Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2025 – 04:09 pm BST

PDB ID	:	9G8F / pdb_00009g8f
Title	:	Carotenoid cleavage oxygenase from Moesziomyces aphidis bound to orto vanillin
Authors	:	Plewka, J.; Schorber, L.; Magiera-Mularz, K.; Rudroff, F.; Winkler, M.
Deposited on	:	2024-07-23
Resolution	:	1.84 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:

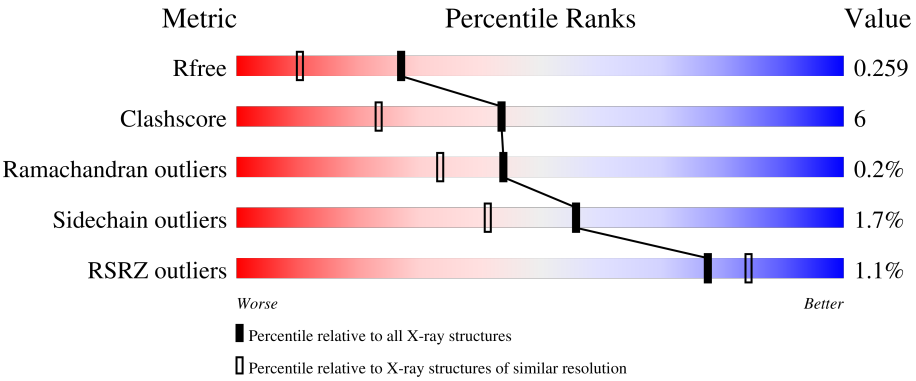
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.84 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}	164625	1150 (1.84-1.84)
Clashscore	180529	1248 (1.84-1.84)
Ramachandran outliers	177936	1240 (1.84-1.84)
Sidechain outliers	177891	1240 (1.84-1.84)
RSRZ outliers	164620	1149 (1.84-1.84)

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

Mol	Chain	Length	Quality of chain
1	A	556	2% 79% 14% • 6%
1	B	556	% 79% 13% • 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9440 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.

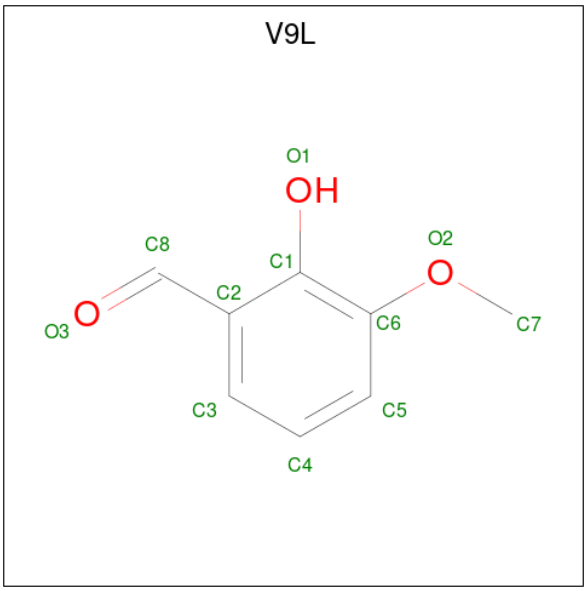
- Molecule 1 is a protein called Lignostilbene dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4210	2689	722	783	16			
1	B	525	Total	C	N	O	S	0	0	0
			4210	2689	722	783	16			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP W3VHW6
A	-6	TRP	-	expression tag	UNP W3VHW6
A	-5	SER	-	expression tag	UNP W3VHW6
A	-4	HIS	-	expression tag	UNP W3VHW6
A	-3	PRO	-	expression tag	UNP W3VHW6
A	-2	GLN	-	expression tag	UNP W3VHW6
A	-1	PHE	-	expression tag	UNP W3VHW6
A	0	GLU	-	expression tag	UNP W3VHW6
A	1	LYS	-	expression tag	UNP W3VHW6
B	-7	MET	-	initiating methionine	UNP W3VHW6
B	-6	TRP	-	expression tag	UNP W3VHW6
B	-5	SER	-	expression tag	UNP W3VHW6
B	-4	HIS	-	expression tag	UNP W3VHW6
B	-3	PRO	-	expression tag	UNP W3VHW6
B	-2	GLN	-	expression tag	UNP W3VHW6
B	-1	PHE	-	expression tag	UNP W3VHW6
B	0	GLU	-	expression tag	UNP W3VHW6
B	1	LYS	-	expression tag	UNP W3VHW6

- Molecule 2 is ortho-vanillin (CCD ID: V9L) (formula: $C_8H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 11 8 3	0	0
2	B	1	Total C O 11 8 3	0	0

- Molecule 3 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is water.

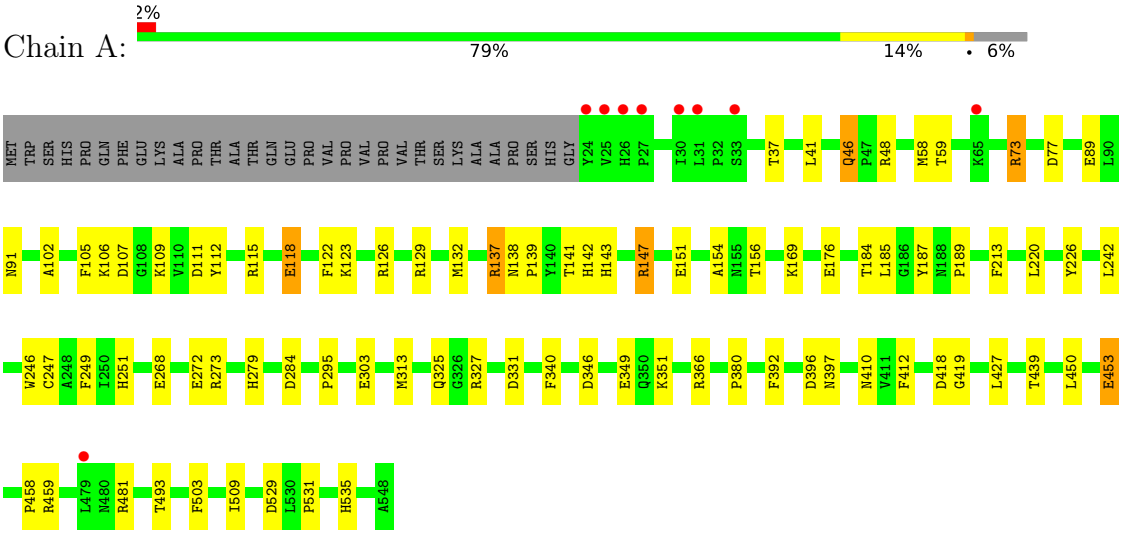
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	486	Total O 486 486	0	0
4	B	510	Total O 510 510	0	0

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.

