



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 01:07 AM UTC

PDB ID : 7OBW / pdb_00007obw
Title : Crystal structure of the ferric enterobactin receptor (PfeA) from *Pseudomonas aeruginosa* in complex with TCV-L6
Authors : Moynie, L.; Naismith, J.H.
Deposited on : 2021-04-23
Resolution : 2.66 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	:	FAILED
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

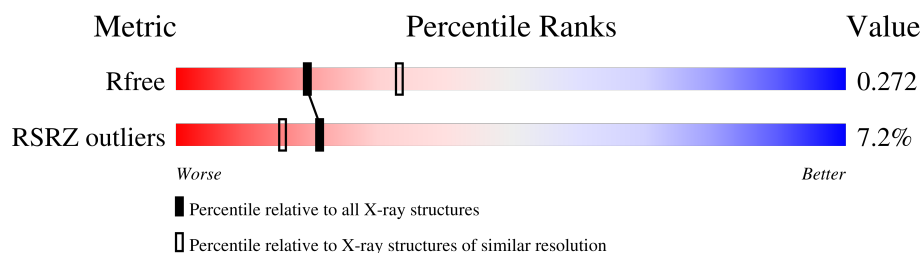
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1110 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

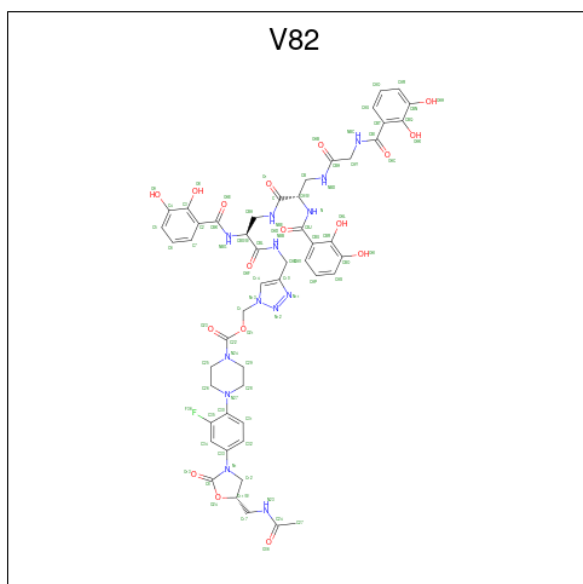
There are 4 unique types of molecules in this entry. The entry contains 5496 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ferric enterobactin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	697	Total	C	N	O	S	0	0	0
			5363	3318	962	1072	11			

- Molecule 2 is [4-[[[(2 {S})-2-[[2,3-bis(oxidanyl)phenyl]carbonylamino]-3-[[[(2 {S})-2-[[2,3-bis(oxidanyl)phenyl]carbonylamino]-3-[2-[[2,3-bis(oxidanyl)phenyl]carbonylamino]ethanoylamino]propanoyl]amino]propanoyl]amino]methyl]-1,2,3-triazol-1-yl]methyl 4-[4-[(5 {S})-5-(acetamidomethyl)-2-oxidanylidene-1,3-oxazolidin-3-yl]-2-fluoranyl-phenyl]piperazine-1-carboxylate (CCD ID: V82) (formula: C₅₀H₅₄FN₁₃O₁₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	N	O		0	0
			49	31	6	12			
2	AAA	1	Total	C	F	N	O	0	0
			81	50	1	13	17		

- 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	AAA	2	Total 2	Fe 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total 1	O 1	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	87.41Å 157.11Å 77.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.43 – 2.66 58.43 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.8 (58.43-2.66) 99.9 (58.43-2.66)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.231 , 0.277 0.232 , 0.272	Depositor DCC
R_{free} test set	1539 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	81.7	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5496	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 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	V82	AAA	802	3	87,87,87	1.46	5 (5%)	118,122,122	1.59	21 (17%)
2	V82	AAA	801	3	51,51,87	0.47	0	67,70,122	0.75	0

