Full wwPDB X-ray Structure Validation Report ⓘ

Jan 6, 2025 – 04:55 PM EST

PDB ID	:	9AUV
Title	:	Crystal structure of A. baumannii GuaB dCBS with inhibitor GNE9123
Authors	:	Harris, S.F.; Wu, P.
Deposited on	:	2024-03-01
Resolution	:	1.83 Å(reported)

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

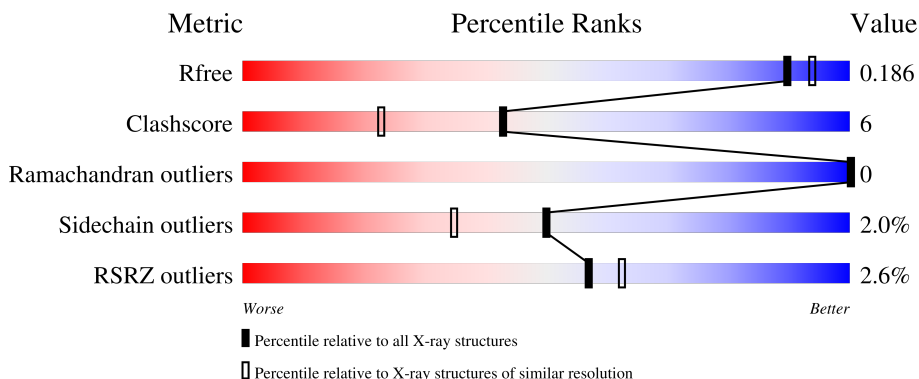|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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.
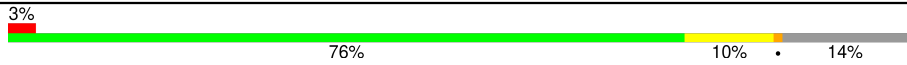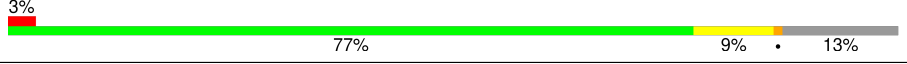
Metric	Percentile Ranks	Value
Rfree		0.186
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		2.0%
RSRZ outliers		2.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1150 (1.84-1.84)
Clashscore	180529	1248 (1.84-1.84)
Ramachandran outliers	177936	1240 (1.84-1.84)
Sidechain outliers	177891	1240 (1.84-1.84)
RSRZ outliers	164620	1149 (1.84-1.84)

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	A	395	% 77% 10% • 13%
1	B	395	2% 74% 12% • 13%
1	C	395	% 77% 10% • 13%
1	D	395	2% 78% 9% • 13%
1	E	395	3% 74% 12% 14%

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Mol	Chain	Length	Quality of chain
1	F	395	3% 76% 10% · 14%
1	G	395	3% 75% 11% · 14%
1	H	395	3% 77% 9% · 13%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 22919 atoms, of which 112 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 Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total 2544	C 1590	N 451	O 486	S 17	0	6	0
1	B	342	Total 2533	C 1584	N 447	O 485	S 17	0	7	0
1	C	344	Total 2541	C 1589	N 448	O 486	S 18	0	6	0
1	D	343	Total 2537	C 1587	N 447	O 485	S 18	0	6	0
1	E	341	Total 2531	C 1585	N 446	O 483	S 17	0	7	0
1	F	341	Total 2531	C 1585	N 446	O 483	S 17	0	7	0
1	G	341	Total 2523	C 1579	N 445	O 482	S 17	0	6	0
1	H	343	Total 2537	C 1587	N 447	O 485	S 18	0	6	0

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP D0CF46
A	-14	HIS	-	expression tag	UNP D0CF46
A	-13	HIS	-	expression tag	UNP D0CF46
A	-12	HIS	-	expression tag	UNP D0CF46
A	-11	HIS	-	expression tag	UNP D0CF46
A	-10	HIS	-	expression tag	UNP D0CF46
A	-9	HIS	-	expression tag	UNP D0CF46
A	-8	GLY	-	expression tag	UNP D0CF46
A	-7	GLU	-	expression tag	UNP D0CF46
A	-6	ASN	-	expression tag	UNP D0CF46
A	-5	LEU	-	expression tag	UNP D0CF46
A	-4	TYR	-	expression tag	UNP D0CF46
A	-3	PHE	-	expression tag	UNP D0CF46

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLN	-	expression tag	UNP D0CF46
A	-1	GLY	-	expression tag	UNP D0CF46
A	0	SER	-	expression tag	UNP D0CF46
B	-15	MET	-	initiating methionine	UNP D0CF46
B	-14	HIS	-	expression tag	UNP D0CF46
B	-13	HIS	-	expression tag	UNP D0CF46
B	-12	HIS	-	expression tag	UNP D0CF46
B	-11	HIS	-	expression tag	UNP D0CF46
B	-10	HIS	-	expression tag	UNP D0CF46
B	-9	HIS	-	expression tag	UNP D0CF46
B	-8	GLY	-	expression tag	UNP D0CF46
B	-7	GLU	-	expression tag	UNP D0CF46
B	-6	ASN	-	expression tag	UNP D0CF46
B	-5	LEU	-	expression tag	UNP D0CF46
B	-4	TYR	-	expression tag	UNP D0CF46
B	-3	PHE	-	expression tag	UNP D0CF46
B	-2	GLN	-	expression tag	UNP D0CF46
B	-1	GLY	-	expression tag	UNP D0CF46
B	0	SER	-	expression tag	UNP D0CF46
C	-15	MET	-	initiating methionine	UNP D0CF46
C	-14	HIS	-	expression tag	UNP D0CF46
C	-13	HIS	-	expression tag	UNP D0CF46
C	-12	HIS	-	expression tag	UNP D0CF46
C	-11	HIS	-	expression tag	UNP D0CF46
C	-10	HIS	-	expression tag	UNP D0CF46
C	-9	HIS	-	expression tag	UNP D0CF46
C	-8	GLY	-	expression tag	UNP D0CF46
C	-7	GLU	-	expression tag	UNP D0CF46
C	-6	ASN	-	expression tag	UNP D0CF46
C	-5	LEU	-	expression tag	UNP D0CF46
C	-4	TYR	-	expression tag	UNP D0CF46
C	-3	PHE	-	expression tag	UNP D0CF46
C	-2	GLN	-	expression tag	UNP D0CF46
C	-1	GLY	-	expression tag	UNP D0CF46
C	0	SER	-	expression tag	UNP D0CF46
D	-15	MET	-	initiating methionine	UNP D0CF46
D	-14	HIS	-	expression tag	UNP D0CF46
D	-13	HIS	-	expression tag	UNP D0CF46
D	-12	HIS	-	expression tag	UNP D0CF46
D	-11	HIS	-	expression tag	UNP D0CF46
D	-10	HIS	-	expression tag	UNP D0CF46
D	-9	HIS	-	expression tag	UNP D0CF46

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	GLY	-	expression tag	UNP D0CF46
D	-7	GLU	-	expression tag	UNP D0CF46
D	-6	ASN	-	expression tag	UNP D0CF46
D	-5	LEU	-	expression tag	UNP D0CF46
D	-4	TYR	-	expression tag	UNP D0CF46
D	-3	PHE	-	expression tag	UNP D0CF46
D	-2	GLN	-	expression tag	UNP D0CF46
D	-1	GLY	-	expression tag	UNP D0CF46
D	0	SER	-	expression tag	UNP D0CF46
E	-15	MET	-	initiating methionine	UNP D0CF46
E	-14	HIS	-	expression tag	UNP D0CF46
E	-13	HIS	-	expression tag	UNP D0CF46
E	-12	HIS	-	expression tag	UNP D0CF46
E	-11	HIS	-	expression tag	UNP D0CF46
E	-10	HIS	-	expression tag	UNP D0CF46
E	-9	HIS	-	expression tag	UNP D0CF46
E	-8	GLY	-	expression tag	UNP D0CF46
E	-7	GLU	-	expression tag	UNP D0CF46
E	-6	ASN	-	expression tag	UNP D0CF46
E	-5	LEU	-	expression tag	UNP D0CF46
E	-4	TYR	-	expression tag	UNP D0CF46
E	-3	PHE	-	expression tag	UNP D0CF46
E	-2	GLN	-	expression tag	UNP D0CF46
E	-1	GLY	-	expression tag	UNP D0CF46
E	0	SER	-	expression tag	UNP D0CF46
F	-15	MET	-	initiating methionine	UNP D0CF46
F	-14	HIS	-	expression tag	UNP D0CF46
F	-13	HIS	-	expression tag	UNP D0CF46
F	-12	HIS	-	expression tag	UNP D0CF46
F	-11	HIS	-	expression tag	UNP D0CF46
F	-10	HIS	-	expression tag	UNP D0CF46
F	-9	HIS	-	expression tag	UNP D0CF46
F	-8	GLY	-	expression tag	UNP D0CF46
F	-7	GLU	-	expression tag	UNP D0CF46
F	-6	ASN	-	expression tag	UNP D0CF46
F	-5	LEU	-	expression tag	UNP D0CF46
F	-4	TYR	-	expression tag	UNP D0CF46
F	-3	PHE	-	expression tag	UNP D0CF46
F	-2	GLN	-	expression tag	UNP D0CF46
F	-1	GLY	-	expression tag	UNP D0CF46
F	0	SER	-	expression tag	UNP D0CF46
G	-15	MET	-	initiating methionine	UNP D0CF46

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-14	HIS	-	expression tag	UNP D0CF46
G	-13	HIS	-	expression tag	UNP D0CF46
G	-12	HIS	-	expression tag	UNP D0CF46
G	-11	HIS	-	expression tag	UNP D0CF46
G	-10	HIS	-	expression tag	UNP D0CF46
G	-9	HIS	-	expression tag	UNP D0CF46
G	-8	GLY	-	expression tag	UNP D0CF46
G	-7	GLU	-	expression tag	UNP D0CF46
G	-6	ASN	-	expression tag	UNP D0CF46
G	-5	LEU	-	expression tag	UNP D0CF46
G	-4	TYR	-	expression tag	UNP D0CF46
G	-3	PHE	-	expression tag	UNP D0CF46
G	-2	GLN	-	expression tag	UNP D0CF46
G	-1	GLY	-	expression tag	UNP D0CF46
G	0	SER	-	expression tag	UNP D0CF46
H	-15	MET	-	initiating methionine	UNP D0CF46
H	-14	HIS	-	expression tag	UNP D0CF46
H	-13	HIS	-	expression tag	UNP D0CF46
H	-12	HIS	-	expression tag	UNP D0CF46
H	-11	HIS	-	expression tag	UNP D0CF46
H	-10	HIS	-	expression tag	UNP D0CF46
H	-9	HIS	-	expression tag	UNP D0CF46
H	-8	GLY	-	expression tag	UNP D0CF46
H	-7	GLU	-	expression tag	UNP D0CF46
H	-6	ASN	-	expression tag	UNP D0CF46
H	-5	LEU	-	expression tag	UNP D0CF46
H	-4	TYR	-	expression tag	UNP D0CF46
H	-3	PHE	-	expression tag	UNP D0CF46
H	-2	GLN	-	expression tag	UNP D0CF46
H	-1	GLY	-	expression tag	UNP D0CF46
H	0	SER	-	expression tag	UNP D0CF46

- Molecule 2 is INOSINIC ACID (three-letter code: IMP) (formula: $C_{10}H_{13}N_4O_8P$).

