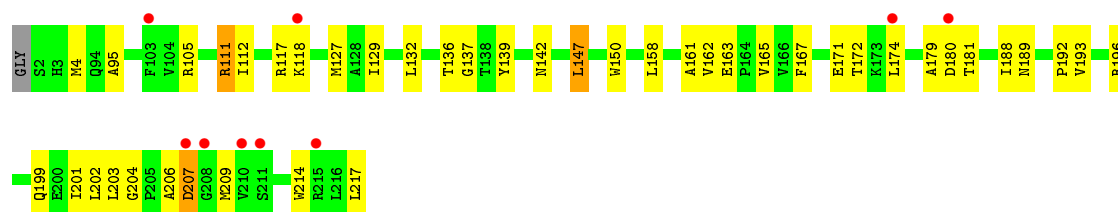




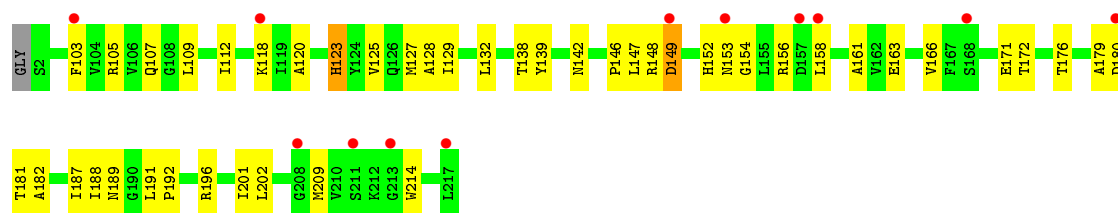
- Molecule 1: Protease NS2-3 (p23)



- Molecule 1: Protease NS2-3 (p23)



- Molecule 1: Protease NS2-3 (p23)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.81Å 68.82Å 125.16Å 90.00° 105.88° 90.00°	Depositor
Resolution (Å)	30.00 – 2.28 29.87 – 2.28	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.28) 98.2 (29.87-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.93 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.268 0.229 , 0.271	Depositor DCC
R_{free} test set	8206 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11930	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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 21.13 % 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 7.4826e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.37	0/994	0.64	0/1347
1	B	0.34	0/978	0.61	0/1329
1	C	0.39	0/986	0.64	0/1338
1	D	0.33	0/978	0.61	0/1327
1	E	0.37	0/984	0.65	0/1335
1	F	0.35	0/970	0.61	0/1320
1	G	0.38	0/971	0.64	0/1320
1	H	0.35	0/978	0.61	0/1328
1	I	0.36	0/972	0.64	0/1322
1	J	0.35	0/990	0.60	0/1343
1	K	0.34	0/968	0.63	0/1317
1	L	0.32	0/972	0.57	0/1321
All	All	0.35	0/11741	0.62	0/15947

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	974	0	1012	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	958	0	979	41	0
1	C	966	0	995	32	0
1	D	958	0	989	30	0
1	E	964	0	997	35	0
1	F	950	0	962	35	0
1	G	951	0	971	32	0
1	H	958	0	984	34	0
1	I	952	0	968	28	0
1	J	970	0	1001	32	0
1	K	948	0	964	49	0
1	L	952	0	973	44	0
2	A	60	0	84	4	0
2	B	20	0	28	1	0
2	C	20	0	28	1	0
2	F	40	0	56	0	0
2	H	20	0	28	4	0
2	I	20	0	28	0	0
2	J	20	0	28	0	0
2	K	20	0	28	0	0
3	I	33	0	37	0	0
4	A	16	0	0	0	0
4	B	10	0	0	0	0
4	C	24	0	0	2	0
4	D	14	0	0	0	0
4	E	29	0	0	1	0
4	F	13	0	0	0	0
4	G	15	0	0	1	0
4	H	13	0	0	0	0
4	I	14	0	0	0	0
4	J	8	0	0	0	0
4	K	13	0	0	0	0
4	L	7	0	0	0	0
All	All	11930	0	12140	359	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 15.

The worst 5 of 359 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:L:179:ALA:HA	1:L:201:ILE:HD11	1.30	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:179:ALA:HA	1:H:201:ILE:HD11	1.23	1.10
1:G:179:ALA:HA	1:G:201:ILE:HD11	1.40	1.02
1:D:111:ARG:HH11	1:D:111:ARG:HA	1.26	0.99
1:F:179:ALA:HA	1:F:201:ILE:HD11	1.43	0.96

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	125/128 (98%)	122 (98%)	3 (2%)	0	100	100
1	B	125/128 (98%)	120 (96%)	4 (3%)	1 (1%)	19	22
1	C	125/128 (98%)	122 (98%)	3 (2%)	0	100	100
1	D	125/128 (98%)	122 (98%)	2 (2%)	1 (1%)	19	22
1	E	125/128 (98%)	122 (98%)	3 (2%)	0	100	100
1	F	125/128 (98%)	123 (98%)	2 (2%)	0	100	100
1	G	125/128 (98%)	119 (95%)	6 (5%)	0	100	100
1	H	126/128 (98%)	116 (92%)	10 (8%)	0	100	100
1	I	125/128 (98%)	122 (98%)	3 (2%)	0	100	100
1	J	125/128 (98%)	122 (98%)	3 (2%)	0	100	100
1	K	125/128 (98%)	120 (96%)	5 (4%)	0	100	100
1	L	125/128 (98%)	117 (94%)	8 (6%)	0	100	100
All	All	1501/1536 (98%)	1447 (96%)	52 (4%)	2 (0%)	51	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	120	ALA
1	D	119	ILE

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	100/100 (100%)	92 (92%)	8 (8%)	12	14
1	B	97/100 (97%)	94 (97%)	3 (3%)	40	53
1	C	98/100 (98%)	93 (95%)	5 (5%)	24	31
1	D	96/100 (96%)	93 (97%)	3 (3%)	40	53
1	E	98/100 (98%)	92 (94%)	6 (6%)	18	23
1	F	95/100 (95%)	94 (99%)	1 (1%)	73	84
1	G	95/100 (95%)	91 (96%)	4 (4%)	30	39
1	H	96/100 (96%)	94 (98%)	2 (2%)	53	68
1	I	96/100 (96%)	91 (95%)	5 (5%)	23	30
1	J	99/100 (99%)	98 (99%)	1 (1%)	76	86
1	K	95/100 (95%)	90 (95%)	5 (5%)	22	29
1	L	96/100 (96%)	91 (95%)	5 (5%)	23	30
All	All	1161/1200 (97%)	1113 (96%)	48 (4%)	30	41

