



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:13 PM UTC

PDB ID : 7K4K / pdb_00007k4k
Title : Human Arginase 1 in complex with compound 52.
Authors : Palte, R.L.
Deposited on : 2020-09-15
Resolution : 2.27 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

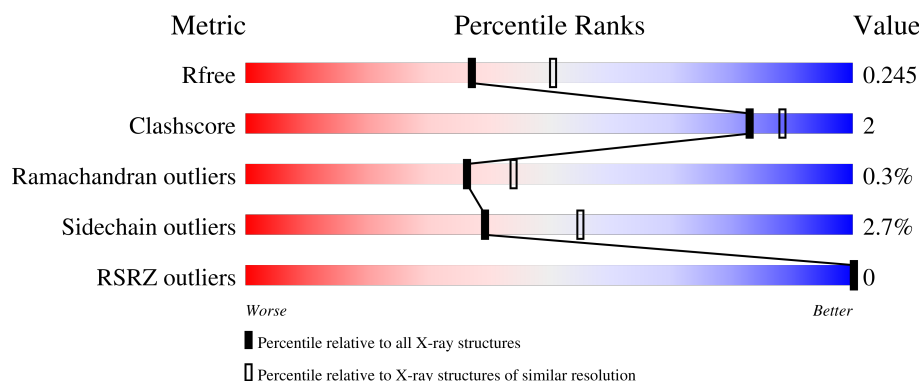
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	89% 10% .
1	B	322	87% 11% ..
1	C	322	86% 12% .
1	D	322	86% 11% ..
1	E	322	89% 9% .

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Mol	Chain	Length	Quality of chain
1	F	322	92% 6% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15739 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.

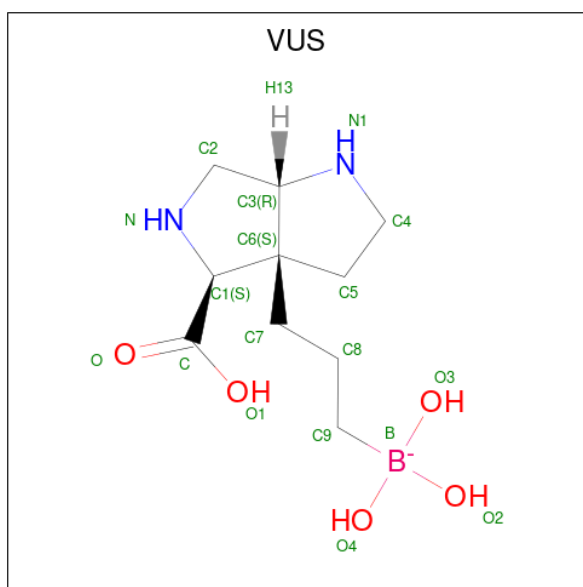
- Molecule 1 is a protein called Arginase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2409	1535	411	457	6			
1	B	317	Total	C	N	O	S	0	0	0
			2409	1535	411	457	6			
1	C	317	Total	C	N	O	S	0	0	0
			2409	1535	411	457	6			
1	D	317	Total	C	N	O	S	0	0	0
			2409	1535	411	457	6			
1	E	317	Total	C	N	O	S	0	0	0
			2409	1535	411	457	6			
1	F	317	Total	C	N	O	S	0	0	0
			2409	1535	411	457	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-[(3 {a} {S},4 {S},6 {a} {R})-4-carboxy-2,3,4,5,6,6 {a}-hexahydro-1 {H}-pyrrolo[2,3-c]pyrrol-3 {a}-yl]propyl-\$l^{\wedge}\$ {3}-oxidanyl-bis(oxidanyl)boranuide (CCD ID: VUS) (formula: C₁₀H₂₀BN₂O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	B	C	N	O	0	0
			18	1	10	2	5		
3	B	1	Total	B	C	N	O	0	0
			18	1	10	2	5		
3	C	1	Total	B	C	N	O	0	0
			18	1	10	2	5		
3	D	1	Total	B	C	N	O	0	0
			18	1	10	2	5		
3	E	1	Total	B	C	N	O	0	0
			18	1	10	2	5		
3	F	1	Total	B	C	N	O	0	0
			18	1	10	2	5		

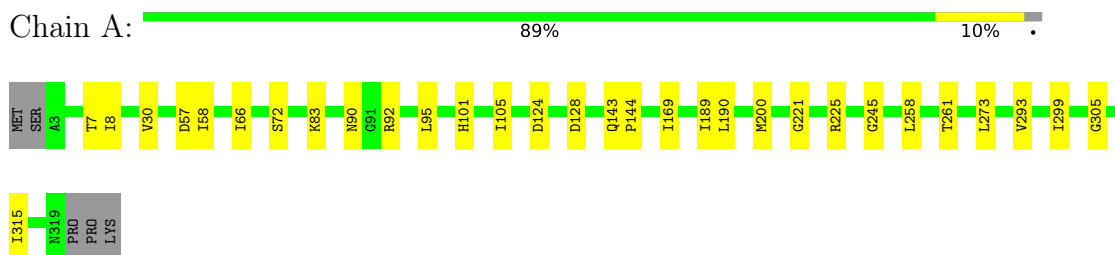
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	212	Total	O	0	0
			212	212		
4	B	222	Total	O	0	0
			222	222		
4	C	211	Total	O	0	0
			211	211		
4	D	196	Total	O	0	0
			196	196		
4	E	172	Total	O	0	0
			172	172		
4	F	152	Total	O	0	0
			152	152		

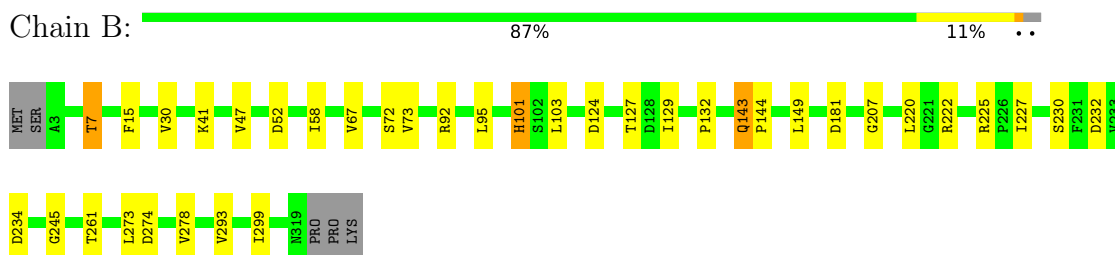
3 Residue-property plots [i](#)

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.

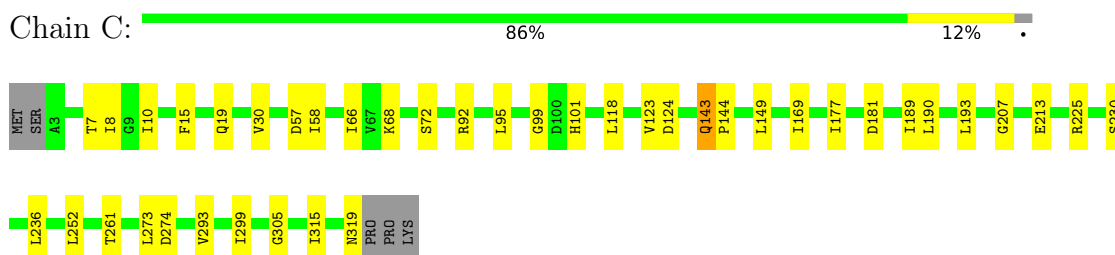
• Molecule 1: Arginase-1



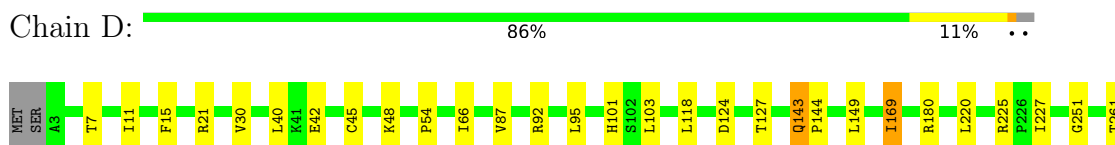
• Molecule 1: Arginase-1



• Molecule 1: Arginase-1

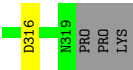
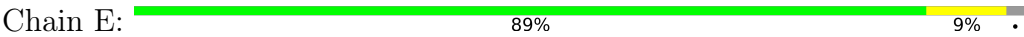


