



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 7, 2026 – 03:16 PM JST

PDB ID : 27DQ / pdb_000027dq
Title : Crystal structure of HPO from Pseudomonas
Authors : Cheng, Z.Y.; Han, X.; Li, Q.; Wei, H.L.; Hu, H.Y.; Xu, P.; Liu, W.; Tang, H.Z.
Deposited on : 2026-05-27
Resolution : 2.56 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

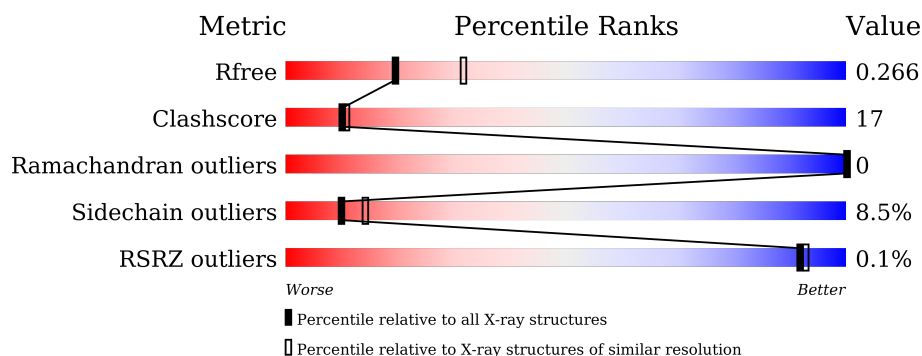
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	343	
1	B	343	
1	C	343	
1	D	343	
1	E	343	
1	F	343	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15099 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 2,5-DHP dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2526	1602	421	481	22			
1	B	333	Total	C	N	O	S	0	0	0
			2518	1593	424	479	22			
1	C	330	Total	C	N	O	S	0	0	0
			2520	1595	426	477	22			
1	D	332	Total	C	N	O	S	0	0	0
			2522	1600	422	478	22			
1	E	332	Total	C	N	O	S	0	0	0
			2492	1575	415	480	22			
1	F	332	Total	C	N	O	S	0	0	0
			2436	1545	400	470	21			

- Molecule 2 is FE (III) ION (CCD ID: FE) (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		
2	E	1	Total	Fe	0	0
			1	1		
2	F	1	Total	Fe	0	0
			1	1		

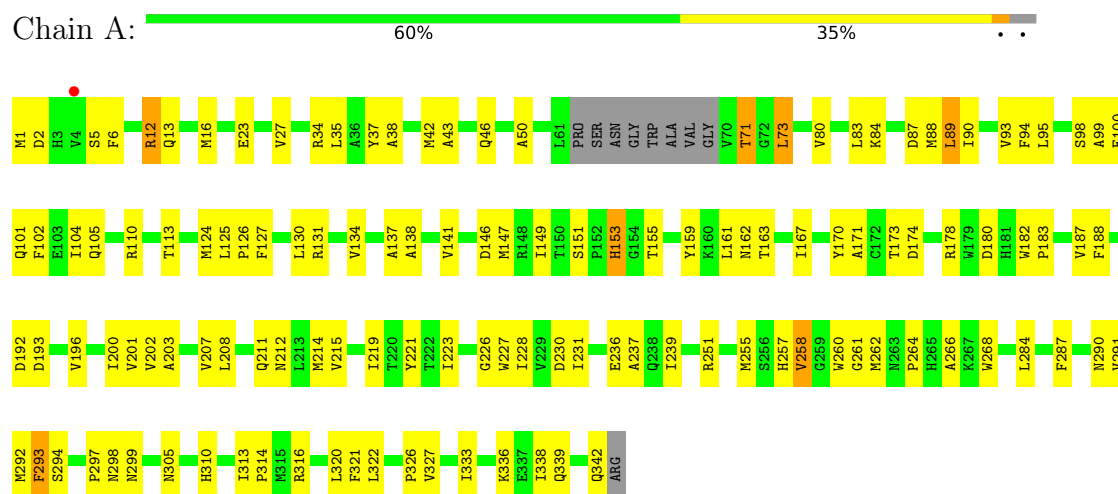
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total 23	O 23	0	0
3	B	13	Total 13	O 13	0	0
3	C	12	Total 12	O 12	0	0
3	D	19	Total 19	O 19	0	0
3	E	7	Total 7	O 7	0	0
3	F	5	Total 5	O 5	0	0

