



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:17 PM UTC

PDB ID : 7K4H / pdb_00007k4h
Title : Human Arginase 1 in complex with compound 04.
Authors : Palte, R.L.
Deposited on : 2020-09-15
Resolution : 1.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

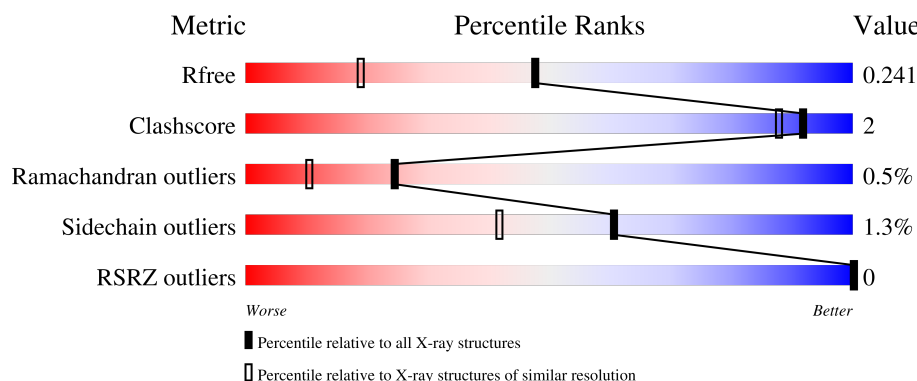
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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

Mol	Chain	Length	Quality of chain
1	A	322	 88% 11% .
1	B	322	 90% 8% ..
1	C	322	 87% 12% .
1	D	322	 88% 9% ..
1	E	322	 84% 14% .

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Mol	Chain	Length	Quality of chain
1	F	322	 A horizontal bar chart showing the quality of the chain. The bar is divided into three segments: a large green segment representing 85%, a smaller yellow segment representing 13%, and a very small grey segment at the end. The percentages '85%' and '13%' are printed below the green and yellow segments respectively. A small black dot is visible at the end of the bar.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16252 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Arginase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2415	1538	412	459	6			
1	B	318	Total	C	N	O	S	0	0	0
			2415	1538	412	459	6			
1	C	318	Total	C	N	O	S	0	0	0
			2415	1538	412	459	6			
1	D	318	Total	C	N	O	S	0	0	0
			2415	1538	412	459	6			
1	E	318	Total	C	N	O	S	0	0	0
			2415	1538	412	459	6			
1	F	318	Total	C	N	O	S	0	0	0
			2415	1538	412	459	6			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

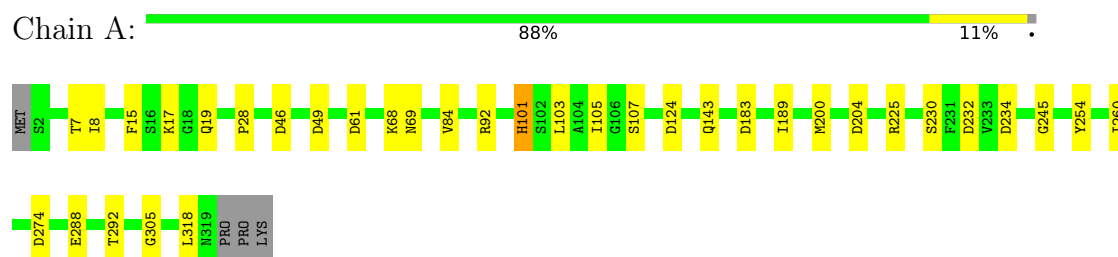
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		
2	D	2	Total	Mn	0	0
			2	2		
2	E	2	Total	Mn	0	0
			2	2		
2	F	2	Total	Mn	0	0
			2	2		

- Molecule 3 is 3-[(1 {R},5 {S},8 {R})-5-carboxy-2,6-diazabicyclo[3.2.1]octan-8-yl]propyl- $\text{B}(\text{O}^-)_3$ -oxidanyl-bis(oxidanyl)boranuide (CCD ID: VV4) (formula: $\text{C}_{10}\text{H}_{20}\text{BN}_2\text{O}_5$) (labeled as "Ligand of Interest" by depositor).

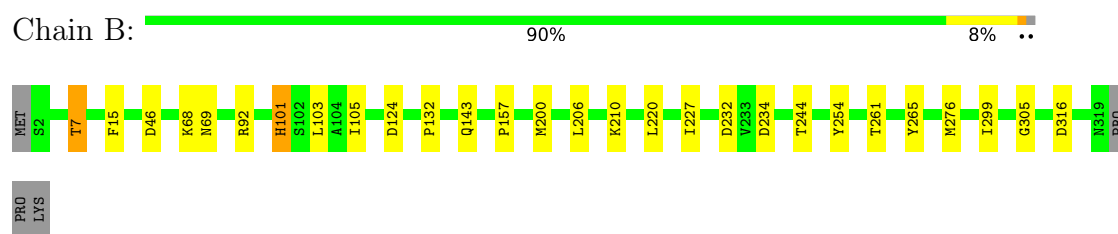
3 Residue-property plots

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.

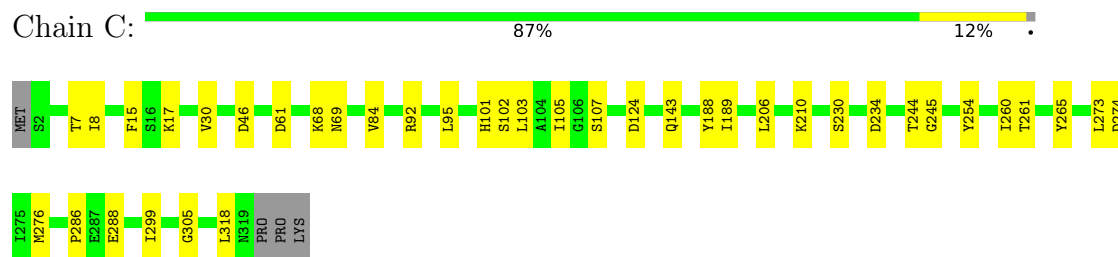
• Molecule 1: Arginase-1



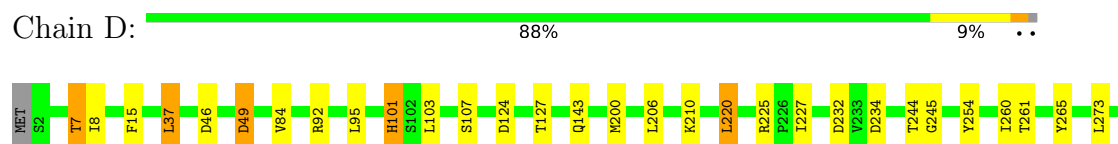
• Molecule 1: Arginase-1



• Molecule 1: Arginase-1



• Molecule 1: Arginase-1





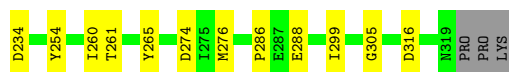
• Molecule 1: Arginase-1

Chain E: 84% 14%



• Molecule 1: Arginase-1

Chain F: 85% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.14Å 286.09Å 66.95Å 90.00° 90.12° 90.00°	Depositor
Resolution (Å)	48.88 – 1.65 48.88 – 1.65	Depositor EDS
% Data completeness (in resolution range)	87.2 (48.88-1.65) 86.7 (48.88-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 1.65Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.210 , 0.235 0.218 , 0.241	Depositor DCC
R_{free} test set	10360 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å ²)	8.4	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 12.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.317 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16252	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, VV4

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	1.10	2/2465 (0.1%)	1.66	28/3344 (0.8%)
1	B	1.10	1/2465 (0.0%)	1.66	19/3344 (0.6%)
1	C	1.10	1/2465 (0.0%)	1.67	30/3344 (0.9%)
1	D	1.10	0/2465	1.66	23/3344 (0.7%)
1	E	1.14	1/2465 (0.0%)	1.72	43/3344 (1.3%)
1	F	1.14	1/2465 (0.0%)	1.73	30/3344 (0.9%)
All	All	1.12	6/14790 (0.0%)	1.69	173/20064 (0.9%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	69	ASN	CA-C	7.43	1.58	1.53
1	C	69	ASN	CA-C	7.25	1.58	1.53
1	B	69	ASN	CA-C	6.86	1.58	1.53
1	F	69	ASN	CA-C	6.45	1.58	1.53
1	A	69	ASN	CA-C	5.92	1.57	1.53
1	A	19	GLN	CA-C	5.02	1.57	1.52

