



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 09:50 PM UTC

PDB ID : 7OMS / pdb_00007oms
Title : Bs164 in complex with mannocyclophellitol aziridine
Authors : McGregor, N.; Beenakker, T.; Kuo, C.L.; Wong, C.S.; Offren, W.A.; Armstrong, Z.; Codee, J.D.C.; Aerts, J.M.F.G.; Florea, B.I.; Overkleeft, H.; Davies, G.J.
Deposited on : 2021-05-24
Resolution : 2.05 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 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

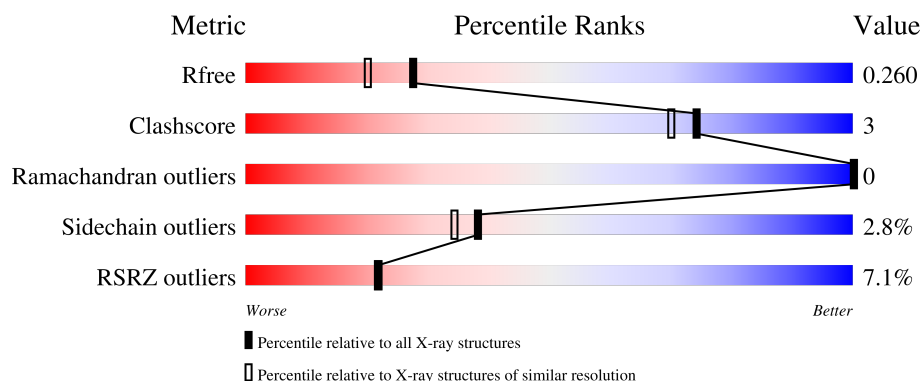
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	AAA	674	10% 88% 8% ..
1	BBB	674	4% 87% 9% .
1	CCC	674	5% 89% 7% ..
1	DDD	674	10% 89% 6% ..

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Mol	Chain	Length	Quality of chain
1	EEE	674	7% 87% 9%
1	FFF	674	5% 88% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 62844 atoms, of which 30640 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 Glyco_hydro_42M domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	655	Total	C	H	N	O	S	291	0	0
			10323	3377	5100	863	964	19			
1	DDD	650	Total	C	H	N	O	S	291	0	0
			10236	3349	5046	857	965	19			
1	CCC	651	Total	C	H	N	O	S	296	0	0
			10225	3346	5036	858	966	19			
1	BBB	651	Total	C	H	N	O	S	288	0	0
			10303	3366	5086	862	970	19			
1	FFF	653	Total	C	H	N	O	S	289	0	0
			10326	3374	5097	864	972	19			
1	EEE	652	Total	C	H	N	O	S	289	0	0
			10328	3373	5101	863	972	19			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	10	MET	-	initiating methionine	UNP I9SUA3
AAA	11	GLY	-	expression tag	UNP I9SUA3
AAA	12	SER	-	expression tag	UNP I9SUA3
AAA	13	SER	-	expression tag	UNP I9SUA3
AAA	14	HIS	-	expression tag	UNP I9SUA3
AAA	15	HIS	-	expression tag	UNP I9SUA3
AAA	16	HIS	-	expression tag	UNP I9SUA3
AAA	17	HIS	-	expression tag	UNP I9SUA3
AAA	18	HIS	-	expression tag	UNP I9SUA3
AAA	19	HIS	-	expression tag	UNP I9SUA3
AAA	20	SER	-	expression tag	UNP I9SUA3
AAA	21	SER	-	expression tag	UNP I9SUA3
AAA	22	GLY	-	expression tag	UNP I9SUA3
AAA	23	LEU	-	expression tag	UNP I9SUA3
AAA	24	GLU	-	expression tag	UNP I9SUA3
AAA	25	VAL	-	expression tag	UNP I9SUA3
AAA	26	LEU	-	expression tag	UNP I9SUA3

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	27	PHE	-	expression tag	UNP I9SUA3
AAA	28	GLN	-	expression tag	UNP I9SUA3
AAA	29	GLY	-	expression tag	UNP I9SUA3
AAA	30	PRO	-	expression tag	UNP I9SUA3
AAA	31	ALA	-	expression tag	UNP I9SUA3
DDD	10	MET	-	initiating methionine	UNP I9SUA3
DDD	11	GLY	-	expression tag	UNP I9SUA3
DDD	12	SER	-	expression tag	UNP I9SUA3
DDD	13	SER	-	expression tag	UNP I9SUA3
DDD	14	HIS	-	expression tag	UNP I9SUA3
DDD	15	HIS	-	expression tag	UNP I9SUA3
DDD	16	HIS	-	expression tag	UNP I9SUA3
DDD	17	HIS	-	expression tag	UNP I9SUA3
DDD	18	HIS	-	expression tag	UNP I9SUA3
DDD	19	HIS	-	expression tag	UNP I9SUA3
DDD	20	SER	-	expression tag	UNP I9SUA3
DDD	21	SER	-	expression tag	UNP I9SUA3
DDD	22	GLY	-	expression tag	UNP I9SUA3
DDD	23	LEU	-	expression tag	UNP I9SUA3
DDD	24	GLU	-	expression tag	UNP I9SUA3
DDD	25	VAL	-	expression tag	UNP I9SUA3
DDD	26	LEU	-	expression tag	UNP I9SUA3
DDD	27	PHE	-	expression tag	UNP I9SUA3
DDD	28	GLN	-	expression tag	UNP I9SUA3
DDD	29	GLY	-	expression tag	UNP I9SUA3
DDD	30	PRO	-	expression tag	UNP I9SUA3
DDD	31	ALA	-	expression tag	UNP I9SUA3
CCC	10	MET	-	initiating methionine	UNP I9SUA3
CCC	11	GLY	-	expression tag	UNP I9SUA3
CCC	12	SER	-	expression tag	UNP I9SUA3
CCC	13	SER	-	expression tag	UNP I9SUA3
CCC	14	HIS	-	expression tag	UNP I9SUA3
CCC	15	HIS	-	expression tag	UNP I9SUA3
CCC	16	HIS	-	expression tag	UNP I9SUA3
CCC	17	HIS	-	expression tag	UNP I9SUA3
CCC	18	HIS	-	expression tag	UNP I9SUA3
CCC	19	HIS	-	expression tag	UNP I9SUA3
CCC	20	SER	-	expression tag	UNP I9SUA3
CCC	21	SER	-	expression tag	UNP I9SUA3
CCC	22	GLY	-	expression tag	UNP I9SUA3
CCC	23	LEU	-	expression tag	UNP I9SUA3
CCC	24	GLU	-	expression tag	UNP I9SUA3

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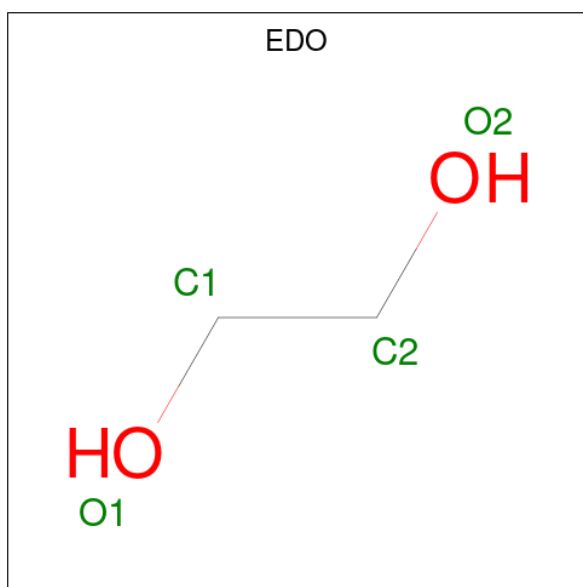
Chain	Residue	Modelled	Actual	Comment	Reference
CCC	25	VAL	-	expression tag	UNP I9SUA3
CCC	26	LEU	-	expression tag	UNP I9SUA3
CCC	27	PHE	-	expression tag	UNP I9SUA3
CCC	28	GLN	-	expression tag	UNP I9SUA3
CCC	29	GLY	-	expression tag	UNP I9SUA3
CCC	30	PRO	-	expression tag	UNP I9SUA3
CCC	31	ALA	-	expression tag	UNP I9SUA3
BBB	10	MET	-	initiating methionine	UNP I9SUA3
BBB	11	GLY	-	expression tag	UNP I9SUA3
BBB	12	SER	-	expression tag	UNP I9SUA3
BBB	13	SER	-	expression tag	UNP I9SUA3
BBB	14	HIS	-	expression tag	UNP I9SUA3
BBB	15	HIS	-	expression tag	UNP I9SUA3
BBB	16	HIS	-	expression tag	UNP I9SUA3
BBB	17	HIS	-	expression tag	UNP I9SUA3
BBB	18	HIS	-	expression tag	UNP I9SUA3
BBB	19	HIS	-	expression tag	UNP I9SUA3
BBB	20	SER	-	expression tag	UNP I9SUA3
BBB	21	SER	-	expression tag	UNP I9SUA3
BBB	22	GLY	-	expression tag	UNP I9SUA3
BBB	23	LEU	-	expression tag	UNP I9SUA3
BBB	24	GLU	-	expression tag	UNP I9SUA3
BBB	25	VAL	-	expression tag	UNP I9SUA3
BBB	26	LEU	-	expression tag	UNP I9SUA3
BBB	27	PHE	-	expression tag	UNP I9SUA3
BBB	28	GLN	-	expression tag	UNP I9SUA3
BBB	29	GLY	-	expression tag	UNP I9SUA3
BBB	30	PRO	-	expression tag	UNP I9SUA3
BBB	31	ALA	-	expression tag	UNP I9SUA3
FFF	10	MET	-	initiating methionine	UNP I9SUA3
FFF	11	GLY	-	expression tag	UNP I9SUA3
FFF	12	SER	-	expression tag	UNP I9SUA3
FFF	13	SER	-	expression tag	UNP I9SUA3
FFF	14	HIS	-	expression tag	UNP I9SUA3
FFF	15	HIS	-	expression tag	UNP I9SUA3
FFF	16	HIS	-	expression tag	UNP I9SUA3
FFF	17	HIS	-	expression tag	UNP I9SUA3
FFF	18	HIS	-	expression tag	UNP I9SUA3
FFF	19	HIS	-	expression tag	UNP I9SUA3
FFF	20	SER	-	expression tag	UNP I9SUA3
FFF	21	SER	-	expression tag	UNP I9SUA3
FFF	22	GLY	-	expression tag	UNP I9SUA3