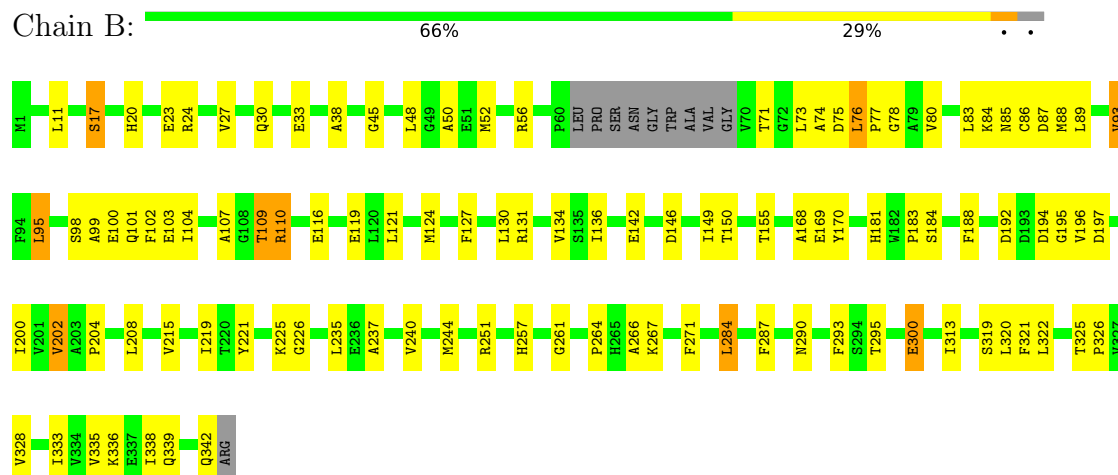
3 Residue-property plots

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: 2,5-DHP dioxygenase

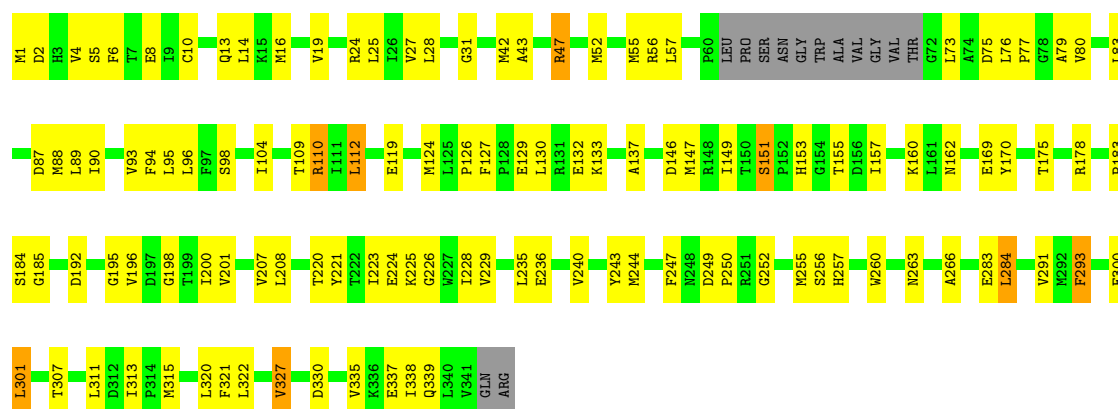


• Molecule 1: 2,5-DHP dioxygenase



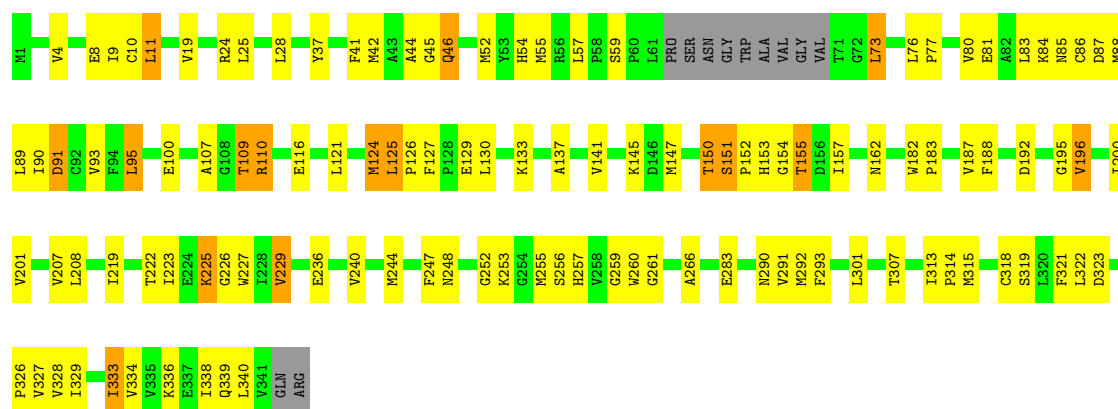
• Molecule 1: 2,5-DHP dioxygenase





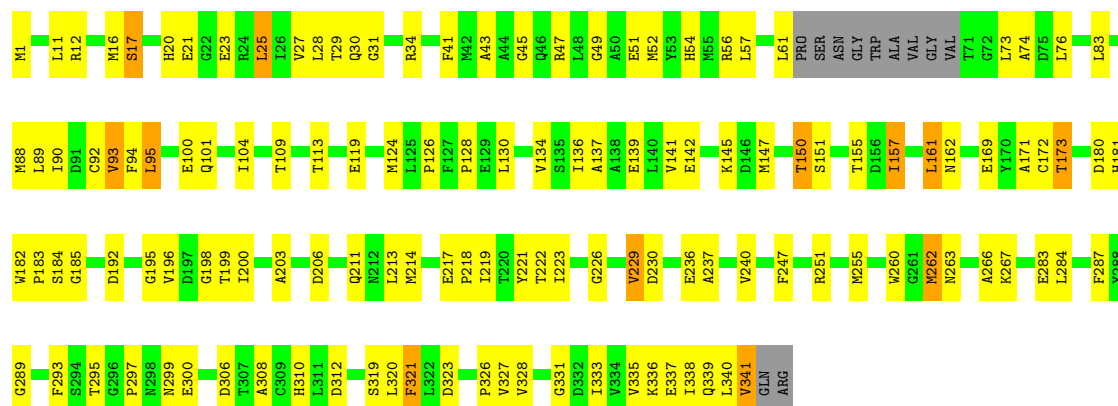
• Molecule 1: 2,5-DHP dioxygenase

Chain D: 62% 30% 5%



• Molecule 1: 2,5-DHP dioxygenase

Chain E: 59% 35%



• Molecule 1: 2,5-DHP dioxygenase

Chain F: 58% 36%

M280	G281	M282	E283	L284	R285	S286	F287	Y288	G289	N290	V291	M292	F293	S294	T295	G296	P297	N298	N299	N305	D306	T307	A308	C309	H310	M315	G318	S319	L320	F321	L322	V327	V328	I333	V334	V335	K336	E337	I338	V341	GLN	ARG						
W1	D2	H3	V4	E8	L11	R12	Q13	L14	K15	M16	V19	E23	R24	L25	I26	V27	L28	T29	D39	G45	M52	L57	L61	P62	SER	ASN	GLY	TRP	ALA	VAL	GLY	VAL	THR	G72	L73	A74	D75	L76	K84	M85	C86	D87	M88	L89	I90	D91	C92	V93
S98	Q101	A106	A107	G108	T109	L112	E116	L121	M124	L125	P126	F127	F128	E129	L130	R131	E132	K133	I136	A137	E142	K145	D146	I149	T150	S151	T155	D156	I157	T158	Y159	K160	L161	T166	E169	Y170	A171	C172	R178	W179	D180	H181	W182	P183	S184			
G185	F186	V187	F188	T189	D193	V196	D197	G198	T199	I200	A203	D206	V207	L208	Q211	V215	I219	T220	Y221	T222	I223	G226	P227	I228	G234	L235	E236	A237	V240	M244	F247	R251	G252	M255	G259	W260	G261	N263	A266	F271								

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.63Å 142.96Å 89.53Å 90.00° 107.72° 90.00°	Depositor
Resolution (Å)	28.14 – 2.56 28.14 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.1 (28.14-2.56) 96.2 (28.14-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.57Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.223 , 0.277 0.236 , 0.266	Depositor DCC
R_{free} test set	3380 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	63.8	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.059 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15099	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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: FE

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	0.50	0/2585	0.82	0/3521
1	B	0.62	0/2577	0.93	0/3511
1	C	0.61	0/2579	0.96	0/3508
1	D	0.54	0/2582	0.86	0/3515
1	E	0.71	0/2549	1.03	0/3475
1	F	0.61	0/2494	0.97	0/3409
All	All	0.60	0/15366	0.93	0/20939

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	2526	0	2420	84	0
1	B	2518	0	2406	77	0
1	C	2520	0	2434	86	0
1	D	2522	0	2424	88	0
1	E	2492	0	2374	87	0
1	F	2436	0	2268	93	0
2	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	23	0	0	1	0
3	B	13	0	0	0	0
3	C	12	0	0	0	0
3	D	19	0	0	1	0
3	E	7	0	0	1	0
3	F	5	0	0	0	0
All	All	15099	0	14326	509	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 17.

