wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 18, 2023 – 07:18 pm BST

PDB ID	:	8CQE
Title	:	pVHL:EloB:EloC in complex with (2S,4R)-1-((S)-2-(1-Fluorocyclopropane-1-carboxamido)-3,3-dimethylbutanoyl)-4-hydroxy-N-((S)-1-(2-methyl-4-(4-met hylthiazol-5-yl)phenyl)ethyl)pyrrolidine-2-carboxamide (Compound 37)
Authors	:	Casement, R.; Phuong Vu, L.; Ciulli, A.; Gutschow, M.
Deposited on	:	2023-03-06
Resolution	:	2.85 Å(reported)

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

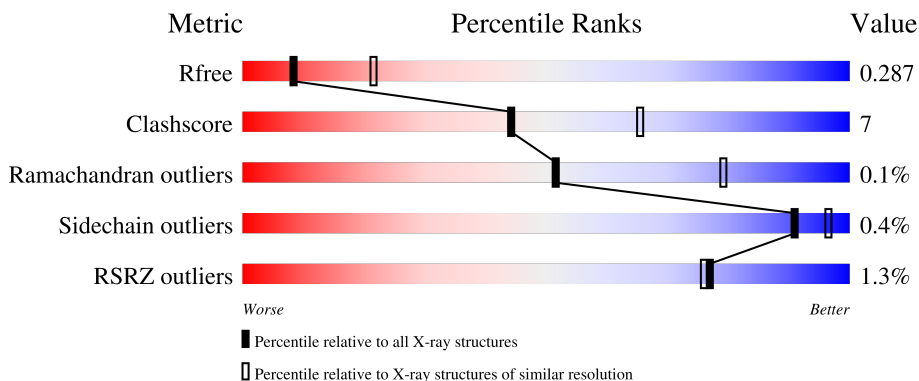|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.85 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		0.287
Clashscore		7
Ramachandran outliers		0.1%
Sidechain outliers		0.4%
RSRZ outliers		1.3%

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$_{free}$	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	104	2% / 76% / 24%
1	D	104	84% / 16%
1	G	104	% / 77% / 21% / •
1	J	104	2% / 76% / 24%

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Mol	Chain	Length	Quality of chain
2	B	97	% 79% 12% 8%
2	E	97	75% 16% 8%
2	H	97	2% 77% 11% 11%
2	K	97	% 85% · 11%
3	C	162	78% 9% 13%
3	F	162	% 75% 12% 13%
3	I	162	3% 76% 12% 12%
3	L	162	% 78% 9% 13%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 10495 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 Elongin-B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	104	Total 809	As 2	C 513	N 133	O 156	S 5	0	0	0
1	D	104	Total 812	As 2	C 516	N 137	O 152	S 5	0	0	0
1	G	104	Total 811	As 2	C 513	N 136	O 156	S 4	0	0	0
1	J	104	Total 772	As 2	C 492	N 125	O 149	S 4	0	0	0

- Molecule 2 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	89	Total 677	C 441	N 106	O 124	S 6	0	0	0
2	E	89	Total 687	C 445	N 112	O 123	S 7	0	0	0
2	H	86	Total 670	C 434	N 105	O 126	S 5	0	0	0
2	K	86	Total 669	C 433	N 106	O 125	S 5	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	initiating methionine	UNP Q15369
E	16	MET	-	initiating methionine	UNP Q15369
H	16	MET	-	initiating methionine	UNP Q15369
K	16	MET	-	initiating methionine	UNP Q15369

- Molecule 3 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	141	Total 1118	As 1	C 712	N 200	O 203	S 2	0	0	0
3	F	141	Total 1102	As 1	C 701	N 199	O 199	S 2	0	0	0
3	I	143	Total 1111	As 1	C 706	N 203	O 199	S 2	0	0	0
3	L	141	Total 1092	As 1	C 697	N 197	O 195	S 2	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	52	GLY	-	expression tag	UNP P40337
C	53	SER	-	expression tag	UNP P40337
F	52	GLY	-	expression tag	UNP P40337
F	53	SER	-	expression tag	UNP P40337
I	52	GLY	-	expression tag	UNP P40337
I	53	SER	-	expression tag	UNP P40337
L	52	GLY	-	expression tag	UNP P40337
L	53	SER	-	expression tag	UNP P40337