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	GLY	N-CA-C	9.93	124.20	113.58
1	E	305	GLY	N-CA-C	9.47	123.72	113.58
1	C	305	GLY	N-CA-C	9.27	124.63	113.79
1	F	305	GLY	N-CA-C	9.18	123.40	113.58
1	D	124	ASP	CA-CB-CG	8.49	121.09	112.60
1	B	124	ASP	CA-CB-CG	8.45	121.05	112.60
1	C	124	ASP	CA-CB-CG	8.32	120.92	112.60
1	F	124	ASP	CA-CB-CG	7.92	120.52	112.60
1	A	124	ASP	CA-CB-CG	7.83	120.43	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	234	ASP	CA-CB-CG	7.22	119.82	112.60
1	E	124	ASP	CA-CB-CG	7.10	119.70	112.60
1	C	234	ASP	CA-CB-CG	7.03	119.63	112.60
1	E	234	ASP	CA-CB-CG	6.96	119.56	112.60
1	E	105	ILE	N-CA-C	-6.95	103.56	110.30
1	F	105	ILE	N-CA-C	-6.82	103.87	110.42
1	F	118	LEU	CA-C-N	6.79	127.29	122.33
1	F	118	LEU	C-N-CA	6.79	127.29	122.33
1	D	305	GLY	N-CA-C	6.78	122.91	114.37
1	F	276	MET	CA-C-N	6.71	132.41	122.74
1	F	276	MET	C-N-CA	6.71	132.41	122.74
1	E	276	MET	CA-C-N	6.66	132.33	122.74
1	E	276	MET	C-N-CA	6.66	132.33	122.74
1	B	305	GLY	N-CA-C	6.64	122.38	114.48
1	A	105	ILE	N-CA-C	-6.62	104.06	110.42
1	D	234	ASP	CA-CB-CG	6.59	119.19	112.60
1	B	234	ASP	CA-CB-CG	6.58	119.18	112.60
1	A	234	ASP	CA-CB-CG	6.47	119.07	112.60
1	F	46	ASP	CA-CB-CG	6.38	118.98	112.60
1	E	221	GLY	CA-C-N	6.16	128.86	120.54
1	E	221	GLY	C-N-CA	6.16	128.86	120.54
1	F	254	TYR	CA-C-N	5.90	128.12	120.44
1	F	254	TYR	C-N-CA	5.90	128.12	120.44
1	E	260	ILE	CA-C-N	5.90	128.18	120.28
1	E	260	ILE	C-N-CA	5.90	128.18	120.28
1	A	189	ILE	CA-C-N	5.89	128.49	120.54
1	A	189	ILE	C-N-CA	5.89	128.49	120.54
1	B	68	LYS	CA-C-N	5.84	128.71	123.10
1	B	68	LYS	C-N-CA	5.84	128.71	123.10
1	C	254	TYR	CA-C-N	5.82	128.01	120.44
1	C	254	TYR	C-N-CA	5.82	128.01	120.44
1	E	68	LYS	CA-C-N	5.81	128.68	123.10
1	E	68	LYS	C-N-CA	5.81	128.68	123.10
1	C	244	THR	CA-C-N	5.81	126.39	119.94
1	C	244	THR	C-N-CA	5.81	126.39	119.94
1	D	254	TYR	CA-C-N	5.75	127.92	120.44
1	D	254	TYR	C-N-CA	5.75	127.92	120.44
1	E	207	GLY	N-CA-C	-5.74	105.53	112.48
1	F	260	ILE	CA-C-N	5.69	128.37	120.29
1	F	260	ILE	C-N-CA	5.69	128.37	120.29
1	C	105	ILE	N-CA-C	-5.68	104.97	110.42
1	C	61	ASP	CA-C-N	5.67	128.26	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	61	ASP	C-N-CA	5.67	128.26	120.39
1	D	276	MET	CA-C-N	5.62	132.07	123.47
1	D	276	MET	C-N-CA	5.62	132.07	123.47
1	F	207	GLY	N-CA-C	-5.61	104.66	112.18
1	E	254	TYR	CA-C-N	5.60	127.72	120.44
1	E	254	TYR	C-N-CA	5.60	127.72	120.44
1	A	49	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	46	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	254	TYR	CA-C-N	5.57	128.01	120.44
1	A	254	TYR	C-N-CA	5.57	128.01	120.44
1	C	46	ASP	CA-CB-CG	5.55	118.16	112.60
1	D	46	ASP	CA-CB-CG	5.55	118.15	112.60
1	E	288	GLU	CA-C-N	5.54	127.48	120.72
1	E	288	GLU	C-N-CA	5.54	127.48	120.72
1	E	164	TRP	CA-C-N	5.53	127.98	120.63
1	E	164	TRP	C-N-CA	5.53	127.98	120.63
1	B	316	ASP	CA-CB-CG	5.50	118.10	112.60
1	B	265	TYR	CA-C-N	5.50	128.40	120.38
1	B	265	TYR	C-N-CA	5.50	128.40	120.38
1	F	149	LEU	CA-C-N	5.50	127.64	120.28
1	F	149	LEU	C-N-CA	5.50	127.64	120.28
1	B	46	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	200	MET	CA-C-N	5.47	127.56	120.44
1	A	200	MET	C-N-CA	5.47	127.56	120.44
1	C	245	GLY	N-CA-C	5.46	118.84	112.50
1	A	68	LYS	CA-C-N	5.46	128.34	123.10
1	A	68	LYS	C-N-CA	5.46	128.34	123.10
1	F	68	LYS	CA-C-N	5.42	128.68	122.83
1	F	68	LYS	C-N-CA	5.42	128.68	122.83
1	F	286	PRO	CA-C-N	5.36	127.47	120.28
1	F	286	PRO	C-N-CA	5.36	127.47	120.28
1	C	260	ILE	CA-C-N	5.35	127.89	120.29
1	C	260	ILE	C-N-CA	5.35	127.89	120.29
1	A	245	GLY	N-CA-C	5.34	119.61	112.77
1	A	260	ILE	CA-C-N	5.34	127.44	120.28
1	A	260	ILE	C-N-CA	5.34	127.44	120.28
1	B	254	TYR	CA-C-N	5.34	127.38	120.44
1	B	254	TYR	C-N-CA	5.34	127.38	120.44
1	D	265	TYR	CA-C-N	5.33	128.16	120.38
1	D	265	TYR	C-N-CA	5.33	128.16	120.38
1	E	248	VAL	CA-C-N	5.33	127.75	120.35
1	E	248	VAL	C-N-CA	5.33	127.75	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	THR	CB-CA-C	5.32	119.30	110.78
1	A	292	THR	CA-C-N	5.31	127.25	120.56
1	A	292	THR	C-N-CA	5.31	127.25	120.56
1	A	61	ASP	CA-C-N	5.31	127.77	120.39
1	A	61	ASP	C-N-CA	5.31	127.77	120.39
1	D	260	ILE	CA-C-N	5.31	127.83	120.29
1	D	260	ILE	C-N-CA	5.31	127.83	120.29
1	E	200	MET	CA-C-N	5.28	127.31	120.44
1	E	200	MET	C-N-CA	5.28	127.31	120.44
1	E	286	PRO	CA-C-N	5.28	127.79	120.29
1	E	286	PRO	C-N-CA	5.28	127.79	120.29
1	D	244	THR	CA-C-N	5.28	125.80	119.94
1	D	244	THR	C-N-CA	5.28	125.80	119.94
1	D	49	ASP	CA-CB-CG	5.28	117.88	112.60
1	F	265	TYR	CA-C-N	5.27	128.07	120.38
1	F	265	TYR	C-N-CA	5.27	128.07	120.38
1	E	37	LEU	CA-C-N	5.27	127.29	120.44
1	E	37	LEU	C-N-CA	5.27	127.29	120.44
1	D	200	MET	CA-C-N	5.26	127.28	120.44
1	D	200	MET	C-N-CA	5.26	127.28	120.44
1	A	28	PRO	CA-C-N	5.25	127.63	120.54
1	A	28	PRO	C-N-CA	5.25	127.63	120.54
1	C	276	MET	CA-C-N	5.24	131.49	123.47
1	C	276	MET	C-N-CA	5.24	131.49	123.47
1	E	105	ILE	CA-C-N	5.24	125.76	119.94
1	E	105	ILE	C-N-CA	5.24	125.76	119.94
1	E	28	PRO	CA-C-N	5.19	128.00	120.79
1	E	28	PRO	C-N-CA	5.19	128.00	120.79
1	C	68	LYS	CA-C-N	5.18	128.07	123.10
1	C	68	LYS	C-N-CA	5.18	128.07	123.10
1	E	86	GLU	CA-C-N	5.17	127.07	120.56
1	E	86	GLU	C-N-CA	5.17	127.07	120.56
1	D	288	GLU	CA-C-N	5.15	127.01	120.72
1	D	288	GLU	C-N-CA	5.15	127.01	120.72
1	B	200	MET	CA-C-N	5.14	127.12	120.44
1	B	200	MET	C-N-CA	5.14	127.12	120.44
1	C	265	TYR	CA-C-N	5.14	127.88	120.38
1	C	265	TYR	C-N-CA	5.14	127.88	120.38
1	F	316	ASP	CA-CB-CG	5.12	117.72	112.60
1	F	128	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	189	ILE	CA-C-N	5.11	127.38	120.38
1	C	189	ILE	C-N-CA	5.11	127.38	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	288	GLU	CA-C-N	5.11	127.10	120.56
1	F	288	GLU	C-N-CA	5.11	127.10	120.56
1	E	265	TYR	CA-C-N	5.10	127.83	120.38
1	E	265	TYR	C-N-CA	5.10	127.83	120.38
1	A	288	GLU	CA-C-N	5.09	127.08	120.56
1	A	288	GLU	C-N-CA	5.09	127.08	120.56
1	C	286	PRO	CA-C-N	5.09	127.10	120.28
1	C	286	PRO	C-N-CA	5.09	127.10	120.28
1	E	291	ARG	CA-C-N	5.09	127.05	120.44
1	E	291	ARG	C-N-CA	5.09	127.05	120.44
1	A	204	ASP	CA-C-N	5.08	127.04	120.44
1	A	204	ASP	C-N-CA	5.08	127.04	120.44
1	E	46	ASP	CA-CB-CG	5.08	117.67	112.60
1	D	245	GLY	N-CA-C	5.07	118.38	112.50
1	F	85	ALA	CA-C-N	5.06	127.06	120.28
1	F	85	ALA	C-N-CA	5.06	127.06	120.28
1	C	102	SER	CA-C-N	5.06	128.70	120.60
1	C	102	SER	C-N-CA	5.06	128.70	120.60
1	B	276	MET	CA-C-N	5.06	131.21	123.47
1	B	276	MET	C-N-CA	5.06	131.21	123.47
1	B	105	ILE	N-CA-C	-5.06	105.56	110.42
1	D	7	THR	CB-CA-C	5.06	118.87	110.78
1	E	61	ASP	CA-CB-CG	5.05	117.66	112.60
1	F	73	VAL	CA-C-N	5.04	125.58	119.98
1	F	73	VAL	C-N-CA	5.04	125.58	119.98
1	C	188	TYR	CA-C-N	5.03	126.90	120.56
1	C	188	TYR	C-N-CA	5.03	126.90	120.56
1	B	244	THR	CA-C-N	5.03	125.52	119.94
1	B	244	THR	C-N-CA	5.03	125.52	119.94
1	A	183	ASP	CA-CB-CG	5.02	117.62	112.60
1	E	244	THR	CA-C-N	5.02	125.55	119.98
1	E	244	THR	C-N-CA	5.02	125.55	119.98
1	C	288	GLU	CA-C-N	5.02	126.84	120.72
1	C	288	GLU	C-N-CA	5.02	126.84	120.72
1	E	78	GLU	CA-C-N	5.01	126.95	120.44
1	E	78	GLU	C-N-CA	5.01	126.95	120.44
1	D	220	LEU	CA-C-N	5.00	125.64	119.99
1	D	220	LEU	C-N-CA	5.00	125.64	119.99

