Full wwPDB X-ray Structure Validation Report (i)

Nov 22, 2023 – 06:13 PM JST

PDB ID	:	7WPY
Title	:	AndA_M119A_N121V variant
Authors	:	Mori, T.; Chen, H.; Abe, I.
Deposited on	:	2022-01-24
Resolution	:	2.25 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 (i) 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 (1)) were used in the production of this report:

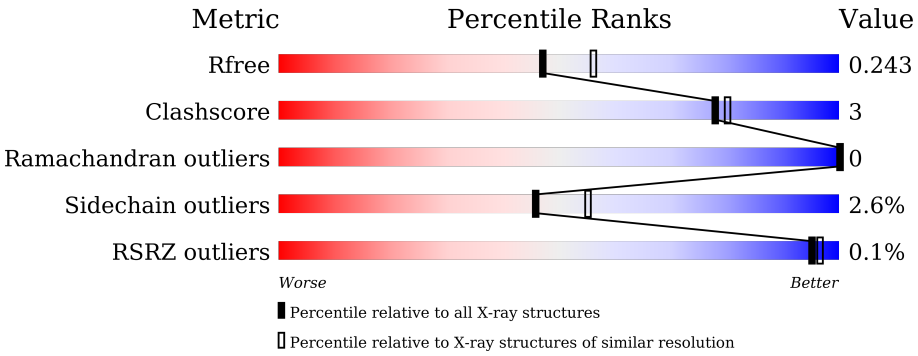
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 <=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	305	81% 7% 12%
1	B	305	78% 9% • 12%
1	C	305	78% 9% 13%
1	D	305	78% 9% 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8613 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 Dioxygenase andA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2074	1300	367	394	13			
1	B	268	Total	C	N	O	S	0	0	0
			2069	1300	363	392	14			
1	C	266	Total	C	N	O	S	0	0	0
			2052	1288	363	388	13			
1	D	265	Total	C	N	O	S	0	0	0
			2039	1280	359	387	13			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP A0A097ZPD5
A	-10	GLY	-	expression tag	UNP A0A097ZPD5
A	-9	SER	-	expression tag	UNP A0A097ZPD5
A	-8	SER	-	expression tag	UNP A0A097ZPD5
A	-7	HIS	-	expression tag	UNP A0A097ZPD5
A	-6	HIS	-	expression tag	UNP A0A097ZPD5
A	-5	HIS	-	expression tag	UNP A0A097ZPD5
A	-4	HIS	-	expression tag	UNP A0A097ZPD5
A	-3	HIS	-	expression tag	UNP A0A097ZPD5
A	-2	HIS	-	expression tag	UNP A0A097ZPD5
A	-1	SER	-	expression tag	UNP A0A097ZPD5
A	0	SER	-	expression tag	UNP A0A097ZPD5
A	1	GLY	-	expression tag	UNP A0A097ZPD5
A	2	LEU	-	expression tag	UNP A0A097ZPD5
A	3	VAL	-	expression tag	UNP A0A097ZPD5
A	4	PRO	-	expression tag	UNP A0A097ZPD5
A	5	ARG	-	expression tag	UNP A0A097ZPD5
A	6	GLY	-	expression tag	UNP A0A097ZPD5
A	7	SER	-	expression tag	UNP A0A097ZPD5
A	8	MET	-	expression tag	UNP A0A097ZPD5
A	119	ALA	MET	variant	UNP A0A097ZPD5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	121	VAL	ASN	variant	UNP A0A097ZPD5
B	-11	MET	-	initiating methionine	UNP A0A097ZPD5
B	-10	GLY	-	expression tag	UNP A0A097ZPD5
B	-9	SER	-	expression tag	UNP A0A097ZPD5
B	-8	SER	-	expression tag	UNP A0A097ZPD5
B	-7	HIS	-	expression tag	UNP A0A097ZPD5
B	-6	HIS	-	expression tag	UNP A0A097ZPD5
B	-5	HIS	-	expression tag	UNP A0A097ZPD5
B	-4	HIS	-	expression tag	UNP A0A097ZPD5
B	-3	HIS	-	expression tag	UNP A0A097ZPD5
B	-2	HIS	-	expression tag	UNP A0A097ZPD5
