



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 23, 2020 – 04:14 PM JST

PDB ID : 7CY4
Title : Crystal Structure of CMD1 in apo form
Authors : Li, W.; Zhang, T.; Sun, M.; Ding, J.
Deposited on : 2020-09-03
Resolution : 2.20 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.16
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) : 2.16

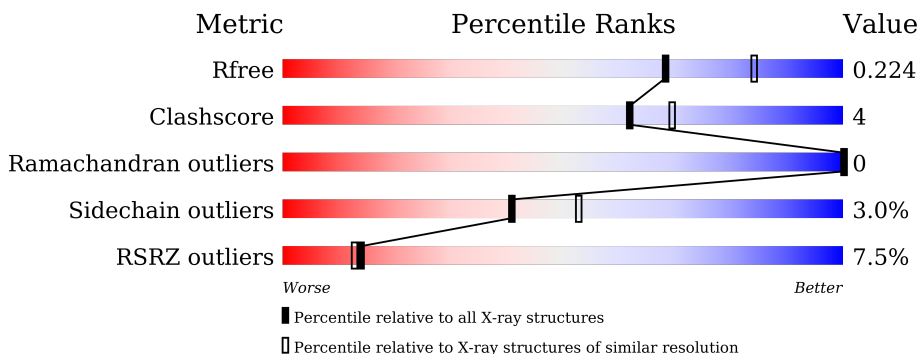
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	917	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6758 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 Maltodextrin-binding protein,5-methylcytosine-modifying enzyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	858	6521	4148	1117	1229	27	0	2	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-373	MET	-	initiating methionine	UNP A0A140NCD0
A	-291	ALA	ASP	engineered mutation	UNP A0A140NCD0
A	-290	ALA	LYS	engineered mutation	UNP A0A140NCD0
A	-201	ALA	GLU	engineered mutation	UNP A0A140NCD0
A	-200	ALA	ASN	engineered mutation	UNP A0A140NCD0
A	-134	ALA	LYS	engineered mutation	UNP A0A140NCD0
A	-14	ALA	GLU	engineered mutation	UNP A0A140NCD0
A	-11	ALA	LYS	engineered mutation	UNP A0A140NCD0
A	-10	ALA	ASP	engineered mutation	UNP A0A140NCD0
A	-6	ASN	-	linker	UNP A0A140NCD0
A	-5	ALA	-	linker	UNP A0A140NCD0
A	-4	ALA	-	linker	UNP A0A140NCD0
A	-3	ARG	-	linker	UNP A0A140NCD0
A	-2	ALA	-	linker	UNP A0A140NCD0
A	-1	ALA	-	linker	UNP A0A140NCD0
A	0	ALA	-	linker	UNP A0A140NCD0
A	533	ALA	-	expression tag	UNP A0A2K3D5Z7
A	534	ALA	-	expression tag	UNP A0A2K3D5Z7
A	535	ALA	-	expression tag	UNP A0A2K3D5Z7
A	536	LEU	-	expression tag	UNP A0A2K3D5Z7
A	537	GLU	-	expression tag	UNP A0A2K3D5Z7
A	538	HIS	-	expression tag	UNP A0A2K3D5Z7
A	539	HIS	-	expression tag	UNP A0A2K3D5Z7
A	540	HIS	-	expression tag	UNP A0A2K3D5Z7
A	541	HIS	-	expression tag	UNP A0A2K3D5Z7
A	542	HIS	-	expression tag	UNP A0A2K3D5Z7

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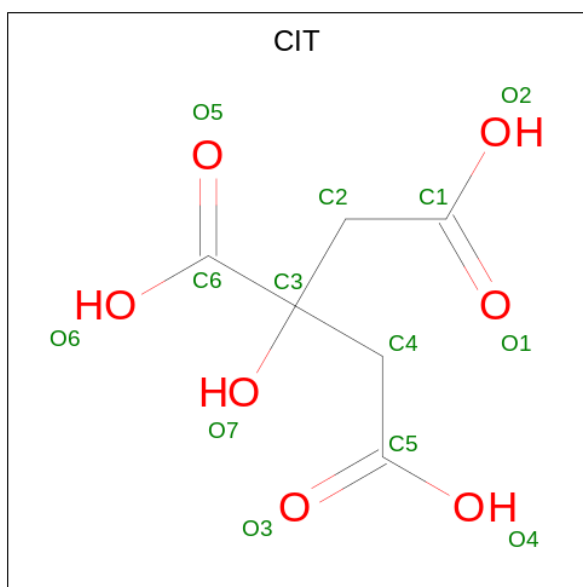
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Chain	Residue	Modelled	Actual	Comment	Reference
A	543	HIS	-	expression tag	UNP A0A2K3D5Z7