- Molecule 4 is (2 {S},4 {R})-1-[(2 {S})-2-[(1-fluoranylcyclopropyl)carbonylamino]-3,3-dime thyl-butanoyl]- {N}-[(1 {S})-7-fluoranyl-6-(4-methyl-1,3-thiazol-5-yl)-1,2,3,4-tetrahydro naphthalen-1-yl]-4-oxidanyl-pyrrolidine-2-carboxamide (three-letter code: VFO) (formula: $C_{29}H_{36}F_2N_4O_4S$) (labeled as "Ligand of Interest" by depositor).
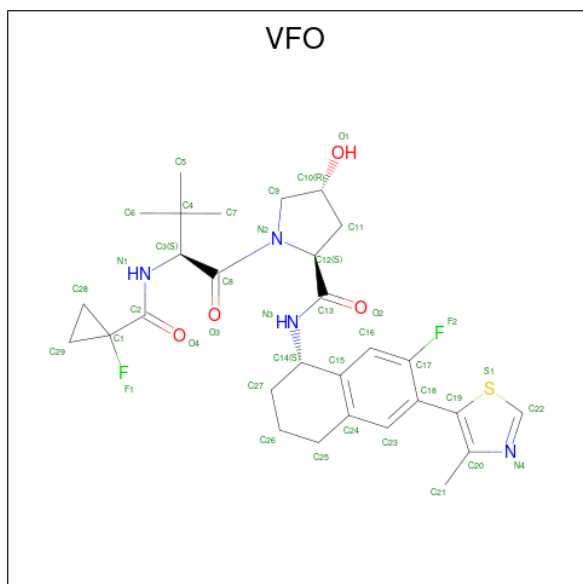
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	C	1	Total	C	F	N	O	S		0	0
			40	29	2	4	4	1			
4	F	1	Total	C	F	N	O	S		0	0
			40	29	2	4	4	1			
4	I	1	Total	C	F	N	O	S		0	0
			40	29	2	4	4	1			
4	L	1	Total	C	F	N	O	S		0	0
			40	29	2	4	4	1			

- Molecule 5 is water.

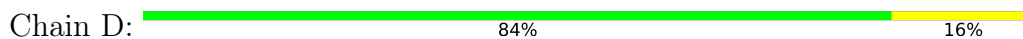| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	1	Total	O	0	0
			1	1		
5	E	1	Total	O	0	0
			1	1		
5	F	1	Total	O	0	0
			1	1		
5	I	1	Total	O	0	0
			1	1		

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.
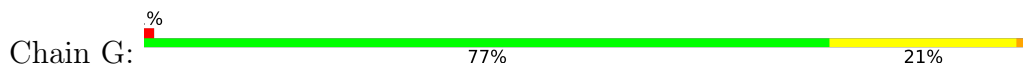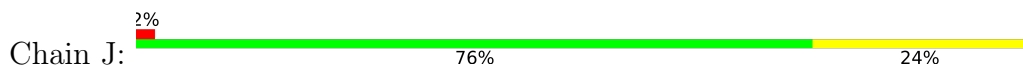
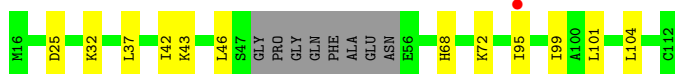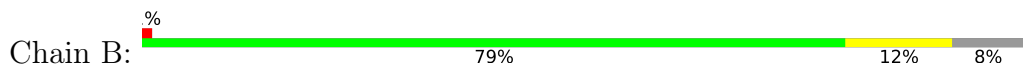- Molecule 1: Elongin-B

Chain A:

- Molecule 1: Elongin-B

Chain D:

- Molecule 1: Elongin-B
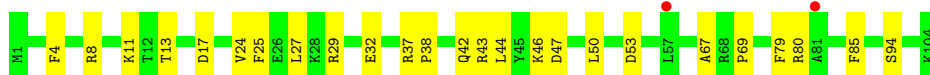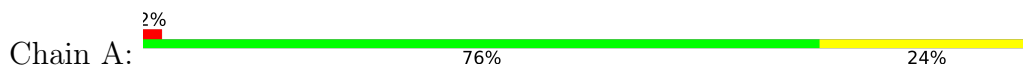
Chain G:

- Molecule 1: Elongin-B

Chain J:

- Molecule 2: Elongin-C

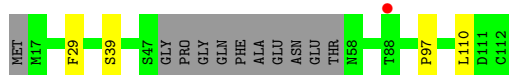Chain B:

- Molecule 2: Elongin-C

Chain E:

75%　　　　　　　　　　16%　　8%

M16 M17 Y18 D25 F29 K32 H35 T38 T41 M45 L46 S47 GLY PRO GLY GLN PHE ALA GLU ASN E56 R63 E64 K80 V81 E98 A107 D111 C112

● Molecule 2: Elongin-C

Chain H:

2%

77%　　　　　　　　11%　　11%
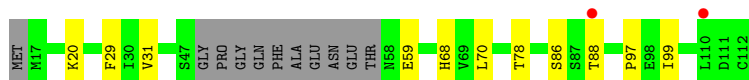
MET M17 K20 F29 I30 V31 S47 GLY PRO GLY GLN PHE ALA GLU ASN GLU THR N58 E59 H68 V69 L70 T78 S86 S87 T88 P97 E98 I99 L110 D111 C112

● Molecule 2: Elongin-C

Chain K:

%

85%　　　　　　　　　　　　　11%

MET M17 F29 S39 S47 GLY PRO GLY GLN PHE ALA GLU ASN GLU THR N58 T88 P97 L110 D111 C112

● Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain C:

78%　　　　　　　　　9%　　13%

GLY SER MET GLU ALA GLY ARG PRO ARG PRO V62 Q73 F76 N90 E94 P95 Q96 R108 I109 V165 N174 R177 L178 R182 S183 L184 Y185 E189 T202 GLN GLU ARG ILE ALA HIS GLN ARG MET GLY ASP

● Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain F:

%

75%　　　　　　　　12%　　13%

GLY SER MET GLU ALA GLY ARG PRO ARG PRO V62 V74 I75 F76 N90 E94 P102 T105 G106 H125 L129 T133 E134 Q145 P146 I147 F148 P154 I180 L184 Y185 E189 V194 D197 T202 GLN GLU ARG ILE ALA HIS GLN ARG MET

GLY ASP

● Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain I:

3%

76%　　　　　　　　12%　　12%

GLY SER MET GLU ALA GLY ARG PRO ARG PRO V62 Q73 F76 P102 P103 G104 T105 R108 I109 Y112 R113 G114 H115 L129 L140 D143 P154 L158 R161 V165 V166 R167 S168 L169 L178 R182 S183 L184 H191 P192 N193 K196 E204

ARG ILE ALA HIS GLN ARG MET GLY ASP
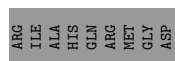
● Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain L:

%

78%　　　　　　　　　9%　　13%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	92.97Å 92.97Å 362.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.05 – 2.85 90.51 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (90.05-2.85) 99.8 (90.51-2.85)	Depositor EDS
R_{merge}	0.90	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.243 , 0.297 0.244 , 0.287	Depositor DCC
R_{free} test set	1924 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	48.8	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 36.0	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	10495	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2248e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: VFO, CAS

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	0.32	0/805	0.58	0/1087
1	D	0.32	0/808	0.56	0/1089
1	G	0.37	0/807	0.54	0/1090
1	J	0.32	0/768	0.54	0/1043
2	B	0.28	0/691	0.48	0/935
2	E	0.27	0/701	0.46	0/947
2	H	0.33	0/684	0.49	0/926
2	K	0.29	0/683	0.49	0/925
3	C	0.33	0/1138	0.57	0/1558
3	F	0.33	0/1121	0.51	0/1535
3	I	0.30	0/1130	0.48	0/1546
3	L	0.34	0/1111	0.55	0/1524
All	All	0.32	0/10447	0.52	0/14205

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	809	0	783	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	812	0	800	11	0
1	G	811	0	785	17	0
1	J	772	0	718	15	0
2	B	677	0	654	11	0
2	E	687	0	672	15	0
2	H	670	0	652	7	0
2	K	669	0	652	3	0
3	C	1118	0	1071	11	0
3	F	1102	0	1053	12	0
3	I	1111	0	1052	19	0
3	L	1092	0	1041	10	0
4	C	40	0	0	1	0
4	F	40	0	0	1	0
4	I	40	0	0	1	0
4	L	40	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	I	1	0	0	0	0
All	All	10495	0	9933	135	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 7.

The worst 5 of 135 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)
3:I:193:ASN:HD22	3:I:196:LYS:H	1.20	0.85
1:A:43:ARG:HG2	1:A:50:LEU:HD11	1.60	0.82
2:E:63:ARG:HD3	3:I:104:GLY:HA3	1.63	0.81
1:J:52:ASP:HB2	1:J:55:LYS:HG2	1.66	0.77
2:B:37:LEU:HD22	2:B:43:LYS:HG3	1.66	0.76

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	100/104 (96%)	96 (96%)	4 (4%)	0	100	100
1	D	100/104 (96%)	97 (97%)	3 (3%)	0	100	100
1	G	100/104 (96%)	97 (97%)	2 (2%)	1 (1%)	15	40
1	J	100/104 (96%)	96 (96%)	4 (4%)	0	100	100
2	B	85/97 (88%)	84 (99%)	1 (1%)	0	100	100
2	E	85/97 (88%)	84 (99%)	1 (1%)	0	100	100
2	H	82/97 (84%)	82 (100%)	0	0	100	100
2	K	82/97 (84%)	82 (100%)	0	0	100	100
3	C	138/162 (85%)	132 (96%)	6 (4%)	0	100	100
3	F	138/162 (85%)	132 (96%)	6 (4%)	0	100	100
3	I	140/162 (86%)	130 (93%)	10 (7%)	0	100	100
3	L	138/162 (85%)	133 (96%)	5 (4%)	0	100	100
All	All	1288/1452 (89%)	1245 (97%)	42 (3%)	1 (0%)	51	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	82	ASP