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	136	THR
1	G	103	PHE
1	L	118	LYS
1	E	155	LEU
1	E	207	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	189	ASN
1	G	152	HIS
1	L	142	ASN
1	G	94	GLN
1	G	153	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	BOG	C	218	-	20,20,20	0.97	2 (10%)	25,25,25	0.65	0
2	BOG	B	218	-	20,20,20	0.83	2 (10%)	25,25,25	0.61	0
2	BOG	A	218	-	20,20,20	0.82	1 (5%)	25,25,25	0.64	0
2	BOG	F	219	-	20,20,20	0.85	1 (5%)	25,25,25	0.63	0
2	BOG	H	218	-	20,20,20	1.10	1 (5%)	25,25,25	0.87	2 (8%)
2	BOG	A	220	-	20,20,20	0.98	2 (10%)	25,25,25	1.46	2 (8%)
2	BOG	I	219	-	20,20,20	0.68	1 (5%)	25,25,25	0.66	0
3	DMU	I	218	-	34,34,34	2.87	9 (26%)	45,45,45	4.27	20 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BOG	K	218	-	20,20,20	0.89	1 (5%)	25,25,25	0.62	0
2	BOG	J	218	-	20,20,20	0.76	0	25,25,25	0.61	0
2	BOG	A	219	-	20,20,20	0.99	2 (10%)	25,25,25	0.64	0
2	BOG	F	218	-	20,20,20	0.91	2 (10%)	25,25,25	0.72	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BOG	C	218	-	-	5/11/31/31	0/1/1/1
2	BOG	B	218	-	-	2/11/31/31	0/1/1/1
2	BOG	A	218	-	-	6/11/31/31	0/1/1/1
2	BOG	F	219	-	-	6/11/31/31	0/1/1/1
2	BOG	H	218	-	-	2/11/31/31	0/1/1/1
2	BOG	A	220	-	-	5/11/31/31	0/1/1/1
2	BOG	I	219	-	-	6/11/31/31	0/1/1/1
3	DMU	I	218	-	5/5/10/10	10/19/59/59	0/2/2/2
2	BOG	K	218	-	-	6/11/31/31	0/1/1/1
2	BOG	J	218	-	-	3/11/31/31	0/1/1/1
2	BOG	A	219	-	-	5/11/31/31	0/1/1/1
2	BOG	F	218	-	-	5/11/31/31	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	218	DMU	O7-C3	-7.20	1.25	1.43
3	I	218	DMU	O5-C4	-6.39	1.28	1.44
3	I	218	DMU	O16-C6	-6.36	1.29	1.40
3	I	218	DMU	O7-C10	-5.82	1.25	1.41
3	I	218	DMU	O1-C9	-5.74	1.30	1.44

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	218	DMU	C10-C5-C7	11.13	133.18	110.00
3	I	218	DMU	C1-C2-C3	10.30	133.20	109.68
3	I	218	DMU	C6-O5-C4	8.74	130.85	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	218	DMU	O1-C9-C8	7.90	124.05	109.69
3	I	218	DMU	O5-C4-C3	7.28	125.09	109.75

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	I	218	DMU	C4
3	I	218	DMU	C6
3	I	218	DMU	C5
3	I	218	DMU	C2
3	I	218	DMU	C9

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	218	BOG	O5-C1-O1-C1'
2	A	218	BOG	C2-C1-O1-C1'
2	A	218	BOG	O5-C1-O1-C1'
2	F	219	BOG	O5-C1-O1-C1'
2	A	220	BOG	O5-C1-O1-C1'

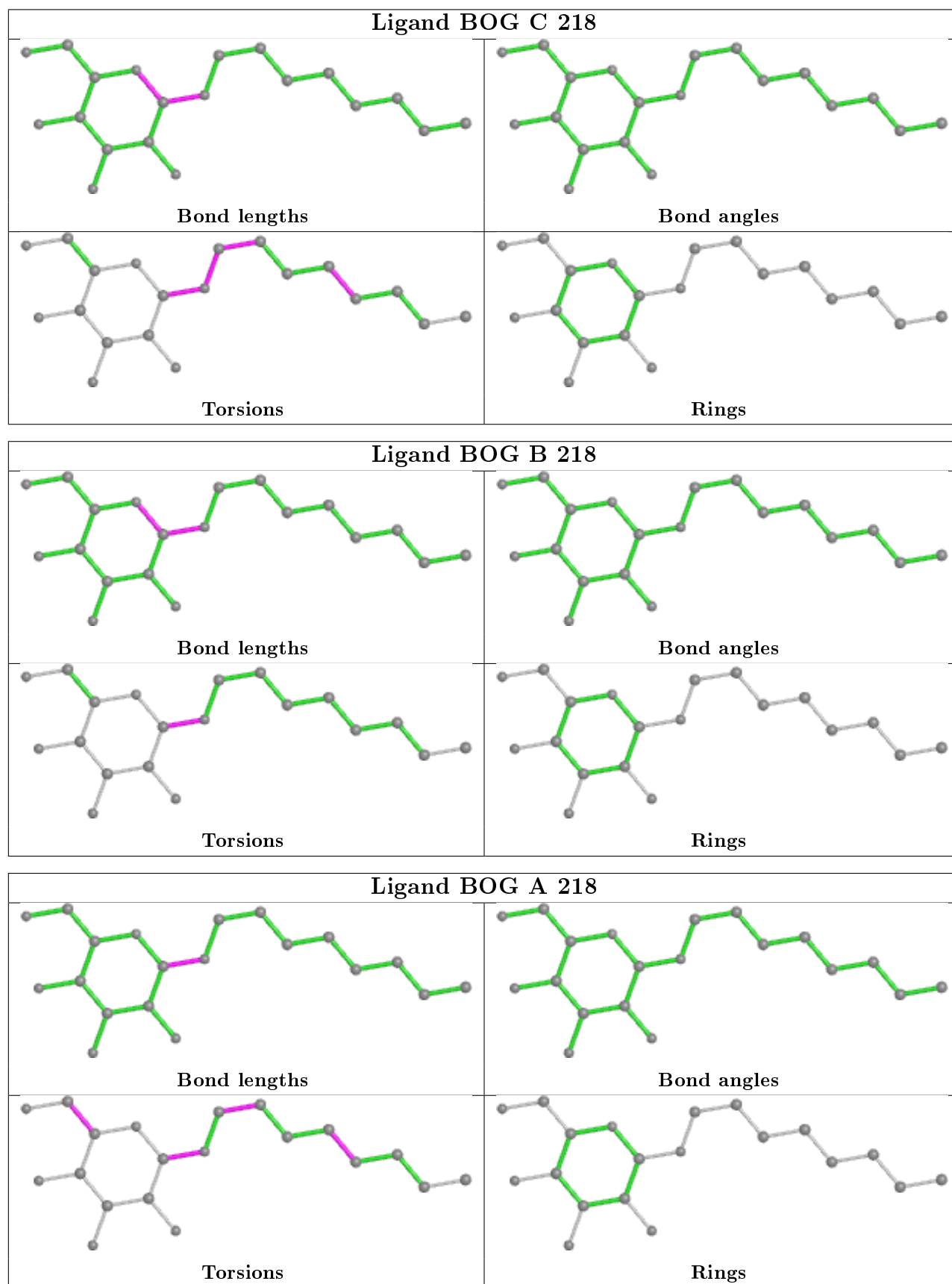
There are no ring outliers.