B	-1	SER	-	expression tag	UNP A0A097ZPD5
B	0	SER	-	expression tag	UNP A0A097ZPD5
B	1	GLY	-	expression tag	UNP A0A097ZPD5
B	2	LEU	-	expression tag	UNP A0A097ZPD5
B	3	VAL	-	expression tag	UNP A0A097ZPD5
B	4	PRO	-	expression tag	UNP A0A097ZPD5
B	5	ARG	-	expression tag	UNP A0A097ZPD5
B	6	GLY	-	expression tag	UNP A0A097ZPD5
B	7	SER	-	expression tag	UNP A0A097ZPD5
B	8	MET	-	expression tag	UNP A0A097ZPD5
B	119	ALA	MET	variant	UNP A0A097ZPD5
B	121	VAL	ASN	variant	UNP A0A097ZPD5
C	-11	MET	-	initiating methionine	UNP A0A097ZPD5
C	-10	GLY	-	expression tag	UNP A0A097ZPD5
C	-9	SER	-	expression tag	UNP A0A097ZPD5
C	-8	SER	-	expression tag	UNP A0A097ZPD5
C	-7	HIS	-	expression tag	UNP A0A097ZPD5
C	-6	HIS	-	expression tag	UNP A0A097ZPD5
C	-5	HIS	-	expression tag	UNP A0A097ZPD5
C	-4	HIS	-	expression tag	UNP A0A097ZPD5
C	-3	HIS	-	expression tag	UNP A0A097ZPD5
C	-2	HIS	-	expression tag	UNP A0A097ZPD5
C	-1	SER	-	expression tag	UNP A0A097ZPD5
C	0	SER	-	expression tag	UNP A0A097ZPD5
C	1	GLY	-	expression tag	UNP A0A097ZPD5
C	2	LEU	-	expression tag	UNP A0A097ZPD5
C	3	VAL	-	expression tag	UNP A0A097ZPD5
C	4	PRO	-	expression tag	UNP A0A097ZPD5
C	5	ARG	-	expression tag	UNP A0A097ZPD5
C	6	GLY	-	expression tag	UNP A0A097ZPD5
C	7	SER	-	expression tag	UNP A0A097ZPD5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	8	MET	-	expression tag	UNP A0A097ZPD5
C	119	ALA	MET	variant	UNP A0A097ZPD5
C	121	VAL	ASN	variant	UNP A0A097ZPD5
D	-11	MET	-	initiating methionine	UNP A0A097ZPD5
D	-10	GLY	-	expression tag	UNP A0A097ZPD5
D	-9	SER	-	expression tag	UNP A0A097ZPD5
D	-8	SER	-	expression tag	UNP A0A097ZPD5
D	-7	HIS	-	expression tag	UNP A0A097ZPD5
D	-6	HIS	-	expression tag	UNP A0A097ZPD5
D	-5	HIS	-	expression tag	UNP A0A097ZPD5
D	-4	HIS	-	expression tag	UNP A0A097ZPD5
D	-3	HIS	-	expression tag	UNP A0A097ZPD5
D	-2	HIS	-	expression tag	UNP A0A097ZPD5
D	-1	SER	-	expression tag	UNP A0A097ZPD5
D	0	SER	-	expression tag	UNP A0A097ZPD5
D	1	GLY	-	expression tag	UNP A0A097ZPD5
D	2	LEU	-	expression tag	UNP A0A097ZPD5
D	3	VAL	-	expression tag	UNP A0A097ZPD5
D	4	PRO	-	expression tag	UNP A0A097ZPD5
D	5	ARG	-	expression tag	UNP A0A097ZPD5
D	6	GLY	-	expression tag	UNP A0A097ZPD5
D	7	SER	-	expression tag	UNP A0A097ZPD5
D	8	MET	-	expression tag	UNP A0A097ZPD5
D	119	ALA	MET	variant	UNP A0A097ZPD5
D	121	VAL	ASN	variant	UNP A0A097ZPD5