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	V82	AAA	802	3	-	11/70/92/92	0/7/7/7
2	V82	AAA	801	3	-	5/46/46/92	0/3/3/7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	802	V82	O24-C8	7.55	1.46	1.35
2	AAA	802	V82	O21-C22	6.02	1.46	1.34
2	AAA	802	V82	N11-N12	5.79	1.41	1.32
2	AAA	802	V82	C8-N1	-3.46	1.32	1.36
2	AAA	802	V82	N13-N12	3.35	1.40	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	802	V82	O21-C22-N24	5.89	122.05	111.77
2	AAA	802	V82	C11-O24-C8	-4.56	106.46	110.10
2	AAA	802	V82	O21-C22-O23	-4.51	116.92	124.76
2	AAA	802	V82	C12-N1-C8	4.49	114.49	111.17
2	AAA	802	V82	C34-C35-C30	-3.70	120.08	123.35
2	AAA	802	V82	O24-C11-C12	3.58	107.96	104.50
2	AAA	802	V82	C2-CBK-NBG	3.54	124.34	116.67
2	AAA	802	V82	C28-C29-N24	-3.37	103.71	110.42
2	AAA	802	V82	C29-C28-N27	-3.30	103.85	110.78
2	AAA	802	V82	C28-N27-C26	3.17	118.71	111.57
2	AAA	802	V82	C31-C30-N27	-3.08	117.60	122.42
2	AAA	802	V82	C26-N27-C30	2.97	123.23	116.19
2	AAA	802	V82	C33-N1-C8	-2.93	122.91	125.98
2	AAA	802	V82	F36-C35-C30	2.83	121.07	118.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	802	V82	N13-N12-N11	-2.79	104.51	107.02
2	AAA	802	V82	OAE-CBK-C2	-2.70	116.08	121.03
2	AAA	802	V82	C1-O21-C22	2.66	120.14	115.76
2	AAA	802	V82	C35-C30-N27	2.44	123.27	120.42
2	AAA	802	V82	O24-C11-C17	2.35	111.79	109.13
2	AAA	802	V82	CAX-C10-N11	2.21	125.95	121.61
2	AAA	802	V82	CAX-C10-C14	-2.09	126.16	130.03

There are no chirality outliers.

All (16) torsion outliers are listed below:

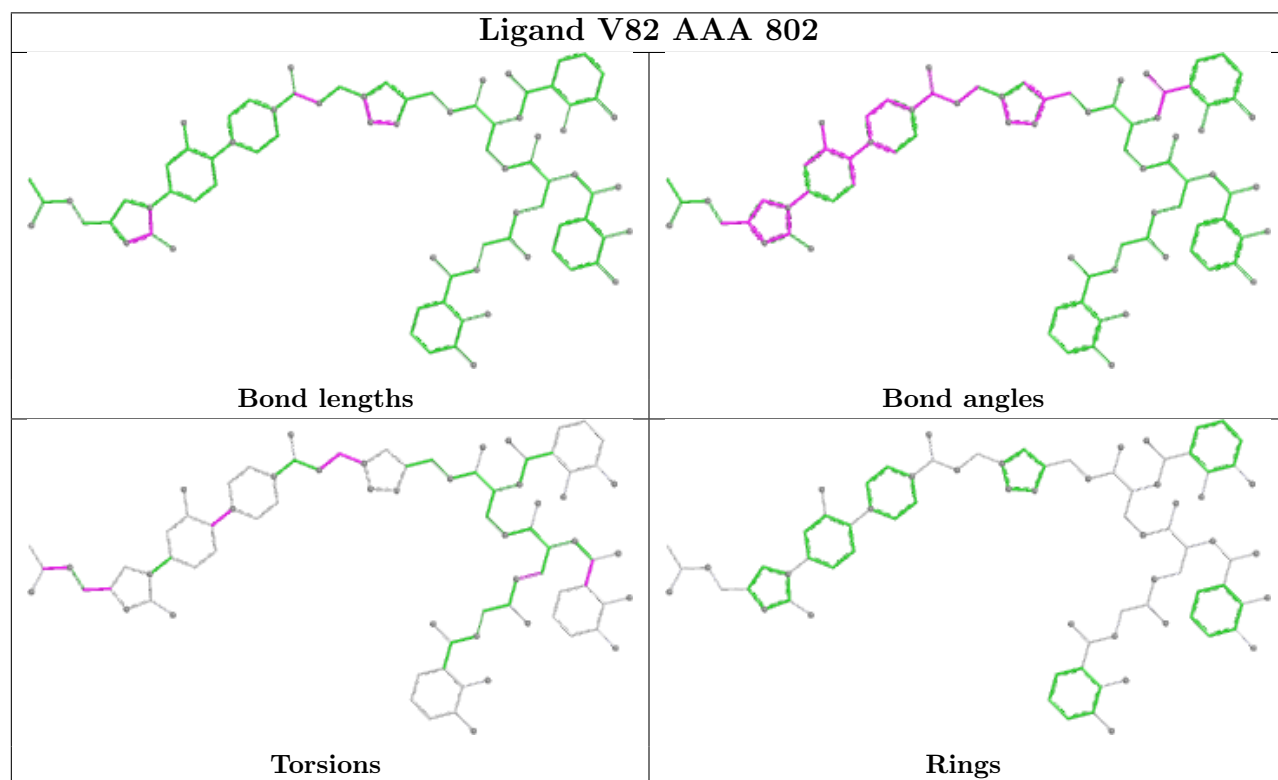
Mol	Chain	Res	Type	Atoms
2	AAA	802	V82	C12-C11-C17-N23
2	AAA	802	V82	O24-C11-C17-N23
2	AAA	802	V82	O21-C1-N13-C14
2	AAA	802	V82	O21-C1-N13-N12
2	AAA	802	V82	N13-C1-O21-C22
2	AAA	802	V82	C27-C24-N23-C17
2	AAA	802	V82	O36-C24-N23-C17
2	AAA	802	V82	C35-C30-N27-C28
2	AAA	801	V82	OAF-CBL-CBX-NBG
2	AAA	801	V82	NBC-CAY-CBH-OAB
2	AAA	801	V82	NBB-CBL-CBX-NBG
2	AAA	801	V82	NBC-CAY-CBH-NBD
2	AAA	802	V82	OAD-CBJ-CBU-CBR
2	AAA	802	V82	N-CBJ-CBU-CBR
2	AAA	802	V82	CA-CB-NBD-CBH
2	AAA	801	V82	OAF-CBL-CBX-CBA