IMP
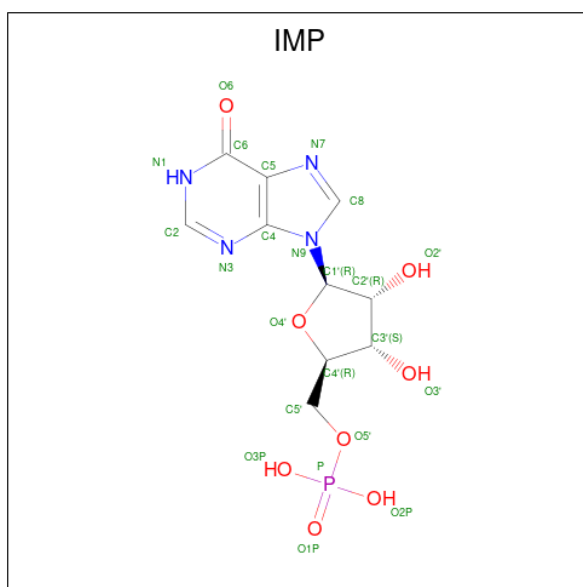
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			36	10	13	4	8	1		
2	B	1	Total	C	H	N	O	P	0	0
			36	10	13	4	8	1		
2	C	1	Total	C	H	N	O	P	0	0
			36	10	13	4	8	1		
2	D	1	Total	C	H	N	O	P	0	0
			36	10	13	4	8	1		
2	E	1	Total	C	H	N	O	P	0	0
			36	10	13	4	8	1		
2	F	1	Total	C	H	N	O	P	0	0
			36	10	13	4	8	1		
2	G	1	Total	C	H	N	O	P	0	0
			36	10	13	4	8	1		
2	H	1	Total	C	H	N	O	P	0	0
			36	10	13	4	8	1		

- Molecule 3 is N-(6-chloropyridin-3-yl)-N 2 -(1,4-dihydro-2H-pyrano[3,4-c]quinolin-9-yl) -L-alaninamide (three-letter code: VOA) (formula: $C_{20}H_{19}ClN_4O_2$) (labeled as "Ligand of Interest" by depositor).

VOA

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	H	N	O	0	0
			28	20	1	1	4	2		
3	B	1	Total	C	Cl	H	N	O	0	0
			28	20	1	1	4	2		
3	C	1	Total	C	Cl	H	N	O	0	0
			28	20	1	1	4	2		
3	D	1	Total	C	Cl	H	N	O	0	0
			28	20	1	1	4	2		
3	E	1	Total	C	Cl	H	N	O	0	0
			28	20	1	1	4	2		
3	F	1	Total	C	Cl	H	N	O	0	0
			28	20	1	1	4	2		
3	G	1	Total	C	Cl	H	N	O	0	0
			28	20	1	1	4	2		
3	H	1	Total	C	Cl	H	N	O	0	0
			28	20	1	1	4	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	319	Total	O	0	0
			319	319		
4	B	295	Total	O	0	0
			295	295		
4	C	275	Total	O	0	0
			275	275		
4	D	279	Total	O	0	0
			279	279		

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	243	Total 243	O 243	0	0
4	F	253	Total 253	O 253	0	0
4	G	236	Total 236	O 236	0	0
4	H	230	Total 230	O 230	0	0

3 Residue-property plots ⓘ

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.
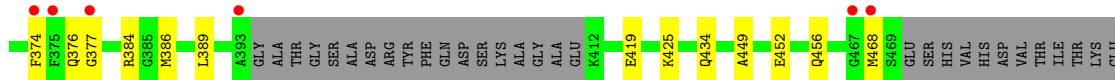
- Molecule 1: Inosine-5'-monophosphate dehydrogenase
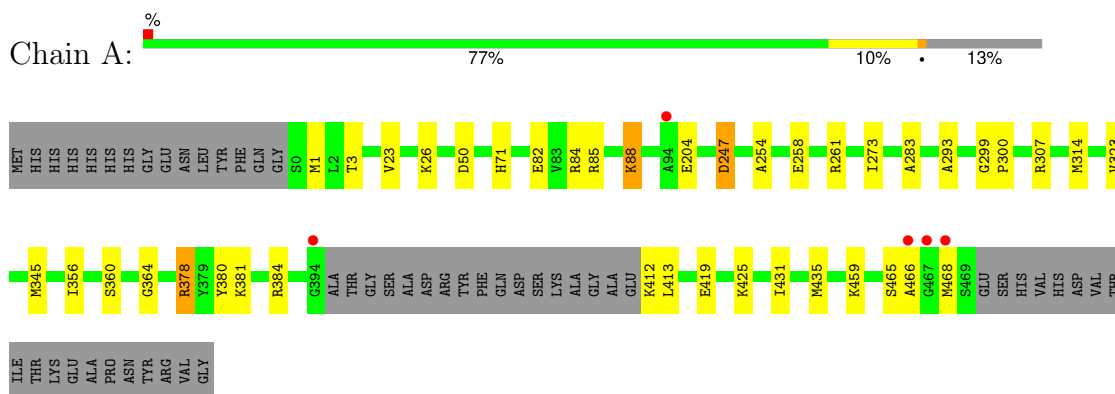
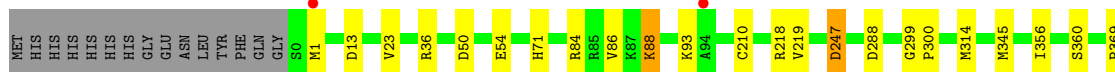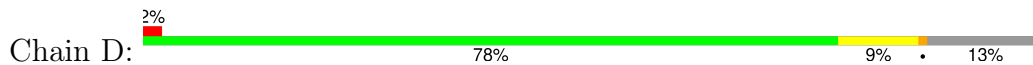- Molecule 1: Inosine-5'-monophosphate dehydrogenase
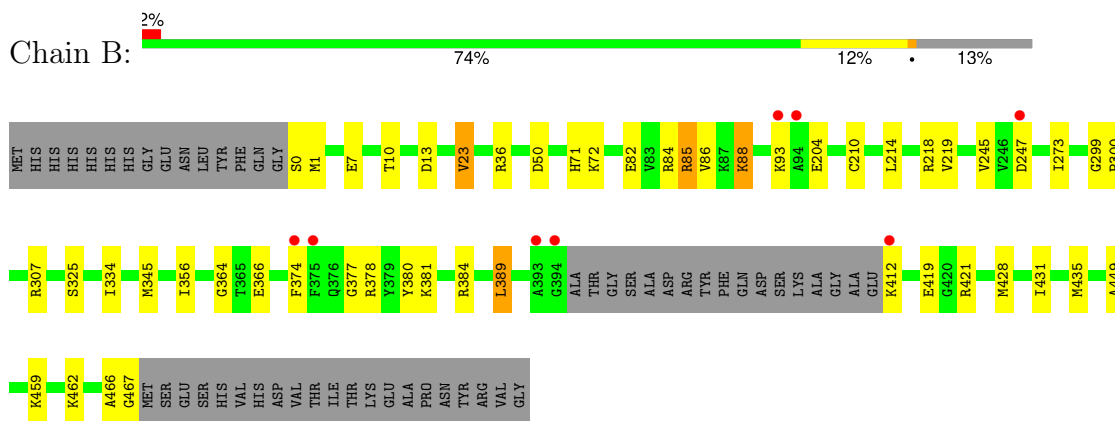
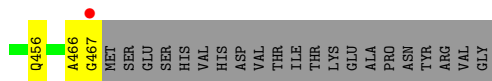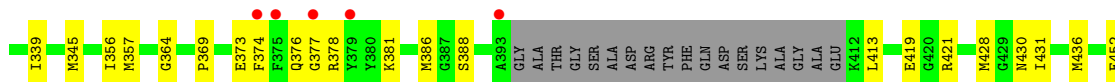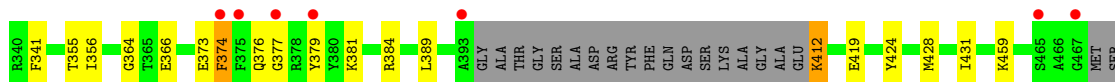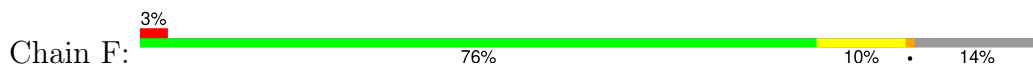- Molecule 1: Inosine-5'-monophosphate dehydrogenase
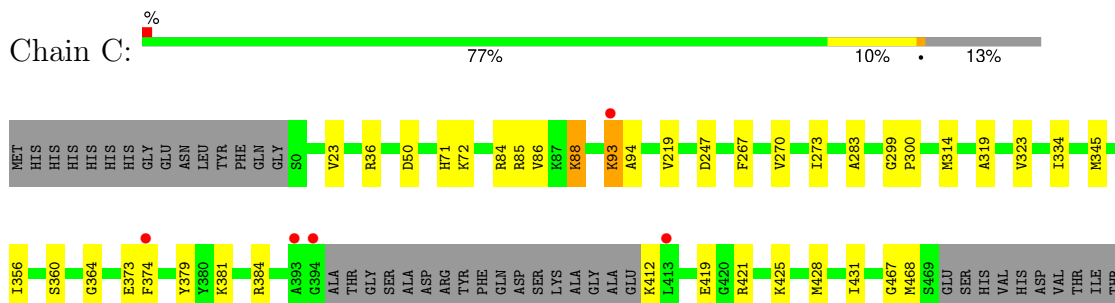
LYS GLU ALA PRO ASN TYR ARG VAL GLY

• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain D:

• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain E:

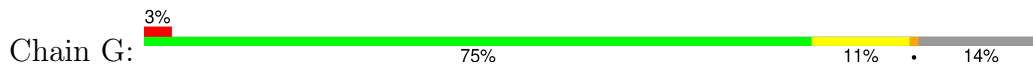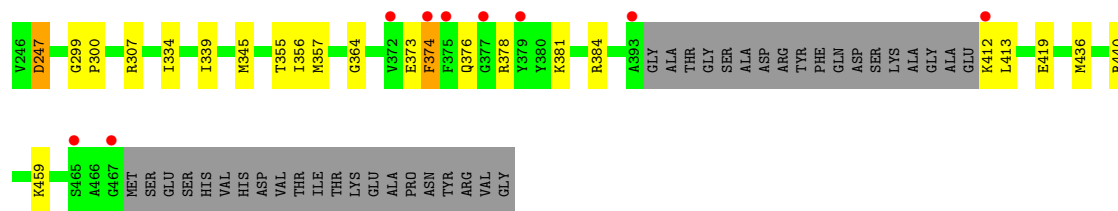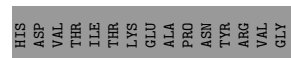• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain F:

• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain G:

• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain H:
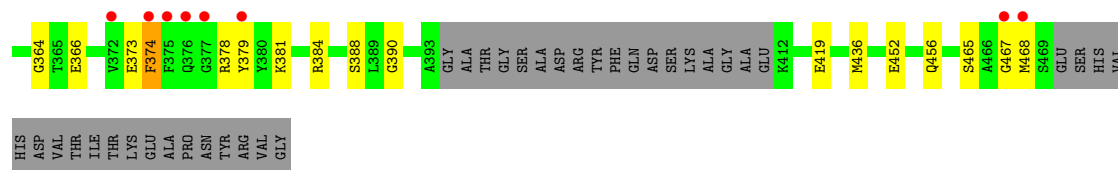
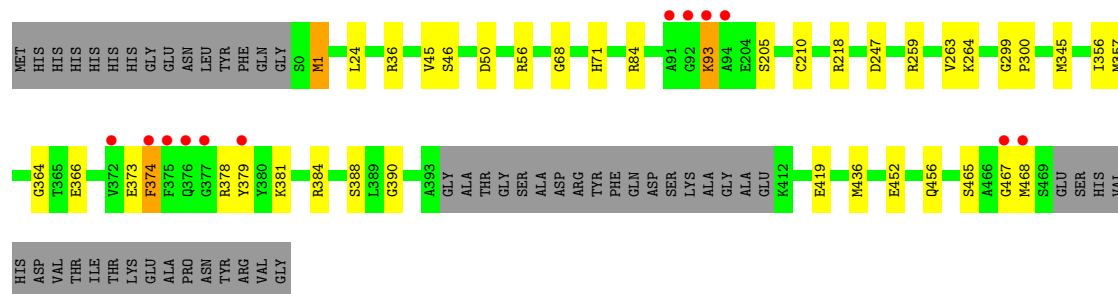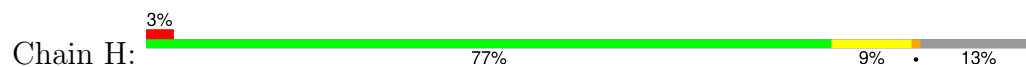# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.73Å 127.28Å 126.70Å 90.00° 104.78° 90.00°	Depositor
Resolution (Å)	46.54 – 1.83 46.54 – 1.83	Depositor EDS
% Data completeness (in resolution range)	88.3 (46.54-1.83) 91.4 (46.54-1.83)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 1.83Å)	Xtriage
Refinement program	PHENIX 1.18.2-3874_final	Depositor
R, R_{free}	0.135 , 0.186 0.136 , 0.186	Depositor DCC
R_{free} test set	13763 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	23.2	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.9	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	22919	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: VOA, IMP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.28	0/2576	0.49	0/3477
1	B	0.28	0/2565	0.48	0/3463
1	C	0.28	0/2573	0.48	0/3473
1	D	0.27	0/2569	0.48	0/3468
1	E	0.27	0/2563	0.48	0/3461
1	F	0.27	0/2563	0.47	0/3461
1	G	0.27	0/2555	0.48	0/3450
1	H	0.27	0/2569	0.48	0/3468
All	All	0.27	0/20533	0.48	0/27721