- 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
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0

- Molecule 3 is water.

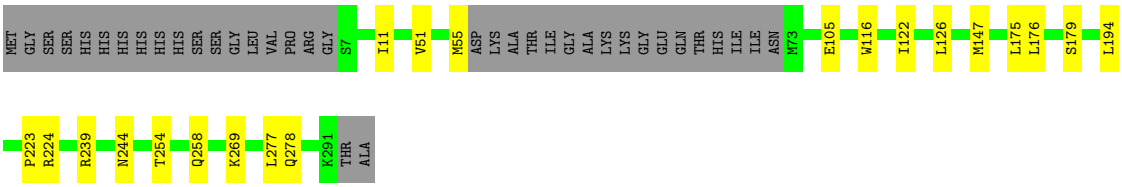
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	97	Total O 97 97	0	0
3	B	92	Total O 92 92	0	0
3	C	100	Total O 100 100	0	0
3	D	86	Total O 86 86	0	0

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.

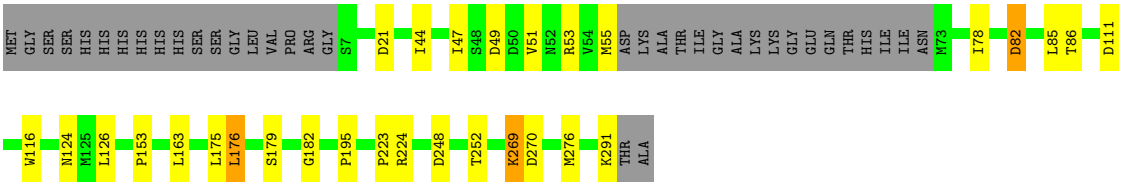
• Molecule 1: Dioxygenase andA

Chain A:



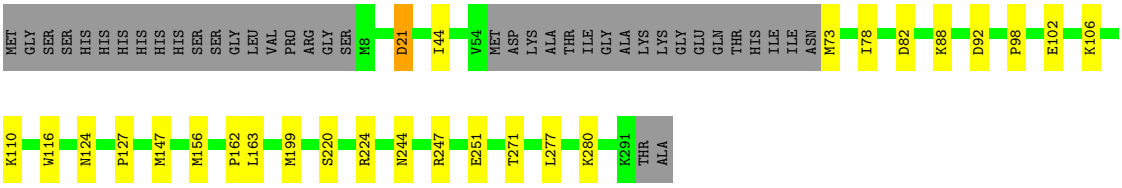
• Molecule 1: Dioxygenase andA

Chain B:



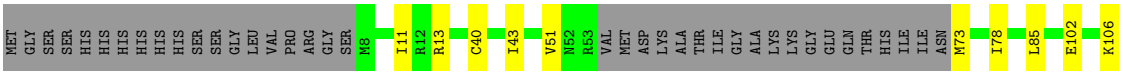
• Molecule 1: Dioxygenase andA

Chain C:



• Molecule 1: Dioxygenase andA

Chain D:




W116
I122
L123
N124
S144
L155
P162
L175
M199
S220
R224
R247
E251
T254
P255
L256
A257
Q258
R259
M260
Y272
Q278
D279
K280
K291
THR
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.52Å 73.76Å 97.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.45 – 2.25 48.74 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.45-2.25) 99.8 (48.74-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.188 , 0.241 0.189 , 0.243	Depositor DCC
R_{free} test set	2017 reflections (4.12%)	wwPDB-VP
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 28.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l 0.017 for k,h,-l 0.469 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8613	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.38	0/2118	0.61	0/2877
1	B	0.38	0/2113	0.61	0/2869
1	C	0.35	0/2096	0.60	0/2849
1	D	0.37	0/2083	0.60	0/2832
All	All	0.37	0/8410	0.61	0/11427

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

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	2074	0	2035	10	0
1	B	2069	0	2034	14	0
1	C	2052	0	2009	15	0
1	D	2039	0	1989	14	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	97	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	92	0	0	2	0
3	C	100	0	0	1	0
3	D	86	0	0	0	0
All	All	8613	0	8067	48	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 3.