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	85/90 (94%)	85 (100%)	0	100	100
1	D	85/90 (94%)	85 (100%)	0	100	100
1	G	85/90 (94%)	83 (98%)	2 (2%)	49	77
1	J	76/90 (84%)	76 (100%)	0	100	100
2	B	71/86 (83%)	71 (100%)	0	100	100
2	E	73/86 (85%)	73 (100%)	0	100	100
2	H	73/86 (85%)	73 (100%)	0	100	100
2	K	73/86 (85%)	73 (100%)	0	100	100
3	C	121/147 (82%)	120 (99%)	1 (1%)	81	93
3	F	118/147 (80%)	117 (99%)	1 (1%)	81	93
3	I	116/147 (79%)	116 (100%)	0	100	100
3	L	116/147 (79%)	116 (100%)	0	100	100
All	All	1092/1292 (84%)	1088 (100%)	4 (0%)	91	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	96	GLN
3	F	148	PHE
1	G	40	ASP
1	G	85	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	65	GLN
3	I	191	HIS
3	L	191	HIS
3	I	193	ASN
3	C	174	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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	#$|Z| > 2$
3	CAS	I	77	3	5,8,9	1.16	0	1,9,11	0.99	0
1	CAS	J	60	1	5,8,9	1.04	0	1,9,11	0.90	0
1	CAS	A	60	1	5,8,9	1.07	0	1,9,11	0.92	0
1	CAS	G	60	1	5,8,9	0.90	0	1,9,11	1.60	0
1	CAS	G	89	1	5,8,9	1.19	0	1,9,11	0.86	0
1	CAS	A	89	1	5,8,9	1.14	0	1,9,11	0.41	0
1	CAS	J	89	1	5,8,9	1.17	0	1,9,11	1.34	0
3	CAS	C	77	3	5,8,9	1.18	0	1,9,11	0.68	0
3	CAS	L	77	3	5,8,9	1.22	0	1,9,11	1.10	0
3	CAS	F	77	3	5,8,9	1.23	0	1,9,11	0.62	0
1	CAS	D	60	1	5,8,9	1.08	0	1,9,11	0.83	0
1	CAS	D	89	1	5,8,9	1.15	0	1,9,11	0.84	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CAS	I	77	3	-	0/0/7/9	-
1	CAS	J	60	1	-	0/0/7/9	-
1	CAS	A	60	1	-	0/0/7/9	-
1	CAS	G	60	1	-	0/0/7/9	-
1	CAS	G	89	1	-	0/0/7/9	-
1	CAS	A	89	1	-	0/0/7/9	-
1	CAS	J	89	1	-	0/0/7/9	-
3	CAS	C	77	3	-	0/0/7/9	-
3	CAS	L	77	3	-	0/0/7/9	-
3	CAS	F	77	3	-	0/0/7/9	-
1	CAS	D	60	1	-	0/0/7/9	-
1	CAS	D	89	1	-	0/0/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	60	CAS	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	$\#|Z| > 2$
4	VFO	L	301	-	37,44,44	0.46	0	51,68,68	0.98	2 (3%)
4	VFO	C	301	-	37,44,44	0.45	0	51,68,68	1.12	5 (9%)
4	VFO	F	301	-	37,44,44	0.44	0	51,68,68	1.04	4 (7%)
4	VFO	I	301	-	37,44,44	0.41	0	51,68,68	0.99	2 (3%)

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
4	VFO	L	301	-	-	3/33/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	VFO	C	301	-	-	5/33/62/62	0/5/5/5
4	VFO	F	301	-	-	3/33/62/62	0/5/5/5
4	VFO	I	301	-	-	2/33/62/62	0/5/5/5

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	301	VFO	C14-N3-C13	-3.71	117.63	123.19
4	F	301	VFO	C14-N3-C13	-3.58	117.83	123.19
4	I	301	VFO	C14-N3-C13	-2.89	118.86	123.19
4	L	301	VFO	C14-N3-C13	-2.36	119.66	123.19
4	C	301	VFO	C4-C3-N1	-2.32	108.94	111.84

