



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 05:13 PM BST

PDB ID : 6N1Y
Title : Structure of L509V CAO1 - growth condition 1
Authors : Khadka, N.; Kiser, P.D.
Deposited on : 2018-11-12
Resolution : 2.15 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

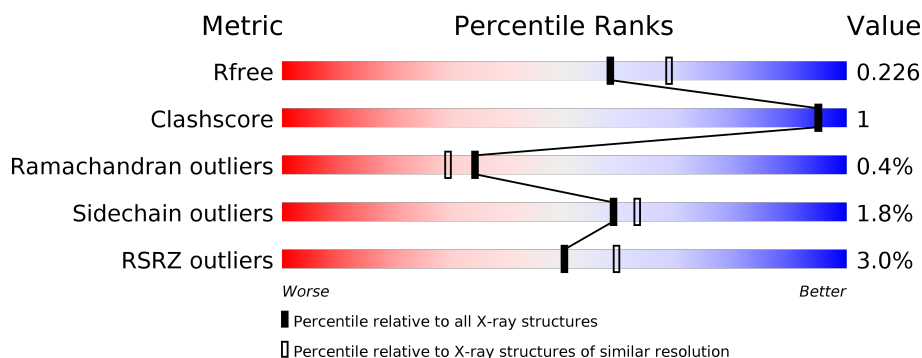
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 on 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	526	<div> <div>0%</div> <div>89%</div> <div>5%</div> <div>6%</div> </div>
1	B	526	<div> <div>3%</div> <div>90%</div> <div>6%</div> </div>
1	C	526	<div> <div>2%</div> <div>91%</div> <div>6%</div> </div>
1	D	526	<div> <div>5%</div> <div>90%</div> <div>6%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16707 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 Carotenoid oxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	2	0
			4002	2565	684	733	20			
1	B	497	Total	C	N	O	S	0	2	0
			3998	2564	682	732	20			
1	C	497	Total	C	N	O	S	0	0	0
			3980	2553	676	731	20			
1	D	497	Total	C	N	O	S	0	1	0
			3989	2561	676	732	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	509	VAL	LEU	engineered mutation	UNP A0A0B0DIC8
B	509	VAL	LEU	engineered mutation	UNP A0A0B0DIC8
C	509	VAL	LEU	engineered mutation	UNP A0A0B0DIC8
D	509	VAL	LEU	engineered mutation	UNP A0A0B0DIC8

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by author).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

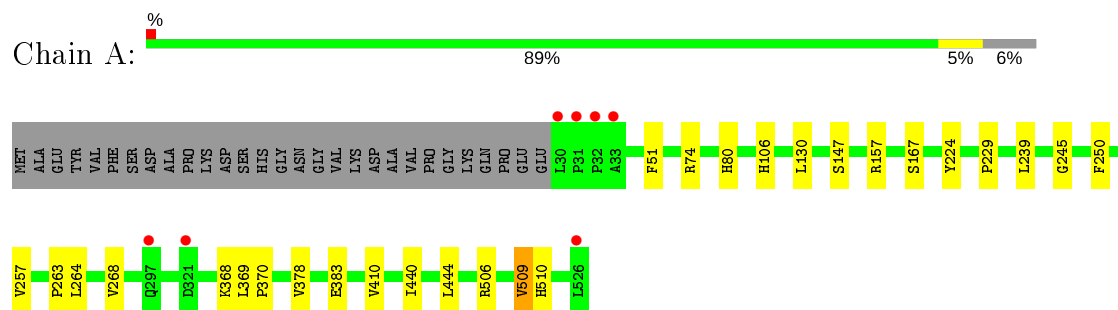
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	242	Total O 242 242	0	0
4	B	174	Total O 174 174	0	0
4	C	162	Total O 162 162	0	0
4	D	152	Total O 152 152	0	0