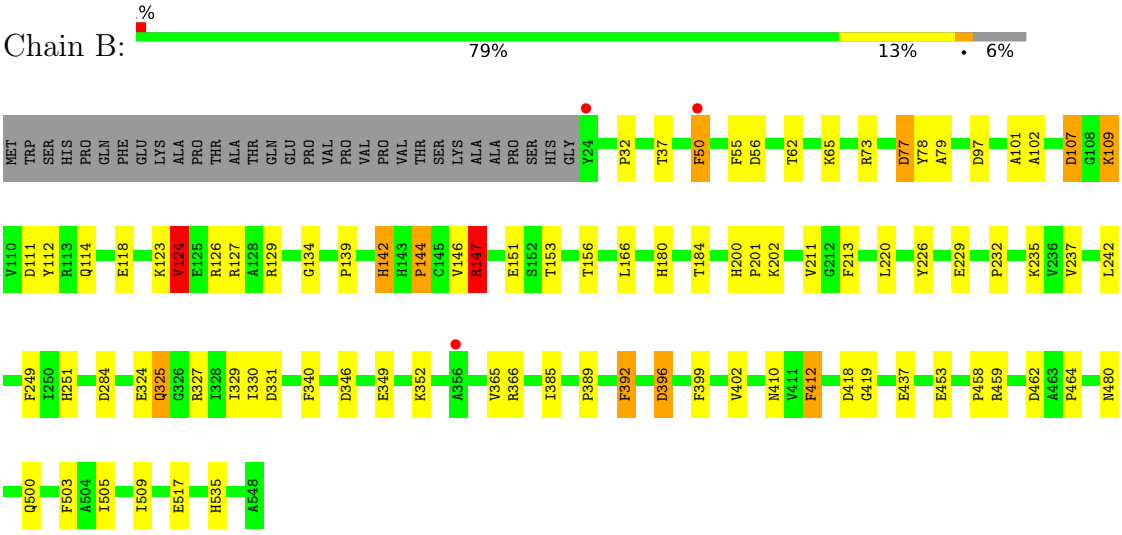
• Molecule 1: Lignostilbene dioxygenase

Chain A:



• Molecule 1: Lignostilbene dioxygenase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.88Å 84.94Å 107.02Å 90.00° 108.40° 90.00°	Depositor
Resolution (Å)	48.76 – 1.84 48.76 – 1.84	Depositor EDS
% Data completeness (in resolution range)	96.3 (48.76-1.84) 96.3 (48.76-1.84)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.23 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.209 , 0.259 0.209 , 0.259	Depositor DCC
R_{free} test set	5083 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	16.1	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.047 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9440	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: V9L, FE2

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	0.93	0/4342	1.53	45/5909 (0.8%)
1	B	0.95	2/4342 (0.0%)	1.48	29/5909 (0.5%)
All	All	0.94	2/8684 (0.0%)	1.50	74/11818 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	7
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	142	HIS	CG-CD2	-5.21	1.30	1.35
1	B	180	HIS	CD2-NE2	5.17	1.43	1.37