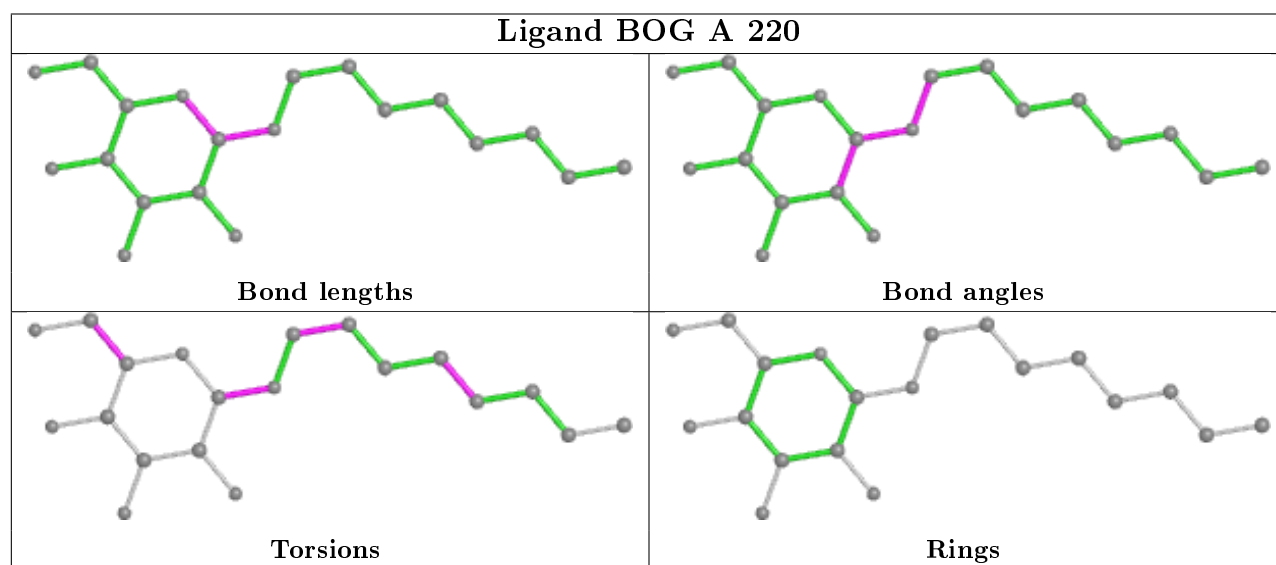
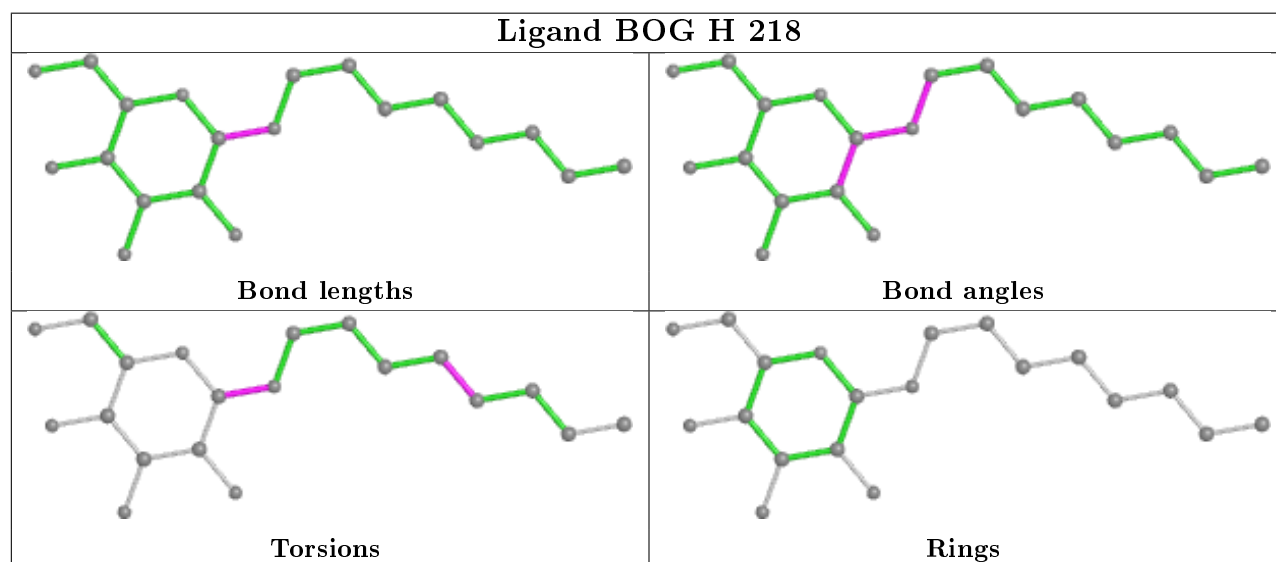
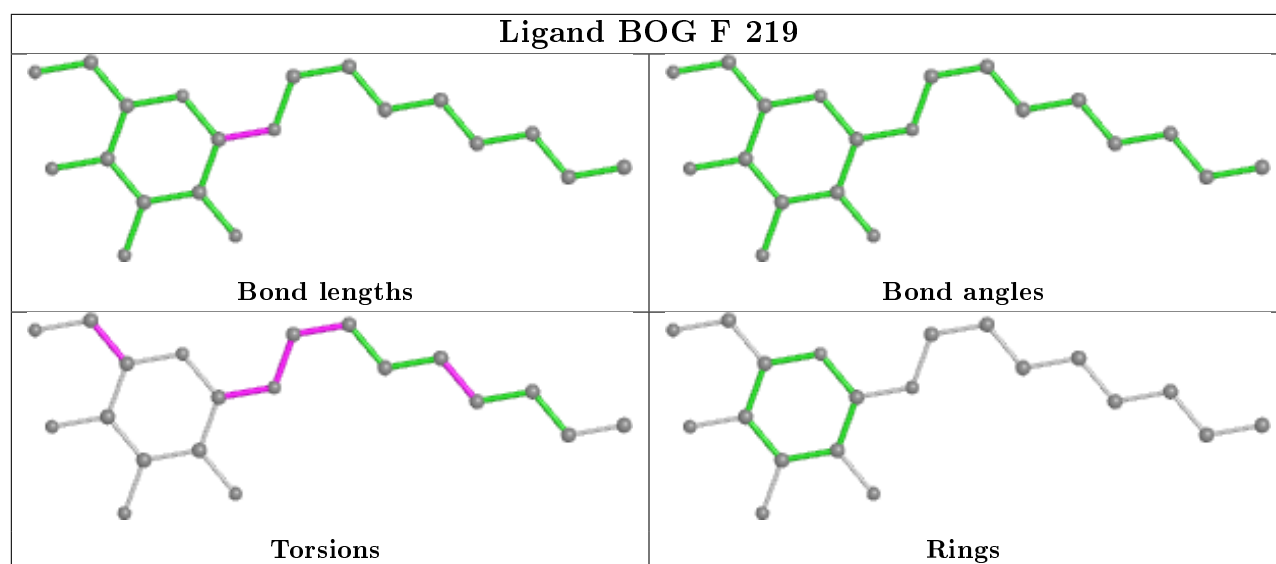
6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	218	BOG	1	0
2	B	218	BOG	1	0
2	A	218	BOG	2	0
2	H	218	BOG	4	0
2	A	220	BOG	1	0
2	A	219	BOG	1	0

