



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:53 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 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:

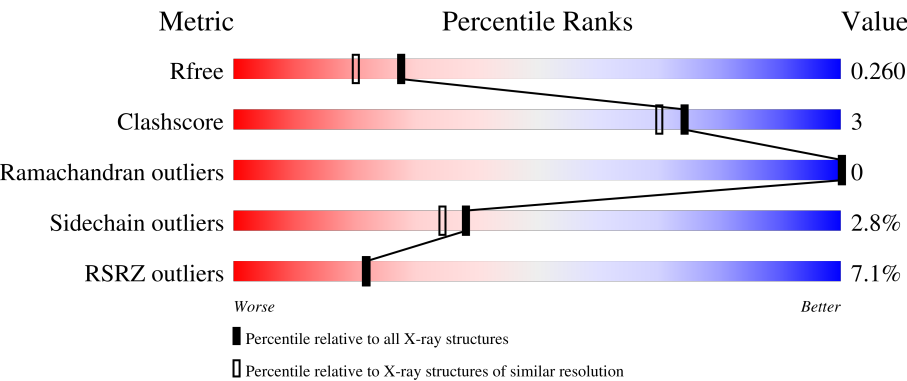
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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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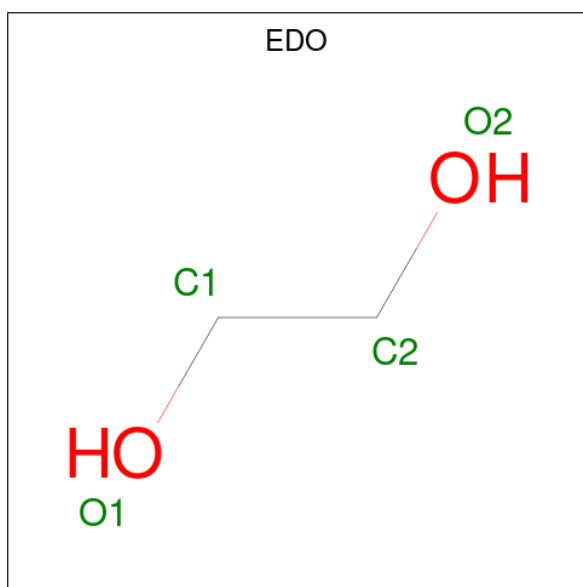
Chain	Residue	Modelled	Actual	Comment	Reference
CCC	25	VAL	-	expression tag	UNP I9SUA3
CCC	26	LEU	-	expression tag	UNP I9SUA3
CCC	27	PHE	-	expression tag	UNP I9SUA3
CCC	28	GLN	-	expression tag	UNP I9SUA3
CCC	29	GLY	-	expression tag	UNP I9SUA3
CCC	30	PRO	-	expression tag	UNP I9SUA3
CCC	31	ALA	-	expression 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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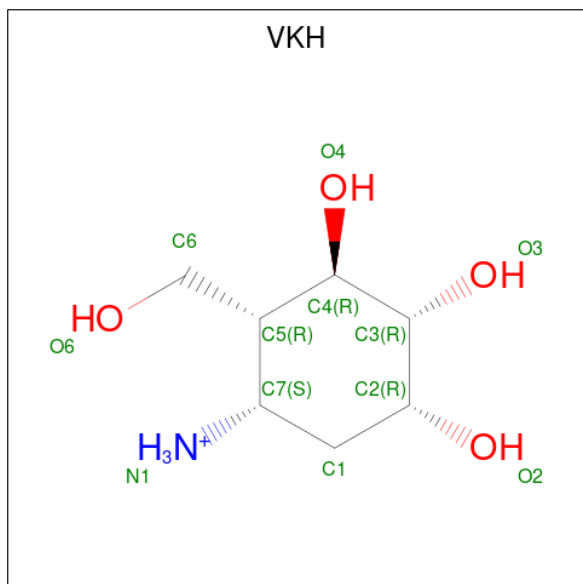
Chain	Residue	Modelled	Actual	Comment	Reference
FFF	23	LEU	-	expression tag	UNP I9SUA3
FFF	24	GLU	-	expression tag	UNP I9SUA3
FFF	25	VAL	-	expression tag	UNP I9SUA3
FFF	26	LEU	-	expression tag	UNP I9SUA3
FFF	27	PHE	-	expression tag	UNP I9SUA3
FFF	28	GLN	-	expression tag	UNP I9SUA3
FFF	29	GLY	-	expression 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

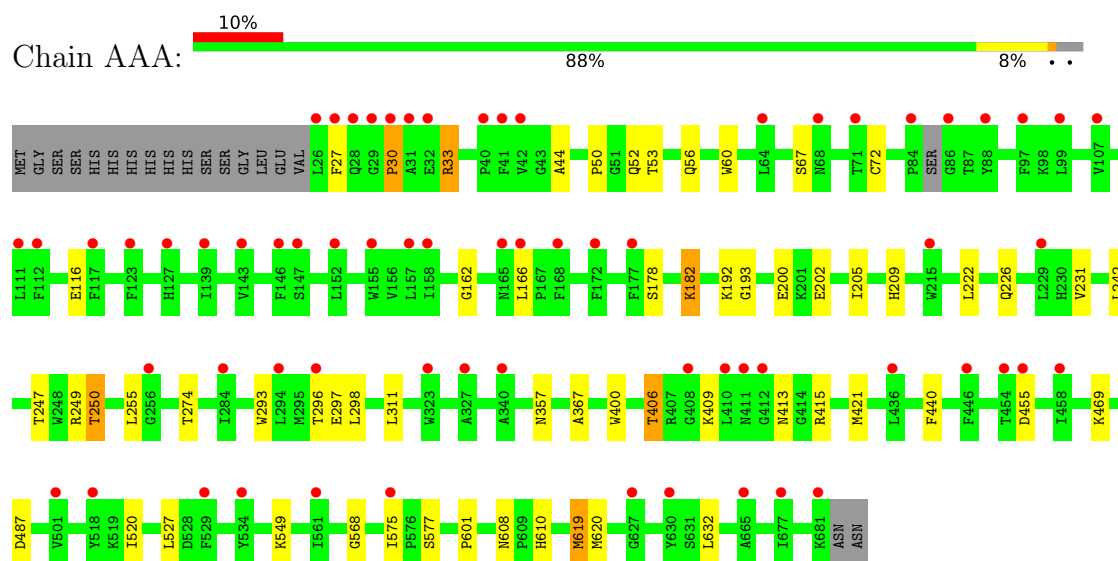
- Molecule 5 is water.

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

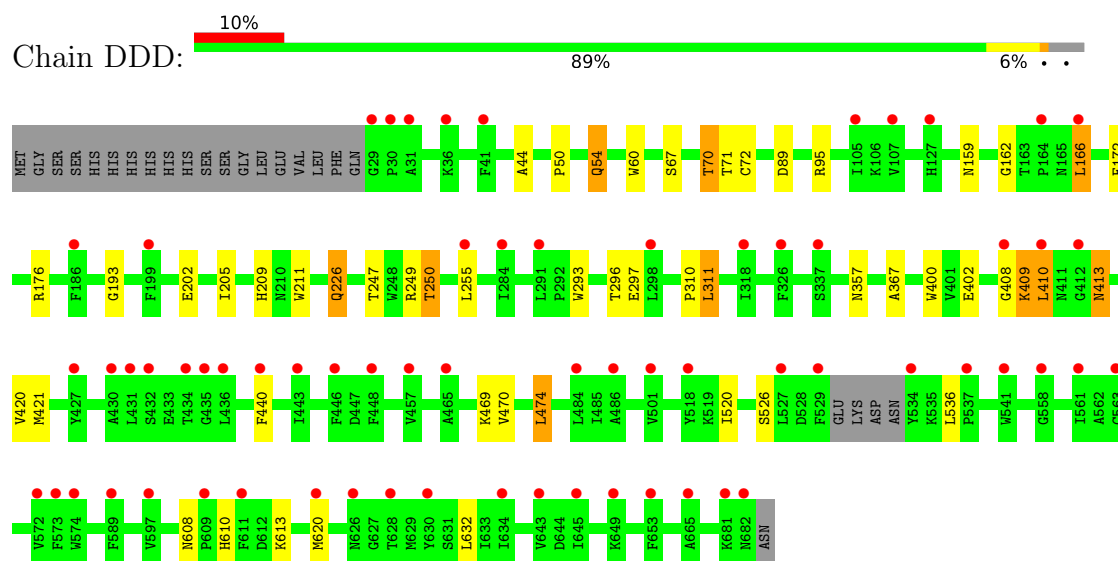
3 Residue-property plots [i](#)

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.

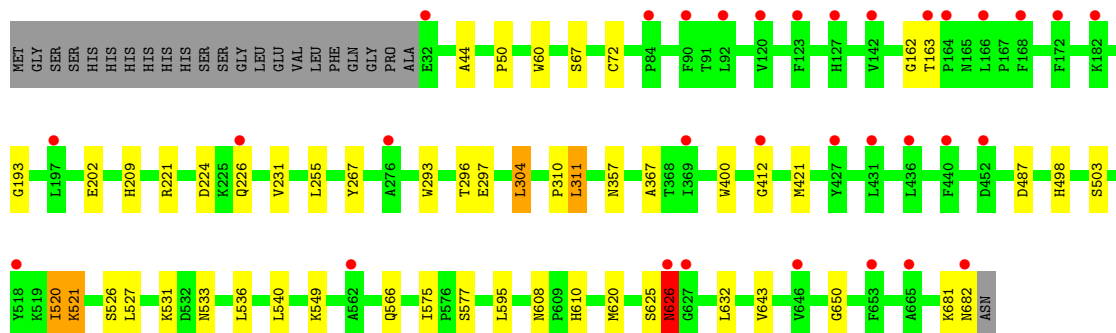
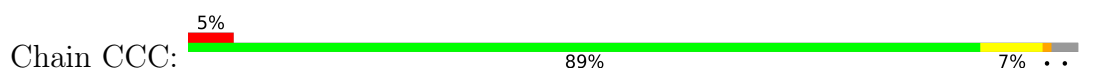
- Molecule 1: Glyco_hydro_42M domain-containing protein