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	109	LYS	CB-CG-CD	9.85	133.95	111.30
1	B	220	LEU	N-CA-CB	-9.45	95.23	109.69
1	A	418	ASP	CB-CA-C	9.10	124.97	110.96
1	B	418	ASP	CB-CA-C	9.02	124.92	110.95
1	A	349	GLU	CB-CG-CD	8.94	127.79	112.60
1	A	410	ASN	CA-CB-CG	8.22	120.82	112.60
1	B	109	LYS	CB-CG-CD	7.78	129.20	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	346	ASP	CA-CB-CG	7.68	120.28	112.60
1	A	73	ARG	CG-CD-NE	-7.62	95.24	112.00
1	A	147	ARG	CG-CD-NE	-7.55	95.39	112.00
1	A	249	PHE	CA-CB-CG	7.49	121.29	113.80
1	B	147	ARG	CG-CD-NE	-7.47	95.56	112.00
1	A	346	ASP	CB-CA-C	-7.37	99.26	110.90
1	A	380	PRO	CB-CA-C	7.16	120.39	111.23
1	B	37	THR	CA-CB-OG1	-6.80	99.40	109.60
1	B	346	ASP	CB-CA-C	-6.73	100.27	110.90
1	A	251	HIS	CB-CG-CD2	6.72	139.94	131.20
1	A	531	PRO	CB-CA-C	6.69	121.32	111.22
1	A	41	LEU	N-CA-CB	6.66	120.66	110.14
1	A	396	ASP	CA-CB-CG	6.65	119.25	112.60
1	A	272	GLU	CB-CA-C	6.61	122.09	110.85
1	B	462	ASP	CA-CB-CG	6.51	119.11	112.60
1	A	397	ASN	CA-CB-CG	-6.43	106.17	112.60
1	A	137	ARG	CA-C-N	-6.42	114.19	122.98
1	A	137	ARG	C-N-CA	-6.42	114.19	122.98
1	B	249	PHE	N-CA-CB	-6.36	101.02	110.24
1	B	458	PRO	CB-CA-C	6.34	119.28	110.98
1	B	284	ASP	CA-CB-CG	6.31	118.91	112.60
1	A	77	ASP	CA-CB-CG	6.29	118.89	112.60
1	A	37	THR	CA-CB-OG1	-6.28	100.18	109.60
1	B	340	PHE	CA-CB-CG	6.17	119.97	113.80
1	B	412	PHE	CA-CB-CG	6.13	119.93	113.80
1	B	325	GLN	N-CA-CB	6.12	119.82	110.70
1	B	124	VAL	N-CA-CB	-6.04	104.28	110.62
1	B	249	PHE	CA-CB-CG	6.02	119.82	113.80
1	B	392	PHE	N-CA-CB	-6.00	105.00	111.66
1	A	105	PHE	CA-CB-CG	5.99	119.79	113.80
1	A	251	HIS	CB-CG-ND1	-5.91	113.84	122.70
1	A	325	GLN	CB-CA-C	-5.88	100.27	110.09
1	A	46	GLN	CB-CA-C	5.79	117.72	109.38
1	B	251	HIS	CB-CG-CD2	5.75	138.67	131.20
1	B	324	GLU	CB-CG-CD	5.73	122.34	112.60
1	A	331	ASP	CA-CB-CG	5.68	118.28	112.60
1	B	126	ARG	CA-CB-CG	-5.66	102.78	114.10
1	B	111	ASP	CA-CB-CG	5.64	118.24	112.60
1	B	410	ASN	CA-CB-CG	5.64	118.24	112.60
1	A	118	GLU	CB-CG-CD	-5.63	103.02	112.60
1	B	349	GLU	CB-CG-CD	5.63	122.18	112.60
1	B	77	ASP	CA-CB-CG	5.62	118.22	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	126	ARG	NE-CZ-NH1	-5.57	115.93	121.50
1	A	220	LEU	N-CA-CB	-5.56	100.16	109.28
1	B	396	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	351	LYS	N-CA-CB	5.47	118.17	110.12
1	A	412	PHE	CA-CB-CG	5.47	119.27	113.80
1	A	107	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	111	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	453	GLU	CA-C-O	5.33	124.19	119.71
1	A	106	LYS	CB-CA-C	5.32	118.39	110.62
1	A	118	GLU	CG-CD-OE1	5.32	130.64	118.40
1	B	437	GLU	CB-CG-CD	5.26	121.54	112.60
1	A	458	PRO	CB-CA-C	5.25	117.86	110.98
1	A	439	THR	OG1-CB-CG2	5.24	119.79	109.30
1	A	284	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	91	ASN	CB-CA-C	5.11	118.20	109.72
1	B	517	GLU	N-CA-CB	-5.08	102.40	110.22
1	B	107	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	132	MET	O-C-N	5.07	127.75	122.23
1	B	201	PRO	CB-CA-C	5.06	117.61	110.98
1	A	59	THR	CA-CB-OG1	-5.04	102.04	109.60
1	A	115	ARG	CB-CG-CD	-5.04	99.70	111.30
1	A	122	PHE	O-C-N	5.04	127.26	122.07
1	A	529	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	327	ARG	N-CA-CB	5.02	117.64	110.06
1	B	331	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	ARG	Sidechain
1	A	366	ARG	Sidechain
1	A	459	ARG	Sidechain
1	A	73	ARG	Sidechain
1	B	127	ARG	Sidechain
1	B	129	ARG	Sidechain
1	B	147	ARG	Sidechain
1	B	327	ARG	Sidechain
1	B	366	ARG	Sidechain
1	B	459	ARG	Sidechain
1	B	73	ARG	Sidechain

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	4210	0	4034	45	0
1	B	4210	0	4034	51	0
2	A	11	0	0	1	0
2	B	11	0	0	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	486	0	0	33	1
4	B	510	0	0	32	1
All	All	9440	0	8068	99	1