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

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

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0

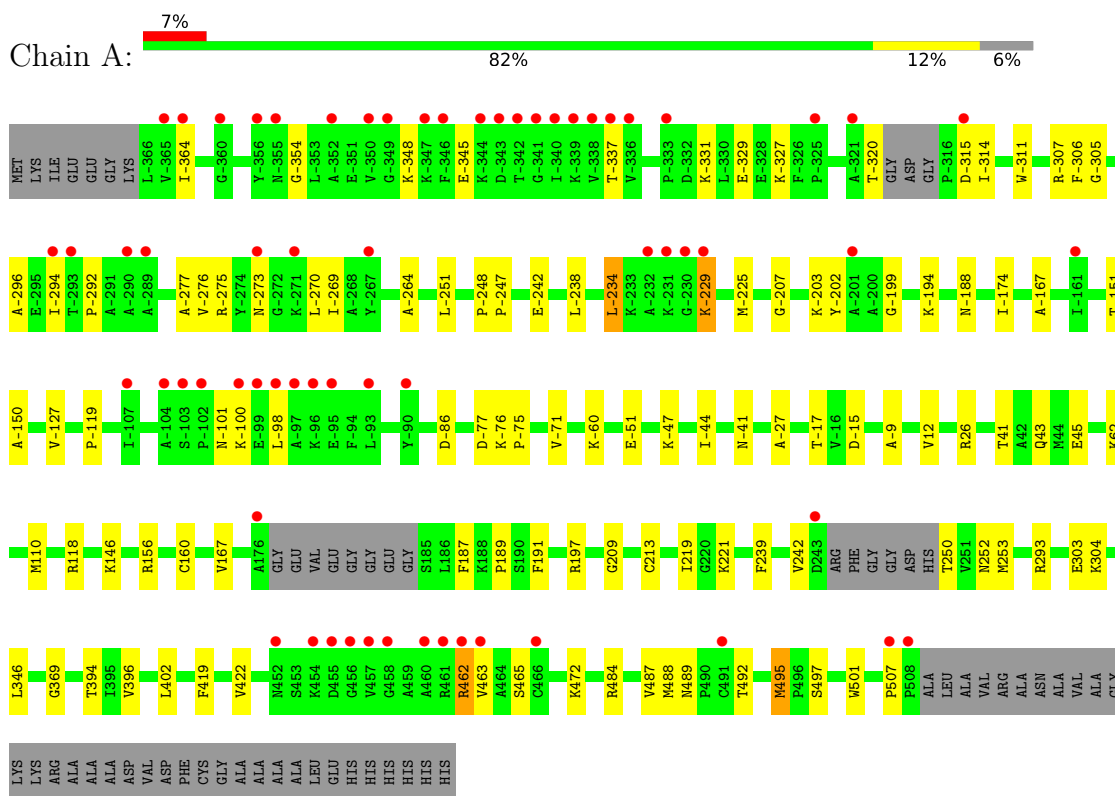
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	223	Total O 223 223	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: Maltodextrin-binding protein,5-methylcytosine-modifying enzyme 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.68Å 123.57Å 64.21Å 90.00° 103.16° 90.00°	Depositor
Resolution (Å)	47.77 – 2.20 47.77 – 2.20	Depositor EDS
% Data completeness (in resolution range)	80.0 (47.77-2.20) 79.7 (47.77-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.180 , 0.223 0.180 , 0.224	Depositor DCC
R_{free} test set	2000 reflections (4.19%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtrriage
Anisotropy	0.053	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6758	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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, CIT

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	0.48	0/6667	0.59	0/9068

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	6521	0	6463	57	0
2	A	1	0	0	0	0
3	A	13	0	5	0	0
4	A	223	0	0	1	0
All	All	6758	0	6468	57	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 4.