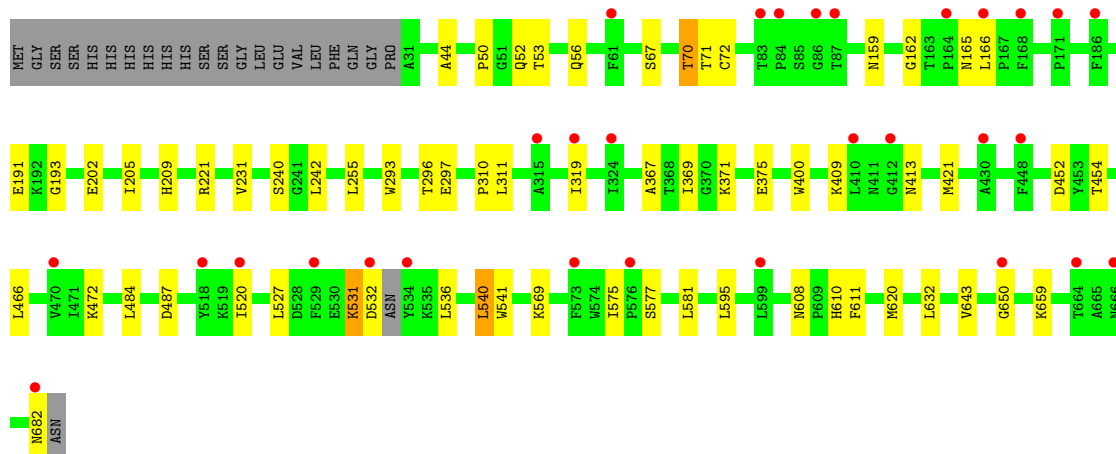
- Molecule 1: Glyco_hydro_42M domain-containing protein



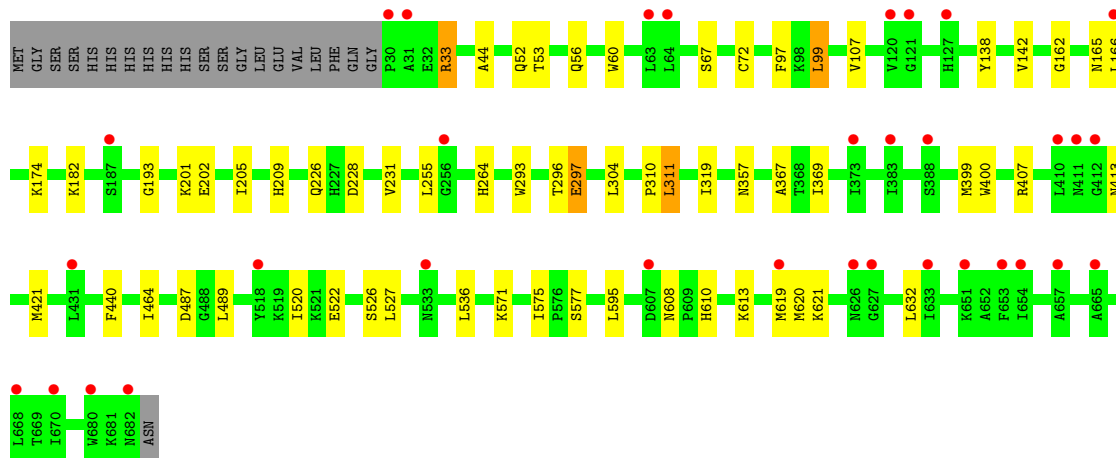
- Molecule 1: Glyco_hydro_42M domain-containing protein



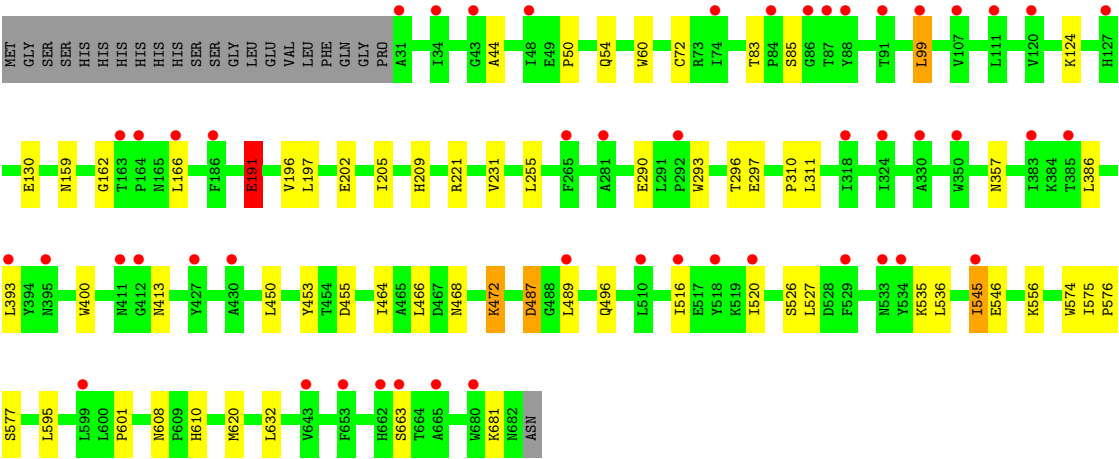
- Molecule 1: Glyco_hydro_42M domain-containing protein



- 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%)

All (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
1	DDD	297	GLU	CD-OE1	8.95	1.42	1.25
1	BBB	650	GLY	C-O	5.75	1.28	1.23

All (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
1	DDD	249	ARG	CA-C-N	5.28	127.88	120.28
1	DDD	249	ARG	C-N-CA	5.28	127.88	120.28
1	AAA	249	ARG	CA-C-N	5.16	127.91	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	249	ARG	C-N-CA	5.16	127.91	120.38
1	AAA	30	PRO	CB-CA-C	-5.15	104.17	111.68
1	EEE	221	ARG	CB-CG-CD	5.02	122.84	111.30

