



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:34 AM UTC

PDB ID : 7T8Q / pdb_00007t8q
Title : CRYSTAL STRUCTURE OF T151G CAO1
Authors : Daruwalla, A.; Kiser, P.D.
Deposited on : 2021-12-16
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 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

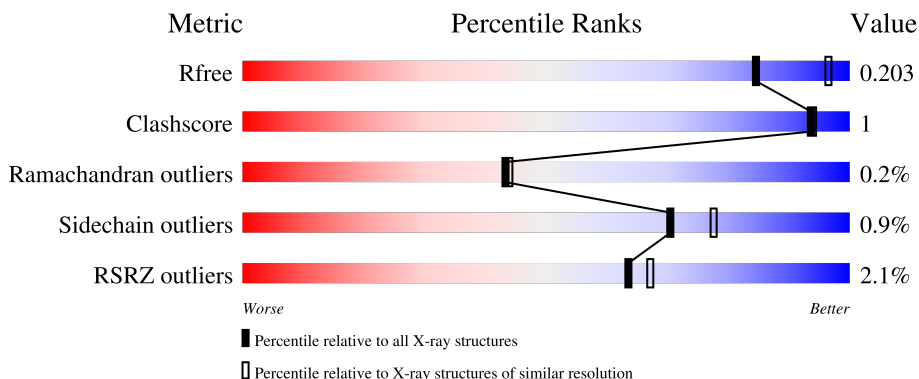
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	526	2% 92% 6%
1	B	526	4% 89% 5% 6%
1	C	526	% 92% 5%
1	D	526	% 90% 5% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17178 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			3974	2550	675	729	20			
1	B	497	Total	C	N	O	S	0	1	0
			3978	2553	677	728	20			
1	C	500	Total	C	N	O	S	0	0	0
			4003	2567	679	737	20			
1	D	497	Total	C	N	O	S	0	0	0
			3974	2549	675	730	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	GLY	THR	engineered mutation	UNP Q7S860
B	151	GLY	THR	engineered mutation	UNP Q7S860
C	151	GLY	THR	engineered mutation	UNP Q7S860
D	151	GLY	THR	engineered mutation	UNP Q7S860

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Cl 3	0	0
3	B	2	Total 2	Cl 2	0	0
3	C	2	Total 2	Cl 2	0	0
3	D	3	Total 3	Cl 3	0	0

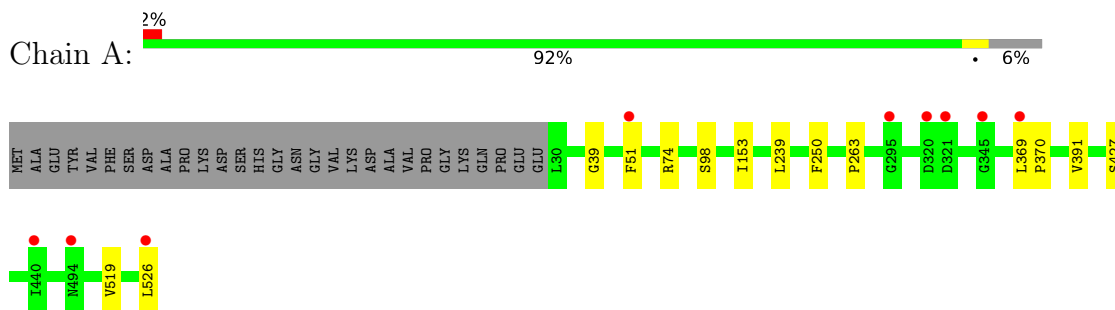
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	290	Total 290	O 290	0	0
4	B	305	Total 305	O 305	0	0
4	C	309	Total 309	O 309	0	0
4	D	331	Total 331	O 331	0	0

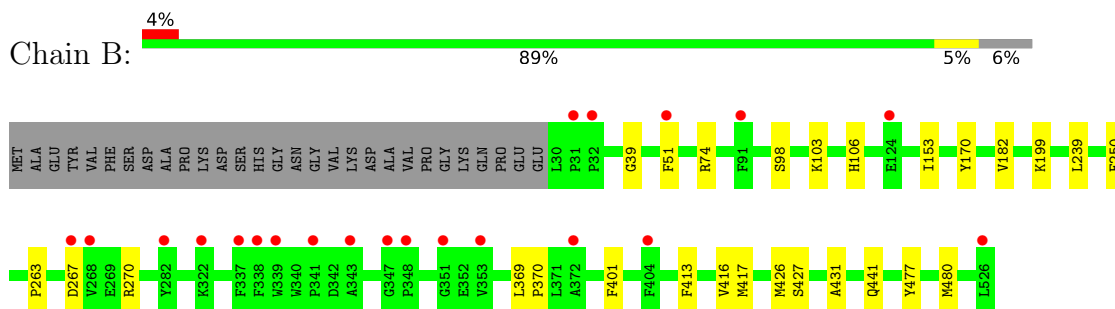
3 Residue-property plots [i](#)

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.