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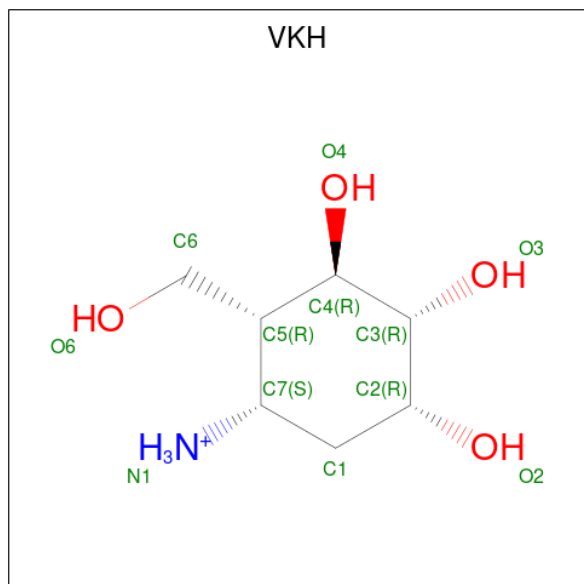
Chain	Residue	Modelled	Actual	Comment	Reference
FFF	23	LEU	-	expression tag	UNP I9SUA3
FFF	24	GLU	-	expression tag	UNP I9SUA3
FFF	25	VAL	-	expression tag	UNP I9SUA3
FFF	26	LEU	-	expression tag	UNP I9SUA3
FFF	27	PHE	-	expression tag	UNP I9SUA3
FFF	28	GLN	-	expression tag	UNP I9SUA3
FFF	29	GLY	-	expression tag	UNP I9SUA3
FFF	30	PRO	-	expression tag	UNP I9SUA3
FFF	31	ALA	-	expression tag	UNP I9SUA3
EEE	10	MET	-	initiating methionine	UNP I9SUA3
EEE	11	GLY	-	expression tag	UNP I9SUA3
EEE	12	SER	-	expression tag	UNP I9SUA3
EEE	13	SER	-	expression tag	UNP I9SUA3
EEE	14	HIS	-	expression tag	UNP I9SUA3
EEE	15	HIS	-	expression tag	UNP I9SUA3
EEE	16	HIS	-	expression tag	UNP I9SUA3
EEE	17	HIS	-	expression tag	UNP I9SUA3
EEE	18	HIS	-	expression tag	UNP I9SUA3
EEE	19	HIS	-	expression tag	UNP I9SUA3
EEE	20	SER	-	expression tag	UNP I9SUA3
EEE	21	SER	-	expression tag	UNP I9SUA3
EEE	22	GLY	-	expression tag	UNP I9SUA3
EEE	23	LEU	-	expression tag	UNP I9SUA3
EEE	24	GLU	-	expression tag	UNP I9SUA3
EEE	25	VAL	-	expression tag	UNP I9SUA3
EEE	26	LEU	-	expression tag	UNP I9SUA3
EEE	27	PHE	-	expression tag	UNP I9SUA3
EEE	28	GLN	-	expression tag	UNP I9SUA3
EEE	29	GLY	-	expression tag	UNP I9SUA3
EEE	30	PRO	-	expression tag	UNP I9SUA3
EEE	31	ALA	-	expression tag	UNP I9SUA3

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
2	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
2	DDD	1	Total	C	H	O	1	0
			10	2	6	2		
2	DDD	1	Total	C	H	O	1	0
			10	2	6	2		
2	DDD	1	Total	C	H	O	1	0
			10	2	6	2		
2	CCC	1	Total	C	H	O	1	0
			10	2	6	2		
2	CCC	1	Total	C	H	O	1	0
			10	2	6	2		
2	CCC	1	Total	C	H	O	1	0
			10	2	6	2		
2	CCC	1	Total	C	H	O	1	0
			10	2	6	2		
2	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
2	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
2	FFF	1	Total	C	H	O	1	0
			10	2	6	2		
2	EEE	1	Total	C	H	O	1	0
			10	2	6	2		
2	EEE	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 3 is (1 {R},2 {R},3 {S},4 {R},5 {R},6 {R})-5-(hydroxymethyl)-7-azabicyclo[4.1.0]heptane-2,3,4-triol (CCD ID: VKH) (formula: $C_7H_{16}NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total 27	C 7	H 15	N 1	O 4	3	0
3	DDD	1	Total 27	C 7	H 15	N 1	O 4	3	0
3	CCC	1	Total 27	C 7	H 15	N 1	O 4	3	0
3	BBB	1	Total 27	C 7	H 15	N 1	O 4	3	0
3	FFF	1	Total 27	C 7	H 15	N 1	O 4	3	0
3	EEE	1	Total 27	C 7	H 15	N 1	O 4	3	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	Cl	0	0
			1	1		
4	DDD	1	Total	Cl	0	0
			1	1		
4	CCC	1	Total	Cl	0	0
			1	1		
4	BBB	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	FFF	1	Total 1	Cl 1	0	0
4	EEE	1	Total 1	Cl 1	0	0

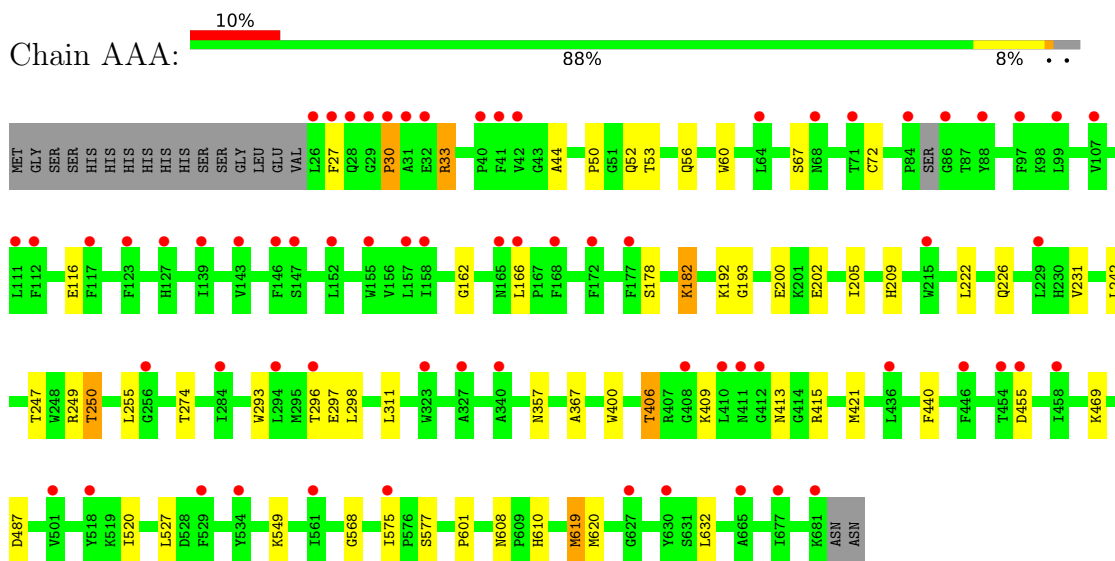
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	154	Total 154	O 154	0	0
5	DDD	82	Total 82	O 82	0	0
5	CCC	146	Total 146	O 146	0	0
5	BBB	142	Total 142	O 142	0	0
5	FFF	151	Total 151	O 151	0	0
5	EEE	120	Total 120	O 120	0	0

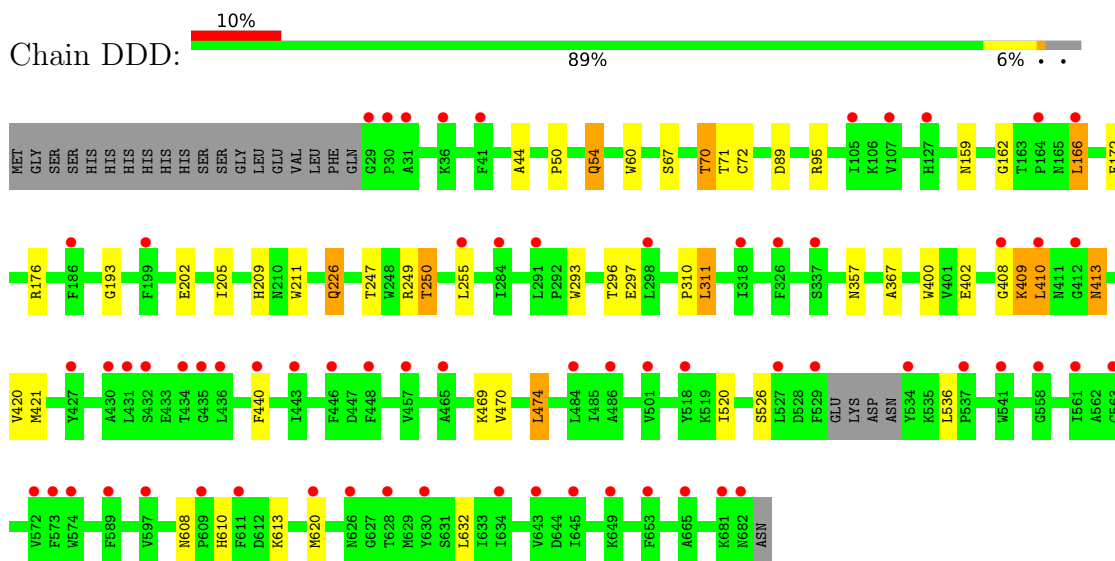
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