All (57) 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:A:-364:ILE:HG12	1:A:-314:ILE:HB	1.47	0.96
1:A:-277:ALA:HA	1:A:-44:ILE:HD11	1.65	0.77
1:A:-329:GLU:HG3	1:A:-311:TRP:CZ2	2.29	0.68
1:A:-348:LYS:NZ	1:A:-345:GLU:OE1	2.28	0.66
1:A:-234:LEU:HD12	1:A:-229:LYS:HB2	1.81	0.63
1:A:110:MET:HE1	1:A:209:GLY:HA2	1.81	0.61
1:A:-247:PRO:HB3	1:A:-242:GLU:HG3	1.82	0.61
1:A:484:ARG:HD2	1:A:488:MET:HE1	1.83	0.61
1:A:-101:ASN:HB3	1:A:-98:LEU:HD11	1.83	0.59
1:A:-225:MET:HB2	1:A:-151:THR:HG21	1.85	0.59
1:A:-174:ILE:HG21	1:A:-167:ALA:HB2	1.83	0.58
1:A:-17:THR:HG22	1:A:-15:ASP:N	2.19	0.58
1:A:-354:GLY:N	1:A:-77:ASP:OD2	2.35	0.57
1:A:242:VAL:O	1:A:250:THR:HB	2.05	0.57
1:A:12:VAL:HG21	1:A:487:VAL:HG11	1.89	0.55
1:A:-294:ILE:HG22	1:A:-292:PRO:HD3	1.89	0.55
1:A:-277:ALA:CA	1:A:-44:ILE:HD11	2.35	0.55
1:A:-305:GLY:HA3	1:A:-41:ASN:O	2.09	0.53
1:A:197:ARG:NH2	1:A:507:PRO:O	2.41	0.52
1:A:-251:LEU:CD2	1:A:-248:PRO:HA	2.40	0.52
1:A:-329:GLU:HB3	1:A:-307:ARG:NH1	2.25	0.52
1:A:-364:ILE:CG1	1:A:-314:ILE:HB	2.30	0.50
1:A:-119:PRO:HB3	1:A:-47:LYS:HD3	1.94	0.49
1:A:187:PHE:HB3	1:A:501:TRP:CZ2	2.48	0.49
1:A:-202:TYR:OH	1:A:-199:GLY:HA2	2.11	0.49
1:A:-17:THR:HG22	1:A:-15:ASP:H	1.77	0.49
1:A:41:THR:O	1:A:45:GLU:HG2	2.12	0.49
1:A:-251:LEU:HD21	1:A:-248:PRO:HA	1.95	0.48
1:A:369:GLY:HA3	1:A:402:LEU:HG	1.95	0.47
1:A:-251:LEU:HD12	1:A:-150:ALA:HB1	1.96	0.47
1:A:-364:ILE:HG12	1:A:-314:ILE:CB	2.32	0.47
1:A:239:PHE:HB3	1:A:252:ASN:HB3	1.97	0.47
1:A:-127:VAL:HB	1:A:-51:GLU:OE1	2.15	0.47
1:A:419:PHE:HB3	1:A:495:MET:HE1	1.98	0.46
1:A:242:VAL:HG21	1:A:253:MET:HG3	1.98	0.46
1:A:-207:GLY:HA2	1:A:-188:ASN:HD21	1.80	0.45
1:A:-275:ARG:HG3	1:A:-270:LEU:HD12	1.99	0.45
1:A:-276:VAL:O	1:A:-269:ILE:HG13	2.17	0.45
1:A:-76:LYS:HG3	1:A:-75:PRO:HD2	2.00	0.44
1:A:489:ASN:HB3	1:A:492:THR:OG1	2.18	0.43
1:A:-296:ALA:HB2	1:A:-100:LYS:HE3	2.00	0.43
1:A:394:THR:HG21	1:A:497:SER:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-331:LYS:HE3	1:A:-327:LYS:HD2	2.01	0.43
1:A:419:PHE:HA	1:A:422:VAL:HG12	2.01	0.43
1:A:-203:LYS:HA	1:A:-203:LYS:HD3	1.77	0.42
1:A:-306:PHE:HB3	1:A:-269:ILE:HD13	2.01	0.42
1:A:-194:LYS:HE3	1:A:-194:LYS:HB2	1.89	0.42
1:A:62:LYS:HG3	1:A:160:CYS:HB2	2.01	0.42
1:A:167:VAL:HG23	1:A:213[B]:CYS:SG	2.60	0.42
1:A:43:GLN:HG3	1:A:118:ARG:HH22	1.85	0.41
1:A:-264:ALA:HA	1:A:-71:VAL:HA	2.02	0.41
1:A:462:ARG:HG2	1:A:463:VAL:N	2.36	0.41
1:A:189:PRO:HG2	1:A:191:PHE:CE2	2.56	0.41
1:A:-27:ALA:HB2	1:A:-9:ALA:HB2	2.02	0.40
1:A:-348:LYS:HA	1:A:-348:LYS:HD2	1.82	0.40
1:A:346:LEU:HG	1:A:396:VAL:HG22	2.03	0.40
1:A:293:ARG:NH1	4:A:720:HOH:O	2.55	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	852/917 (93%)	833 (98%)	19 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	671/711 (94%)	651 (97%)	20 (3%)	41 53