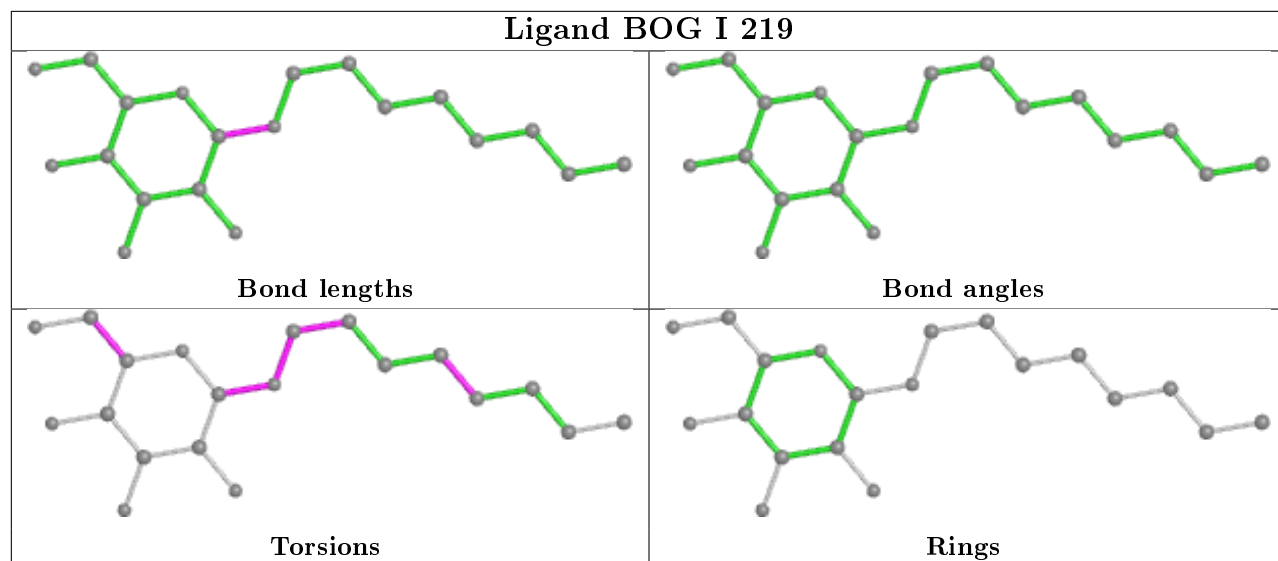
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