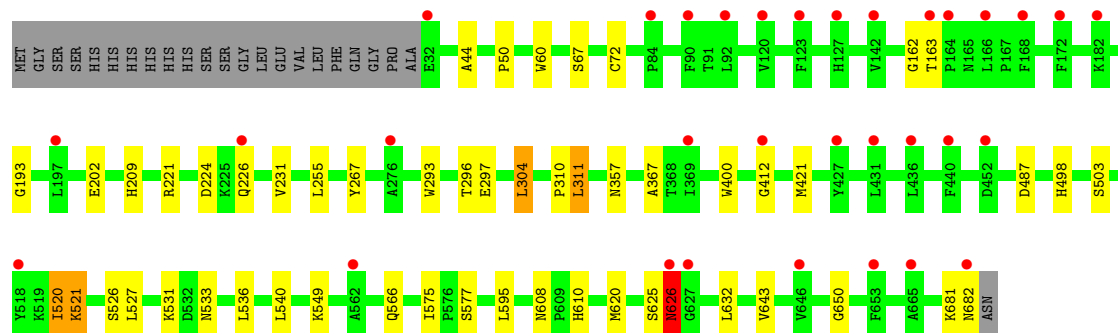
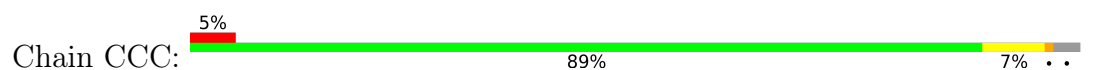
- Molecule 1: Glyco_hydro_42M domain-containing protein



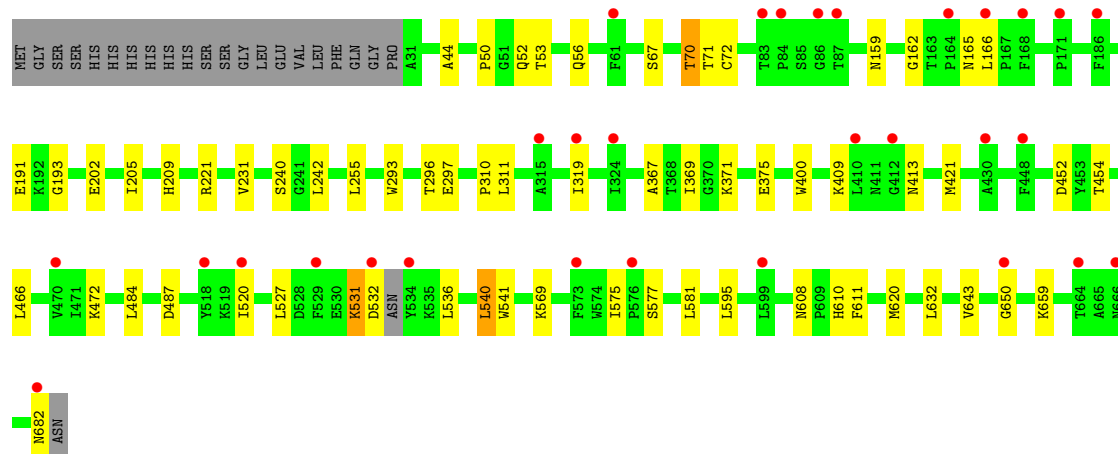
- Molecule 1: Glyco_hydro_42M domain-containing protein



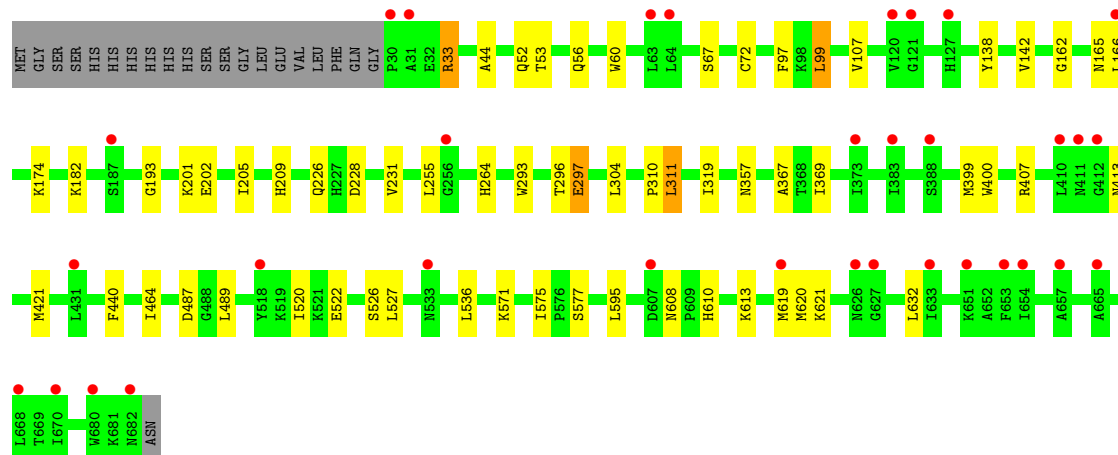
- Molecule 1: Glyco_hydro_42M domain-containing protein



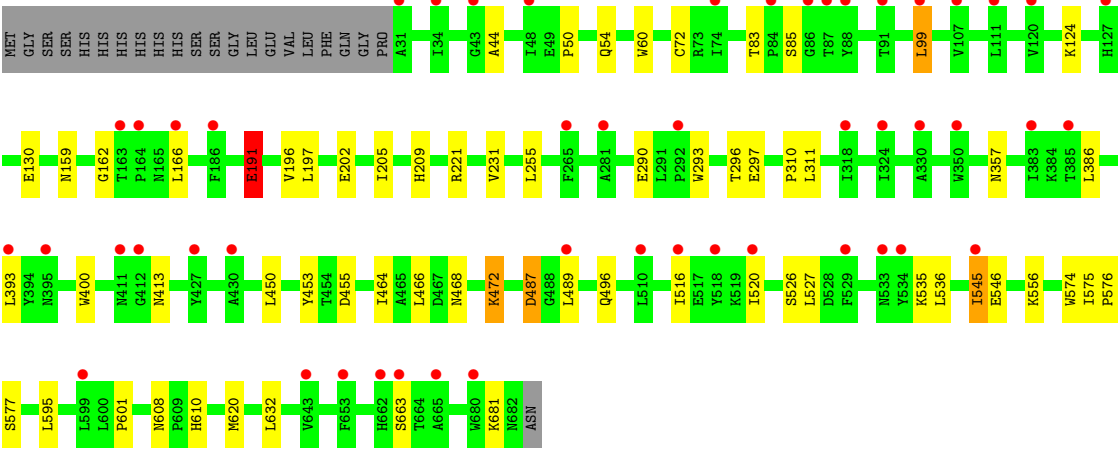
- Molecule 1: Glyco_hydro_42M domain-containing protein



- Molecule 1: Glyco_hydro_42M domain-containing protein



- Molecule 1: Glyco_hydro_42M domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.33Å 103.96Å 170.13Å 92.27° 97.71° 106.40°	Depositor
Resolution (Å)	99.40 – 2.05 99.40 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.8 (99.40-2.05) 97.8 (99.40-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.223 , 0.258 0.225 , 0.260	Depositor DCC
R_{free} test set	13624 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 25.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	62844	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: EDO, VKH, 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	AAA	1.00	1/5368 (0.0%)	1.29	4/7274 (0.1%)
1	BBB	1.01	2/5360 (0.0%)	1.28	1/7261 (0.0%)
1	CCC	1.01	1/5333 (0.0%)	1.29	2/7233 (0.0%)
1	DDD	0.99	1/5334 (0.0%)	1.29	2/7232 (0.0%)
1	EEE	1.00	1/5371 (0.0%)	1.29	2/7276 (0.0%)
1	FFF	1.01	1/5374 (0.0%)	1.29	0/7282
All	All	1.00	7/32140 (0.0%)	1.29	11/43558 (0.0%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	EEE	297	GLU	CD-OE1	10.18	1.44	1.25
1	BBB	297	GLU	CD-OE1	9.79	1.44	1.25
1	FFF	297	GLU	CD-OE1	9.79	1.44	1.25
1	AAA	297	GLU	CD-OE1	9.76	1.44	1.25
1	CCC	297	GLU	CD-OE1	9.21	1.42	1.25

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	626	ASN	CB-CA-C	8.09	126.52	110.42
1	BBB	70	THR	N-CA-CB	-6.74	101.63	110.59
1	EEE	191	GLU	CB-CG-CD	6.17	123.10	112.60
1	AAA	33	ARG	CB-CA-C	5.71	119.60	109.72
1	CCC	650	GLY	CA-C-O	-5.28	118.05	122.33

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	AAA	5223	5100	5056	30	2
1	BBB	5217	5086	5056	35	0
1	CCC	5189	5036	4991	36	0
1	DDD	5190	5046	5010	33	0
1	EEE	5227	5101	5074	36	0
1	FFF	5229	5097	5067	37	2
2	AAA	8	12	12	0	0
2	BBB	8	12	12	1	0
2	CCC	16	24	24	4	0
2	DDD	12	18	18	3	0
2	EEE	8	12	12	0	0
2	FFF	4	6	6	1	0
3	AAA	12	15	0	0	0
3	BBB	12	15	0	1	0
3	CCC	12	15	0	0	0
3	DDD	12	15	0	1	0
3	EEE	12	15	0	1	0
3	FFF	12	15	0	0	0
4	AAA	1	0	0	0	0
4	BBB	1	0	0	0	0
4	CCC	1	0	0	0	0
4	DDD	1	0	0	0	0
4	EEE	1	0	0	0	0
4	FFF	1	0	0	0	0
5	AAA	154	0	0	2	0
5	BBB	142	0	0	1	0
5	CCC	146	0	0	2	0
5	DDD	82	0	0	0	0
5	EEE	120	0	0	1	0
5	FFF	151	0	0	4	0
All	All	32204	30640	30338	191	2

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 3.

