

wwPDB X-ray Structure Validation Summary Report (i)

Feb 21, 2024 – 02:38 PM EST

PDB ID	:	40MF
Title	:	The F420-reducing [NiFe]-hydrogenase complex from Methanothermobacter
		marburgensis, the first X-ray structure of a group 3 family member
Authors	:	Vitt, S.; Ma, K.; Warkentin, E.; Moll, J.; Pierik, A.; Shima, S.; Ermler, U.
Deposited on	:	2014-01-27
Resolution	:	1.71 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 (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:

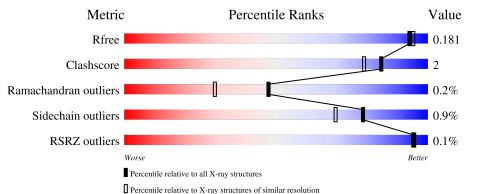
MolProbity Mogul Xtriage (Phenix) EDS	:	4.02b-467 1.8.5 (274361), CSD as541be (2020) 1.13 2.36
buster-report Percentile statistics Refmac	: : :	1.1.7 (2018) 20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		Parkinson et al. (1996) 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 1.71 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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	5722(1.74-1.70)
Clashscore	141614	6152(1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629(1.74-1.70)

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	G	275	78% 6%	16%
2	А	405	92%	• 5%
3	В	281	92%	7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	KEN	В	403	-	-	Х	-
6	UNL	G	305	-	-	Х	-



2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 7815 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 F420-reducing hydrogenase, subunit gamma.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	G	231	Total 1784	C 1118	N 296	0 345	$\begin{array}{c} \mathrm{S} \\ \mathrm{25} \end{array}$	0	6	0

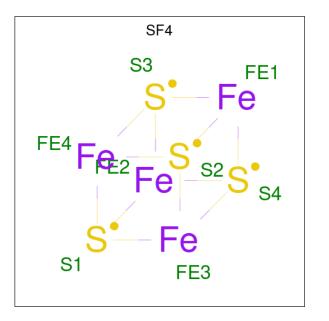
• Molecule 2 is a protein called F420-reducing hydrogenase, subunit alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	А	385	Total 2989	C 1880	N 532	O 560	S 17	0	1	0

• Molecule 3 is a protein called F420-reducing hydrogenase, subunit beta.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	В	280	Total 2167	C 1389	N 351	0 412	S 15	0	3	0

• Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

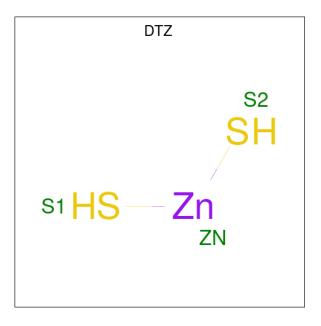






Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	TotalFeS844	0	0
4	G	1	TotalFeS844	0	0
4	G	1	TotalFeS844	0	0
4	В	1	TotalFeS844	0	0

• Molecule 5 is zinc(II) hydrogensulfide (three-letter code: DTZ) (formula: H_2S_2Zn).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total 3	S 1	Zn 2	0	1

• Molecule 6 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atom	s	ZeroOcc	AltConf
6	G	1	Total C 5 4	S 1	0	0

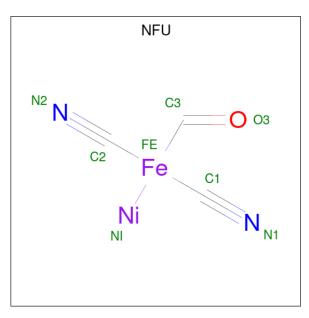
 $\bullet\,$ Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	3	Total Mg 3 3	0	0



[Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	7	В	1	Total Mg 1 1	0	0

• Molecule 8 is formyl[bis(hydrocyanato-1kappaC)]ironnickel(Fe-Ni) (three-letter code: NFU) (formula: C₃HFeN₂NiO).