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	301	VFO	C17-C18-C19-S1
4	C	301	VFO	C23-C18-C19-C20
4	C	301	VFO	C28-C1-C2-O4
4	F	301	VFO	C17-C18-C19-S1
4	I	301	VFO	C17-C18-C19-S1

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	301	VFO	1	0
4	C	301	VFO	1	0
4	F	301	VFO	1	0
4	I	301	VFO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 VFO L 301

Bond lengths

Bond angles

Torsions

Rings

Ligand VFO C 301

Bond lengths

Bond angles

Torsions

Rings

Ligand VFO F 301

Bond lengths

Bond angles

Torsions

Rings

Ligand VFO I 301

Bond lengths

Bond angles

Torsions

Rings
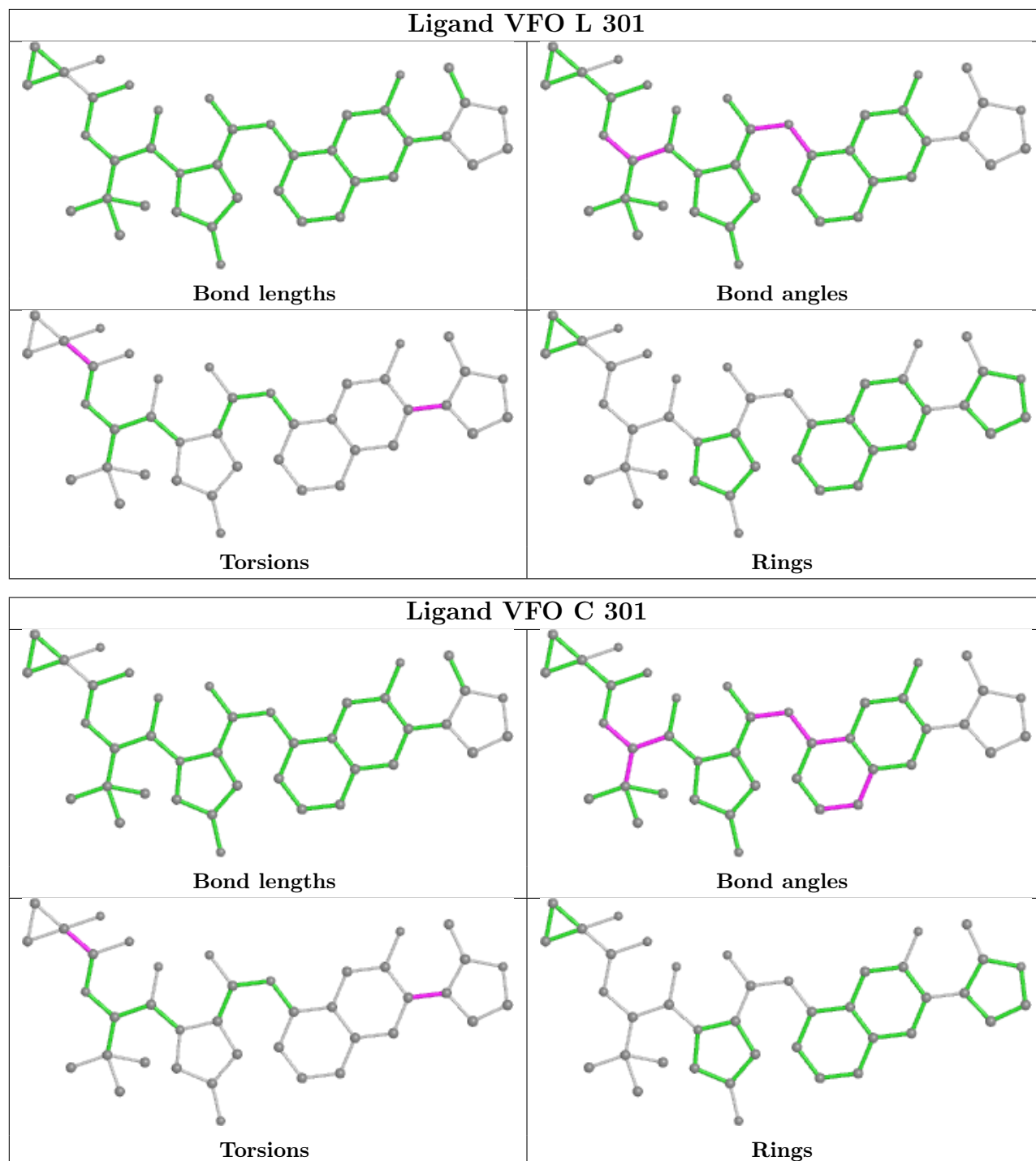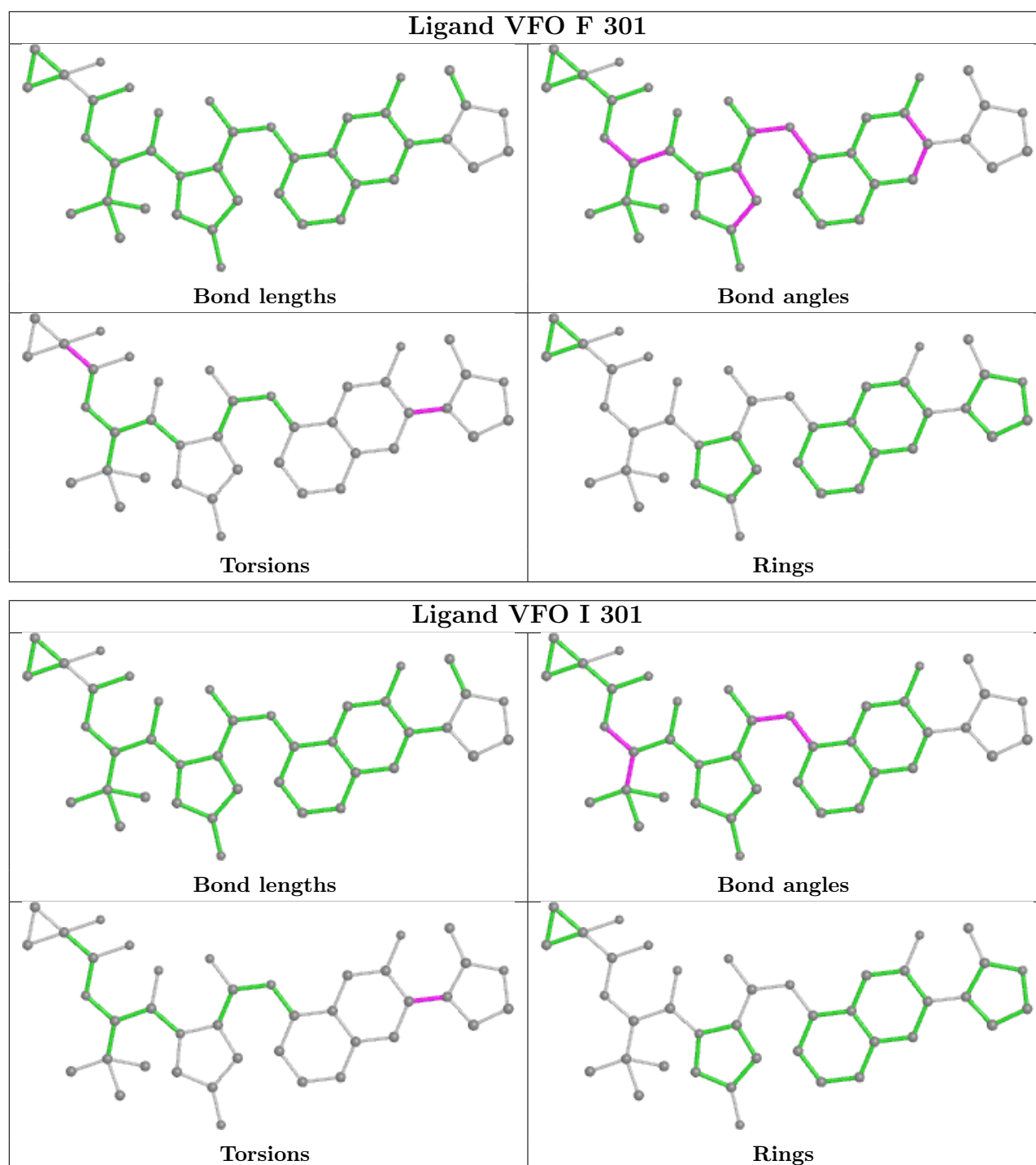
5.7 Other polymers ⓘ

