



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 01:14 AM UTC

PDB ID : 9PCL / pdb\_00009pcl  
Title : Crystal structure of Rv0097 with 10 mM CADA soaked (CADA bound)  
Authors : Ye, N.; Drennan, C.L.  
Deposited on : 2025-06-27  
Resolution : 1.76 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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

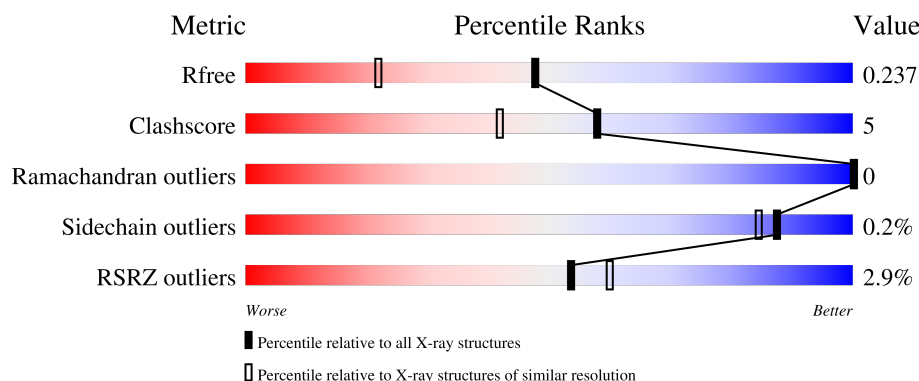
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

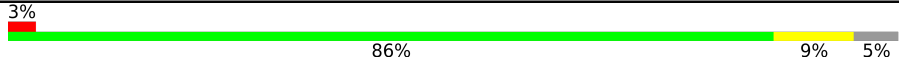


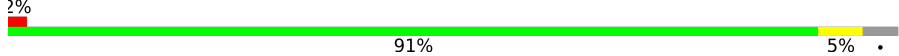
The reported resolution of this entry is 1.76 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	302	
1	B	302	
1	C	302	
1	D	302	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEG	C	401	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10013 atoms, of which 20 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 (3R)-3-[(carboxymethyl)amino]fatty acid oxygenase/decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	63	3	0
			2300	1473	396	423	8			
1	B	285	Total	C	N	O	S	40	1	0
			2281	1461	394	418	8			
1	C	283	Total	C	N	O	S	36	2	0
			2273	1456	394	415	8			
1	D	289	Total	C	N	O	S	27	1	0
			2307	1476	399	424	8			

There are 52 discrepancies between the modelled and reference sequences:

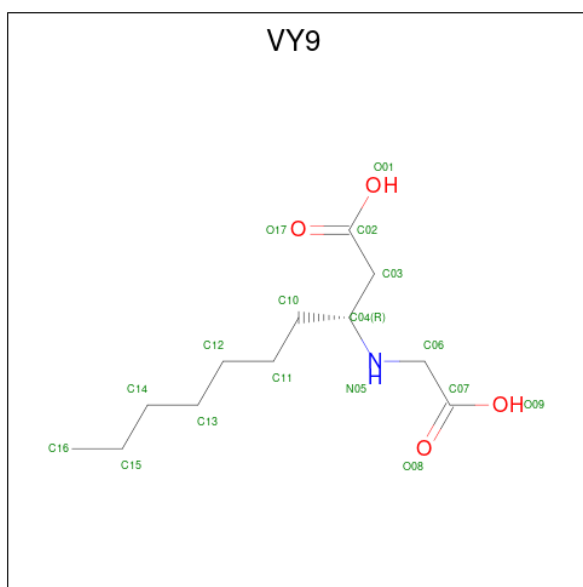
Chain	Residue	Modelled	Actual	Comment	Reference
A	290	LYS	-	expression tag	UNP P9WG83
A	291	LEU	-	expression tag	UNP P9WG83
A	292	ALA	-	expression tag	UNP P9WG83
A	293	ALA	-	expression tag	UNP P9WG83
A	294	ALA	-	expression tag	UNP P9WG83
A	295	LEU	-	expression tag	UNP P9WG83
A	296	GLU	-	expression tag	UNP P9WG83
A	297	HIS	-	expression tag	UNP P9WG83
A	298	HIS	-	expression tag	UNP P9WG83
A	299	HIS	-	expression tag	UNP P9WG83
A	300	HIS	-	expression tag	UNP P9WG83
A	301	HIS	-	expression tag	UNP P9WG83
A	302	HIS	-	expression tag	UNP P9WG83
B	290	LYS	-	expression tag	UNP P9WG83
B	291	LEU	-	expression tag	UNP P9WG83
B	292	ALA	-	expression tag	UNP P9WG83
B	293	ALA	-	expression tag	UNP P9WG83
B	294	ALA	-	expression tag	UNP P9WG83
B	295	LEU	-	expression tag	UNP P9WG83
B	296	GLU	-	expression tag	UNP P9WG83

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	297	HIS	-	expression tag	UNP P9WG83
B	298	HIS	-	expression tag	UNP P9WG83
B	299	HIS	-	expression tag	UNP P9WG83
B	300	HIS	-	expression tag	UNP P9WG83
B	301	HIS	-	expression tag	UNP P9WG83
B	302	HIS	-	expression tag	UNP P9WG83
C	290	LYS	-	expression tag	UNP P9WG83
C	291	LEU	-	expression tag	UNP P9WG83
C	292	ALA	-	expression tag	UNP P9WG83
C	293	ALA	-	expression tag	UNP P9WG83
C	294	ALA	-	expression tag	UNP P9WG83
C	295	LEU	-	expression tag	UNP P9WG83
C	296	GLU	-	expression tag	UNP P9WG83
C	297	HIS	-	expression tag	UNP P9WG83
C	298	HIS	-	expression tag	UNP P9WG83
C	299	HIS	-	expression tag	UNP P9WG83
C	300	HIS	-	expression tag	UNP P9WG83
C	301	HIS	-	expression tag	UNP P9WG83
C	302	HIS	-	expression tag	UNP P9WG83
D	290	LYS	-	expression tag	UNP P9WG83
D	291	LEU	-	expression tag	UNP P9WG83
D	292	ALA	-	expression tag	UNP P9WG83
D	293	ALA	-	expression tag	UNP P9WG83
D	294	ALA	-	expression tag	UNP P9WG83
D	295	LEU	-	expression tag	UNP P9WG83
D	296	GLU	-	expression tag	UNP P9WG83
D	297	HIS	-	expression tag	UNP P9WG83
D	298	HIS	-	expression tag	UNP P9WG83
D	299	HIS	-	expression tag	UNP P9WG83
D	300	HIS	-	expression tag	UNP P9WG83
D	301	HIS	-	expression tag	UNP P9WG83
D	302	HIS	-	expression tag	UNP P9WG83