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	2415	0	2461	7	0
1	B	2415	0	2461	7	0
1	C	2415	0	2461	9	0
1	D	2415	0	2461	9	0
1	E	2415	0	2461	8	0
1	F	2415	0	2461	9	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	18	0	0	0	0
3	B	18	0	0	0	0
3	C	18	0	0	0	0
3	D	18	0	0	0	0
3	E	18	0	0	0	0
3	F	18	0	0	0	0
4	A	302	0	0	0	0
4	B	301	0	0	0	0
4	C	277	0	0	0	0
4	D	311	0	0	0	0
4	E	228	0	0	0	0
4	F	223	0	0	0	0
All	All	16252	0	14766	47	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (47) 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:E:15:PHE:HB3	1:E:103:LEU:HD11	1.89	0.55
1:C:7:THR:HG22	1:C:92:ARG:HG2	1.89	0.53
1:C:15:PHE:CZ	1:C:17:LYS:HB2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:PHE:HB3	1:B:103:LEU:HD11	1.92	0.52
1:B:220:LEU:HD11	1:B:227:ILE:HD11	1.92	0.52
1:F:206:LEU:HB3	1:F:210:LYS:HB3	1.93	0.51
1:D:220:LEU:HD11	1:D:227:ILE:HD11	1.91	0.51
1:E:206:LEU:HB3	1:E:210:LYS:HB3	1.91	0.51
1:A:7:THR:HG22	1:A:92:ARG:HG2	1.95	0.48
1:E:220:LEU:HD11	1:E:227:ILE:HD11	1.94	0.48
1:D:15:PHE:HB3	1:D:103:LEU:HD11	1.96	0.48
1:F:261:THR:HG21	1:F:299:ILE:HG23	1.96	0.47
1:C:15:PHE:HB3	1:C:103:LEU:HD11	1.95	0.47
1:A:230:SER:HA	1:A:274:ASP:HB2	1.96	0.47
1:F:220:LEU:HD11	1:F:227:ILE:HD11	1.97	0.47
1:F:7:THR:HG22	1:F:92:ARG:HG2	1.96	0.47
1:E:230:SER:HA	1:E:274:ASP:HB2	1.96	0.47
1:A:84:VAL:HG21	1:A:107:SER:HA	1.96	0.46
1:C:206:LEU:HB3	1:C:210:LYS:HB3	1.99	0.45
1:C:230:SER:HA	1:C:274:ASP:HB2	1.98	0.44
1:C:261:THR:HG21	1:C:299:ILE:HG23	2.00	0.44
1:D:37:LEU:HD21	1:D:49:ASP:HB2	1.98	0.44
1:E:7:THR:HG22	1:E:92:ARG:HG2	1.99	0.44
1:B:261:THR:HG21	1:B:299:ILE:HG23	2.00	0.44
1:A:15:PHE:HB3	1:A:103:LEU:HD11	1.99	0.44
1:D:206:LEU:HB3	1:D:210:LYS:HB3	2.01	0.43
1:C:95:LEU:HD13	1:C:273:LEU:HD23	2.01	0.43
1:B:206:LEU:HB3	1:B:210:LYS:HB3	2.00	0.43
1:C:84:VAL:HG21	1:C:107:SER:HA	2.00	0.43
1:D:101:HIS:CE1	1:D:232:ASP:HB2	2.54	0.42
1:F:58:ILE:HD12	1:F:72:SER:HA	2.00	0.42
1:C:318:LEU:HB3	1:E:155:LYS:HD2	2.01	0.42
1:E:58:ILE:HD12	1:E:72:SER:HA	2.01	0.42
1:E:261:THR:HG21	1:E:299:ILE:HG23	2.01	0.42
1:D:261:THR:HG21	1:D:299:ILE:HG23	2.01	0.42
1:B:101:HIS:CE1	1:B:232:ASP:HB2	2.55	0.41
1:D:7:THR:HG22	1:D:92:ARG:HG2	2.02	0.41
1:B:132:PRO:HD2	1:B:157:PRO:HD2	2.01	0.41
1:D:84:VAL:HG21	1:D:107:SER:HA	2.03	0.41
1:D:95:LEU:HD13	1:D:273:LEU:HD23	2.01	0.41
1:B:7:THR:HG22	1:B:92:ARG:HG2	2.02	0.41
1:F:84:VAL:HG21	1:F:107:SER:HA	2.03	0.41
1:A:318:LEU:HB3	1:F:155:LYS:HD2	2.03	0.41
1:F:101:HIS:CE1	1:F:232:ASP:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:SER:HA	1:F:274:ASP:HB2	2.02	0.40
1:A:15:PHE:CZ	1:A:17:LYS:HB2	2.56	0.40
1:A:101:HIS:CE1	1:A:232:ASP:HB2	2.57	0.40

There are no symmetry-related clashes.