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	102/104 (98%)	-0.10	2 (1%)	65	62	29, 47, 66, 80	0
1	D	102/104 (98%)	-0.22	0	100	100	26, 37, 65, 90	0
1	G	102/104 (98%)	-0.02	1 (0%)	82	81	29, 43, 74, 82	0
1	J	102/104 (98%)	0.04	2 (1%)	65	62	33, 56, 79, 96	0
2	B	89/97 (91%)	-0.04	1 (1%)	80	80	24, 38, 56, 72	0
2	E	89/97 (91%)	-0.05	0	100	100	25, 34, 52, 63	0
2	H	86/97 (88%)	0.07	2 (2%)	60	57	26, 42, 62, 81	0
2	K	86/97 (88%)	0.04	1 (1%)	79	78	31, 46, 62, 72	0
3	C	140/162 (86%)	-0.11	0	100	100	23, 39, 57, 75	0
3	F	140/162 (86%)	-0.13	1 (0%)	87	87	22, 38, 59, 71	0
3	I	142/162 (87%)	-0.07	5 (3%)	44	38	20, 37, 67, 88	0
3	L	140/162 (86%)	0.00	2 (1%)	75	74	22, 38, 65, 92	0
All	All	1320/1452 (90%)	-0.05	17 (1%)	77	76	20, 41, 67, 96	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	27	LEU	3.7
2	H	110	LEU	3.5
1	A	81	ALA	3.3
3	I	158	LEU	2.7
3	I	143	ASP	2.7