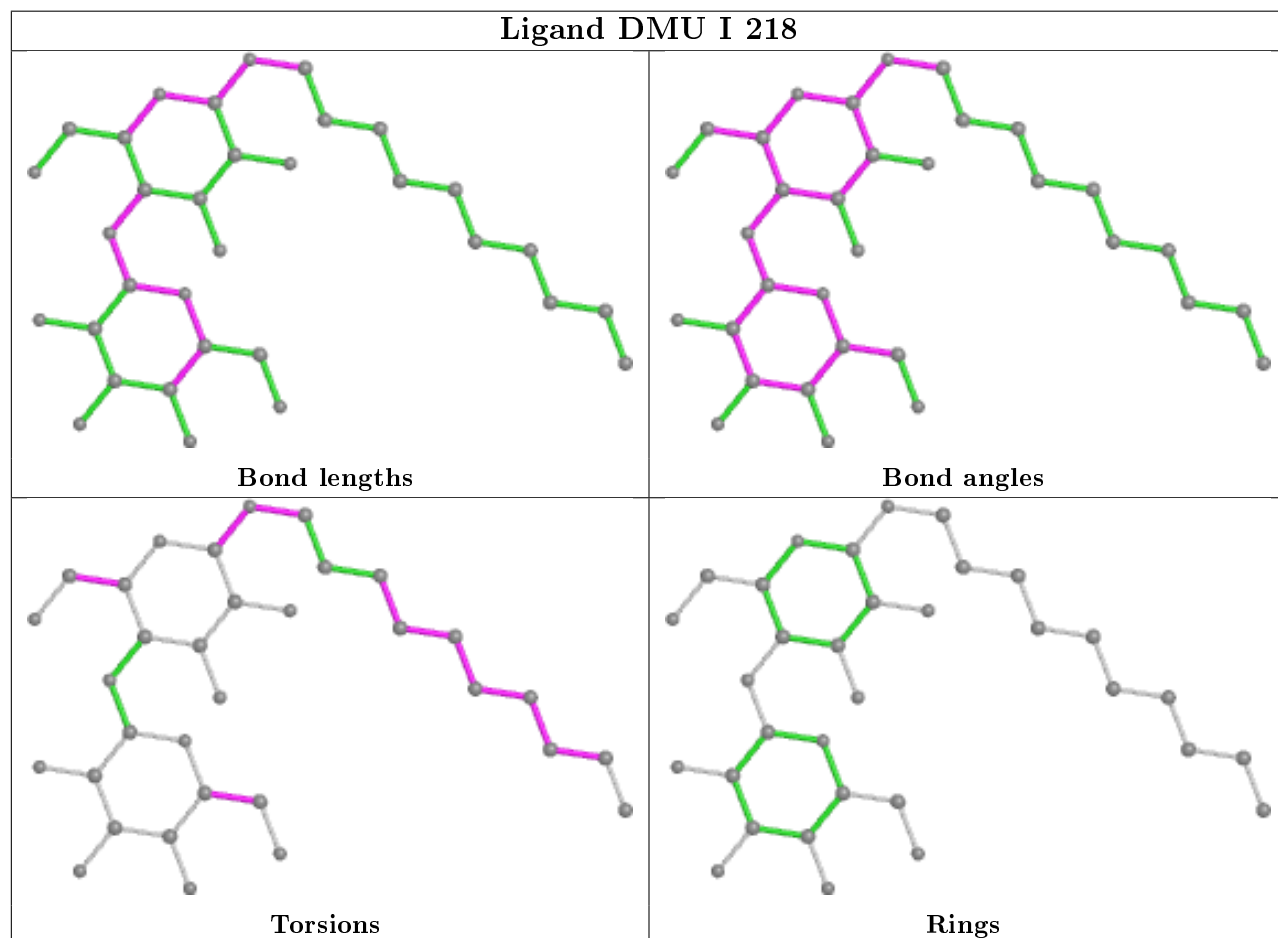


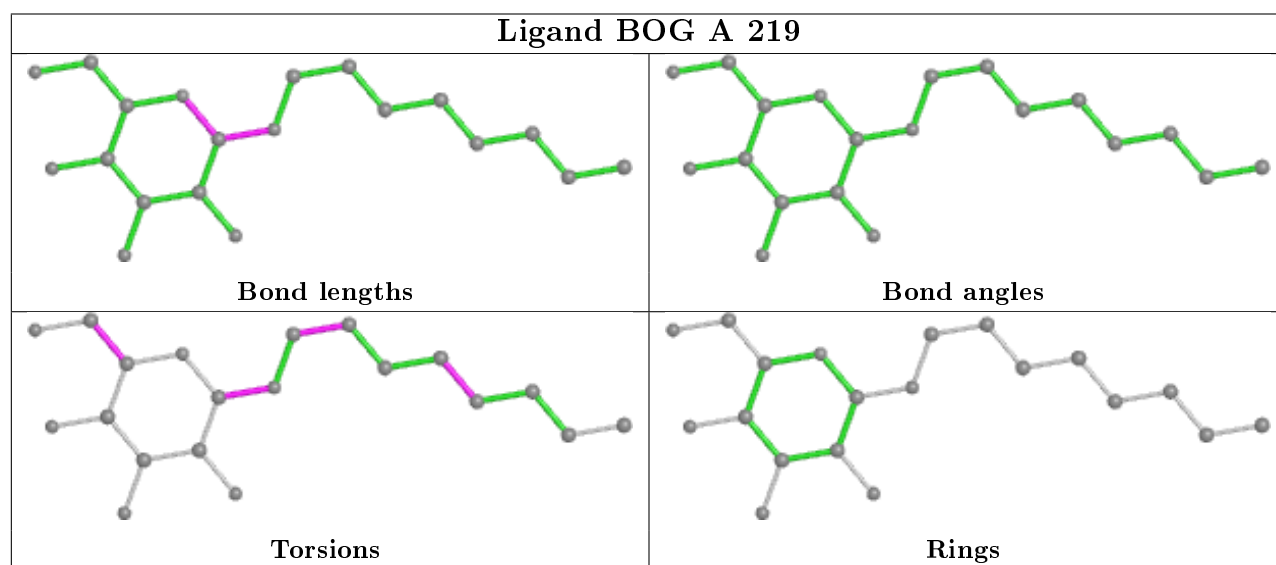
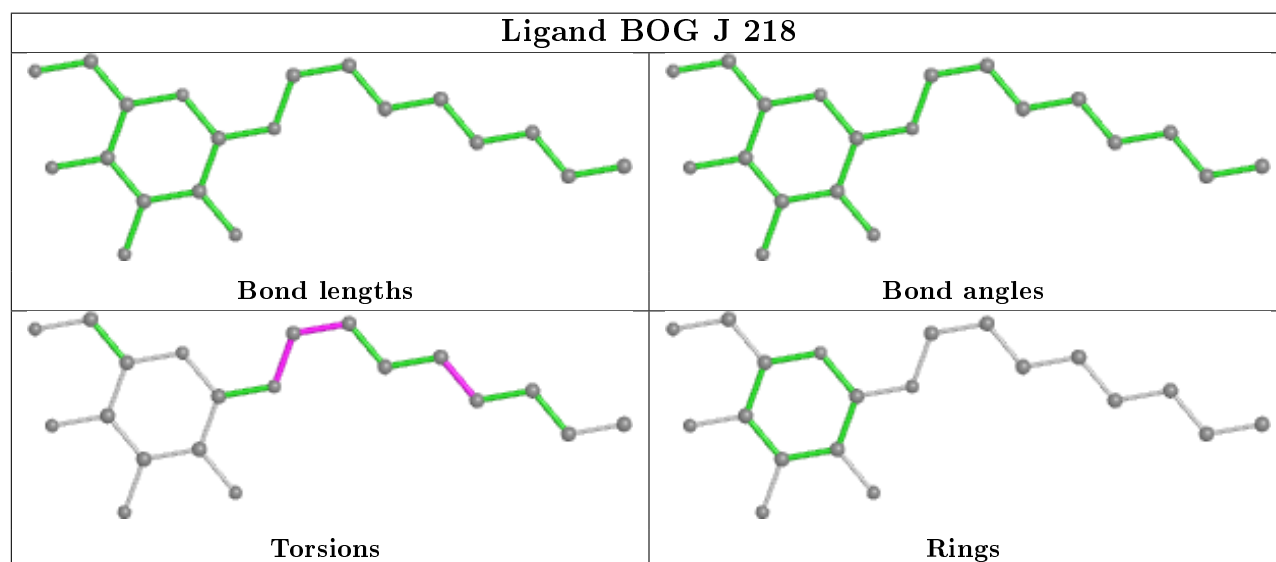
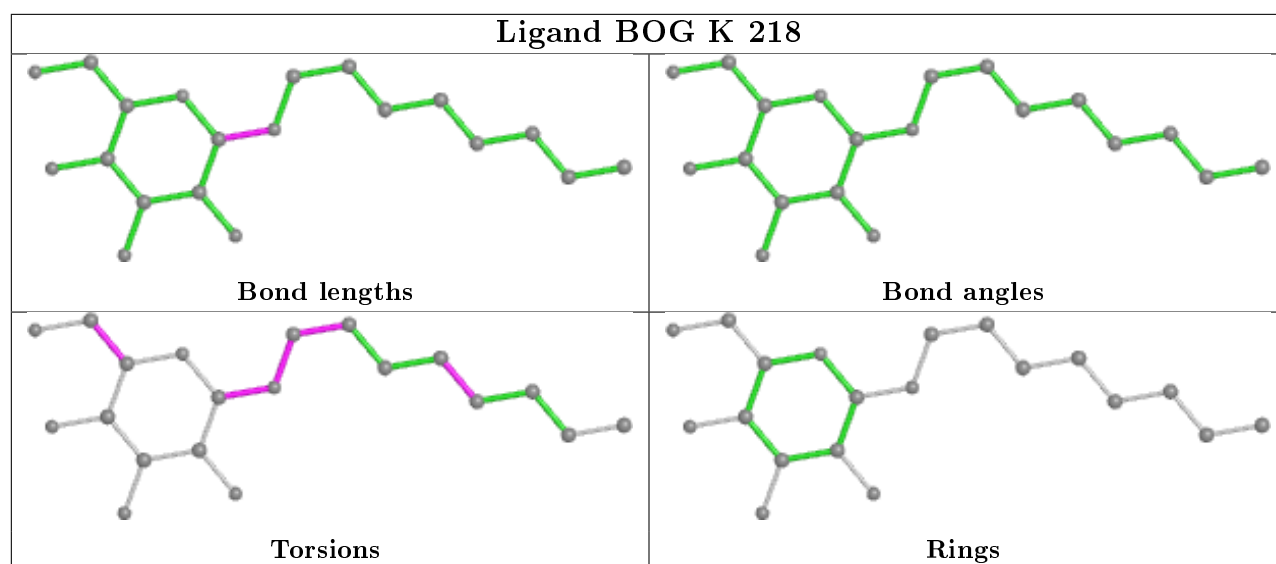