All (48) 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:271:THR:HG21	1:D:13:ARG:HD3	1.76	0.67
1:C:21:ASP:OD2	1:C:106:LYS:HE2	1.98	0.64
1:C:162:PRO:HG3	1:C:199:MET:HG3	1.80	0.64
1:D:73:MET:HB2	1:D:78:ILE:HD13	1.81	0.63
1:C:78:ILE:HB	1:C:124:ASN:HB3	1.82	0.61
1:B:176:LEU:HG	1:B:179:SER:HB3	1.83	0.60
1:C:110:LYS:NZ	3:C:401:HOH:O	2.33	0.60
1:D:78:ILE:HB	1:D:124:ASN:HB3	1.85	0.59
1:B:78:ILE:HB	1:B:124:ASN:HB3	1.87	0.56
1:C:44:ILE:HG23	1:C:163:LEU:HD22	1.88	0.56
1:A:244:ASN:HB2	1:C:277:LEU:HD22	1.88	0.54
1:D:102:GLU:O	1:D:106:LYS:HG3	2.09	0.53
1:A:11:ILE:HD13	1:A:175:LEU:HD12	1.90	0.52
1:D:247:ARG:O	1:D:251:GLU:HG3	2.09	0.52
1:C:73:MET:HB2	1:C:78:ILE:HD13	1.91	0.52
1:C:88:LYS:NZ	1:C:92:ASP:OD2	2.36	0.51
1:B:126:LEU:HD23	1:B:223:PRO:HB3	1.93	0.50
1:A:147:MET:HG2	1:C:147:MET:HG2	1.95	0.48
1:B:49:ASP:O	1:B:53:ARG:HG3	2.12	0.48
1:B:175:LEU:O	1:B:195:PRO:HD2	2.12	0.48
1:A:254:THR:O	1:A:258:GLN:HG3	2.15	0.47
1:B:82:ASP:O	1:B:86:THR:HG23	2.14	0.47
1:D:144:SER:HB3	1:D:155:LEU:HD12	1.98	0.45
1:D:40:CYS:HB3	1:D:43:ILE:HD12	1.98	0.45
1:D:51:VAL:HG21	1:D:122:ILE:HD11	1.97	0.45
1:B:47:ILE:O	1:B:51:VAL:HG13	2.17	0.45
1:D:162:PRO:HG3	1:D:199:MET:HG3	1.99	0.44
1:C:247:ARG:O	1:C:251:GLU:HG3	2.18	0.44
1:D:256:LEU:O	1:D:260:MET:HG2	2.17	0.43
1:B:248:ASP:O	1:B:252:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LEU:HD22	1:C:244:ASN:HB2	2.01	0.43
1:A:51:VAL:HG21	1:A:122:ILE:HD11	2.00	0.43
1:B:44:ILE:HG23	1:B:163:LEU:HD22	2.01	0.43
1:D:278:GLN:O	1:D:280:LYS:HG3	2.18	0.43
1:A:176:LEU:HG	1:A:179:SER:HB3	2.01	0.42
1:A:194:LEU:HD23	1:A:194:LEU:HA	1.80	0.42
1:B:21:ASP:HB2	3:B:458:HOH:O	2.19	0.42
1:B:182:GLY:N	3:B:408:HOH:O	2.53	0.42
1:D:254:THR:O	1:D:258:GLN:HG3	2.20	0.42
1:B:111:ASP:HB3	1:B:153:PRO:HB3	2.02	0.41
1:D:51:VAL:HG21	1:D:122:ILE:CD1	2.50	0.41
1:D:11:ILE:HD13	1:D:175:LEU:HD12	2.02	0.41
1:A:278:GLN:HA	1:C:82:ASP:OD2	2.21	0.41
1:C:98:PRO:O	1:C:102:GLU:HG3	2.21	0.41
1:A:126:LEU:HD23	1:A:223:PRO:HB3	2.02	0.40
1:B:85:LEU:HD23	1:B:85:LEU:HA	1.92	0.40
1:B:269:LYS:HD2	1:B:270:ASP:CG	2.41	0.40
1:C:127:PRO:HB3	1:C:220:SER:O	2.21	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	264/305 (87%)	256 (97%)	8 (3%)	0	100	100
1	B	264/305 (87%)	258 (98%)	6 (2%)	0	100	100
1	C	262/305 (86%)	256 (98%)	6 (2%)	0	100	100
1	D	261/305 (86%)	254 (97%)	7 (3%)	0	100	100
All	All	1051/1220 (86%)	1024 (97%)	27 (3%)	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	225/256 (88%)	219 (97%)	6 (3%)	44	54
1	B	224/256 (88%)	216 (96%)	8 (4%)	35	42
1	C	221/256 (86%)	216 (98%)	5 (2%)	50	59
1	D	219/256 (86%)	215 (98%)	4 (2%)	59	68
All	All	889/1024 (87%)	866 (97%)	23 (3%)	46	55

