Full wwPDB X-ray Structure Validation Report (i)

Jan 20, 2024 – 08:27 pm GMT

PDB ID	:	7OMI
Title	:	Bs164 in complex with mannocyclophellitol epoxide
Authors	:	Armstrong, Z.; Mcgregor, N.; Davies, G.
Deposited on	:	2021-05-24
Resolution	:	1.76 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 (i) 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 (i)) were used in the production of this report:

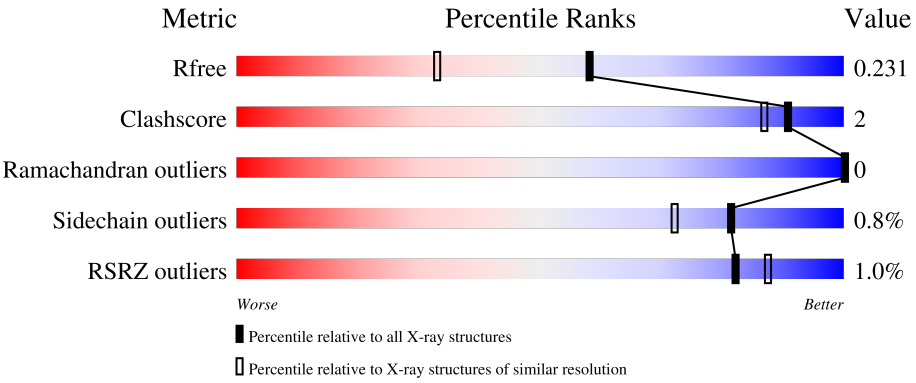
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.76 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 <=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	93% 5%
1	BBB	674	2% 93%
1	CCC	674	91% 6%
1	DDD	674	92% 5%
1	EEE	674	91% 5%

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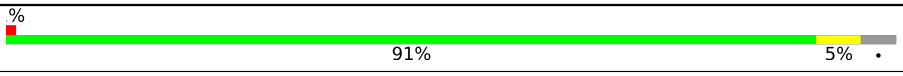
Mol	Chain	Length	Quality of chain
1	FFF	674	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 65224 atoms, of which 31210 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	661	Total	C	H	N	O	S	289	1	0
			10514	3430	5200	879	986	19			
1	BBB	658	Total	C	H	N	O	S	286	0	0
			10467	3416	5180	874	978	19			
1	CCC	651	Total	C	H	N	O	S	286	1	0
			10383	3385	5136	871	972	19			
1	DDD	652	Total	C	H	N	O	S	286	0	0
			10369	3382	5128	868	972	19			
1	EEE	652	Total	C	H	N	O	S	284	1	0
			10393	3389	5143	869	973	19			
1	FFF	650	Total	C	H	N	O	S	280	0	0
			10349	3376	5123	864	967	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
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
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
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
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

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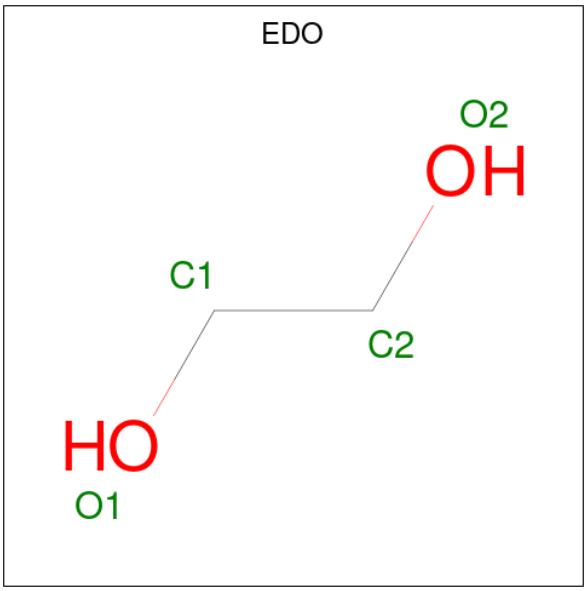
Chain	Residue	Modelled	Actual	Comment	Reference
EEE	23	LEU	-	expression tag	UNP I9SUA3
EEE	24	GLU	-	expression tag	UNP I9SUA3
EEE	25	VAL	-	expression tag	UNP I9SUA3
EEE	26	LEU	-	expression tag	UNP I9SUA3
EEE	27	PHE	-	expression tag	UNP I9SUA3
EEE	28	GLN	-	expression tag	UNP I9SUA3
EEE	29	GLY	-	expression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

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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	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	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	BBB	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	CCC	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		

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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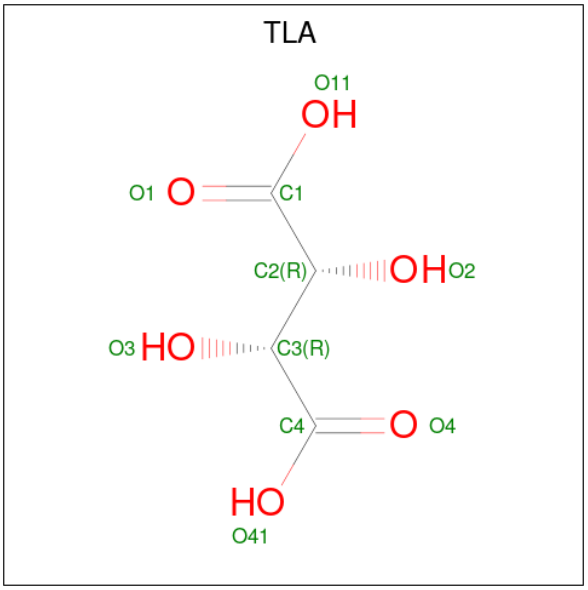
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	EEE	1	Total Cl 1 1	0	0
3	FFF	1	Total Cl 1 1	0	0

- Molecule 4 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C H O 14 4 4 6	2	0
4	AAA	1	Total C H O 14 4 4 6	2	0
4	BBB	1	Total C H O 14 4 4 6	2	0
4	BBB	1	Total C H O 14 4 4 6	2	0
4	CCC	1	Total C H O 14 4 4 6	2	0
4	CCC	1	Total C H O 14 4 4 6	2	0
4	DDD	1	Total C H O 14 4 4 6	2	0
4	DDD	1	Total C H O 14 4 4 6	2	0
4	EEE	1	Total C H O 14 4 4 6	2	0

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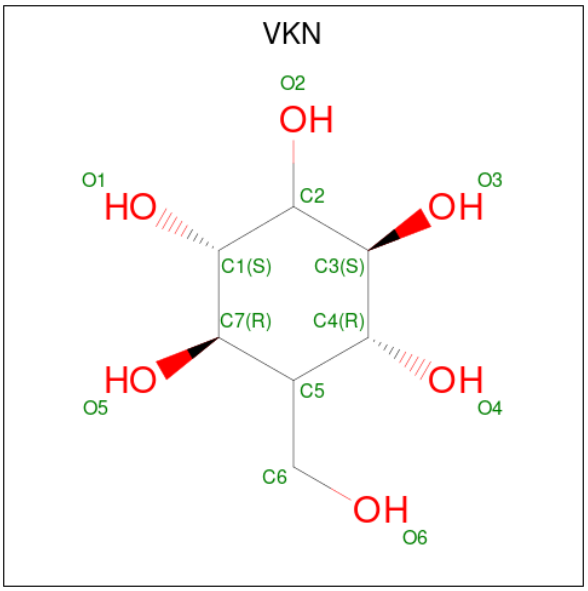
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	EEE	1	Total C H O 14 4 4 6	2	0
4	FFF	1	Total C H O 14 4 4 6	2	0
4	FFF	1	Total C H O 14 4 4 6	2	0

- Molecule 5 is (1R,2S,4S,5R)-6-(hydroxymethyl)cyclohexane-1,2,3,4,5-pentol (three-letter code: VKN) (formula: $C_7H_{14}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C H O 25 7 13 5	4	0
5	BBB	1	Total C H O 25 7 13 5	4	0
5	CCC	1	Total C H O 25 7 13 5	4	0
5	DDD	1	Total C H O 25 7 13 5	4	0
5	EEE	1	Total C H O 25 7 13 5	4	0
5	FFF	1	Total C H O 25 7 13 5	4	0

- Molecule 6 is water.

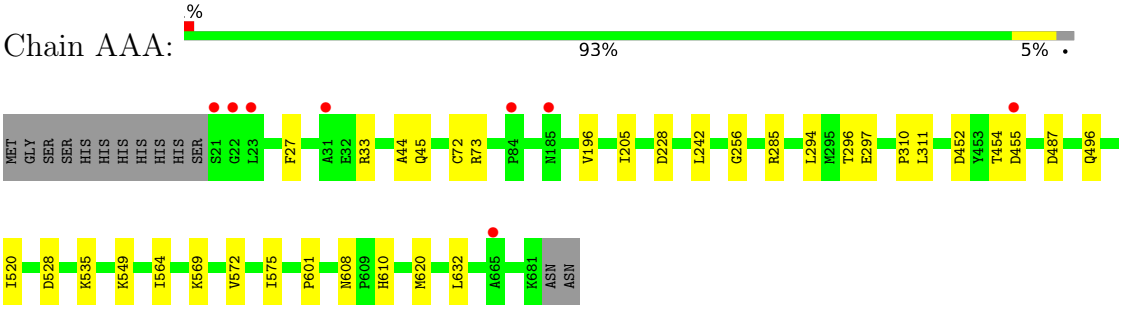
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	307	Total O 307 307	0	0
6	BBB	322	Total O 322 322	0	0
6	CCC	399	Total O 399 399	0	0
6	DDD	415	Total O 415 415	0	0
6	EEE	360	Total O 360 360	0	0
6	FFF	332	Total O 332 332	0	0

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.

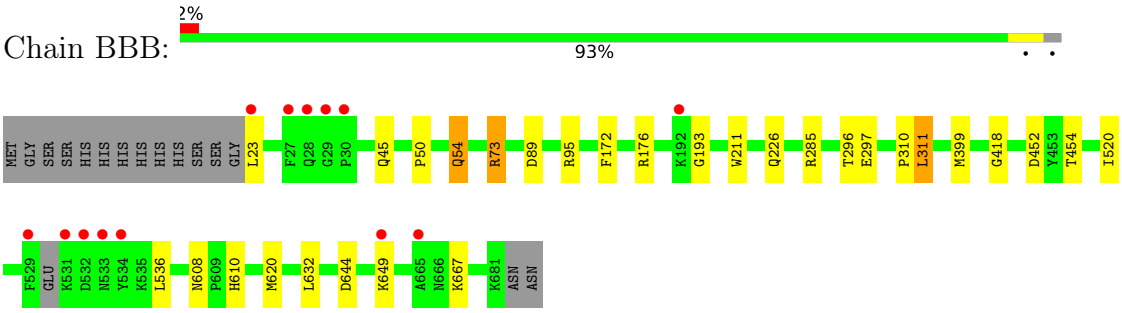
• Molecule 1: Glyco_hydro_42M domain-containing protein

Chain AAA:



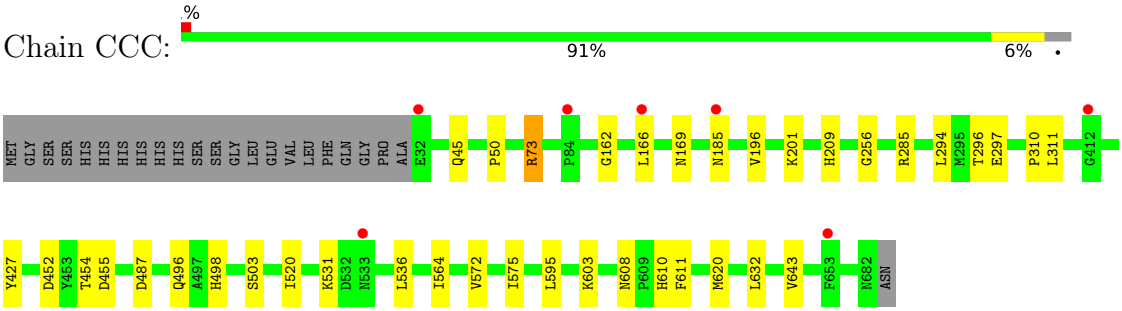
• Molecule 1: Glyco_hydro_42M domain-containing protein