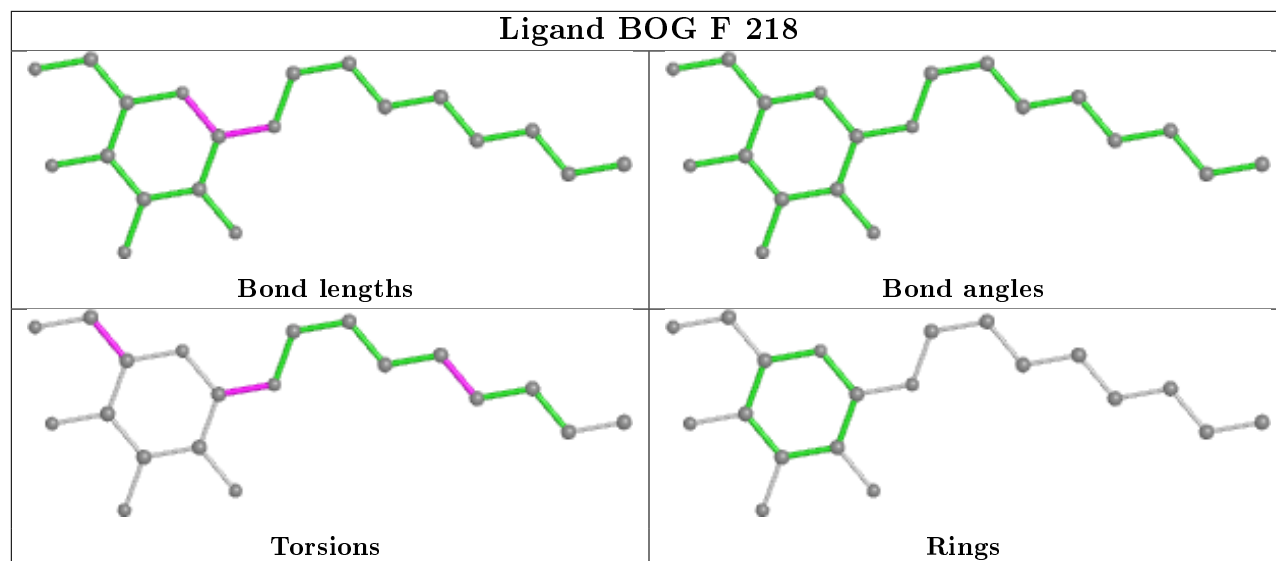
Ligand BOG I 219



Ligand DMU I 218







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	127/128 (99%)	0.26	6 (4%) 31 37	14, 26, 46, 54	0
1	B	127/128 (99%)	0.33	4 (3%) 49 54	19, 31, 42, 47	0
1	C	127/128 (99%)	0.18	4 (3%) 49 54	13, 24, 42, 49	0
1	D	127/128 (99%)	0.28	6 (4%) 31 37	16, 31, 46, 51	0
1	E	127/128 (99%)	0.09	1 (0%) 86 89	14, 22, 35, 42	0
1	F	127/128 (99%)	0.07	2 (1%) 72 77	17, 27, 40, 47	0
1	G	127/128 (99%)	0.19	3 (2%) 59 65	12, 24, 45, 55	0
1	H	128/128 (100%)	0.34	5 (3%) 39 44	15, 30, 48, 53	0
1	I	127/128 (99%)	0.18	4 (3%) 49 54	15, 26, 42, 48	0
1	J	127/128 (99%)	0.35	6 (4%) 31 37	20, 30, 47, 53	0
1	K	127/128 (99%)	0.47	9 (7%) 16 19	18, 31, 60, 65	0
1	L	127/128 (99%)	0.56	12 (9%) 8 10	23, 38, 51, 60	0
All	All	1525/1536 (99%)	0.28	62 (4%) 37 42	12, 29, 47, 65	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	119	ILE	5.0
1	K	180	ASP	4.2
1	L	103	PHE	4.2
1	A	174	LEU	4.1
1	L	208	GLY	4.0

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

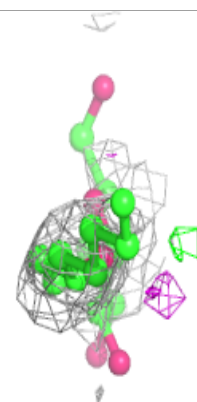
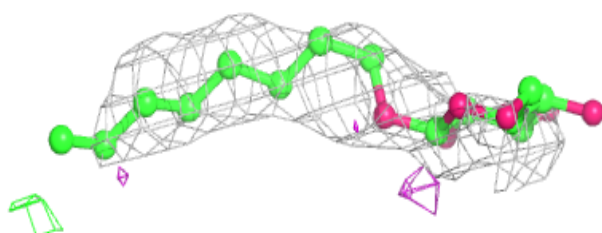
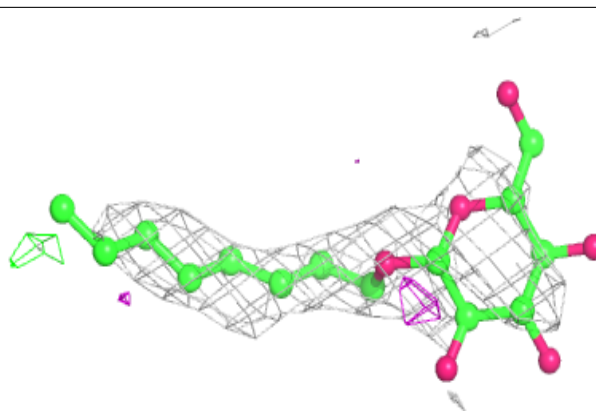
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BOG	H	218	20/20	0.49	0.50	64,77,81,81	0
2	BOG	J	218	20/20	0.55	0.33	55,65,68,68	0
2	BOG	A	218	20/20	0.58	0.34	41,60,65,65	0
2	BOG	C	218	20/20	0.61	0.31	40,57,63,64	0
2	BOG	A	219	20/20	0.61	0.29	46,59,63,64	0
2	BOG	I	219	20/20	0.62	0.32	48,61,64,65	0
2	BOG	F	218	20/20	0.63	0.31	53,66,70,71	0
2	BOG	K	218	20/20	0.72	0.26	47,58,63,64	0
2	BOG	A	220	20/20	0.75	0.28	55,61,63,63	0
2	BOG	B	218	20/20	0.78	0.22	58,61,63,64	0
2	BOG	F	219	20/20	0.82	0.24	58,61,64,64	0
3	DMU	I	218	33/33	0.86	0.18	29,35,38,39	0

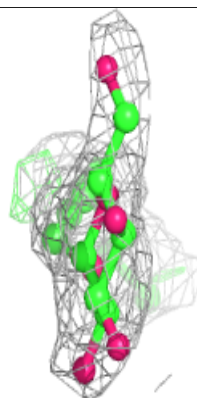
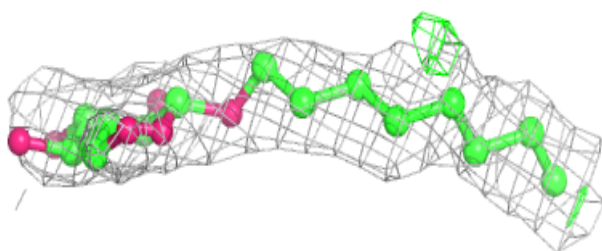
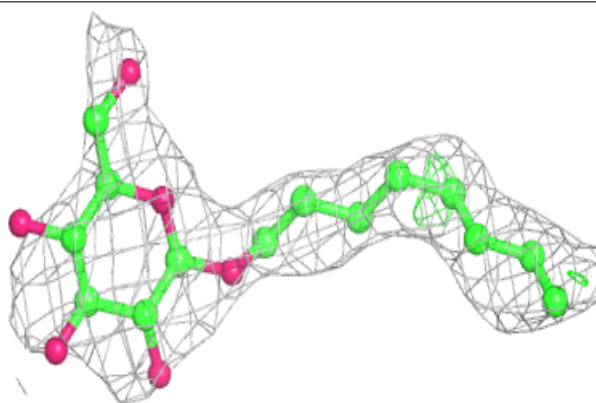
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BOG H 218:

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

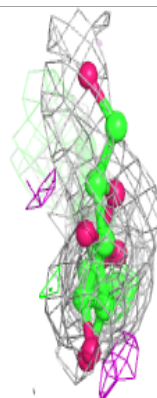
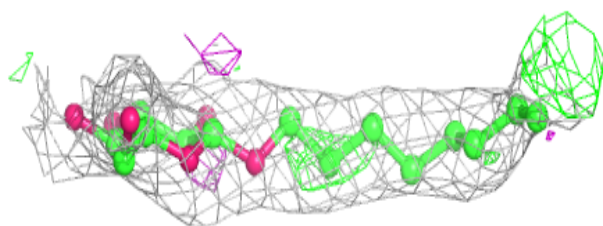
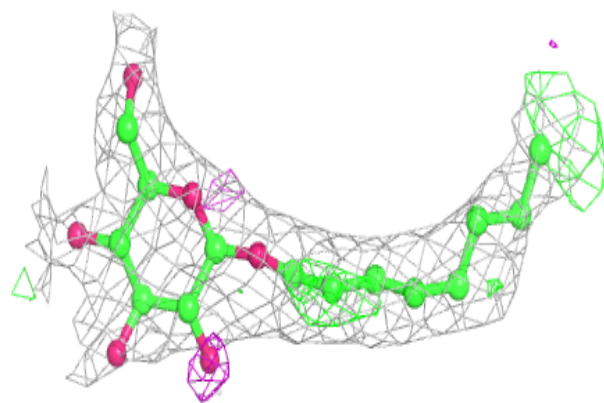
**Electron density around BOG J 218:**