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	A	316/322 (98%)	304 (96%)	11 (4%)	1 (0%)	36	21
1	B	316/322 (98%)	306 (97%)	9 (3%)	1 (0%)	36	21
1	C	316/322 (98%)	304 (96%)	11 (4%)	1 (0%)	36	21
1	D	316/322 (98%)	304 (96%)	11 (4%)	1 (0%)	36	21
1	E	316/322 (98%)	305 (96%)	9 (3%)	2 (1%)	21	8
1	F	316/322 (98%)	303 (96%)	10 (3%)	3 (1%)	14	3
All	All	1896/1932 (98%)	1826 (96%)	61 (3%)	9 (0%)	24	10

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	65	GLN
1	F	17	LYS
1	F	65	GLN
1	A	143	GLN
1	C	143	GLN
1	D	143	GLN
1	E	143	GLN
1	F	143	GLN
1	B	143	GLN

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	266/270 (98%)	263 (99%)	3 (1%)	65	48
1	B	266/270 (98%)	265 (100%)	1 (0%)	84	77
1	C	266/270 (98%)	263 (99%)	3 (1%)	65	48
1	D	266/270 (98%)	261 (98%)	5 (2%)	50	28
1	E	266/270 (98%)	262 (98%)	4 (2%)	57	37
1	F	266/270 (98%)	262 (98%)	4 (2%)	57	37
All	All	1596/1620 (98%)	1576 (99%)	20 (1%)	61	42

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	101	HIS
1	A	225	ARG
1	B	101	HIS
1	C	8	ILE
1	C	30	VAL
1	C	101	HIS
1	D	8	ILE
1	D	37	LEU
1	D	101	HIS
1	D	127	THR
1	D	225	ARG
1	E	8	ILE
1	E	101	HIS
1	E	140	LEU
1	E	225	ARG
1	F	8	ILE
1	F	101	HIS
1	F	140	LEU
1	F	225	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	79	GLN
1	A	130	ASN
1	B	90	ASN
1	B	130	ASN
1	C	90	ASN
1	C	143	GLN
1	D	130	ASN
1	E	115	HIS
1	E	130	ASN
1	E	139	ASN
1	F	79	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	$\# Z > 2$
3	VV4	A	403	2	16,19,19	1.83	4 (25%)	14,29,29	2.43	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	VV4	F	403	2	16,19,19	1.85	4 (25%)	14,29,29	2.42	4 (28%)
3	VV4	E	403	2	16,19,19	1.59	2 (12%)	14,29,29	2.00	2 (14%)
3	VV4	C	403	2	16,19,19	1.51	2 (12%)	14,29,29	2.09	2 (14%)
3	VV4	B	403	2	16,19,19	1.87	4 (25%)	14,29,29	2.47	4 (28%)
3	VV4	D	403	2	16,19,19	1.61	2 (12%)	14,29,29	2.03	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
3	VV4	A	403	2	-	0/10/36/36	1/3/2/2
3	VV4	F	403	2	-	1/10/36/36	1/3/2/2
3	VV4	E	403	2	-	2/10/36/36	1/3/2/2
3	VV4	C	403	2	-	2/10/36/36	1/3/2/2
3	VV4	B	403	2	-	0/10/36/36	1/3/2/2
3	VV4	D	403	2	-	1/10/36/36	1/3/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	VV4	C1-N1	5.27	1.55	1.47
3	F	403	VV4	C1-N1	5.19	1.55	1.47
3	D	403	VV4	C1-N1	5.17	1.55	1.47
3	E	403	VV4	C1-N1	5.09	1.55	1.47
3	B	403	VV4	C1-N1	5.07	1.55	1.47
3	C	403	VV4	C1-N1	4.81	1.54	1.47
3	B	403	VV4	O1-C	3.21	1.32	1.22
3	F	403	VV4	O1-C	2.96	1.31	1.22
3	A	403	VV4	O1-C	2.76	1.30	1.22
3	B	403	VV4	O-C	-2.46	1.21	1.30
3	A	403	VV4	C5-N	2.36	1.51	1.47
3	B	403	VV4	C5-N	2.32	1.51	1.47
3	F	403	VV4	C5-N	2.28	1.51	1.47
3	C	403	VV4	C5-N	2.28	1.51	1.47
3	F	403	VV4	O-C	-2.27	1.22	1.30
3	A	403	VV4	O-C	-2.25	1.22	1.30
3	E	403	VV4	C5-N	2.25	1.51	1.47
3	D	403	VV4	C5-N	2.25	1.51	1.47

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	403	VV4	C3-N-C5	6.47	115.66	111.62
3	B	403	VV4	C3-N-C5	6.43	115.64	111.62
3	E	403	VV4	C3-N-C5	6.27	115.53	111.62
3	F	403	VV4	C3-N-C5	6.21	115.50	111.62
3	D	403	VV4	C3-N-C5	6.15	115.46	111.62
3	A	403	VV4	C3-N-C5	6.00	115.37	111.62
3	A	403	VV4	O-C-C1	3.94	124.11	113.66
3	F	403	VV4	O-C-C1	3.90	124.01	113.66
3	B	403	VV4	O-C-C1	3.73	123.56	113.66
3	A	403	VV4	O1-C-C1	-3.53	112.85	122.48
3	F	403	VV4	O1-C-C1	-3.50	112.94	122.48
3	B	403	VV4	O1-C-C1	-3.34	113.36	122.48
3	C	403	VV4	C8-C7-C6	3.06	120.76	114.08
3	B	403	VV4	C8-C7-C6	3.01	120.65	114.08
3	D	403	VV4	C8-C7-C6	2.88	120.36	114.08
3	A	403	VV4	C8-C7-C6	2.67	119.91	114.08
3	E	403	VV4	C8-C7-C6	2.64	119.82	114.08
3	F	403	VV4	C8-C7-C6	2.37	119.24	114.08

There are no chirality outliers.

All (6) torsion outliers are listed below:

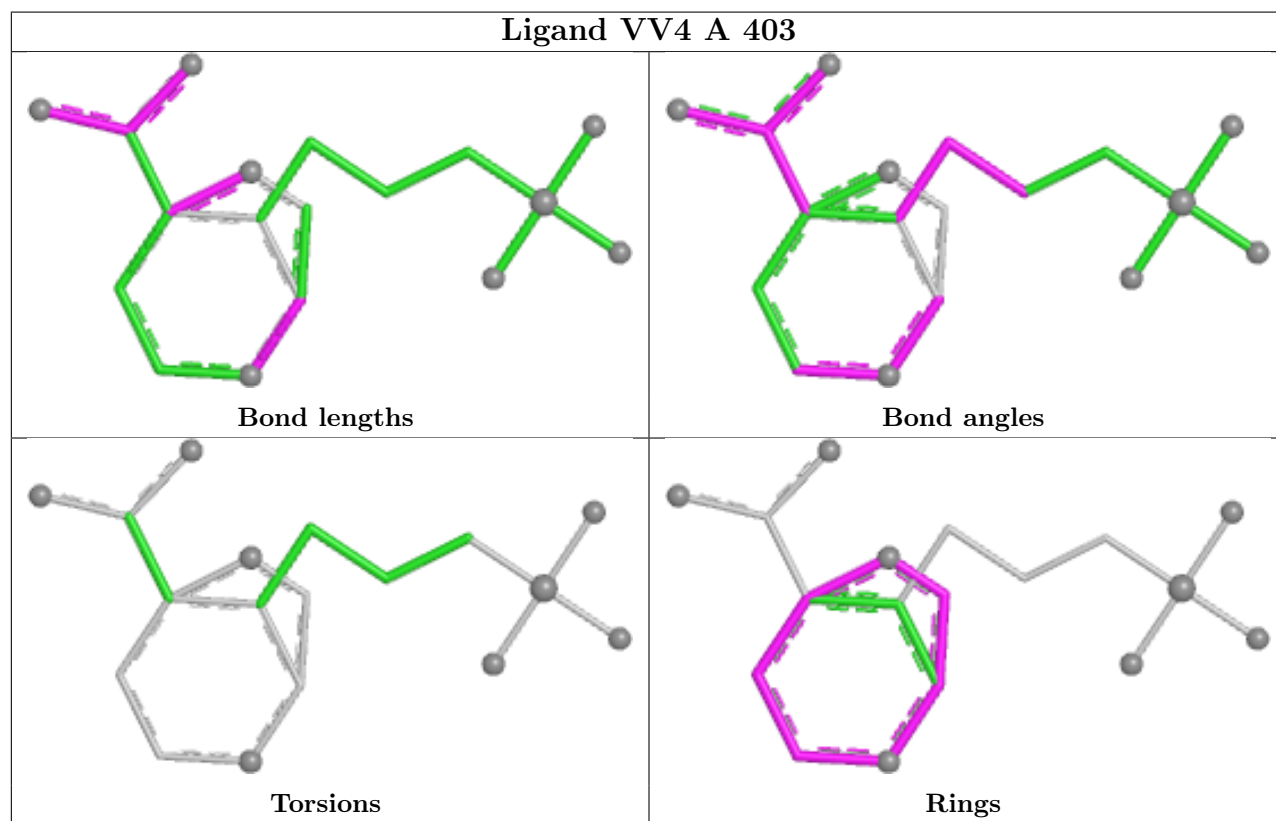
Mol	Chain	Res	Type	Atoms
3	F	403	VV4	C7-C8-C9-B
3	E	403	VV4	C7-C8-C9-B
3	D	403	VV4	O-C-C1-C2
3	C	403	VV4	C7-C8-C9-B
3	C	403	VV4	O-C-C1-C2
3	E	403	VV4	O-C-C1-C2

All (6) ring outliers are listed below:

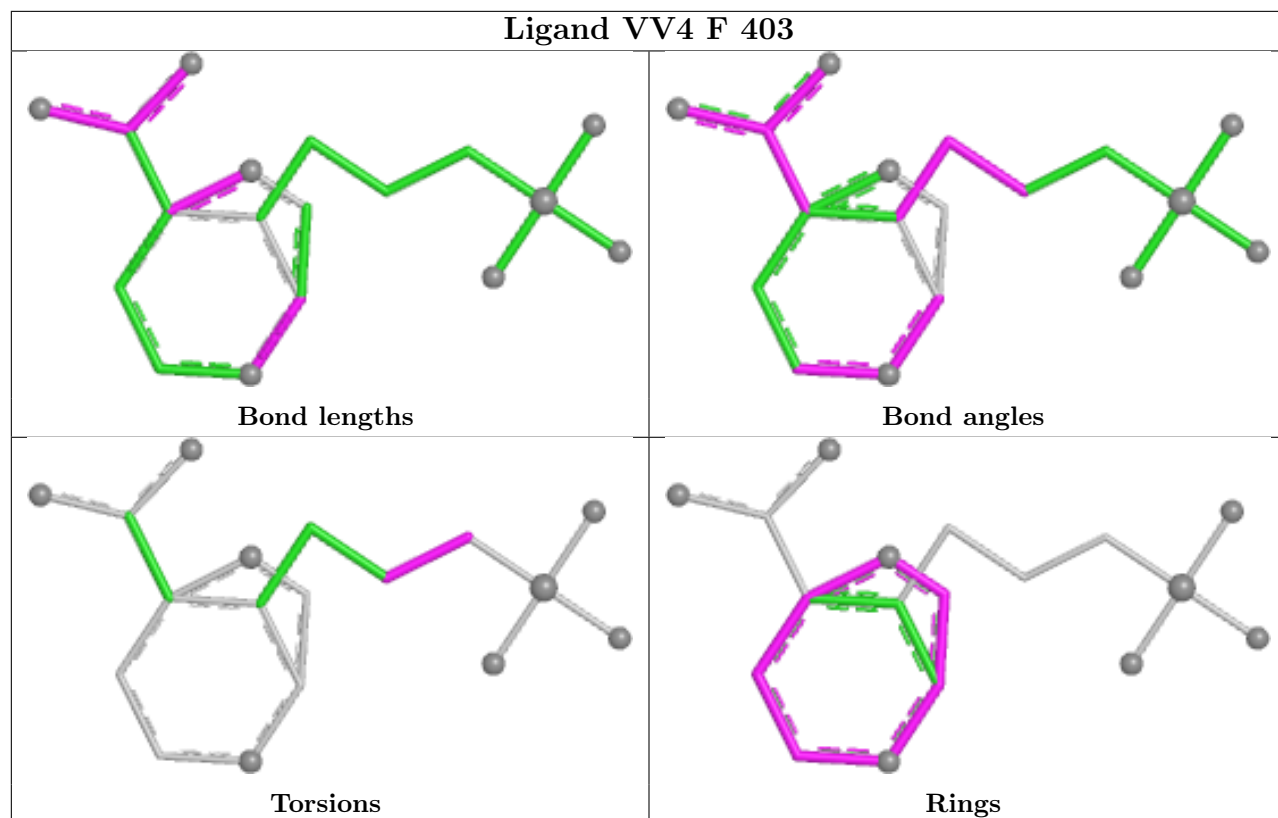
Mol	Chain	Res	Type	Atoms
3	B	403	VV4	C1-C2-C3-C4-C5-N-N1
3	E	403	VV4	C1-C2-C3-C4-C5-N-N1
3	F	403	VV4	C1-C2-C3-C4-C5-N-N1
3	C	403	VV4	C1-C2-C3-C4-C5-N-N1
3	A	403	VV4	C1-C2-C3-C4-C5-N-N1
3	D	403	VV4	C1-C2-C3-C4-C5-N-N1

No monomer is involved in short contacts.

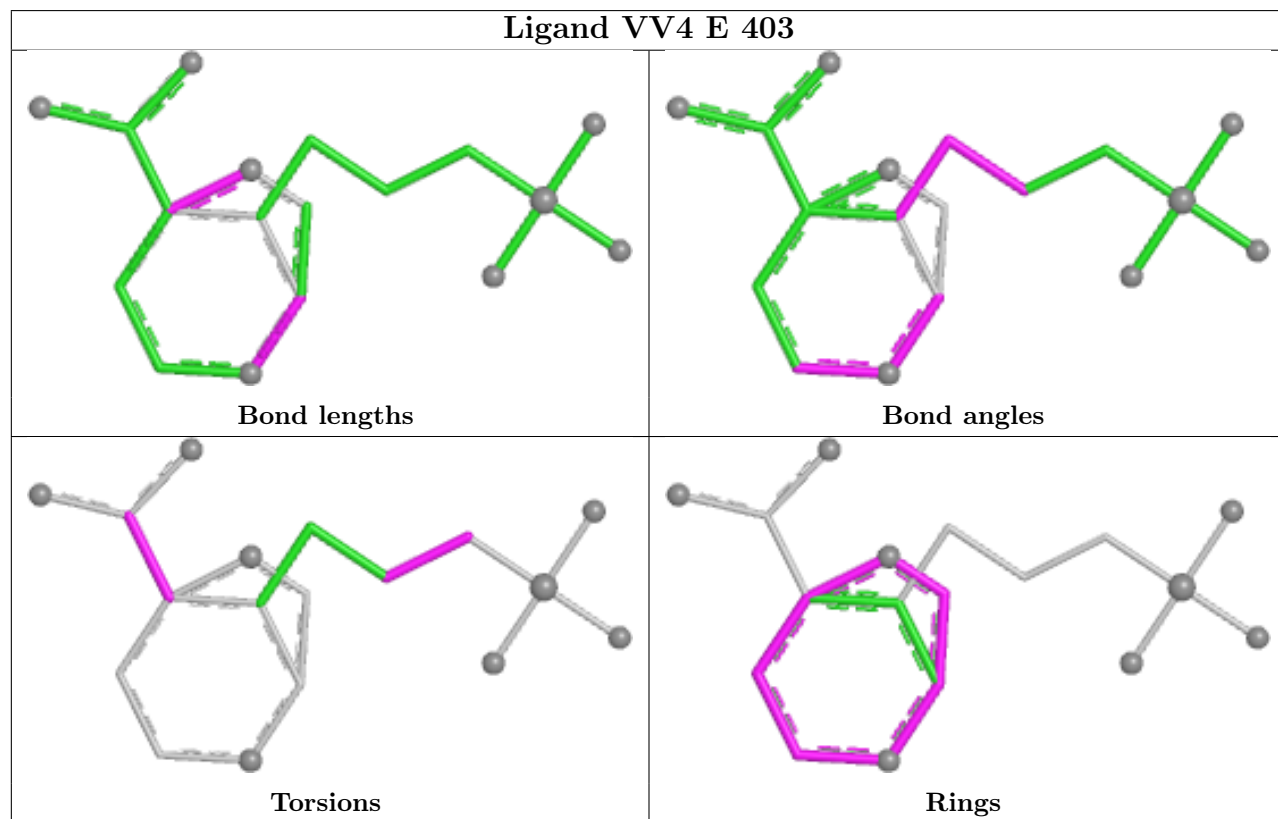
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