• Molecule 1: Arginase-1

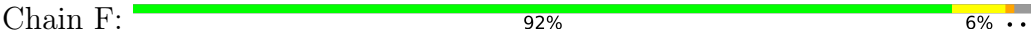




● Molecule 1: Arginase-1



● Molecule 1: Arginase-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.55Å 287.10Å 67.00Å 90.00° 90.26° 90.00°	Depositor
Resolution (Å)	71.78 – 2.27 71.78 – 2.27	Depositor EDS
% Data completeness (in resolution range)	98.8 (71.78-2.27) 97.9 (71.78-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.27Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.170 , 0.233 0.181 , 0.245	Depositor DCC
R_{free} test set	4542 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	1.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.217 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15739	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: VUS, MN

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	0.89	0/2459	1.35	11/3336 (0.3%)
1	B	0.87	0/2459	1.33	8/3336 (0.2%)
1	C	0.87	1/2459 (0.0%)	1.32	12/3336 (0.4%)
1	D	0.88	0/2459	1.32	9/3336 (0.3%)
1	E	0.86	0/2459	1.35	11/3336 (0.3%)
1	F	0.87	0/2459	1.33	5/3336 (0.1%)
All	All	0.87	1/14754 (0.0%)	1.33	56/20016 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	19	GLN	CA-C	5.12	1.57	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	305	GLY	N-CA-C	7.97	122.11	113.58
1	F	124	ASP	CA-CB-CG	7.26	119.86	112.60
1	D	124	ASP	CA-CB-CG	6.53	119.13	112.60
1	B	124	ASP	CA-CB-CG	6.34	118.94	112.60
1	F	125	ALA	N-CA-C	-6.17	105.71	113.18
1	D	118	LEU	CA-C-N	6.12	126.41	122.18
1	D	118	LEU	C-N-CA	6.12	126.41	122.18
1	D	305	GLY	N-CA-C	5.96	122.99	114.64
1	E	207	GLY	N-CA-C	-5.88	105.36	112.48
1	C	305	GLY	N-CA-C	5.85	122.52	114.92
1	B	278	VAL	N-CA-CB	5.84	117.30	110.82
1	A	221	GLY	CA-C-N	5.83	128.09	120.28
1	A	221	GLY	C-N-CA	5.83	128.09	120.28
1	A	305	GLY	N-CA-C	5.79	121.67	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	ILE	N-CA-C	5.73	116.73	108.48
1	D	316	ASP	CA-CB-CG	5.69	118.29	112.60
1	F	200	MET	CA-C-N	5.68	127.82	120.44
1	F	200	MET	C-N-CA	5.68	127.82	120.44
1	B	245	GLY	N-CA-C	5.65	119.33	112.49
1	A	105	ILE	N-CA-C	-5.62	105.03	110.42
1	E	183	ASP	CA-CB-CG	5.61	118.21	112.60
1	D	54	PRO	CA-C-N	-5.61	114.59	123.12
1	D	54	PRO	C-N-CA	-5.61	114.59	123.12
1	C	213	GLU	CA-C-N	5.61	128.25	120.29
1	C	213	GLU	C-N-CA	5.61	128.25	120.29
1	B	181	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	245	GLY	N-CA-C	5.47	119.77	112.77
1	A	189	ILE	CA-C-N	5.47	127.61	120.28
1	A	189	ILE	C-N-CA	5.47	127.61	120.28
1	D	42	GLU	CA-C-N	5.43	131.16	122.86
1	D	42	GLU	C-N-CA	5.43	131.16	122.86
1	B	234	ASP	CA-CB-CG	5.40	118.00	112.60
1	B	207	GLY	N-CA-C	-5.39	105.96	112.48
1	E	125	ALA	N-CA-C	-5.38	106.22	112.89
1	C	207	GLY	CA-C-O	-5.33	118.55	122.23
1	B	7	THR	CB-CA-C	5.27	118.72	110.19
1	E	46	ASP	CA-CB-CG	5.26	117.86	112.60
1	F	234	ASP	CA-CB-CG	5.23	117.83	112.60
1	C	118	LEU	CA-C-N	5.22	126.14	122.33
1	C	118	LEU	C-N-CA	5.22	126.14	122.33
1	C	8	ILE	N-CA-C	5.18	115.95	108.48
1	B	52	ASP	CA-CB-CG	5.17	117.77	112.60
1	E	316	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	124	ASP	CA-CB-CG	5.16	117.76	112.60
1	E	19	GLN	N-CA-C	5.15	112.65	108.07
1	A	124	ASP	CA-CB-CG	5.15	117.75	112.60
1	E	200	MET	CA-C-N	5.07	127.03	120.44
1	E	200	MET	C-N-CA	5.07	127.03	120.44
1	C	68	LYS	CA-C-N	5.07	127.97	123.10
1	C	68	LYS	C-N-CA	5.07	127.97	123.10
1	E	28	PRO	CA-C-N	5.06	127.32	120.65
1	E	28	PRO	C-N-CA	5.06	127.32	120.65
1	A	200	MET	CA-C-N	5.05	127.05	120.28
1	A	200	MET	C-N-CA	5.05	127.05	120.28
1	C	181	ASP	CA-CB-CG	5.03	117.63	112.60
1	C	319	ASN	CA-CB-CG	5.02	117.62	112.60