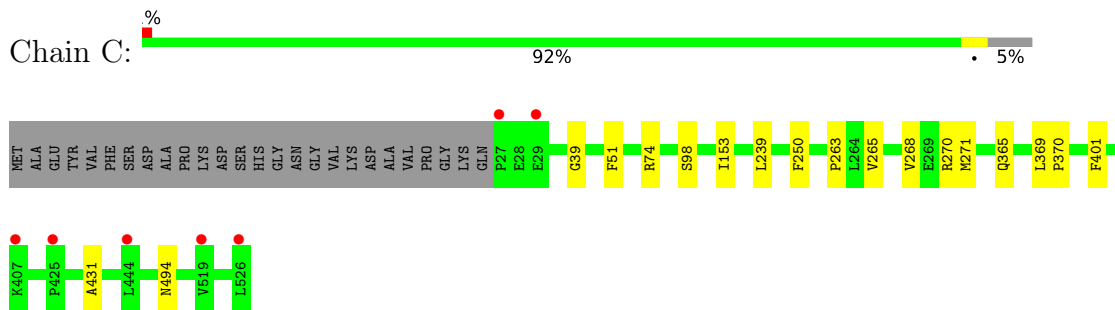
- Molecule 1: Carotenoid oxygenase 1



- Molecule 1: Carotenoid oxygenase 1

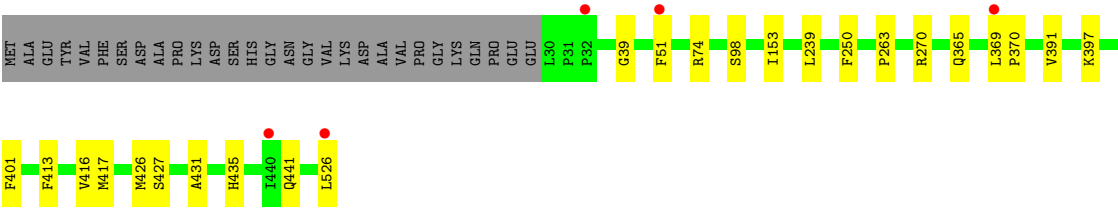


- Molecule 1: Carotenoid oxygenase 1



- Molecule 1: Carotenoid oxygenase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	100.63Å 100.63Å 447.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.09 – 2.15 49.09 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.09-2.15) 99.0 (49.09-2.15)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.190 , 0.211 (Not available) , 0.203	Depositor DCC
R_{free} test set	6063 reflections (4.26%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17178	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: CL, 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	0.96	0/4098	1.22	1/5569 (0.0%)
1	B	0.96	0/4106	1.22	1/5581 (0.0%)
1	C	0.96	0/4128	1.22	1/5609 (0.0%)
1	D	0.96	0/4098	1.22	1/5570 (0.0%)
All	All	0.96	0/16430	1.22	4/22329 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	39	GLY	CA-C-O	-5.67	118.53	122.22
1	A	39	GLY	CA-C-O	-5.53	118.47	122.45
1	B	39	GLY	CA-C-O	-5.34	118.61	122.45
1	D	39	GLY	CA-C-O	-5.14	118.75	122.45