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	MET
1	A	105	GLU
1	A	116	TRP
1	A	224	ARG
1	A	239	ARG
1	A	269	LYS
1	B	55	MET
1	B	82	ASP
1	B	116	TRP
1	B	176	LEU
1	B	224	ARG
1	B	269	LYS
1	B	276	MET
1	B	291	LYS
1	C	21	ASP
1	C	116	TRP
1	C	156	MET
1	C	224	ARG
1	C	280	LYS
1	D	85	LEU
1	D	116	TRP
1	D	220	SER
1	D	224	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 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, 95^{th} 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	268/305 (87%)	-0.44	0	100	100	25, 35, 49, 68	0
1	B	268/305 (87%)	-0.48	0	100	100	25, 35, 50, 65	0
1	C	266/305 (87%)	-0.55	0	100	100	26, 37, 50, 58	0
1	D	265/305 (86%)	-0.49	1 (0%)	92	93	25, 37, 49, 57	0
All	All	1067/1220 (87%)	-0.49	1 (0%)	95	96	25, 36, 50, 68	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	272	TYR	2.3

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, 95^{th} 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
2	FE	B	301	1/1	0.95	0.07	63,63,63,63	0

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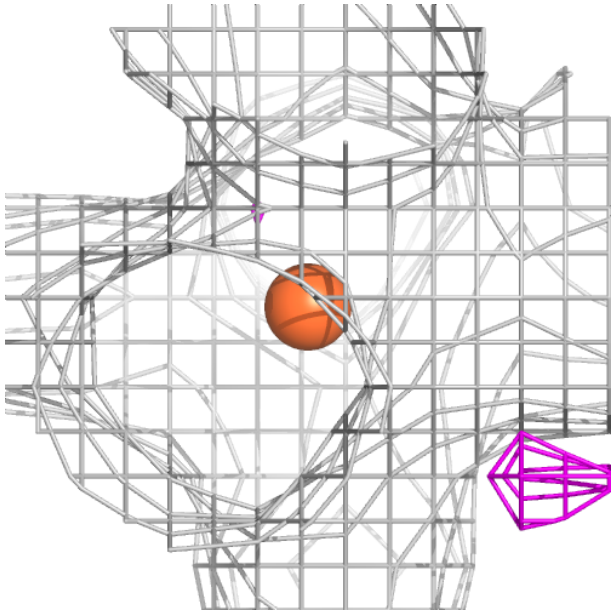
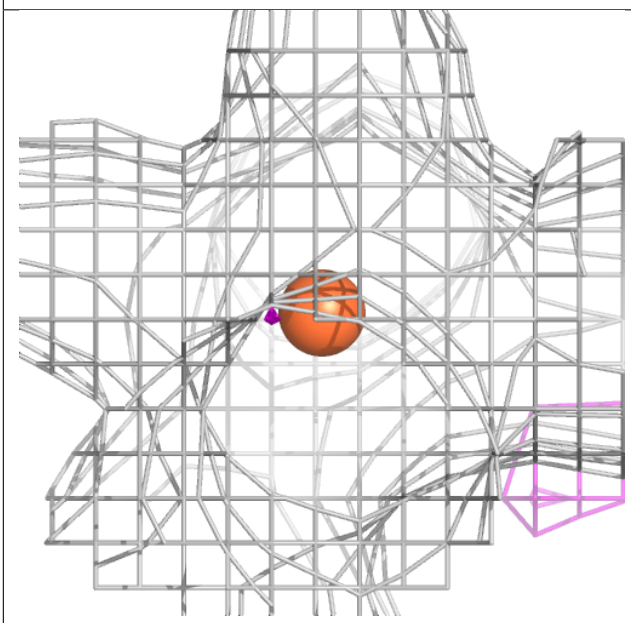
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE	C	301	1/1	0.95	0.04	57,57,57,57	0
2	FE	D	301	1/1	0.98	0.12	61,61,61,61	0
2	FE	A	301	1/1	0.99	0.09	63,63,63,63	0