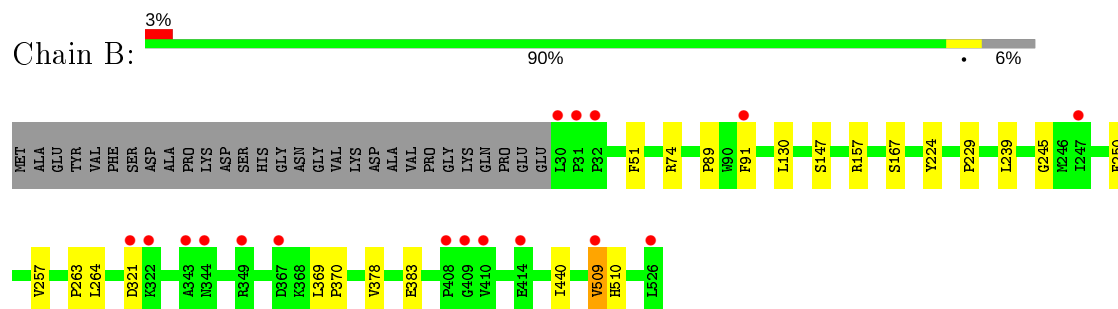
3 Residue-property plots

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.

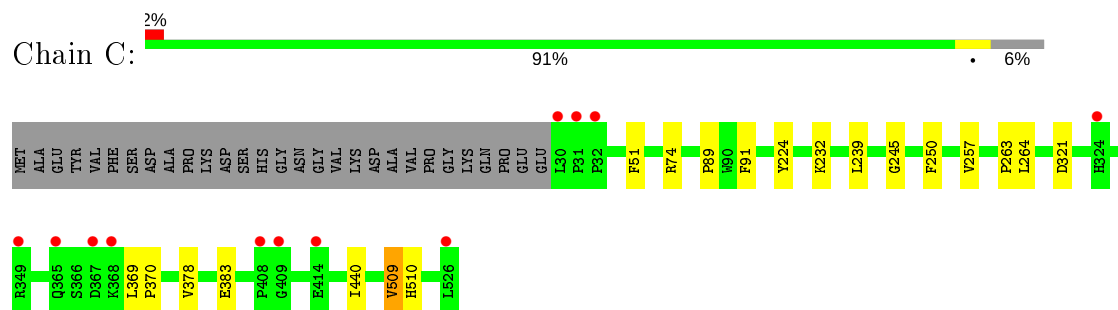
- Molecule 1: Carotenoid oxygenase



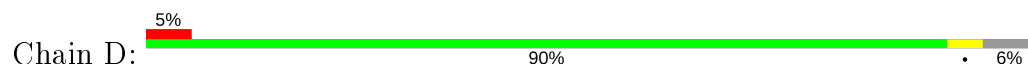
- Molecule 1: Carotenoid oxygenase

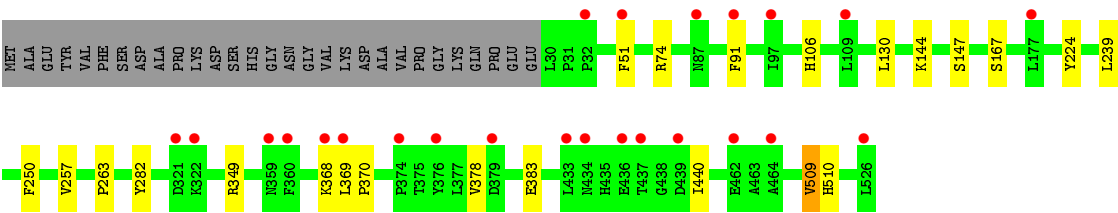


- Molecule 1: Carotenoid oxygenase



- Molecule 1: Carotenoid oxygenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.21Å 101.21Å 450.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.37 – 2.15 49.37 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.37-2.15) 99.9 (49.37-2.15)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.198 , 0.218 0.208 , 0.226	Depositor DCC
R_{free} test set	6490 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16707	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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: FE2, CL