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:EEE:545:ILE:HD11	1:EEE:576:PRO:HG3	1.65	0.76
1:EEE:196:VAL:HG11	1:EEE:496:GLN:NE2	2.04	0.73
1:FFF:60:TRP:HE1	1:FFF:357:ASN:ND2	1.88	0.71
1:CCC:412:GLY:HA2	2:CCC:802:EDO:O1	1.91	0.71
1:FFF:297:GLU:HG3	5:FFF:983:HOH:O	1.90	0.71
1:CCC:60:TRP:HE1	1:CCC:357:ASN:ND2	1.88	0.71
1:FFF:60:TRP:HE1	1:FFF:357:ASN:HD22	1.39	0.71
1:AAA:60:TRP:HE1	1:AAA:357:ASN:ND2	1.89	0.70
1:DDD:60:TRP:HE1	1:DDD:357:ASN:ND2	1.89	0.70
1:EEE:60:TRP:HE1	1:EEE:357:ASN:ND2	1.88	0.70
1:DDD:247:THR:O	1:DDD:250:THR:HB	1.91	0.70
1:AAA:247:THR:O	1:AAA:250:THR:HB	1.92	0.70
1:FFF:52:GLN:HA	1:FFF:56:GLN:HE21	1.57	0.69
1:BBB:52:GLN:HA	1:BBB:56:GLN:HE21	1.57	0.69
1:CCC:60:TRP:HE1	1:CCC:357:ASN:HD22	1.40	0.69
1:EEE:60:TRP:HE1	1:EEE:357:ASN:HD22	1.39	0.68
1:AAA:60:TRP:HE1	1:AAA:357:ASN:HD22	1.42	0.68
1:FFF:399:MET:HE3	5:FFF:991:HOH:O	1.93	0.68
1:AAA:52:GLN:HA	1:AAA:56:GLN:HE21	1.56	0.68
1:DDD:60:TRP:HE1	1:DDD:357:ASN:HD22	1.44	0.65
1:EEE:166:LEU:HD22	1:EEE:205:ILE:HG12	1.79	0.64
1:FFF:264:HIS:NE2	2:FFF:801:EDO:O1	2.20	0.64
1:CCC:310:PRO:HB2	1:BBB:520:ILE:HD13	1.80	0.63
1:DDD:54:GLN:HG2	1:DDD:95:ARG:HD2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:166:LEU:CD2	1:BBB:205:ILE:HG12	2.29	0.61
1:BBB:611:PHE:CE1	1:BBB:643:VAL:HG11	2.36	0.61
1:EEE:166:LEU:CD2	1:EEE:205:ILE:HG12	2.31	0.61
1:DDD:310:PRO:HB2	1:FFF:520:ILE:HD13	1.82	0.60
1:AAA:30:PRO:HD2	1:AAA:226:GLN:NE2	2.16	0.60
1:CCC:549:LYS:HE3	1:CCC:566:GLN:O	2.04	0.58
1:FFF:536:LEU:HD11	1:FFF:595:LEU:HD22	1.84	0.58
1:EEE:191:GLU:H	1:EEE:191:GLU:CD	2.13	0.57
1:EEE:545:ILE:CG1	1:EEE:574:TRP:CZ3	2.87	0.57
1:DDD:193:GLY:O	1:EEE:50:PRO:HB2	2.05	0.56
1:DDD:402:GLU:CD	1:DDD:420:VAL:HG12	2.30	0.56
1:BBB:536:LEU:HD11	1:BBB:595:LEU:HD22	1.88	0.56
1:DDD:89:ASP:OD2	1:BBB:659:LYS:HA	2.05	0.56
1:FFF:608:ASN:O	1:FFF:610:HIS:HD2	1.89	0.56
1:DDD:520:ILE:HD13	1:EEE:310:PRO:HB2	1.88	0.55
1:AAA:608:ASN:O	1:AAA:610:HIS:HD2	1.90	0.55
1:EEE:608:ASN:O	1:EEE:610:HIS:HD2	1.90	0.55
1:BBB:608:ASN:O	1:BBB:610:HIS:HD2	1.88	0.55
1:AAA:620:MET:HA	1:AAA:632:LEU:O	2.07	0.55
1:EEE:83:THR:O	1:EEE:85:SER:O	2.25	0.55
1:EEE:620:MET:HA	1:EEE:632:LEU:O	2.07	0.54
1:CCC:620:MET:HA	1:CCC:632:LEU:O	2.07	0.54
1:BBB:620:MET:HA	1:BBB:632:LEU:O	2.08	0.54
1:DDD:620:MET:HA	1:DDD:632:LEU:O	2.07	0.54
1:CCC:520:ILE:HD13	1:CCC:521:LYS:O	2.08	0.53
1:CCC:608:ASN:O	1:CCC:610:HIS:HD2	1.90	0.53
1:FFF:310:PRO:HB2	1:EEE:520:ILE:HD13	1.90	0.53
1:FFF:620:MET:HA	1:FFF:632:LEU:O	2.08	0.53
1:DDD:608:ASN:O	1:DDD:610:HIS:HD2	1.89	0.53
1:CCC:520:ILE:HD13	1:CCC:521:LYS:N	2.23	0.53
1:AAA:311:LEU:HA	1:CCC:520:ILE:CG2	2.39	0.53
1:DDD:50:PRO:HB2	1:FFF:193:GLY:O	2.09	0.53
1:DDD:413:ASN:HA	2:DDD:803:EDO:C1	2.38	0.53
1:AAA:193:GLY:O	1:BBB:50:PRO:HB2	2.08	0.53
1:BBB:221:ARG:HD2	5:BBB:1039:HOH:O	2.08	0.53
1:DDD:408:GLY:O	1:DDD:410:LEU:HD13	2.09	0.52
1:CCC:221:ARG:NH2	5:CCC:902:HOH:O	2.42	0.52
1:EEE:536:LEU:HD11	1:EEE:595:LEU:HD22	1.91	0.52
1:BBB:531:LYS:O	1:BBB:532:ASP:C	2.52	0.52
1:DDD:409:LYS:C	1:DDD:410:LEU:HD13	2.35	0.52
1:EEE:159:ASN:ND2	3:EEE:803:VKH:O2	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:124:LYS:HB3	5:EEE:990:HOH:O	2.10	0.52
1:EEE:516:ILE:HD11	1:EEE:546:GLU:HB2	1.92	0.52
1:FFF:399:MET:CE	5:FFF:991:HOH:O	2.56	0.51
1:AAA:406:THR:OG1	1:AAA:415:ARG:O	2.28	0.51
1:AAA:200:GLU:HG3	5:AAA:1045:HOH:O	2.11	0.50
1:FFF:311:LEU:HA	1:EEE:520:ILE:CG2	2.41	0.50
1:FFF:52:GLN:HA	1:FFF:56:GLN:NE2	2.25	0.50
1:EEE:196:VAL:HG22	1:EEE:496:GLN:HB3	1.93	0.50
1:CCC:267:TYR:O	2:CCC:804:EDO:O2	2.30	0.50
1:DDD:159:ASN:ND2	3:DDD:804:VKH:O2	2.42	0.50
1:BBB:70:THR:HG22	1:BBB:71:THR:OG1	2.11	0.50
1:CCC:520:ILE:HD11	1:CCC:540:LEU:HD12	1.94	0.49
1:AAA:52:GLN:HA	1:AAA:56:GLN:NE2	2.25	0.49
1:AAA:205:ILE:HG21	1:AAA:242:LEU:HD22	1.95	0.49
1:BBB:52:GLN:HA	1:BBB:56:GLN:NE2	2.26	0.48
1:CCC:626:ASN:ND2	1:CCC:626:ASN:N	2.60	0.48
1:DDD:421:MET:HE1	1:DDD:440:PHE:CE1	2.49	0.48
1:FFF:527:LEU:HD11	1:FFF:577:SER:HB2	1.94	0.48
1:EEE:54:GLN:NE2	1:EEE:99:LEU:HD21	2.29	0.48
1:CCC:536:LEU:HD11	1:CCC:595:LEU:HD22	1.95	0.48
1:AAA:520:ILE:HD13	1:BBB:310:PRO:HB2	1.96	0.48
1:FFF:522:GLU:H	1:FFF:522:GLU:CD	2.21	0.48
1:CCC:527:LEU:HD11	1:CCC:577:SER:HB2	1.96	0.47
1:FFF:202:GLU:HB3	1:FFF:400:TRP:CE2	2.50	0.47
1:FFF:319:ILE:HD12	1:FFF:369:ILE:HD11	1.96	0.47
1:BBB:202:GLU:HB3	1:BBB:400:TRP:CE2	2.50	0.47
1:CCC:498:HIS:CE1	1:CCC:503:SER:OG	2.67	0.47
1:CCC:311:LEU:HA	1:BBB:520:ILE:CG2	2.45	0.47
1:BBB:371:LYS:HE2	1:BBB:375:GLU:OE2	2.15	0.47
1:EEE:196:VAL:HG13	1:EEE:197:LEU:O	2.15	0.47
1:CCC:224:ASP:CG	5:CCC:902:HOH:O	2.57	0.47
1:BBB:162:GLY:HA2	1:BBB:209:HIS:NE2	2.30	0.47
1:BBB:581:LEU:HD22	2:BBB:802:EDO:H12	1.95	0.46
1:CCC:625:SER:C	1:CCC:626:ASN:ND2	2.73	0.46
1:DDD:202:GLU:HB3	1:DDD:400:TRP:CE2	2.50	0.46
1:BBB:452:ASP:OD1	1:BBB:454:THR:OG1	2.23	0.46
1:CCC:520:ILE:CD1	1:CCC:521:LYS:O	2.64	0.46
1:AAA:162:GLY:HA2	1:AAA:209:HIS:NE2	2.30	0.46
1:DDD:70:THR:HG22	1:DDD:71:THR:OG1	2.16	0.46
1:AAA:202:GLU:HB3	1:AAA:400:TRP:CE2	2.50	0.46
1:FFF:621:LYS:HE2	5:FFF:1011:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:311:LEU:HA	1:FFF:520:ILE:CG2	2.46	0.46
1:CCC:202:GLU:HB3	1:CCC:400:TRP:CE2	2.51	0.46
1:CCC:412:GLY:HA2	2:CCC:802:EDO:H22	1.98	0.46
1:EEE:202:GLU:HB3	1:EEE:400:TRP:CE2	2.51	0.46
1:CCC:625:SER:C	1:CCC:626:ASN:HD22	2.24	0.46
1:FFF:138:TYR:CE2	1:FFF:142:VAL:HG21	2.51	0.46
1:EEE:162:GLY:HA2	1:EEE:209:HIS:NE2	2.31	0.46
1:EEE:464:ILE:HG22	1:EEE:489:LEU:HB2	1.98	0.46
1:BBB:611:PHE:CD1	1:BBB:643:VAL:CG1	2.98	0.45
1:EEE:450:LEU:HB2	1:EEE:453:TYR:CZ	2.51	0.45
1:AAA:421:MET:HE1	1:AAA:440:PHE:CE1	2.51	0.45
1:BBB:319:ILE:HD12	1:BBB:369:ILE:HD11	1.99	0.45
1:DDD:162:GLY:HA2	1:DDD:209:HIS:NE2	2.31	0.45
1:AAA:53:THR:H	1:AAA:56:GLN:NE2	2.15	0.44
1:DDD:413:ASN:HA	2:DDD:803:EDO:H12	1.99	0.44
1:BBB:240:SER:OG	1:BBB:421:MET:HE2	2.17	0.44
1:BBB:44:ALA:O	1:BBB:72:CYS:HA	2.17	0.44
1:FFF:44:ALA:O	1:FFF:72:CYS:HA	2.18	0.44
1:FFF:53:THR:H	1:FFF:56:GLN:NE2	2.15	0.44
1:BBB:527:LEU:HD11	1:BBB:577:SER:HB2	1.98	0.44
1:FFF:522:GLU:CD	1:FFF:522:GLU:N	2.76	0.44
1:DDD:172:PHE:O	1:DDD:176:ARG:HG2	2.17	0.44
1:CCC:412:GLY:CA	2:CCC:802:EDO:O1	2.64	0.44
1:BBB:53:THR:H	1:BBB:56:GLN:NE2	2.15	0.44
1:FFF:33:ARG:NH2	1:FFF:226:GLN:O	2.48	0.44
1:EEE:527:LEU:HD11	1:EEE:577:SER:HB2	1.99	0.44
1:AAA:30:PRO:HD2	1:AAA:226:GLN:HE21	1.82	0.44
1:AAA:44:ALA:O	1:AAA:72:CYS:HA	2.18	0.43
1:FFF:162:GLY:HA2	1:FFF:209:HIS:NE2	2.33	0.43
1:CCC:44:ALA:O	1:CCC:72:CYS:HA	2.17	0.43
1:DDD:176:ARG:NH2	1:DDD:211:TRP:CE2	2.86	0.43
1:DDD:226:GLN:NE2	1:DDD:226:GLN:HA	2.34	0.43
1:BBB:205:ILE:HG21	1:BBB:242:LEU:HD22	2.00	0.43
1:AAA:33:ARG:NH1	5:AAA:921:HOH:O	2.52	0.43
1:FFF:464:ILE:HG22	1:FFF:489:LEU:HB2	1.99	0.43
1:EEE:545:ILE:HD13	1:EEE:576:PRO:CG	2.41	0.43
1:AAA:520:ILE:CG2	1:BBB:311:LEU:HA	2.49	0.43
1:AAA:527:LEU:HD11	1:AAA:577:SER:HB2	2.01	0.43
1:FFF:255:LEU:O	1:FFF:293:TRP:HA	2.19	0.43
1:EEE:44:ALA:O	1:EEE:72:CYS:HA	2.18	0.43
1:DDD:166:LEU:HD13	1:DDD:205:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FFF:67:SER:O	1:FFF:367:ALA:HA	2.19	0.43
1:DDD:470:VAL:O	1:DDD:474:LEU:HD22	2.20	0.42
1:CCC:162:GLY:HA2	1:CCC:209:HIS:NE2	2.34	0.42
1:CCC:682:ASN:OD1	1:CCC:682:ASN:C	2.63	0.42
1:AAA:50:PRO:HB2	1:CCC:193:GLY:O	2.20	0.42
1:DDD:44:ALA:O	1:DDD:72:CYS:HA	2.19	0.42
1:DDD:413:ASN:CA	2:DDD:803:EDO:H12	2.49	0.42
1:EEE:455:ASP:HA	1:EEE:601:PRO:HG2	2.01	0.42
1:DDD:255:LEU:O	1:DDD:293:TRP:HA	2.19	0.42
1:AAA:487:ASP:HA	1:AAA:575:ILE:O	2.20	0.42
1:DDD:54:GLN:HE21	1:DDD:54:GLN:HB3	1.75	0.42
1:CCC:487:ASP:HA	1:CCC:575:ILE:O	2.20	0.42
1:FFF:304:LEU:HD23	1:FFF:304:LEU:HA	1.93	0.42
1:AAA:178:SER:O	1:AAA:182:LYS:HD2	2.20	0.42
1:CCC:255:LEU:O	1:CCC:293:TRP:HA	2.19	0.42
1:BBB:255:LEU:O	1:BBB:293:TRP:HA	2.19	0.42
1:AAA:255:LEU:O	1:AAA:293:TRP:HA	2.20	0.41
1:BBB:487:ASP:HA	1:BBB:575:ILE:O	2.20	0.41
1:CCC:67:SER:O	1:CCC:367:ALA:HA	2.20	0.41
1:EEE:487:ASP:HA	1:EEE:575:ILE:O	2.20	0.41
1:AAA:455:ASP:HA	1:AAA:601:PRO:HG2	2.02	0.41
1:DDD:166:LEU:HD13	1:DDD:205:ILE:CD1	2.50	0.41
1:FFF:166:LEU:HD22	1:FFF:205:ILE:HG12	2.02	0.41
1:FFF:487:ASP:HA	1:FFF:575:ILE:O	2.19	0.41
1:CCC:304:LEU:HD23	1:CCC:304:LEU:HA	1.98	0.41
1:FFF:421:MET:HE1	1:FFF:440:PHE:CE2	2.55	0.41
1:AAA:274:THR:HB	1:AAA:619:MET:HE3	2.01	0.41
1:CCC:520:ILE:HD13	1:CCC:521:LYS:H	1.85	0.41
1:EEE:468:ASN:HB3	1:EEE:472:LYS:HE2	2.02	0.41
1:CCC:50:PRO:HB2	1:BBB:193:GLY:O	2.20	0.41
1:CCC:226:GLN:NE2	1:CCC:226:GLN:HA	2.36	0.41
1:DDD:67:SER:O	1:DDD:367:ALA:HA	2.21	0.41
1:BBB:67:SER:O	1:BBB:367:ALA:HA	2.21	0.41
1:FFF:97:PHE:CZ	1:FFF:107:VAL:HG11	2.56	0.41
1:BBB:159:ASN:ND2	3:BBB:803:VKH:O2	2.54	0.41
1:EEE:255:LEU:O	1:EEE:293:TRP:HA	2.20	0.40
1:AAA:67:SER:O	1:AAA:367:ALA:HA	2.21	0.40
1:BBB:540:LEU:HD13	1:BBB:541:TRP:CE2	2.56	0.40
1:FFF:99:LEU:HD12	1:FFF:99:LEU:HA	1.89	0.40