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2544	0	2605	37	0
1	B	2533	0	2591	41	0
1	C	2541	0	2601	27	0
1	D	2537	0	2598	26	0
1	E	2531	0	2594	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2531	0	2594	34	0
1	G	2523	0	2584	32	1
1	H	2537	0	2598	32	0
2	A	23	13	11	0	0
2	B	23	13	11	0	0
2	C	23	13	11	0	0
2	D	23	13	11	0	0
2	E	23	13	11	0	0
2	F	23	13	11	0	0
2	G	23	13	11	0	0
2	H	23	13	11	0	0
3	A	27	1	0	0	0
3	B	27	1	0	0	0
3	C	27	1	0	0	0
3	D	27	1	0	0	0
3	E	27	1	0	0	0
3	F	27	1	0	0	0
3	G	27	1	0	0	0
3	H	27	1	0	0	0
4	A	319	0	0	12	2
4	B	295	0	0	14	1
4	C	275	0	0	6	1
4	D	279	0	0	6	2
4	E	243	0	0	6	1
4	F	253	0	0	9	2
4	G	236	0	0	8	2
4	H	230	0	0	7	2
All	All	22807	112	20853	253	7

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (253) 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:D:345[A]:MET:HG2	1:D:356:ILE:HD13	1.47	0.95
1:C:345[A]:MET:HG2	1:C:356:ILE:HD13	1.48	0.95
1:A:465:SER:HA	1:A:468:MET:HE2	1.47	0.94
1:B:345[A]:MET:HG2	1:B:356:ILE:HD13	1.49	0.94
1:H:345[B]:MET:HG2	1:H:356:ILE:HD13	1.51	0.93
1:A:345:MET:HG2	1:A:356:ILE:HD13	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:345[A]:MET:HG2	1:H:356:ILE:HD13	1.55	0.84
1:B:345[B]:MET:HG2	1:B:356:ILE:HD13	1.61	0.81
1:A:88:LYS:HE3	4:A:1139:HOH:O	1.80	0.81
1:D:84:ARG:O	1:D:88:LYS:HG3	1.81	0.80
1:E:456:GLN:HG3	4:E:1106:HOH:O	1.81	0.80
1:B:307[A]:ARG:NH1	1:C:467:GLY:O	2.14	0.80
1:B:412:LYS:HA	4:B:1131:HOH:O	1.83	0.79
1:D:345[B]:MET:HG2	1:D:356:ILE:HD13	1.63	0.79
1:C:345[B]:MET:HG2	1:C:356:ILE:HD13	1.63	0.78
1:E:373:GLU:OE2	1:E:421:ARG:NE	2.16	0.77
1:B:459:LYS:NZ	4:B:902:HOH:O	2.17	0.77
1:A:84:ARG:O	1:A:88:LYS:HG3	1.86	0.76
1:D:288:ASP:HB3	4:D:1140:HOH:O	1.86	0.76
1:B:23:VAL:HG13	4:B:965:HOH:O	1.84	0.75
1:C:84:ARG:O	1:C:88:LYS:HG3	1.87	0.74
1:E:467:GLY:HA3	4:H:1077:HOH:O	1.88	0.73
1:C:384:ARG:HB3	1:C:419:GLU:HG3	1.72	0.72
1:E:307[B]:ARG:NH2	4:E:901:HOH:O	2.20	0.72
1:A:465:SER:HA	1:A:468:MET:CE	2.19	0.72
1:E:43:PRO:O	1:E:356[B]:ILE:HD13	1.90	0.72
1:A:459:LYS:HE3	4:A:977:HOH:O	1.88	0.71
1:A:378:ARG:HH21	1:E:378:ARG:HH21	1.38	0.71
1:A:1:MET:HG2	4:B:1171:HOH:O	1.91	0.71
1:F:43:PRO:O	1:F:356[B]:ILE:HD13	1.91	0.71
1:D:345[A]:MET:HG2	1:D:356:ILE:CD1	2.19	0.70
1:A:88:LYS:HB3	4:A:1165:HOH:O	1.92	0.70
1:C:345[A]:MET:HG2	1:C:356:ILE:CD1	2.22	0.70
1:A:247:ASP:OD1	4:A:901:HOH:O	2.11	0.69
1:F:374:PHE:HE1	1:F:377:GLY:HA2	1.57	0.68
1:B:72:LYS:NZ	4:B:903:HOH:O	2.23	0.68
1:D:23:VAL:HG22	4:D:923:HOH:O	1.94	0.67
1:D:23:VAL:HG13	4:D:1081:HOH:O	1.94	0.67
1:F:261:ARG:NH1	4:F:903:HOH:O	2.28	0.66
1:C:428:MET:O	1:C:431:ILE:HG22	1.94	0.66
1:G:459:LYS:HE2	4:G:1056:HOH:O	1.95	0.66
1:G:84:ARG:HD3	4:G:1086:HOH:O	1.94	0.66
1:H:384:ARG:HB2	1:H:419:GLU:HG2	1.78	0.66
1:C:85:ARG:HD2	4:C:1134:HOH:O	1.97	0.64
1:E:374:PHE:CE2	1:E:377:GLY:HA2	2.33	0.64
1:B:85:ARG:HD2	4:B:1091:HOH:O	1.97	0.64
1:G:384:ARG:HB3	1:G:419:GLU:HG3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:374:PHE:HA	1:H:378:ARG:O	1.97	0.63
1:F:3:THR:HG21	1:G:459:LYS:HD2	1.80	0.63
1:E:466:ALA:HB2	1:H:468:MET:CE	2.29	0.63
1:E:84:ARG:O	1:E:88:LYS:HG2	1.99	0.63
1:D:386:MET:HE2	4:D:1101:HOH:O	2.00	0.62
1:A:3:THR:HG21	1:B:459:LYS:HD3	1.81	0.62
1:G:374:PHE:HA	1:G:378:ARG:O	1.99	0.62
1:C:36:ARG:NH2	4:C:901:HOH:O	2.25	0.62
1:G:412:LYS:HE2	4:G:997:HOH:O	1.99	0.62
1:H:345[B]:MET:HG2	1:H:356:ILE:CD1	2.27	0.62
1:H:364:GLY:HA2	1:H:381:LYS:HB2	1.81	0.62
1:F:374:PHE:HE1	1:F:377:GLY:CA	2.13	0.61
1:A:261:ARG:NH1	4:A:904:HOH:O	2.33	0.61
1:G:339:ILE:HG13	1:G:356:ILE:CG2	2.30	0.61
1:F:384:ARG:HB3	1:F:419:GLU:HG3	1.82	0.61
1:A:466:ALA:HB2	1:D:468:MET:SD	2.40	0.61
1:B:366:GLU:HG3	4:B:919:HOH:O	2.01	0.61
1:E:466:ALA:HB2	1:H:468:MET:SD	2.41	0.61
1:B:378:ARG:HD3	4:B:1035:HOH:O	2.00	0.60
1:A:435:MET:HE1	4:A:1091:HOH:O	2.02	0.59
1:B:36:ARG:NH2	4:B:905:HOH:O	2.31	0.59
1:E:374:PHE:CZ	1:E:377:GLY:HA2	2.37	0.59
1:G:91:ALA:HB1	1:G:204:GLU:HG2	1.84	0.58
1:A:82:GLU:OE1	1:A:85:ARG:NH1	2.36	0.58
1:A:384:ARG:HB3	1:A:419:GLU:HG3	1.83	0.58
1:A:412:LYS:N	4:A:905:HOH:O	2.36	0.58
1:A:345:MET:HG2	1:A:356:ILE:CD1	2.29	0.58
1:B:36:ARG:NH1	4:B:907:HOH:O	2.31	0.57
1:H:56:ARG:NH1	1:H:366:GLU:OE1	2.36	0.57
1:H:373:GLU:O	1:H:373:GLU:HG3	2.04	0.57
1:F:459:LYS:HE3	4:F:951:HOH:O	2.05	0.57
1:E:50:ASP:HA	1:E:71:HIS:CD2	2.40	0.56
1:D:384:ARG:HB3	1:D:419:GLU:HG3	1.87	0.56
1:A:88:LYS:HD2	4:A:922:HOH:O	2.06	0.56
1:B:245:VAL:HG12	1:B:247:ASP:HB3	1.86	0.56
1:H:93:LYS:H	1:H:93:LYS:HD3	1.71	0.55
1:F:85:ARG:HD3	4:F:918:HOH:O	2.06	0.55
4:A:1042:HOH:O	1:D:1:MET:HE1	2.05	0.55
1:C:384:ARG:CB	1:C:419:GLU:HG3	2.36	0.55
1:H:50:ASP:HA	1:H:71:HIS:CD2	2.42	0.55
1:D:247:ASP:OD2	4:D:901:HOH:O	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:GLU:HG3	1:E:369:PRO:HG3	1.89	0.55
1:E:364:GLY:HA2	1:E:381:LYS:HB2	1.88	0.55
1:B:435:MET:HE1	4:B:1046:HOH:O	2.07	0.54
1:B:345[A]:MET:HG2	1:B:356:ILE:CD1	2.29	0.54
1:E:345[B]:MET:HE3	1:E:356[B]:ILE:HD11	1.89	0.54
1:H:36:ARG:NH2	4:H:906:HOH:O	2.37	0.54
1:B:384:ARG:HB3	1:B:419:GLU:HG3	1.89	0.54
1:B:86:VAL:HG11	1:B:219:VAL:HB	1.89	0.54
1:B:299:GLY:N	1:B:300:PRO:CD	2.71	0.54
1:D:384:ARG:CB	1:D:419:GLU:HG3	2.38	0.54
1:F:364:GLY:HA2	1:F:381:LYS:HB2	1.90	0.54
1:C:364:GLY:HA2	1:C:381:LYS:HB2	1.90	0.53
1:A:258:GLU:HG2	4:A:904:HOH:O	2.09	0.53
1:B:459:LYS:HG3	4:B:1175:HOH:O	2.08	0.53
1:A:431:ILE:N	1:A:431:ILE:HD12	2.24	0.53
1:C:299:GLY:N	1:C:300:PRO:CD	2.72	0.53
1:G:376:GLN:O	1:G:376:GLN:HG3	2.08	0.53
1:F:339:ILE:HG13	1:F:356[A]:ILE:CG2	2.39	0.53
1:G:307[A]:ARG:NH1	1:H:467:GLY:O	2.42	0.53
1:F:93:LYS:HG2	4:F:902:HOH:O	2.09	0.52
1:C:345[B]:MET:HG2	1:C:356:ILE:CD1	2.37	0.52
1:A:23:VAL:HB	4:A:972:HOH:O	2.08	0.52
1:F:384:ARG:CB	1:F:419:GLU:HG3	2.40	0.52
1:G:364:GLY:HA2	1:G:381:LYS:HB2	1.91	0.52
1:D:54:GLU:HG3	1:D:369:PRO:HG3	1.91	0.52
1:E:339:ILE:HG13	1:E:356[A]:ILE:CG2	2.39	0.52
1:D:374:PHE:CZ	1:D:377:GLY:HA2	2.44	0.52
1:G:50:ASP:HA	1:G:71:HIS:CD2	2.44	0.52
1:G:204:GLU:HG3	1:G:206:TYR:CE1	2.44	0.52
1:A:431:ILE:HD12	1:A:431:ILE:H	1.75	0.51
1:A:364:GLY:HA2	1:A:381:LYS:HB2	1.93	0.51
1:H:345[A]:MET:HG2	1:H:356:ILE:CD1	2.32	0.51
1:F:299:GLY:N	1:F:300:PRO:CD	2.73	0.51
1:A:307[A]:ARG:NH1	1:B:467:GLY:O	2.44	0.51