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	0.61	0/4126	0.71	0/5606
1	B	0.61	0/4126	0.72	0/5607
1	C	0.61	0/4104	0.71	0/5578
1	D	0.61	0/4117	0.72	0/5596
All	All	0.61	0/16473	0.72	0/22387

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	4002	0	3829	12	0
1	B	3998	0	3824	10	0
1	C	3980	0	3805	7	0
1	D	3989	0	3814	7	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	242	0	0	4	0
4	B	174	0	0	0	0
4	C	162	0	0	0	0
4	D	152	0	0	1	0
All	All	16707	0	15272	36	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 1.

All (36) 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:106:HIS:HB2	4:D:811:HOH:O	2.02	0.59
1:B:157[B]:ARG:NH1	1:B:229:PRO:O	2.35	0.59
1:A:157[B]:ARG:NH1	1:A:229:PRO:O	2.37	0.57
1:B:89:PRO:HB2	1:B:91:PHE:CZ	2.44	0.52
1:C:509:VAL:HG12	1:C:510:HIS:CD2	2.46	0.51
1:B:509:VAL:HG12	1:B:510:HIS:CD2	2.46	0.51
1:A:80:HIS:CE1	4:A:795:HOH:O	2.63	0.50
1:A:509:VAL:HG12	1:A:510:HIS:CD2	2.47	0.50
1:D:509:VAL:HG12	1:D:510:HIS:CD2	2.46	0.50
1:A:369:LEU:HB2	1:A:370:PRO:HD3	1.98	0.46
1:A:410:VAL:HG13	1:A:444:LEU:HD12	1.98	0.45
1:D:369:LEU:HB2	1:D:370:PRO:HD3	1.97	0.45
1:C:89:PRO:HB2	1:C:91:PHE:CZ	2.52	0.45
1:B:369:LEU:HB2	1:B:370:PRO:HD3	1.98	0.45
1:C:369:LEU:HB2	1:C:370:PRO:HD3	1.98	0.44
1:B:89:PRO:CB	1:B:91:PHE:CZ	3.01	0.44
1:A:106:HIS:HB2	4:A:900:HOH:O	2.18	0.44
1:B:157[B]:ARG:HG2	1:B:157[B]:ARG:HH11	1.82	0.44
1:A:268:VAL:HG23	4:A:752:HOH:O	2.18	0.43
1:A:378:VAL:HG12	1:A:440:ILE:HD11	1.99	0.43
1:A:506:ARG:NH2	4:A:704:HOH:O	2.43	0.43
1:B:378:VAL:HG12	1:B:440:ILE:HD11	2.01	0.43
1:C:245:GLY:HA2	1:C:264:LEU:O	2.19	0.43
1:C:378:VAL:HG12	1:C:440:ILE:HD11	2.01	0.42
1:D:378:VAL:HG12	1:D:440:ILE:HD11	2.02	0.42
1:B:147:SER:HB2	1:B:167:SER:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:TYR:CE1	1:A:257:VAL:HG11	2.55	0.41
1:A:245:GLY:HA2	1:A:264:LEU:O	2.19	0.41
1:B:245:GLY:HA2	1:B:264:LEU:O	2.20	0.41
1:A:147:SER:HB2	1:A:167:SER:CB	2.50	0.41
1:C:224:TYR:CE1	1:C:257:VAL:HG11	2.55	0.41
1:B:224:TYR:CE1	1:B:257:VAL:HG11	2.56	0.41
1:C:232:LYS:HD3	1:C:232:LYS:HA	1.94	0.41
1:D:147:SER:HB2	1:D:167:SER:CB	2.50	0.41
1:D:224:TYR:CE1	1:D:257:VAL:HG11	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	497/526 (94%)	485 (98%)	10 (2%)	2 (0%)	34	29
1	B	497/526 (94%)	486 (98%)	9 (2%)	2 (0%)	34	29
1	C	495/526 (94%)	483 (98%)	10 (2%)	2 (0%)	34	29
1	D	496/526 (94%)	483 (97%)	11 (2%)	2 (0%)	34	29
All	All	1985/2104 (94%)	1937 (98%)	40 (2%)	8 (0%)	34	29