Chain BBB:



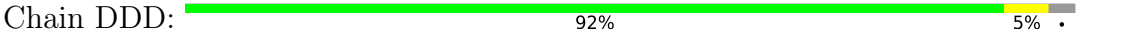
• Molecule 1: Glyco_hydro_42M domain-containing protein

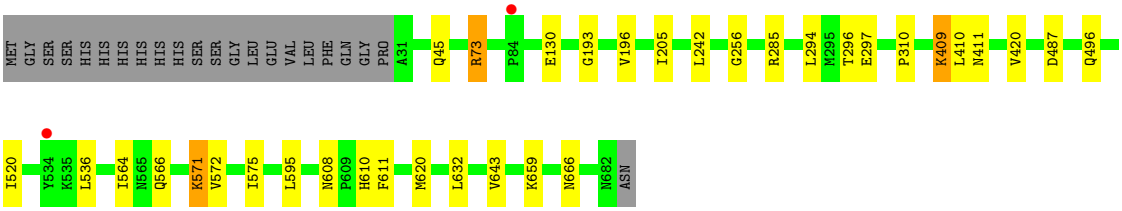
Chain CCC:



• Molecule 1: Glyco_hydro_42M domain-containing protein

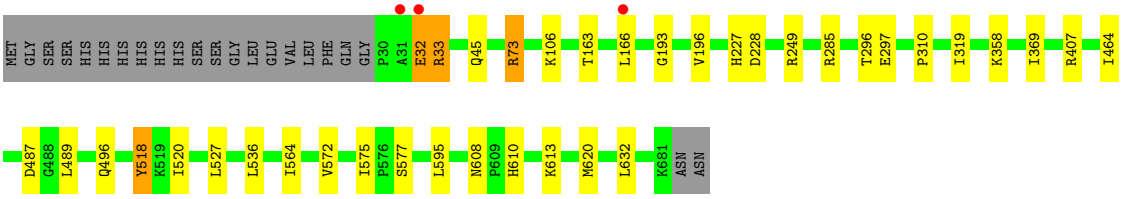
Chain DDD:





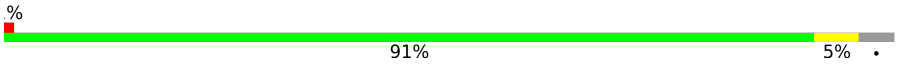
• Molecule 1: Glyco_hydro_42M domain-containing protein

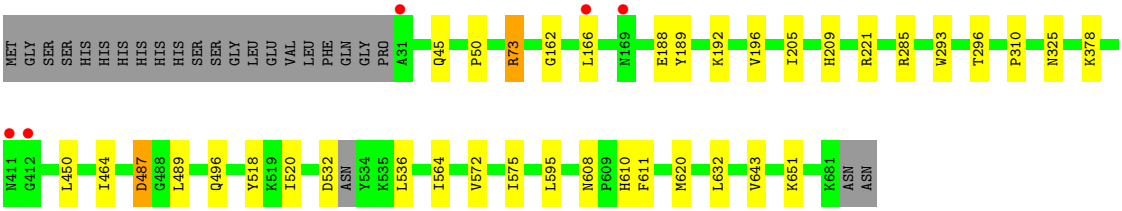
Chain EEE:



• Molecule 1: Glyco_hydro_42M domain-containing protein

Chain FFF:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	69.45Å 104.43Å 170.78Å 92.29° 97.35° 106.55°	Depositor
Resolution (Å)	65.87 – 1.76 65.87 – 1.76	Depositor EDS
% Data completeness (in resolution range)	97.2 (65.87-1.76) 97.2 (65.87-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.231 , 0.261 0.204 , 0.231	Depositor DCC
R_{free} test set	22062 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 55.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	65224	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.70	1/5460 (0.0%)	0.77	2/7393 (0.0%)
1	BBB	0.69	2/5432 (0.0%)	0.77	3/7354 (0.0%)
1	CCC	0.70	1/5391 (0.0%)	0.78	5/7298 (0.1%)
1	DDD	0.70	1/5385 (0.0%)	0.77	4/7291 (0.1%)
1	EEE	0.69	2/5395 (0.0%)	0.78	5/7303 (0.1%)
1	FFF	0.68	0/5369	0.76	4/7266 (0.1%)
All	All	0.70	7/32432 (0.0%)	0.77	23/43905 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	EEE	297	GLU	CD-OE1	8.17	1.34	1.25
1	AAA	297	GLU	CD-OE1	7.97	1.34	1.25
1	BBB	297	GLU	CD-OE2	-6.46	1.18	1.25
1	CCC	297	GLU	CD-OE1	6.39	1.32	1.25
1	DDD	297	GLU	CD-OE1	6.24	1.32	1.25
1	BBB	297	GLU	CD-OE1	6.06	1.32	1.25
1	EEE	297	GLU	CD-OE2	-5.01	1.20	1.25

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	EEE	285	ARG	NE-CZ-NH2	-8.59	116.01	120.30
1	CCC	73	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	FFF	73	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	BBB	285	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	CCC	285	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	BBB	73	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	EEE	73	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	DDD	285	ARG	NE-CZ-NH2	-7.28	116.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	285	ARG	NE-CZ-NH2	-7.27	116.66	120.30
1	DDD	285	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	BBB	285	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	FFF	285	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	EEE	518	TYR	CB-CG-CD1	-7.02	116.79	121.00
1	AAA	285	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	FFF	285	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	DDD	73	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	EEE	285	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	CCC	285	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	EEE	518	TYR	CB-CG-CD2	5.70	124.42	121.00
1	FFF	73	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	CCC	427	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	DDD	666	ASN	CB-CA-C	5.18	120.76	110.40
1	CCC	73	ARG	NE-CZ-NH1	5.12	122.86	120.30

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	AAA	5314	5200	5178	20	2
1	BBB	5287	5180	5158	22	0
1	CCC	5247	5136	5114	19	0
1	DDD	5241	5128	5107	18	1
1	EEE	5250	5143	5124	23	1
1	FFF	5226	5123	5101	21	0
2	AAA	16	24	24	0	0
2	BBB	12	18	18	0	0
2	CCC	20	30	30	0	0
2	DDD	28	42	42	0	0
2	EEE	24	36	36	0	0
2	FFF	16	24	24	0	0
3	AAA	1	0	0	0	0
3	BBB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CCC	1	0	0	0	0
3	DDD	1	0	0	0	0
3	EEE	1	0	0	0	0
3	FFF	1	0	0	0	0
4	AAA	20	8	8	0	0
4	BBB	20	8	8	0	0
4	CCC	20	8	8	0	0
4	DDD	20	8	8	0	0
4	EEE	20	8	8	0	0
4	FFF	20	8	8	0	0
5	AAA	12	13	0	0	0
5	BBB	12	13	0	0	0
5	CCC	12	13	0	0	0
5	DDD	12	13	0	0	0
5	EEE	12	13	0	0	0
5	FFF	12	13	0	0	0
6	AAA	307	0	0	0	0
6	BBB	322	0	0	3	0
6	CCC	399	0	0	0	0
6	DDD	415	0	0	1	0
6	EEE	360	0	0	4	0
6	FFF	332	0	0	2	0
All	All	34014	31210	31004	109	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 2.