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	2409	0	2456	8	0
1	B	2409	0	2456	18	0
1	C	2409	0	2456	14	0
1	D	2409	0	2456	17	0
1	E	2409	0	2456	7	0
1	F	2409	0	2456	7	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	212	0	0	0	0
4	B	222	0	0	0	0
4	C	211	0	0	0	0
4	D	196	0	0	0	0
4	E	172	0	0	0	0
4	F	152	0	0	0	0
All	All	15739	0	14736	71	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 (71) 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:15:PHE:HB3	1:D:103:LEU:HD11	1.75	0.67
1:B:30:VAL:CG1	1:B:293:VAL:HG21	2.27	0.65
1:B:220:LEU:HD11	1:B:227:ILE:HD11	1.80	0.63
1:C:30:VAL:HG12	1:C:293:VAL:HG21	1.80	0.62
1:C:10:ILE:HD13	1:C:95:LEU:HD23	1.83	0.60
1:D:7:THR:HG22	1:D:92:ARG:HG2	1.85	0.58
1:E:150:LYS:O	1:E:153:LYS:HB2	2.03	0.57
1:C:7:THR:HG22	1:C:92:ARG:HG2	1.86	0.57
1:F:261:THR:HG21	1:F:299:ILE:HG23	1.86	0.56
1:B:15:PHE:HB3	1:B:103:LEU:HD11	1.90	0.53
1:C:30:VAL:CG1	1:C:293:VAL:HG21	2.37	0.53
1:D:261:THR:HG21	1:D:299:ILE:HG23	1.90	0.52
1:B:41:LYS:HE3	1:B:47:VAL:HB	1.90	0.52
1:F:143:GLN:N	1:F:144:PRO:HD2	2.25	0.52
1:A:7:THR:HG22	1:A:92:ARG:HG2	1.92	0.52
1:B:30:VAL:HG12	1:B:293:VAL:HG21	1.93	0.51
1:B:30:VAL:HG11	1:B:293:VAL:HG21	1.93	0.51
1:B:261:THR:HG21	1:B:299:ILE:HG23	1.92	0.50
1:D:103:LEU:HB2	1:D:276:MET:HE1	1.94	0.49
1:E:101:HIS:CE1	1:E:232:ASP:HB2	2.48	0.49
1:E:220:LEU:HD11	1:E:227:ILE:HD11	1.93	0.49
1:E:10:ILE:HD13	1:E:95:LEU:HD23	1.94	0.49
1:B:143:GLN:N	1:B:144:PRO:HD2	2.28	0.49
1:F:230:SER:HA	1:F:274:ASP:HB2	1.94	0.49
1:D:143:GLN:N	1:D:144:PRO:HD2	2.28	0.48
1:E:230:SER:HA	1:E:274:ASP:HB2	1.96	0.47
1:B:230:SER:HA	1:B:274:ASP:HB2	1.96	0.47
1:D:95:LEU:HD13	1:D:273:LEU:HD23	1.97	0.47
1:D:30:VAL:HG12	1:D:293:VAL:HG21	1.95	0.47
1:B:101:HIS:CE1	1:B:232:ASP:HB2	2.50	0.47
1:C:261:THR:HG21	1:C:299:ILE:HG23	1.96	0.47
1:A:30:VAL:CG1	1:A:293:VAL:HG21	2.46	0.46
1:A:261:THR:HG21	1:A:299:ILE:HG23	1.96	0.46
1:A:58:ILE:HD12	1:A:72:SER:HA	1.97	0.46
1:D:30:VAL:CG1	1:D:293:VAL:HG21	2.46	0.46
1:F:220:LEU:HD11	1:F:227:ILE:HD11	1.98	0.46
1:F:101:HIS:CE1	1:F:232:ASP:HB2	2.52	0.45
1:D:21:ARG:HD3	1:D:282:LEU:HD11	1.98	0.45
1:D:30:VAL:HG21	1:D:280:PRO:HG3	1.97	0.45
1:C:230:SER:HA	1:C:274:ASP:HB2	1.98	0.45
1:D:40:LEU:O	1:D:45:CYS:HB2	2.17	0.45
1:A:95:LEU:HD13	1:A:273:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ILE:HD12	1:B:72:SER:HA	1.99	0.45
1:D:180:ARG:CZ	1:D:251:GLY:HA2	2.47	0.45
1:A:30:VAL:HG12	1:A:293:VAL:HG21	1.97	0.44
1:D:11:ILE:HD11	1:D:87:VAL:HG21	1.99	0.44
1:D:48:LYS:HB2	1:D:92:ARG:CZ	2.48	0.44
1:E:40:LEU:O	1:E:45:CYS:HB2	2.17	0.44
1:B:143:GLN:N	1:B:144:PRO:CD	2.81	0.43
1:F:67:VAL:HG21	1:F:132:PRO:HB3	2.00	0.43
1:B:95:LEU:HD13	1:B:273:LEU:HD23	2.00	0.43
1:C:189:ILE:HG23	1:C:193:LEU:HD12	1.99	0.43
1:C:58:ILE:HD12	1:C:72:SER:HA	2.01	0.43
1:C:123:VAL:HG22	1:C:177:ILE:HB	2.01	0.43
1:C:143:GLN:N	1:C:144:PRO:HD2	2.34	0.43
1:E:30:VAL:HG12	1:E:293:VAL:HG21	2.01	0.43
1:D:143:GLN:N	1:D:144:PRO:CD	2.82	0.43
1:C:95:LEU:HD13	1:C:273:LEU:HD23	2.01	0.43
1:D:220:LEU:HD11	1:D:227:ILE:HD11	2.01	0.43
1:A:258:LEU:HD23	1:A:299:ILE:HD13	2.00	0.42
1:B:143:GLN:H	1:B:144:PRO:CD	2.32	0.42
1:F:143:GLN:N	1:F:144:PRO:CD	2.82	0.41
1:B:129:ILE:HD11	1:B:149:LEU:HD11	2.01	0.41
1:C:15:PHE:O	1:C:99:GLY:HA2	2.20	0.41
1:A:128:ASP:HB3	1:A:144:PRO:HD2	2.02	0.41
1:B:7:THR:HG22	1:B:92:ARG:HG2	2.02	0.40
1:C:236:LEU:HD23	1:C:252:LEU:HB2	2.04	0.40
1:C:10:ILE:CD1	1:C:95:LEU:HD23	2.51	0.40
1:B:15:PHE:CZ	1:B:73:VAL:HA	2.56	0.40
1:B:67:VAL:HG21	1:B:132:PRO:HB3	2.03	0.40
1:D:149:LEU:HD23	1:D:169:ILE:HG13	2.03	0.40

There are no symmetry-related clashes.

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	315/322 (98%)	306 (97%)	8 (2%)	1 (0%)	36	44
1	B	315/322 (98%)	305 (97%)	9 (3%)	1 (0%)	36	44
1	C	315/322 (98%)	305 (97%)	9 (3%)	1 (0%)	36	44
1	D	315/322 (98%)	304 (96%)	10 (3%)	1 (0%)	36	44
1	E	315/322 (98%)	304 (96%)	10 (3%)	1 (0%)	36	44
1	F	315/322 (98%)	303 (96%)	11 (4%)	1 (0%)	36	44
All	All	1890/1932 (98%)	1827 (97%)	57 (3%)	6 (0%)	36	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	143	GLN
1	E	143	GLN
1	F	143	GLN
1	A	143	GLN
1	D	143	GLN
1	C	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	265/270 (98%)	256 (97%)	9 (3%)	32	46
1	B	265/270 (98%)	261 (98%)	4 (2%)	57	72
1	C	265/270 (98%)	257 (97%)	8 (3%)	36	51
1	D	265/270 (98%)	258 (97%)	7 (3%)	40	56
1	E	265/270 (98%)	257 (97%)	8 (3%)	36	51
1	F	265/270 (98%)	258 (97%)	7 (3%)	40	56
All	All	1590/1620 (98%)	1547 (97%)	43 (3%)	39	55

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ASP
1	A	66	ILE
1	A	83	LYS
1	A	90	ASN
1	A	101	HIS
1	A	169	ILE
1	A	190	LEU
1	A	225	ARG
1	A	315	ILE
1	B	101	HIS
1	B	127	THR
1	B	222	ARG
1	B	225	ARG
1	C	57	ASP
1	C	66	ILE
1	C	101	HIS
1	C	149	LEU
1	C	169	ILE
1	C	190	LEU
1	C	225	ARG
1	C	315	ILE
1	D	66	ILE
1	D	101	HIS
1	D	127	THR
1	D	169	ILE
1	D	225	ARG
1	D	284	LYS
1	D	315	ILE
1	E	8	ILE
1	E	29	THR
1	E	66	ILE
1	E	68	LYS
1	E	86	GLU
1	E	101	HIS
1	E	172	LYS
1	E	225	ARG
1	F	8	ILE
1	F	24	VAL
1	F	66	ILE
1	F	101	HIS
1	F	140	LEU
1	F	220	LEU
1	F	225	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	130	ASN
1	B	19	GLN
1	B	65	GLN
1	B	79	GLN
1	B	143	GLN
1	C	115	HIS
1	D	90	ASN
1	D	130	ASN
1	D	319	ASN
1	E	79	GLN
1	F	19	GLN
1	F	65	GLN
1	F	115	HIS
1	F	143	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	VUS	D	1003	2	15,19,19	1.38	2 (13%)	8,29,29	1.15	1 (12%)
3	VUS	C	1003	2	15,19,19	1.52	3 (20%)	8,29,29	1.11	1 (12%)
3	VUS	E	1003	2	15,19,19	0.87	0	8,29,29	1.26	1 (12%)
3	VUS	B	1003	2	15,19,19	0.80	0	8,29,29	1.11	0
3	VUS	A	1003	2	15,19,19	0.78	0	8,29,29	1.32	2 (25%)
3	VUS	F	1003	2	15,19,19	1.34	2 (13%)	8,29,29	1.20	2 (25%)

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	VUS	D	1003	2	-	2/9/36/36	0/2/2/2
3	VUS	C	1003	2	-	1/9/36/36	0/2/2/2
3	VUS	E	1003	2	-	2/9/36/36	0/2/2/2
3	VUS	B	1003	2	-	3/9/36/36	0/2/2/2
3	VUS	A	1003	2	-	0/9/36/36	0/2/2/2
3	VUS	F	1003	2	-	2/9/36/36	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1003	VUS	O-C	3.09	1.31	1.22
3	C	1003	VUS	O-C	3.04	1.31	1.22
3	F	1003	VUS	O-C	3.02	1.31	1.22
3	C	1003	VUS	O1-C	-2.90	1.21	1.30
3	F	1003	VUS	O1-C	-2.85	1.21	1.30
3	D	1003	VUS	O1-C	-2.61	1.22	1.30
3	C	1003	VUS	B-O4	2.41	1.52	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	VUS	C2-C3-C6	2.38	106.88	103.36
3	C	1003	VUS	C2-C3-C6	2.32	106.79	103.36
3	E	1003	VUS	C2-C3-C6	2.21	106.63	103.36
3	F	1003	VUS	B-C9-C8	-2.15	108.14	115.56
3	A	1003	VUS	O2-B-O4	-2.05	101.11	108.94
3	D	1003	VUS	C2-C3-C6	2.01	106.33	103.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1003	VUS	C2-C3-C6	2.00	106.33	103.36

There are no chirality outliers.