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	509	VAL
1	B	509	VAL
1	C	509	VAL
1	D	509	VAL
1	A	263	PRO
1	B	263	PRO

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Mol	Chain	Res	Type
1	C	263	PRO
1	D	263	PRO

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	424/445 (95%)	417 (98%)	7 (2%)	60	65
1	B	424/445 (95%)	417 (98%)	7 (2%)	60	65
1	C	422/445 (95%)	416 (99%)	6 (1%)	67	72
1	D	423/445 (95%)	413 (98%)	10 (2%)	49	51
All	All	1693/1780 (95%)	1663 (98%)	30 (2%)	59	63

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	PHE
1	A	74	ARG
1	A	130	LEU
1	A	239	LEU
1	A	250	PHE
1	A	368	LYS
1	A	383	GLU
1	B	51	PHE
1	B	74	ARG
1	B	130	LEU
1	B	239	LEU
1	B	250	PHE
1	B	321	ASP
1	B	383	GLU
1	C	51	PHE
1	C	74	ARG
1	C	239	LEU
1	C	250	PHE
1	C	321	ASP

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Mol	Chain	Res	Type
1	C	383	GLU
1	D	51	PHE
1	D	74	ARG
1	D	91	PHE
1	D	130	LEU
1	D	144	LYS
1	D	239	LEU
1	D	250	PHE
1	D	349	ARG
1	D	368	LYS
1	D	383	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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, 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	497/526 (94%)	-0.09	7 (1%) 75 80	35, 50, 69, 90	0
1	B	497/526 (94%)	0.09	17 (3%) 45 53	37, 52, 80, 108	0
1	C	497/526 (94%)	0.04	12 (2%) 59 67	35, 58, 85, 107	0
1	D	497/526 (94%)	0.22	24 (4%) 30 39	39, 59, 83, 99	0
All	All	1988/2104 (94%)	0.07	60 (3%) 50 59	35, 54, 81, 108	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	32	PRO	5.1
1	D	526	LEU	5.0
1	C	30	LEU	4.7
1	C	526	LEU	4.6
1	A	526	LEU	4.4
1	B	408	PRO	4.2
1	C	31	PRO	4.1
1	B	31	PRO	4.0
1	B	409	GLY	4.0
1	B	30	LEU	4.0
1	A	32	PRO	3.7
1	C	409	GLY	3.6
1	D	439	ASP	3.2
1	D	321	ASP	3.2
1	D	32	PRO	3.1
1	D	462	GLU	3.1
1	C	365	GLN	3.0
1	B	343	ALA	3.0
1	B	349	ARG	2.9
1	B	526	LEU	2.9
1	B	322	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	324	HIS	2.8
1	B	32	PRO	2.8
1	A	33	ALA	2.8
1	B	344	ASN	2.7
1	C	414	GLU	2.7
1	A	30	LEU	2.7
1	D	433	LEU	2.7
1	D	437	THR	2.6
1	C	408	PRO	2.6
1	D	376	TYR	2.6
1	D	91	PHE	2.6
1	B	410	VAL	2.4
1	D	368	LYS	2.4
1	D	436	GLU	2.3
1	D	51	PHE	2.3
1	D	379	ASP	2.3
1	B	91	PHE	2.3
1	D	109	LEU	2.3
1	A	31	PRO	2.3
1	B	321	ASP	2.2
1	D	360	PHE	2.2
1	A	297	GLN	2.2
1	D	369	LEU	2.2
1	B	509	VAL	2.2
1	C	368	LYS	2.2
1	D	322	LYS	2.2
1	D	374	PRO	2.2
1	D	359	ASN	2.1
1	C	367	ASP	2.1
1	D	177	LEU	2.1
1	D	434	ASN	2.1
1	B	247	ILE	2.1
1	B	367	ASP	2.1
1	D	464	ALA	2.1
1	A	321	ASP	2.1
1	C	349	ARG	2.1
1	B	414	GLU	2.0
1	D	97	ILE	2.0
1	D	87	ASN	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 monosaccharides in this entry.