All (109) 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:FFF:221:ARG:HD2	6:FFF:1116:HOH:O	1.90	0.72
1:BBB:54:GLN:HG2	1:BBB:95:ARG:HD2	1.73	0.70
1:EEE:32:GLU:OE2	1:EEE:106:LYS:HD2	1.94	0.66
1:AAA:33:ARG:HD3	1:AAA:228:ASP:OD1	2.01	0.60
1:BBB:176:ARG:HD3	6:BBB:1076:HOH:O	2.02	0.59
1:BBB:310:PRO:HB2	1:EEE:520:ILE:HD13	1.83	0.59
1:AAA:310:PRO:HB2	1:CCC:520:ILE:HD13	1.83	0.59
1:BBB:644:ASP:CG	1:BBB:667:LYS:HD2	2.21	0.59
1:FFF:489:LEU:CD2	1:FFF:518:TYR:CZ	2.86	0.58
1:AAA:564:ILE:HD11	1:BBB:23:LEU:HD21	1.85	0.58
1:AAA:454:THR:O	1:AAA:455:ASP:OD1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:611:PHE:CE1	1:DDD:643:VAL:HG11	2.39	0.58
1:EEE:319:ILE:HD12	1:EEE:369:ILE:HD11	1.84	0.57
1:FFF:611:PHE:CE1	1:FFF:643:VAL:HG11	2.39	0.57
1:CCC:611:PHE:CE1	1:CCC:643:VAL:HG11	2.39	0.57
1:EEE:33:ARG:HD3	1:EEE:228:ASP:OD1	2.04	0.56
1:CCC:310:PRO:HB2	1:DDD:520:ILE:HD13	1.89	0.55
1:EEE:45:GLN:OE1	1:EEE:73:ARG:HD3	2.07	0.55
1:BBB:45:GLN:OE1	1:BBB:73:ARG:HD3	2.07	0.55
1:DDD:45:GLN:OE1	1:DDD:73:ARG:HD3	2.07	0.55
1:FFF:45:GLN:OE1	1:FFF:73:ARG:HD3	2.07	0.54
1:FFF:608:ASN:O	1:FFF:610:HIS:HD2	1.91	0.54
1:AAA:608:ASN:O	1:AAA:610:HIS:HD2	1.91	0.54
1:CCC:45:GLN:OE1	1:CCC:73:ARG:HD3	2.07	0.54
1:EEE:608:ASN:O	1:EEE:610:HIS:HD2	1.90	0.54
1:AAA:45:GLN:OE1	1:AAA:73:ARG:HD3	2.09	0.53
1:DDD:608:ASN:O	1:DDD:610:HIS:HD2	1.90	0.53
1:CCC:608:ASN:O	1:CCC:610:HIS:HD2	1.92	0.53
1:FFF:378:LYS:NZ	6:FFF:803:HOH:O	2.42	0.53
1:BBB:418:GLY:HA2	6:BBB:1079:HOH:O	2.09	0.52
1:BBB:89:ASP:OD2	1:DDD:659:LYS:HA	2.09	0.52
1:EEE:310:PRO:HB2	1:FFF:520:ILE:HD13	1.92	0.52
1:BBB:608:ASN:O	1:BBB:610:HIS:HD2	1.92	0.51
1:BBB:226:GLN:NE2	1:BBB:226:GLN:HA	2.26	0.51
1:BBB:520:ILE:HD13	1:FFF:310:PRO:HB2	1.94	0.50
1:AAA:620:MET:HA	1:AAA:632:LEU:O	2.12	0.49
1:EEE:163:THR:HG23	1:EEE:166:LEU:HD13	1.95	0.49
1:EEE:358:LYS:HD2	6:EEE:827:HOH:O	2.13	0.49
1:EEE:536:LEU:HD11	1:EEE:595:LEU:HD22	1.93	0.49
1:FFF:620:MET:HA	1:FFF:632:LEU:O	2.13	0.48
1:DDD:536:LEU:HD11	1:DDD:595:LEU:HD22	1.96	0.48
1:AAA:520:ILE:HD13	1:DDD:310:PRO:HB2	1.96	0.48
1:DDD:620:MET:HA	1:DDD:632:LEU:O	2.14	0.48
1:BBB:620:MET:HA	1:BBB:632:LEU:O	2.13	0.48
1:BBB:644:ASP:OD1	1:BBB:667:LYS:HD2	2.12	0.48
1:CCC:620:MET:HA	1:CCC:632:LEU:O	2.14	0.48
1:EEE:620:MET:HA	1:EEE:632:LEU:O	2.14	0.48
1:EEE:227:HIS:NE2	6:EEE:802:HOH:O	2.36	0.47
1:AAA:452:ASP:OD1	1:AAA:454:THR:OG1	2.23	0.47
1:EEE:166:LEU:H	1:EEE:166:LEU:HD22	1.78	0.47
1:EEE:407:ARG:NH2	6:EEE:810:HOH:O	2.48	0.47
1:BBB:50:PRO:HB2	1:EEE:193:GLY:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:166:LEU:HD22	1:CCC:166:LEU:N	2.30	0.46
1:FFF:464:ILE:HG22	1:FFF:489:LEU:HB2	1.98	0.46
1:EEE:464:ILE:HG22	1:EEE:489:LEU:HB2	1.97	0.46
1:EEE:166:LEU:HD22	1:EEE:166:LEU:N	2.31	0.46
1:FFF:536:LEU:HD11	1:FFF:595:LEU:HD22	1.97	0.45
1:BBB:193:GLY:O	1:FFF:50:PRO:HB2	2.18	0.44
1:DDD:566:GLN:HE22	1:DDD:571:LYS:CE	2.29	0.44
1:EEE:518:TYR:OH	6:EEE:801:HOH:O	2.20	0.44
1:DDD:566:GLN:HE22	1:DDD:571:LYS:HE2	1.83	0.44
1:BBB:311:LEU:HA	1:EEE:520:ILE:CG2	2.49	0.43
1:AAA:487:ASP:HA	1:AAA:575:ILE:O	2.19	0.43
1:FFF:293:TRP:HH2	1:FFF:325:ASN:HD22	1.66	0.43
1:CCC:487:ASP:HA	1:CCC:575:ILE:O	2.19	0.43
1:CCC:50:PRO:HB2	1:DDD:193:GLY:O	2.19	0.43
1:BBB:176:ARG:NH2	1:BBB:211:TRP:CE2	2.87	0.42
1:FFF:192:LYS:HA	1:FFF:192:LYS:HE2	2.01	0.42
1:DDD:205:ILE:HG21	1:DDD:242:LEU:HD22	2.00	0.42
1:FFF:166:LEU:HD13	1:FFF:205:ILE:HD13	2.01	0.42
1:AAA:564:ILE:HD11	1:BBB:23:LEU:CD2	2.47	0.42
1:CCC:455:ASP:OD2	1:CCC:603:LYS:HD3	2.20	0.42
1:CCC:611:PHE:CD1	1:CCC:643:VAL:CG1	3.03	0.42
1:CCC:498:HIS:HE1	1:CCC:503:SER:OG	2.03	0.42
1:AAA:196:VAL:HB	1:AAA:496:GLN:HB3	2.01	0.42
1:DDD:487:ASP:HA	1:DDD:575:ILE:O	2.20	0.42
1:FFF:487:ASP:HA	1:FFF:575:ILE:O	2.20	0.42
1:AAA:528:ASP:OD1	1:AAA:535:LYS:HE3	2.20	0.41
1:CCC:564:ILE:HA	1:CCC:572:VAL:O	2.20	0.41
1:EEE:487:ASP:HA	1:EEE:575:ILE:O	2.19	0.41
1:CCC:162:GLY:HA2	1:CCC:209:HIS:NE2	2.36	0.41
1:FFF:564:ILE:HA	1:FFF:572:VAL:O	2.20	0.41
1:EEE:564:ILE:HA	1:EEE:572:VAL:O	2.20	0.41
1:FFF:196:VAL:HB	1:FFF:496:GLN:HB3	2.01	0.41
1:AAA:205:ILE:HG21	1:AAA:242:LEU:HD22	2.03	0.41
1:AAA:311:LEU:HA	1:CCC:520:ILE:CG2	2.51	0.41
1:AAA:256:GLY:HA2	1:AAA:294:LEU:O	2.20	0.41
1:AAA:455:ASP:OD1	1:AAA:455:ASP:C	2.59	0.41
1:DDD:420:VAL:HG22	6:DDD:1160:HOH:O	2.21	0.41
1:CCC:536:LEU:HD11	1:CCC:595:LEU:HD22	2.02	0.41
1:DDD:196:VAL:HB	1:DDD:496:GLN:HB3	2.02	0.41
1:EEE:196:VAL:HB	1:EEE:496:GLN:HB3	2.02	0.41
1:EEE:527:LEU:HD11	1:EEE:577:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FFF:162:GLY:HA2	1:FFF:209:HIS:NE2	2.35	0.41
1:FFF:489:LEU:HD22	1:FFF:518:TYR:CZ	2.55	0.41
1:BBB:226:GLN:HA	1:BBB:226:GLN:HE21	1.85	0.41
1:CCC:196:VAL:HB	1:CCC:496:GLN:HB3	2.03	0.41
1:DDD:409:LYS:HE3	1:DDD:411:ASN:HD22	1.86	0.41
1:AAA:564:ILE:HA	1:AAA:572:VAL:O	2.21	0.40
1:BBB:452:ASP:OD1	1:BBB:454:THR:OG1	2.25	0.40
1:FFF:188:GLU:HG3	1:FFF:189:TYR:CE2	2.56	0.40
1:AAA:44:ALA:O	1:AAA:72:CYS:HA	2.22	0.40
1:AAA:455:ASP:HA	1:AAA:601:PRO:HG2	2.04	0.40
1:DDD:564:ILE:HA	1:DDD:572:VAL:O	2.21	0.40
1:BBB:172:PHE:O	1:BBB:176:ARG:HG2	2.21	0.40
1:BBB:399:MET:HE3	6:BBB:951:HOH:O	2.21	0.40
1:CCC:256:GLY:HA2	1:CCC:294:LEU:O	2.21	0.40
1:CCC:452:ASP:OD1	1:CCC:454:THR:OG1	2.26	0.40
1:DDD:256:GLY:HA2	1:DDD:294:LEU:O	2.22	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:27:PHE:HZ	1:DDD:566:GLN:HE22[1_565]	1.18	0.42
1:AAA:569:LYS:HZ1	1:EEE:249:ARG:O[1_565]	1.59	0.01

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	660/674 (98%)	643 (97%)	17 (3%)	0	100	100
1	BBB	654/674 (97%)	634 (97%)	20 (3%)	0	100	100
1	CCC	650/674 (96%)	629 (97%)	21 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DDD	650/674 (96%)	629 (97%)	21 (3%)	0	100	100
1	EEE	651/674 (97%)	633 (97%)	18 (3%)	0	100	100
1	FFF	646/674 (96%)	627 (97%)	19 (3%)	0	100	100
All	All	3911/4044 (97%)	3795 (97%)	116 (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	570/582 (98%)	568 (100%)	2 (0%)	91	87
1	BBB	567/582 (97%)	562 (99%)	5 (1%)	78	67
1	CCC	563/582 (97%)	557 (99%)	6 (1%)	73	60
1	DDD	562/582 (97%)	557 (99%)	5 (1%)	78	67
1	EEE	564/582 (97%)	560 (99%)	4 (1%)	84	75
1	FFF	560/582 (96%)	555 (99%)	5 (1%)	78	67
All	All	3386/3492 (97%)	3359 (99%)	27 (1%)	81	72

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	296	THR
1	AAA	549	LYS
1	BBB	54	GLN
1	BBB	296	THR
1	BBB	311	LEU
1	BBB	536	LEU
1	BBB	649	LYS
1	CCC	169	ASN
1	CCC	185	ASN
1	CCC	201	LYS

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Mol	Chain	Res	Type
1	CCC	296	THR
1	CCC	311	LEU
1	CCC	531	LYS
1	DDD	130	GLU
1	DDD	296	THR
1	DDD	409	LYS
1	DDD	410	LEU
1	DDD	571	LYS
1	EEE	32	GLU
1	EEE	33	ARG
1	EEE	296	THR
1	EEE	613	LYS
1	FFF	296	THR
1	FFF	450	LEU
1	FFF	487	ASP
1	FFF	532	ASP
1	FFF	651	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 53 ligands modelled in this entry, 6 are monoatomic - leaving 47 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	$\#\|Z\| > 2$
5	VKN	DDD	711	-	12,12,13	0.40	0	14,17,19	1.24	2 (14%)
4	TLA	FFF	704	-	9,9,9	1.08	0	12,12,12	1.55	2 (16%)
4	TLA	BBB	706	-	9,9,9	1.10	0	12,12,12	1.17	1 (8%)
5	VKN	FFF	708	-	12,12,13	0.39	0	14,17,19	0.86	0
2	EDO	AAA	701	-	3,3,3	0.12	0	2,2,2	0.34	0
2	EDO	EEE	701	-	3,3,3	0.22	0	2,2,2	0.13	0
2	EDO	DDD	706	-	3,3,3	0.14	0	2,2,2	0.21	0
5	VKN	BBB	707	-	12,12,13	0.46	0	14,17,19	1.19	1 (7%)
2	EDO	FFF	702	-	3,3,3	0.19	0	2,2,2	0.11	0
2	EDO	CCC	701	-	3,3,3	0.07	0	2,2,2	0.08	0
2	EDO	DDD	710	-	3,3,3	0.26	0	2,2,2	0.23	0
2	EDO	DDD	701	-	3,3,3	0.39	0	2,2,2	0.12	0
2	EDO	CCC	702	-	3,3,3	0.05	0	2,2,2	0.28	0
2	EDO	EEE	709	-	3,3,3	0.32	0	2,2,2	0.25	0
2	EDO	DDD	702	-	3,3,3	0.34	0	2,2,2	0.28	0
2	EDO	BBB	701	-	3,3,3	0.06	0	2,2,2	0.04	0
2	EDO	EEE	707	-	3,3,3	0.30	0	2,2,2	0.25	0
2	EDO	FFF	705	-	3,3,3	0.25	0	2,2,2	0.38	0
2	EDO	CCC	705	-	3,3,3	0.42	0	2,2,2	0.47	0
2	EDO	CCC	707	-	3,3,3	0.23	0	2,2,2	0.19	0
5	VKN	EEE	710	-	12,12,13	0.55	0	14,17,19	1.14	2 (14%)
4	TLA	FFF	706	-	9,9,9	1.08	0	12,12,12	0.79	0
2	EDO	AAA	707	-	3,3,3	0.60	0	2,2,2	0.45	0
2	EDO	EEE	705	-	3,3,3	0.16	0	2,2,2	0.40	0
4	TLA	DDD	707	-	9,9,9	0.97	0	12,12,12	1.51	3 (25%)
2	EDO	DDD	705	-	3,3,3	0.46	0	2,2,2	0.58	0
2	EDO	AAA	704	-	3,3,3	0.14	0	2,2,2	0.02	0
2	EDO	DDD	709	-	3,3,3	0.12	0	2,2,2	0.25	0
4	TLA	EEE	706	-	9,9,9	0.94	0	12,12,12	1.47	3 (25%)
2	EDO	FFF	701	-	3,3,3	0.28	0	2,2,2	0.13	0
4	TLA	BBB	703	-	9,9,9	1.04	0	12,12,12	1.67	3 (25%)
2	EDO	BBB	704	-	3,3,3	0.14	0	2,2,2	0.72	0
2	EDO	BBB	705	-	3,3,3	0.23	0	2,2,2	0.52	0
2	EDO	FFF	707	-	3,3,3	0.28	0	2,2,2	0.62	0
4	TLA	AAA	705	-	9,9,9	1.09	0	12,12,12	1.24	2 (16%)
4	TLA	EEE	708	-	9,9,9	1.19	0	12,12,12	1.87	5 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	EDO	EEE	703	-	3,3,3	0.12	0	2,2,2	0.14	0
4	TLA	CCC	706	-	9,9,9	1.10	0	12,12,12	1.44	3 (25%)
4	TLA	CCC	708	-	9,9,9	1.01	0	12,12,12	1.43	2 (16%)
4	TLA	DDD	708	-	9,9,9	1.10	0	12,12,12	1.76	3 (25%)
4	TLA	AAA	706	-	9,9,9	1.29	1 (11%)	12,12,12	1.24	2 (16%)
2	EDO	AAA	702	-	3,3,3	0.34	0	2,2,2	0.80	0
2	EDO	CCC	703	-	3,3,3	0.37	0	2,2,2	0.28	0
5	VKN	AAA	708	-	12,12,13	0.43	0	14,17,19	1.66	4 (28%)
2	EDO	DDD	703	-	3,3,3	0.30	0	2,2,2	0.49	0
2	EDO	EEE	702	-	3,3,3	0.12	0	2,2,2	0.24	0
5	VKN	CCC	709	-	12,12,13	0.67	0	14,17,19	1.28	2 (14%)