All (10) torsion outliers are listed below:

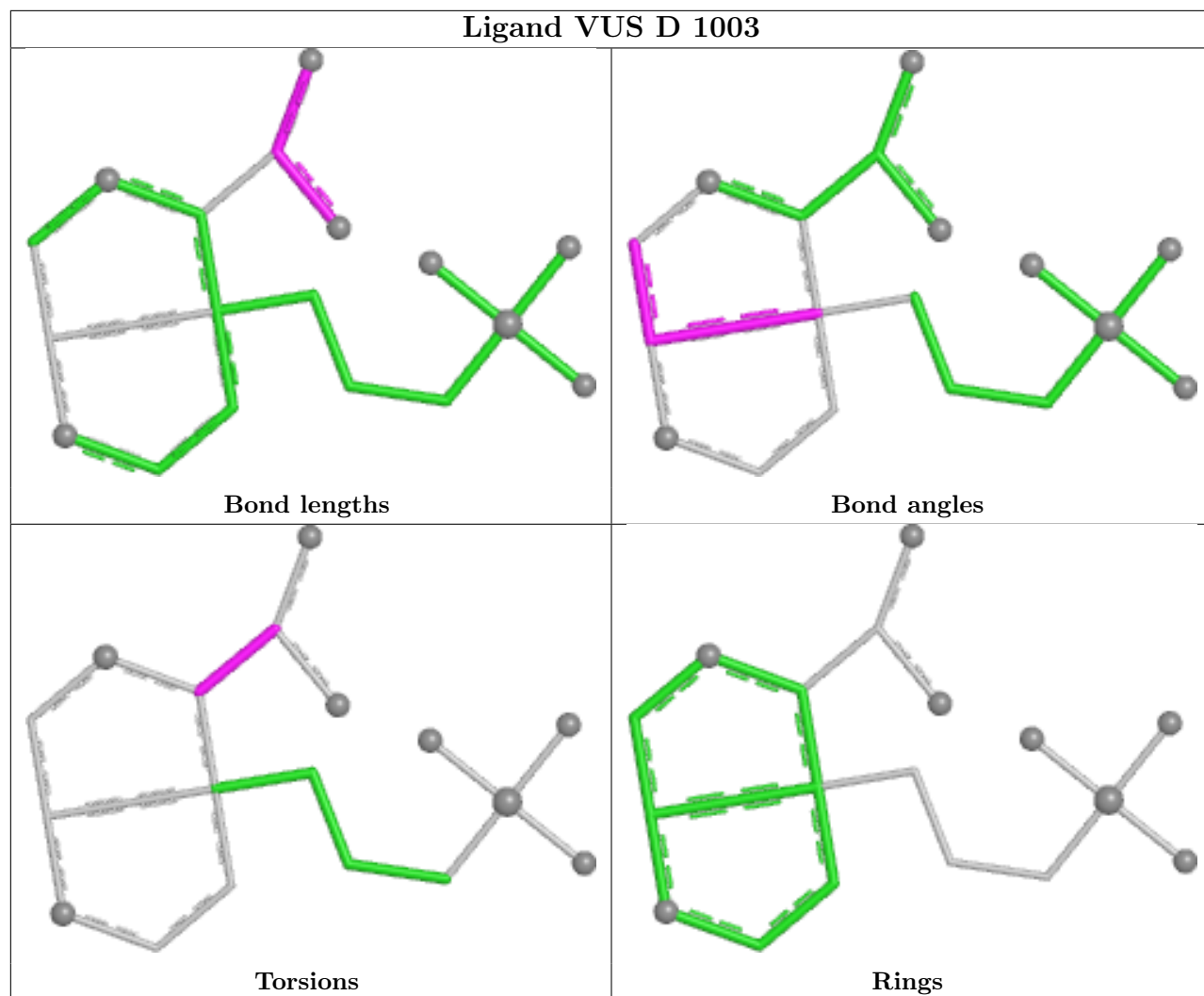
Mol	Chain	Res	Type	Atoms
3	B	1003	VUS	C3-C6-C7-C8
3	B	1003	VUS	O-C-C1-C6
3	F	1003	VUS	O-C-C1-C6
3	F	1003	VUS	O1-C-C1-C6
3	B	1003	VUS	O1-C-C1-C6
3	D	1003	VUS	O-C-C1-C6
3	D	1003	VUS	O1-C-C1-C6
3	E	1003	VUS	O-C-C1-C6
3	E	1003	VUS	O1-C-C1-C6
3	C	1003	VUS	O-C-C1-C6

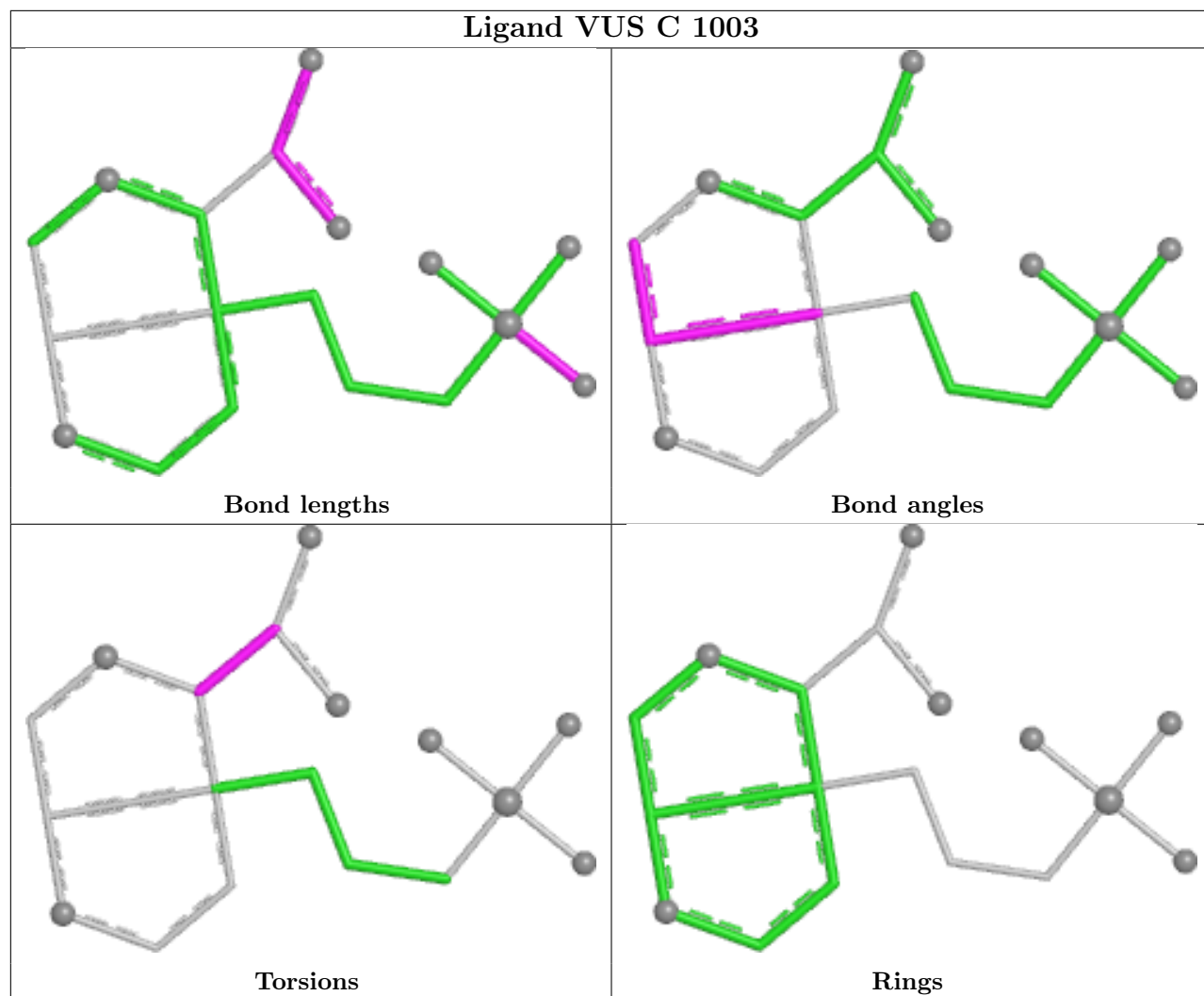
There are no ring outliers.