1:E:345[B]:MET:HE3	1:E:436:MET:HE1	1.92	0.50
1:A:299:GLY:N	1:A:300:PRO:CD	2.74	0.50
1:E:299:GLY:N	1:E:300:PRO:CD	2.74	0.50
1:H:299:GLY:N	1:H:300:PRO:CD	2.74	0.50
1:G:225:THR:O	4:G:901:HOH:O	2.19	0.50
1:D:299:GLY:N	1:D:300:PRO:CD	2.75	0.50
1:B:428:MET:O	1:B:431:ILE:HG22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:374:PHE:CE1	1:F:377:GLY:HA2	2.43	0.49
1:G:299:GLY:N	1:G:300:PRO:CD	2.75	0.49
1:B:364:GLY:HA2	1:B:381:LYS:HB2	1.94	0.49
1:H:36:ARG:NH2	4:H:912:HOH:O	2.46	0.49
1:G:31:LYS:HD2	4:G:1037:HOH:O	2.12	0.49
1:C:412:LYS:N	4:C:910:HOH:O	2.45	0.49
1:A:1:MET:HB2	1:B:325:SER:OG	2.13	0.49
1:B:23:VAL:HG11	1:B:449:ALA:HB2	1.94	0.49
1:D:345[B]:MET:HE2	1:D:356:ILE:HD11	1.94	0.49
1:E:245:VAL:HG12	1:E:247:ASP:HB3	1.94	0.49
1:F:355:THR:O	1:F:356[A]:ILE:HD13	2.13	0.49
1:B:0:SER:HB2	4:B:1160:HOH:O	2.11	0.49
1:G:24:LEU:HD12	4:G:1065:HOH:O	2.12	0.48
1:B:1:MET:HG3	4:C:1157:HOH:O	2.13	0.48
1:C:23:VAL:HB	4:C:909:HOH:O	2.12	0.48
1:A:378:ARG:HB2	1:A:380:TYR:CE2	2.49	0.48
1:F:412:LYS:HD3	1:F:412:LYS:N	2.28	0.48
1:D:23:VAL:HG11	1:D:449:ALA:HB2	1.95	0.48
1:E:345[B]:MET:CE	1:E:356[B]:ILE:HD11	2.43	0.48
1:B:210:CYS:SG	1:B:218:ARG:HG3	2.54	0.48
1:A:283:ALA:HB2	1:A:323:VAL:HG13	1.95	0.47
1:G:373:GLU:O	1:G:373:GLU:HG3	2.13	0.47
1:F:50:ASP:HA	1:F:71:HIS:CD2	2.49	0.47
1:G:345[A]:MET:HE3	1:G:436:MET:HE1	1.97	0.47
1:C:86:VAL:HG11	1:C:219:VAL:HB	1.96	0.47
1:H:24:LEU:HD12	4:H:1099:HOH:O	2.15	0.47
1:G:54:GLU:HB3	1:G:82:GLU:OE2	2.15	0.46
1:G:384:ARG:CB	1:G:419:GLU:HG3	2.44	0.46
1:E:430:ASN:ND2	4:E:903:HOH:O	2.25	0.46
1:H:345[B]:MET:HE3	1:H:436:MET:HE1	1.97	0.46
1:A:384:ARG:CB	1:A:419:GLU:HG3	2.45	0.46
1:E:452:GLU:O	1:E:456:GLN:HG2	2.15	0.46
1:B:7:GLU:OE1	1:B:462:LYS:HE3	2.15	0.46
1:E:247:ASP:HB2	4:E:1035:HOH:O	2.15	0.46
1:H:264:LYS:HA	4:H:985:HOH:O	2.15	0.46
1:A:254:ALA:O	1:A:258:GLU:HG3	2.16	0.46
1:D:86:VAL:HG11	1:D:219:VAL:HB	1.98	0.46
1:E:356[B]:ILE:HG12	1:E:356[B]:ILE:O	2.16	0.46
1:B:82:GLU:OE1	1:B:85:ARG:NH2	2.49	0.46
1:G:345[A]:MET:HE2	1:G:345[A]:MET:HB3	1.72	0.46
1:F:428:MET:O	1:F:431:ILE:HG22	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345[B]:MET:SD	1:D:356:ILE:HD11	2.56	0.45
1:E:325:SER:OG	1:H:1:MET:HB2	2.16	0.45
1:F:373:GLU:O	1:F:373:GLU:HG3	2.16	0.45
1:G:86:VAL:HG11	1:G:219:VAL:HB	1.97	0.45
1:H:356:ILE:O	1:H:356:ILE:HG13	2.17	0.45
1:H:210:CYS:SG	1:H:218:ARG:HG3	2.56	0.45
1:G:45:VAL:O	1:G:357:MET:HA	2.17	0.45
1:G:214:LEU:HD13	4:G:1096:HOH:O	2.16	0.45
1:F:288:ASP:OD2	4:F:901:HOH:O	2.21	0.45
1:E:299:GLY:O	1:E:307[B]:ARG:HD3	2.17	0.45
1:F:379:TYR:N	4:F:912:HOH:O	2.48	0.45
1:H:390:GLY:HA3	1:H:419:GLU:OE2	2.16	0.45
1:B:50:ASP:HA	1:B:71:HIS:CD2	2.52	0.45
1:D:36:ARG:NH2	4:D:905:HOH:O	2.47	0.44
1:B:389:LEU:HD23	1:B:389:LEU:HA	1.77	0.44
1:F:33:ARG:HA	1:F:39:TYR:HA	1.99	0.44
1:H:46:SER:OG	1:H:68:GLY:HA2	2.18	0.44
1:F:24:LEU:HD12	4:F:1108:HOH:O	2.17	0.44
1:A:50:ASP:HA	1:A:71:HIS:CD2	2.52	0.44
1:E:45:VAL:O	1:E:357:MET:HA	2.18	0.44
1:F:307[B]:ARG:NH2	4:F:916:HOH:O	2.50	0.43
1:B:374:PHE:CZ	1:B:377:GLY:HA2	2.54	0.43
1:D:50:ASP:HA	1:D:71:HIS:CD2	2.53	0.43
1:C:93:LYS:O	1:C:94:ALA:HB3	2.19	0.43
1:F:3:THR:CG2	1:G:459:LYS:HD2	2.48	0.43
1:B:84:ARG:O	1:B:88:LYS:HG3	2.19	0.43
1:E:24:LEU:HD12	4:E:1095:HOH:O	2.17	0.43
1:F:366:GLU:OE1	1:F:424:TYR:OH	2.27	0.43
1:H:205:SER:HA	4:H:941:HOH:O	2.18	0.43
1:H:388:SER:HB2	1:H:419:GLU:HG3	2.01	0.43
1:H:452:GLU:O	1:H:456:GLN:HG2	2.19	0.43
1:A:468:MET:SD	1:B:466:ALA:HB2	2.58	0.43
1:A:26:LYS:HE3	4:A:979:HOH:O	2.18	0.43
1:C:267:PHE:O	1:C:270:VAL:HG12	2.18	0.43
1:D:360[A]:SER:O	1:D:425:LYS:NZ	2.52	0.43
1:E:33:ARG:HA	1:E:39:TYR:HA	2.01	0.43
1:F:93:LYS:HE2	1:F:93:LYS:HB3	1.86	0.43
1:G:334:ILE:HG12	1:G:355:THR:OG1	2.19	0.43
1:C:360[A]:SER:O	1:C:425:LYS:NZ	2.53	0.42
1:D:210:CYS:SG	1:D:218:ARG:HG3	2.59	0.42
1:F:264:LYS:HD2	1:F:264:LYS:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360[A]:SER:O	1:A:425:LYS:NZ	2.52	0.42
1:F:86:VAL:HG11	1:F:219:VAL:HB	2.01	0.42
1:F:93:LYS:HD2	1:F:93:LYS:O	2.20	0.42
1:B:10:THR:HG22	1:B:13:ASP:OD2	2.18	0.42
1:C:374:PHE:HD1	1:C:379:TYR:CZ	2.37	0.42
1:H:259:ARG:O	1:H:263:VAL:HG23	2.19	0.42
1:A:345:MET:HB3	1:A:345:MET:HE2	1.62	0.42
1:C:283:ALA:HB2	1:C:323:VAL:HG13	2.01	0.42
1:F:334:ILE:HG12	1:F:355:THR:OG1	2.19	0.42
1:C:72:LYS:NZ	4:C:906:HOH:O	2.40	0.41
1:E:376:GLN:HG3	1:E:376:GLN:O	2.20	0.41
1:F:264:LYS:HD2	4:F:957:HOH:O	2.20	0.41
1:B:273:ILE:HD13	1:B:334:ILE:HD11	2.01	0.41
1:B:384:ARG:CB	1:B:419:GLU:HG3	2.49	0.41
1:C:50:ASP:HA	1:C:71:HIS:CD2	2.55	0.41
1:E:73:ASN:HB2	1:E:386:MET:HE1	2.03	0.41
1:E:419:GLU:OE1	4:E:902:HOH:O	2.22	0.41
1:D:452:GLU:O	1:D:456:GLN:HG2	2.20	0.41
1:H:374:PHE:HA	1:H:379:TYR:HA	2.03	0.41
1:G:307[B]:ARG:NH2	4:G:918:HOH:O	2.53	0.41
1:C:273:ILE:HD13	1:C:334:ILE:HD11	2.02	0.41
1:C:345[A]:MET:HB3	1:C:345[A]:MET:HE3	1.74	0.41
1:G:33:ARG:HA	1:G:39:TYR:HA	2.03	0.41
1:D:13:ASP:HA	1:D:468:MET:HE1	2.01	0.41
1:E:388:SER:HB2	1:E:419:GLU:HG2	2.03	0.41
1:B:345[A]:MET:HE2	1:B:345[A]:MET:HB3	1.48	0.41
1:B:345[A]:MET:SD	1:B:356:ILE:HD11	2.61	0.41
1:E:54:GLU:HG3	1:E:369:PRO:CG	2.49	0.41
1:E:308:ILE:HG23	1:F:341:PHE:CG	2.55	0.41
1:G:245:VAL:HG12	1:G:247:ASP:HB2	2.02	0.41
1:E:345[B]:MET:HE2	1:E:345[B]:MET:HB3	1.60	0.41
1:E:83:VAL:O	1:E:87:LYS:HG2	2.20	0.40
1:E:428:MET:O	1:E:431:ILE:HG22	2.21	0.40
1:G:28:VAL:CG2	1:G:440:ARG:HG2	2.50	0.40
1:A:273:ILE:HG12	1:A:293:ALA:HB3	2.03	0.40
1:C:314:MET:HG3	1:C:319:ALA:HB2	2.02	0.40
1:E:54:GLU:HB3	1:E:82:GLU:OE2	2.21	0.40
1:F:254:ALA:HB2	1:G:22:THR:HG22	2.04	0.40
1:H:45:VAL:O	1:H:357:MET:HA	2.22	0.40
1:H:84:ARG:HD3	4:H:1052:HOH:O	2.21	0.40
4:B:929:HOH:O	1:C:468:MET:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:TYR:CG	1:B:421:ARG:HD3	2.57	0.40

All (7) 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)
4:D:1088:HOH:O	4:G:1017:HOH:O[2_545]	1.94	0.26
1:G:92:GLY:O	4:F:902:HOH:O[2_555]	1.95	0.25
4:C:1111:HOH:O	4:F:920:HOH:O[2_555]	1.97	0.23
4:A:1054:HOH:O	4:H:1031:HOH:O[2_546]	1.98	0.22
4:D:1088:HOH:O	4:G:1006:HOH:O[2_545]	1.99	0.21
4:A:1054:HOH:O	4:H:908:HOH:O[2_546]	2.08	0.12
4:B:1051:HOH:O	4:E:1062:HOH:O[2_556]	2.13	0.07