The worst 5 of 191 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:EEE:545:ILE:CD1	1:EEE:576:PRO:HG3	1.91	0.99
1:BBB:166:LEU:HD22	1:BBB:205:ILE:HG12	1.54	0.88
1:FFF:33:ARG:HD3	1:FFF:228:ASP:OD1	1.78	0.82
1:EEE:545:ILE:HG12	1:EEE:574:TRP:CZ3	2.18	0.77
1:EEE:545:ILE:HD13	1:EEE:576:PRO:HG3	1.66	0.76

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:568:GLY:O	1:FFF:33:ARG:HH12[1_565]	1.51	0.09
1:AAA:568:GLY:O	1:FFF:33:ARG:NH1[1_565]	2.13	0.07

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	AAA	651/674 (97%)	632 (97%)	19 (3%)	0	100	100
1	BBB	647/674 (96%)	629 (97%)	18 (3%)	0	100	100
1	CCC	649/674 (96%)	626 (96%)	23 (4%)	0	100	100
1	DDD	646/674 (96%)	624 (97%)	22 (3%)	0	100	100
1	EEE	650/674 (96%)	627 (96%)	23 (4%)	0	100	100
1	FFF	651/674 (97%)	631 (97%)	20 (3%)	0	100	100
All	All	3894/4044 (96%)	3769 (97%)	125 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	553/582 (95%)	537 (97%)	16 (3%)	37	33
1	BBB	557/582 (96%)	544 (98%)	13 (2%)	44	42
1	CCC	550/582 (94%)	536 (98%)	14 (2%)	42	39
1	DDD	552/582 (95%)	537 (97%)	15 (3%)	39	36
1	EEE	559/582 (96%)	540 (97%)	19 (3%)	32	27
1	FFF	558/582 (96%)	543 (97%)	15 (3%)	39	36
All	All	3329/3492 (95%)	3237 (97%)	92 (3%)	38	34

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	682	ASN
1	FFF	613	LYS
1	FFF	99	LEU
1	FFF	296	THR
1	EEE	191	GLU

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 26 ligands modelled in this entry, 6 are monoatomic - leaving 20 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$
2	EDO	CCC	802	-	3,3,3	0.39	0	2,2,2	0.53	0
3	VKH	BBB	803	1	12,12,12	1.27	2 (16%)	14,17,17	2.20	3 (21%)
2	EDO	FFF	801	-	3,3,3	0.23	0	2,2,2	0.39	0
3	VKH	AAA	803	1	12,12,12	1.11	1 (8%)	14,17,17	2.47	5 (35%)
2	EDO	AAA	801	-	3,3,3	0.36	0	2,2,2	0.30	0
3	VKH	FFF	802	1	12,12,12	1.10	0	14,17,17	2.38	4 (28%)
3	VKH	DDD	804	1	12,12,12	1.21	3 (25%)	14,17,17	2.42	4 (28%)
3	VKH	CCC	805	1	12,12,12	1.04	0	14,17,17	2.22	6 (42%)
2	EDO	AAA	802	-	3,3,3	0.45	0	2,2,2	0.40	0
2	EDO	CCC	801	-	3,3,3	0.30	0	2,2,2	0.18	0
2	EDO	EEE	802	-	3,3,3	0.14	0	2,2,2	0.10	0
2	EDO	BBB	801	-	3,3,3	0.24	0	2,2,2	0.06	0
2	EDO	BBB	802	-	3,3,3	0.64	0	2,2,2	0.63	0
3	VKH	EEE	803	1	12,12,12	1.14	1 (8%)	14,17,17	2.40	3 (21%)
2	EDO	EEE	801	-	3,3,3	0.21	0	2,2,2	0.16	0
2	EDO	CCC	803	-	3,3,3	0.16	0	2,2,2	0.16	0
2	EDO	DDD	803	-	3,3,3	0.25	0	2,2,2	0.56	0
2	EDO	CCC	804	-	3,3,3	0.43	0	2,2,2	0.23	0
2	EDO	DDD	802	-	3,3,3	0.34	0	2,2,2	0.31	0
2	EDO	DDD	801	-	3,3,3	0.19	0	2,2,2	0.20	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	EDO	CCC	802	-	-	0/1/1/1	-
3	VKH	BBB	803	1	-	0/2/22/22	0/1/1/1
2	EDO	FFF	801	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	VKH	AAA	803	1	-	0/2/22/22	0/1/1/1
2	EDO	AAA	801	-	-	0/1/1/1	-
3	VKH	FFF	802	1	-	0/2/22/22	0/1/1/1
3	VKH	DDD	804	1	-	0/2/22/22	0/1/1/1
3	VKH	CCC	805	1	-	0/2/22/22	0/1/1/1
2	EDO	AAA	802	-	-	0/1/1/1	-
2	EDO	CCC	801	-	-	0/1/1/1	-
2	EDO	EEE	802	-	-	0/1/1/1	-
2	EDO	BBB	801	-	-	1/1/1/1	-
2	EDO	BBB	802	-	-	1/1/1/1	-
3	VKH	EEE	803	1	-	0/2/22/22	0/1/1/1
2	EDO	EEE	801	-	-	1/1/1/1	-
2	EDO	CCC	803	-	-	0/1/1/1	-
2	EDO	DDD	803	-	-	0/1/1/1	-
2	EDO	CCC	804	-	-	1/1/1/1	-
2	EDO	DDD	802	-	-	0/1/1/1	-
2	EDO	DDD	801	-	-	0/1/1/1	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	EEE	803	VKH	C2-C3	2.88	1.56	1.52
3	BBB	803	VKH	C5-C4	-2.77	1.50	1.53
3	BBB	803	VKH	C2-C3	2.71	1.56	1.52
3	DDD	804	VKH	C5-C7	-2.19	1.50	1.54
3	DDD	804	VKH	C2-C3	2.13	1.55	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	DDD	804	VKH	C1-C2-C3	7.22	121.08	110.67
3	FFF	802	VKH	C1-C2-C3	6.85	120.54	110.67
3	EEE	803	VKH	C1-C2-C3	6.67	120.28	110.67
3	BBB	803	VKH	C1-C2-C3	6.63	120.22	110.67
3	AAA	803	VKH	C1-C2-C3	6.30	119.75	110.67

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	CCC	804	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	EEE	801	EDO	O1-C1-C2-O2
2	BBB	802	EDO	O1-C1-C2-O2
2	BBB	801	EDO	O1-C1-C2-O2
2	FFF	801	EDO	O1-C1-C2-O2