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

All (99) 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)
2:B:601:V9L:C5	4:B:716:HOH:O	1.71	1.32
1:B:97:ASP:HB2	4:B:704:HOH:O	1.36	1.23
1:B:365:VAL:HA	4:B:707:HOH:O	1.36	1.21
1:B:500:GLN:NE2	4:B:701:HOH:O	1.78	1.15
1:A:313:MET:HE1	4:A:757:HOH:O	1.47	1.14
1:B:399:PHE:HD1	4:B:702:HOH:O	1.31	1.12
1:A:185:LEU:HB2	4:A:701:HOH:O	1.55	1.05
1:A:176:GLU:O	4:A:701:HOH:O	1.80	0.98
1:A:189:PRO:HD3	4:A:767:HOH:O	1.62	0.96
1:A:141:THR:N	4:A:702:HOH:O	1.93	0.96
1:B:419:GLY:N	4:B:703:HOH:O	1.98	0.94
1:B:101:ALA:HB2	4:B:711:HOH:O	1.70	0.91
1:B:134:GLY:H	1:B:142:HIS:HD2	1.16	0.89
1:A:176:GLU:C	4:A:701:HOH:O	2.15	0.89
1:A:147:ARG:NE	4:A:703:HOH:O	2.09	0.86
1:A:450:LEU:HD22	4:A:724:HOH:O	1.75	0.84
1:B:396:ASP:O	4:B:702:HOH:O	1.98	0.80
1:B:50:PHE:CZ	1:B:505:ILE:HG22	2.16	0.80
1:B:402:VAL:HG13	4:B:710:HOH:O	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ASP:O	4:B:704:HOH:O	1.99	0.79
1:A:313:MET:SD	4:A:757:HOH:O	2.41	0.78
1:A:185:LEU:CB	4:A:701:HOH:O	2.19	0.77
1:A:419:GLY:N	4:A:704:HOH:O	2.11	0.76
1:B:147:ARG:NH2	4:B:705:HOH:O	2.23	0.72
1:B:134:GLY:H	1:B:142:HIS:CD2	2.04	0.71
1:B:480:ASN:ND2	4:B:706:HOH:O	2.23	0.70
1:A:247:CYS:N	4:A:706:HOH:O	2.25	0.70
1:A:138:ASN:CG	4:A:702:HOH:O	2.35	0.69
1:A:313:MET:CE	4:A:757:HOH:O	2.14	0.69
1:A:142:HIS:O	4:A:703:HOH:O	2.11	0.68
1:B:385:ILE:HG12	4:B:707:HOH:O	1.93	0.67
1:A:268:GLU:HG3	4:A:706:HOH:O	1.95	0.67
1:A:147:ARG:HG3	4:A:703:HOH:O	1.96	0.66
4:A:868:HOH:O	1:B:56:ASP:HB3	1.94	0.65
1:B:329:ILE:HG22	4:B:722:HOH:O	1.96	0.64
1:B:101:ALA:CB	4:B:711:HOH:O	2.37	0.64
1:A:279:HIS:HE1	4:A:861:HOH:O	1.80	0.64
1:B:144:PRO:HG3	4:B:705:HOH:O	1.98	0.64
1:A:141:THR:HG23	4:A:702:HOH:O	1.96	0.63
1:A:279:HIS:HD2	4:A:837:HOH:O	1.81	0.63
1:B:399:PHE:CD1	4:B:702:HOH:O	2.20	0.63
1:B:330:ILE:C	4:B:722:HOH:O	2.43	0.62
1:B:50:PHE:HZ	1:B:505:ILE:HG22	1.65	0.61
1:A:185:LEU:N	4:A:701:HOH:O	2.24	0.61
1:A:138:ASN:O	4:A:702:HOH:O	2.17	0.60
1:A:156:THR:HG23	4:A:884:HOH:O	2.03	0.59
1:B:156:THR:HG23	4:B:999:HOH:O	2.02	0.59
1:A:139:PRO:HA	1:A:142:HIS:CD2	2.39	0.58
1:B:65:LYS:HE3	1:B:107:ASP:HA	1.85	0.58
1:B:32:PRO:HB2	4:B:1073:HOH:O	2.04	0.58
1:B:385:ILE:N	4:B:707:HOH:O	2.32	0.58
1:A:187:TYR:O	4:A:705:HOH:O	2.16	0.57
1:B:50:PHE:CD2	1:B:50:PHE:N	2.71	0.55
1:A:535:HIS:HD2	4:B:889:HOH:O	1.90	0.55
1:A:46:GLN:OE1	4:B:701:HOH:O	2.19	0.53
1:A:340:PHE:HB2	4:A:757:HOH:O	2.08	0.53
1:A:138:ASN:OD1	4:A:702:HOH:O	2.19	0.53
1:B:464:PRO:HD3	4:B:1034:HOH:O	2.08	0.53
1:B:142:HIS:HE1	1:B:151:GLU:OE1	1.92	0.52
1:A:392:PHE:HB3	1:A:453:GLU:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ALA:N	4:B:704:HOH:O	2.42	0.52
1:B:235:LYS:HE2	1:B:237:VAL:HG12	1.93	0.49
1:A:143:HIS:C	4:A:703:HOH:O	2.56	0.49
1:B:213:PHE:HA	1:B:226:TYR:O	2.13	0.49
1:A:427:LEU:N	4:A:724:HOH:O	2.45	0.49
1:A:46:GLN:NE2	4:A:730:HOH:O	2.46	0.47
1:B:392:PHE:HB3	1:B:453:GLU:HG3	1.95	0.47
4:A:887:HOH:O	1:B:535:HIS:HD2	1.97	0.47
1:B:330:ILE:N	4:B:722:HOH:O	2.47	0.47
1:B:399:PHE:N	4:B:702:HOH:O	2.48	0.46
1:A:137:ARG:HA	1:A:151:GLU:OE2	2.15	0.46
1:A:102:ALA:O	1:A:112:TYR:HA	2.16	0.46
1:B:55:PHE:CZ	1:B:109:LYS:HE2	2.51	0.46
1:B:139:PRO:HA	1:B:142:HIS:ND1	2.30	0.46
1:A:147:ARG:CZ	4:A:703:HOH:O	2.56	0.45
1:A:58:MET:HE2	1:A:58:MET:HB2	1.88	0.45
1:A:295:PRO:HG2	1:A:303:GLU:HB3	1.99	0.45
1:B:65:LYS:HG2	4:B:763:HOH:O	2.15	0.45
2:B:601:V9L:C7	2:B:601:V9L:O1	2.65	0.45
1:B:114:GLN:CD	4:B:711:HOH:O	2.60	0.45
1:B:77:ASP:O	1:B:78:TYR:C	2.61	0.44
1:A:213:PHE:HA	1:A:226:TYR:O	2.17	0.44
1:A:246:TRP:HB2	4:A:706:HOH:O	2.16	0.44
1:B:97:ASP:HA	1:B:153:THR:HB	2.00	0.43
1:B:124:VAL:HG11	1:B:146:VAL:HG11	2.00	0.43
1:B:102:ALA:O	1:B:112:TYR:HA	2.18	0.43
1:A:48:ARG:HD2	4:B:745:HOH:O	2.17	0.43
1:B:235:LYS:HD3	4:B:799:HOH:O	2.19	0.43
1:B:200:HIS:O	1:B:202:LYS:HE2	2.20	0.42
1:B:352:LYS:HE3	4:B:1124:HOH:O	2.19	0.42
1:A:273:ARG:HH11	1:A:273:ARG:HD3	1.75	0.42
2:A:601:V9L:O1	2:A:601:V9L:C7	2.67	0.42
1:B:389:PRO:HB2	1:B:412:PHE:CG	2.55	0.41
1:A:118:GLU:HB2	1:A:184:THR:HB	2.01	0.41
1:B:118:GLU:HB2	1:B:184:THR:HB	2.02	0.41
1:A:154:ALA:HA	1:A:169:LYS:HB2	2.03	0.41
1:B:389:PRO:HB2	1:B:412:PHE:CD1	2.56	0.40
1:B:211:VAL:HG13	1:B:229:GLU:HG2	2.03	0.40
1:A:481:ARG:HH11	1:A:481:ARG:HD3	1.67	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:775:HOH:O	4:B:705:HOH:O[1_455]	2.07	0.13

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	523/556 (94%)	509 (97%)	13 (2%)	1 (0%)	44	33
1	B	523/556 (94%)	503 (96%)	19 (4%)	1 (0%)	44	33
All	All	1046/1112 (94%)	1012 (97%)	32 (3%)	2 (0%)	44	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	509	ILE
1	B	509	ILE

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	449/475 (94%)	444 (99%)	5 (1%)	70	60
1	B	449/475 (94%)	439 (98%)	10 (2%)	47	31
All	All	898/950 (94%)	883 (98%)	15 (2%)	56	41