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

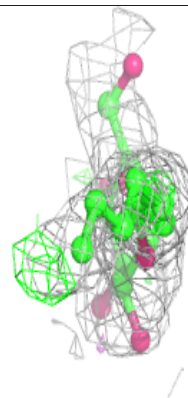
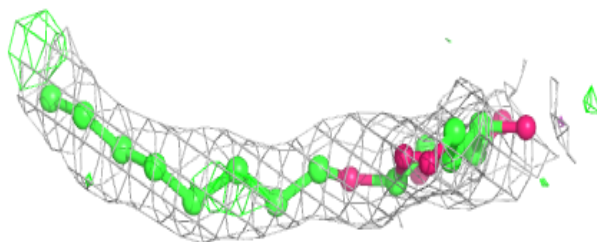
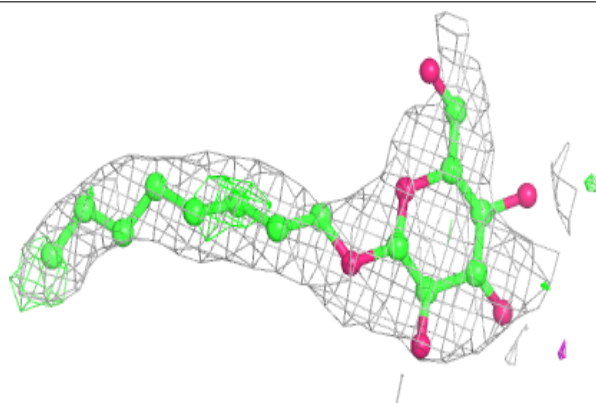


Electron density around BOG A 218:

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

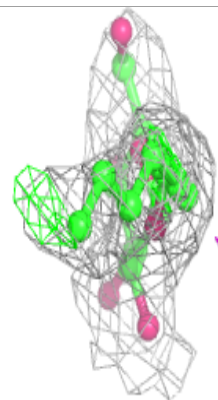
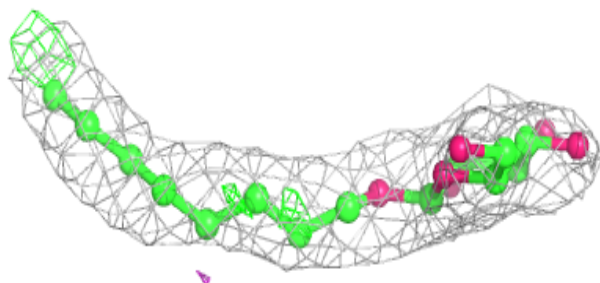
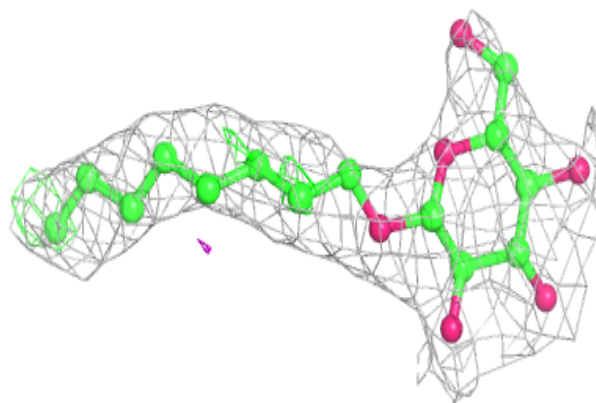
**Electron density around BOG C 218:**

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

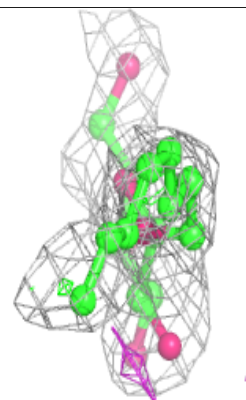
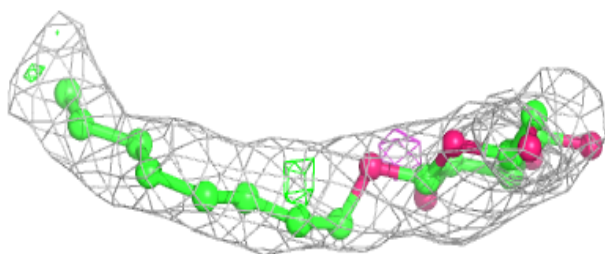
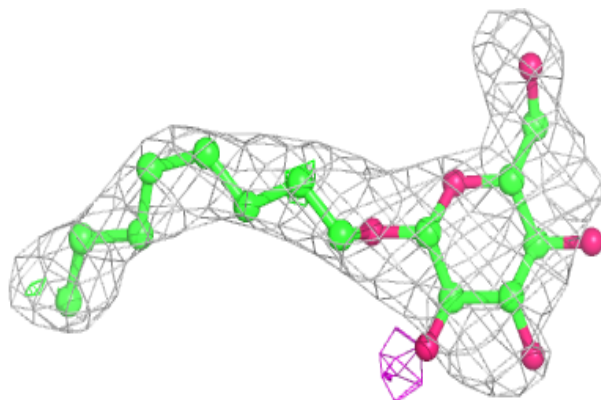


Electron density around BOG A 219:

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

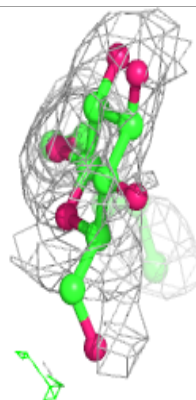
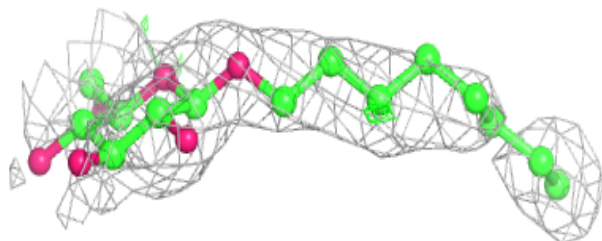
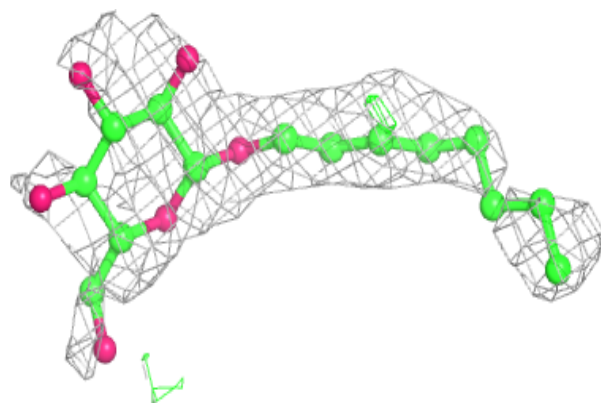
**Electron density around BOG I 219:**