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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	27	PHE
1	AAA	116	GLU
1	AAA	166	LEU
1	AAA	182	LYS
1	AAA	192	LYS
1	AAA	222	LEU
1	AAA	231	VAL
1	AAA	250	THR
1	AAA	296	THR
1	AAA	298	LEU
1	AAA	406	THR
1	AAA	409	LYS
1	AAA	413	ASN
1	AAA	469	LYS
1	AAA	549	LYS
1	AAA	619	MET
1	DDD	54	GLN
1	DDD	70	THR
1	DDD	166	LEU
1	DDD	226	GLN
1	DDD	250	THR
1	DDD	296	THR
1	DDD	311	LEU
1	DDD	409	LYS
1	DDD	410	LEU
1	DDD	413	ASN
1	DDD	469	LYS
1	DDD	474	LEU
1	DDD	526	SER
1	DDD	536	LEU
1	DDD	613	LYS
1	CCC	163	THR
1	CCC	231	VAL

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Mol	Chain	Res	Type
1	CCC	296	THR
1	CCC	304	LEU
1	CCC	311	LEU
1	CCC	421	MET
1	CCC	520	ILE
1	CCC	521	LYS
1	CCC	526	SER
1	CCC	531	LYS
1	CCC	533	ASN
1	CCC	626	ASN
1	CCC	643	VAL
1	CCC	681	LYS
1	BBB	165	ASN
1	BBB	191	GLU
1	BBB	231	VAL
1	BBB	296	THR
1	BBB	409	LYS
1	BBB	413	ASN
1	BBB	466	LEU
1	BBB	472	LYS
1	BBB	484	LEU
1	BBB	531	LYS
1	BBB	540	LEU
1	BBB	569	LYS
1	BBB	682	ASN
1	FFF	33	ARG
1	FFF	99	LEU
1	FFF	165	ASN
1	FFF	174	LYS
1	FFF	182	LYS
1	FFF	201	LYS
1	FFF	231	VAL
1	FFF	296	THR
1	FFF	311	LEU
1	FFF	407	ARG
1	FFF	413	ASN
1	FFF	526	SER
1	FFF	571	LYS
1	FFF	613	LYS
1	FFF	619	MET
1	EEE	99	LEU
1	EEE	130	GLU

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Mol	Chain	Res	Type
1	EEE	191	GLU
1	EEE	231	VAL
1	EEE	290	GLU
1	EEE	296	THR
1	EEE	311	LEU
1	EEE	386	LEU
1	EEE	393	LEU
1	EEE	413	ASN
1	EEE	466	LEU
1	EEE	472	LYS
1	EEE	487	ASP
1	EEE	526	SER
1	EEE	535	LYS
1	EEE	545	ILE
1	EEE	556	LYS
1	EEE	663	SER
1	EEE	681	LYS

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 [i](#)

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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-

All (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
3	AAA	803	VKH	C5-C4	2.04	1.55	1.53
3	DDD	804	VKH	C5-C4	2.01	1.55	1.53

All (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
3	EEE	803	VKH	C2-C3-C4	4.31	118.45	110.86
3	AAA	803	VKH	O2-C2-C3	-4.27	101.31	110.15
3	CCC	805	VKH	C1-C2-C3	3.98	116.40	110.67
3	CCC	805	VKH	O3-C3-C4	-3.72	101.61	110.38
3	CCC	805	VKH	C2-C3-C4	3.45	116.93	110.86
3	DDD	804	VKH	C2-C3-C4	3.19	116.47	110.86
3	BBB	803	VKH	C2-C3-C4	3.14	116.39	110.86
3	FFF	802	VKH	C2-C3-C4	3.02	116.17	110.86
3	CCC	805	VKH	O2-C2-C1	-2.94	102.55	109.86
3	FFF	802	VKH	O2-C2-C1	-2.77	102.96	109.86
3	DDD	804	VKH	C1-C7-C5	-2.69	108.30	111.67
3	CCC	805	VKH	O6-C6-C5	2.64	117.45	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	FFF	802	VKH	O3-C3-C2	-2.30	105.35	110.05
3	EEE	803	VKH	C5-C7-N1	2.28	116.34	111.73
3	DDD	804	VKH	O2-C2-C1	-2.26	104.23	109.86
3	AAA	803	VKH	C2-C3-C4	2.13	114.61	110.86
3	CCC	805	VKH	O4-C4-C5	2.08	114.18	109.94
3	BBB	803	VKH	O6-C6-C5	-2.07	106.35	111.22
3	AAA	803	VKH	O2-C2-C1	-2.06	104.74	109.86
3	AAA	803	VKH	C5-C4-C3	2.05	114.21	110.77

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
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

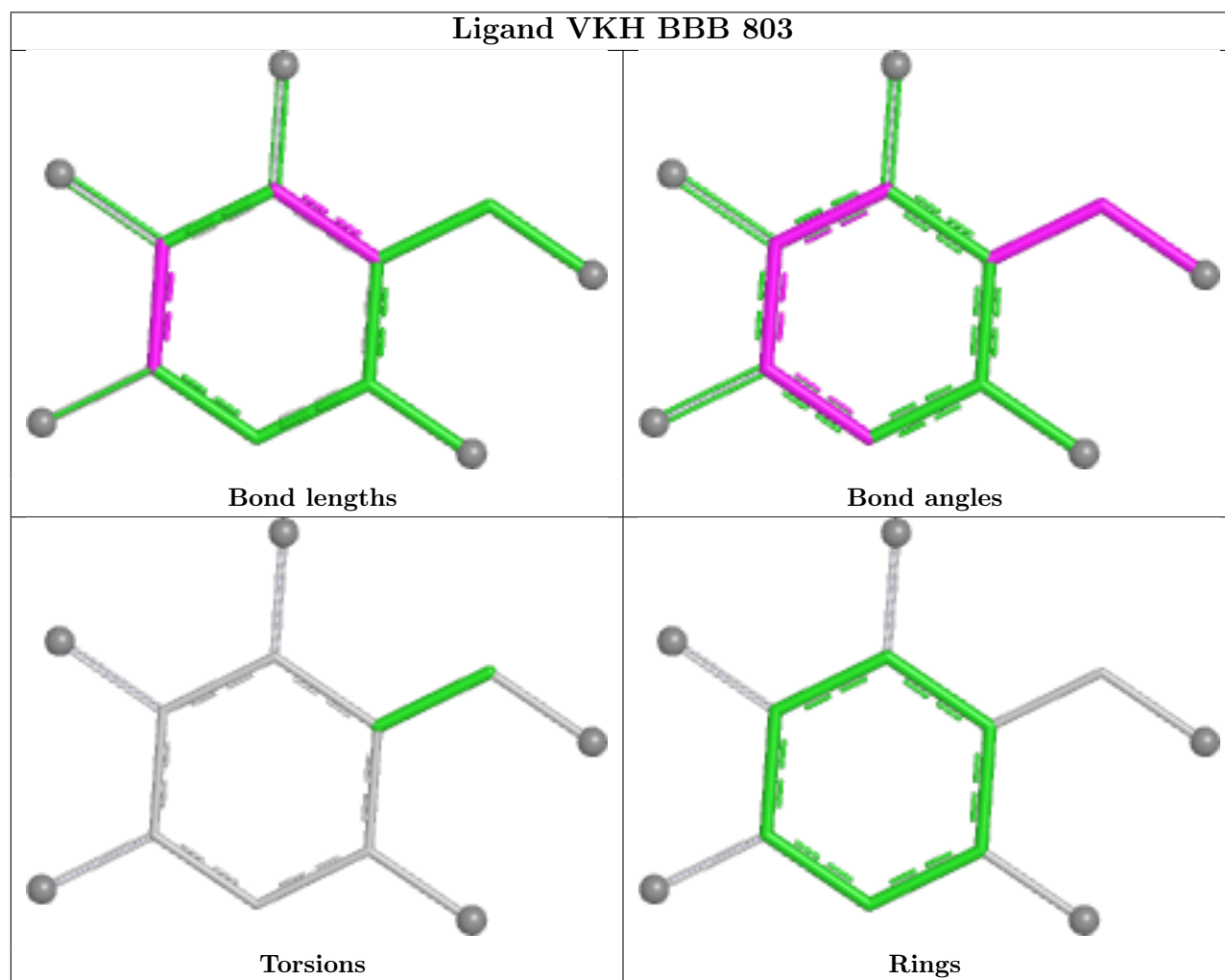
There are no ring outliers.