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	A	123	LYS
1	A	242	LEU
1	A	493	THR
1	A	503	PHE
1	B	50	PHE
1	B	62	THR
1	B	123	LYS
1	B	124	VAL
1	B	144	PRO
1	B	166	LEU
1	B	232	PRO
1	B	242	LEU
1	B	325	GLN
1	B	503	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	46	GLN
1	A	279	HIS
1	A	378	GLN
1	A	410	ASN
1	A	512	GLN
1	A	535	HIS
1	B	142	HIS
1	B	258	ASN
1	B	308	HIS
1	B	397	ASN
1	B	410	ASN
1	B	535	HIS

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	V9L	A	601	-	11,11,11	1.16	1 (9%)	14,14,14	2.67	4 (28%)
2	V9L	B	601	-	11,11,11	1.02	1 (9%)	14,14,14	2.46	3 (21%)

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	V9L	A	601	-	-	4/4/4/4	0/1/1/1
2	V9L	B	601	-	-	2/4/4/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	V9L	C6-C1	2.70	1.44	1.40
2	B	601	V9L	C6-C1	2.04	1.43	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	V9L	O2-C6-C1	7.08	121.69	114.54
2	B	601	V9L	O2-C6-C1	6.88	121.48	114.54
2	A	601	V9L	C7-O2-C6	4.03	123.61	117.53
2	B	601	V9L	C7-O2-C6	3.62	122.99	117.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	V9L	C5-C6-C1	-3.30	116.92	119.97
2	B	601	V9L	C5-C6-C1	-3.12	117.09	119.97
2	A	601	V9L	O1-C1-C2	-2.48	117.10	121.22

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	V9L	C1-C6-O2-C7
2	A	601	V9L	C5-C6-O2-C7
2	B	601	V9L	C5-C6-O2-C7
2	B	601	V9L	C1-C6-O2-C7
2	A	601	V9L	C1-C2-C8-O3
2	A	601	V9L	C3-C2-C8-O3

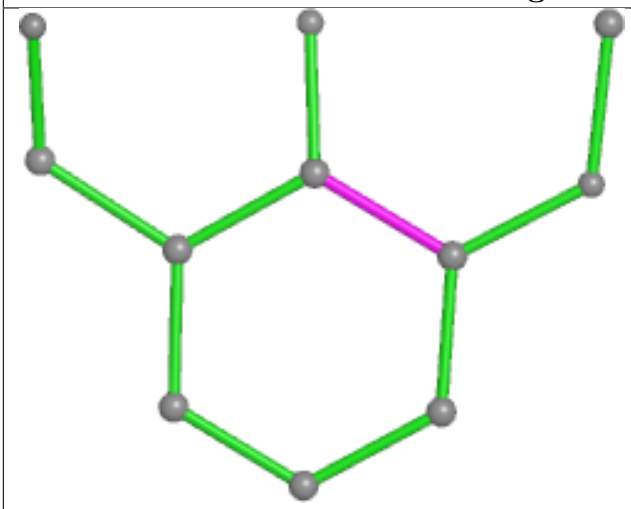
There are no ring outliers.

2 monomers are involved in 3 short contacts:

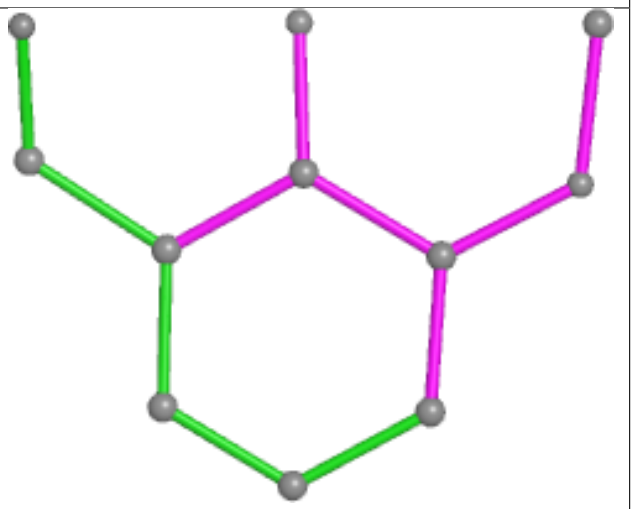
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	V9L	1	0
2	B	601	V9L	2	0

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 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.