The worst 5 of 509 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:88:MET:HB2	1:C:110:ARG:HE	1.06	1.15
1:B:104:ILE:O	1:B:109:THR:HG23	1.55	1.07
1:E:73:LEU:HD12	1:E:95:LEU:HD21	1.35	1.01
1:B:74:ALA:HB2	1:B:100:GLU:OE1	1.63	0.99
1:B:169:GLU:HB3	1:B:184:SER:HB3	1.47	0.95

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	330/343 (96%)	319 (97%)	11 (3%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	329/343 (96%)	321 (98%)	8 (2%)	0	100	100
1	C	326/343 (95%)	317 (97%)	9 (3%)	0	100	100
1	D	328/343 (96%)	314 (96%)	14 (4%)	0	100	100
1	E	328/343 (96%)	317 (97%)	11 (3%)	0	100	100
1	F	328/343 (96%)	319 (97%)	9 (3%)	0	100	100
All	All	1969/2058 (96%)	1907 (97%)	62 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	267/285 (94%)	246 (92%)	21 (8%)	11	16
1	B	266/285 (93%)	247 (93%)	19 (7%)	13	19
1	C	269/285 (94%)	247 (92%)	22 (8%)	10	15
1	D	268/285 (94%)	242 (90%)	26 (10%)	8	10
1	E	263/285 (92%)	236 (90%)	27 (10%)	7	8
1	F	249/285 (87%)	229 (92%)	20 (8%)	11	16
All	All	1582/1710 (92%)	1447 (92%)	135 (8%)	10	14

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	11	LEU
1	F	93	VAL
1	F	293	PHE
1	C	175	THR
1	C	151	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	238	GLN
1	E	30	GLN
1	F	238	GLN
1	D	290	ASN
1	E	101	GLN

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 6 ligands modelled in this entry, 6 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	334/343 (97%)	-1.29	1 (0%) 90 91	47, 69, 87, 103	0
1	B	333/343 (97%)	-1.26	0 100 100	49, 69, 86, 102	0
1	C	330/343 (96%)	-1.24	0 100 100	42, 65, 86, 105	0
1	D	332/343 (96%)	-1.30	0 100 100	46, 67, 86, 101	0
1	E	332/343 (96%)	-1.24	0 100 100	48, 76, 99, 108	0
1	F	332/343 (96%)	-1.22	0 100 100	51, 83, 108, 120	0
All	All	1993/2058 (96%)	-1.26	1 (0%) 92 93	42, 71, 96, 120	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	VAL	2.3

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](#)