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
5	VKN	DDD	711	-	-	0/2/22/26	0/1/1/1
4	TLA	FFF	704	-	-	0/12/12/12	-
4	TLA	BBB	706	-	-	0/12/12/12	-
5	VKN	FFF	708	-	-	0/2/22/26	0/1/1/1
2	EDO	AAA	701	-	-	1/1/1/1	-
2	EDO	EEE	701	-	-	1/1/1/1	-
2	EDO	DDD	706	-	-	0/1/1/1	-
5	VKN	BBB	707	-	-	0/2/22/26	0/1/1/1
2	EDO	FFF	702	-	-	1/1/1/1	-
2	EDO	CCC	701	-	-	0/1/1/1	-
2	EDO	DDD	710	-	-	0/1/1/1	-
2	EDO	DDD	701	-	-	1/1/1/1	-
2	EDO	CCC	702	-	-	1/1/1/1	-
2	EDO	EEE	709	-	-	0/1/1/1	-
2	EDO	DDD	702	-	-	0/1/1/1	-
2	EDO	BBB	701	-	-	1/1/1/1	-
2	EDO	EEE	707	-	-	0/1/1/1	-
2	EDO	FFF	705	-	-	0/1/1/1	-
2	EDO	CCC	705	-	-	1/1/1/1	-
2	EDO	CCC	707	-	-	0/1/1/1	-
5	VKN	EEE	710	-	-	0/2/22/26	0/1/1/1
4	TLA	FFF	706	-	-	0/12/12/12	-
2	EDO	AAA	707	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	EEE	705	-	-	0/1/1/1	-
4	TLA	DDD	707	-	-	0/12/12/12	-
2	EDO	DDD	705	-	-	0/1/1/1	-
2	EDO	AAA	704	-	-	0/1/1/1	-
2	EDO	DDD	709	-	-	0/1/1/1	-
4	TLA	EEE	706	-	-	0/12/12/12	-
2	EDO	FFF	701	-	-	0/1/1/1	-
4	TLA	BBB	703	-	-	0/12/12/12	-
2	EDO	BBB	704	-	-	1/1/1/1	-
2	EDO	BBB	705	-	-	0/1/1/1	-
2	EDO	FFF	707	-	-	0/1/1/1	-
4	TLA	AAA	705	-	-	0/12/12/12	-
4	TLA	EEE	708	-	-	0/12/12/12	-
2	EDO	EEE	703	-	-	1/1/1/1	-
4	TLA	CCC	706	-	-	0/12/12/12	-
4	TLA	CCC	708	-	-	2/12/12/12	-
4	TLA	DDD	708	-	-	3/12/12/12	-
4	TLA	AAA	706	-	-	2/12/12/12	-
2	EDO	AAA	702	-	-	0/1/1/1	-
2	EDO	CCC	703	-	-	1/1/1/1	-
5	VKN	AAA	708	-	-	0/2/22/26	0/1/1/1
2	EDO	DDD	703	-	-	1/1/1/1	-
2	EDO	EEE	702	-	-	0/1/1/1	-
5	VKN	CCC	709	-	-	0/2/22/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	AAA	706	TLA	O4-C4	2.28	1.29	1.22

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	BBB	703	TLA	O41-C4-C3	3.70	123.26	113.27
5	AAA	708	VKN	C1-C2-C3	3.66	116.01	110.69
4	DDD	708	TLA	O11-C1-C2	3.50	122.75	113.27
4	CCC	708	TLA	O41-C4-C3	3.06	121.54	113.27
5	CCC	709	VKN	C1-C2-C3	3.05	115.11	110.69
5	DDD	711	VKN	C1-C2-C3	2.93	114.94	110.69
4	EEE	708	TLA	O11-C1-C2	2.92	121.17	113.27
4	FFF	704	TLA	O11-C1-C2	2.90	121.12	113.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	FFF	704	TLA	O41-C4-C3	2.88	121.05	113.27
4	EEE	706	TLA	O11-C1-C2	2.87	121.02	113.27
5	AAA	708	VKN	O2-C2-C3	-2.75	104.63	110.14
4	EEE	708	TLA	O41-C4-C3	2.69	120.54	113.27
5	BBB	707	VKN	C1-C2-C3	2.62	114.49	110.69
4	BBB	703	TLA	O41-C4-O4	-2.60	118.18	124.09
4	CCC	708	TLA	O11-C1-C2	2.47	119.95	113.27
4	EEE	708	TLA	O3-C3-C4	2.45	115.80	110.66
4	DDD	707	TLA	O11-C1-C2	2.38	119.70	113.27
4	DDD	708	TLA	O1-C1-C2	-2.30	115.58	121.63
5	EEE	710	VKN	C1-C2-C3	2.27	113.99	110.69
4	CCC	706	TLA	O11-C1-O1	-2.27	118.94	124.09
4	AAA	705	TLA	O41-C4-C3	2.25	119.36	113.27
4	BBB	706	TLA	O41-C4-C3	2.20	119.21	113.27
4	EEE	706	TLA	O11-C1-O1	-2.20	119.10	124.09
5	CCC	709	VKN	O2-C2-C3	-2.19	105.75	110.14
4	AAA	705	TLA	O11-C1-C2	2.19	119.18	113.27
4	AAA	706	TLA	O4-C4-C3	-2.18	115.89	121.63
4	DDD	708	TLA	O41-C4-C3	2.18	119.16	113.27
5	AAA	708	VKN	O5-C7-C1	-2.15	104.61	109.94
4	EEE	708	TLA	O1-C1-C2	-2.15	115.98	121.63
4	BBB	703	TLA	C3-C2-C1	2.14	114.66	109.87
4	AAA	706	TLA	O11-C1-C2	2.12	118.99	113.27
4	CCC	706	TLA	O41-C4-C3	2.11	118.98	113.27
5	AAA	708	VKN	C2-C3-C4	2.10	114.53	110.89
4	EEE	708	TLA	O3-C3-C2	-2.09	106.08	110.23
4	DDD	707	TLA	O41-C4-C3	2.07	118.87	113.27
5	EEE	710	VKN	O2-C2-C3	-2.05	106.03	110.14
4	DDD	707	TLA	O3-C3-C2	2.03	114.27	110.23
4	CCC	706	TLA	O2-C2-C3	-2.03	106.20	110.23
4	EEE	706	TLA	O41-C4-C3	2.02	118.72	113.27
5	DDD	711	VKN	O3-C3-C4	-2.02	105.69	110.35

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	DDD	703	EDO	O1-C1-C2-O2
2	EEE	701	EDO	O1-C1-C2-O2
4	DDD	708	TLA	C2-C3-C4-O4
4	DDD	708	TLA	C2-C3-C4-O41
2	BBB	704	EDO	O1-C1-C2-O2

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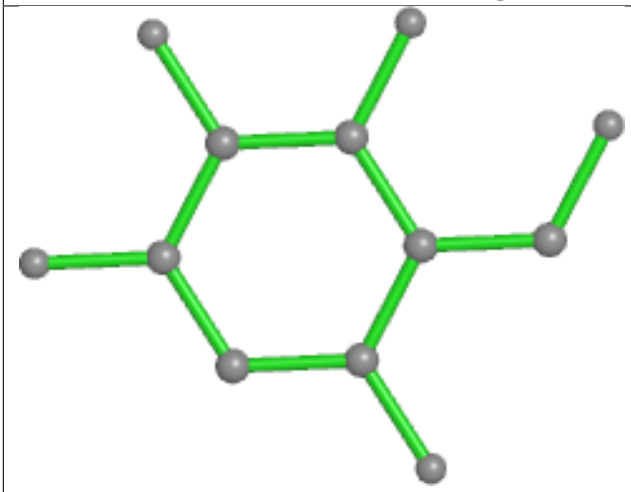
Mol	Chain	Res	Type	Atoms
2	CCC	703	EDO	O1-C1-C2-O2
4	DDD	708	TLA	O3-C3-C4-O4
2	CCC	705	EDO	O1-C1-C2-O2
2	EEE	703	EDO	O1-C1-C2-O2
2	AAA	701	EDO	O1-C1-C2-O2
2	DDD	701	EDO	O1-C1-C2-O2
4	AAA	706	TLA	O1-C1-C2-C3
4	CCC	708	TLA	C2-C3-C4-O4
2	BBB	701	EDO	O1-C1-C2-O2
2	CCC	702	EDO	O1-C1-C2-O2
2	FFF	702	EDO	O1-C1-C2-O2
4	AAA	706	TLA	O11-C1-C2-C3
4	CCC	708	TLA	C2-C3-C4-O41

There are no ring outliers.

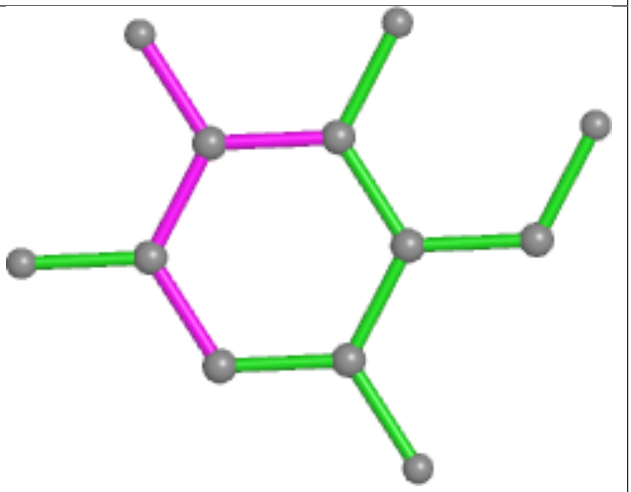
No monomer is involved in short contacts.