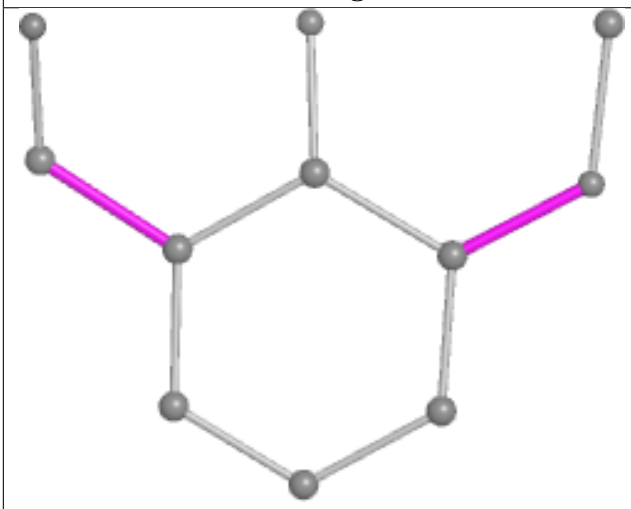
Ligand V9L A 601



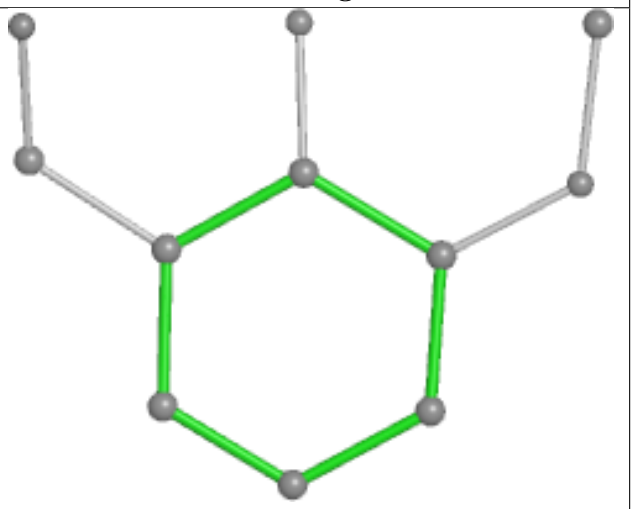
Bond lengths



Bond angles

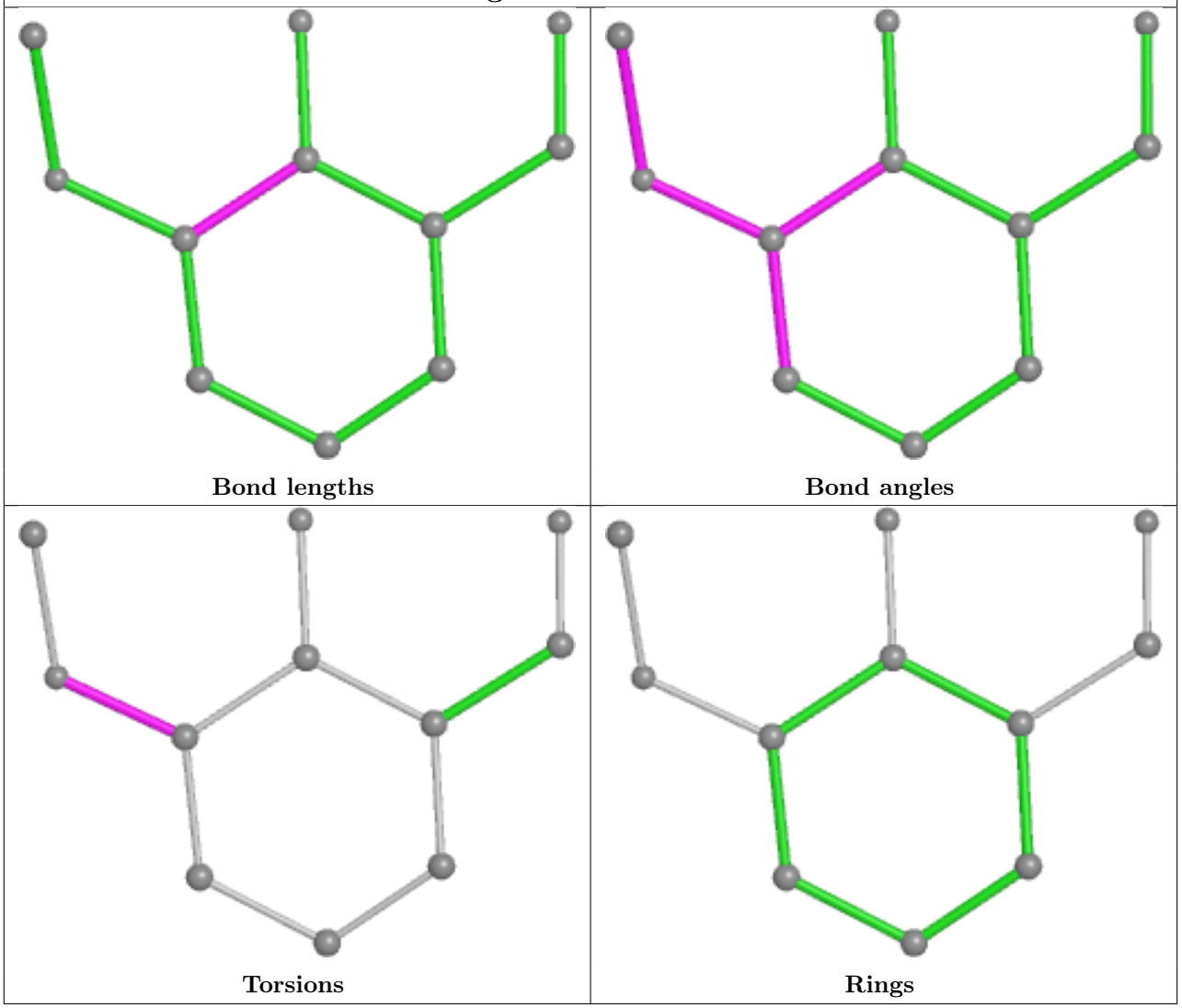


Torsions



Rings

Ligand V9L B 601



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, 95^{th} 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	525/556 (94%)	0.21	9 (1%) 69 75	11, 18, 32, 53	0
1	B	525/556 (94%)	0.22	3 (0%) 85 91	12, 18, 31, 53	0
All	All	1050/1112 (94%)	0.21	12 (1%) 77 84	11, 18, 32, 53	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	30	ILE	3.7
1	A	33	SER	2.8
1	B	50	PHE	2.7
1	A	25	VAL	2.6
1	B	356	ALA	2.4
1	A	27	PRO	2.4
1	B	24	TYR	2.4
1	A	24	TYR	2.3
1	A	65	LYS	2.2
1	A	479	LEU	2.2
1	A	26	HIS	2.2
1	A	31	LEU	2.1

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands (i)

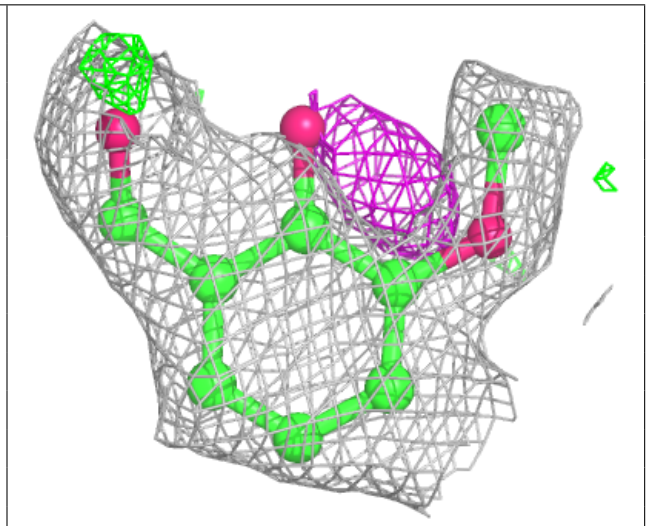
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