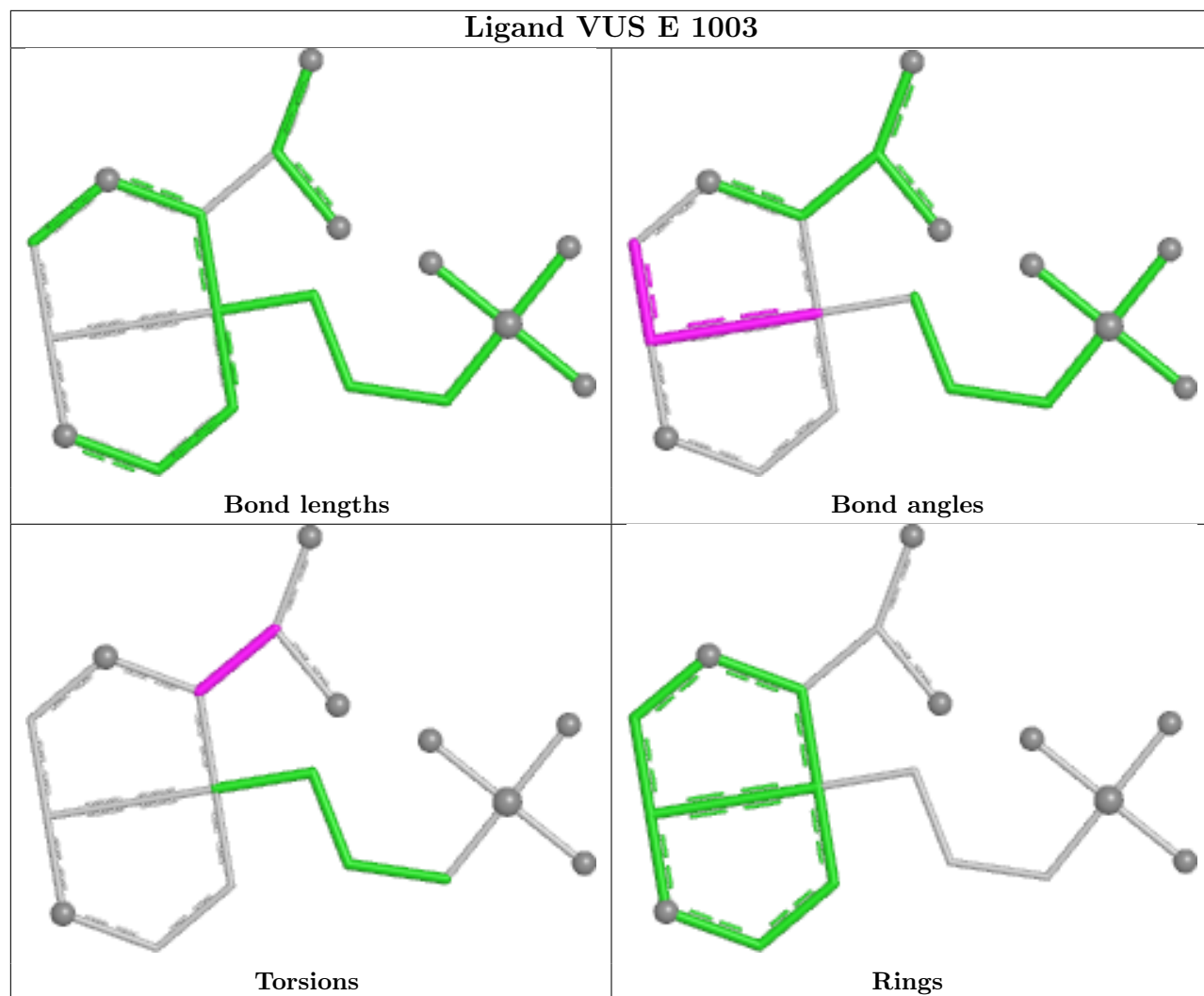
No monomer is involved in short contacts.

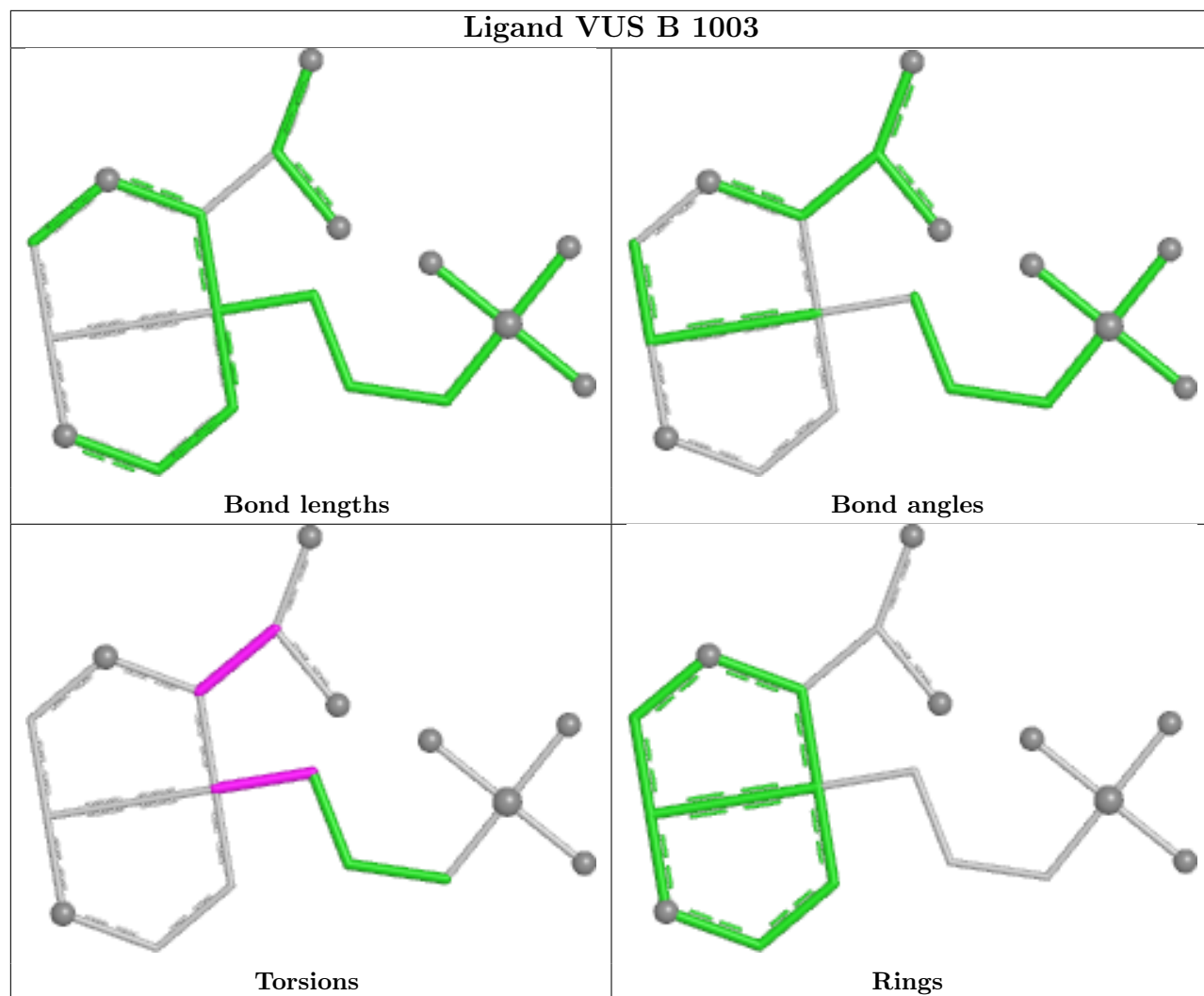
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