- Molecule 2 is (3R)-3-(2-hydroxy-2-oxoethylamino)decanoic acid (CCD ID: VY9) (formula: C<sub>12</sub>H<sub>23</sub>NO<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	12	1	4		
2	B	1	Total	C	N	O	0	0
			17	12	1	4		
2	D	1	Total	C	N	O	0	0
			17	12	1	4		

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	B	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		
3	D	1	Total	Fe	0	0
			1	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	0	0
			17	4	10	3		
4	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	136	Total	O	0	0
			136	136		
5	B	116	Total	O	0	0
			116	116		
5	C	246	Total	O	0	0
			246	246		
5	D	265	Total	O	0	0
			265	265		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.46Å 63.65Å 107.84Å 90.00° 98.04° 90.00°	Depositor
Resolution (Å)	45.10 – 1.76 45.10 – 1.76	Depositor EDS
% Data completeness (in resolution range)	98.2 (45.10-1.76) 98.1 (45.10-1.76)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.198 , 0.237 0.198 , 0.237	Depositor DCC
$R_{free}$ test set	5838 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.2	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 32.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10013	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	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 28.55 % 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 1.8076e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: FE, PEG, VY9

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	0.26	0/2376	0.48	0/3241
1	B	0.23	0/2350	0.46	0/3204
1	C	0.29	0/2345	0.50	0/3195
1	D	0.32	0/2377	0.54	0/3241
All	All	0.28	0/9448	0.50	0/12881

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2300	0	2277	23	0
1	B	2281	0	2255	22	0
1	C	2273	0	2251	16	0
1	D	2307	0	2284	18	0
2	A	17	0	0	0	0
2	B	17	0	0	0	0
2	D	17	0	0	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	C	7	10	10	5	0
4	D	7	10	10	0	0
5	A	136	0	0	4	0
5	B	116	0	0	5	0
5	C	246	0	0	5	0
5	D	265	0	0	6	0
All	All	9993	20	9087	81	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 5.

All (81) 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:A:157:ILE:HD13	1:A:175:ILE:HG23	1.49	0.94
1:C:8:GLU:H	4:C:401:PEG:H32	1.44	0.81
1:A:154:ARG:HA	1:A:157:ILE:HD12	1.62	0.80
1:D:133:TRP:CH2	1:D:141:ARG:HB2	2.22	0.74
1:C:85:GLU:HA	5:C:511:HOH:O	1.86	0.74
1:C:86:GLY:C	1:C:122:ARG:HE	1.95	0.74
1:B:50:ARG:HG3	5:B:599:HOH:O	1.86	0.74
1:A:219:GLU:O	1:A:223:GLU:HG2	1.88	0.72
1:D:45:VAL:HG12	1:D:47:PRO:HD3	1.72	0.72
1:B:95:PHE:HB2	1:B:203:THR:HG21	1.72	0.71
1:A:157:ILE:HD13	1:A:175:ILE:CG2	2.21	0.70
1:A:69:MET:HE2	1:A:160:ARG:HG2	1.73	0.69
1:B:251:ILE:HD11	5:B:549:HOH:O	1.93	0.68
1:C:8:GLU:H	4:C:401:PEG:C3	2.08	0.67
1:B:8:GLU:HB3	5:B:560:HOH:O	1.95	0.66
1:B:237:SER:HB3	1:B:240:ILE:HG13	1.77	0.66
1:A:154:ARG:HA	1:A:157:ILE:CD1	2.28	0.63
1:A:6:LYS:HG3	5:A:605:HOH:O	1.99	0.63
1:D:133:TRP:CZ3	1:D:141:ARG:HB2	2.34	0.63
1:A:69:MET:CE	1:A:160:ARG:HG2	2.28	0.63
1:C:234:GLU:HB3	5:C:612:HOH:O	1.99	0.62
1:C:268:ALA:HA	5:C:511:HOH:O	2.01	0.60
1:B:174:GLU:O	1:B:178:THR:HG23	2.05	0.57
1:B:105:GLU:HG3	5:B:553:HOH:O	2.05	0.56
1:A:122:ARG:HD3	1:A:265:GLY:HA3	1.88	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:LYS:HG3	5:D:615:HOH:O	2.06	0.54
1:D:133:TRP:CE2	1:D:141:ARG:HD2	2.44	0.53
1:C:122:ARG:HD2	1:C:263:LYS:O	2.08	0.53
1:B:19:PRO:HA	1:B:22:LEU:HD21	1.92	0.52
1:B:129:LEU:HD11	1:B:259:MET:HB2	1.92	0.51
4:C:401:PEG:H11	5:C:682:HOH:O	2.10	0.51
1:A:13:GLN:HG3	5:A:537:HOH:O	2.11	0.50
1:A:112[B]:VAL:CG2	1:A:251:ILE:HB	2.43	0.49
1:A:39:LEU:HD11	1:A:251:ILE:HG23	1.93	0.49
1:D:35:TYR:CD2	1:D:192:LYS:HG2	2.48	0.49
1:C:161:PRO:O	1:C:164:VAL:HG12	2.13	0.48
1:D:145:ARG:CD	5:D:718:HOH:O	2.61	0.48
1:B:211:LYS:HB2	1:B:211:LYS:NZ	2.28	0.48
1:D:264:HIS:HE1	5:D:559:HOH:O	1.96	0.48
1:D:65:TYR:OH	2:D:401:VY9:N05	2.47	0.47
1:A:122:ARG:HG2	5:A:581:HOH:O	2.14	0.47
1:A:52:PHE:CE1	1:A:111:MET:HE3	2.50	0.47
1:B:224:LEU:O	1:B:228:THR:HG23	2.14	0.47
1:D:145:ARG:HD2	5:D:718:HOH:O	2.14	0.47
1:B:46:HIS:CE1	1:B:248:GLY:HA3	2.50	0.47
1:B:142:ASP:N	1:B:143:PRO:HD2	2.31	0.46
1:D:45:VAL:CG1	1:D:47:PRO:HD3	2.44	0.46
1:A:209:GLU:HG2	5:A:534:HOH:O	2.15	0.46
1:B:203:THR:CG2	5:B:578:HOH:O	2.64	0.46
1:C:7:GLY:CA	4:C:401:PEG:H31	2.45	0.46
1:A:39:LEU:HD11	1:A:251:ILE:CG2	2.46	0.45
1:B:115:LEU:HD11	1:B:274:TYR:CE2	2.52	0.45
1:B:39:LEU:HD11	1:B:251:ILE:HG23	1.98	0.44
1:C:69:MET:HE3	1:C:69:MET:HB2	1.74	0.44
2:D:401:VY9:C04	5:D:504:HOH:O	2.65	0.44
1:D:142:ASP:HA	1:D:145:ARG:HD2	2.00	0.44
1:A:107:PHE:CG	1:A:277:THR:HB	2.53	0.44
1:B:105:GLU:HG3	1:B:105:GLU:O	2.18	0.43
1:D:19:PRO:HG3	1:D:45:VAL:O	2.18	0.43
1:A:209:GLU:HA	1:A:216:VAL:HG23	2.01	0.43
1:D:133:TRP:CZ2	1:D:141:ARG:HD2	2.54	0.43
1:C:142:ASP:N	1:C:143:PRO:HD2	2.34	0.43
1:A:142:ASP:N	1:A:143:PRO:HD2	2.34	0.42
1:C:35:TYR:CD2	1:C:192:LYS:HG2	2.54	0.42
1:A:142:ASP:HB2	1:A:143:PRO:CD	2.50	0.42
1:D:211:LYS:HG2	5:D:630:HOH:O	2.19	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ASP:HA	1:B:244:HIS:CD2	2.55	0.42
1:B:39:LEU:HD11	1:B:251:ILE:CG2	2.50	0.42
1:C:82:SER:HA	1:C:271:LEU:O	2.20	0.42
1:B:284:THR:HA	1:B:285:PRO:C	2.45	0.42
1:A:237:SER:HB3	1:A:240:ILE:HG13	2.01	0.41
1:D:45:VAL:HG12	1:D:47:PRO:CD	2.45	0.41
1:D:262:ALA:HB1	1:D:264:HIS:CD2	2.55	0.41
1:C:7:GLY:HA3	4:C:401:PEG:H31	2.02	0.41
1:A:35:TYR:CD2	1:A:192:LYS:HG2	2.56	0.41
1:C:85:GLU:HA	5:C:689:HOH:O	2.21	0.41
1:D:225:MET:HE2	1:D:225:MET:HB2	1.98	0.41
1:C:237:SER:HB3	1:C:240:ILE:HG13	2.03	0.41
1:A:216:VAL:HG12	1:A:217:ASP:N	2.36	0.40
1:B:37:ASN:O	1:B:38:LYS:HB2	2.21	0.40
1:B:128:ASP:HA	1:B:258:LEU:HD23	2.04	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	288/302 (95%)	283 (98%)	5 (2%)	0	100	100
1	B	282/302 (93%)	277 (98%)	5 (2%)	0	100	100
1	C	281/302 (93%)	277 (99%)	4 (1%)	0	100	100
1	D	288/302 (95%)	282 (98%)	6 (2%)	0	100	100
All	All	1139/1208 (94%)	1119 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	252/261 (97%)	252 (100%)	0	100	100
1	B	249/261 (95%)	247 (99%)	2 (1%)	73	64
1	C	248/261 (95%)	248 (100%)	0	100	100
1	D	252/261 (97%)	252 (100%)	0	100	100
All	All	1001/1044 (96%)	999 (100%)	2 (0%)	87	84