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

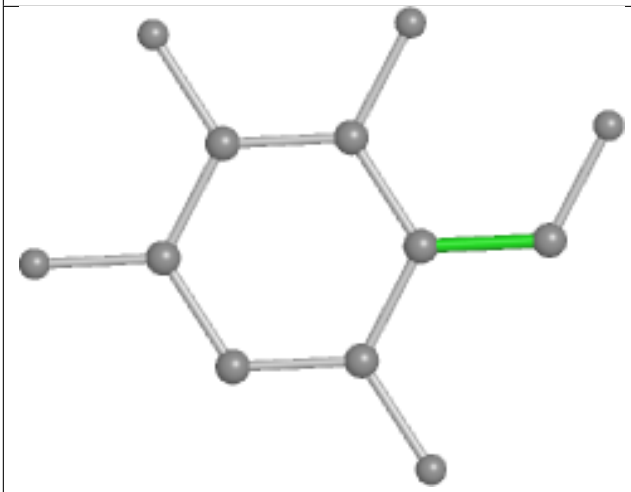
Ligand VKN DDD 711



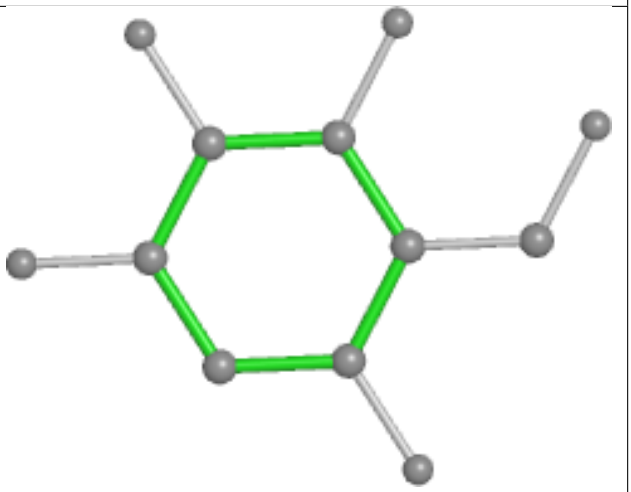
Bond lengths



Bond angles

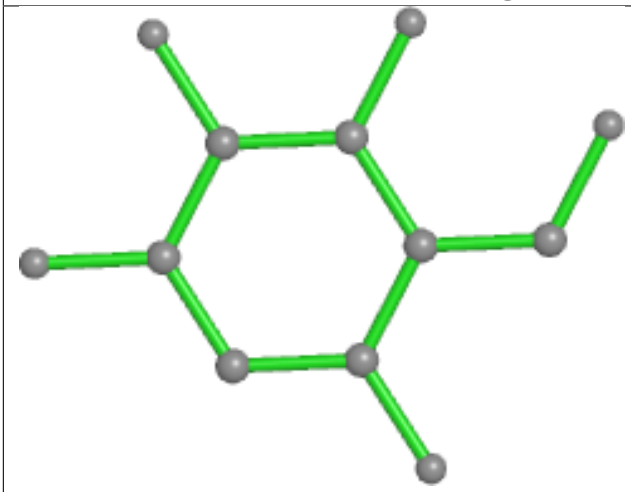


Torsions

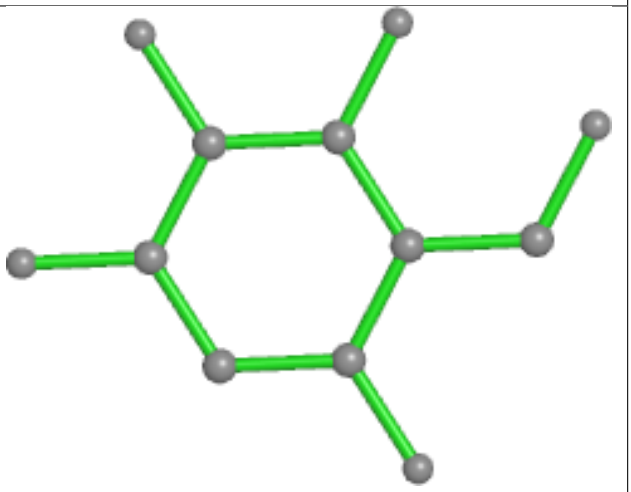


Rings

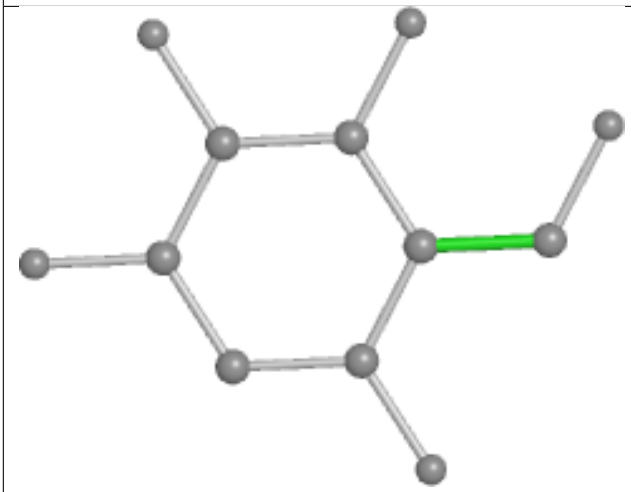
Ligand VKN FFF 708



Bond lengths



Bond angles



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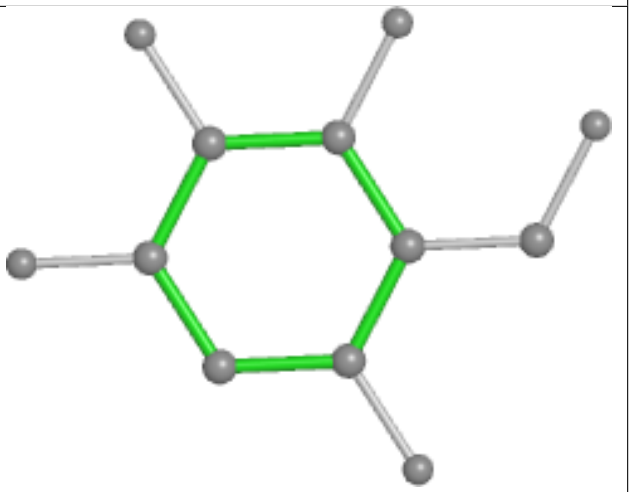
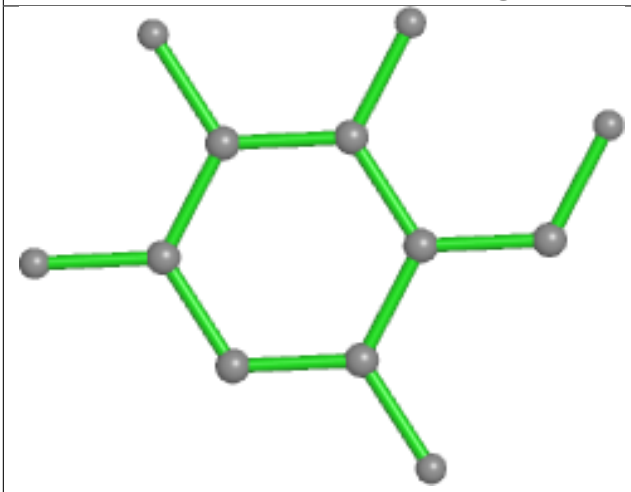
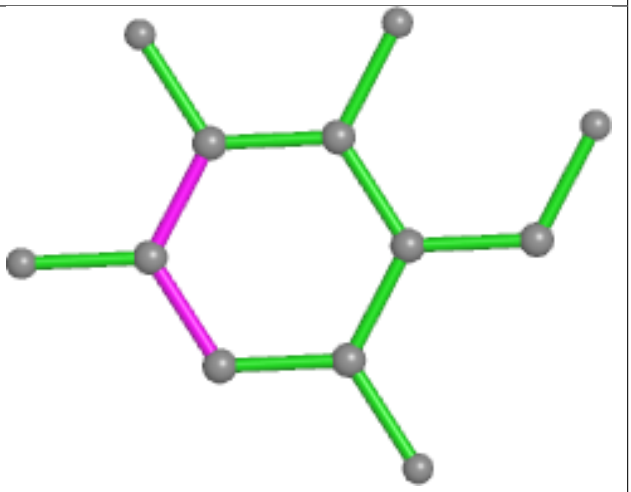