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-337	THR
1	A	-320	THR
1	A	-315	ASP
1	A	-273	ASN
1	A	-238	LEU
1	A	-234	LEU
1	A	-229	LYS
1	A	-86	ASP
1	A	-60	LYS
1	A	26	ARG
1	A	146	LYS
1	A	156	ARG
1	A	219	ILE
1	A	221	LYS
1	A	303	GLU
1	A	304	LYS
1	A	462	ARG
1	A	465	SER
1	A	472	LYS
1	A	495	MET

Sometimes 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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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
3	CIT	A	602	-	3,12,12	0.61	0	3,17,17	0.99	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CIT	A	602	-	-	6/6/16/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	CIT	C1-C2-C3-O7
3	A	602	CIT	C1-C2-C3-C4
3	A	602	CIT	C1-C2-C3-C6
3	A	602	CIT	C2-C3-C4-C5
3	A	602	CIT	O7-C3-C4-C5
3	A	602	CIT	C6-C3-C4-C5

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	858/917 (93%)	0.17	64 (7%) 14 13	17, 49, 109, 152	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-340	ILE	7.5
1	A	-321	ALA	7.4
1	A	-232	ALA	5.8
1	A	-98	LEU	5.6
1	A	-346	PHE	5.2
1	A	-107	ILE	4.9
1	A	176	ALA	4.7
1	A	-365	VAL	4.2
1	A	-100	LYS	4.0
1	A	-336	VAL	4.0
1	A	-347	LYS	3.9
1	A	-95	GLU	3.8
1	A	457	VAL	3.7
1	A	-103	SER	3.7
1	A	-315	ASP	3.6
1	A	-293	THR	3.6
1	A	-338	VAL	3.6
1	A	-342	THR	3.6
1	A	462	ARG	3.5
1	A	-337	THR	3.5
1	A	-294	ILE	3.5
1	A	-360	GLY	3.4
1	A	-99	GLU	3.4
1	A	508	PRO	3.4
1	A	-96	LYS	3.3
1	A	463	VAL	3.2
1	A	456	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	-289	ALA	3.1
1	A	243	ASP	3.1
1	A	-343	ASP	3.1
1	A	-290	ALA	3.0
1	A	-341	GLY	3.0
1	A	-350	VAL	3.0
1	A	-230	GLY	3.0
1	A	-339	LYS	2.9
1	A	491	CYS	2.9
1	A	-344	LYS	2.9
1	A	460	ALA	2.8
1	A	-267	TYR	2.8
1	A	-356	TYR	2.7
1	A	-349	GLY	2.7
1	A	-231	LYS	2.7
1	A	-97	ALA	2.7
1	A	-93	LEU	2.6
1	A	-364	ILE	2.5
1	A	-325	PRO	2.5
1	A	461	ARG	2.5
1	A	452	ASN	2.5
1	A	-161	ILE	2.5
1	A	507	PRO	2.4
1	A	-90	TYR	2.4
1	A	-104	ALA	2.4
1	A	-355	ASN	2.4
1	A	-229	LYS	2.3
1	A	-273	ASN	2.3
1	A	-102	PRO	2.3
1	A	455	ASP	2.3
1	A	-201	ALA	2.3
1	A	454	LYS	2.2
1	A	-271	LYS	2.2
1	A	-333	PRO	2.1
1	A	-352	ALA	2.1
1	A	458	GLY	2.1
1	A	466	CYS	2.0