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	3974	0	3797	5	0
1	B	3978	0	3797	16	0
1	C	4003	0	3823	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3974	0	3792	12	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	3	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
4	A	290	0	0	0	0
4	B	305	0	0	3	0
4	C	309	0	0	3	0
4	D	331	0	0	2	0
All	All	17178	0	15209	43	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 (43) 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:C:268:VAL:HA	1:C:271:MET:HE3	1.72	0.72
1:B:103:LYS:O	1:B:106[B]:HIS:CD2	2.47	0.67
1:D:416:VAL:HG12	1:D:417:MET:HE2	1.83	0.60
1:B:416:VAL:HG12	1:B:417:MET:HE2	1.84	0.60
1:B:477:TYR:HA	1:B:480:MET:CE	2.34	0.57
1:B:199:LYS:HE3	4:B:880:HOH:O	2.04	0.57
1:C:268:VAL:HA	1:C:271:MET:CE	2.37	0.54
1:B:477:TYR:HA	1:B:480:MET:HE2	1.90	0.53
1:C:270:ARG:NH2	4:C:704:HOH:O	2.43	0.51
1:D:441:GLN:NE2	4:D:702:HOH:O	2.45	0.49
1:B:417:MET:HE1	1:B:426:MET:SD	2.52	0.49
1:B:74:ARG:HG2	1:B:98:SER:HB2	1.96	0.48
1:B:170:TYR:CZ	1:B:182:VAL:HG22	2.49	0.47
1:A:74:ARG:HG2	1:A:98:SER:HB2	1.97	0.47
1:A:391:VAL:CG1	1:A:526:LEU:HD12	2.45	0.47
1:D:417:MET:HE1	1:D:426:MET:SD	2.54	0.47
1:D:365:GLN:HA	1:D:365:GLN:OE1	2.15	0.46
1:D:391:VAL:CG1	1:D:526:LEU:HD12	2.45	0.46
1:C:74:ARG:HG2	1:C:98:SER:HB2	1.97	0.46
1:C:365:GLN:OE1	1:C:365:GLN:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:ARG:HG2	1:D:98:SER:HB2	1.97	0.46
1:B:369:LEU:HB2	1:B:370:PRO:HD3	1.96	0.46
1:C:369:LEU:HB2	1:C:370:PRO:HD3	1.98	0.45
1:C:494:ASN:HB2	4:C:934:HOH:O	2.17	0.44
1:A:369:LEU:HB2	1:A:370:PRO:HD3	1.99	0.44
1:D:369:LEU:HB2	1:D:370:PRO:HD3	1.99	0.44
1:B:480:MET:HE2	1:B:480:MET:HA	2.00	0.43
1:B:441:GLN:NE2	4:B:715:HOH:O	2.51	0.43
1:B:477:TYR:O	1:B:480:MET:HE3	2.19	0.42
1:C:153:ILE:O	1:C:153:ILE:HG23	2.19	0.42
1:D:413:PHE:HD1	1:D:417:MET:HE3	1.85	0.42
1:B:267:ASP:HB3	1:B:270:ARG:NH1	2.35	0.42
1:B:153:ILE:O	1:B:153:ILE:HG23	2.20	0.42
1:D:401:PHE:CE1	1:D:431:ALA:HB3	2.55	0.41
1:A:153:ILE:HG23	1:A:153:ILE:O	2.19	0.41
1:D:153:ILE:HG23	1:D:153:ILE:O	2.20	0.41
1:B:401:PHE:CE2	1:B:431:ALA:HB3	2.56	0.41
1:C:401:PHE:CE2	1:C:431:ALA:HB3	2.56	0.41
1:A:519:VAL:HG11	4:B:1004:HOH:O	2.21	0.41
1:B:413:PHE:HD1	1:B:417:MET:HE3	1.86	0.41
1:C:265:VAL:HB	4:C:823:HOH:O	2.20	0.40
1:D:397:LYS:HA	1:D:435:HIS:HB2	2.04	0.40
1:D:270:ARG:NH2	4:D:726:HOH:O	2.54	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	495/526 (94%)	485 (98%)	9 (2%)	1 (0%)	43 44
1	B	496/526 (94%)	489 (99%)	6 (1%)	1 (0%)	43 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	498/526 (95%)	487 (98%)	10 (2%)	1 (0%)	43	44
1	D	495/526 (94%)	487 (98%)	7 (1%)	1 (0%)	43	44
All	All	1984/2104 (94%)	1948 (98%)	32 (2%)	4 (0%)	43	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	263	PRO
1	C	263	PRO
1	D	263	PRO
1	A	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	420/444 (95%)	416 (99%)	4 (1%)	68	75
1	B	420/444 (95%)	416 (99%)	4 (1%)	68	75
1	C	424/444 (96%)	421 (99%)	3 (1%)	76	82
1	D	420/444 (95%)	416 (99%)	4 (1%)	68	75
All	All	1684/1776 (95%)	1669 (99%)	15 (1%)	70	77