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	57	ARG
1	B	211	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	B	46	HIS
1	B	214	ASN
1	B	264	HIS
1	C	236	GLN
1	D	176	ASN

### 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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\# Z  > 2$
2	VY9	B	401	-	16,16,16	0.71	0	14,18,18	1.22	1 (7%)
2	VY9	A	401	-	16,16,16	0.84	0	14,18,18	0.98	1 (7%)
4	PEG	C	401	-	6,6,6	0.23	0	5,5,5	0.73	0
4	PEG	D	402	-	6,6,6	0.25	0	5,5,5	0.36	0
2	VY9	D	401	-	16,16,16	0.85	0	14,18,18	1.19	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
2	VY9	B	401	-	-	7/16/16/16	-
2	VY9	A	401	-	-	2/16/16/16	-
4	PEG	C	401	-	-	2/4/4/4	-
4	PEG	D	402	-	-	0/4/4/4	-
2	VY9	D	401	-	-	6/16/16/16	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	VY9	C06-N05-C04	-2.91	109.02	113.84
2	D	401	VY9	C06-N05-C04	-2.21	110.18	113.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	VY9	O01-C02-C03	2.11	120.55	114.00
2	A	401	VY9	O09-C07-C06	2.09	120.74	112.81

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	VY9	C03-C04-C10-C11
2	B	401	VY9	C03-C04-C10-C11
2	D	401	VY9	C10-C04-N05-C06
2	D	401	VY9	C03-C04-N05-C06
2	B	401	VY9	N05-C04-C10-C11
2	D	401	VY9	N05-C06-C07-O09
4	C	401	PEG	O2-C3-C4-O4
2	B	401	VY9	C04-C10-C11-C12
4	C	401	PEG	O1-C1-C2-O2
2	D	401	VY9	N05-C06-C07-O08
2	D	401	VY9	C10-C11-C12-C13
2	D	401	VY9	C12-C13-C14-C15
2	B	401	VY9	C10-C11-C12-C13
2	B	401	VY9	N05-C06-C07-O08
2	A	401	VY9	N05-C04-C10-C11
2	B	401	VY9	N05-C06-C07-O09
2	B	401	VY9	C11-C12-C13-C14

There are no ring outliers.