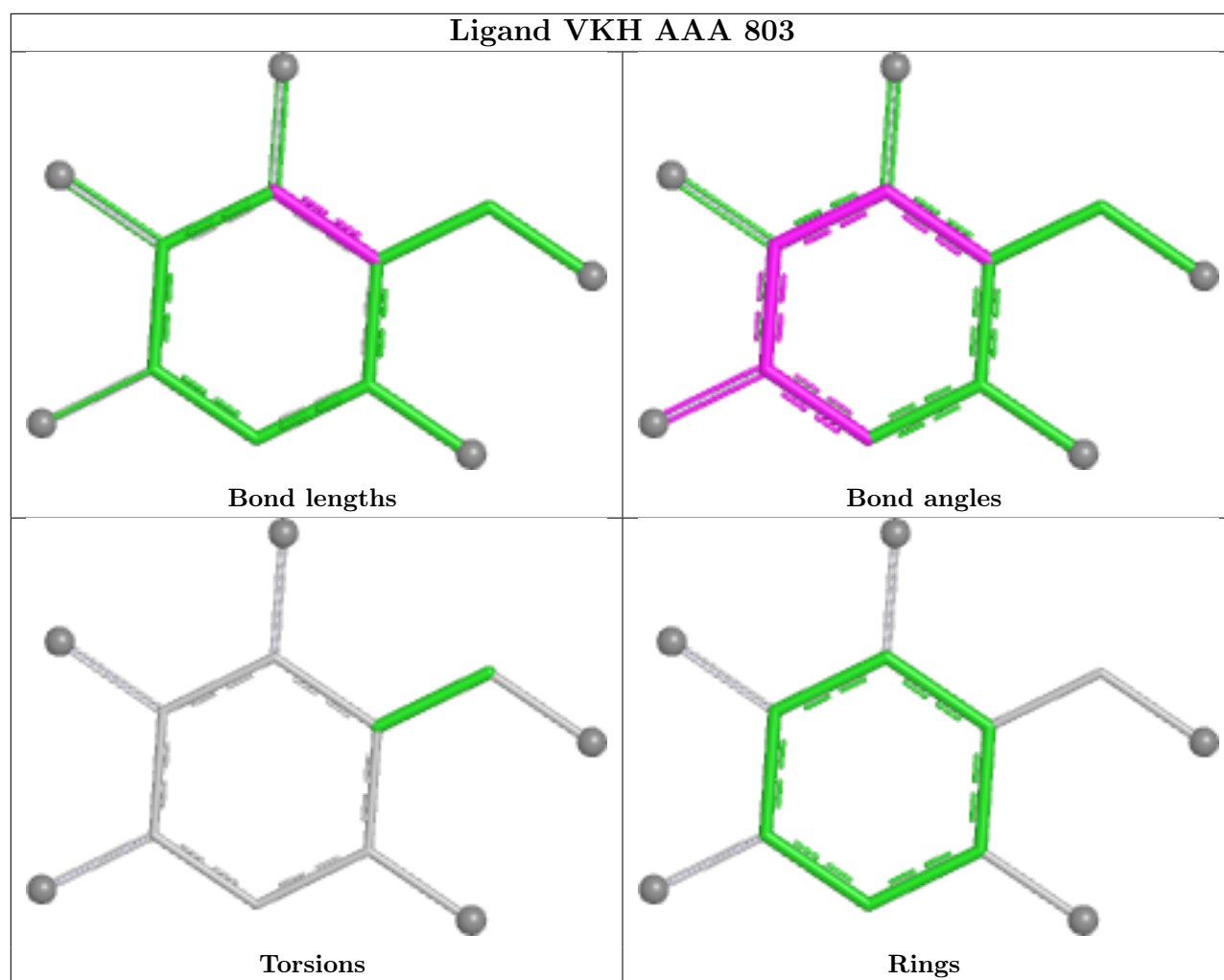
8 monomers are involved in 12 short contacts:

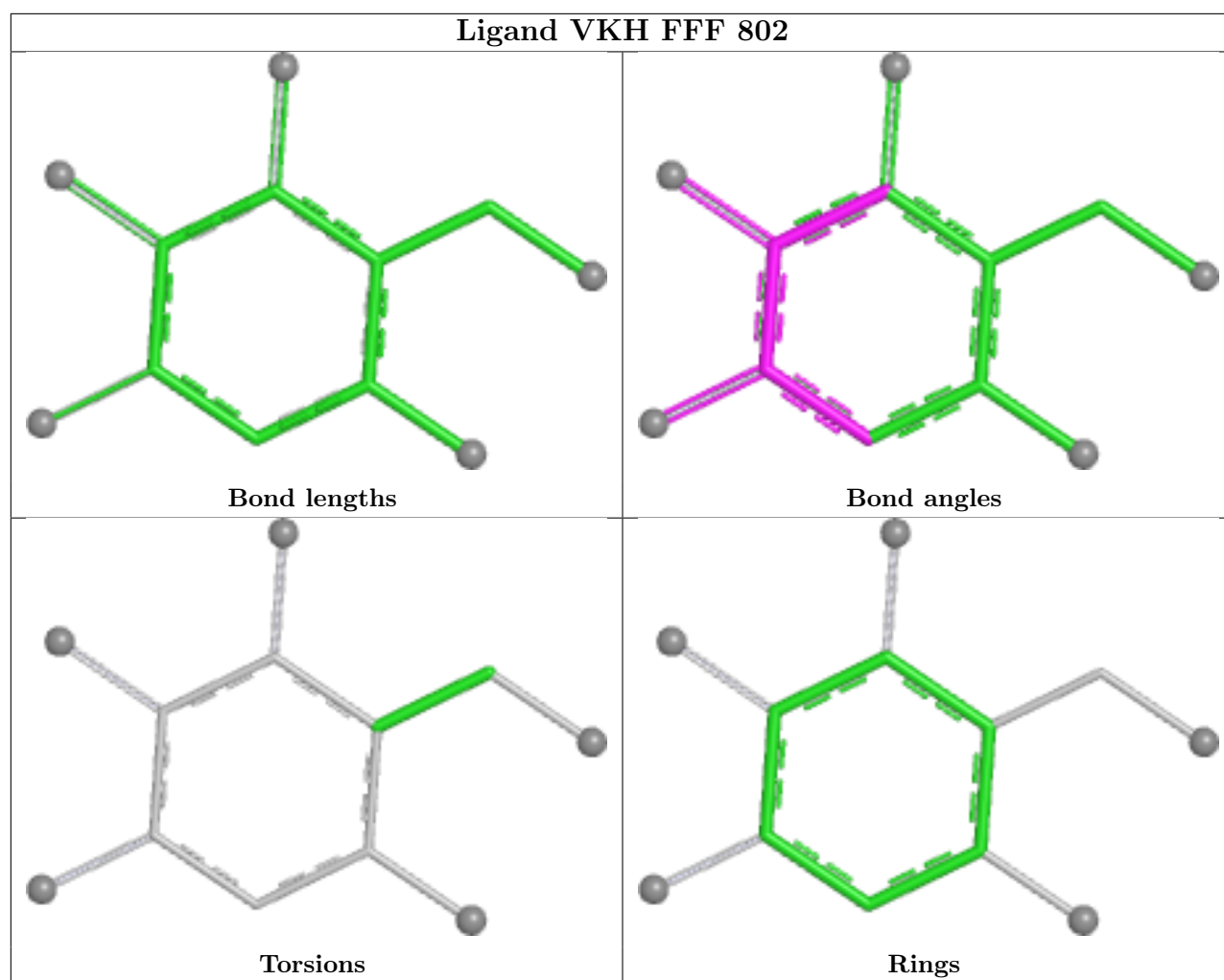
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	CCC	802	EDO	3	0
3	BBB	803	VKH	1	0
2	FFF	801	EDO	1	0
3	DDD	804	VKH	1	0
2	BBB	802	EDO	1	0
3	EEE	803	VKH	1	0
2	DDD	803	EDO	3	0
2	CCC	804	EDO	1	0

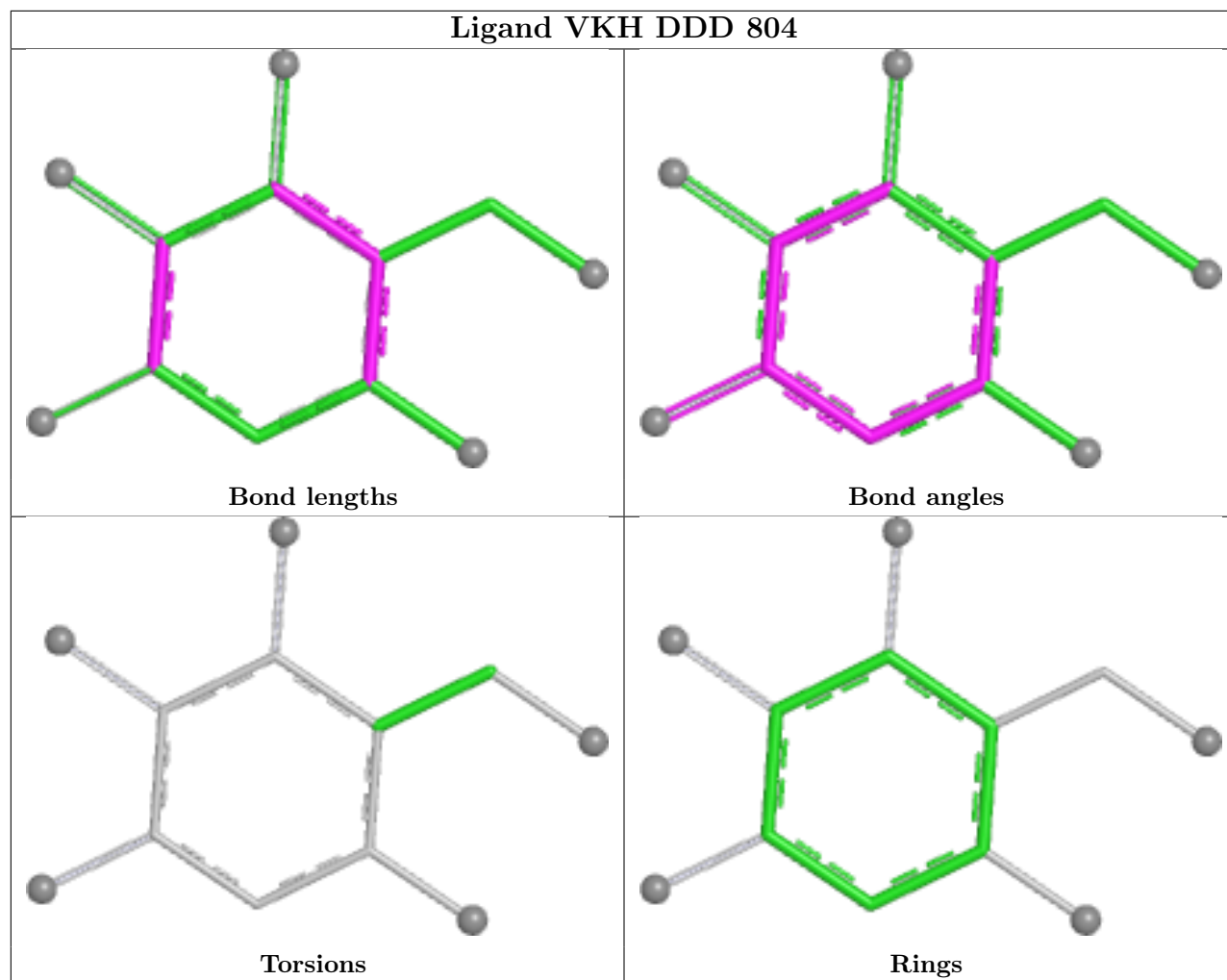
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