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

Mol	Chain	Res	Type
1	A	51	PHE
1	A	239	LEU
1	A	250	PHE
1	A	427	SER
1	B	51	PHE
1	B	239	LEU
1	B	250	PHE
1	B	427	SER

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Mol	Chain	Res	Type
1	C	51	PHE
1	C	239	LEU
1	C	250	PHE
1	D	51	PHE
1	D	239	LEU
1	D	250	PHE
1	D	427	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	A	356	HIS
1	B	356	HIS
1	D	106	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 14 ligands modelled in this entry, 14 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

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	497/526 (94%)	0.32	9 (1%) 67 71	34, 48, 69, 90	0
1	B	497/526 (94%)	0.29	21 (4%) 40 45	23, 45, 72, 107	1 (0%)
1	C	500/526 (95%)	0.24	7 (1%) 73 77	34, 47, 66, 108	0
1	D	497/526 (94%)	0.09	5 (1%) 79 82	33, 44, 62, 81	0
All	All	1991/2104 (94%)	0.24	42 (2%) 63 67	23, 46, 68, 108	1 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	27	PRO	4.3
1	C	425	PRO	4.1
1	B	343	ALA	3.7
1	D	526	LEU	3.4
1	B	348	PRO	3.2
1	D	440	ILE	3.0
1	B	282	TYR	2.9
1	B	337	PHE	2.9
1	B	372	ALA	2.7
1	B	267	ASP	2.6
1	B	526	LEU	2.6
1	B	341	PRO	2.6
1	A	369	LEU	2.6
1	B	51	PHE	2.5
1	A	295	GLY	2.4
1	B	347	GLY	2.3
1	B	339	TRP	2.3
1	B	91	PHE	2.2
1	A	321	ASP	2.2
1	A	51	PHE	2.2
1	D	51	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	353	VAL	2.2
1	C	519	VAL	2.2
1	C	29	GLU	2.1
1	C	526	LEU	2.1
1	B	31	PRO	2.1
1	A	440	ILE	2.1
1	B	268	VAL	2.1
1	B	351	GLY	2.1
1	C	444	LEU	2.1
1	D	369	LEU	2.1
1	B	404	PHE	2.1
1	B	124	GLU	2.1
1	B	32	PRO	2.1
1	A	345	GLY	2.1
1	B	338	PHE	2.1
1	D	32	PRO	2.0
1	C	407	LYS	2.0
1	A	494	ASN	2.0
1	A	526	LEU	2.0
1	A	320	ASP	2.0
1	B	322	LYS	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, 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($\text{\AA}^2$)	Q<0.9
3	CL	D	603	1/1	0.89	0.17	86,86,86,86	0
3	CL	A	603	1/1	0.90	0.20	70,70,70,70	0