Rings

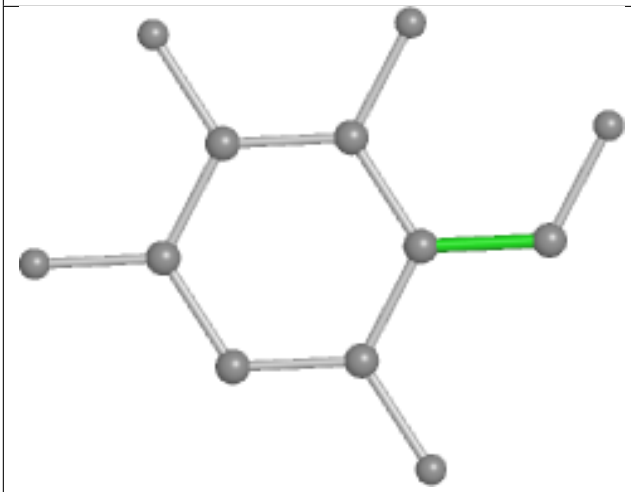
Ligand VKN BBB 707



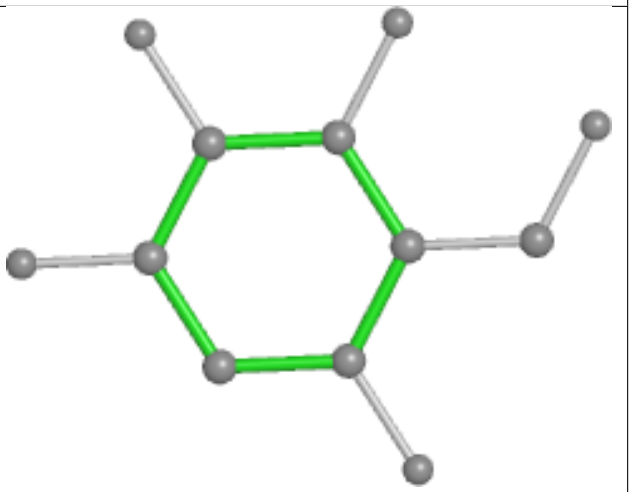
Bond lengths



Bond angles

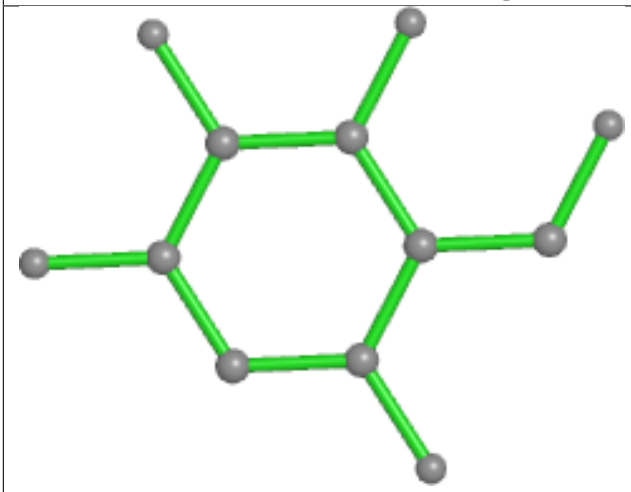


Torsions

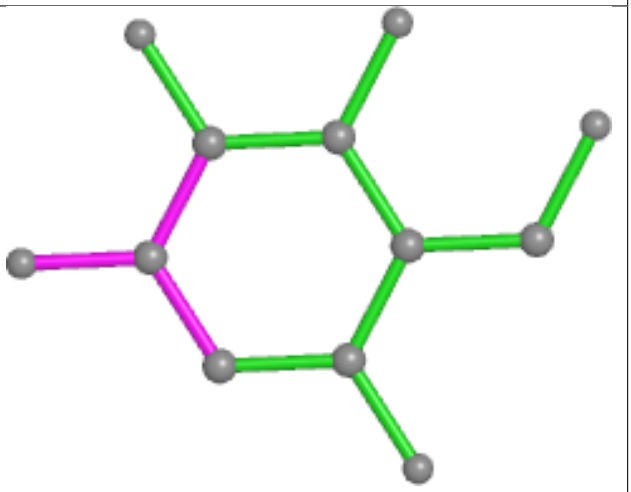


Rings

Ligand VKN EEE 710



Bond lengths



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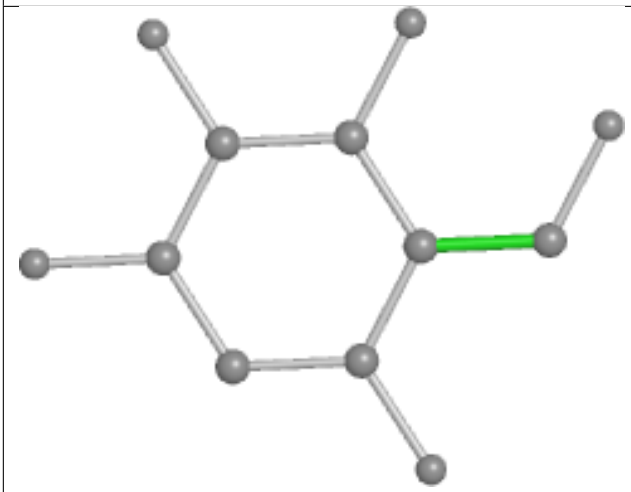
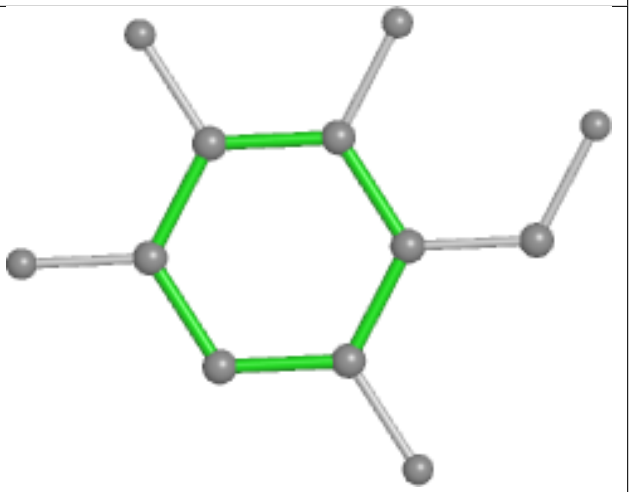
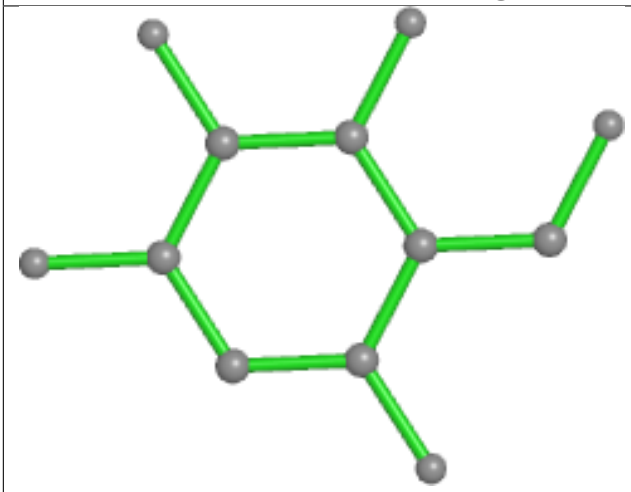


Torsions



Rings

Ligand VKN AAA 708



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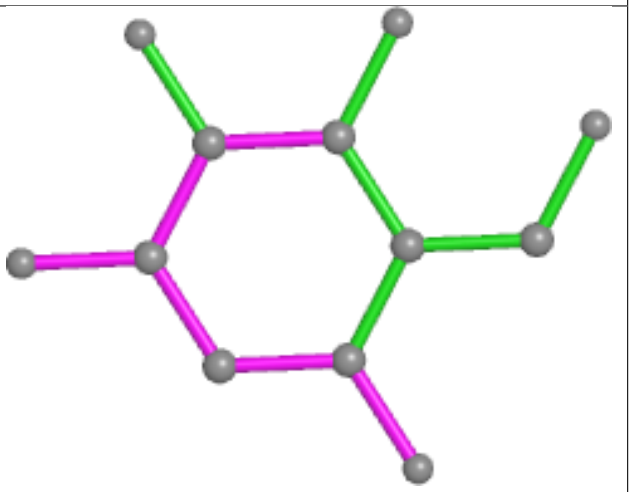
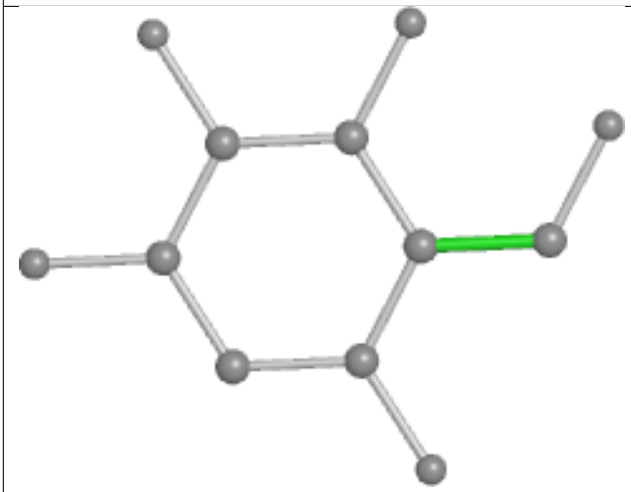


Bond angles



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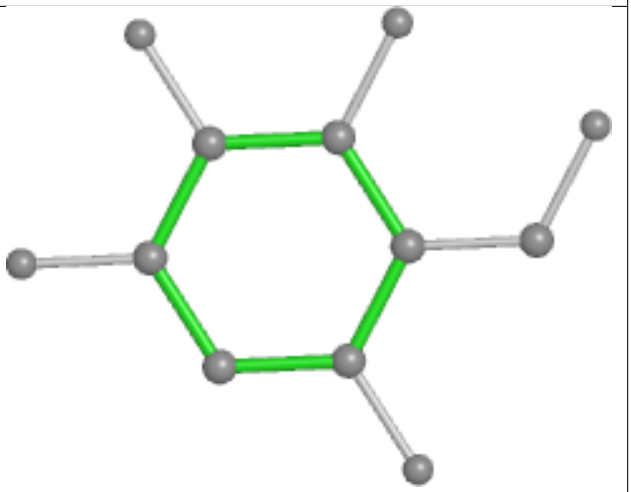
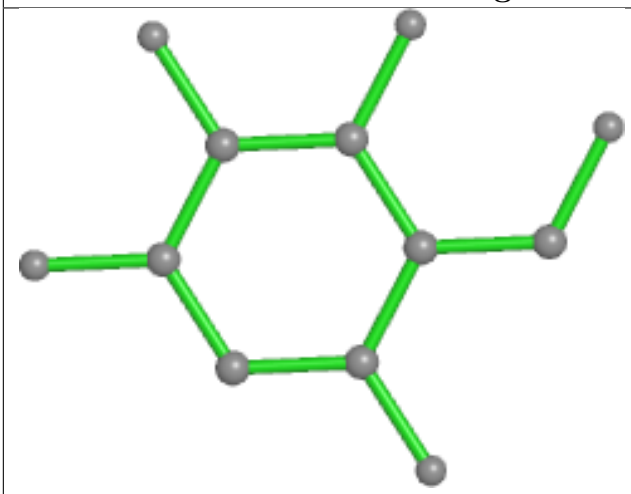
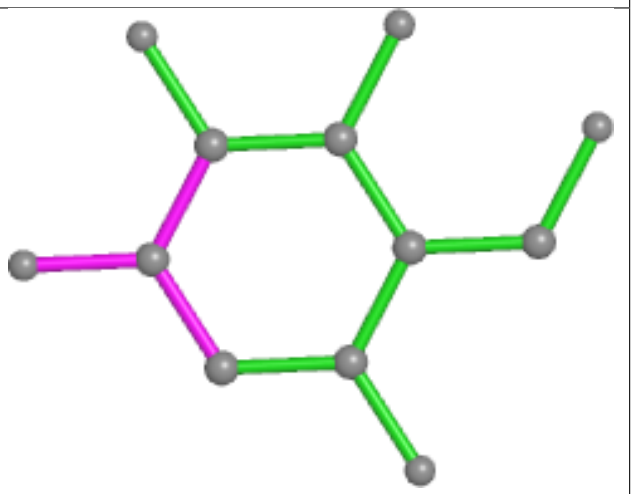