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

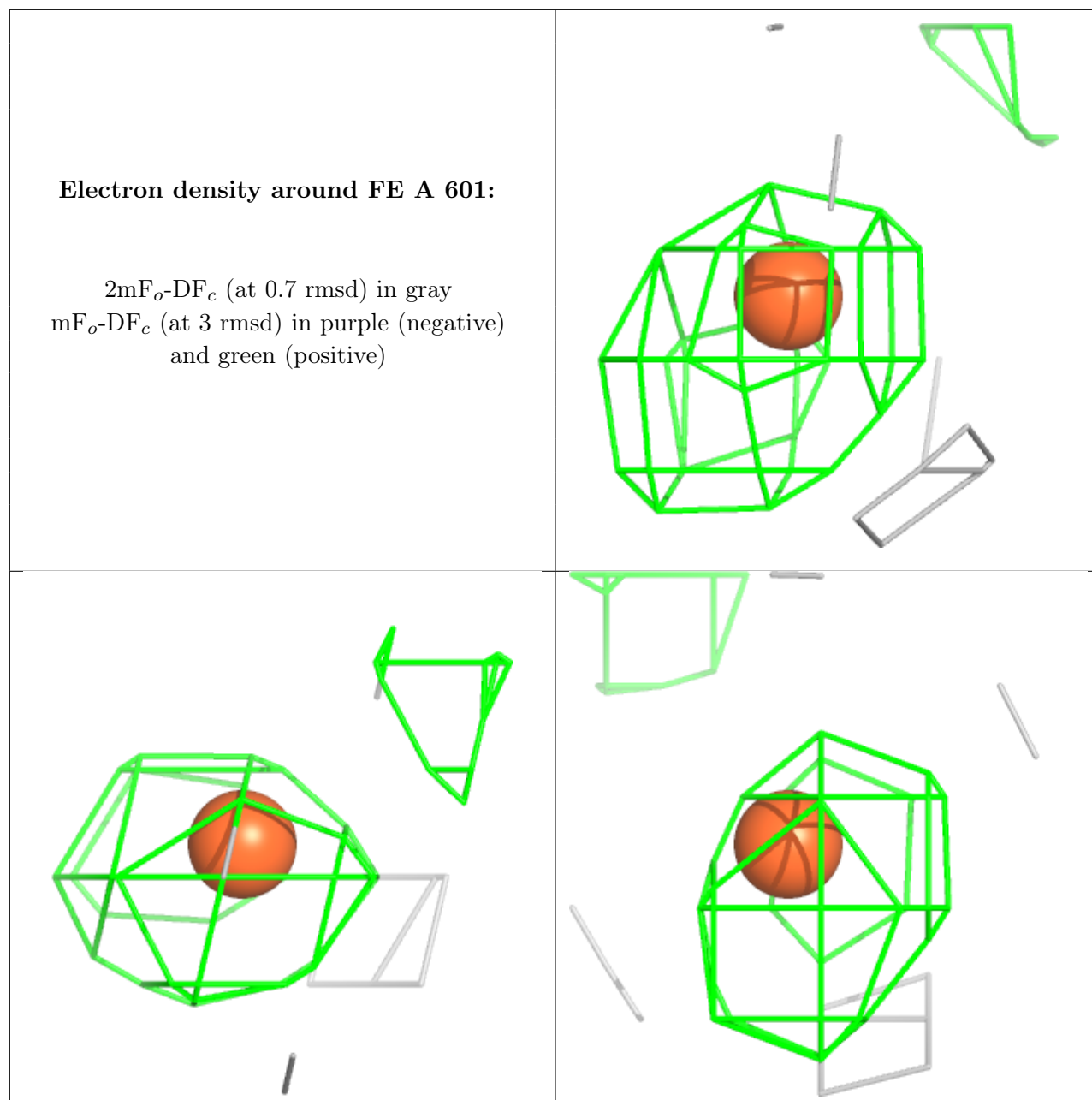
There are no monosaccharides in this entry.

6.4 Ligands

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(Å ²)	Q<0.9
3	CIT	A	602	13/13	0.66	0.27	71,101,111,128	0
2	FE	A	601	1/1	0.98	0.21	66,66,66,66	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.