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	346/395 (88%)	337 (97%)	9 (3%)	0	100	100
1	B	345/395 (87%)	338 (98%)	7 (2%)	0	100	100
1	C	346/395 (88%)	338 (98%)	8 (2%)	0	100	100
1	D	345/395 (87%)	338 (98%)	7 (2%)	0	100	100
1	E	344/395 (87%)	336 (98%)	8 (2%)	0	100	100
1	F	344/395 (87%)	335 (97%)	9 (3%)	0	100	100
1	G	343/395 (87%)	333 (97%)	10 (3%)	0	100	100
1	H	345/395 (87%)	337 (98%)	8 (2%)	0	100	100
All	All	2758/3160 (87%)	2692 (98%)	66 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/298 (88%)	257 (98%)	6 (2%)	45	29
1	B	262/298 (88%)	255 (97%)	7 (3%)	40	22
1	C	263/298 (88%)	258 (98%)	5 (2%)	52	36
1	D	263/298 (88%)	256 (97%)	7 (3%)	40	22
1	E	262/298 (88%)	260 (99%)	2 (1%)	79	72
1	F	262/298 (88%)	257 (98%)	5 (2%)	52	36
1	G	261/298 (88%)	257 (98%)	4 (2%)	60	47
1	H	263/298 (88%)	258 (98%)	5 (2%)	52	36
All	All	2099/2384 (88%)	2058 (98%)	41 (2%)	50	35

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	LYS
1	A	204	GLU
1	A	247	ASP
1	A	314	MET
1	A	378	ARG
1	A	413	LEU
1	B	23	VAL
1	B	85	ARG
1	B	88	LYS
1	B	93	LYS
1	B	204	GLU
1	B	214	LEU
1	B	389	LEU
1	C	88	LYS
1	C	93	LYS
1	C	247	ASP
1	C	373	GLU
1	C	421	ARG
1	D	88	LYS

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Mol	Chain	Res	Type
1	D	93	LYS
1	D	247	ASP
1	D	314	MET
1	D	376	GLN
1	D	389	LEU
1	D	434	GLN
1	E	314	MET
1	E	413	LEU
1	F	247	ASP
1	F	374	PHE
1	F	376	GLN
1	F	389	LEU
1	F	412	LYS
1	G	7	GLU
1	G	247	ASP
1	G	374	PHE
1	G	413	LEU
1	H	1	MET
1	H	93	LYS
1	H	247	ASP
1	H	374	PHE
1	H	465	SER

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

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	IMP	B	801	-	21,25,25	0.80	0	22,38,38	0.72	0
2	IMP	F	801	-	21,25,25	0.74	0	22,38,38	0.71	0
3	VOA	B	802	-	29,30,30	0.61	0	38,42,42	1.71	7 (18%)
2	IMP	C	801	-	21,25,25	0.78	0	22,38,38	0.73	0
3	VOA	F	802	-	29,30,30	0.64	1 (3%)	38,42,42	1.63	6 (15%)
2	IMP	E	801	-	21,25,25	0.78	0	22,38,38	0.70	0
2	IMP	D	801	-	21,25,25	0.76	0	22,38,38	0.68	0
3	VOA	C	802	-	29,30,30	0.61	0	38,42,42	1.65	6 (15%)
2	IMP	H	801	-	21,25,25	0.82	0	22,38,38	0.74	0
2	IMP	G	801	-	21,25,25	0.78	1 (4%)	22,38,38	0.71	0
3	VOA	E	802	-	29,30,30	0.61	0	38,42,42	1.60	6 (15%)
3	VOA	D	802	-	29,30,30	0.60	0	38,42,42	1.67	7 (18%)
3	VOA	A	802	-	29,30,30	0.61	0	38,42,42	1.71	7 (18%)
2	IMP	A	801	-	21,25,25	0.82	0	22,38,38	0.68	0
3	VOA	G	802	-	29,30,30	0.62	1 (3%)	38,42,42	1.71	7 (18%)
3	VOA	H	802	-	29,30,30	0.63	0	38,42,42	1.60	7 (18%)

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	IMP	B	801	-	-	0/6/26/26	0/3/3/3
2	IMP	F	801	-	-	0/6/26/26	0/3/3/3
3	VOA	B	802	-	-	0/12/19/19	0/4/4/4
2	IMP	C	801	-	-	0/6/26/26	0/3/3/3
3	VOA	F	802	-	-	0/12/19/19	0/4/4/4
2	IMP	E	801	-	-	0/6/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMP	D	801	-	-	0/6/26/26	0/3/3/3
3	VOA	C	802	-	-	0/12/19/19	0/4/4/4
2	IMP	H	801	-	-	0/6/26/26	0/3/3/3
2	IMP	G	801	-	-	0/6/26/26	0/3/3/3
3	VOA	E	802	-	-	0/12/19/19	0/4/4/4
3	VOA	D	802	-	-	0/12/19/19	0/4/4/4
3	VOA	A	802	-	-	0/12/19/19	0/4/4/4
2	IMP	A	801	-	-	0/6/26/26	0/3/3/3
3	VOA	G	802	-	-	0/12/19/19	0/4/4/4
3	VOA	H	802	-	-	0/12/19/19	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	802	VOA	C18-N24	-2.15	1.33	1.37
3	G	802	VOA	C18-N24	-2.05	1.34	1.37
2	G	801	IMP	C8-N7	-2.04	1.31	1.34

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	802	VOA	C12-N11-C10	5.29	122.68	116.33
3	A	802	VOA	C12-N11-C10	5.23	122.61	116.33
3	C	802	VOA	C12-N11-C10	4.92	122.24	116.33
3	D	802	VOA	C12-N11-C10	4.85	122.16	116.33
3	G	802	VOA	C12-N11-C10	4.84	122.14	116.33
3	E	802	VOA	C12-N11-C10	4.83	122.13	116.33
3	F	802	VOA	C12-N11-C10	4.72	122.00	116.33
3	H	802	VOA	C12-N11-C10	4.69	121.96	116.33
3	G	802	VOA	C7-C12-N11	-4.59	120.27	124.07
3	A	802	VOA	C7-C12-N11	-4.56	120.30	124.07
3	C	802	VOA	C7-C12-N11	-4.56	120.30	124.07
3	B	802	VOA	C7-C12-N11	-4.53	120.32	124.07
3	D	802	VOA	C7-C12-N11	-4.39	120.44	124.07
3	F	802	VOA	C7-C12-N11	-4.34	120.48	124.07
3	H	802	VOA	C7-C12-N11	-4.33	120.48	124.07
3	E	802	VOA	C7-C12-N11	-4.26	120.55	124.07
3	G	802	VOA	C23-N24-C18	3.93	121.51	116.96
3	H	802	VOA	C23-N24-C18	3.89	121.46	116.96
3	C	802	VOA	C23-N24-C18	3.87	121.44	116.96
3	F	802	VOA	C23-N24-C18	3.85	121.41	116.96
3	E	802	VOA	C23-N24-C18	3.83	121.40	116.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	802	VOA	C23-N24-C18	3.81	121.37	116.96
3	A	802	VOA	C23-N24-C18	3.67	121.21	116.96
3	D	802	VOA	C23-N24-C18	3.61	121.13	116.96
3	A	802	VOA	C9-C10-N11	-3.10	120.36	124.87
3	B	802	VOA	C9-C10-N11	-3.02	120.49	124.87
3	C	802	VOA	C9-C10-N11	-2.95	120.59	124.87
3	G	802	VOA	C9-C10-N11	-2.94	120.60	124.87
3	D	802	VOA	C9-C10-N11	-2.90	120.65	124.87
3	E	802	VOA	C9-C10-N11	-2.83	120.76	124.87
3	F	802	VOA	C9-C10-N11	-2.79	120.82	124.87
3	B	802	VOA	C23-C22-C21	2.68	120.09	118.06
3	F	802	VOA	C19-C18-N24	-2.66	120.00	122.82
3	H	802	VOA	C19-C18-N24	-2.64	120.02	122.82
3	A	802	VOA	C19-C18-N24	-2.61	120.05	122.82
3	C	802	VOA	C19-C18-N24	-2.59	120.08	122.82
3	D	802	VOA	CL13-C10-N11	2.56	120.77	115.98
3	H	802	VOA	C9-C10-N11	-2.55	121.16	124.87
3	G	802	VOA	CL13-C10-N11	2.54	120.73	115.98
3	D	802	VOA	C23-C22-C21	2.53	119.97	118.06
3	A	802	VOA	CL13-C10-N11	2.47	120.60	115.98
3	G	802	VOA	C19-C18-N24	-2.46	120.21	122.82
3	F	802	VOA	CL13-C10-N11	2.46	120.59	115.98
3	E	802	VOA	C19-C18-N24	-2.40	120.28	122.82
3	C	802	VOA	CL13-C10-N11	2.40	120.47	115.98
3	G	802	VOA	C23-C22-C21	2.30	119.80	118.06
3	B	802	VOA	C19-C18-N24	-2.30	120.39	122.82
3	B	802	VOA	CL13-C10-N11	2.22	120.14	115.98
3	E	802	VOA	CL13-C10-N11	2.22	120.13	115.98
3	D	802	VOA	C19-C18-N24	-2.20	120.49	122.82
3	H	802	VOA	CL13-C10-N11	2.16	120.03	115.98
3	H	802	VOA	C23-C22-C21	2.14	119.68	118.06
3	A	802	VOA	C23-C22-C21	2.08	119.63	118.06