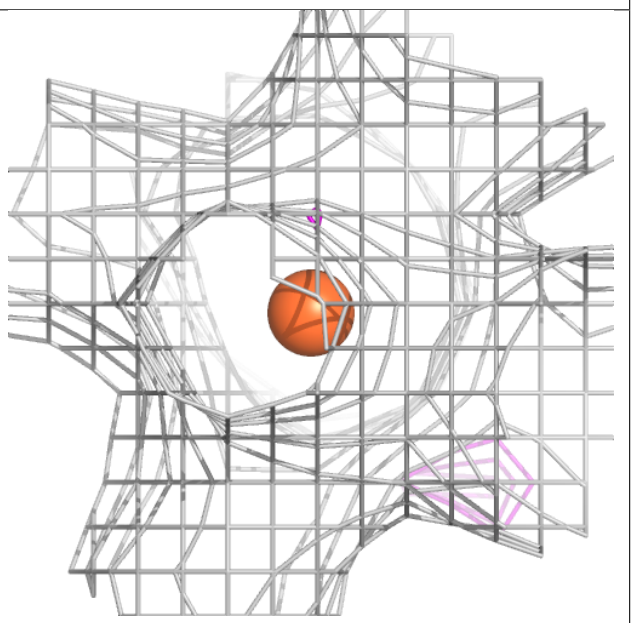
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FE B 301:

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

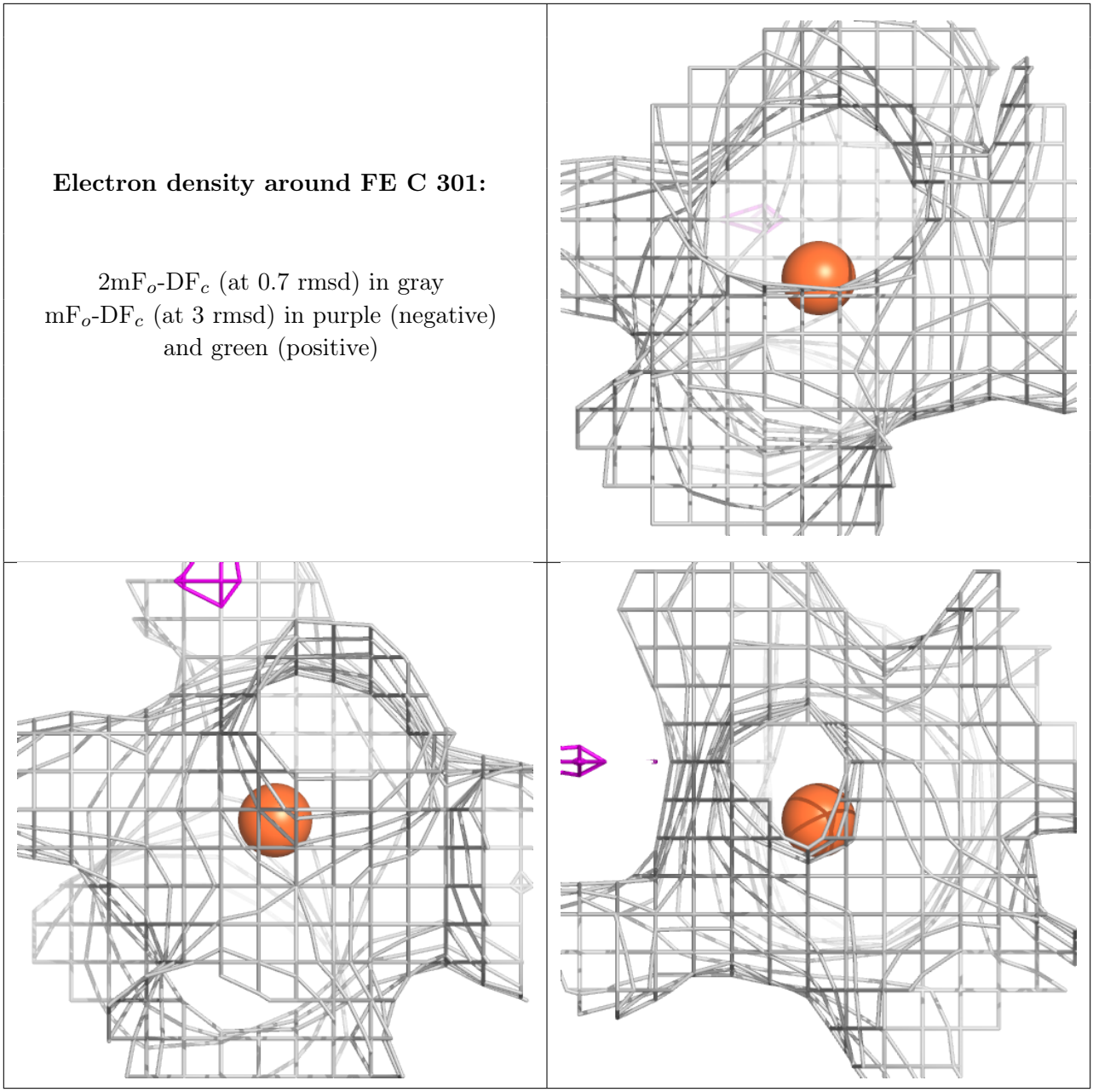






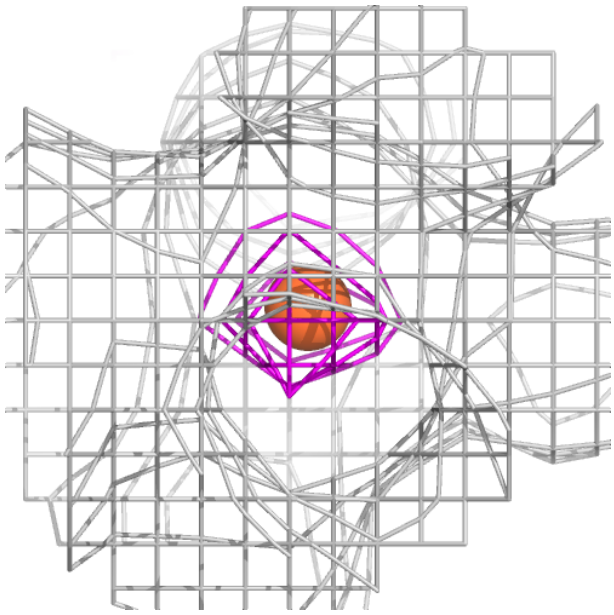
Electron density around FE C 301:

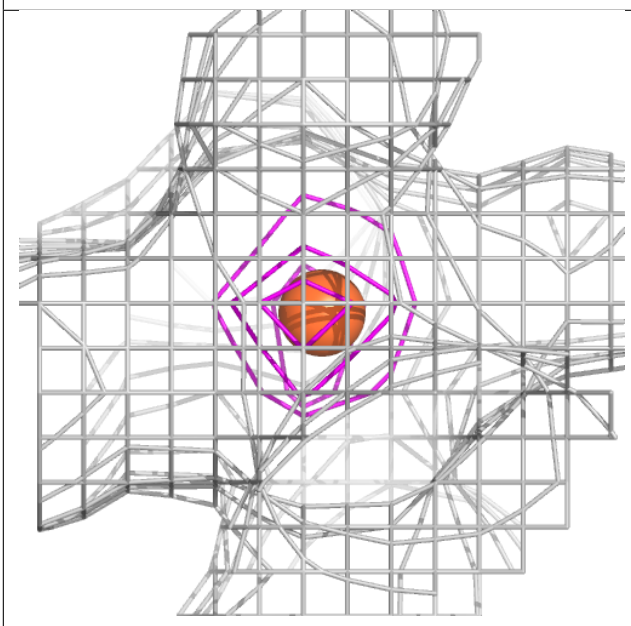
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

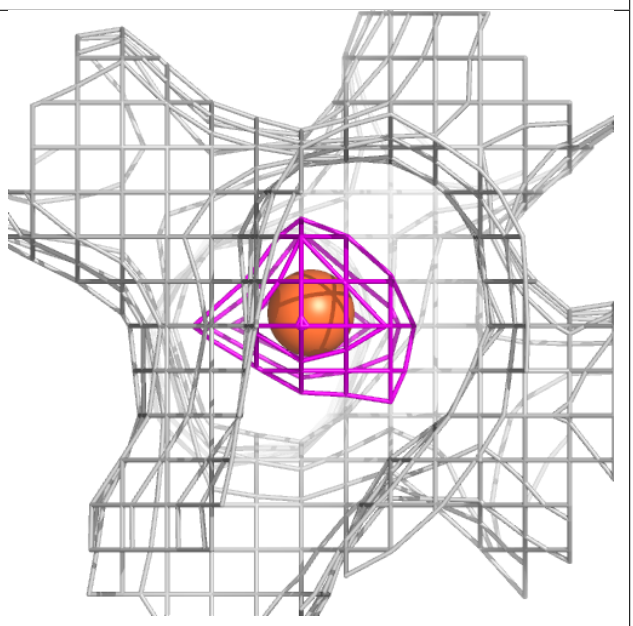


Electron density around FE D 301:

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

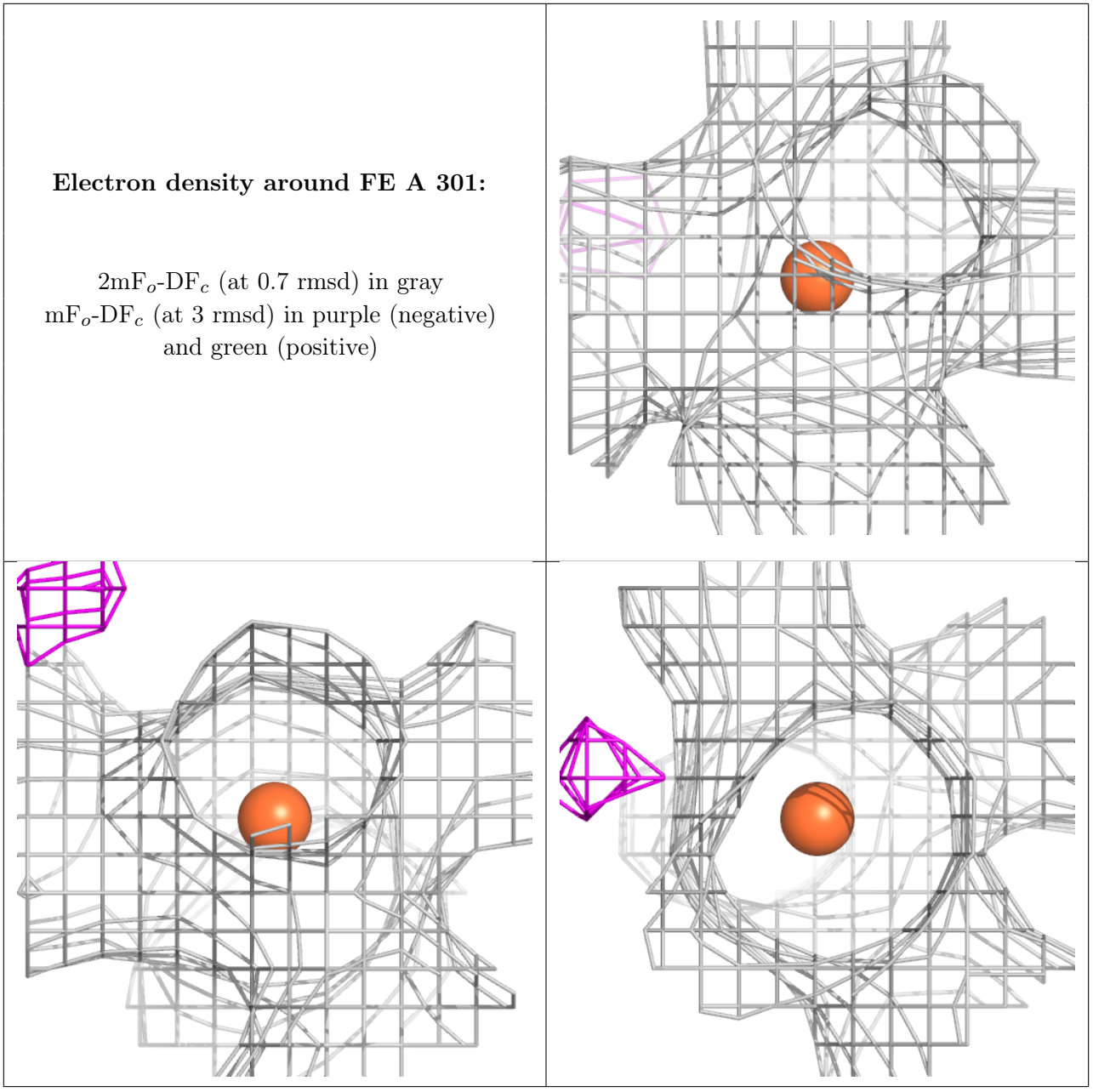






Electron density around FE A 301:

$2mF_o$-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.