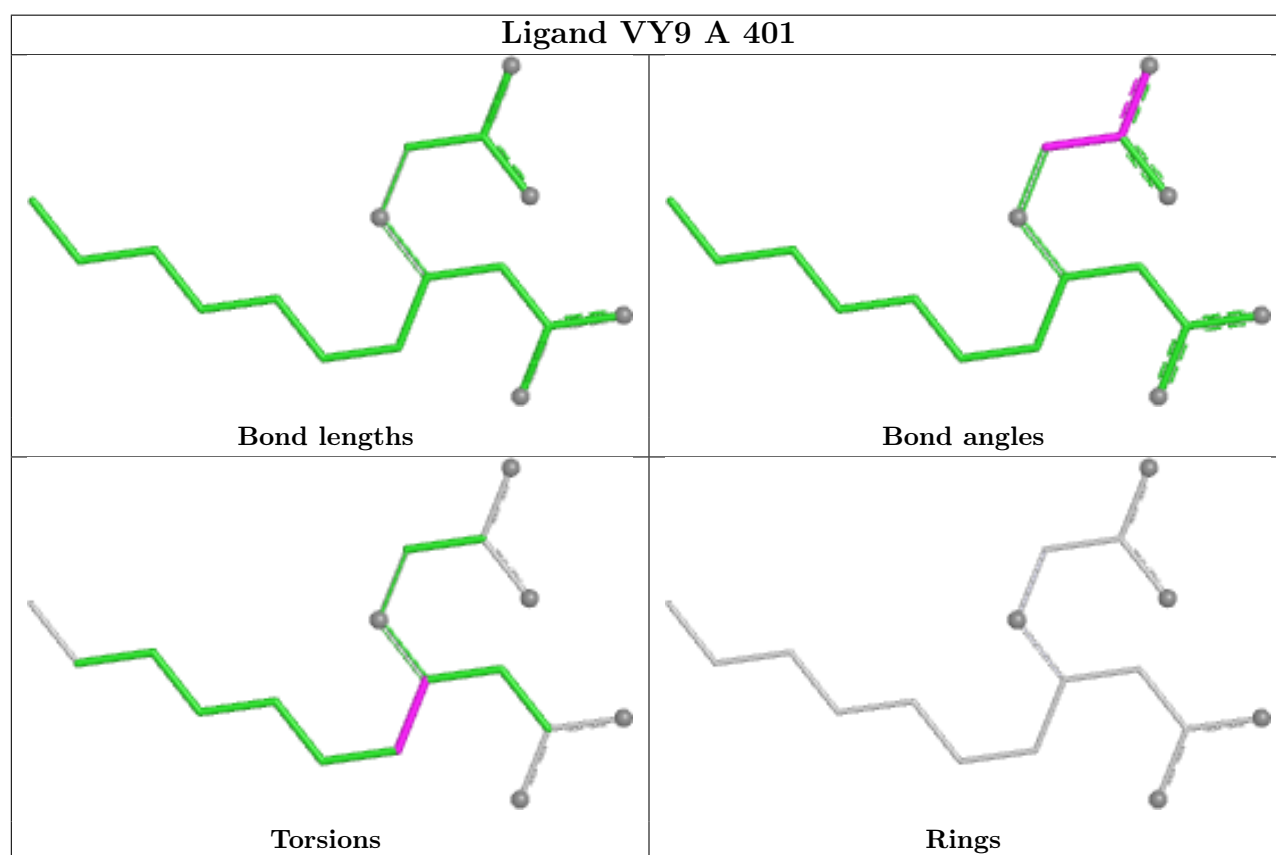
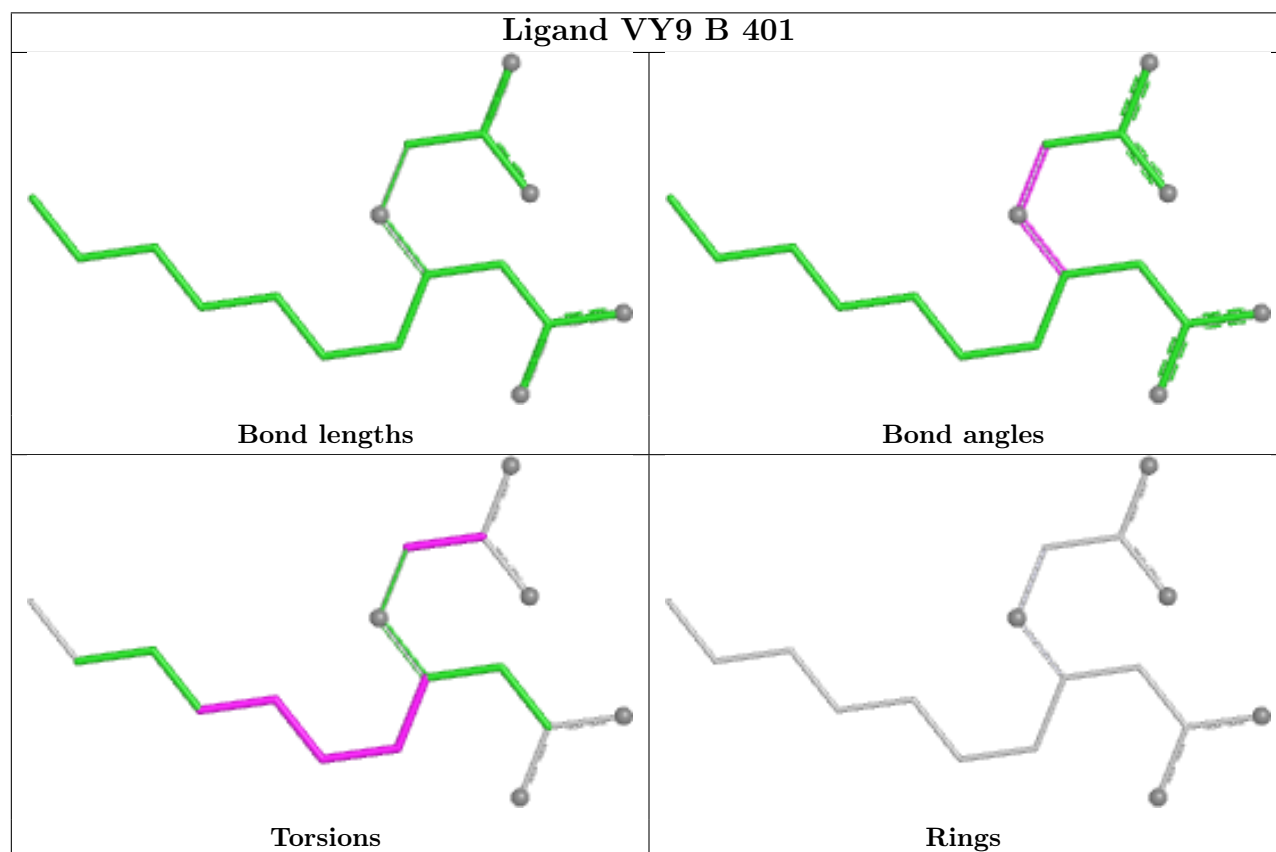
2 monomers are involved in 7 short contacts:

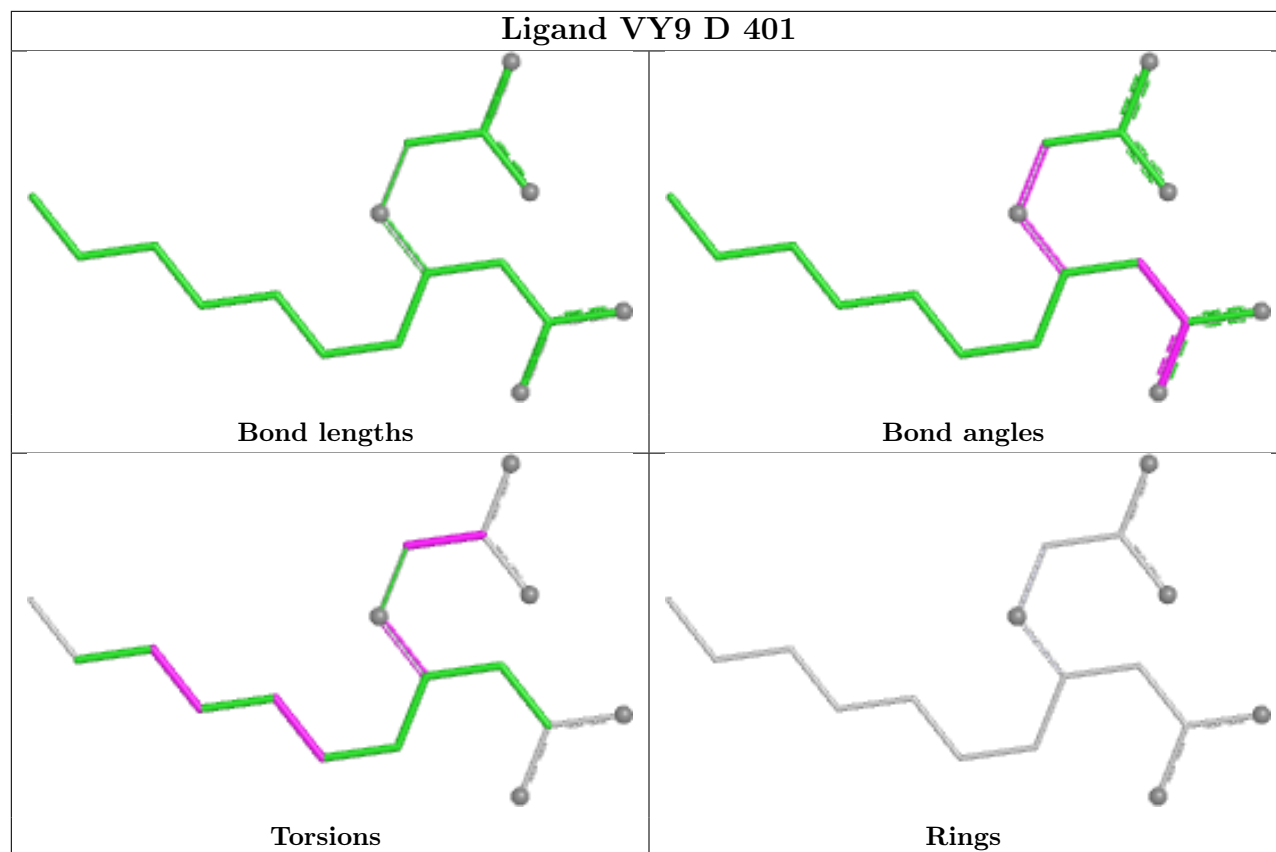
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	401	PEG	5	0
2	D	401	VY9	2	0

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 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.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	287/302 (95%)	0.52	9 (3%)	51	58	13, 27, 45, 52	18 (6%)
1	B	285/302 (94%)	0.50	8 (2%)	55	61	14, 28, 44, 55	11 (3%)
1	C	283/302 (93%)	0.03	9 (3%)	50	57	11, 21, 37, 51	11 (3%)
1	D	289/302 (95%)	0.01	7 (2%)	59	66	12, 20, 36, 49	8 (2%)
All	All	1144/1208 (94%)	0.27	33 (2%)	53	60	11, 24, 42, 55	48 (4%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	86	GLY	4.5
1	A	212	ASP	4.2
1	D	211	LYS	3.8
1	D	120	HIS	3.1
1	B	267	ALA	2.9
1	B	264	HIS	2.8
1	B	203	THR	2.7
1	B	144	ALA	2.7
1	C	143	PRO	2.7
1	C	85	GLU	2.6
1	B	178	THR	2.5
1	D	267	ALA	2.4
1	D	2	THR	2.4
1	A	3	LEU	2.3
1	C	2	THR	2.3
1	C	211	LYS	2.3
1	D	264	HIS	2.2
1	D	143	PRO	2.2
1	A	289	ALA	2.2
1	B	289	ALA	2.2
1	B	268	ALA	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	267	ALA	2.1
1	B	57	ARG	2.1
1	A	139	ALA	2.1
1	A	216	VAL	2.1
1	C	138	ALA	2.1
1	C	268	ALA	2.1
1	A	161	PRO	2.1
1	A	213	GLY	2.1
1	C	142	ASP	2.1
1	D	17	VAL	2.0
1	A	268	ALA	2.0
1	A	264	HIS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

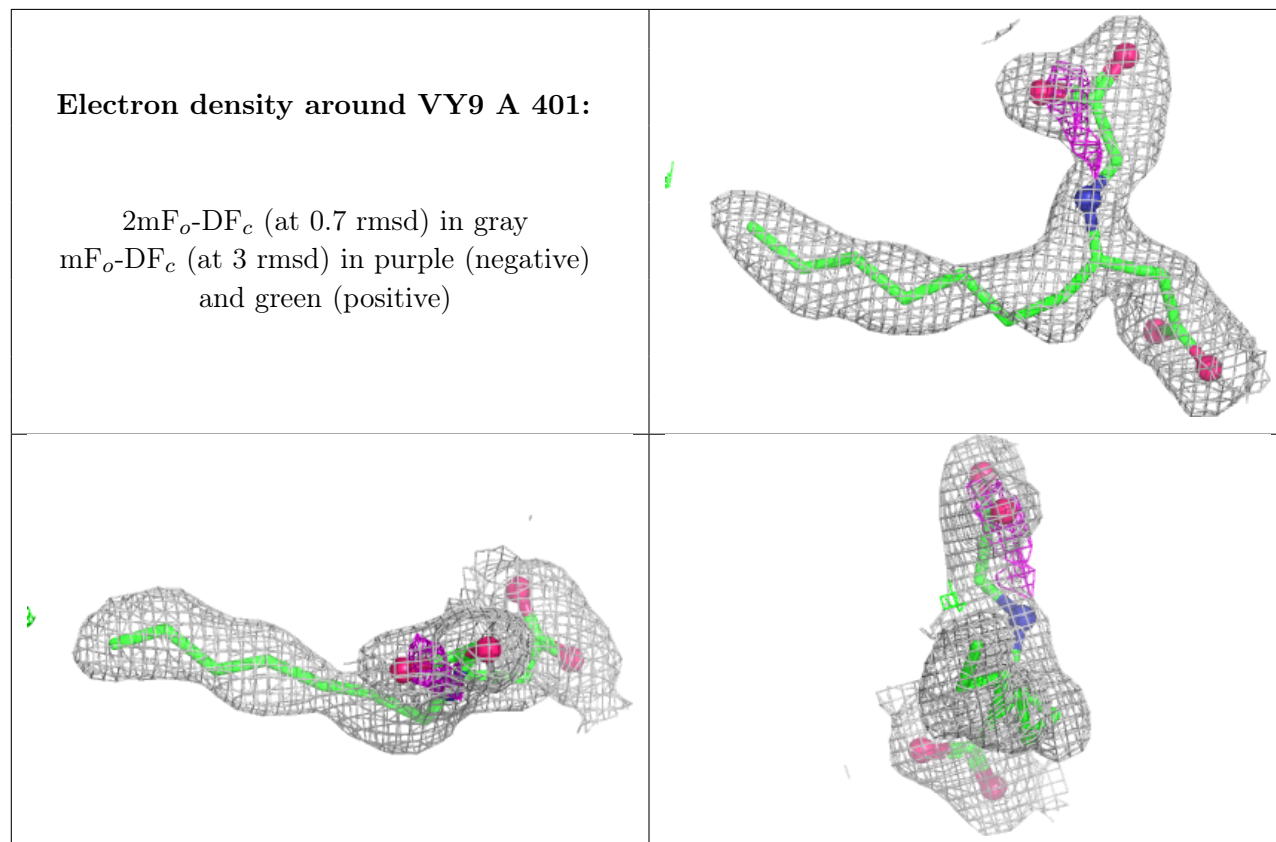
## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	PEG	C	401	7/7	0.60	0.16	37,48,58,58	0
4	PEG	D	402	7/7	0.82	0.10	30,38,49,53	0
2	VY9	A	401	17/17	0.87	0.12	27,34,41,44	0
2	VY9	D	401	17/17	0.90	0.10	18,26,32,36	0
2	VY9	B	401	17/17	0.91	0.10	21,31,36,36	0
3	FE	B	402	1/1	0.99	0.02	22,22,22,22	0
3	FE	C	402	1/1	0.99	0.03	16,16,16,16	0
3	FE	A	402	1/1	1.00	0.01	21,21,21,21	0
3	FE	D	403	1/1	1.00	0.01	15,15,15,15	0