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
1	CAS	J	89	9/10	0.86	0.14	69,76,86,124	0
1	CAS	G	60	9/10	0.89	0.25	30,42,74,98	0
1	CAS	A	60	9/10	0.90	0.21	45,49,72,89	0
1	CAS	D	60	9/10	0.90	0.26	33,33,61,88	0
1	CAS	J	60	9/10	0.91	0.17	37,47,57,85	0
3	CAS	L	77	9/10	0.91	0.17	32,40,70,89	0
1	CAS	A	89	9/10	0.92	0.15	46,60,81,134	0
1	CAS	G	89	9/10	0.95	0.10	43,51,75,117	0
3	CAS	C	77	9/10	0.96	0.15	38,41,62,75	0
3	CAS	I	77	9/10	0.97	0.15	26,36,60,66	0
1	CAS	D	89	9/10	0.97	0.08	32,39,72,93	0
3	CAS	F	77	9/10	0.98	0.15	24,30,53,63	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
4	VFO	C	301	40/40	0.93	0.20	20,35,40,43	0
4	VFO	L	301	40/40	0.93	0.21	26,37,45,59	0
4	VFO	F	301	40/40	0.94	0.22	22,33,41,45	0
4	VFO	I	301	40/40	0.95	0.20	20,32,47,66	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 VFO C 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