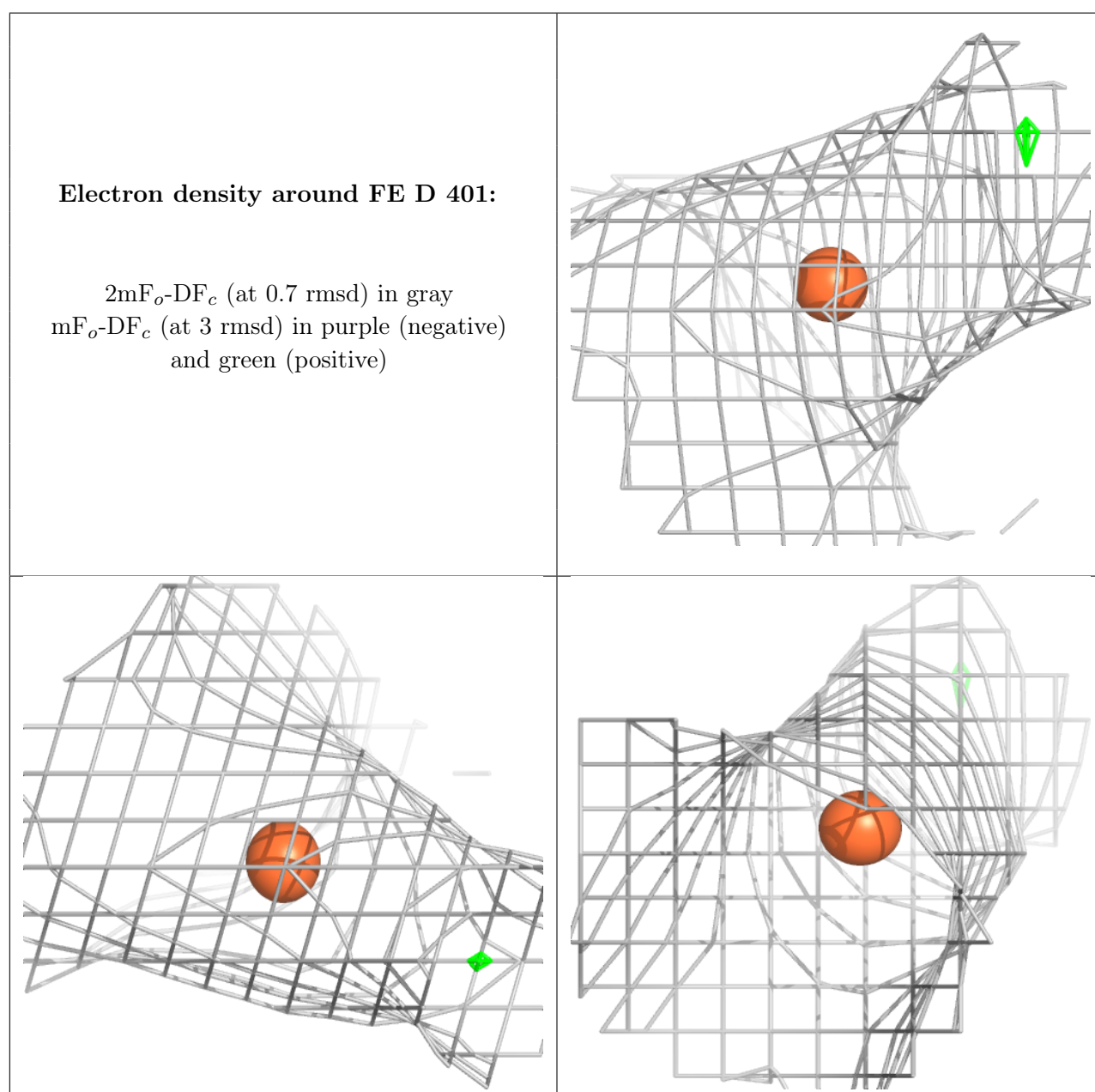
There are no oligosaccharides in this entry.

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.

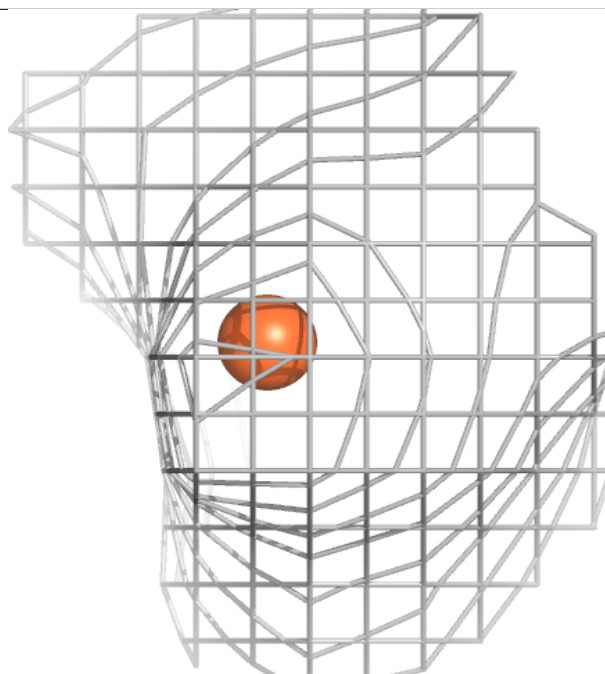
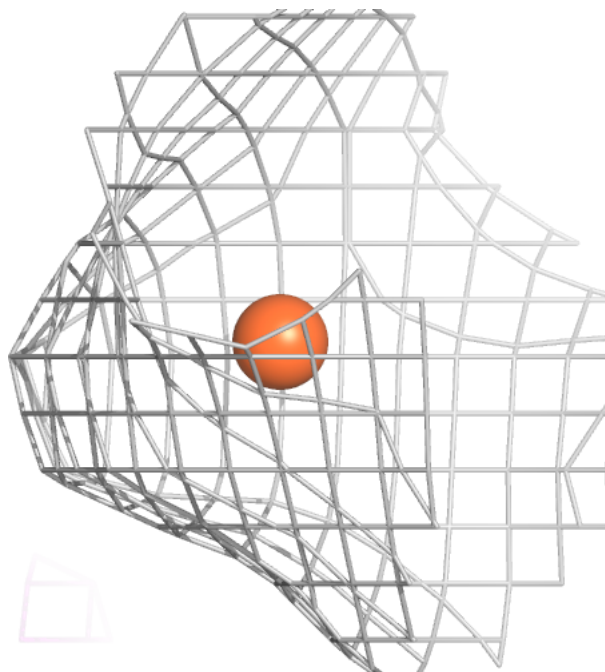
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FE	D	401	1/1	0.98	0.04	108,108,108,108	0
2	FE	B	401	1/1	0.99	0.02	157,157,157,157	0
2	FE	C	401	1/1	0.99	0.04	131,131,131,131	0
2	FE	A	401	1/1	0.99	0.03	121,121,121,121	0
2	FE	E	401	1/1	0.99	0.03	147,147,147,147	0
2	FE	F	401	1/1	0.99	0.03	160,160,160,160	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.