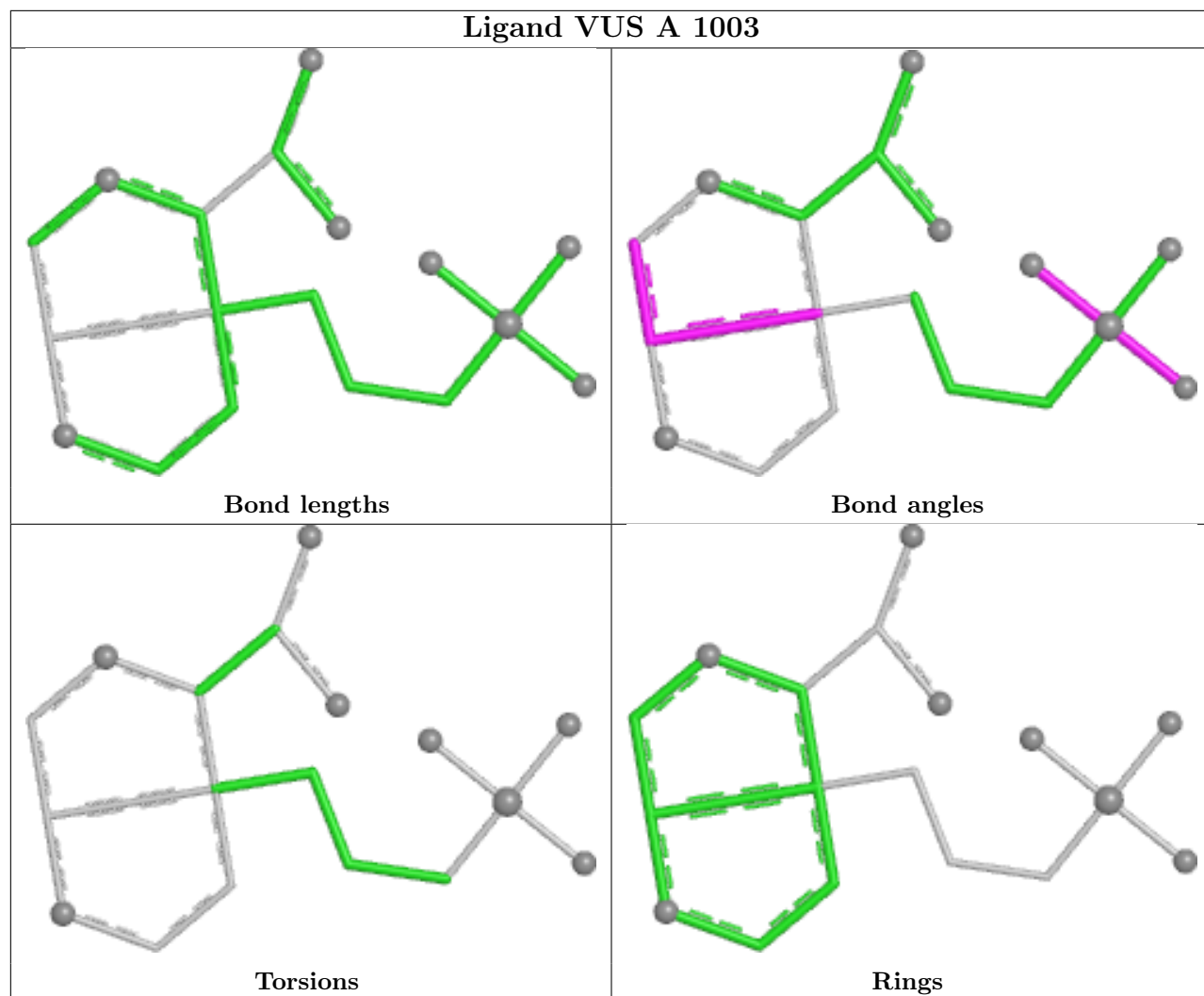
Ligand VUS D 1003

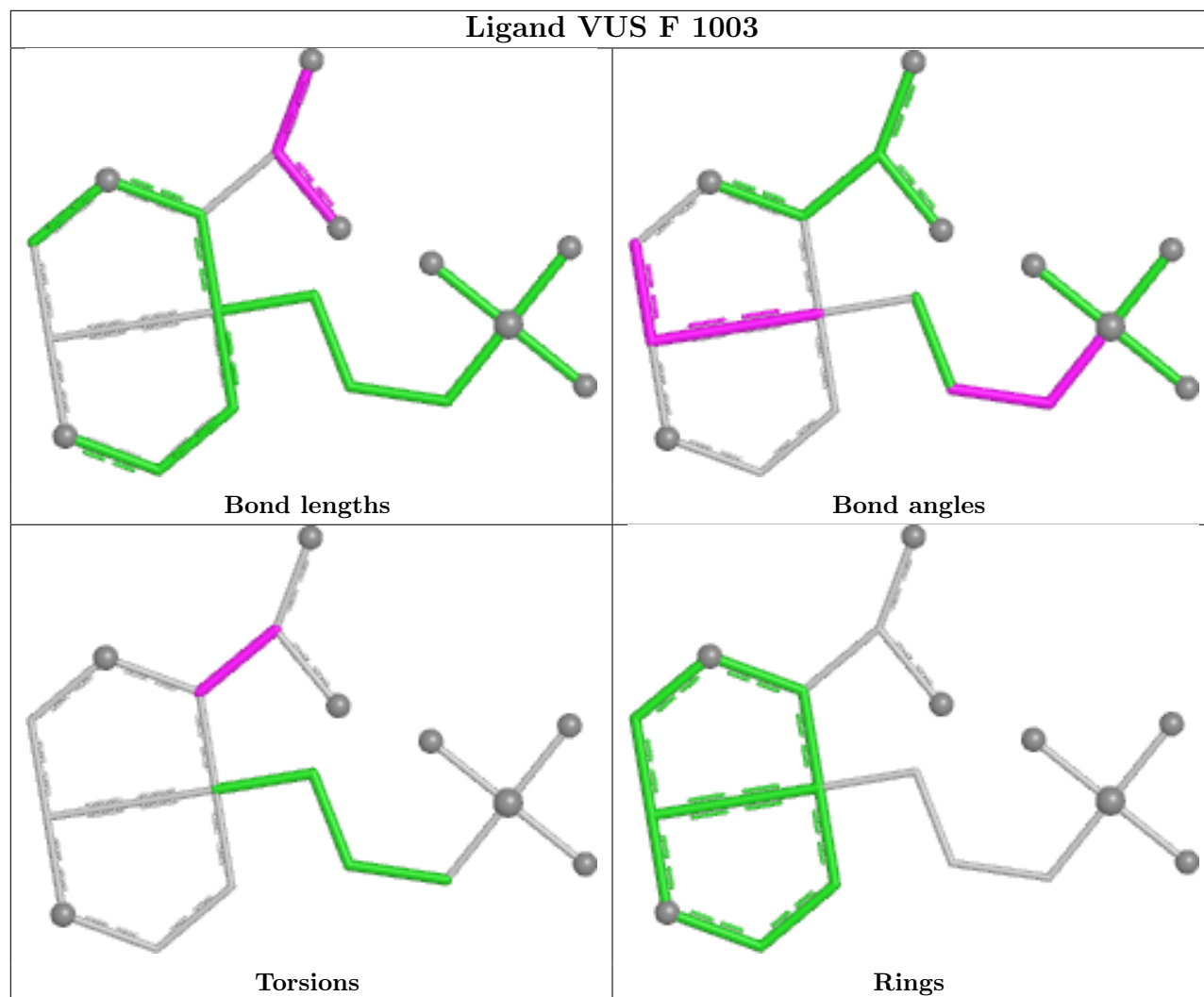












5.7 Other polymers [i](#)

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	317/322 (98%)	-1.57	0 100 100	13, 21, 39, 91	0
1	B	317/322 (98%)	-1.52	0 100 100	13, 22, 39, 70	0
1	C	317/322 (98%)	-1.57	0 100 100	13, 22, 41, 76	0
1	D	317/322 (98%)	-1.50	0 100 100	15, 22, 40, 71	0
1	E	317/322 (98%)	-1.41	0 100 100	15, 29, 48, 83	0
1	F	317/322 (98%)	-1.37	0 100 100	14, 31, 52, 84	0
All	All	1902/1932 (98%)	-1.49	0 100 100	13, 24, 45, 91	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	VUS	B	1003	18/18	0.99	0.03	13,18,22,24	0

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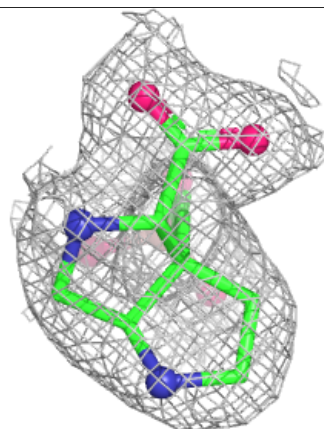
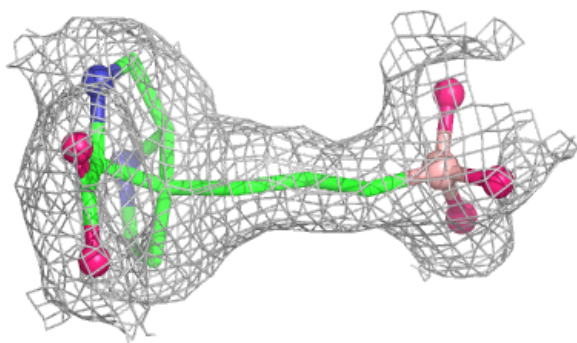
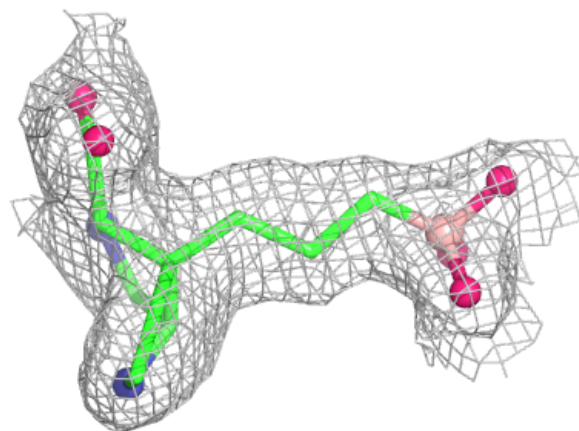
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	VUS	D	1003	18/18	0.99	0.02	14,22,24,27	0