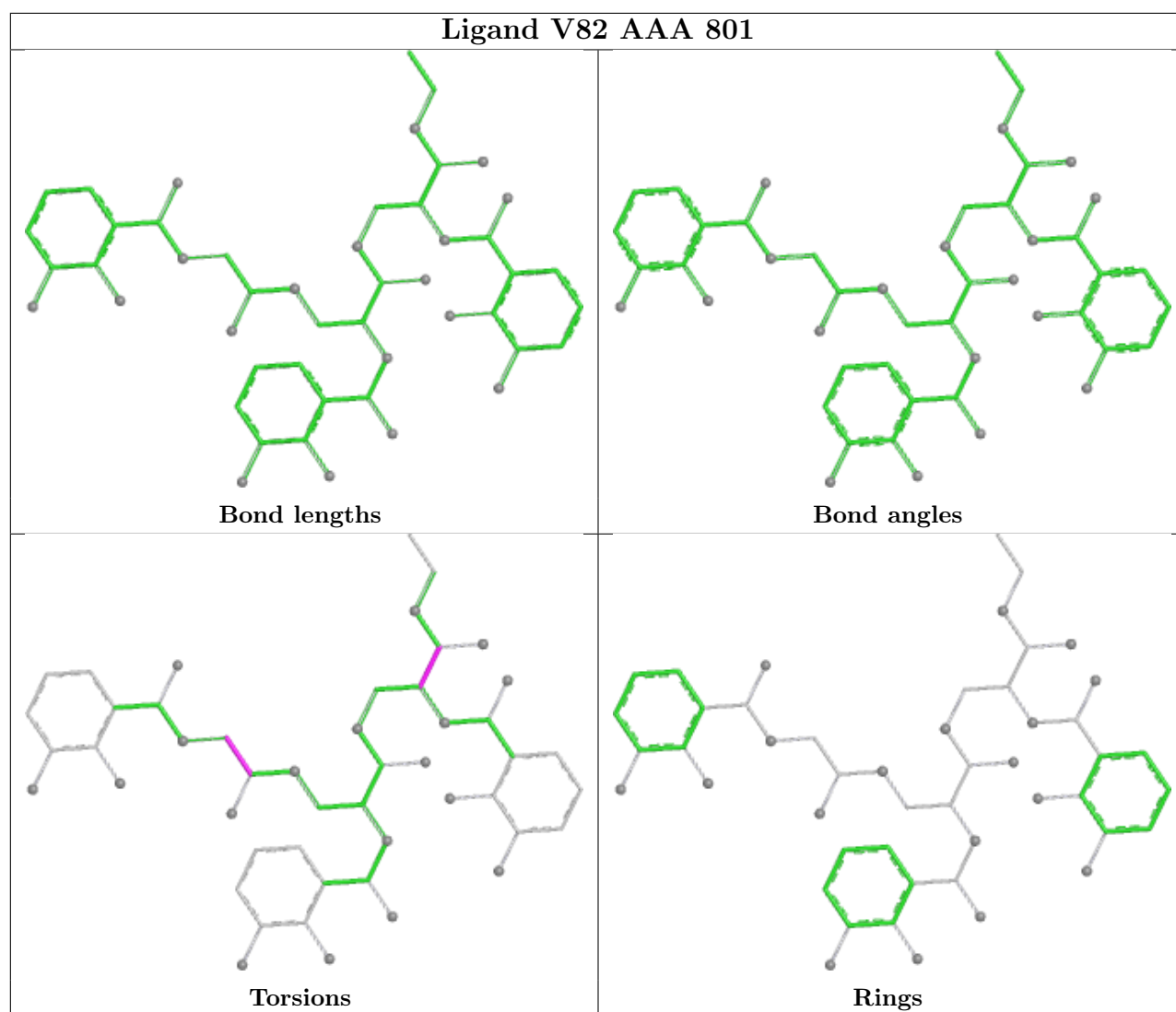
There are no ring outliers.

No monomer is involved in short contacts.

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.





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 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	AAA	697/721 (96%)	0.53	50 (7%) 21 16	60, 94, 131, 163	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	273	ASN	5.5
1	AAA	473	PRO	5.0
1	AAA	475	TYR	4.4
1	AAA	393	LEU	4.2
1	AAA	497	ASP	4.0
1	AAA	469	TYR	3.9
1	AAA	679	ASP	3.8
1	AAA	373	LYS	3.8
1	AAA	301	PHE	3.7
1	AAA	299	TRP	3.6
1	AAA	392	GLY	3.5
1	AAA	522	LEU	3.4
1	AAA	151	ALA	3.1
1	AAA	603	SER	3.1
1	AAA	353	LEU	2.8
1	AAA	181	LEU	2.8
1	AAA	472	ASN	2.8
1	AAA	60	THR	2.8
1	AAA	591	LEU	2.7
1	AAA	101	TYR	2.7
1	AAA	165	PHE	2.7
1	AAA	471	LEU	2.6
1	AAA	662	LEU	2.6
1	AAA	61	GLY	2.6
1	AAA	100	ARG	2.5
1	AAA	245	PRO	2.5
1	AAA	62	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	AAA	427	LEU	2.5
1	AAA	105	GLY	2.5
1	AAA	153	ALA	2.5
1	AAA	605	THR	2.5
1	AAA	604	VAL	2.4
1	AAA	467	ASN	2.4
1	AAA	517	GLY	2.4
1	AAA	275	VAL	2.4
1	AAA	563	LYS	2.3
1	AAA	144	VAL	2.3
1	AAA	185	LEU	2.3
1	AAA	197	ILE	2.3
1	AAA	449	LEU	2.3
1	AAA	243	LEU	2.2
1	AAA	355	LEU	2.2
1	AAA	468	LEU	2.2
1	AAA	439	TRP	2.1
1	AAA	391	PRO	2.1
1	AAA	293	VAL	2.1
1	AAA	490	SER	2.0
1	AAA	233	LYS	2.0
1	AAA	294	THR	2.0
1	AAA	713	PHE	2.0

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 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.