Rings

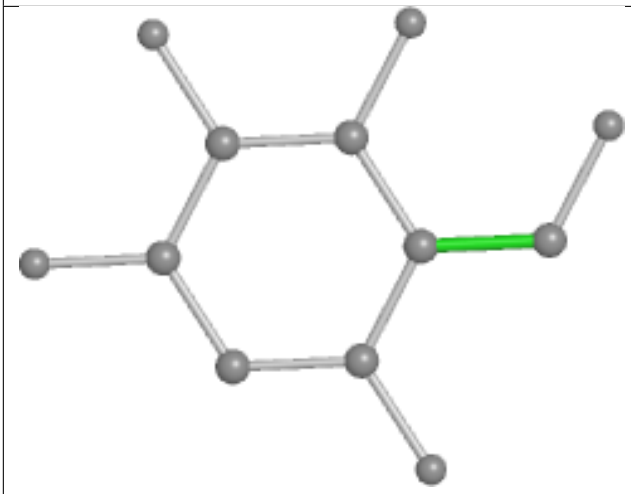
Ligand VKN CCC 709



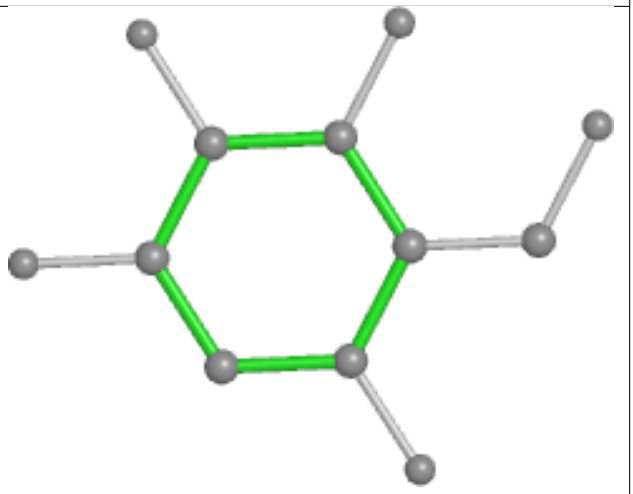
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	661/674 (98%)	-0.07	8 (1%) 79 84	24, 36, 60, 93	0
1	BBB	658/674 (97%)	0.01	13 (1%) 65 72	27, 38, 62, 96	0
1	CCC	651/674 (96%)	-0.20	7 (1%) 80 86	23, 32, 55, 78	0
1	DDD	652/674 (96%)	-0.16	2 (0%) 94 95	23, 31, 52, 92	0
1	EEE	652/674 (96%)	-0.09	3 (0%) 91 93	24, 34, 55, 78	0
1	FFF	650/674 (96%)	-0.18	5 (0%) 86 90	27, 36, 58, 92	0
All	All	3924/4044 (97%)	-0.11	38 (0%) 82 87	23, 35, 58, 96	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	529	PHE	4.5
1	BBB	649	LYS	4.2
1	AAA	21	SER	3.9
1	BBB	29	GLY	3.8
1	BBB	27	PHE	3.5
1	AAA	23	LEU	3.5
1	EEE	31	ALA	3.3
1	AAA	455	ASP	3.3
1	FFF	411	ASN	3.3
1	AAA	665	ALA	3.2
1	BBB	532	ASP	3.1
1	EEE	166	LEU	3.1
1	BBB	30	PRO	2.8
1	CCC	533	ASN	2.7
1	EEE	32	GLU	2.7
1	BBB	531	LYS	2.7
1	CCC	166	LEU	2.6
1	BBB	28	GLN	2.6
1	FFF	31	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	AAA	185	ASN	2.5
1	BBB	665	ALA	2.5
1	BBB	23	LEU	2.5
1	BBB	534	TYR	2.4
1	FFF	412	GLY	2.4
1	AAA	22	GLY	2.3
1	AAA	31	ALA	2.3
1	DDD	534	TYR	2.3
1	BBB	533	ASN	2.3
1	FFF	166	LEU	2.2
1	BBB	192	LYS	2.2
1	CCC	653	PHE	2.2
1	CCC	32	GLU	2.2
1	CCC	84	PRO	2.2
1	FFF	169	ASN	2.1
1	DDD	84	PRO	2.1
1	CCC	412	GLY	2.1
1	AAA	84	PRO	2.0
1	CCC	185	ASN	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 monosaccharides 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, 95^{th} 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
4	TLA	EEE	708	10/10	0.84	0.17	41,50,54,54	2
4	TLA	DDD	707	10/10	0.86	0.13	40,49,56,57	2
4	TLA	AAA	705	10/10	0.86	0.11	46,54,63,63	2
4	TLA	BBB	706	10/10	0.88	0.11	39,50,52,53	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	EEE	701	4/4	0.88	0.15	51,58,60,60	1
4	TLA	DDD	708	10/10	0.88	0.19	47,64,73,79	2
2	EDO	DDD	703	4/4	0.88	0.17	52,56,59,59	1
4	TLA	CCC	708	10/10	0.91	0.09	51,56,60,60	2
4	TLA	EEE	706	10/10	0.91	0.09	41,45,52,58	2
2	EDO	CCC	707	4/4	0.91	0.08	43,46,46,46	1
2	EDO	BBB	704	4/4	0.92	0.09	35,35,38,38	1
4	TLA	AAA	706	10/10	0.92	0.13	41,50,53,56	2
2	EDO	BBB	705	4/4	0.93	0.10	33,38,40,40	1
2	EDO	EEE	707	4/4	0.93	0.09	43,46,49,49	1
2	EDO	FFF	702	4/4	0.93	0.10	44,47,49,49	1
2	EDO	FFF	705	4/4	0.93	0.14	46,46,56,56	1
2	EDO	DDD	705	4/4	0.93	0.10	29,36,38,38	1
2	EDO	DDD	706	4/4	0.93	0.07	40,43,50,50	1
4	TLA	FFF	704	10/10	0.93	0.10	37,41,50,53	2
4	TLA	FFF	706	10/10	0.93	0.16	43,52,55,57	2
5	VKN	EEE	710	12/13	0.93	0.09	0,32,34,35	4
4	TLA	BBB	703	10/10	0.94	0.08	45,50,55,61	2
2	EDO	CCC	703	4/4	0.94	0.10	51,53,54,54	1
2	EDO	EEE	705	4/4	0.95	0.10	29,37,39,39	1
4	TLA	CCC	706	10/10	0.95	0.09	35,42,53,54	2
2	EDO	AAA	701	4/4	0.95	0.09	32,34,40,40	1
2	EDO	EEE	709	4/4	0.95	0.09	45,49,51,51	1
5	VKN	AAA	708	12/13	0.95	0.08	0,30,33,33	4
5	VKN	DDD	711	12/13	0.95	0.08	0,26,30,30	4
2	EDO	AAA	707	4/4	0.95	0.14	37,38,40,40	1
5	VKN	FFF	708	12/13	0.95	0.08	28,32,35,37	4
2	EDO	DDD	710	4/4	0.96	0.07	31,32,34,34	1
2	EDO	AAA	704	4/4	0.96	0.10	34,36,38,38	1
5	VKN	CCC	709	12/13	0.96	0.07	0,29,31,32	4
2	EDO	AAA	702	4/4	0.96	0.06	29,33,34,34	1
2	EDO	FFF	707	4/4	0.96	0.12	28,37,38,38	1
2	EDO	DDD	702	4/4	0.96	0.11	44,44,46,46	1
2	EDO	DDD	709	4/4	0.97	0.08	35,37,39,39	1
2	EDO	BBB	701	4/4	0.97	0.12	46,46,49,49	1
5	VKN	BBB	707	12/13	0.97	0.07	0,31,32,33	4
2	EDO	CCC	702	4/4	0.97	0.07	31,32,37,37	1
2	EDO	FFF	701	4/4	0.97	0.09	36,36,39,39	1
2	EDO	EEE	702	4/4	0.97	0.08	39,40,44,44	1
2	EDO	EEE	703	4/4	0.97	0.06	34,34,35,35	1
2	EDO	CCC	705	4/4	0.98	0.06	25,28,35,35	1
3	CL	AAA	703	1/1	0.98	0.08	33,33,33,33	0

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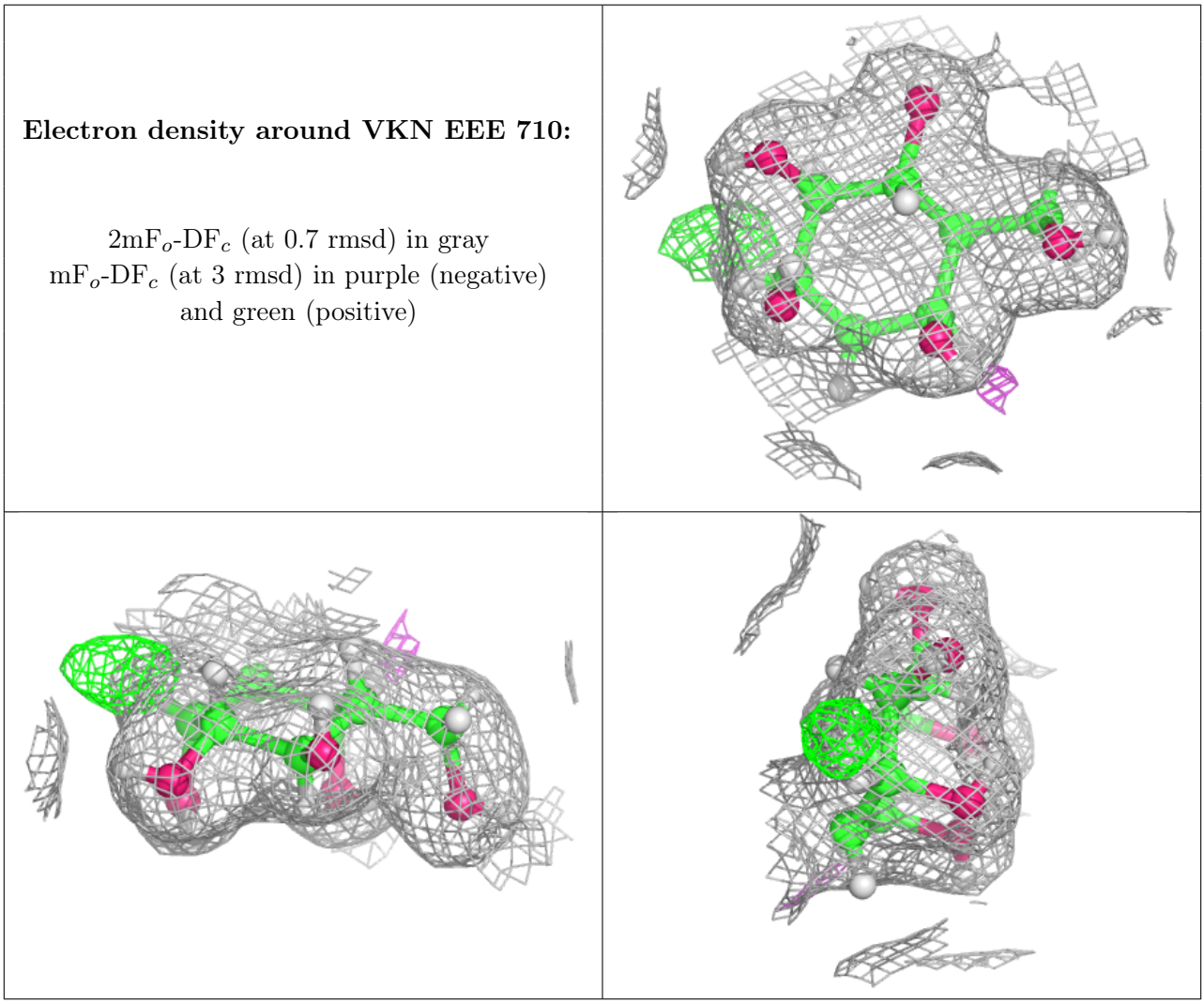
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	CCC	701	4/4	0.98	0.07	35,35,35,35	1
2	EDO	DDD	701	4/4	0.98	0.08	31,33,35,35	1
3	CL	BBB	702	1/1	0.99	0.14	31,31,31,31	0
3	CL	CCC	704	1/1	0.99	0.10	28,28,28,28	0
3	CL	DDD	704	1/1	0.99	0.07	29,29,29,29	0
3	CL	EEE	704	1/1	1.00	0.12	27,27,27,27	0
3	CL	FFF	703	1/1	1.00	0.08	31,31,31,31	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.

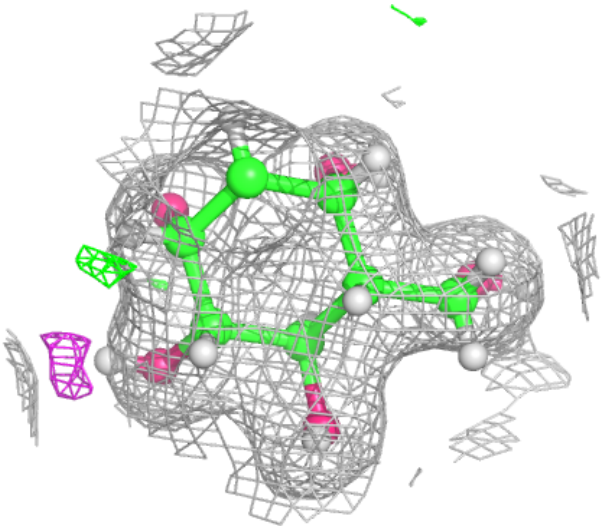
Electron density around VKN EEE 710:

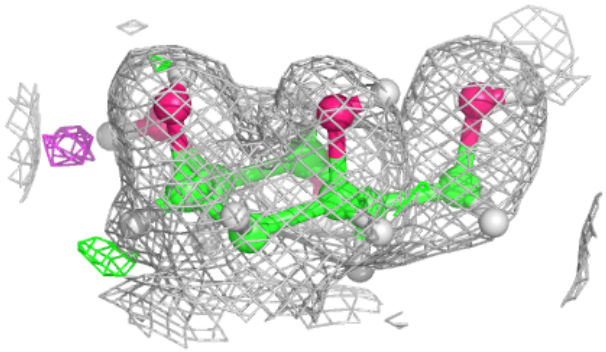
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