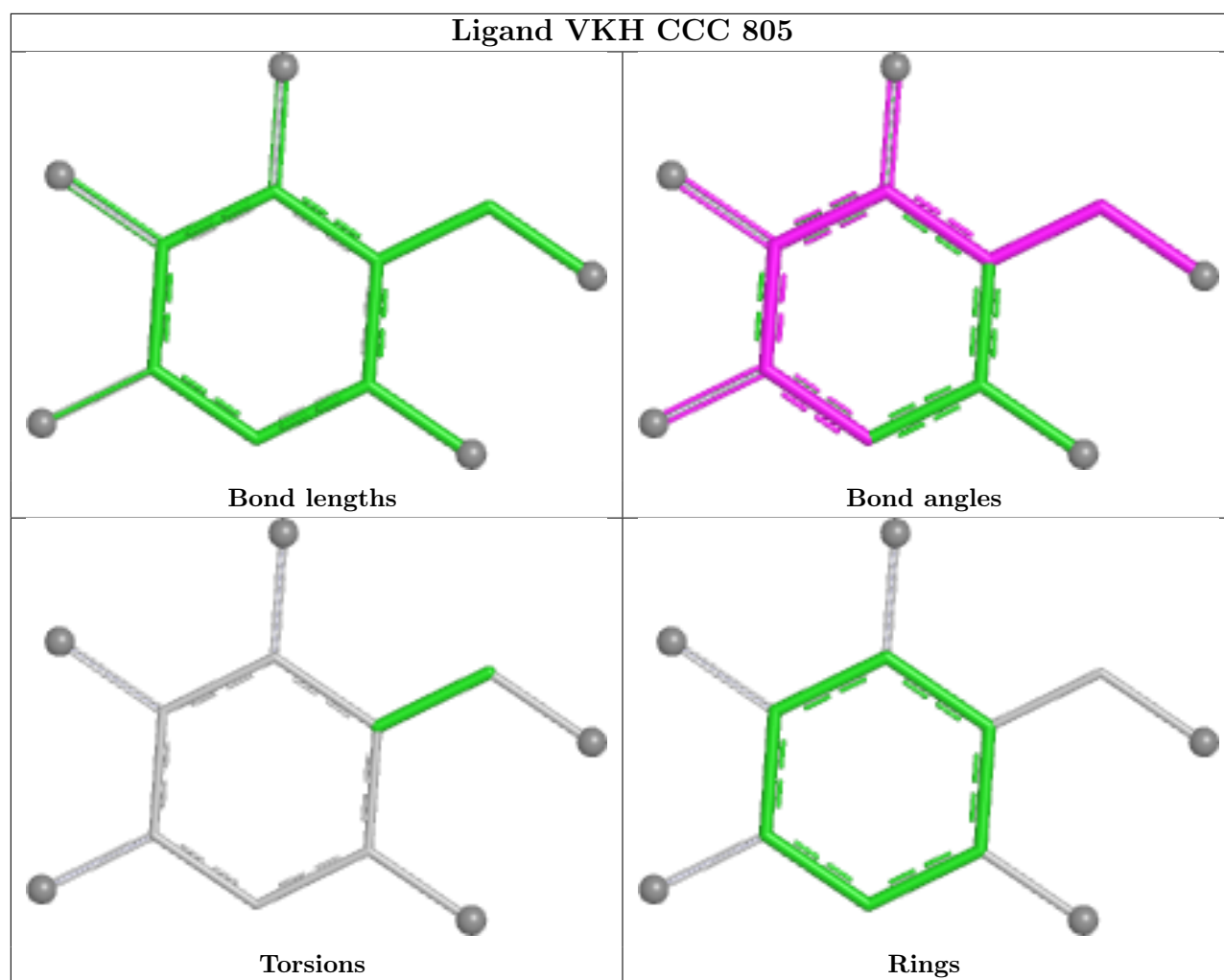
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

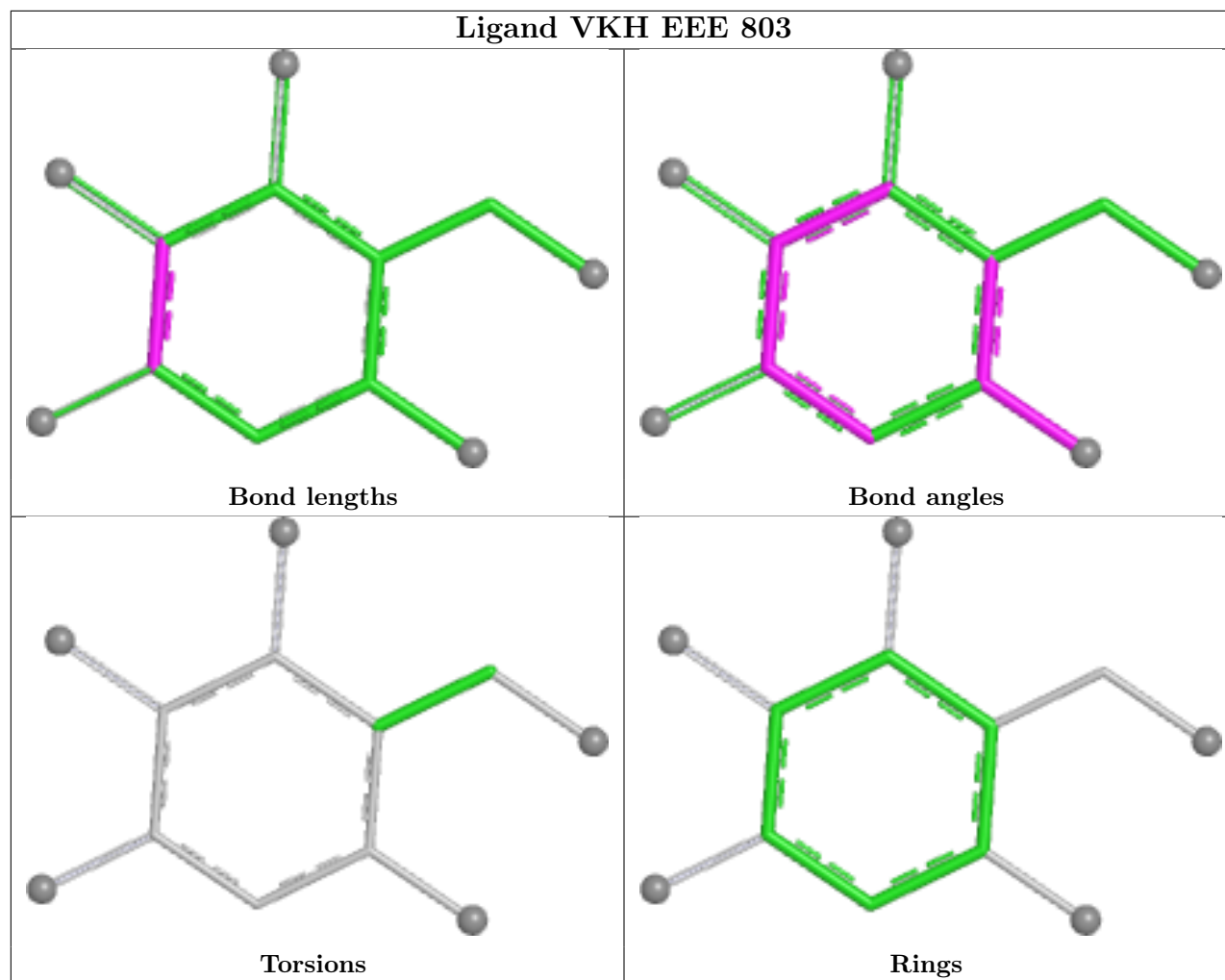












5.7 Other polymers [i](#)

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	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