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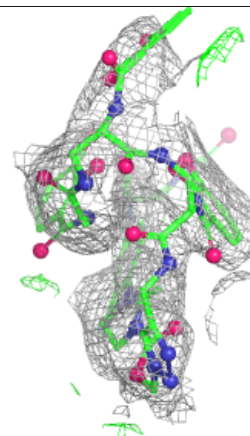
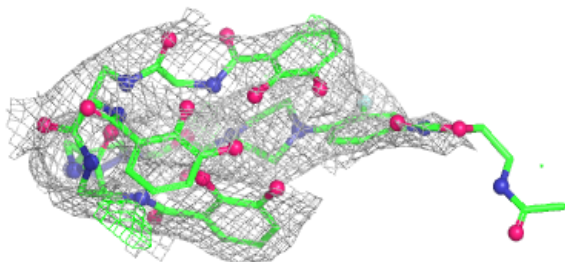
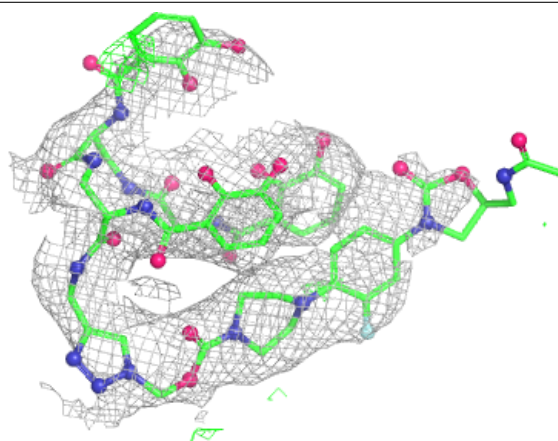
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	V82	AAA	802	81/81	0.78	0.13	102,150,190,201	0
2	V82	AAA	801	49/81	0.92	0.10	74,128,153,156	0
3	FE	AAA	804	1/1	0.96	0.07	145,145,145,145	0
3	FE	AAA	803	1/1	0.99	0.03	114,114,114,114	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.

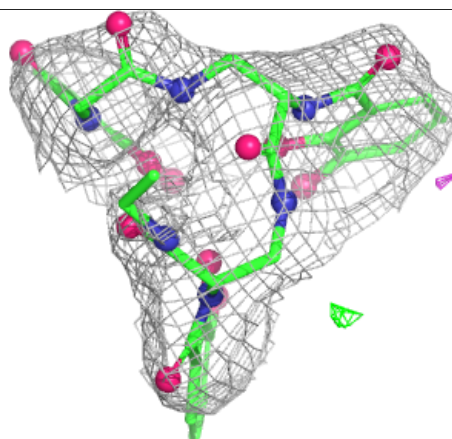
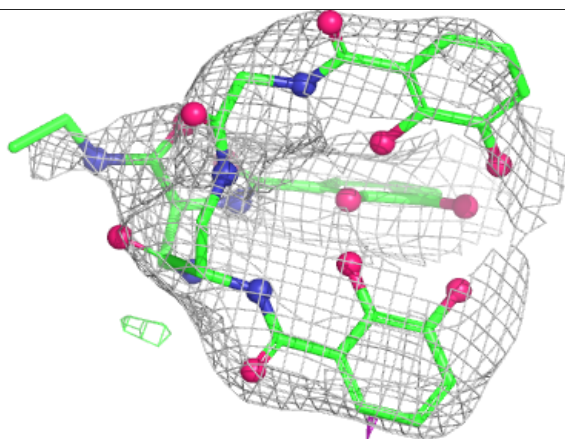
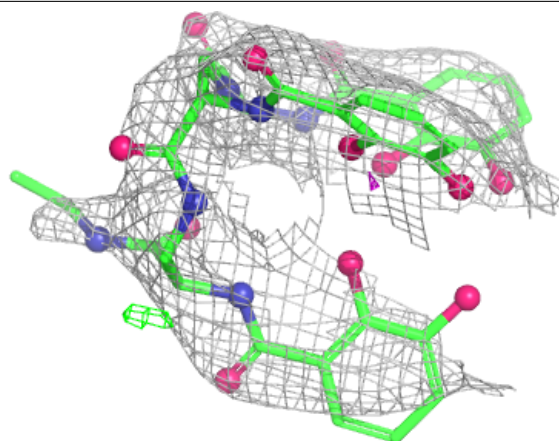
Electron density around V82 AAA 802:

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



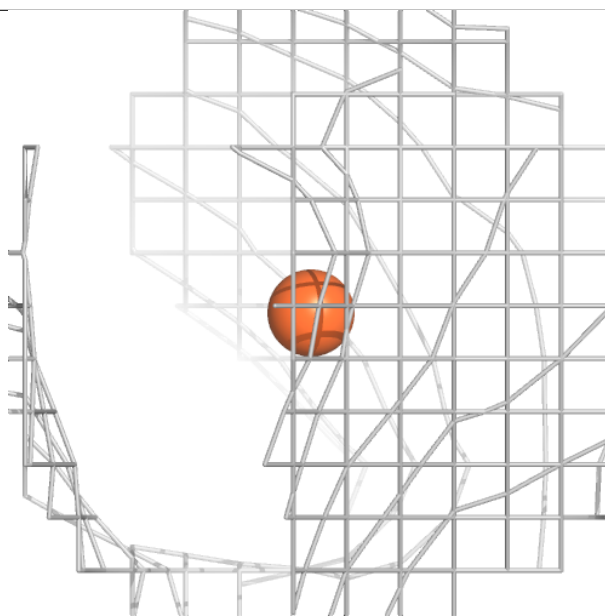
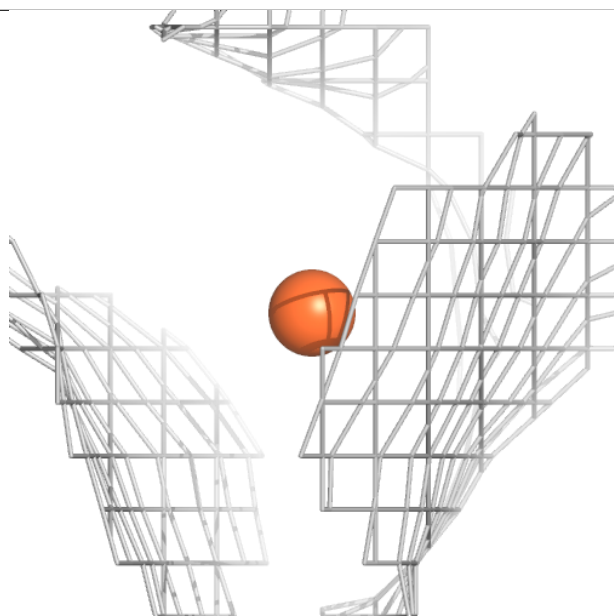
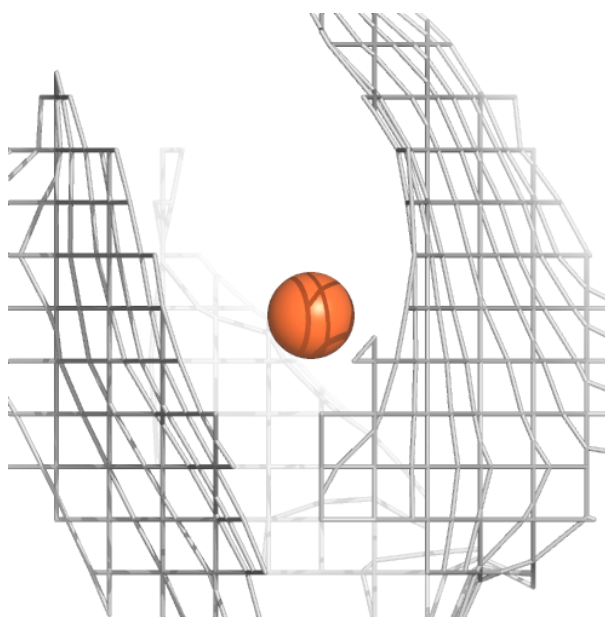
Electron density around V82 AAA 801:

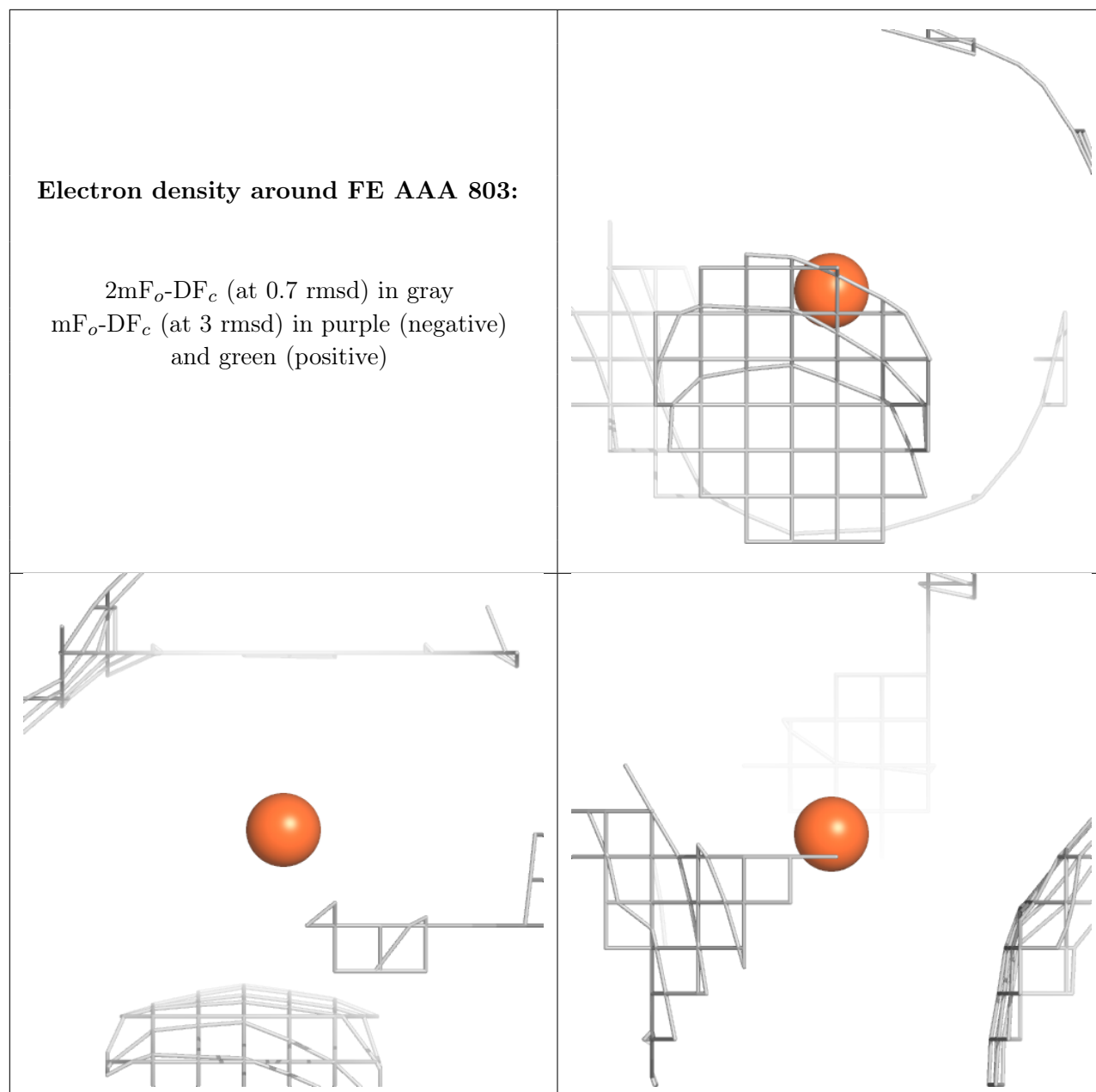
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE AAA 804:

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





5.5 Other polymers ⓘ

There are no such residues in this entry.