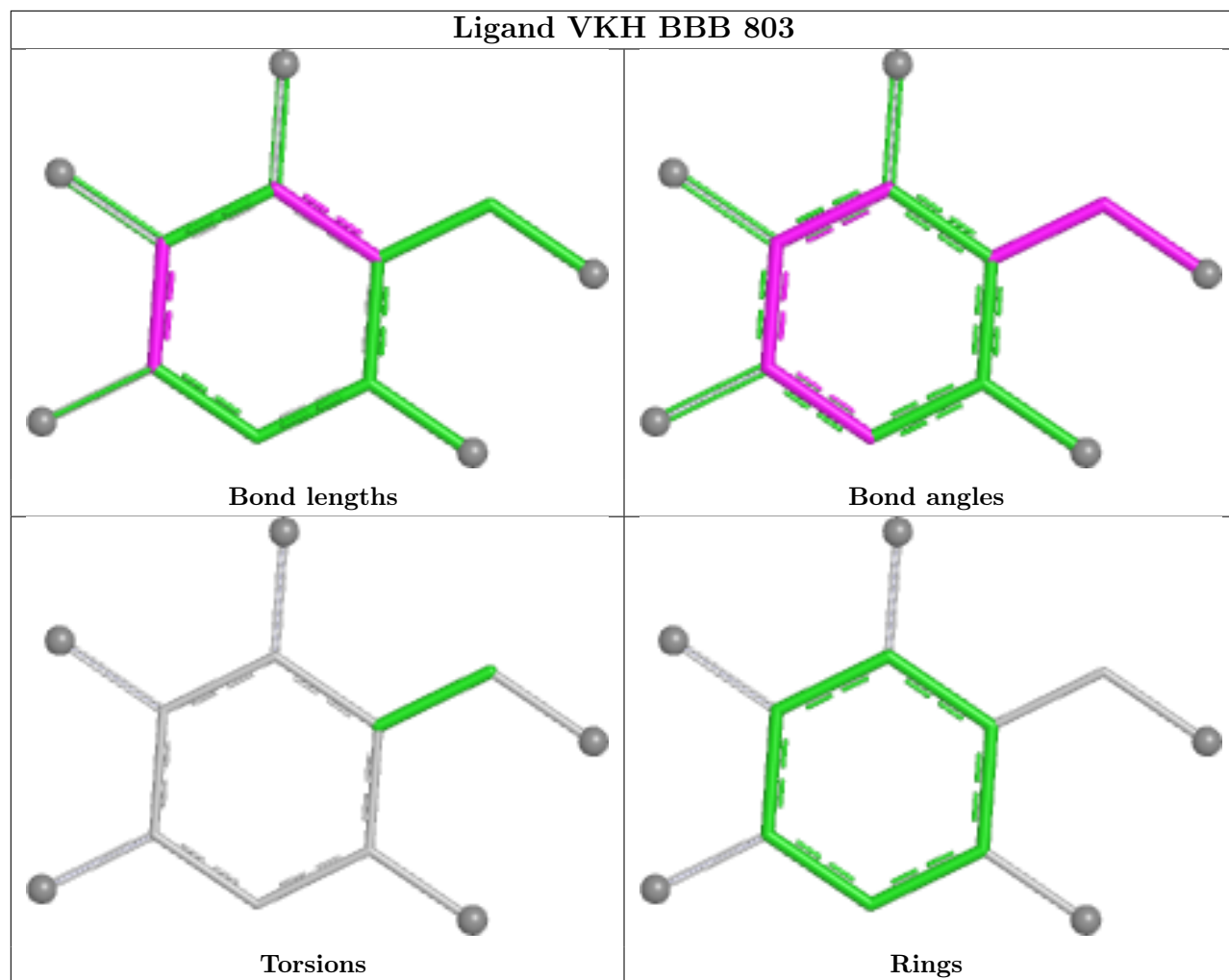
There are no ring outliers.

8 monomers are involved in 12 short contacts:

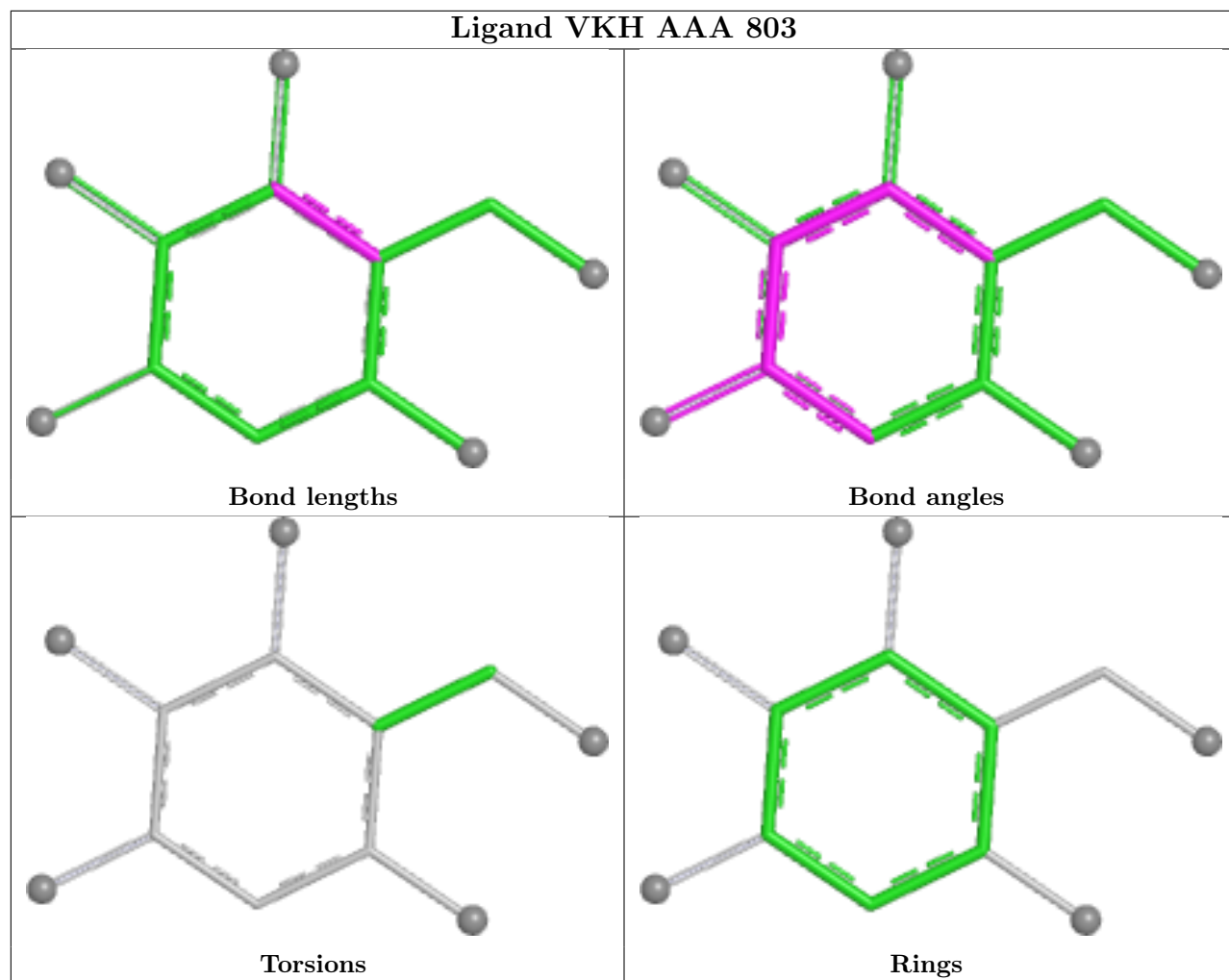
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	CCC	802	EDO	3	0
3	BBB	803	VKH	1	0
2	FFF	801	EDO	1	0
3	DDD	804	VKH	1	0
2	BBB	802	EDO	1	0
3	EEE	803	VKH	1	0
2	DDD	803	EDO	3	0
2	CCC	804	EDO	1	0

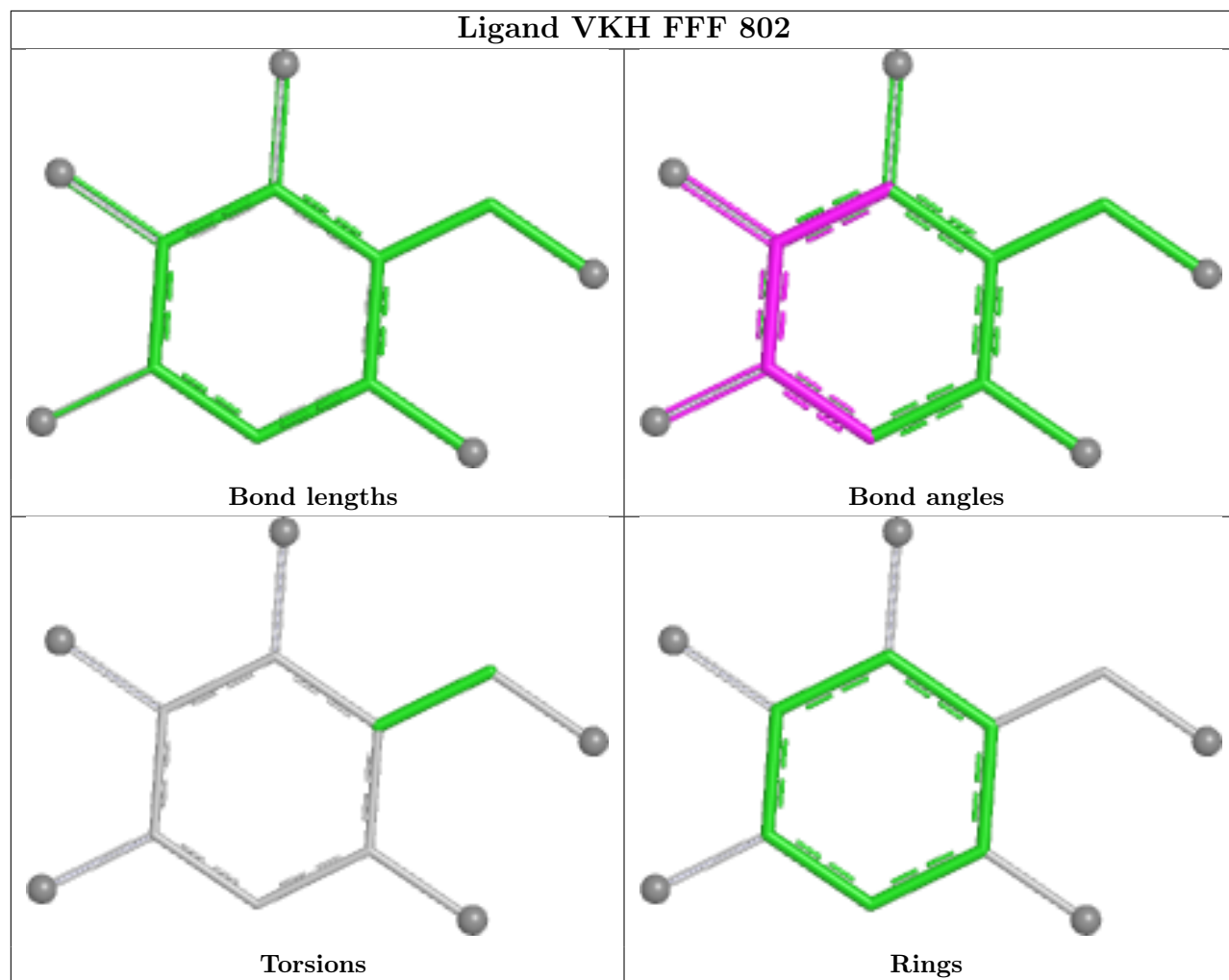
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