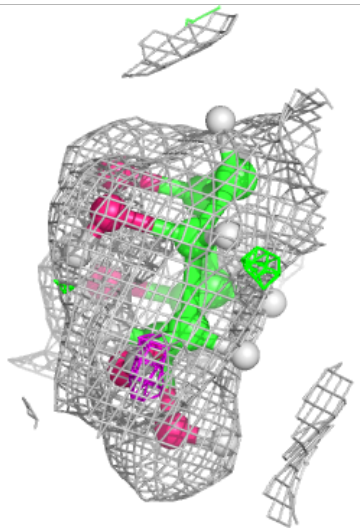


Electron density around VKN AAA 708:

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

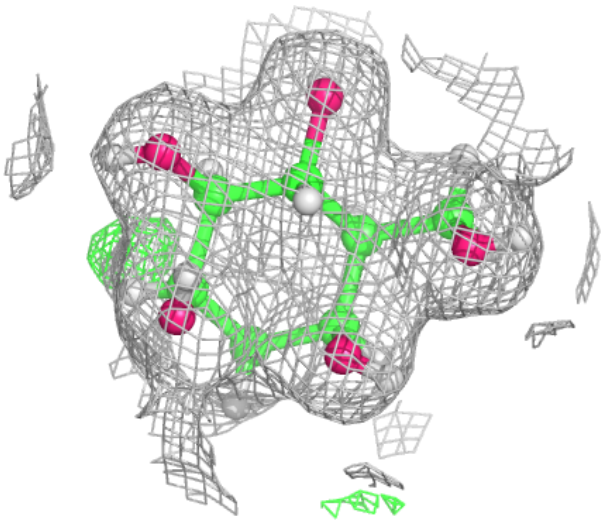


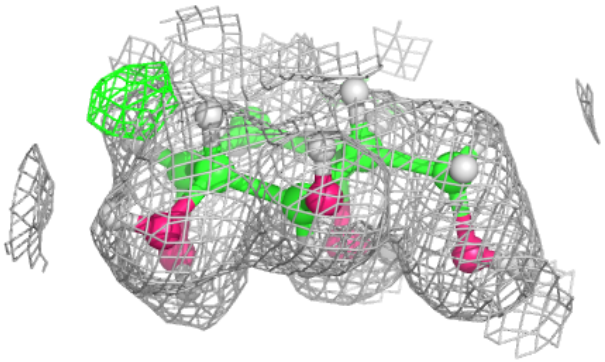


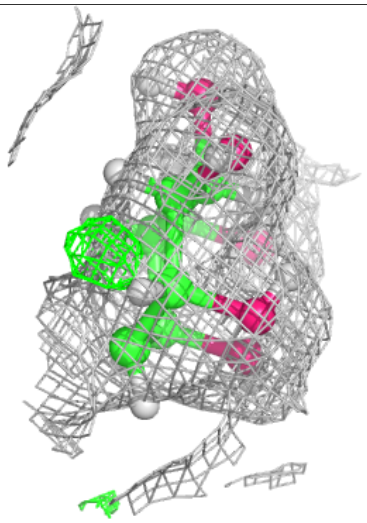


Electron density around VKN DDD 711:

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

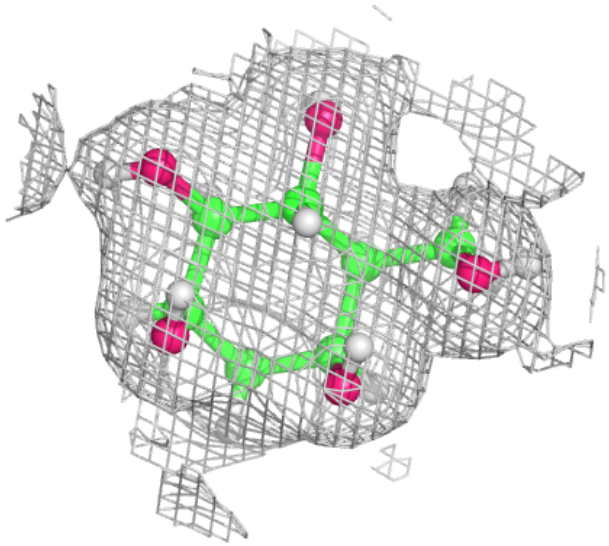


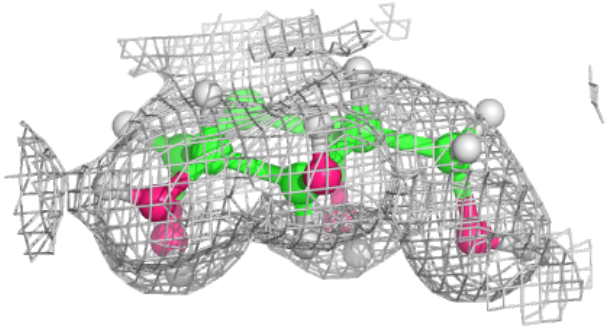


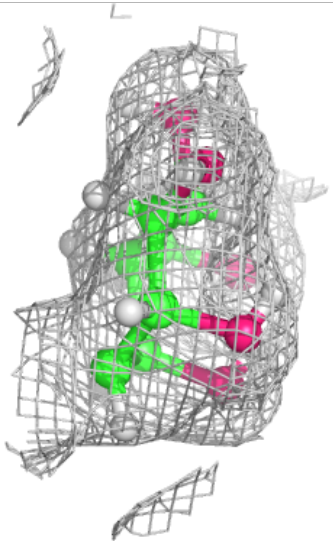


Electron density around VKN FFF 708:

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

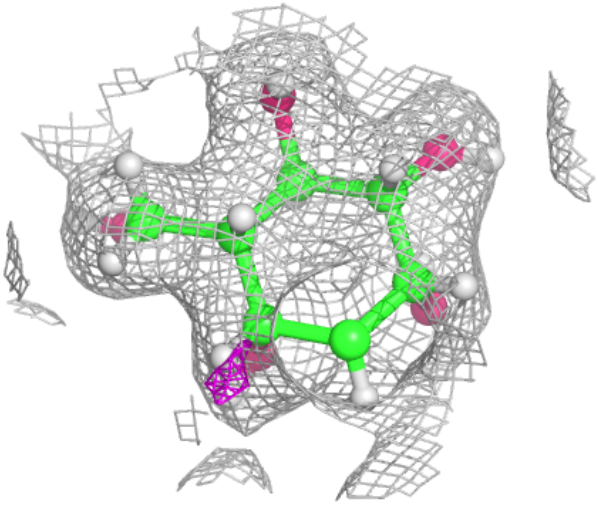


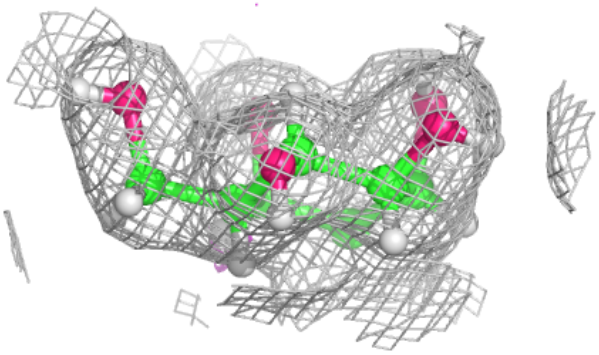


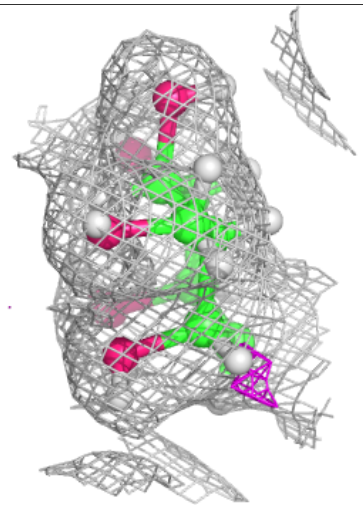


Electron density around VKN CCC 709:

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

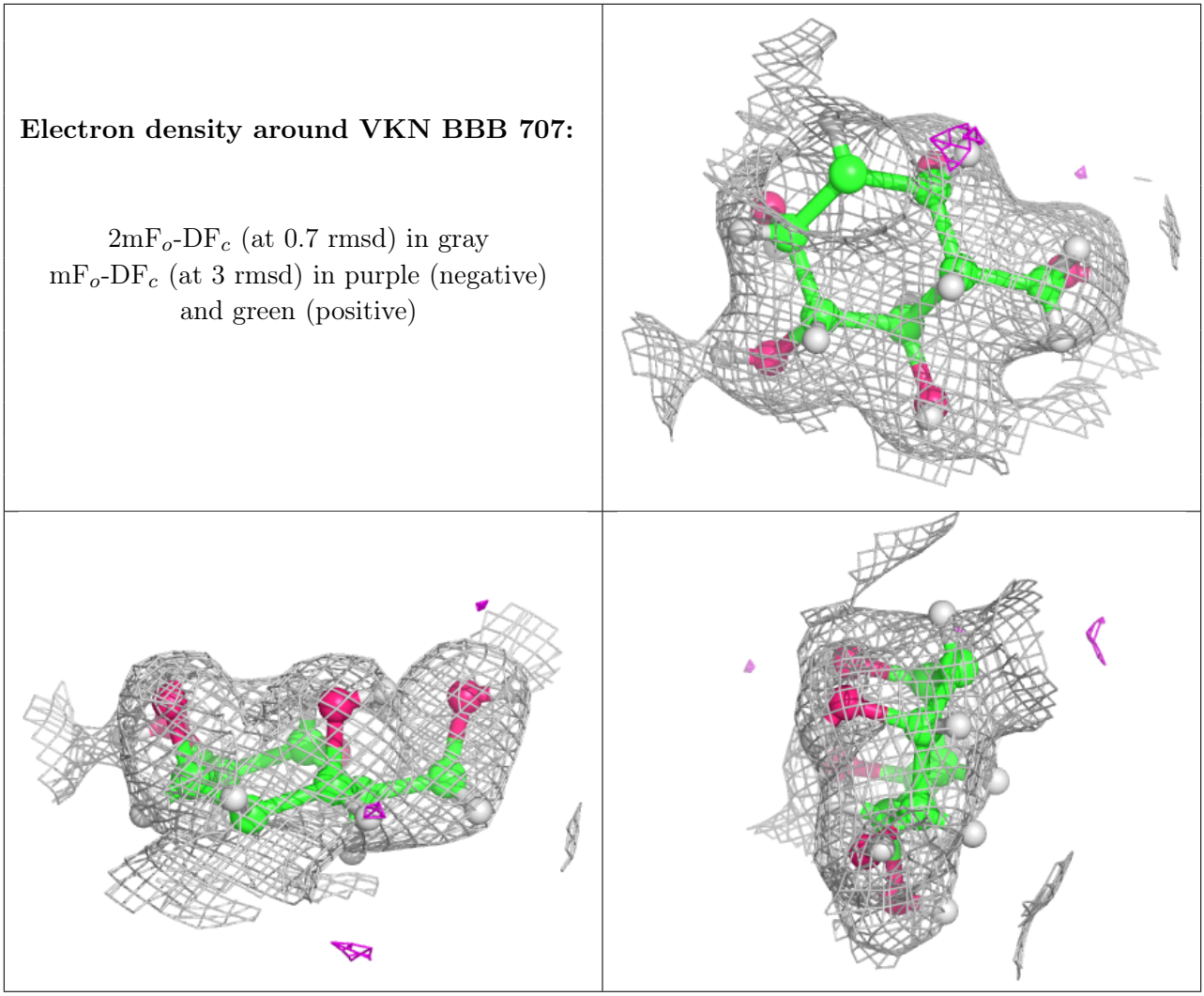






Electron density around VKN BBB 707:

$2mF_o$-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

There are no such residues in this entry.