There are no chirality outliers.
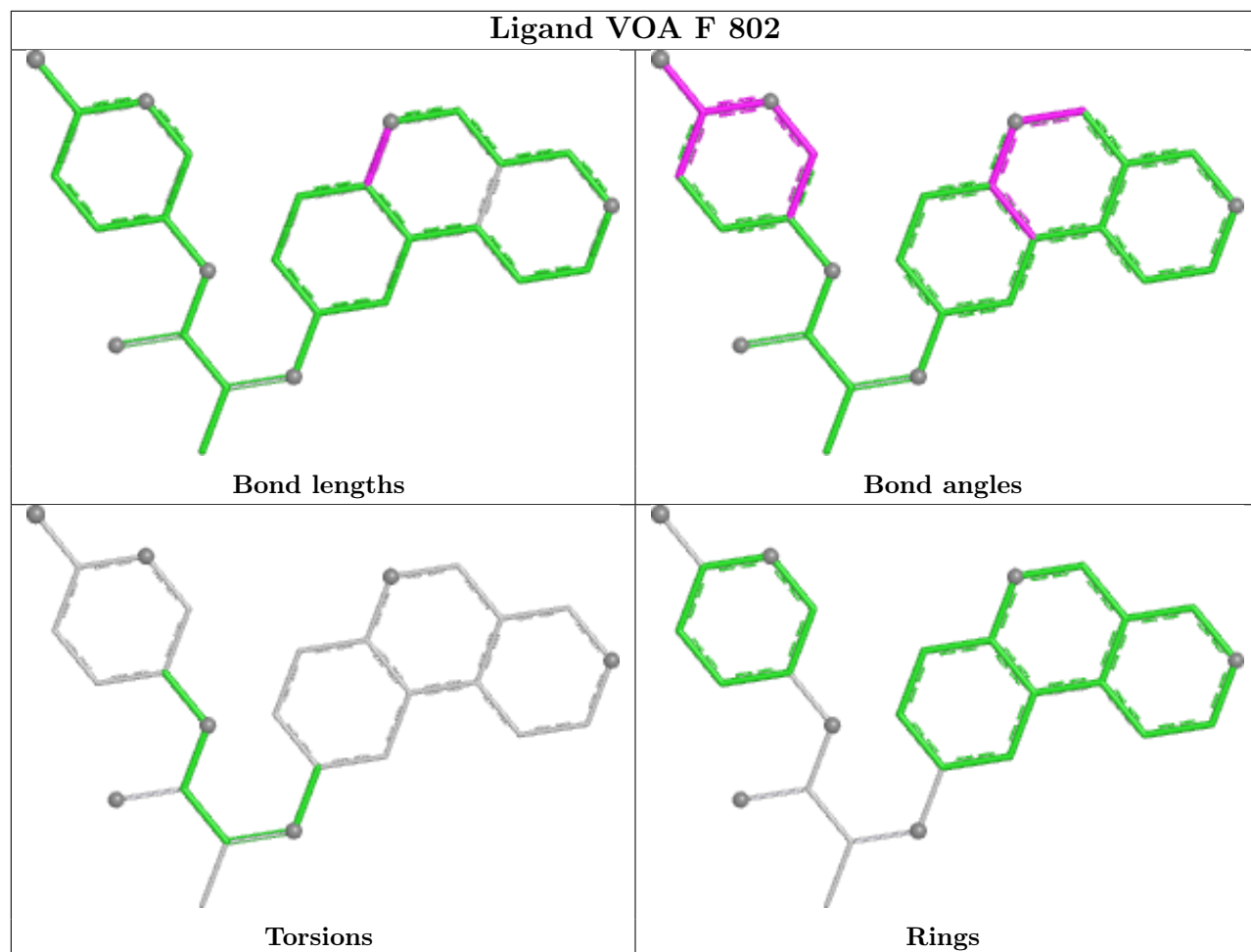
There are no torsion outliers.
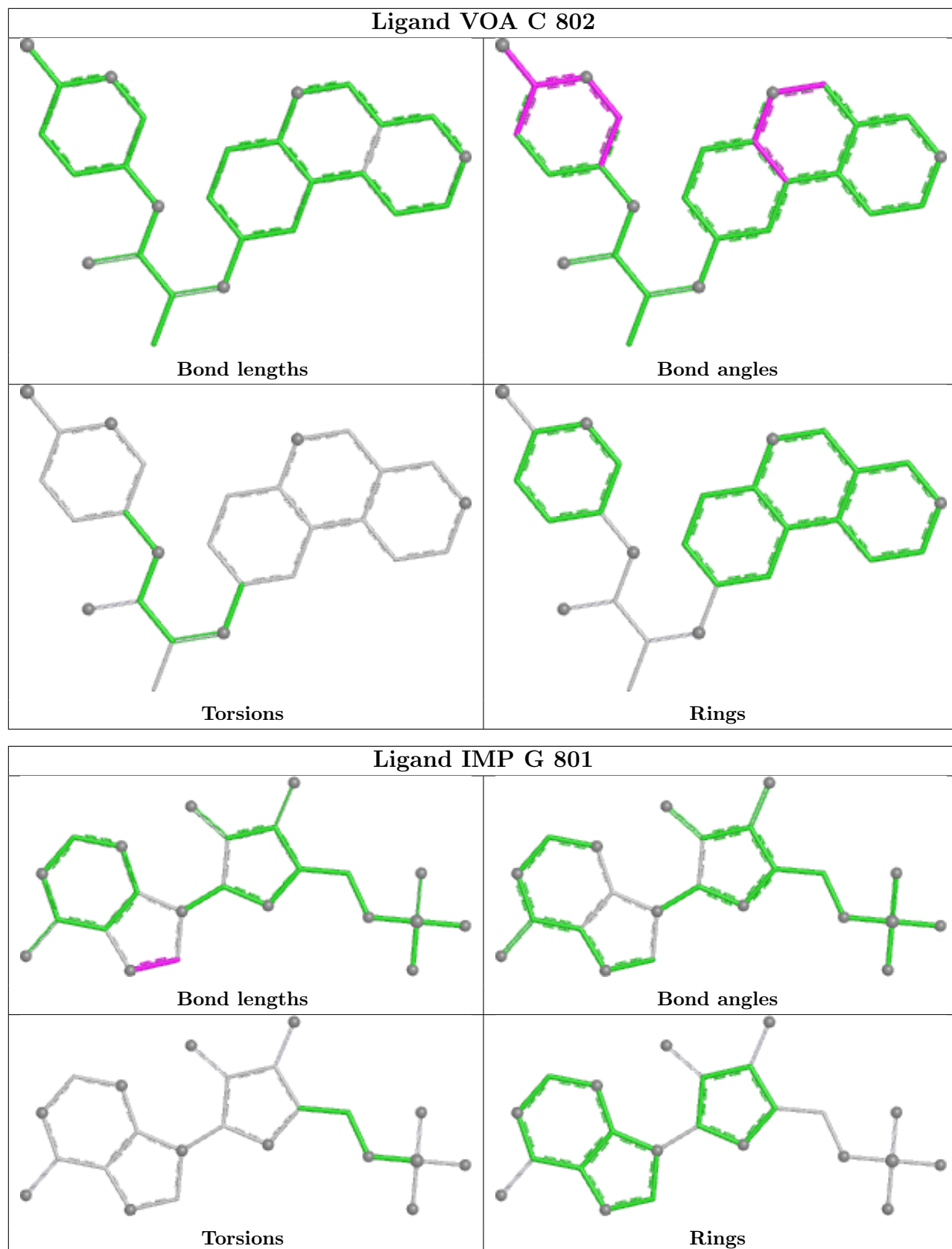
There are no ring outliers.
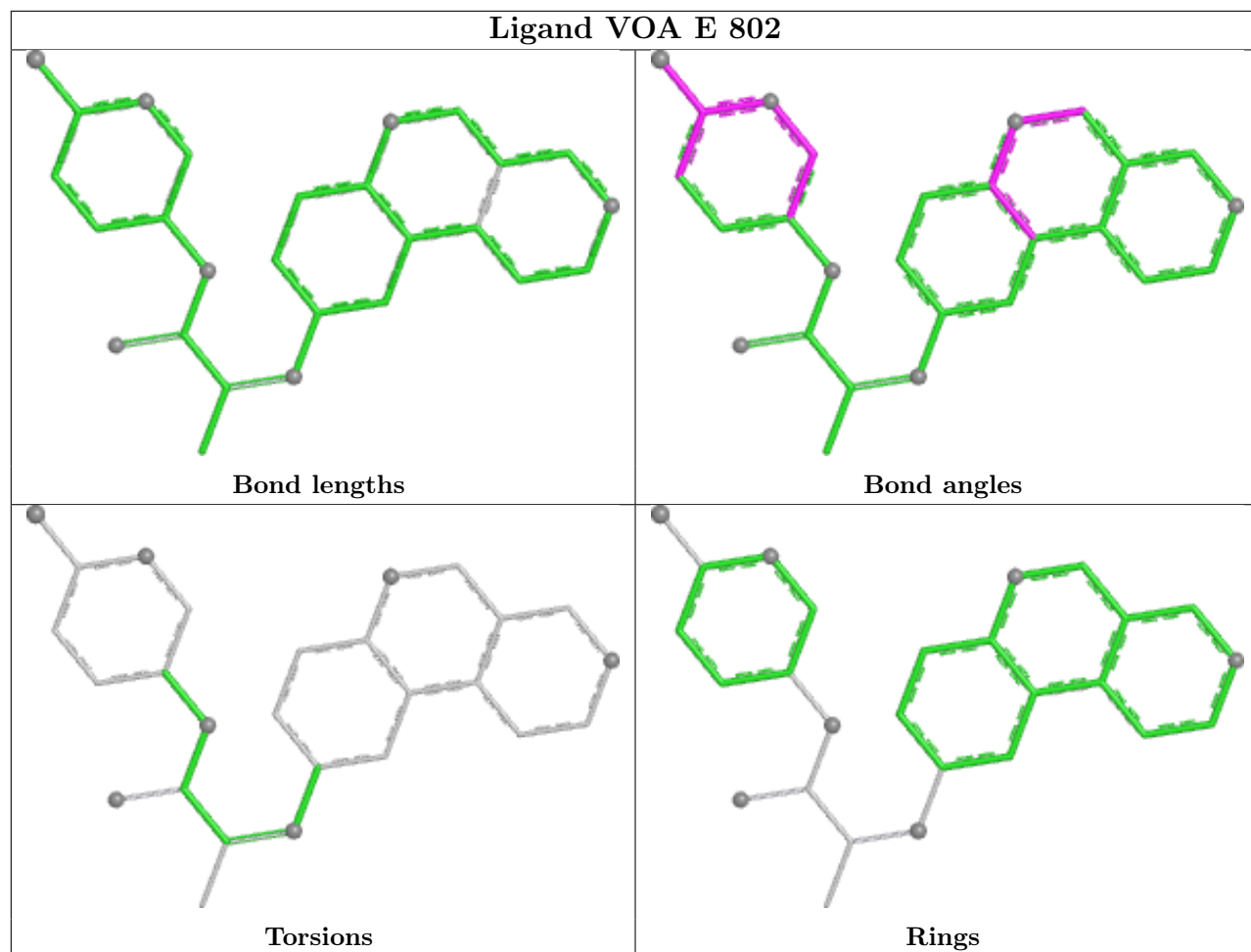
No monomer is involved in short contacts.