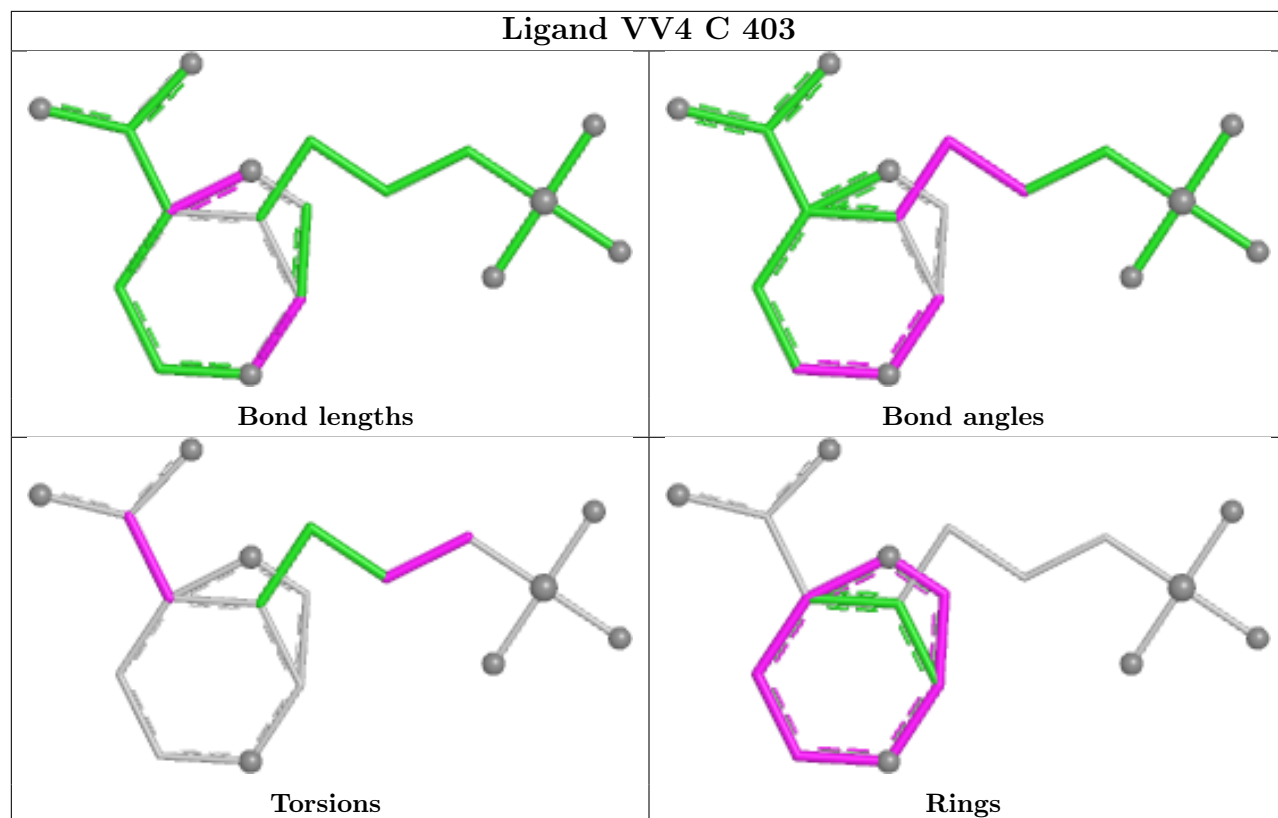
Ligand VV4 F 403



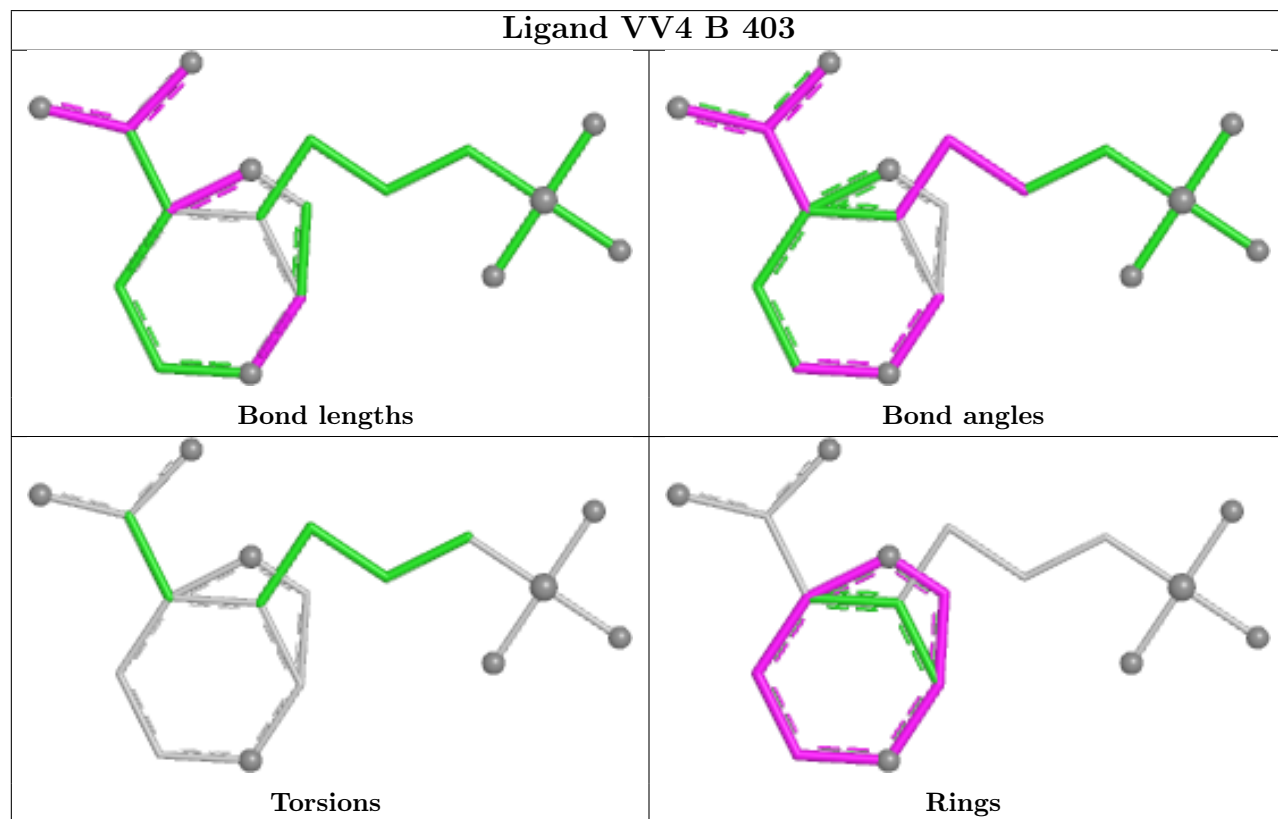
Ligand VV4 E 403

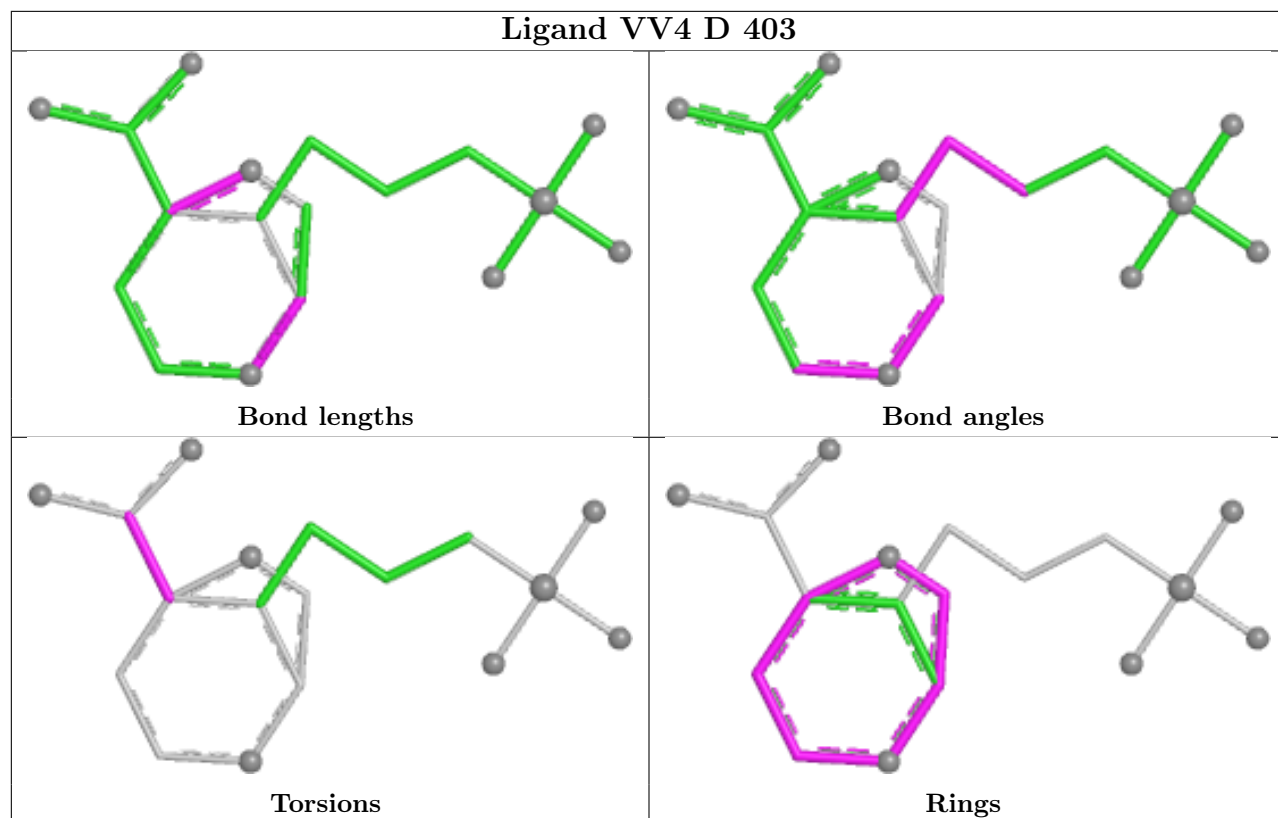


Ligand VV4 C 403



Ligand VV4 B 403





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	318/322 (98%)	-1.20	0 100 100	4, 7, 23, 61	0
1	B	318/322 (98%)	-1.16	0 100 100	5, 8, 21, 54	0
1	C	318/322 (98%)	-1.19	0 100 100	4, 8, 22, 57	0
1	D	318/322 (98%)	-1.14	0 100 100	4, 8, 23, 48	0
1	E	318/322 (98%)	-0.95	0 100 100	5, 16, 33, 54	0
1	F	318/322 (98%)	-0.93	0 100 100	5, 16, 36, 53	0
All	All	1908/1932 (98%)	-1.10	0 100 100	4, 10, 28, 61	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	VV4	A	403	18/18	0.99	0.03	4,5,6,7	0

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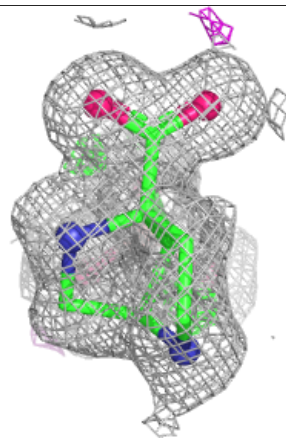