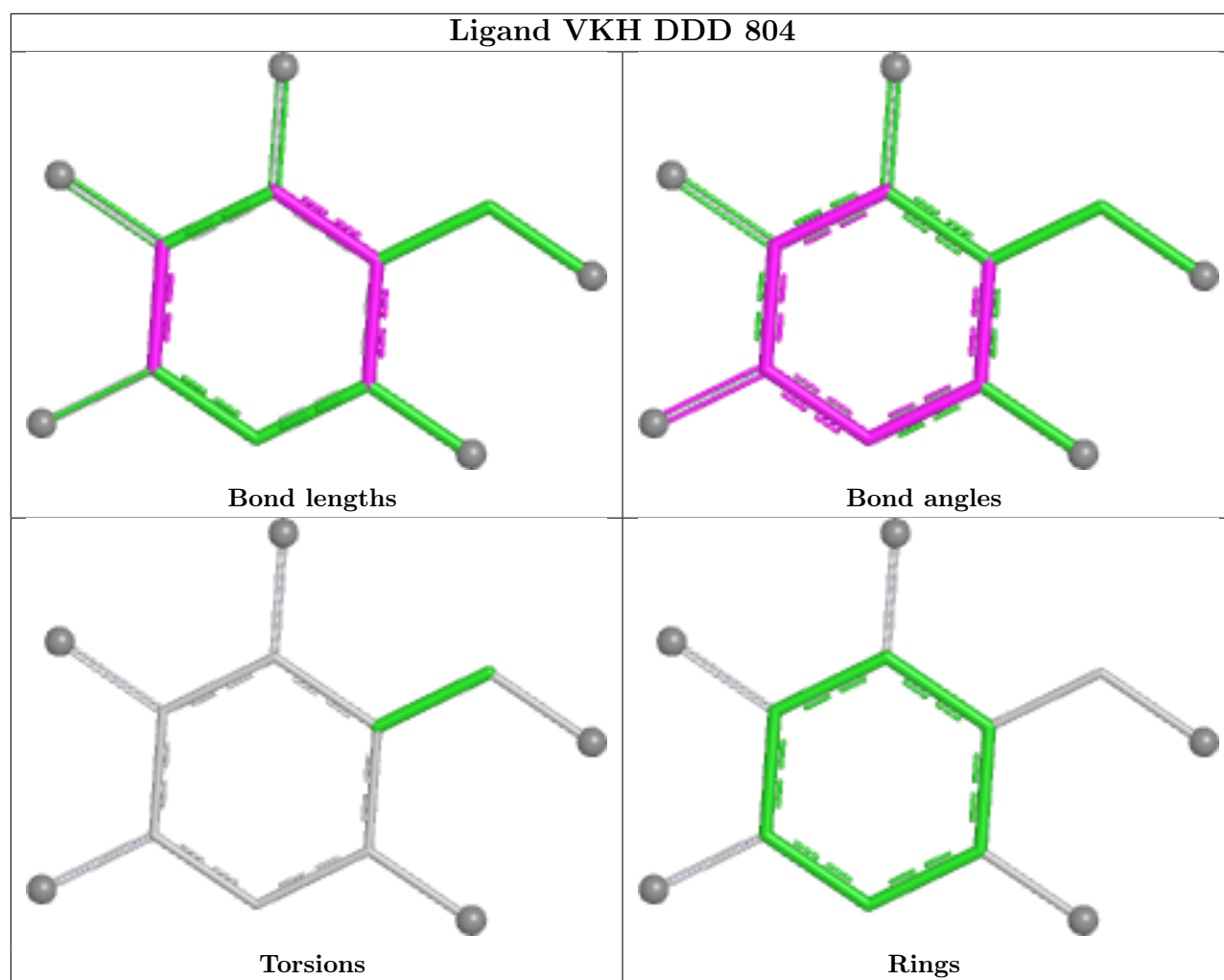
Ligand VKH BBB 803

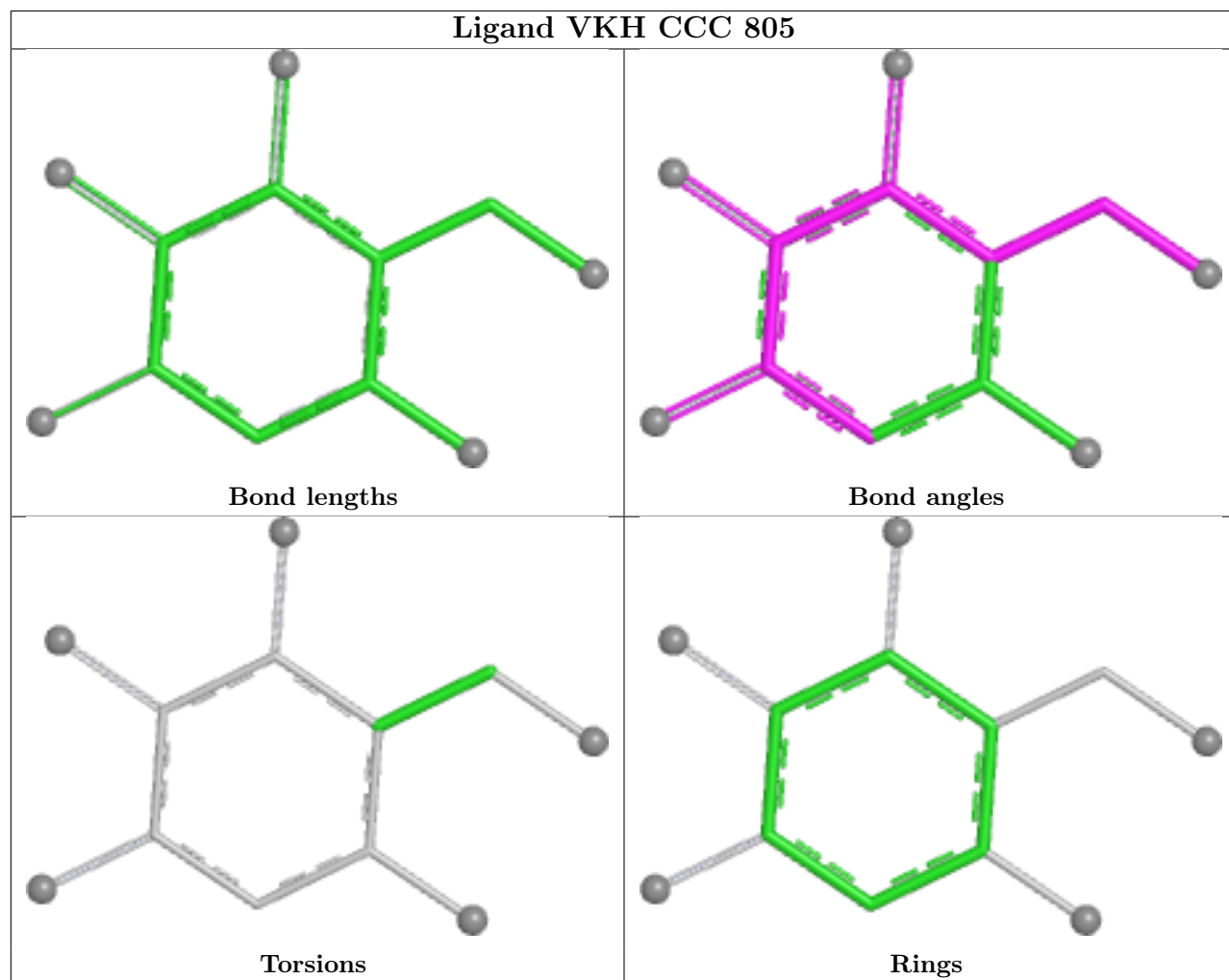


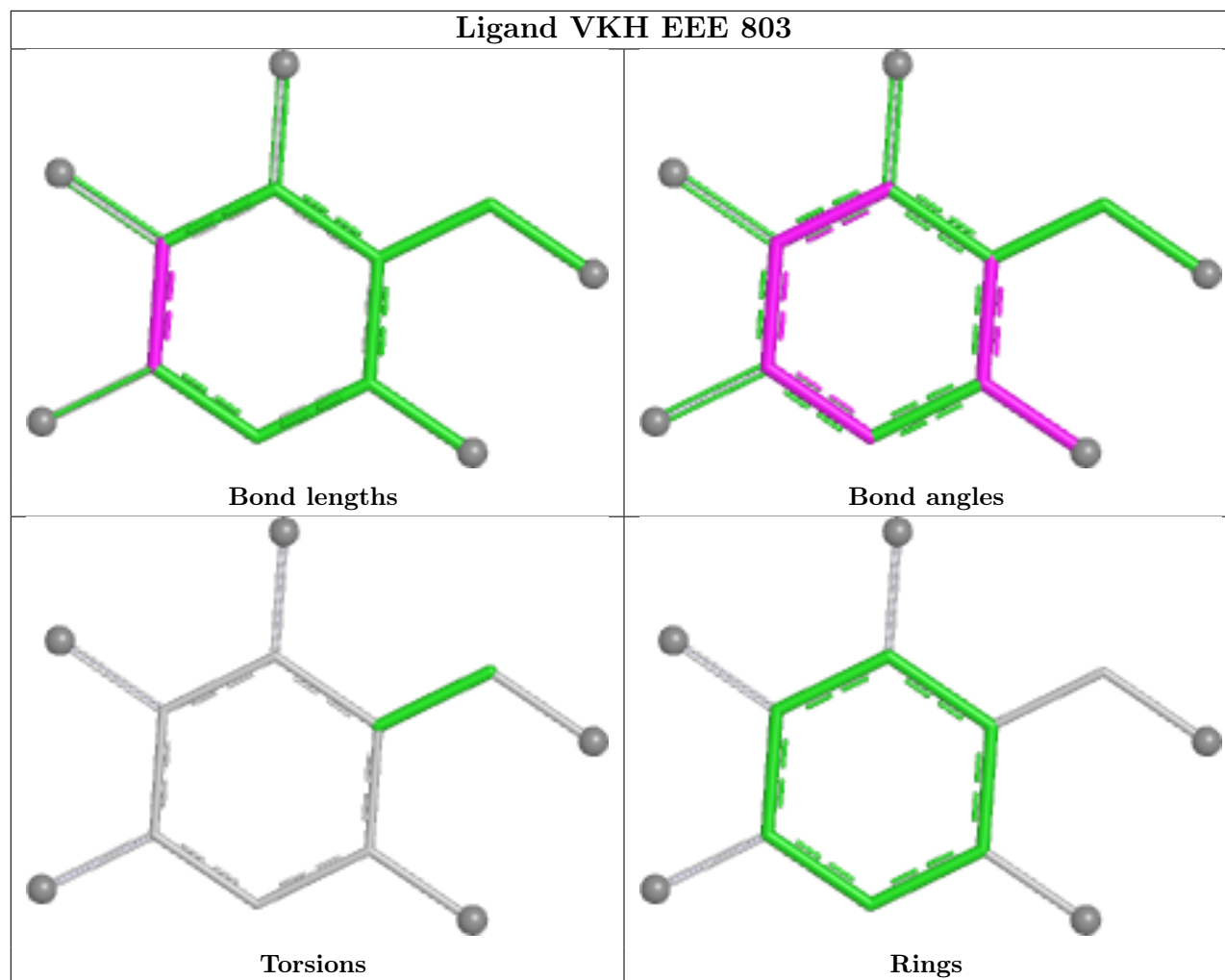
Ligand VKH AAA 803











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	AAA	655/674 (97%)	0.96	66 (10%)	12 12	29, 48, 73, 112	0
1	BBB	651/674 (96%)	0.58	30 (4%)	37 37	29, 43, 69, 94	0
1	CCC	651/674 (96%)	0.72	32 (4%)	35 35	27, 44, 68, 93	0
1	DDD	650/674 (96%)	0.97	66 (10%)	12 12	33, 51, 77, 111	0
1	EEE	652/674 (96%)	0.78	50 (7%)	19 20	31, 48, 73, 97	0
1	FFF	653/674 (96%)	0.70	33 (5%)	33 33	25, 44, 67, 97	0
All	All	3912/4044 (96%)	0.78	277 (7%)	22 22	25, 46, 72, 112	0

The worst 5 of 277 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	534	TYR	5.3
1	AAA	28	GLN	5.1
1	EEE	166	LEU	5.1
1	AAA	27	PHE	4.9
1	DDD	529	PHE	4.9

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 ⓘ

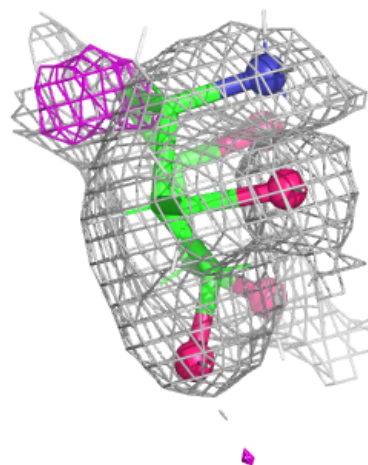
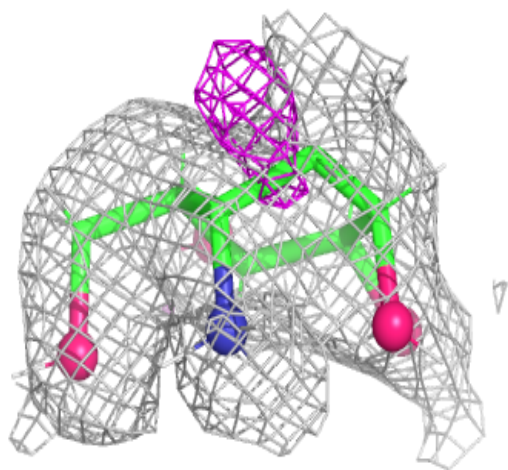
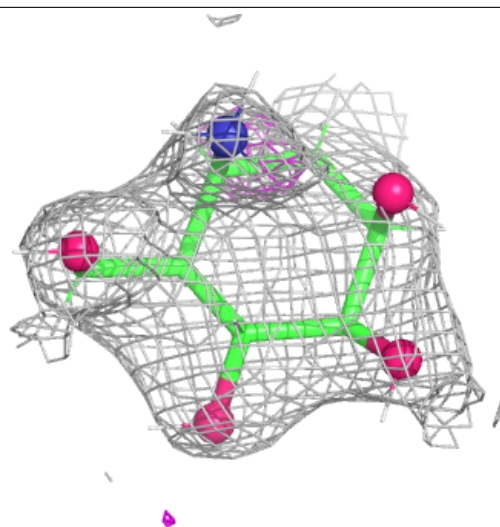
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	EDO	DDD	802	4/4	0.82	0.13	58,66,67,70	1
2	EDO	BBB	801	4/4	0.85	0.17	52,61,63,65	1
3	VKH	AAA	803	12/12	0.86	0.11	45,54,62,68	3