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 VOA B 802

Bond lengths

Bond angles

Torsions

Rings

Ligand VOA F 802

Bond lengths

Bond angles

Torsions

Rings

Ligand VOA C 802

Bond lengths

Bond angles

Torsions

Rings

Ligand IMP G 801

Bond lengths

Bond angles

Torsions

Rings

Ligand VOA E 802

Bond lengths

Bond angles

Torsions

Rings

Ligand VOA D 802

Bond lengths

Bond angles

Torsions

Rings

Ligand VOA A 802

Bond lengths

Bond angles

Torsions

Rings

Ligand VOA G 802

Bond lengths

Bond angles

Torsions

Rings

Ligand VOA H 802

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	344/395 (87%)	-0.56	5 (1%)	71	79	10, 24, 60, 90	6 (1%)
1	B	342/395 (86%)	-0.56	8 (2%)	61	66	10, 23, 56, 92	7 (2%)
1	C	344/395 (87%)	-0.47	5 (1%)	71	79	10, 26, 62, 100	6 (1%)
1	D	343/395 (86%)	-0.48	8 (2%)	61	66	11, 27, 60, 95	6 (1%)
1	E	341/395 (86%)	-0.43	10 (2%)	54	58	10, 27, 66, 105	7 (2%)
1	F	341/395 (86%)	-0.40	11 (3%)	50	54	11, 29, 62, 106	7 (2%)
1	G	341/395 (86%)	-0.39	11 (3%)	50	54	10, 28, 66, 105	6 (1%)
1	H	343/395 (86%)	-0.42	12 (3%)	47	50	10, 28, 71, 103	6 (1%)
All	All	2739/3160 (86%)	-0.46	70 (2%)	57	62	10, 26, 64, 106	51 (1%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	374	PHE	5.0
1	C	394	GLY	4.9
1	G	374	PHE	4.5
1	H	94	ALA	4.4
1	F	374	PHE	4.2
1	A	394	GLY	4.2
1	E	374	PHE	3.5
1	H	377	GLY	3.5
1	G	375	PHE	3.5
1	A	467	GLY	3.3
1	G	377	GLY	3.3
1	F	94	ALA	3.2
1	H	92	GLY	3.2
1	D	467	GLY	3.0
1	E	393	ALA	3.0
1	H	467	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	374	PHE	3.0
1	F	377	GLY	2.9
1	G	379	TYR	2.9
1	E	377	GLY	2.9
1	D	468	MET	2.9
1	A	466	ALA	2.8
1	H	91	ALA	2.8
1	F	93	LYS	2.8
1	E	375	PHE	2.7
1	H	379	TYR	2.7
1	A	468	MET	2.7
1	C	393	ALA	2.7
1	F	375	PHE	2.6
1	B	394	GLY	2.6
1	G	204	GLU	2.6
1	C	93	LYS	2.6
1	G	93	LYS	2.6
1	B	94	ALA	2.6
1	D	393	ALA	2.6
1	G	372	VAL	2.5
1	A	94	ALA	2.5
1	G	393	ALA	2.5
1	E	94	ALA	2.5
1	C	374	PHE	2.5
1	H	375	PHE	2.4
1	F	92	GLY	2.4
1	H	468	MET	2.4
1	E	379	TYR	2.4
1	B	374	PHE	2.3
1	F	467	GLY	2.3
1	F	379	TYR	2.3
1	G	467	GLY	2.2
1	B	393	ALA	2.2
1	E	91	ALA	2.2
1	F	393	ALA	2.2
1	D	377	GLY	2.2
1	B	93	LYS	2.2
1	B	412	LYS	2.2
1	D	1	MET	2.2
1	E	92	GLY	2.2
1	E	467	GLY	2.2
1	E	93	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	375	PHE	2.1
1	F	206	TYR	2.1
1	F	465	SER	2.1
1	D	94	ALA	2.1
1	G	465	SER	2.1
1	H	372	VAL	2.1
1	C	413	LEU	2.1
1	H	93	LYS	2.1
1	B	247	ASP	2.0
1	D	375	PHE	2.0
1	G	412	LYS	2.0
1	H	376	GLN	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, 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	IMP	D	801	23/23	0.98	0.04	19,22,28,35	0
3	VOA	A	802	27/27	0.98	0.04	21,23,26,29	0
3	VOA	B	802	27/27	0.98	0.05	21,23,24,27	0
3	VOA	C	802	27/27	0.98	0.05	22,25,28,30	0
3	VOA	D	802	27/27	0.98	0.05	22,25,27,29	0
3	VOA	E	802	27/27	0.98	0.04	23,25,28,32	0
3	VOA	F	802	27/27	0.98	0.04	22,24,26,30	0
3	VOA	G	802	27/27	0.98	0.04	21,24,26,30	0
3	VOA	H	802	27/27	0.98	0.05	22,24,26,31	0
2	IMP	C	801	23/23	0.99	0.04	19,21,26,27	0
2	IMP	A	801	23/23	0.99	0.03	18,21,24,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	IMP	E	801	23/23	0.99	0.03	20,22,27,27	0
2	IMP	F	801	23/23	0.99	0.03	20,24,29,31	0
2	IMP	G	801	23/23	0.99	0.03	19,22,26,28	0
2	IMP	H	801	23/23	0.99	0.03	20,23,27,28	0
2	IMP	B	801	23/23	0.99	0.04	18,22,27,28	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 VOA A 802:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
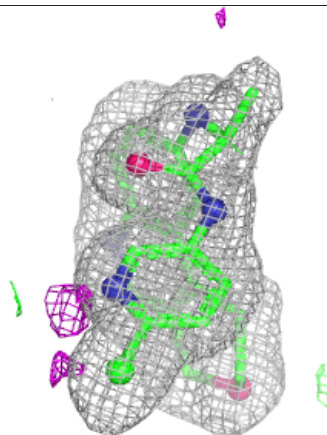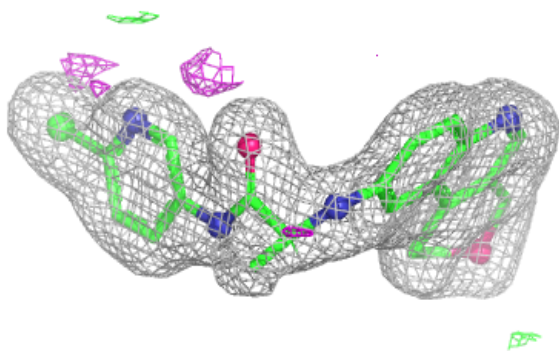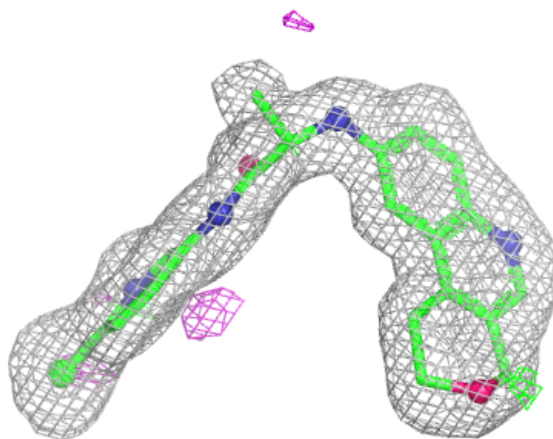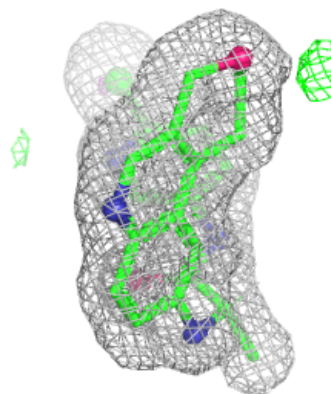and green (positive)

Electron density around VOA B 802:

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

Electron density around VOA C 802:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
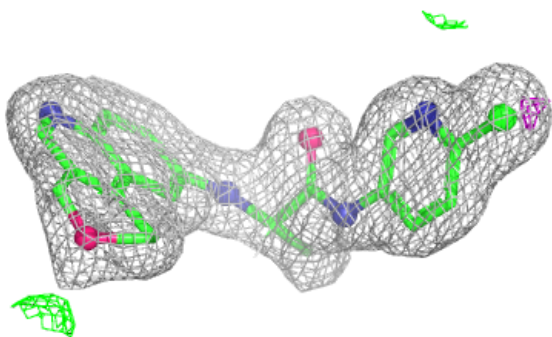mF_o-DF_c (at 3 rmsd) in purple (negative)
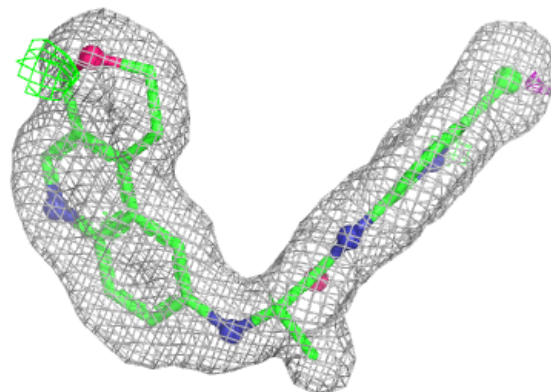and green (positive)
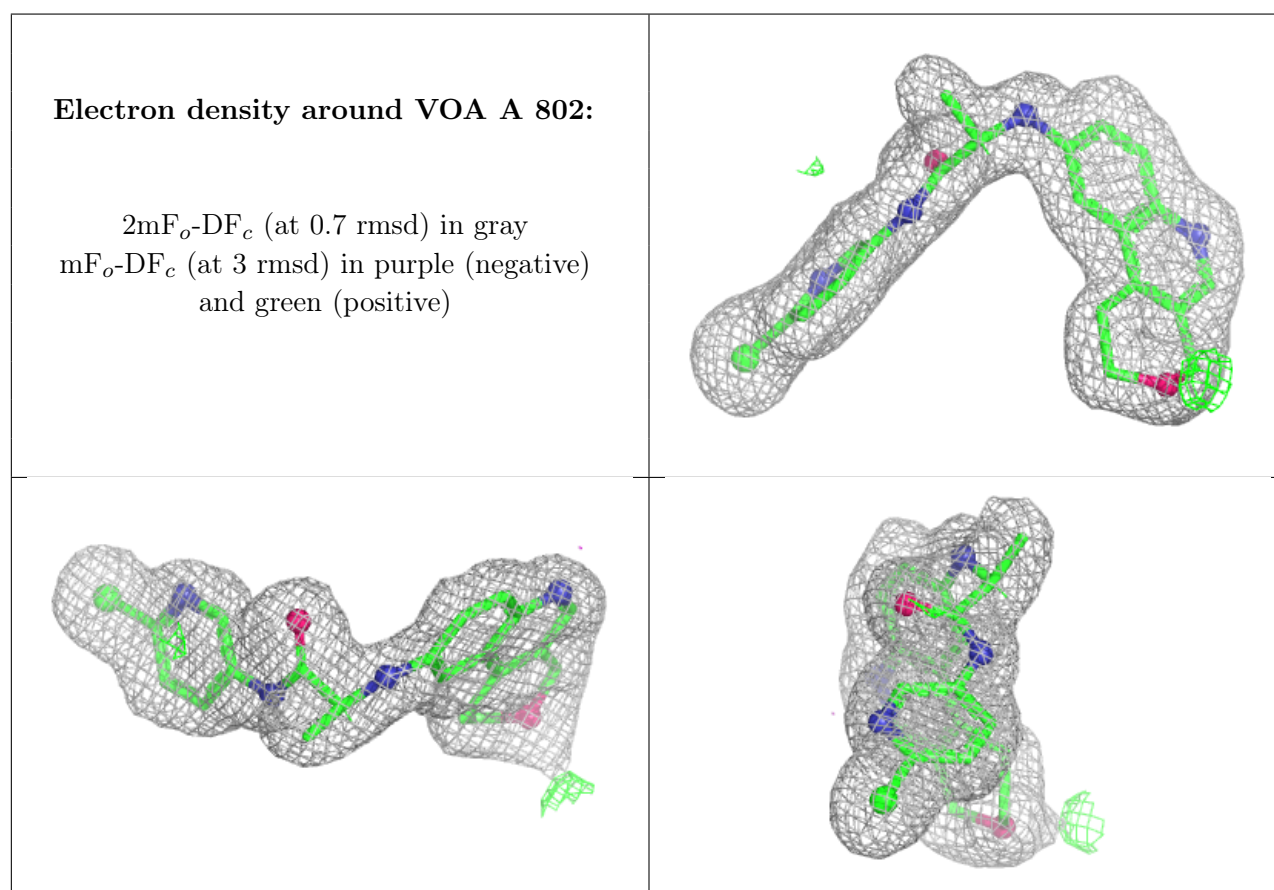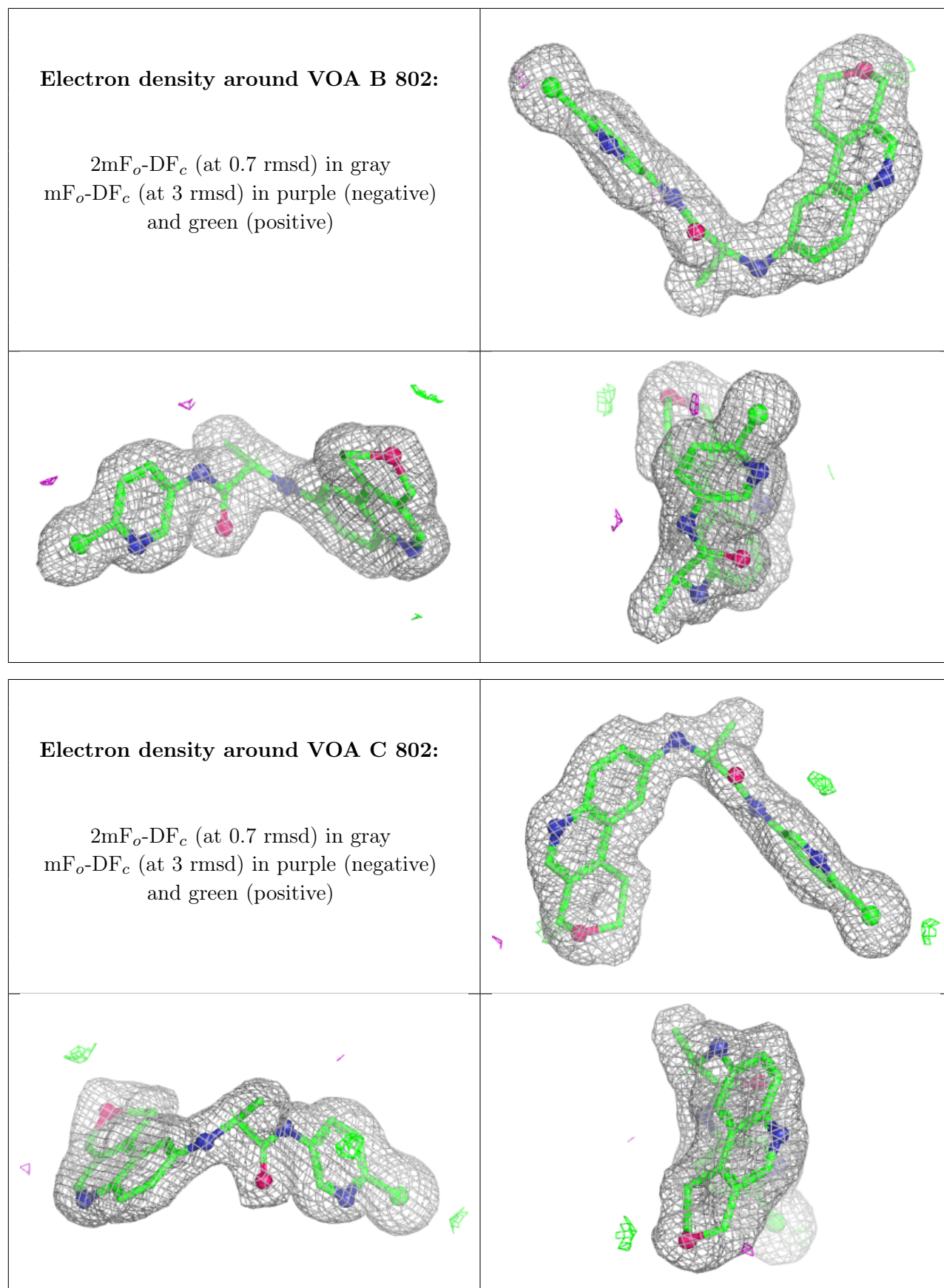
Electron density around VOA D 802:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
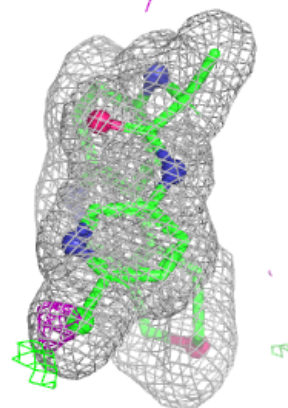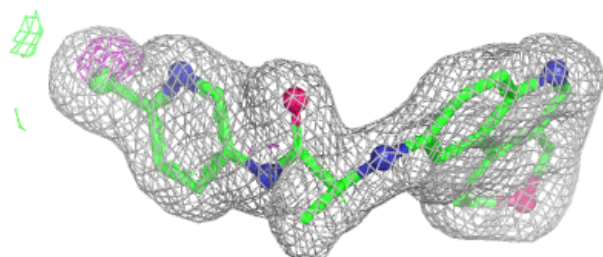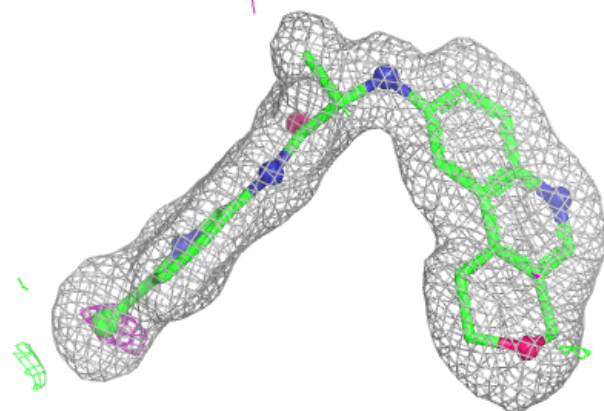
Electron density around VOA E 802:

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 VOA F 802:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
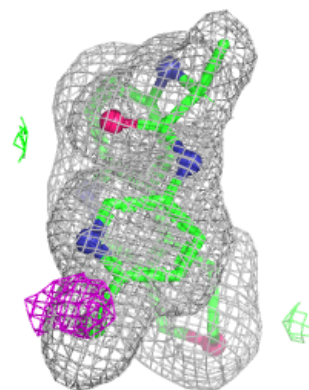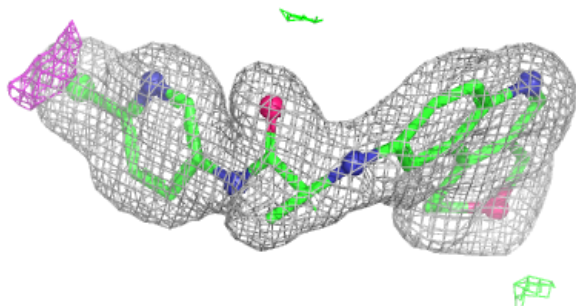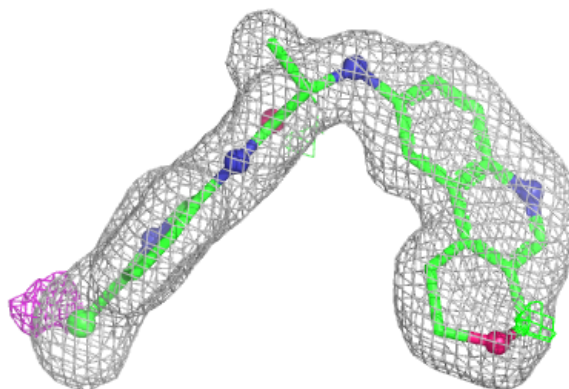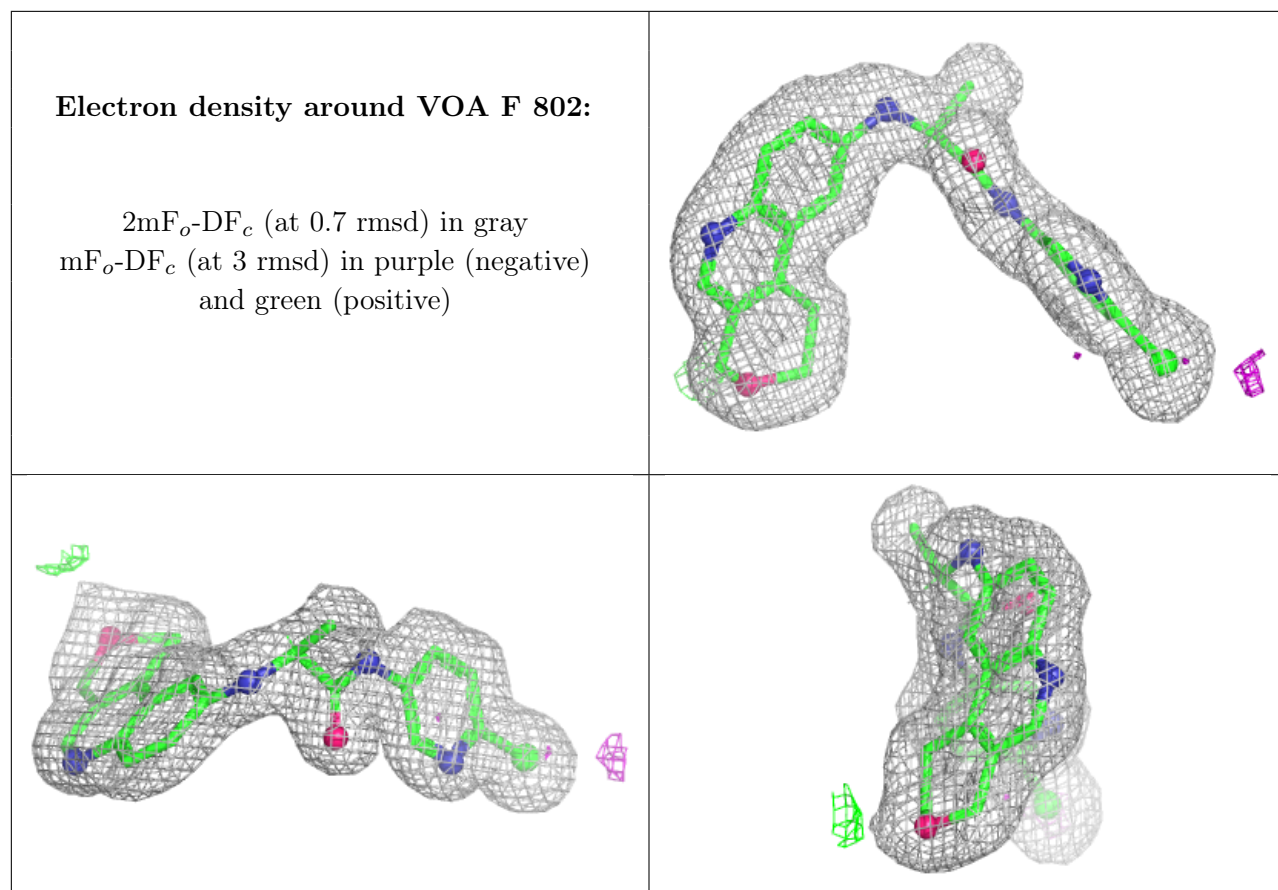
Electron density around VOA G 802:

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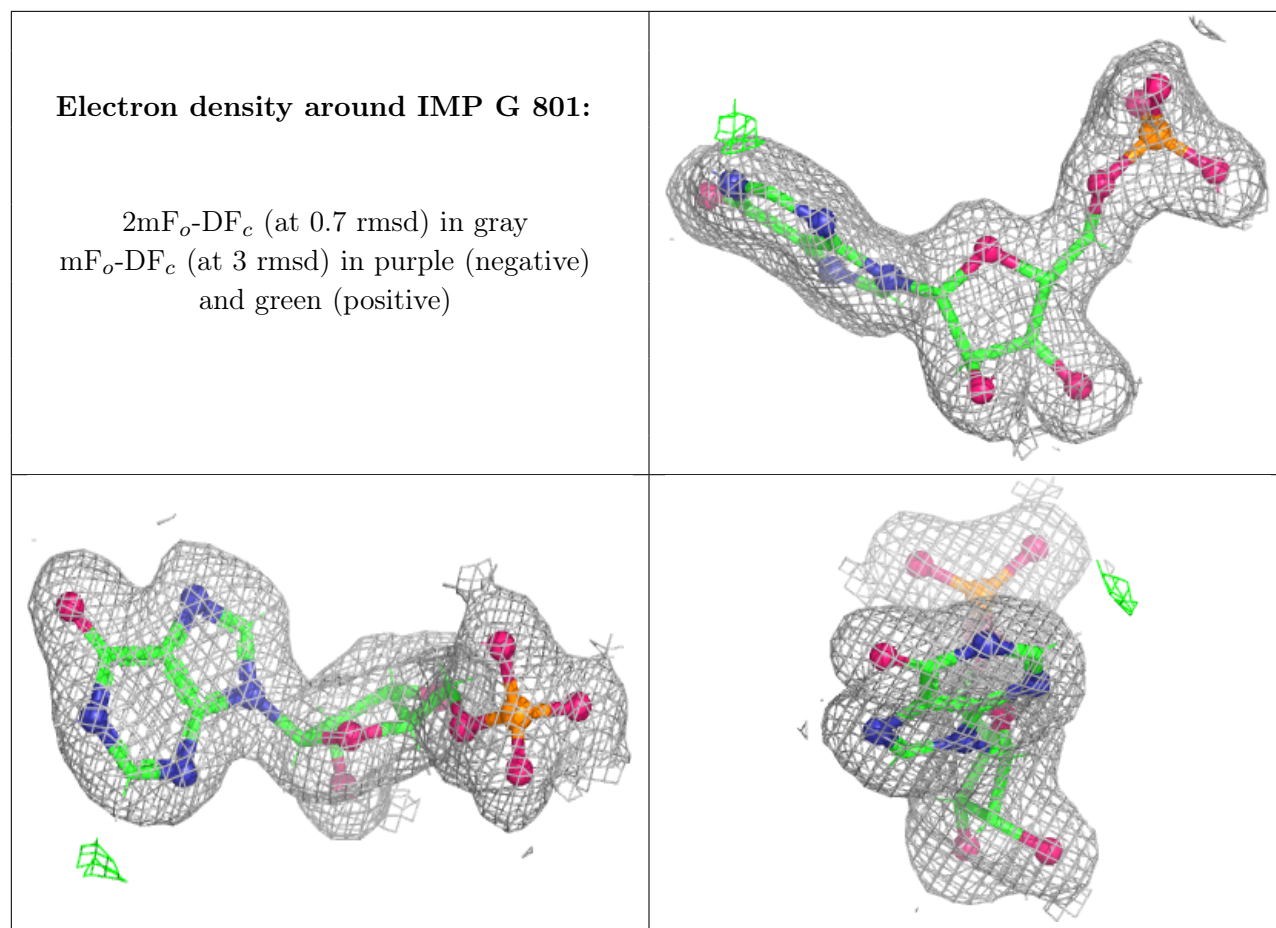mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around VOA H 802:

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

Electron density around IMP G 801:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.