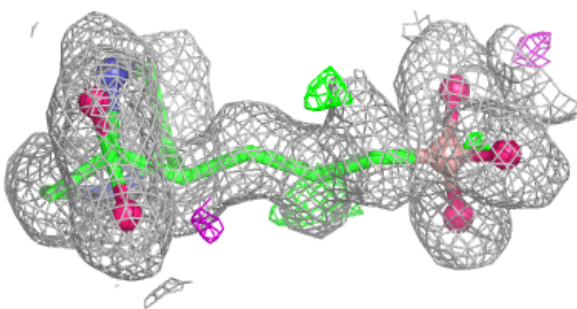
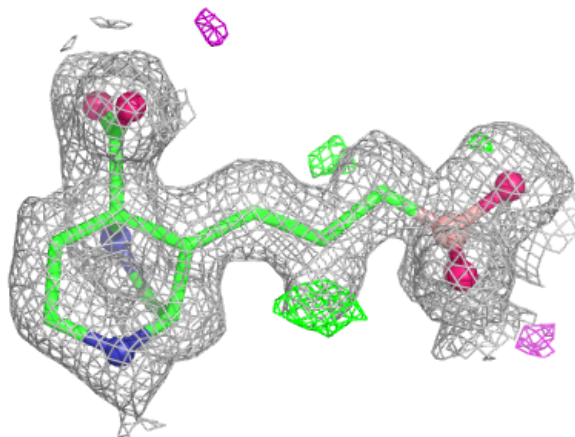
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	VV4	B	403	18/18	0.99	0.03	4,5,6,7	0
3	VV4	C	403	18/18	0.99	0.02	3,4,7,7	0
3	VV4	D	403	18/18	0.99	0.03	3,6,7,7	0
3	VV4	E	403	18/18	0.99	0.03	10,12,13,13	0
3	VV4	F	403	18/18	0.99	0.03	12,12,13,13	0
2	MN	D	401	1/1	1.00	0.01	4,4,4,4	0
2	MN	D	402	1/1	1.00	0.01	6,6,6,6	0
2	MN	E	401	1/1	1.00	0.02	7,7,7,7	0
2	MN	E	402	1/1	1.00	0.01	7,7,7,7	0
2	MN	F	401	1/1	1.00	0.01	10,10,10,10	0
2	MN	F	402	1/1	1.00	0.01	8,8,8,8	0
2	MN	A	401	1/1	1.00	0.01	3,3,3,3	0
2	MN	A	402	1/1	1.00	0.01	3,3,3,3	0
2	MN	B	401	1/1	1.00	0.01	3,3,3,3	0
2	MN	B	402	1/1	1.00	0.01	5,5,5,5	0
2	MN	C	401	1/1	1.00	0.01	3,3,3,3	0
2	MN	C	402	1/1	1.00	0.01	3,3,3,3	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.