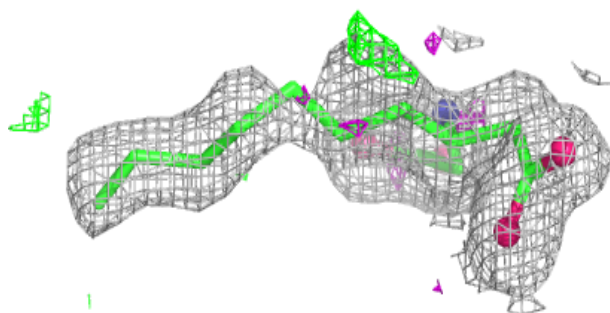
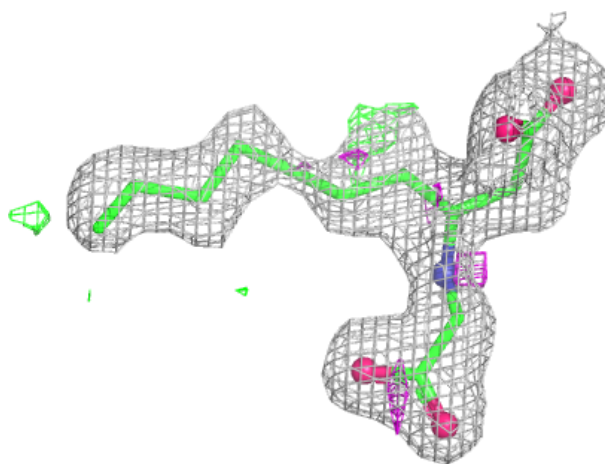
The following is a graphical depiction of the model fit to experimental electron density of all

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.



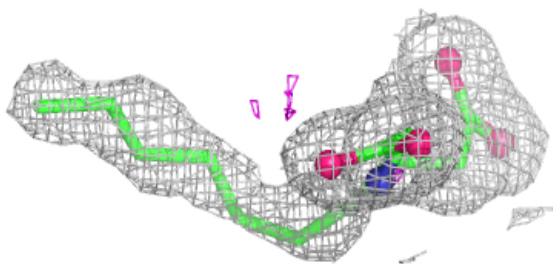
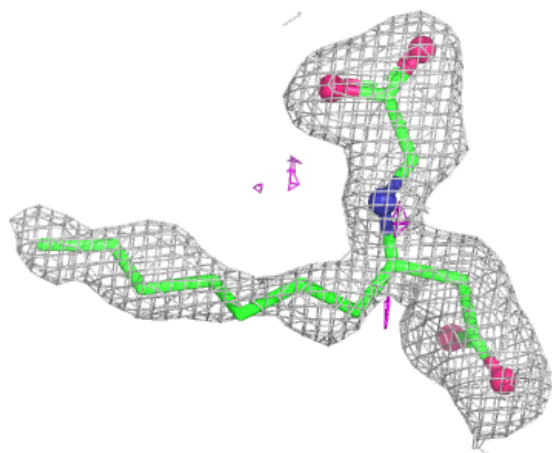
**Electron density around VY9 D 401:**