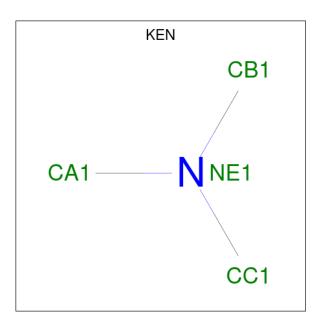
Mol	Chain	Residues		1	Aton	ns			ZeroOcc	AltConf
8	А	1	Total 8	$\begin{array}{c} \mathrm{C} \\ \mathrm{3} \end{array}$	Fe 1	N 2	Ni 1	0 1	0	0

• Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atom	s	ZeroOcc	AltConf
9	А	1	Total 1	Cl 1	0	0

• Molecule 10 is N,N-dimethylmethanamine (three-letter code: KEN) (formula: C₃H₉N).



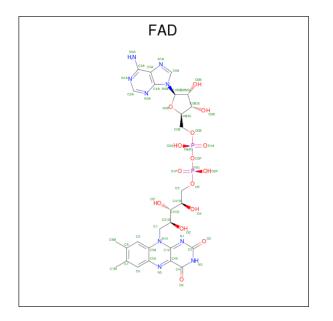


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
10	В	1	Total 4	${ m C} { m 3}$	N 1	0	0

• Molecule 11 is UNKNOWN (three-letter code: UNK) (formula: $C_4H_9NO_2$).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 3 & 1 \end{array}$	0	0

• Molecule 12 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
12	В	1	Total 53			0 15		0	0

• Molecule 13 is water.

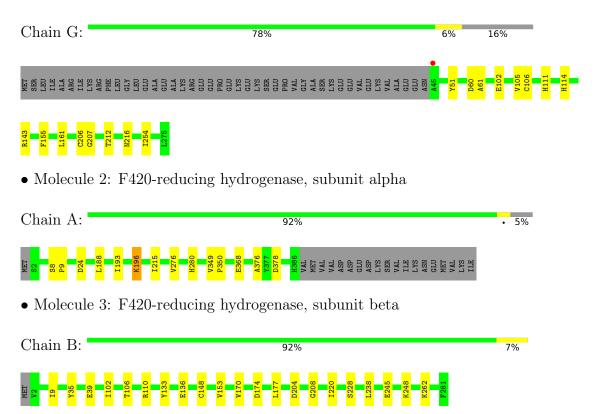
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	G	198	Total O 198 198	0	0
13	А	368	Total O 368 368	0	0
13	В	195	Total O 195 195	0	0



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: F420-reducing hydrogenase, subunit gamma





4 Data and refinement statistics (i)

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants	233.16Å 233.16Å 233.16Å	Denesiton
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 - 1.71	Depositor
Resolution (A)	19.99 - 1.71	EDS
% Data completeness	99.6 (19.99-1.71)	Depositor
(in resolution range)	99.7 (19.99-1.71)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.99 (at 1.70 \text{\AA})$	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.150 , 0.181	Depositor
II, IIfree	0.151 , 0.181	DCC
R_{free} test set	5896 reflections (5.23%)	wwPDB-VP
Wilson B-factor $(Å^2)$	20.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , 34.3	EDS
L-test for twinning ²	$< L >=0.44, < L^2>=0.27$	Xtriage
Estimated twinning fraction	0.109 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7815	wwPDB-VP
Average B, all atoms $(Å^2)$	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.77% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: NFU, CL, DTZ, SF4, MG, KEN, UNL, FAD

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).

Mal	Mol Chain	Bond	lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	G	0.49	0/1835	0.63	0/2488	
2	А	0.52	0/3055	0.64	1/4144~(0.0%)	
3	В	0.43	0/2212	0.55	0/2982	
All	All	0.48	0/7102	0.61	1/9614~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	378	ASP	CB-CG-OD1	5.22	123.00	118.30

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	G	1784	0	1760	13	0
2	А	2989	0	2981	7	0
3	В	2167	0	2215	12	1
4	В	8	0	0	0	0
4	G	24	0	0	0	0
5	G	3	0	0	0	0
6	G	5	0	0	5	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	А	3	0	0	0	0
7	В	1	0	0	0	0
8	А	8	0	0	0	0
9	А	1	0	0	0	0
10	В	4	0	9	4	0
11	В	4	0	0	0	0
12	В	53	0	28	0	0
13	А	368	0	0	3	2
13	В	195	0	0	3	1
13	G	198	0	0	0	0
All	All	7815	0	6993	32	2

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 2.