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

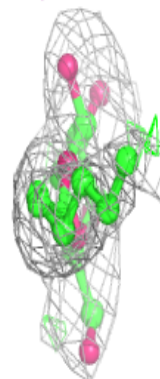
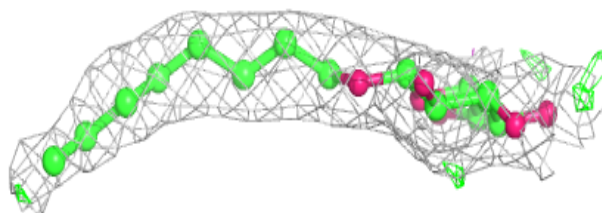
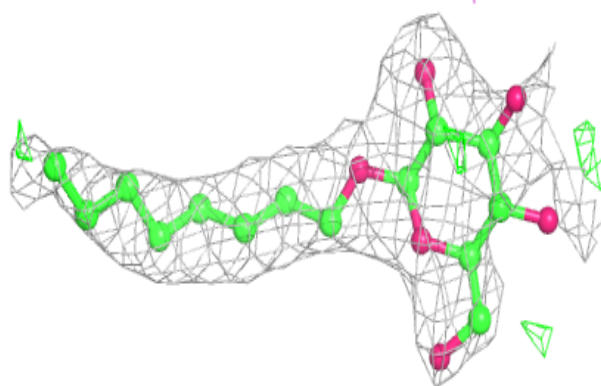


Electron density around BOG F 218:

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

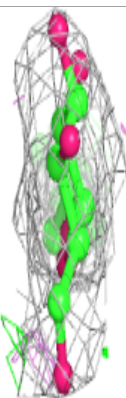
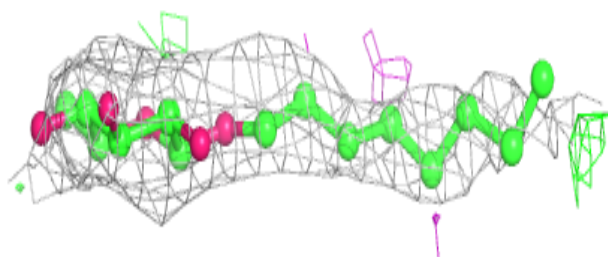
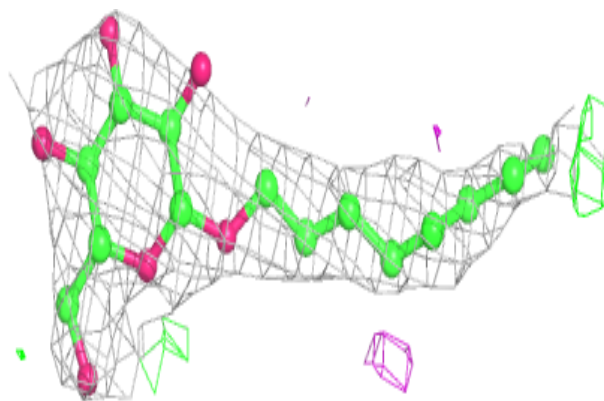
**Electron density around BOG K 218:**

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and green (positive)

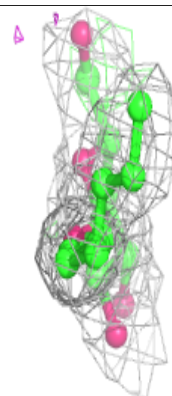
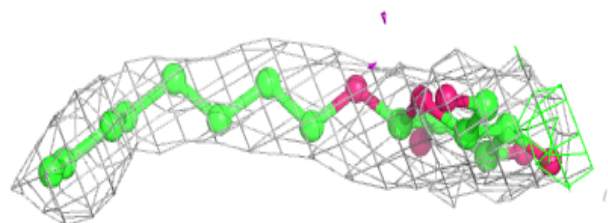
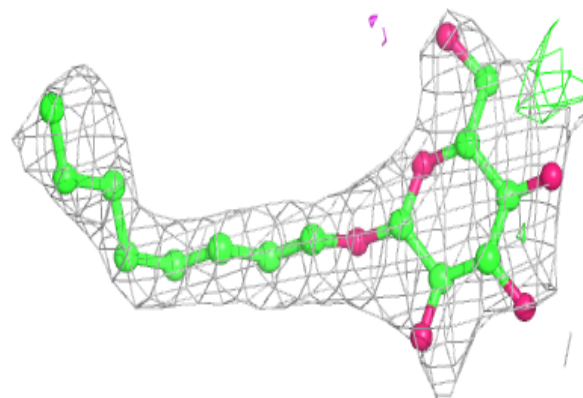


Electron density around BOG A 220:

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

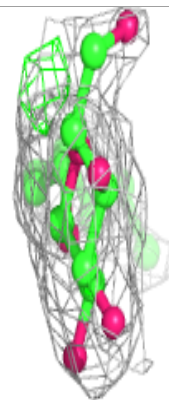
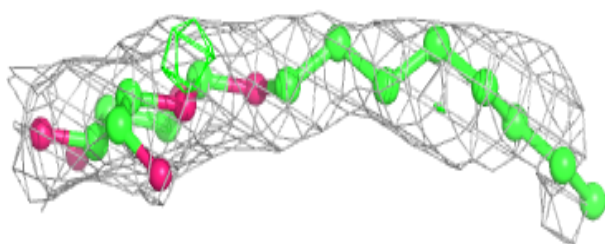
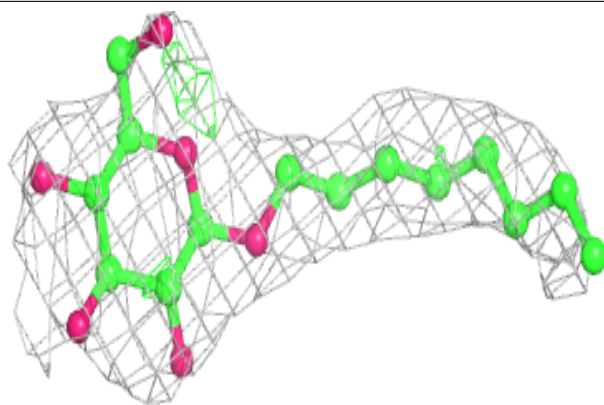
**Electron density around BOG B 218:**

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

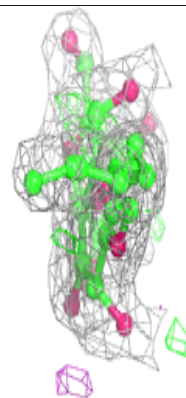
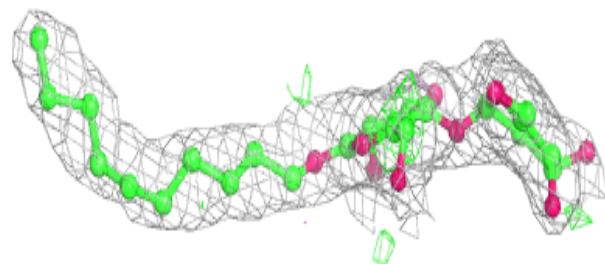
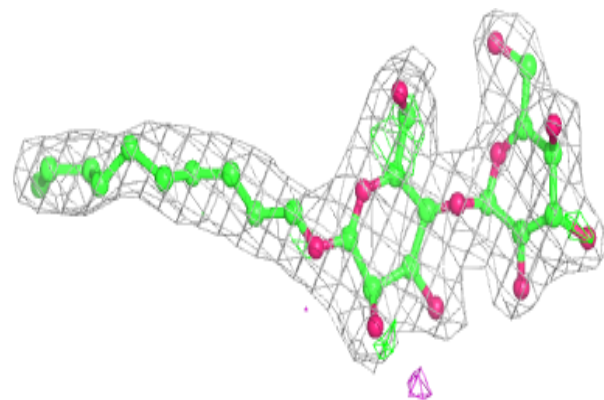


Electron density around BOG F 219:

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

**Electron density around DMU I 218:**

$2mF_o-DF_c$ (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.