All (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
1	AAA	26	LEU	4.8
1	AAA	86	GLY	4.7
1	AAA	455	ASP	4.6
1	DDD	534	TYR	4.5
1	EEE	518	TYR	4.5
1	AAA	139	ILE	4.4
1	EEE	520	ILE	4.1
1	FFF	373	ILE	4.0
1	DDD	465	ALA	3.9
1	AAA	111	LEU	3.9
1	AAA	41	PHE	3.8
1	AAA	155	TRP	3.8
1	AAA	412	GLY	3.8
1	EEE	43	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	DDD	484	LEU	3.8
1	CCC	127	HIS	3.7
1	AAA	529	PHE	3.7
1	DDD	31	ALA	3.7
1	AAA	165	ASN	3.6
1	AAA	166	LEU	3.6
1	FFF	30	PRO	3.6
1	DDD	457	VAL	3.6
1	BBB	529	PHE	3.6
1	CCC	166	LEU	3.6
1	FFF	166	LEU	3.6
1	AAA	665	ALA	3.6
1	DDD	649	LYS	3.5
1	AAA	99	LEU	3.5
1	DDD	558	GLY	3.5
1	BBB	682	ASN	3.5
1	DDD	291	LEU	3.4
1	CCC	163	THR	3.4
1	DDD	436	LEU	3.4
1	CCC	518	TYR	3.3
1	AAA	84	PRO	3.3
1	DDD	410	LEU	3.3
1	DDD	337	SER	3.3
1	DDD	30	PRO	3.2
1	FFF	120	VAL	3.2
1	AAA	88	TYR	3.2
1	DDD	561	ILE	3.2
1	AAA	411	ASN	3.2
1	FFF	31	ALA	3.2
1	EEE	545	ILE	3.2
1	AAA	30	PRO	3.1
1	BBB	520	ILE	3.1
1	AAA	29	GLY	3.1
1	AAA	146	PHE	3.1
1	EEE	107	VAL	3.1
1	FFF	431	LEU	3.1
1	AAA	158	ILE	3.1
1	EEE	516	ILE	3.1
1	FFF	680	TRP	3.0
1	AAA	127	HIS	3.0
1	EEE	120	VAL	3.0
1	AAA	284	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	DDD	681	LYS	3.0
1	DDD	432	SER	3.0
1	CCC	142	VAL	3.0
1	EEE	411	ASN	3.0
1	FFF	256	GLY	3.0
1	CCC	562	ALA	2.9
1	EEE	665	ALA	2.9
1	AAA	143	VAL	2.9
1	AAA	97	PHE	2.9
1	BBB	86	GLY	2.9
1	AAA	40	PRO	2.9
1	DDD	326	PHE	2.9
1	DDD	682	ASN	2.9
1	AAA	31	ALA	2.9
1	CCC	92	LEU	2.8
1	DDD	611	PHE	2.8
1	CCC	123	PHE	2.8
1	DDD	29	GLY	2.8
1	CCC	164	PRO	2.8
1	BBB	186	PHE	2.8
1	DDD	427	TYR	2.8
1	DDD	518	TYR	2.8
1	FFF	412	GLY	2.8
1	EEE	534	TYR	2.8
1	DDD	430	ALA	2.8
1	DDD	563	CYS	2.8
1	AAA	32	GLU	2.8
1	FFF	63	LEU	2.8
1	DDD	284	ILE	2.8
1	EEE	663	SER	2.7
1	BBB	532	ASP	2.7
1	AAA	627	GLY	2.7
1	EEE	31	ALA	2.7
1	CCC	120	VAL	2.7
1	CCC	168	PHE	2.7
1	AAA	157	LEU	2.7
1	AAA	410	LEU	2.7
1	BBB	84	PRO	2.7
1	AAA	458	ILE	2.7
1	AAA	681	LYS	2.7
1	CCC	440	PHE	2.7
1	DDD	537	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	EEE	427	TYR	2.7
1	EEE	412	GLY	2.7
1	DDD	541	TRP	2.7
1	DDD	298	LEU	2.6
1	CCC	682	ASN	2.6
1	BBB	666	ASN	2.6
1	EEE	164	PRO	2.6
1	AAA	501	VAL	2.6
1	FFF	127	HIS	2.6
1	BBB	410	LEU	2.6
1	EEE	88	TYR	2.6
1	AAA	518	TYR	2.6
1	AAA	408	GLY	2.6
1	FFF	411	ASN	2.6
1	AAA	340	ALA	2.6
1	DDD	255	LEU	2.6
1	DDD	434	THR	2.5
1	DDD	486	ALA	2.5
1	EEE	385	THR	2.5
1	DDD	609	PRO	2.5
1	BBB	164	PRO	2.5
1	BBB	171	PRO	2.5
1	AAA	168	PHE	2.5
1	DDD	446	PHE	2.5
1	FFF	654	ILE	2.5
1	DDD	628	THR	2.5
1	BBB	166	LEU	2.5
1	AAA	117	PHE	2.5
1	CCC	627	GLY	2.5
1	DDD	597	VAL	2.5
1	CCC	84	PRO	2.5
1	FFF	668	LEU	2.5
1	DDD	408	GLY	2.5
1	EEE	680	TRP	2.5
1	DDD	572	VAL	2.4
1	FFF	633	ILE	2.5
1	AAA	229	LEU	2.4
1	DDD	127	HIS	2.4
1	DDD	653	PHE	2.4
1	CCC	172	PHE	2.4
1	FFF	533	ASN	2.4
1	EEE	91	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	CCC	197	LEU	2.4
1	EEE	599	LEU	2.4
1	AAA	256	GLY	2.4
1	BBB	61	PHE	2.4
1	AAA	107	VAL	2.4
1	DDD	643	VAL	2.4
1	DDD	645	ILE	2.4
1	BBB	319	ILE	2.4
1	EEE	34	ILE	2.4
1	EEE	643	VAL	2.4
1	FFF	187	SER	2.4
1	AAA	630	TYR	2.4
1	EEE	430	ALA	2.4
1	DDD	186	PHE	2.4
1	DDD	573	PHE	2.4
1	DDD	318	ILE	2.4
1	BBB	324	ILE	2.4
1	EEE	99	LEU	2.3
1	FFF	627	GLY	2.3
1	AAA	123	PHE	2.3
1	DDD	440	PHE	2.3
1	FFF	651	LYS	2.3
1	FFF	653	PHE	2.3
1	AAA	677	ILE	2.3
1	EEE	292	PRO	2.3
1	DDD	412	GLY	2.3
1	DDD	448	PHE	2.3
1	CCC	90	PHE	2.3
1	AAA	561	ILE	2.3
1	EEE	318	ILE	2.3
1	AAA	71	THR	2.3
1	CCC	226	GLN	2.3
1	BBB	576	PRO	2.3
1	EEE	84	PRO	2.3
1	AAA	147	SER	2.3
1	EEE	186	PHE	2.3
1	EEE	48	ILE	2.3
1	FFF	626	ASN	2.3
1	FFF	665	ALA	2.3
1	DDD	166	LEU	2.3
1	DDD	527	LEU	2.3
1	DDD	630	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	BBB	518	TYR	2.3
1	FFF	388	SER	2.2
1	AAA	177	PHE	2.2
1	CCC	653	PHE	2.2
1	DDD	443	ILE	2.2
1	BBB	83	THR	2.2
1	FFF	607	ASP	2.2
1	FFF	121	GLY	2.2
1	AAA	436	LEU	2.2
1	AAA	446	PHE	2.2
1	CCC	182	LYS	2.2
1	EEE	87	THR	2.2
1	DDD	501	VAL	2.2
1	BBB	412	GLY	2.2
1	CCC	32	GLU	2.2
1	FFF	657	ALA	2.2
1	CCC	436	LEU	2.2
1	BBB	599	LEU	2.2
1	AAA	215	TRP	2.2
1	DDD	36	LYS	2.2
1	AAA	68	ASN	2.2
1	EEE	395	ASN	2.2
1	AAA	172	PHE	2.2
1	BBB	448	PHE	2.2
1	EEE	74	ILE	2.2
1	DDD	107	VAL	2.2
1	BBB	430	ALA	2.2
1	EEE	281	ALA	2.2
1	EEE	127	HIS	2.2
1	CCC	431	LEU	2.2
1	FFF	64	LEU	2.2
1	FFF	410	LEU	2.2
1	EEE	533	ASN	2.2
1	AAA	323	TRP	2.2
1	FFF	619	MET	2.2
1	BBB	664	THR	2.2
1	DDD	199	PHE	2.1
1	DDD	589	PHE	2.1
1	BBB	168	PHE	2.1
1	BBB	470	VAL	2.1
1	AAA	294	LEU	2.1
1	EEE	393	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	CCC	452	ASP	2.1
1	EEE	163	THR	2.1
1	EEE	653	PHE	2.1
1	EEE	662	HIS	2.1
1	CCC	276	ALA	2.1
1	CCC	665	ALA	2.1
1	EEE	330	ALA	2.1
1	EEE	111	LEU	2.1
1	FFF	682	ASN	2.1
1	DDD	164	PRO	2.1
1	DDD	634	ILE	2.1
1	FFF	670	ILE	2.1
1	EEE	86	GLY	2.1
1	DDD	41	PHE	2.1
1	EEE	529	PHE	2.1
1	DDD	665	ALA	2.1
1	BBB	315	ALA	2.1
1	CCC	626	ASN	2.1
1	CCC	427	TYR	2.1
1	CCC	412	GLY	2.1
1	BBB	650	GLY	2.1
1	AAA	575	ILE	2.1
1	DDD	105	ILE	2.1
1	FFF	383	ILE	2.1
1	EEE	383	ILE	2.1
1	BBB	573	PHE	2.1
1	DDD	620	MET	2.0
1	AAA	64	LEU	2.0
1	EEE	489	LEU	2.0
1	AAA	296	THR	2.0
1	AAA	454	THR	2.0
1	AAA	534	TYR	2.0
1	DDD	435	GLY	2.0
1	FFF	518	TYR	2.0
1	CCC	369	ILE	2.0
1	EEE	324	ILE	2.0
1	AAA	42	VAL	2.0
1	AAA	112	PHE	2.0
1	CCC	646	VAL	2.0
1	EEE	265	PHE	2.0
1	AAA	327	ALA	2.0
1	DDD	574	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	EEE	350	TRP	2.0
1	DDD	626	ASN	2.0
1	AAA	152	LEU	2.0
1	DDD	431	LEU	2.0
1	EEE	510	LEU	2.0
1	BBB	87	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(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

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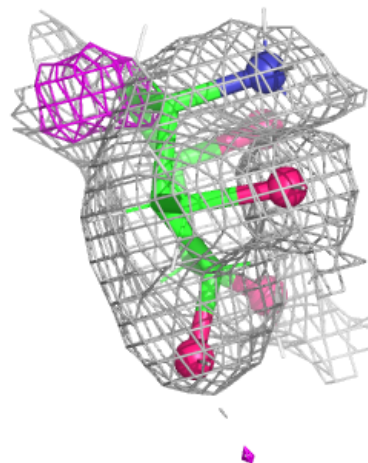
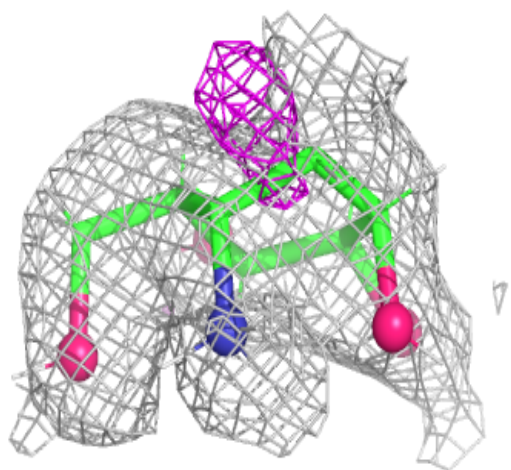
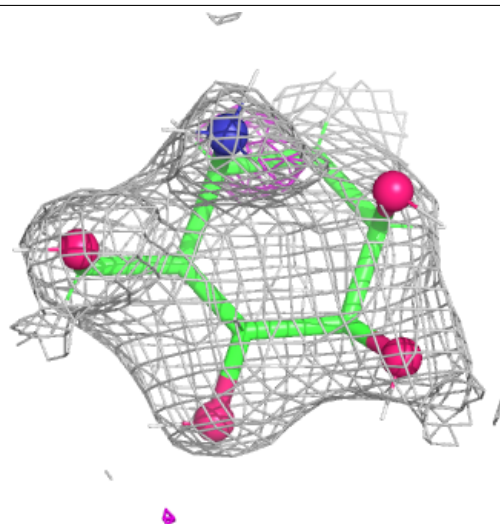
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	AAA	804	1/1	0.95	0.07	38,38,38,38	0
2	EDO	EEE	802	4/4	0.96	0.10	46,49,54,58	1
2	EDO	EEE	801	4/4	0.96	0.10	47,53,57,58	1
2	EDO	CCC	801	4/4	0.97	0.07	41,45,46,46	1
4	CL	BBB	804	1/1	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.