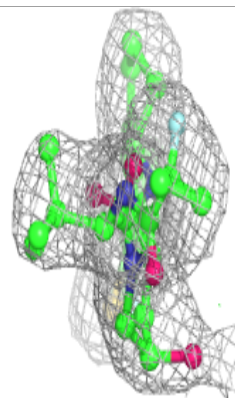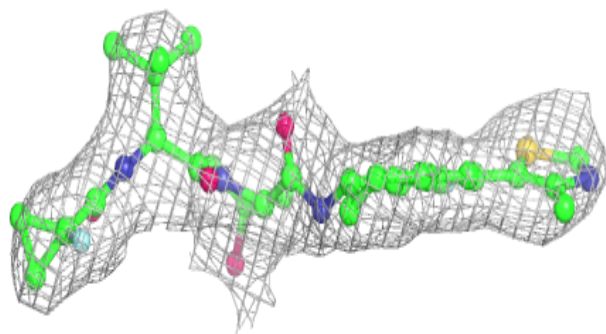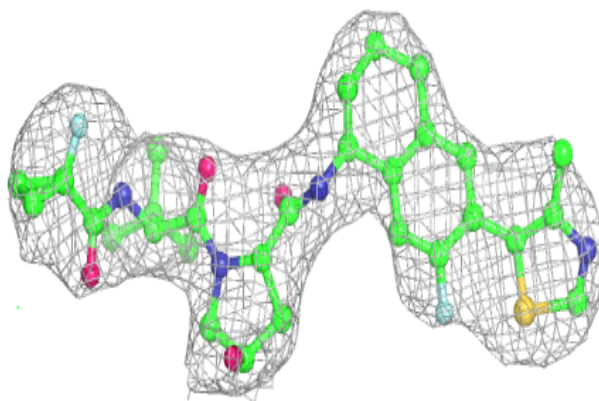and green (positive)
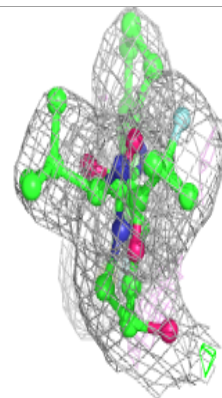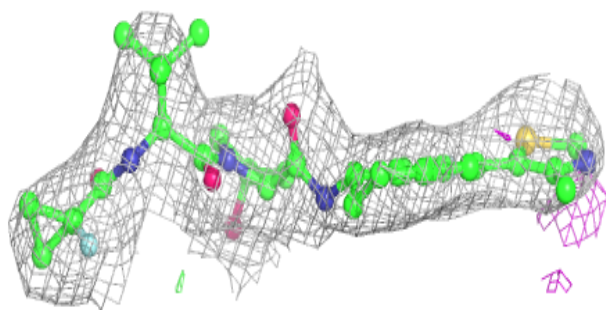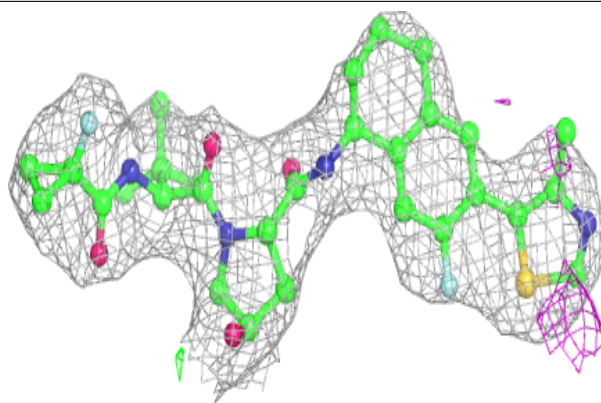
Electron density around VFO L 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
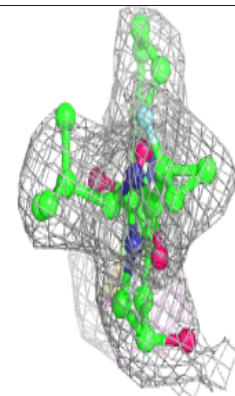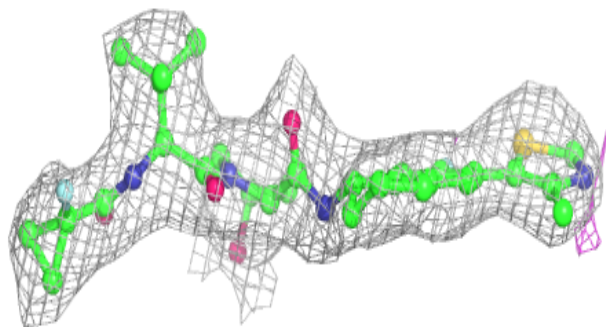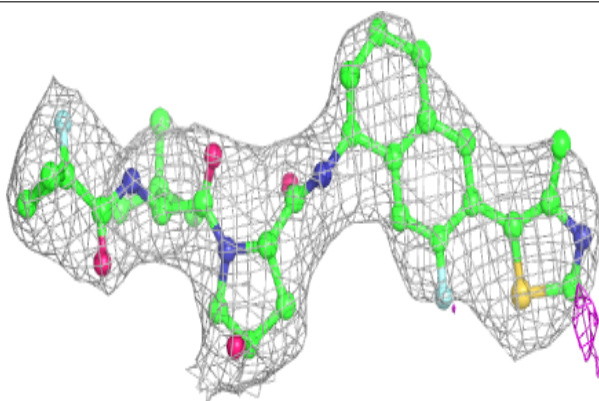and green (positive)
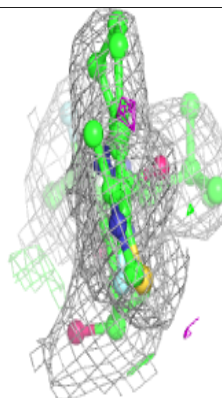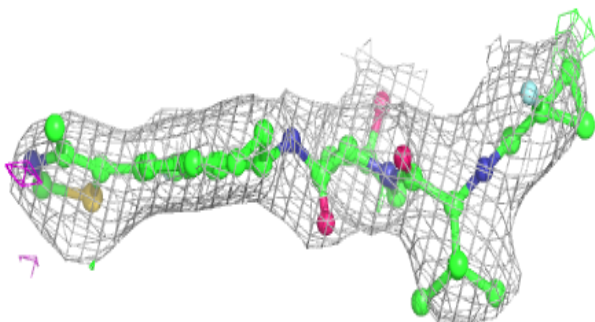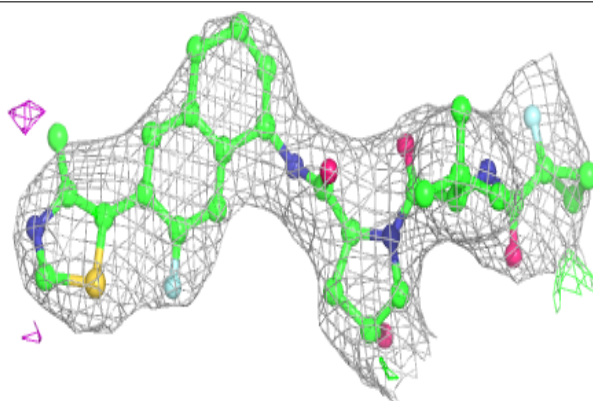
Electron density around VFO F 301:

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

Electron density around VFO I 301:

$2mF_o$-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.