2	EDO	CCC	803	4/4	0.88	0.09	55,61,64,64	1
3	VKH	CCC	805	12/12	0.89	0.09	36,48,55,58	3
3	VKH	DDD	804	12/12	0.90	0.10	41,61,71,75	3
3	VKH	BBB	803	12/12	0.90	0.10	35,43,51,55	3
2	EDO	DDD	801	4/4	0.91	0.15	60,64,65,66	1
2	EDO	DDD	803	4/4	0.91	0.12	67,69,70,73	1
2	EDO	CCC	802	4/4	0.91	0.13	56,58,59,60	1
3	VKH	EEE	803	12/12	0.91	0.09	45,58,64,71	3
2	EDO	BBB	802	4/4	0.92	0.16	57,66,69,73	1
3	VKH	FFF	802	12/12	0.92	0.09	39,55,61,62	3
2	EDO	AAA	801	4/4	0.92	0.11	48,50,58,59	1
2	EDO	AAA	802	4/4	0.93	0.12	41,49,50,50	1
2	EDO	FFF	801	4/4	0.93	0.11	56,59,59,61	1
2	EDO	CCC	804	4/4	0.94	0.10	43,45,46,47	1
4	CL	AAA	804	1/1	0.95	0.07	38,38,38,38	0
2	EDO	EEE	802	4/4	0.96	0.10	46,49,54,58	1
2	EDO	EEE	801	4/4	0.96	0.10	47,53,57,58	1
2	EDO	CCC	801	4/4	0.97	0.07	41,45,46,46	1
4	CL	BBB	804	1/1	0.97	0.06	34,34,34,34	0
4	CL	EEE	804	1/1	0.97	0.06	36,36,36,36	0
4	CL	FFF	803	1/1	0.98	0.07	31,31,31,31	0
4	CL	DDD	805	1/1	0.98	0.07	35,35,35,35	0
4	CL	CCC	806	1/1	0.99	0.08	34,34,34,34	0

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

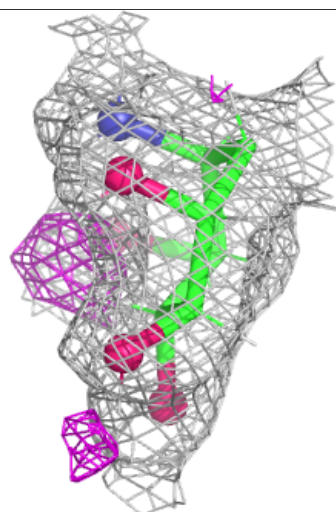
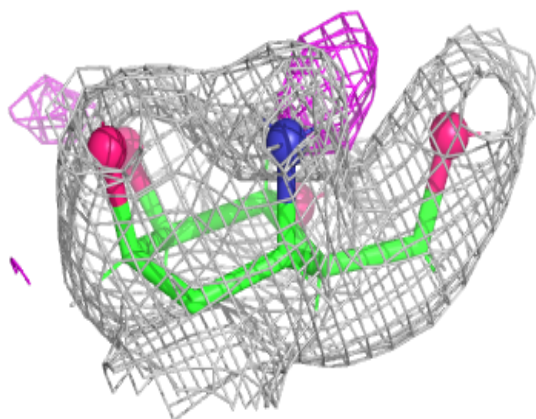
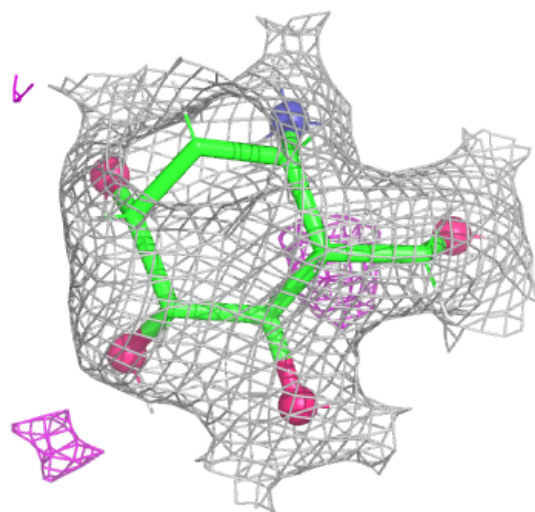
Electron density around VKH AAA 803:

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



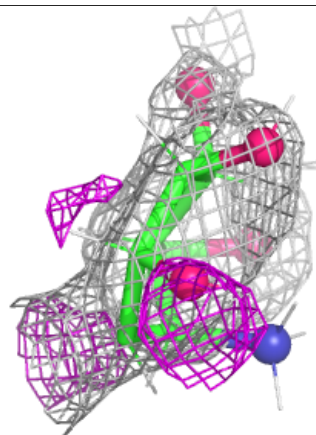
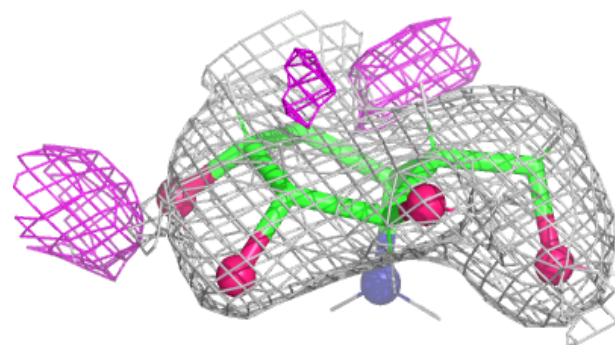
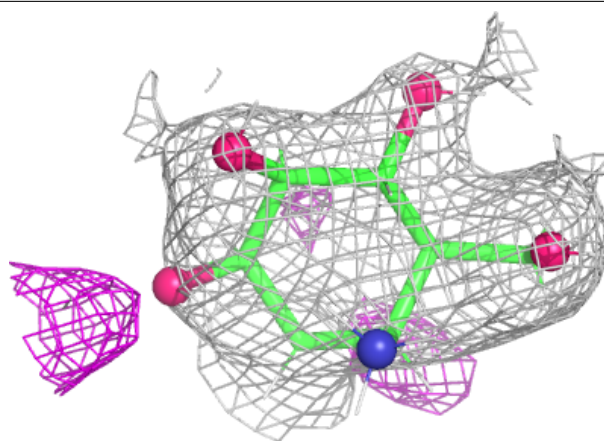
Electron density around VKH CCC 805:

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



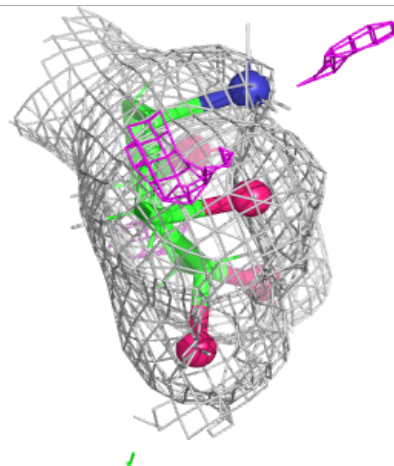
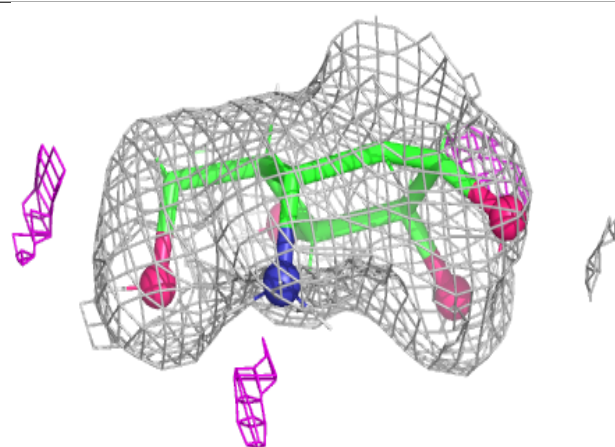
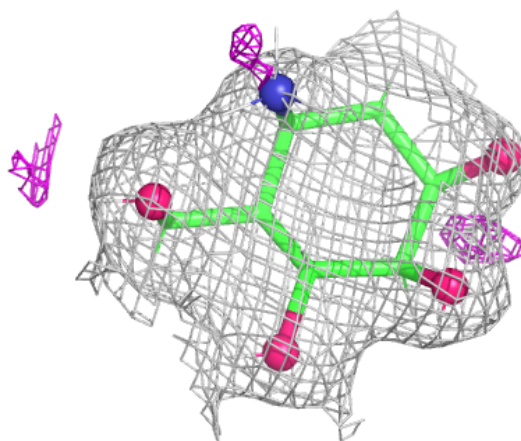
Electron density around VKH DDD 804:

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



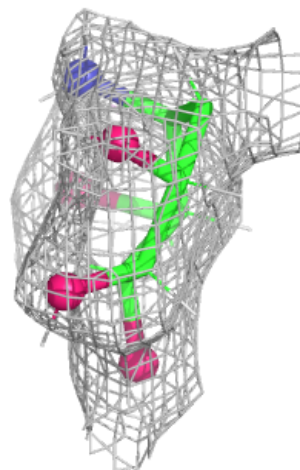
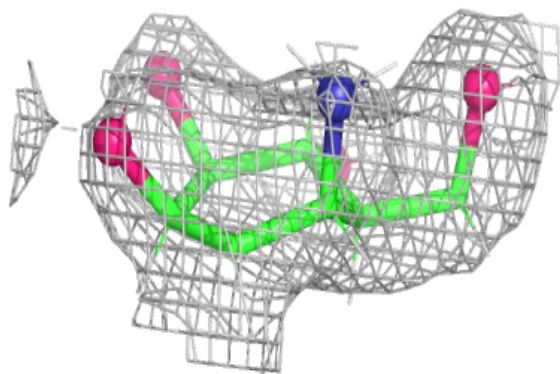
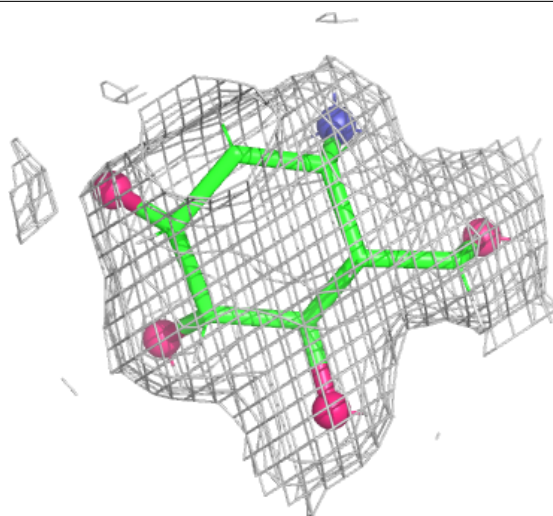
Electron density around VKH BBB 803:

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



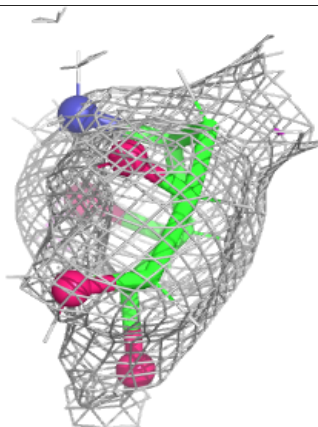
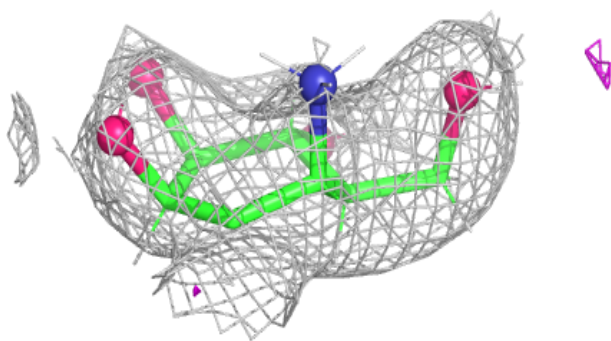
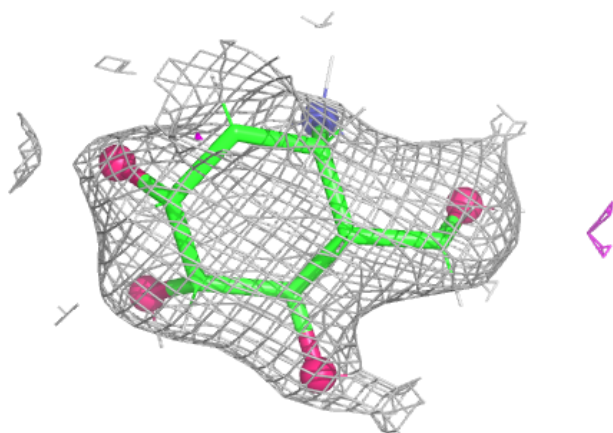
Electron density around VKH EEE 803:

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



Electron density around VKH FFF 802:

$2mF_o-DF_c$ (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.