6.4 Ligands [i](#)

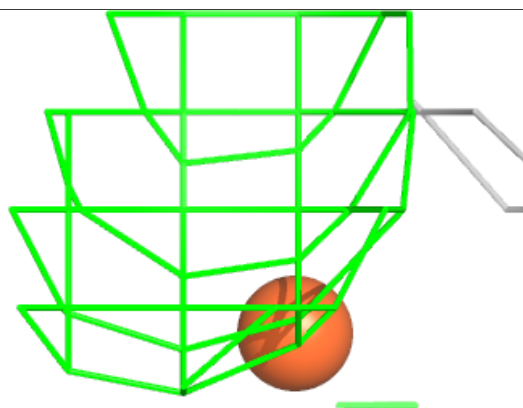
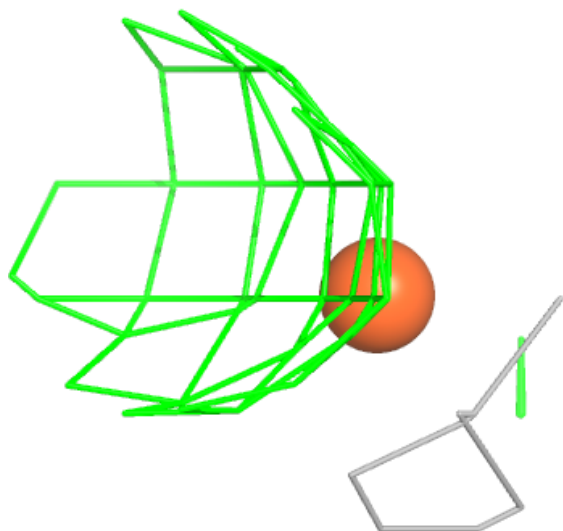
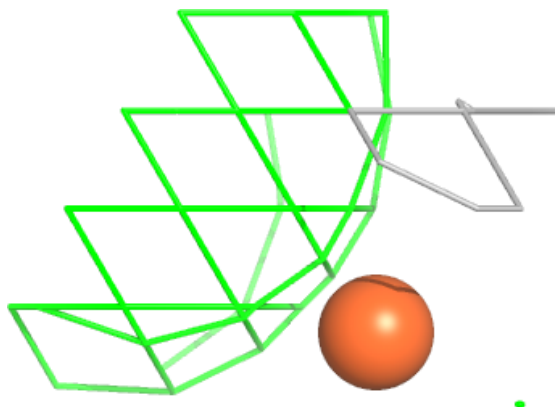
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CL	C	602	1/1	0.94	0.08	59,59,59,59	0
3	CL	A	602	1/1	0.95	0.10	53,53,53,53	0
2	FE2	D	601	1/1	0.96	0.17	50,50,50,50	0
2	FE2	A	601	1/1	0.97	0.15	41,41,41,41	0
2	FE2	C	601	1/1	0.97	0.16	49,49,49,49	0
2	FE2	B	601	1/1	0.97	0.17	42,42,42,42	0
3	CL	D	602	1/1	0.98	0.07	58,58,58,58	0
3	CL	B	602	1/1	0.98	0.09	59,59,59,59	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.