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



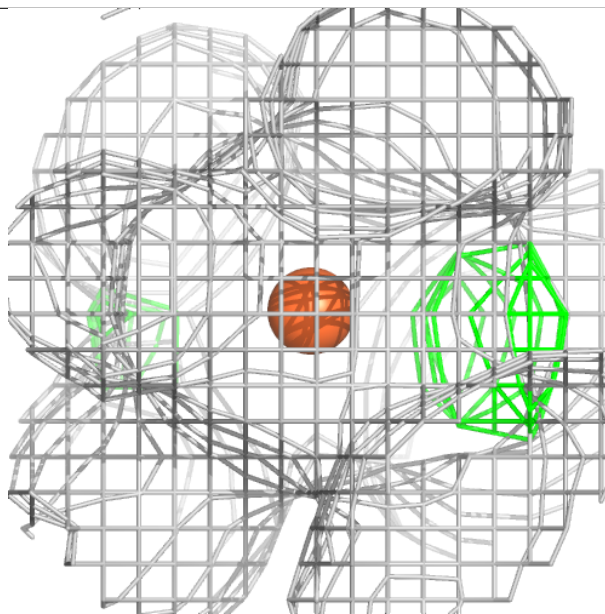
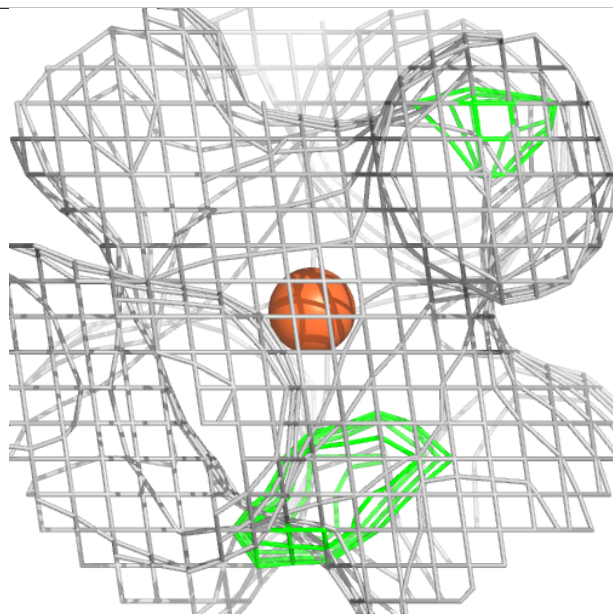
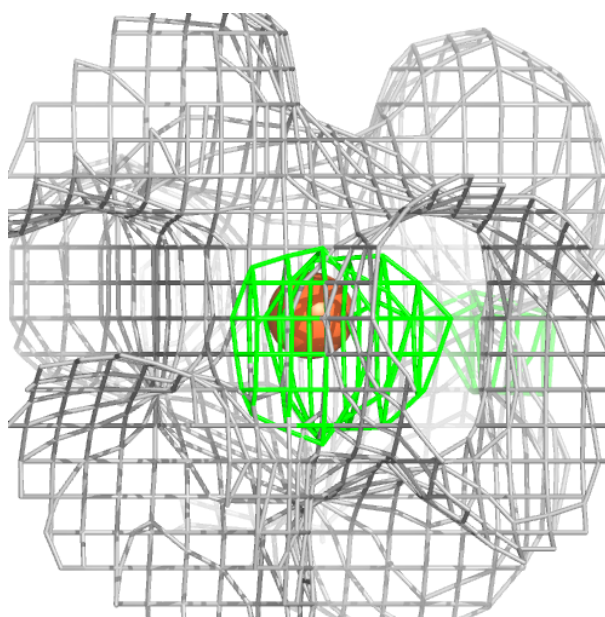
**Electron density around VY9 B 401:**

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



**Electron density around FE B 402:**

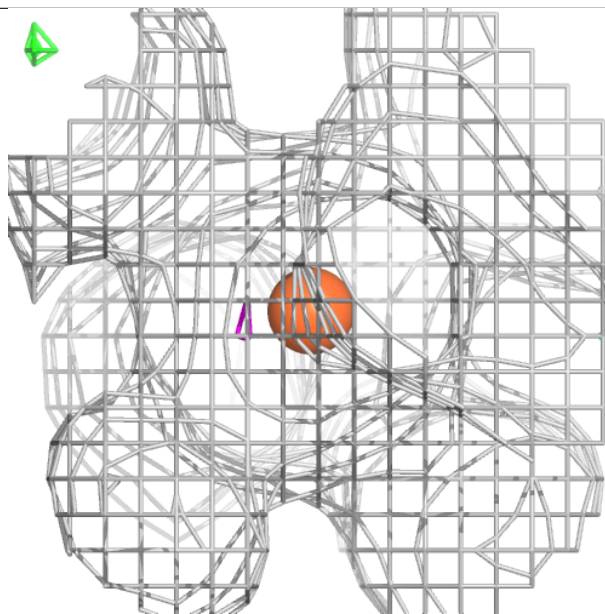
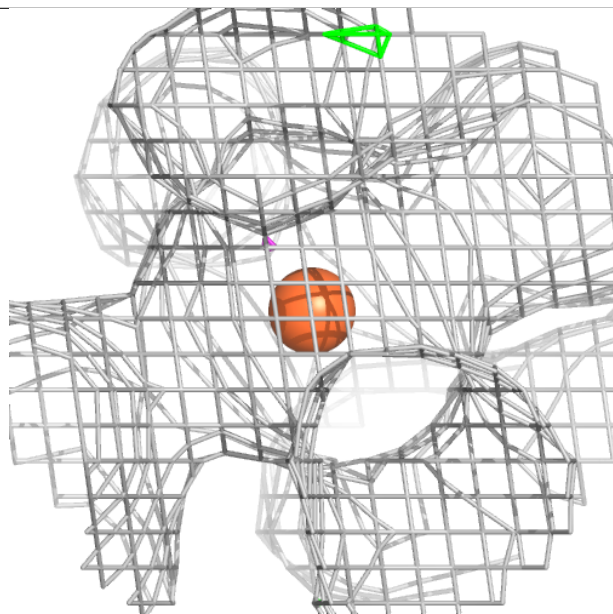
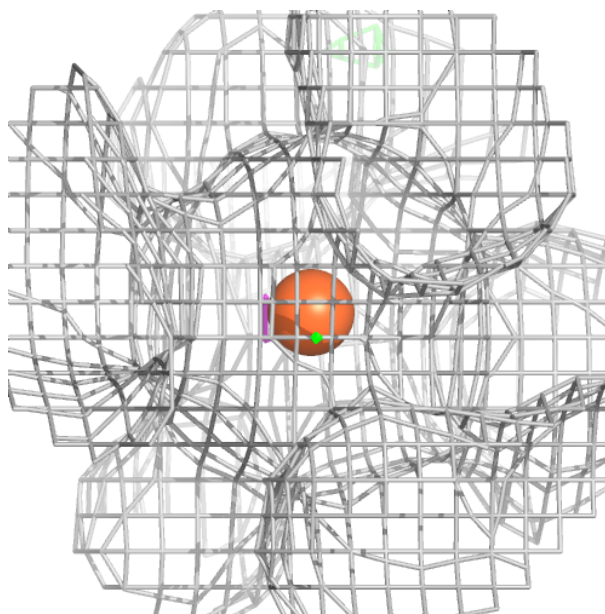
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