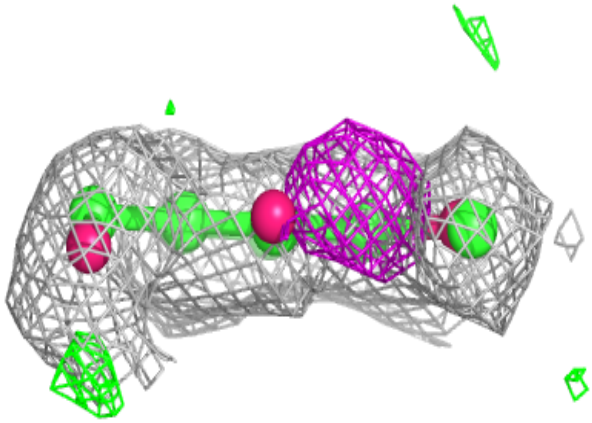
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	V9L	A	601	11/11	0.88	0.12	15,21,25,42	0
2	V9L	B	601	11/11	0.88	0.12	20,22,26,47	0
3	FE2	B	602	1/1	0.99	0.04	14,14,14,14	0
3	FE2	A	602	1/1	1.00	0.03	14,14,14,14	0

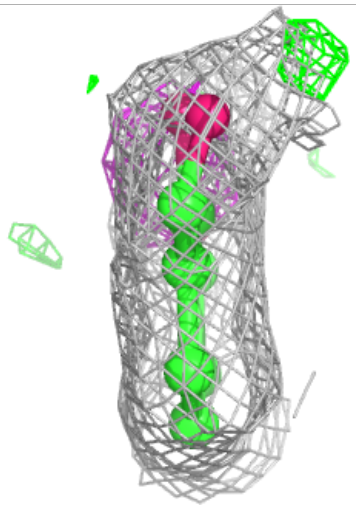
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around V9L A 601:

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

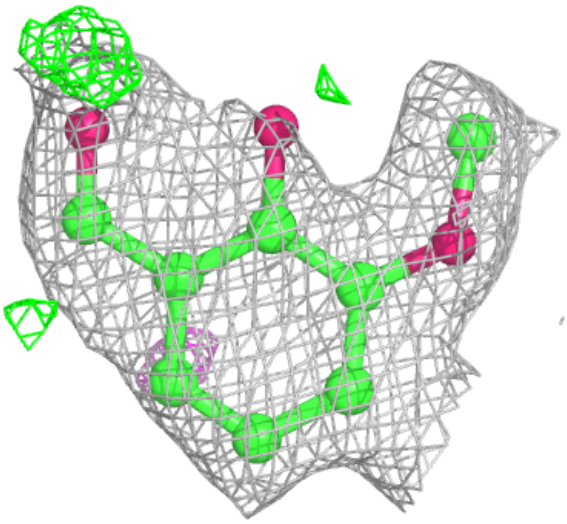


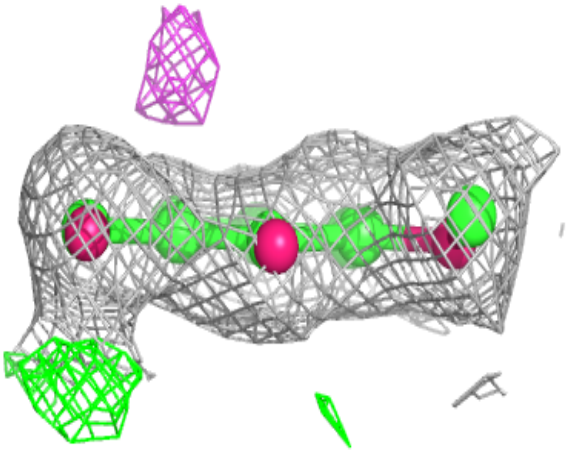


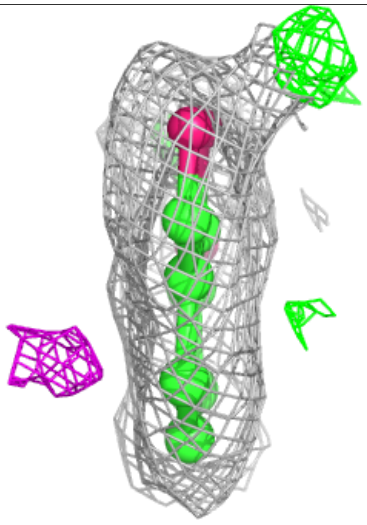


Electron density around V9L B 601:

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

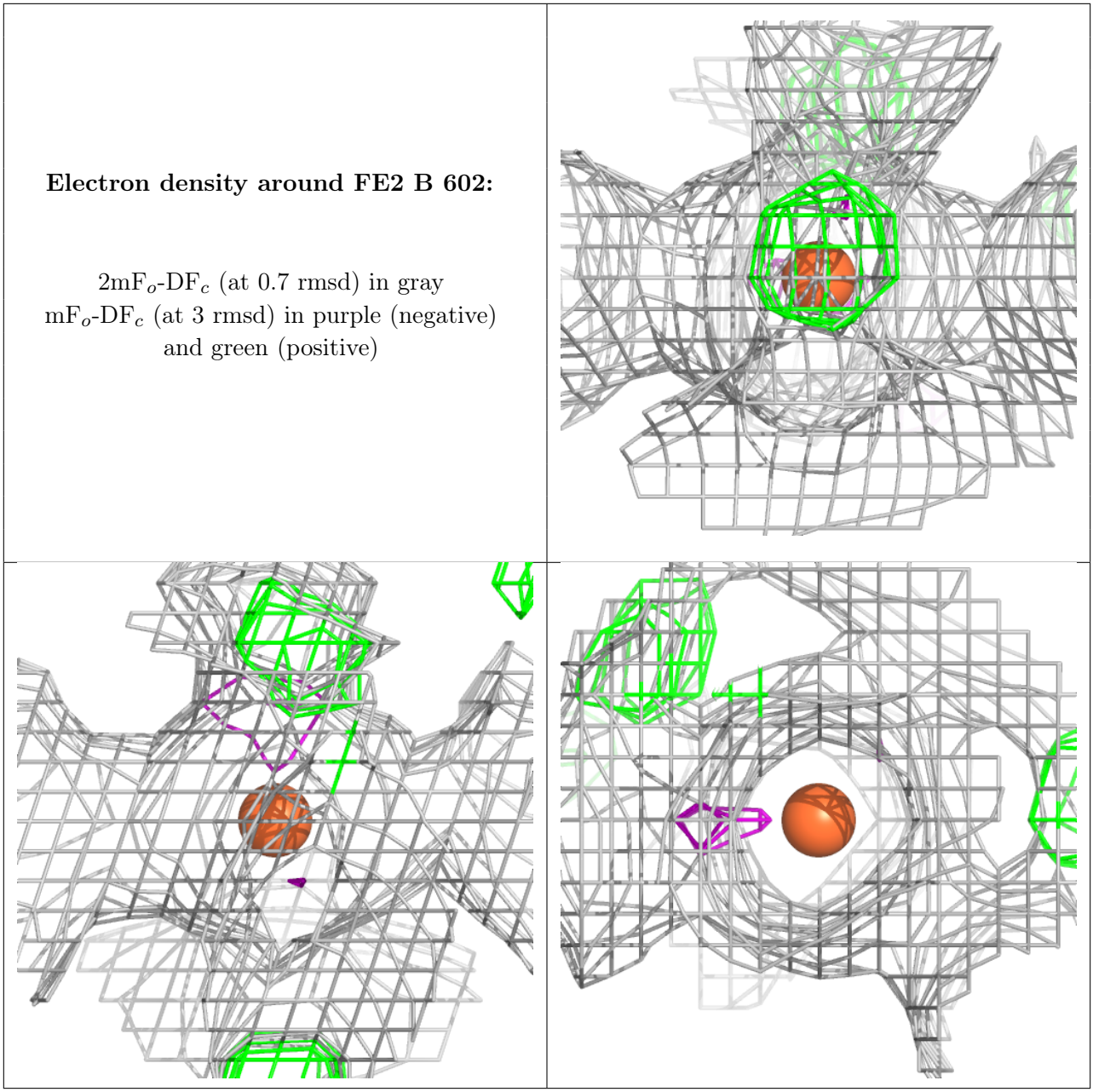






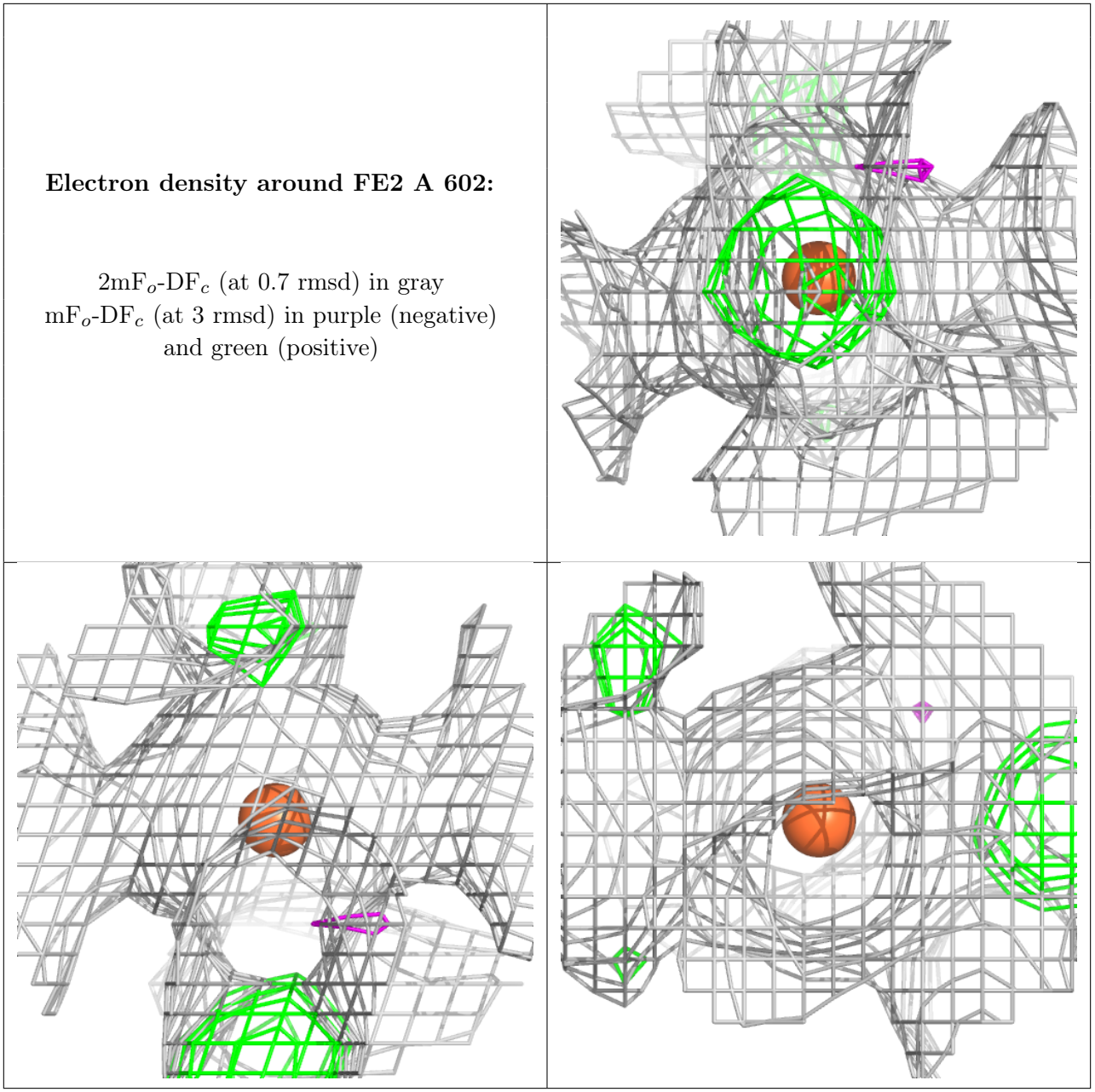
Electron density around FE2 B 602:

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



Electron density around FE2 A 602:

$2mF_o$-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.