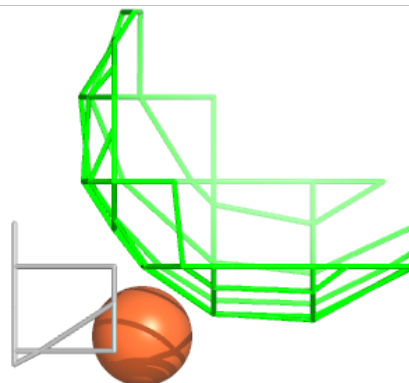
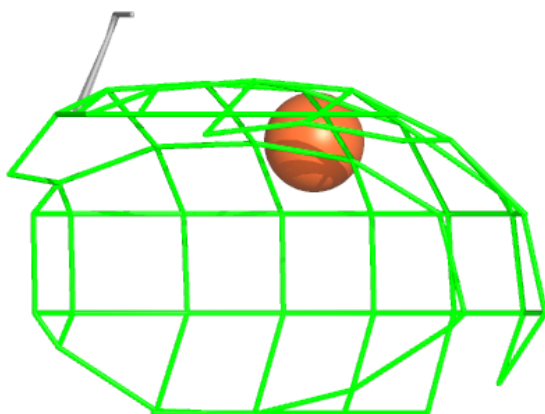
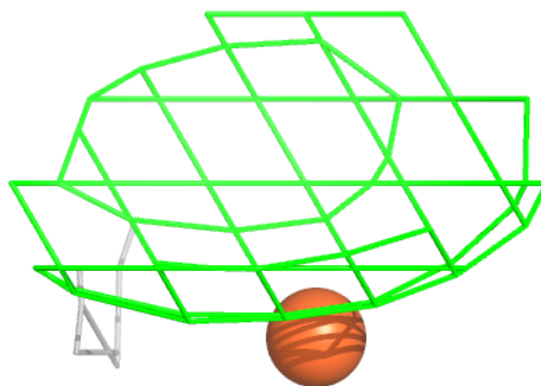
Electron density around FE2 D 601:

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



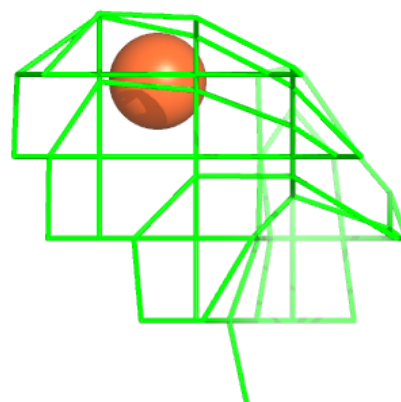
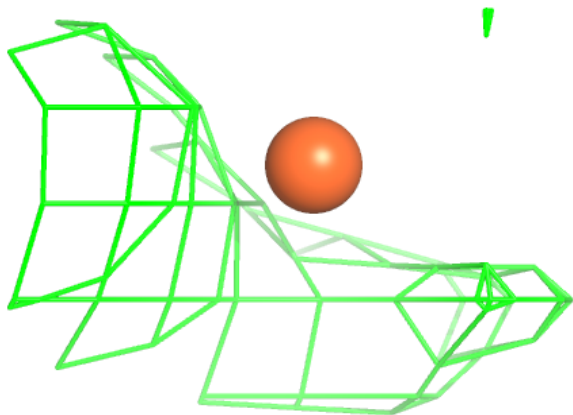
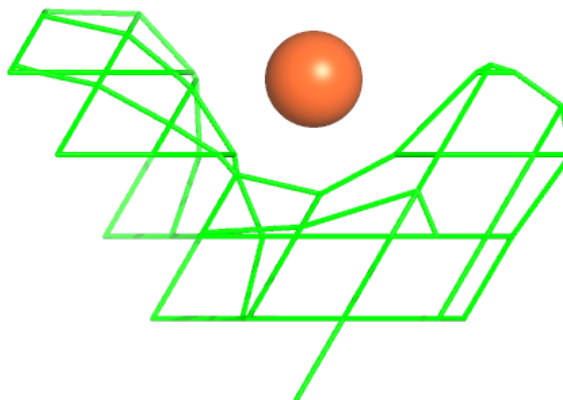
Electron density around FE2 A 601:

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



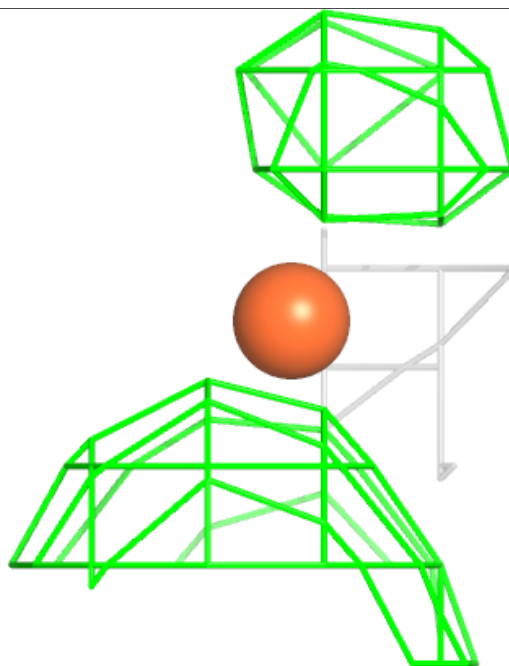
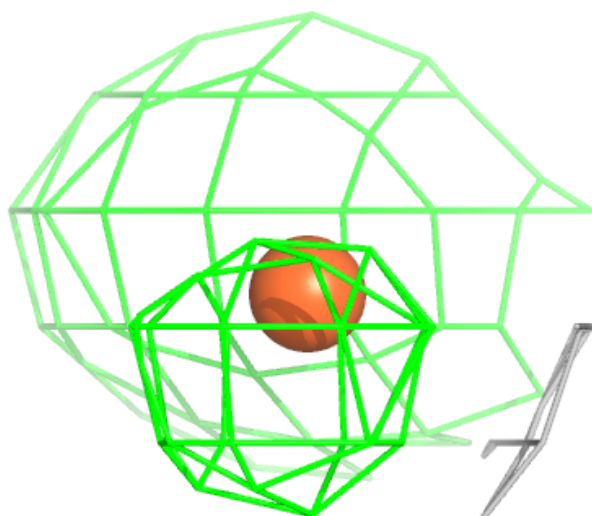
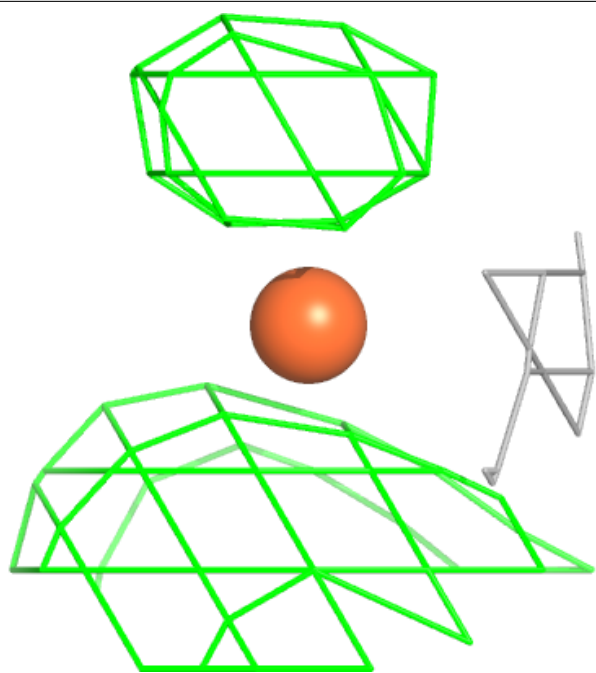
Electron density around FE2 C 601:

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



Electron density around FE2 B 601:

$2mF_o-DF_c$ (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.