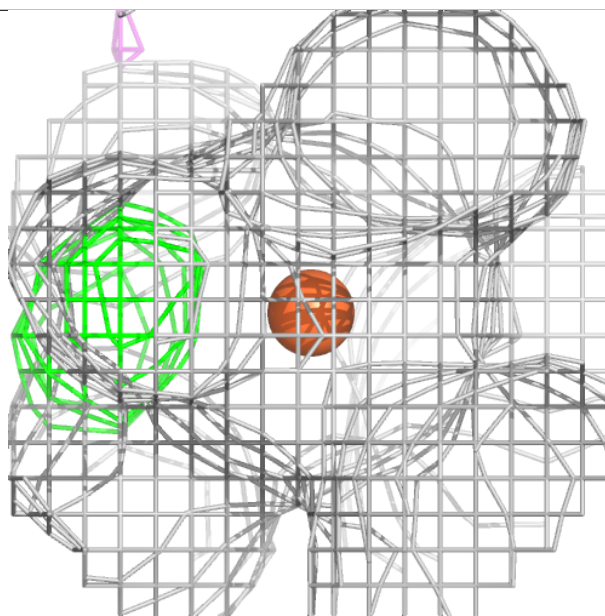
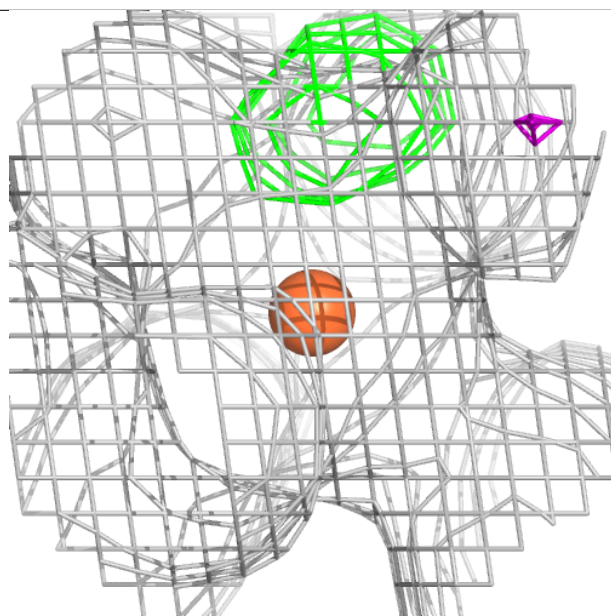
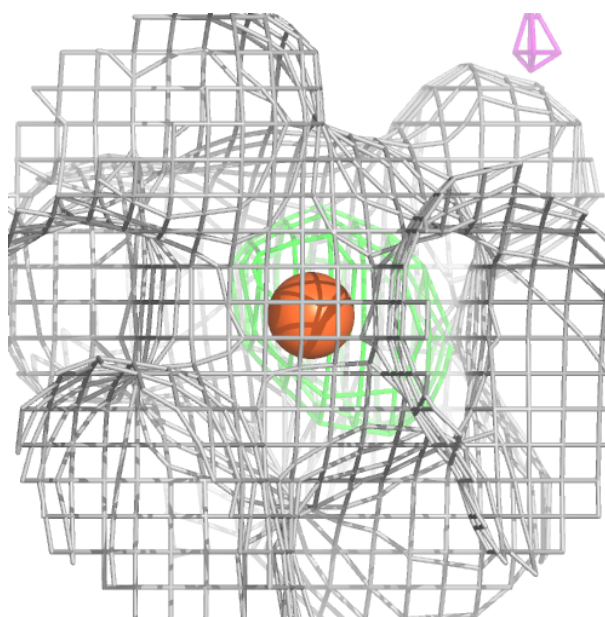
**Electron density around FE C 402:**

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



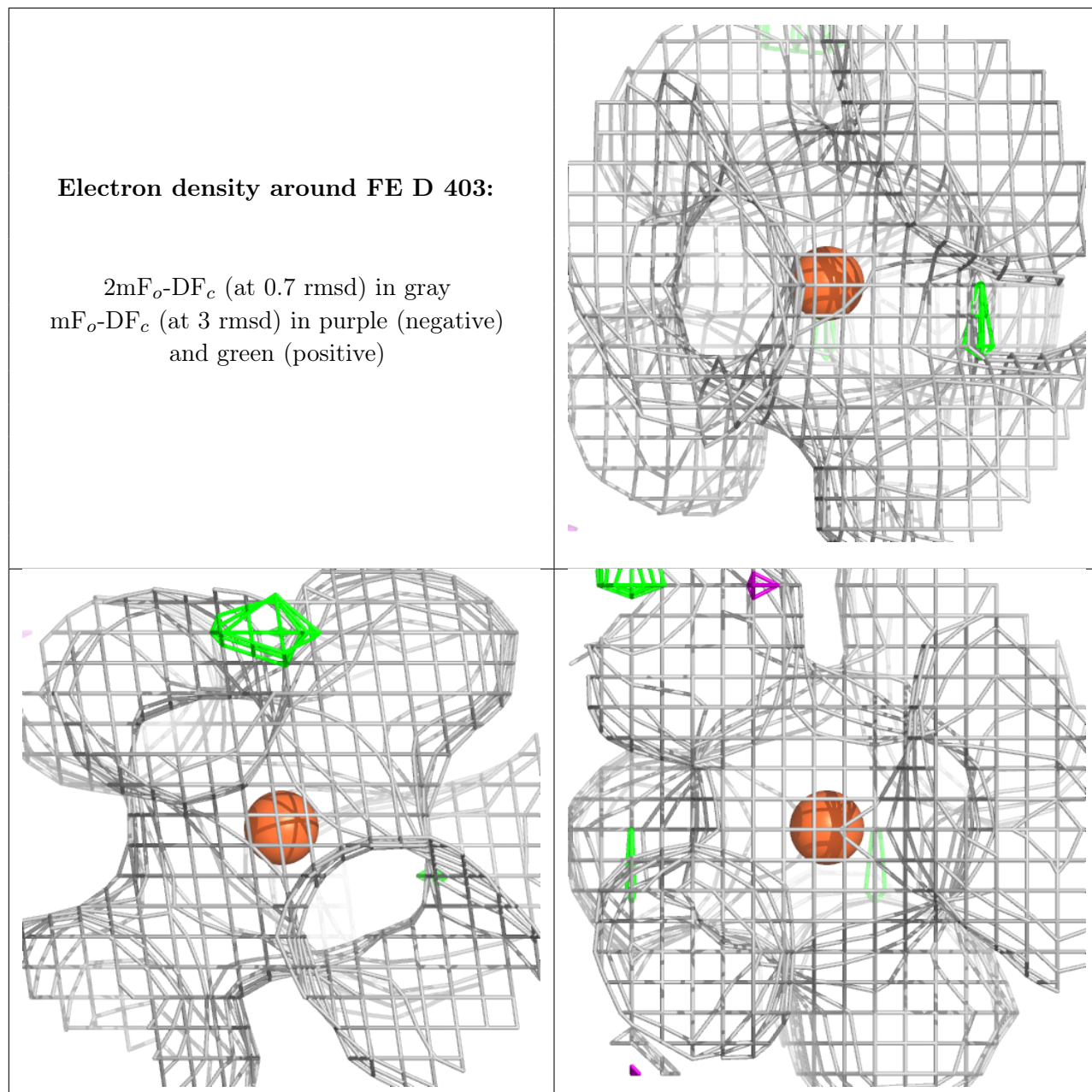
**Electron density around FE A 402:**

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



**Electron density around FE 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)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.