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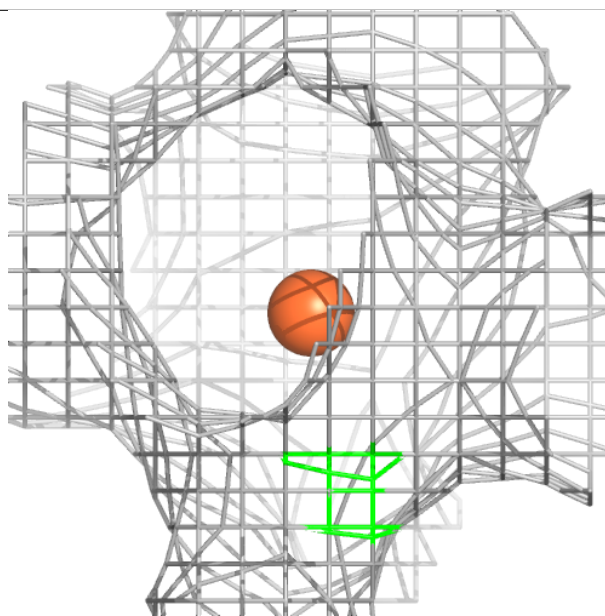
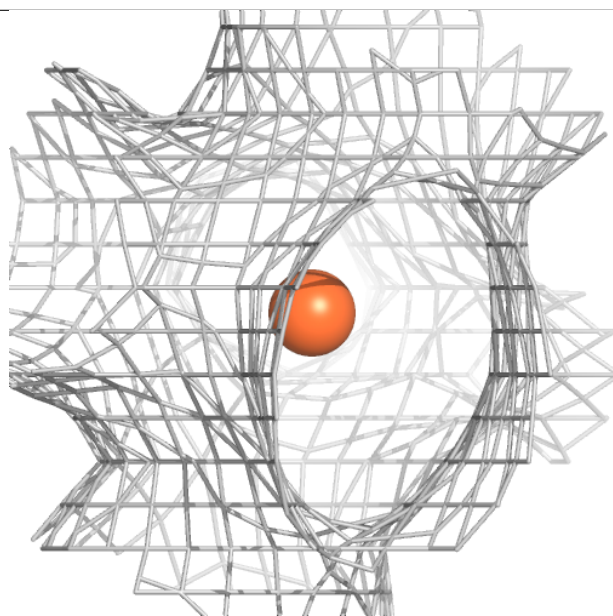
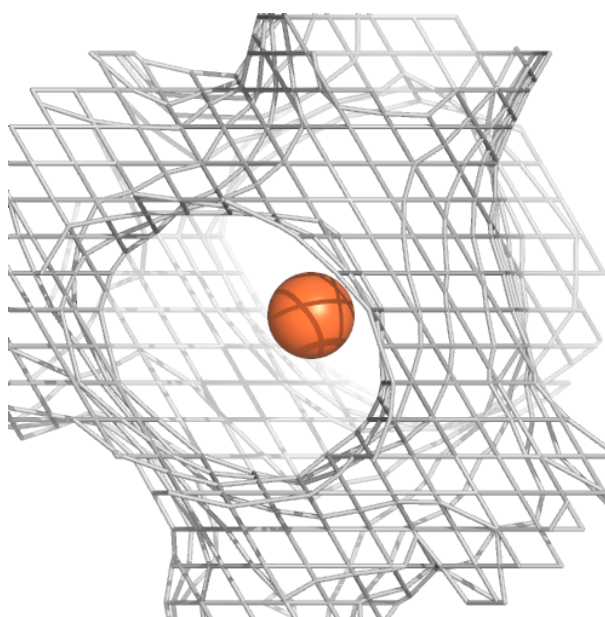
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	A	604	1/1	0.95	0.12	60,60,60,60	0
3	CL	C	603	1/1	0.96	0.10	59,59,59,59	0
3	CL	B	602	1/1	0.97	0.12	56,56,56,56	0
3	CL	C	602	1/1	0.98	0.12	55,55,55,55	0
3	CL	A	602	1/1	0.98	0.15	54,54,54,54	0
3	CL	B	603	1/1	0.98	0.08	61,61,61,61	0
3	CL	D	604	1/1	0.98	0.14	54,54,54,54	0
2	FE2	B	601	1/1	0.99	0.04	43,43,43,43	1
3	CL	D	602	1/1	0.99	0.06	48,48,48,48	0
2	FE2	C	601	1/1	1.00	0.03	42,42,42,42	1
2	FE2	D	601	1/1	1.00	0.02	38,38,38,38	1
2	FE2	A	601	1/1	1.00	0.02	43,43,43,43	1

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.