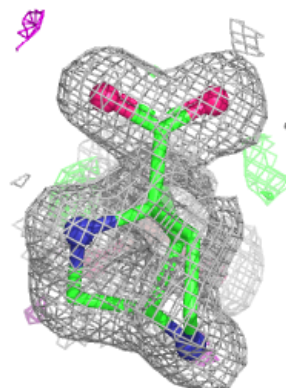
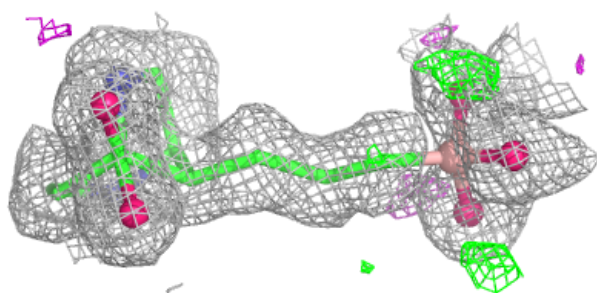
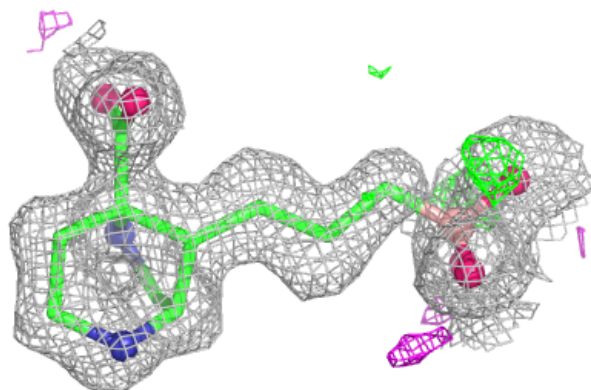
Electron density around VV4 A 403:

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

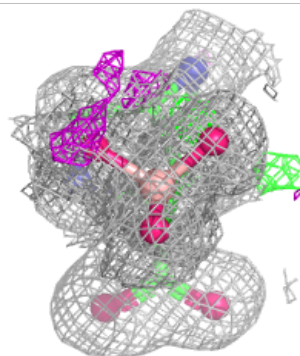
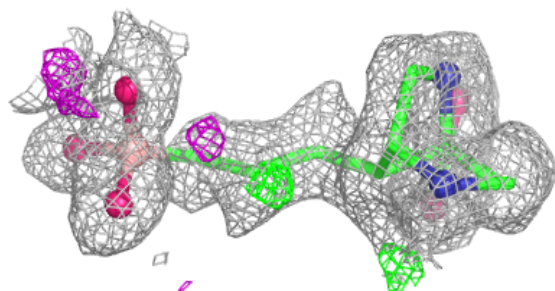
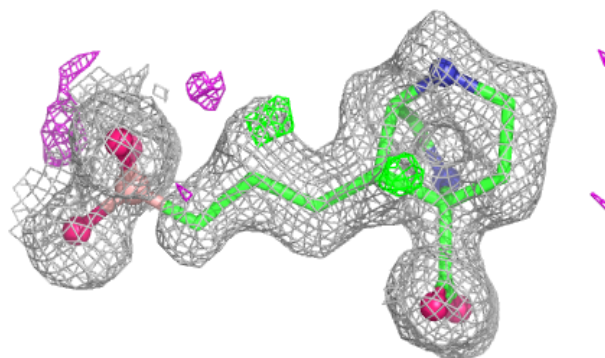


Electron density around VV4 B 403:

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

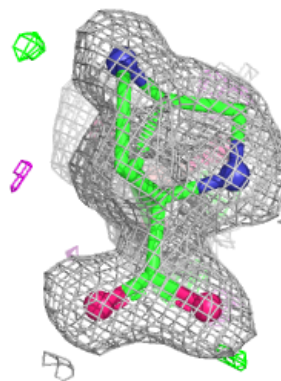
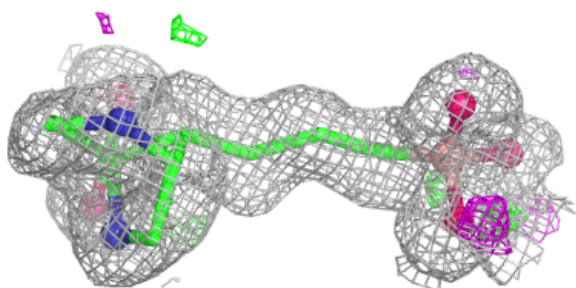
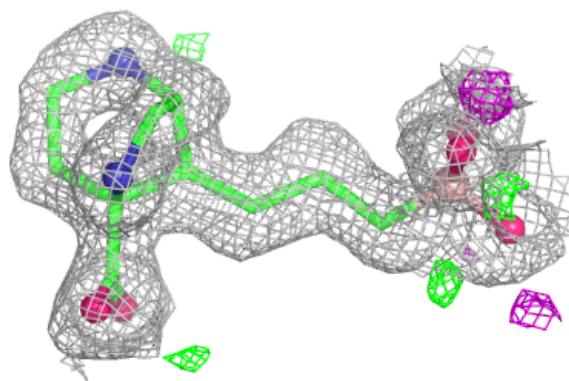
**Electron density around VV4 C 403:**

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

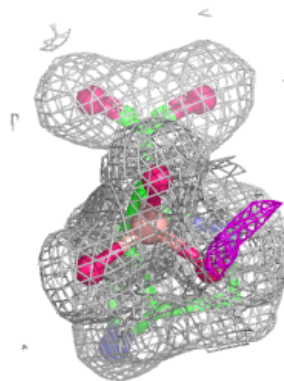
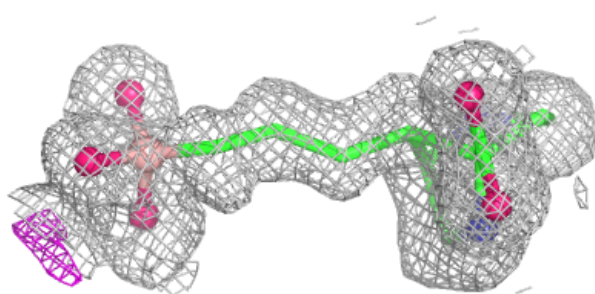
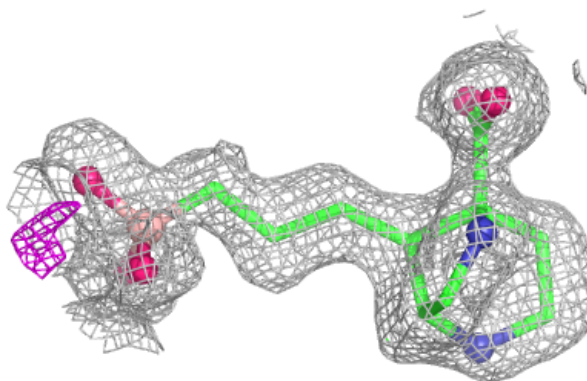


Electron density around VV4 D 403:

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

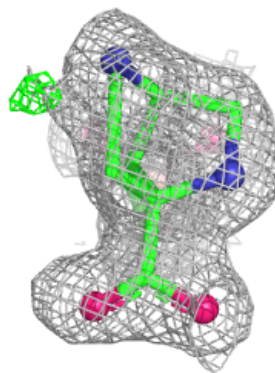
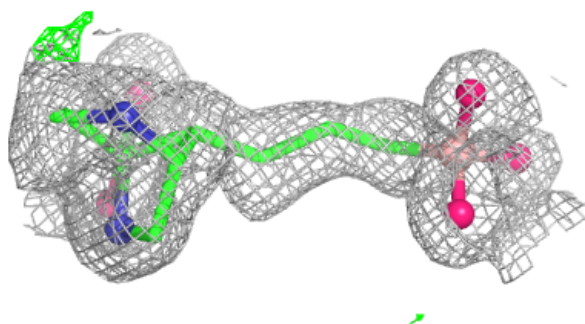
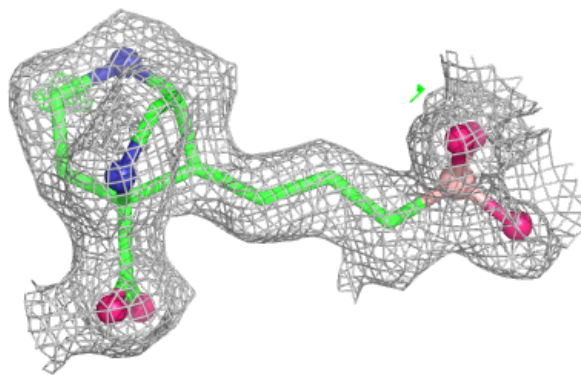
**Electron density around VV4 E 403:**

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



Electron density around VV4 F 403:

$2mF_o - DF_c$ (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.