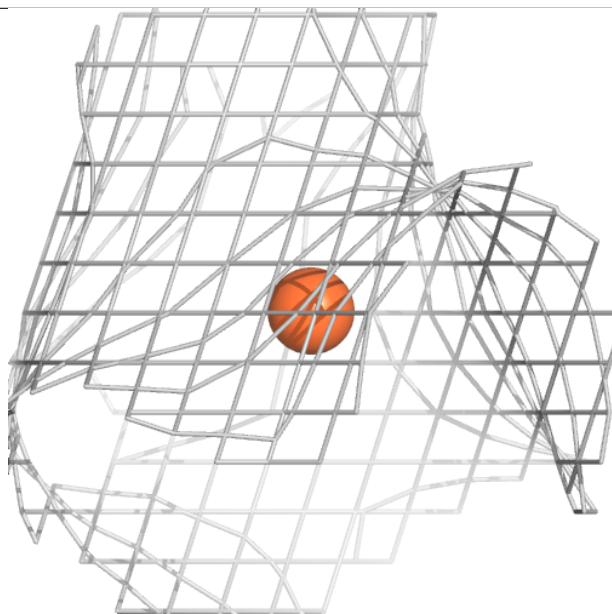
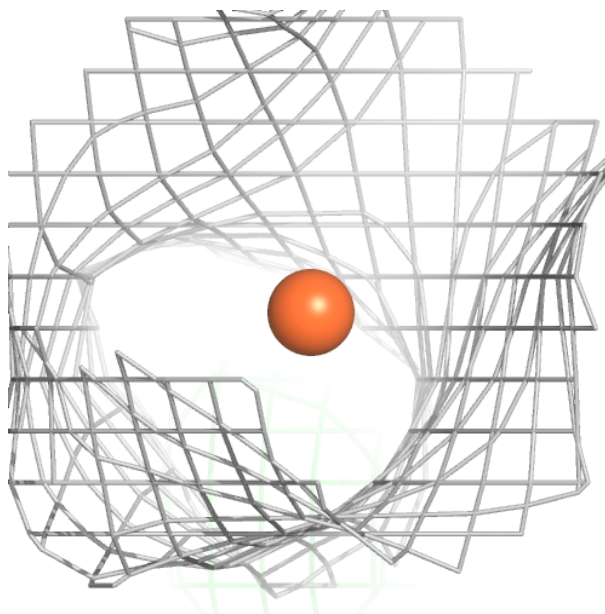
Electron density around FE B 401:

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



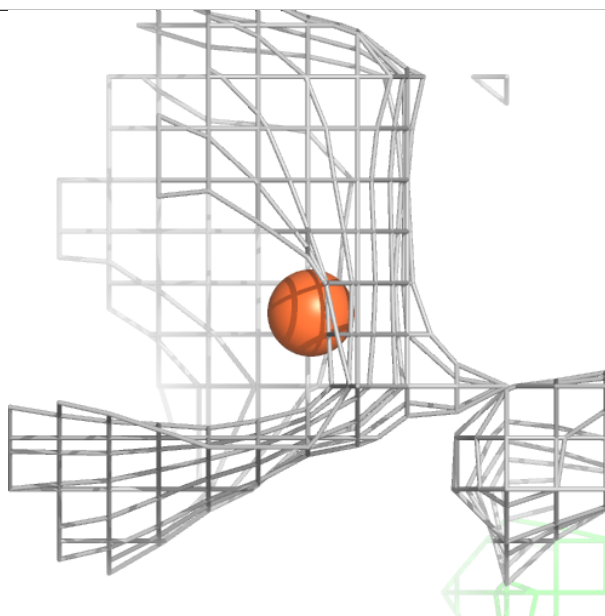
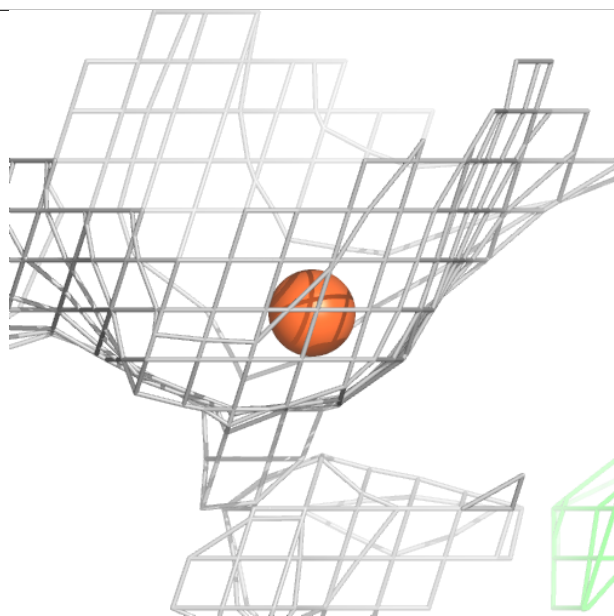
Electron density around FE C 401:

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



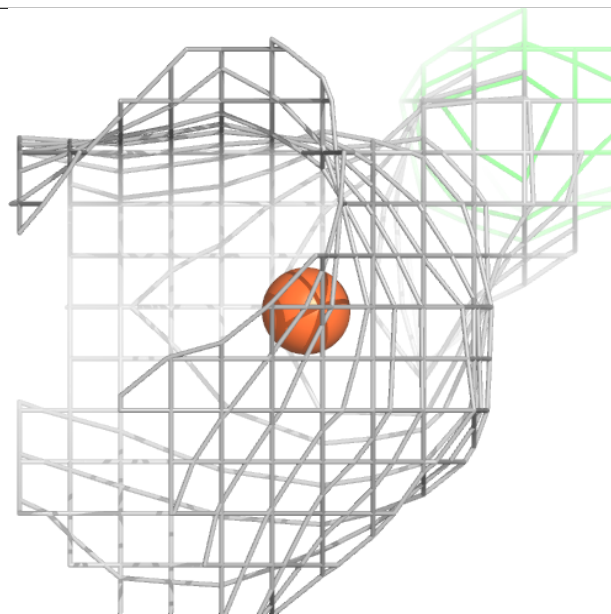
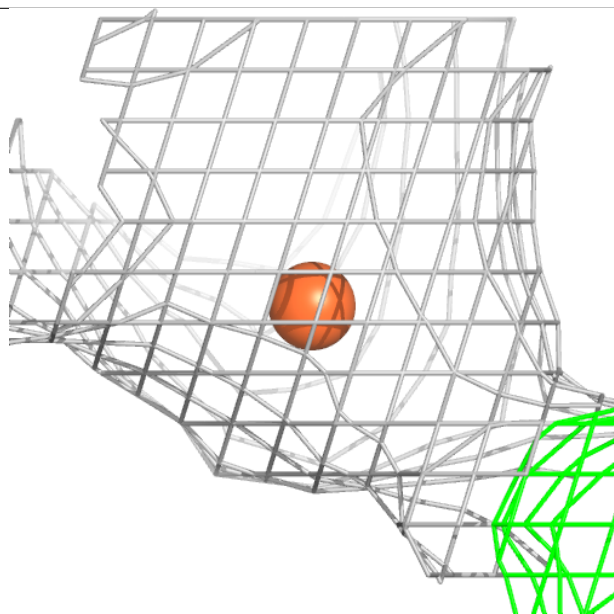
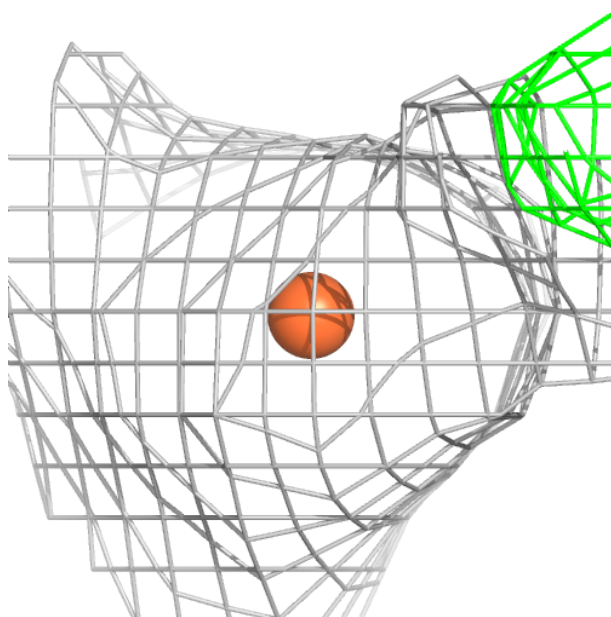
Electron density around FE A 401:

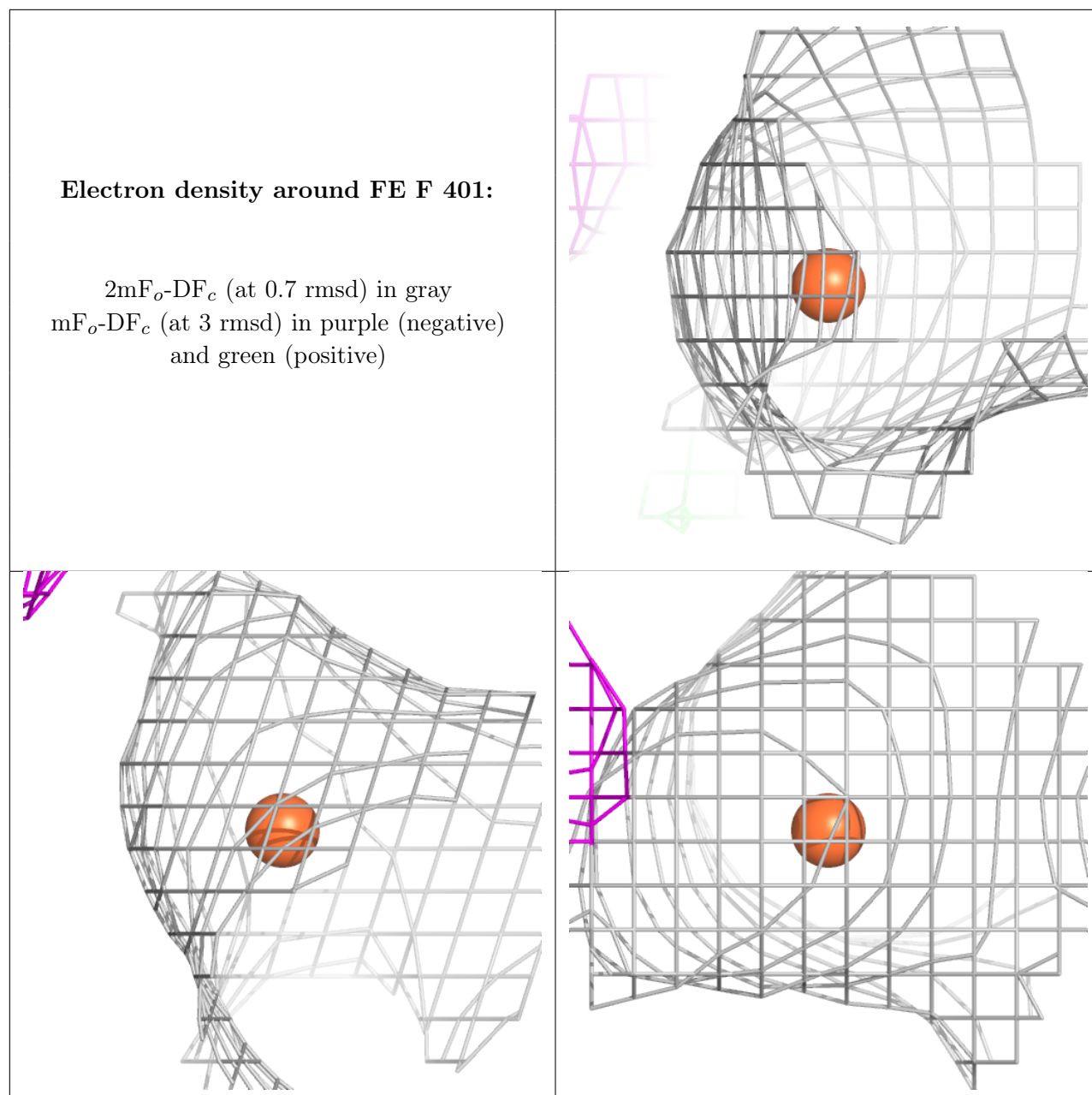
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE E 401:

$2mF_o-DF_c$ (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.