3	VUS	E	1003	18/18	0.99	0.03	26,29,32,34	0
3	VUS	F	1003	18/18	0.99	0.03	26,29,32,35	0
2	MN	C	1001	1/1	1.00	0.01	16,16,16,16	0
2	MN	C	1002	1/1	1.00	0.01	19,19,19,19	0
2	MN	D	1001	1/1	1.00	0.00	18,18,18,18	0
2	MN	D	1002	1/1	1.00	0.01	17,17,17,17	0
2	MN	E	1001	1/1	1.00	0.01	19,19,19,19	0
2	MN	E	1002	1/1	1.00	0.01	20,20,20,20	0
2	MN	F	1001	1/1	1.00	0.01	22,22,22,22	0
2	MN	F	1002	1/1	1.00	0.02	28,28,28,28	0
3	VUS	A	1003	18/18	1.00	0.02	12,18,23,26	0
2	MN	A	1001	1/1	1.00	0.01	18,18,18,18	0
3	VUS	C	1003	18/18	1.00	0.02	8,23,29,32	0
2	MN	A	1002	1/1	1.00	0.00	16,16,16,16	0
2	MN	B	1001	1/1	1.00	0.01	15,15,15,15	0
2	MN	B	1002	1/1	1.00	0.01	20,20,20,20	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.

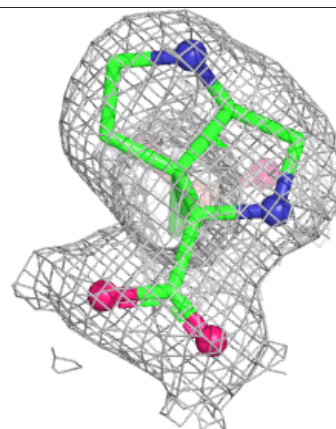
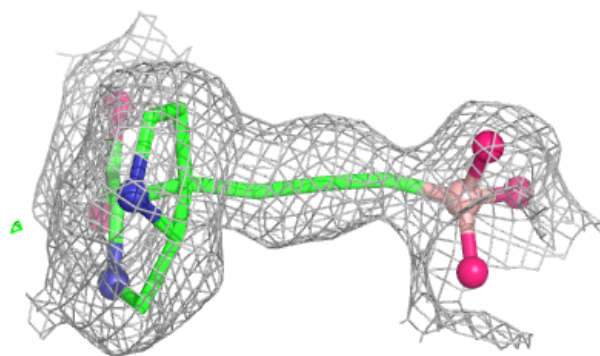
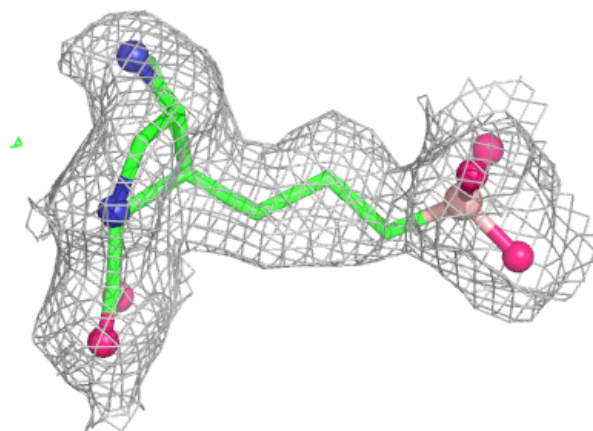
Electron density around VUS B 1003:

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



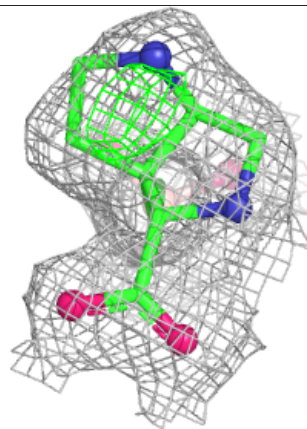
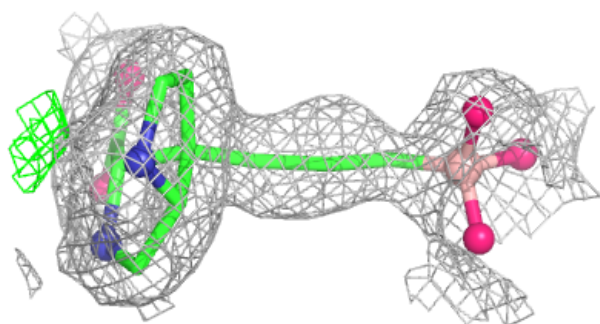
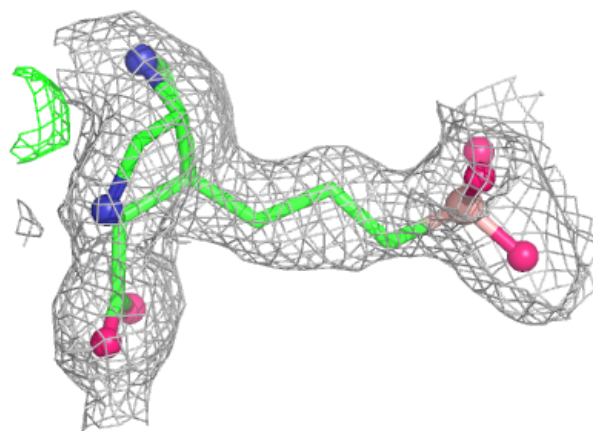
Electron density around VUS D 1003:

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



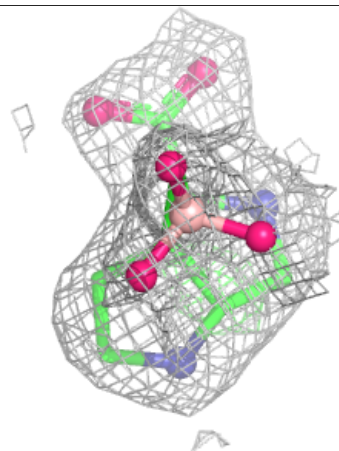
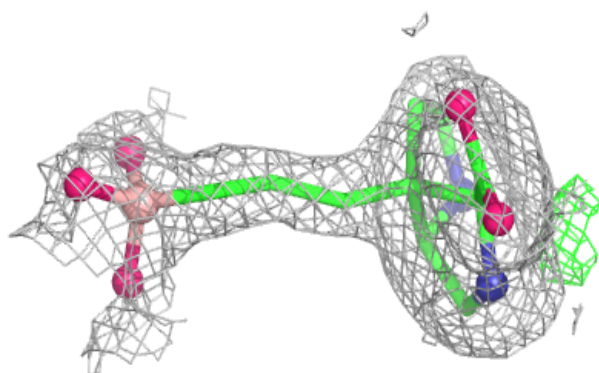
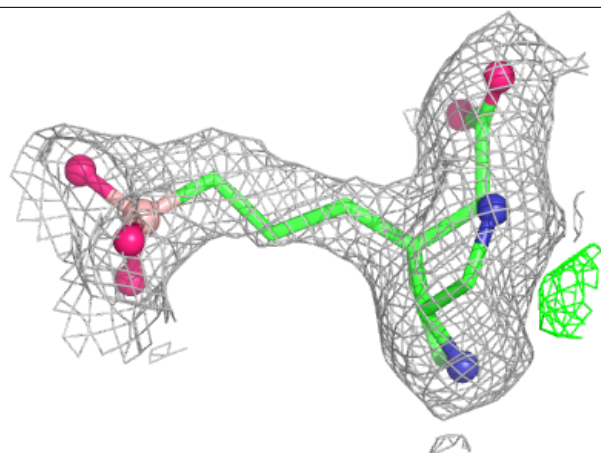
Electron density around VUS E 1003:

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



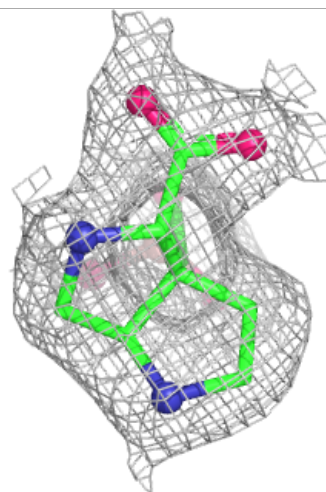
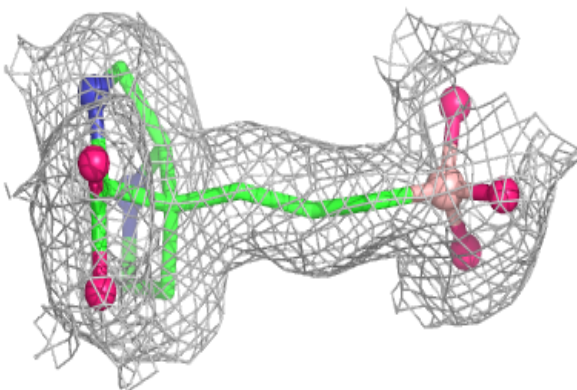
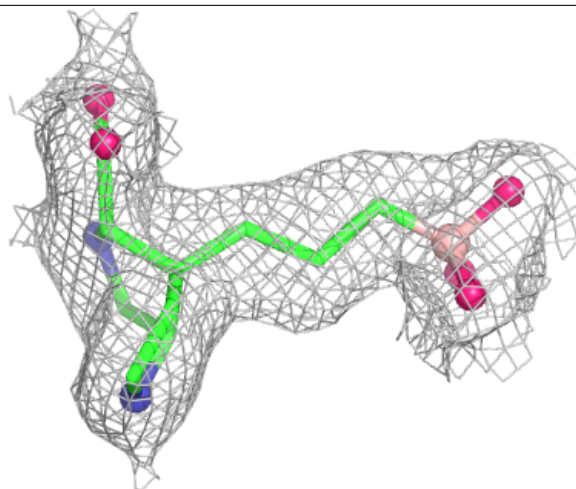
Electron density around VUS F 1003:

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



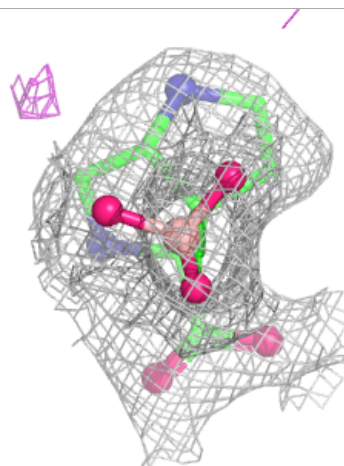
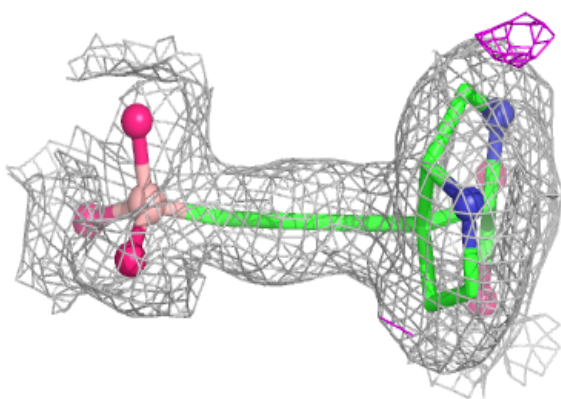
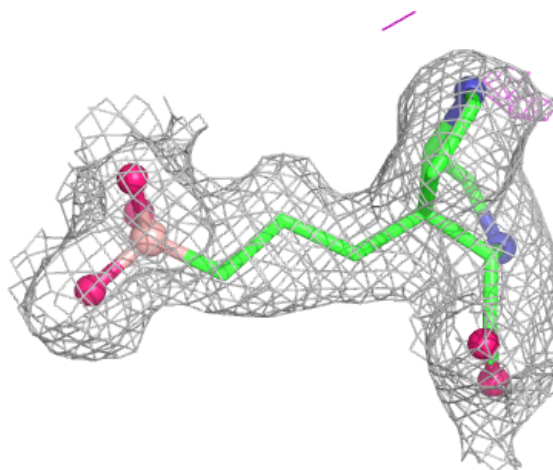
Electron density around VUS A 1003:

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



Electron density around VUS C 1003:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.