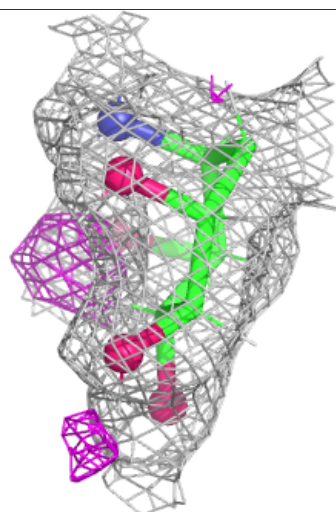
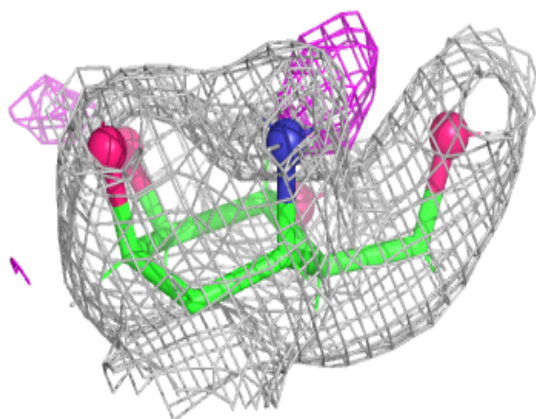
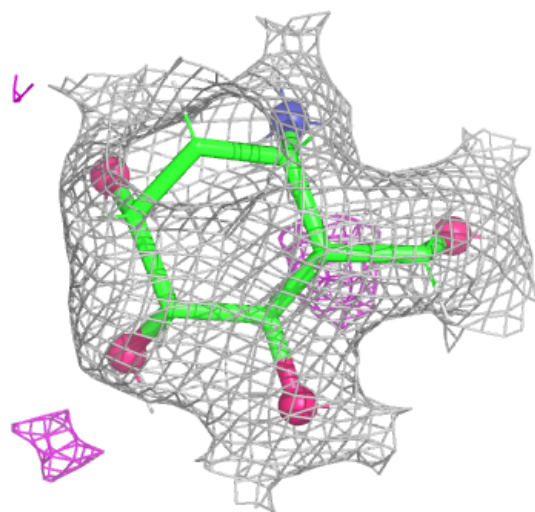
Electron density around VKH AAA 803:

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



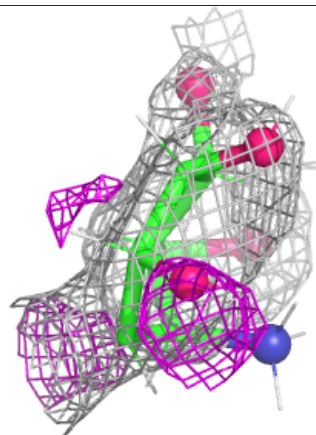
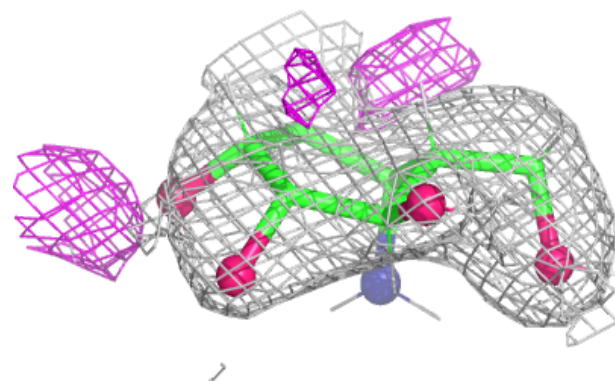
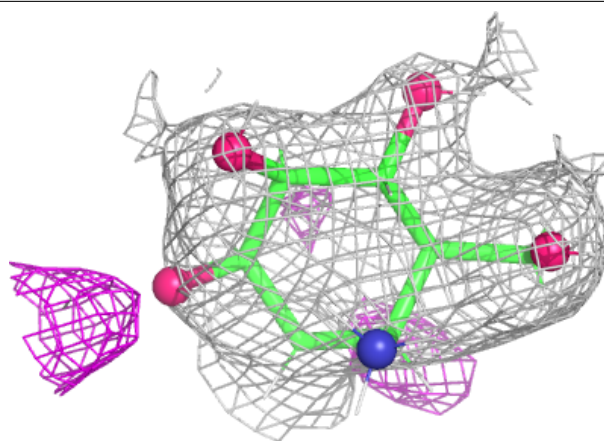
Electron density around VKH CCC 805:

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



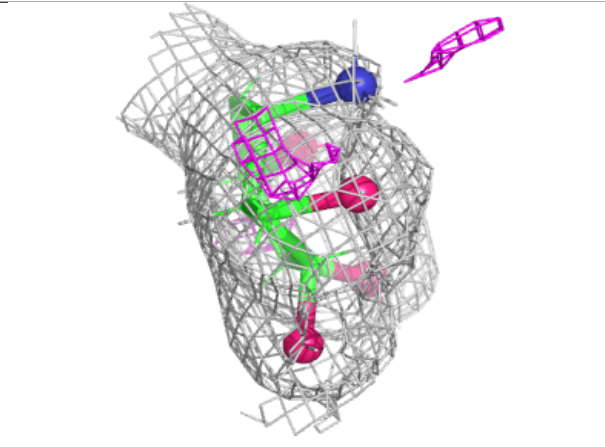
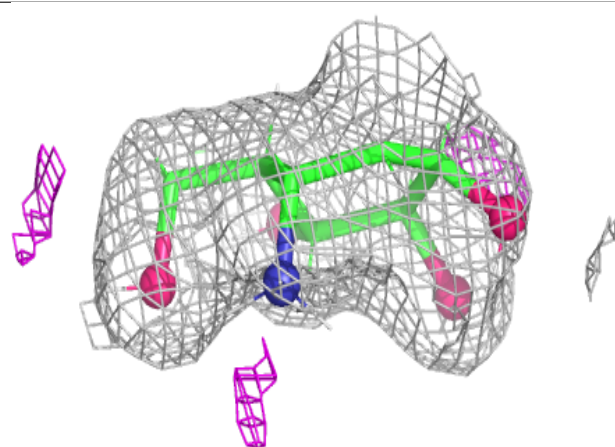
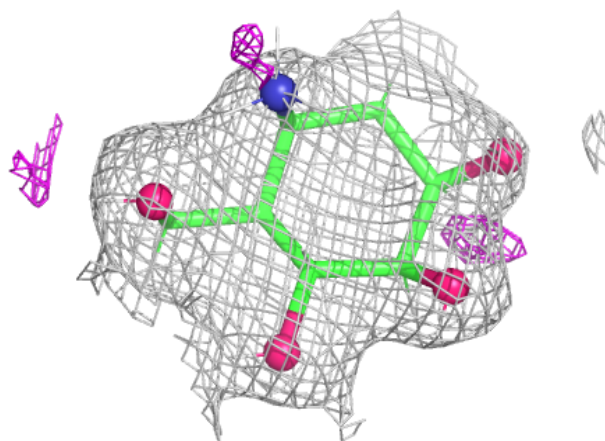
Electron density around VKH DDD 804:

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



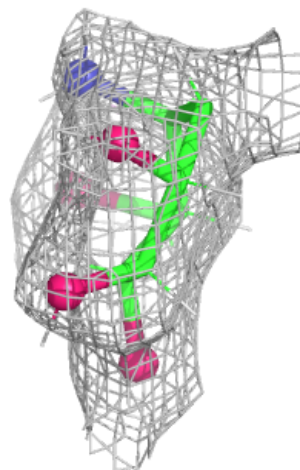
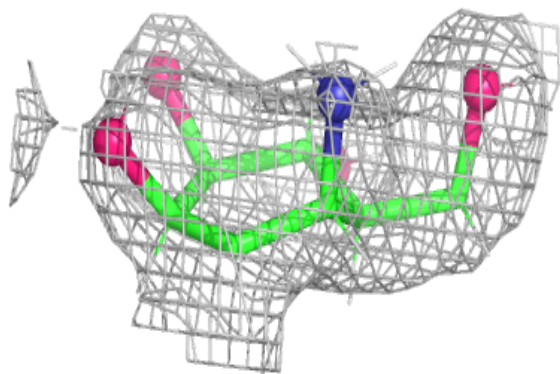
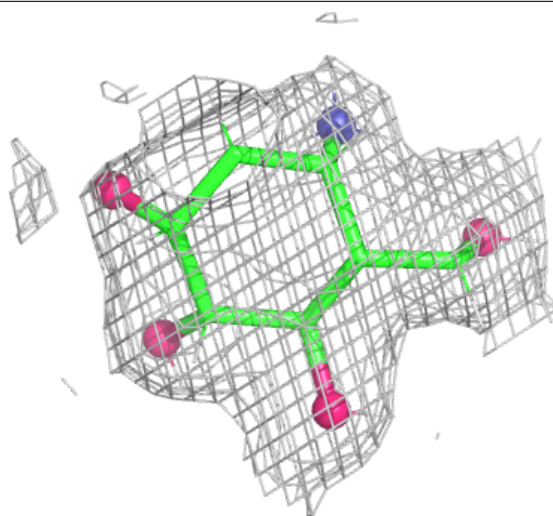
Electron density around VKH BBB 803:

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



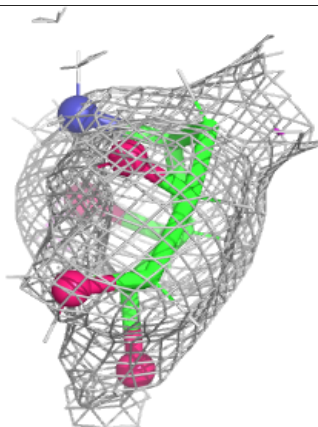
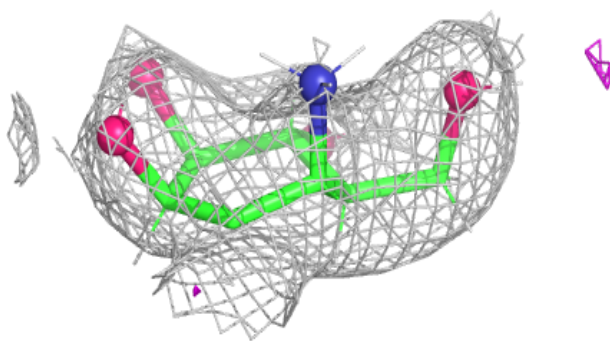
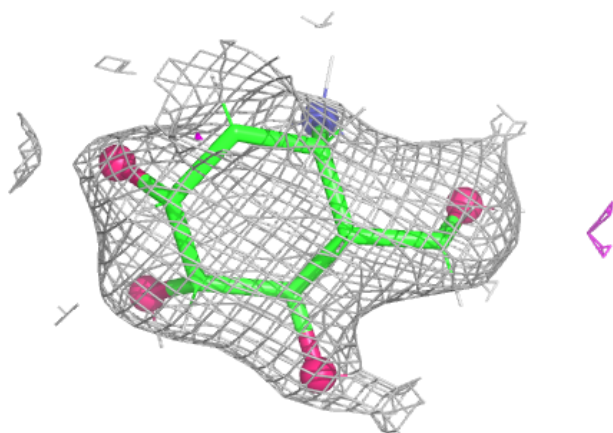
Electron density around VKH EEE 803:

$2mF_o-DF_c$ (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.