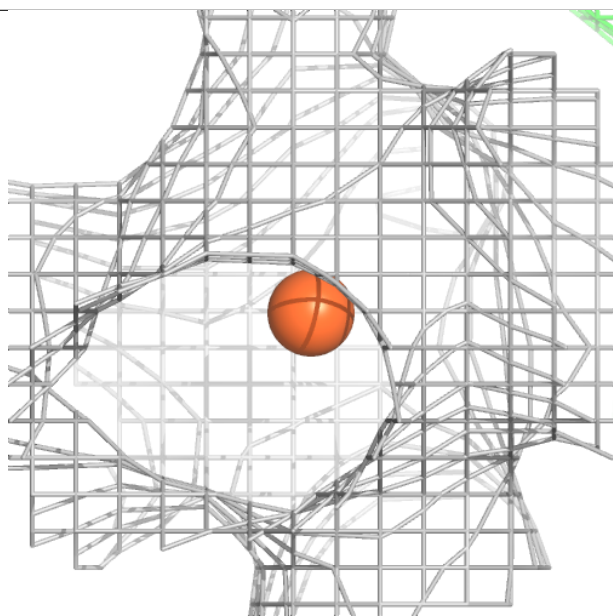
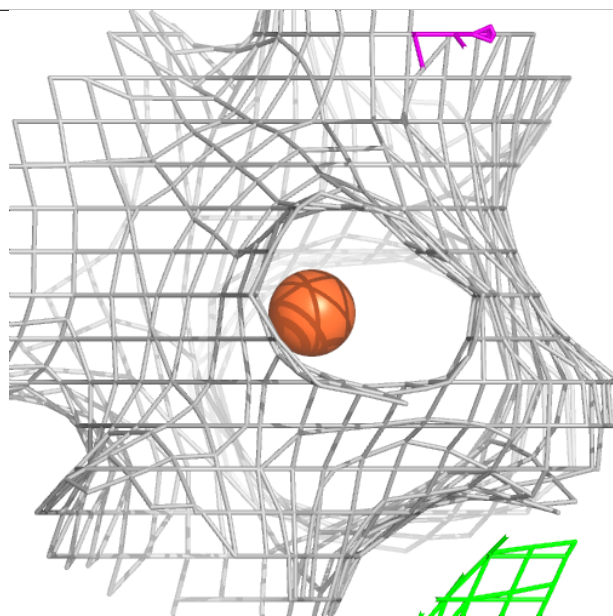
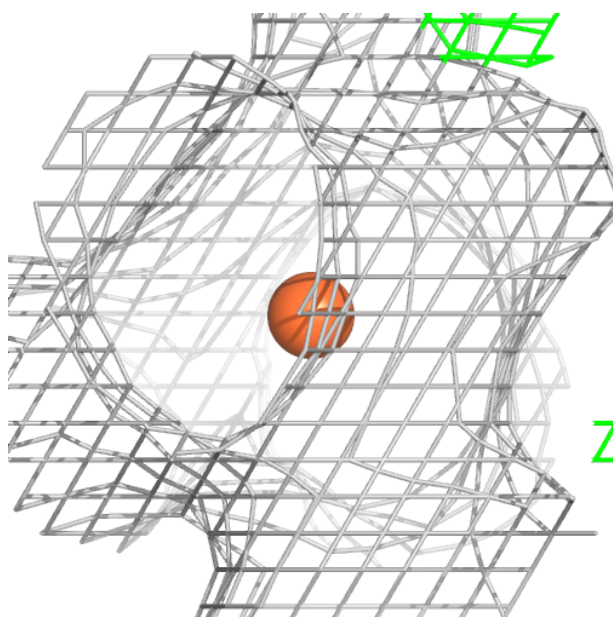
Electron density around FE2 B 601:

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



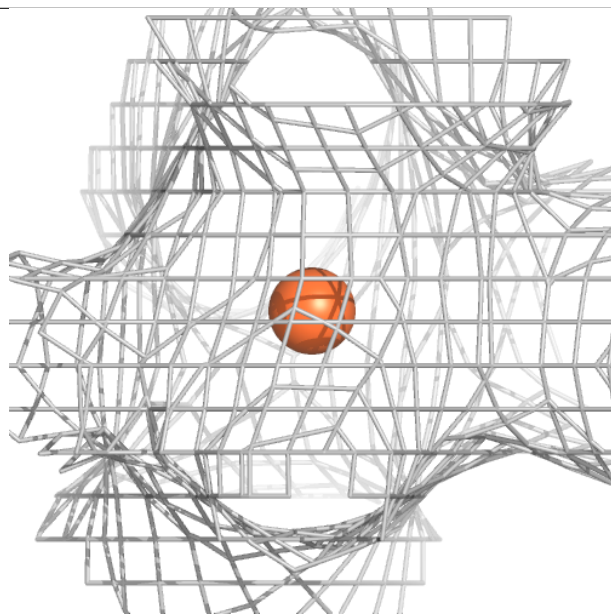
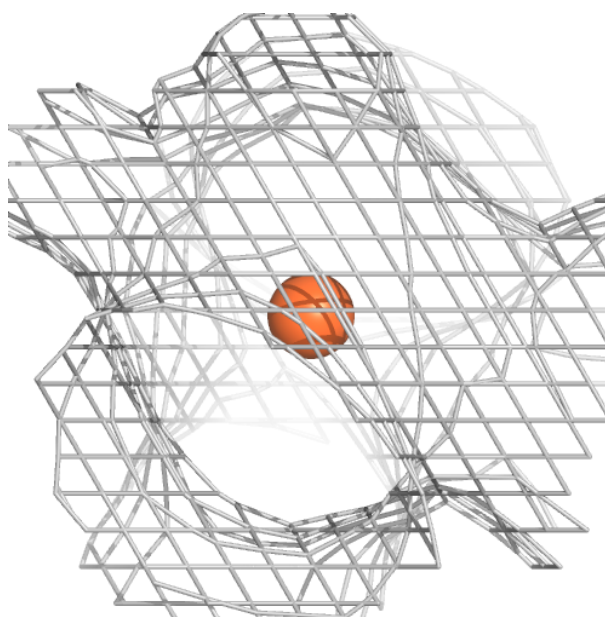
Electron density around FE2 C 601:

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



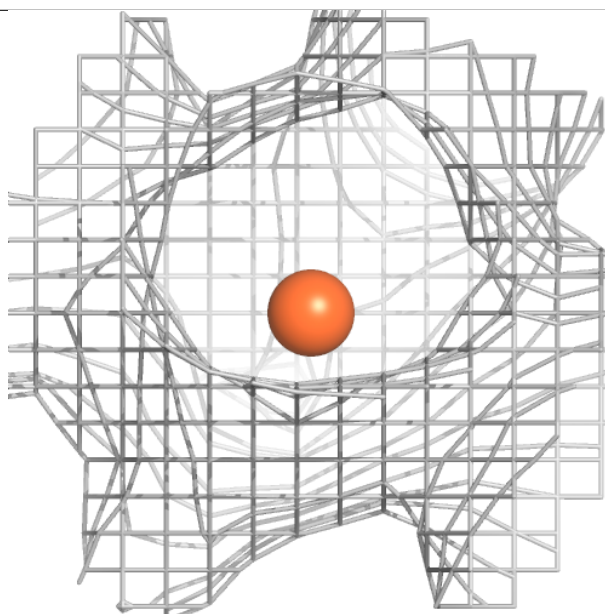
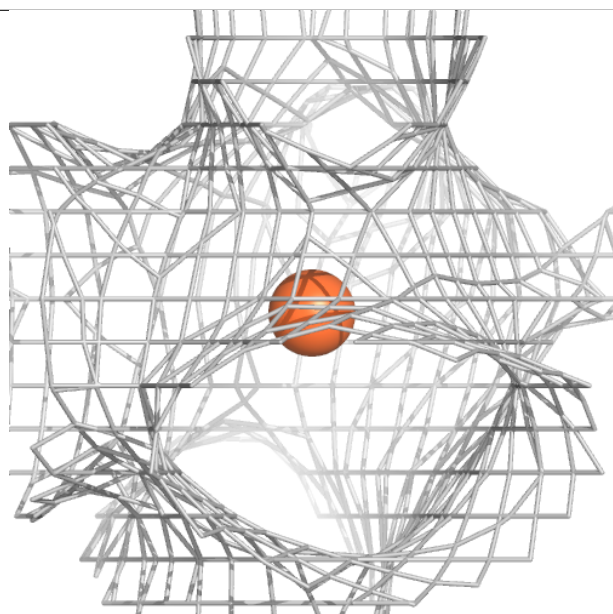
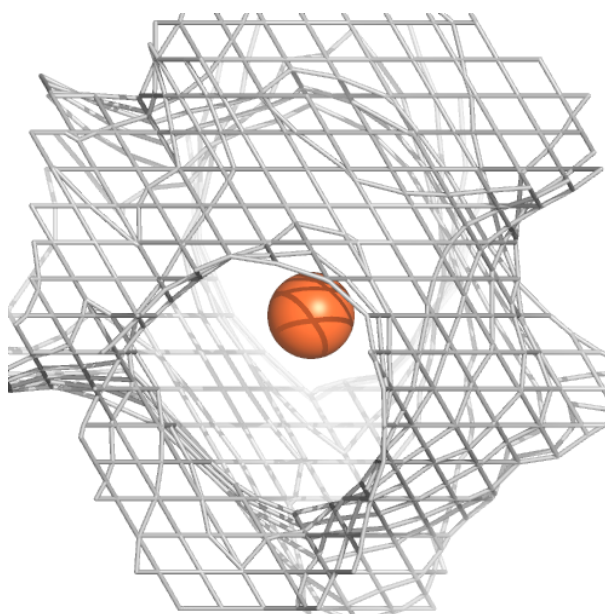
Electron density around FE2 D 601:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.