The worst 5 of 32 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)
3:B:110:ARG:HH22	10:B:403:KEN:HC1B	1.29	0.98
1:G:114[B]:HIS:NE2	6:G:305:UNL:S	2.39	0.95
1:G:111:HIS:ND1	6:G:305:UNL:S	2.42	0.92
1:G:114[B]:HIS:NE2	6:G:305:UNL:C1	2.35	0.90
3:B:204:ASP:OD2	10:B:403:KEN:HC1A	1.86	0.76

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:813:HOH:O	13:B:677:HOH:O[9_555]	2.06	0.14
3:B:174:ASP:OD2	13:A:878:HOH:O[5_555]	2.09	0.11

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	235/275~(86%)	228~(97%)	7 (3%)	0	100 100
2	А	384/405~(95%)	378~(98%)	5 (1%)	1 (0%)	41 24
3	В	281/281 (100%)	273~(97%)	7 (2%)	1 (0%)	34 18
All	All	900/961~(94%)	879~(98%)	19 (2%)	2(0%)	47 30

analysed, and the total number of residues.

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	А	215	ILE
3	В	153	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	G	201/232~(87%)	200 (100%)	1 (0%)	88 83
2	А	322/341~(94%)	320~(99%)	2(1%)	86 80
3	В	232/230~(101%)	228~(98%)	4 (2%)	60 44
All	All	755/803~(94%)	748~(99%)	7 (1%)	78 69

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	В	136	GLU
3	В	228	SER
3	В	248	LYS
3	В	245	GLU
2	А	368	GLU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains 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 16 ligands modelled in this entry, 1 is modelled with single atom, 2 are unknown and 5 are monoatomic - leaving 8 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	Tune	Chain	Res	Link	Bo	ond leng	ths	B	ond ang	gles
	Type	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SF4	G	303	1	$0,\!12,\!12$	-	-	-		
8	NFU	А	502	2	2,7,7	1.82	1 (50%)	-		
5	DTZ	G	304[A]	13,1	$0,\!1,\!2$	-	-	-		
10	KEN	В	403	-	$3,\!3,\!3$	1.91	1 (33%)	$3,\!3,\!3$	0.34	0
4	SF4	В	401	3	0,12,12	-	-	-		
4	SF4	G	301	1	$0,\!12,\!12$	-	-	-		
12	FAD	В	405	-	$53,\!58,\!58$	2.22	8 (15%)	68,89,89	1.60	15 (22%)
4	SF4	G	302	1	0,12,12	-	-	-		

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
4	SF4	G	303	1	-	-	0/6/5/5



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	В	401	3	-	-	0/6/5/5
4	SF4	G	301	1	-	-	0/6/5/5
12	FAD	В	405	-	-	5/30/50/50	0/6/6/6
4	SF4	G	302	1	-	-	0/6/5/5

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	В	405	FAD	C2'- $C3$ '	-9.64	1.35	1.53
12	В	405	FAD	C4X-N5	9.40	1.49	1.30
12	В	405	FAD	C5X-N5	4.06	1.47	1.39
12	В	405	FAD	O2'-C2'	-3.57	1.35	1.43
12	В	405	FAD	O3'-C3'	-2.97	1.36	1.43

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
12	В	405	FAD	O2'-C2'-C3'	3.46	117.52	109.10
12	В	405	FAD	C4-C4X-C10	-3.44	111.02	116.79
12	В	405	FAD	C5X-N5-C4X	-3.39	112.44	118.07
12	В	405	FAD	O4-C4-C4X	-3.35	117.71	126.60
12	В	405	FAD	N3A-C2A-N1A	-3.25	123.60	128.68

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	В	405	FAD	N10-C1'-C2'-O2'
12	В	405	FAD	O2'-C2'-C3'-C4'
12	В	405	FAD	PA-O3P-P-O2P
12	В	405	FAD	O4B-C4B-C5B-O5B
12	В	405	FAD	PA-O3P-P-O1P

There are no ring outliers.

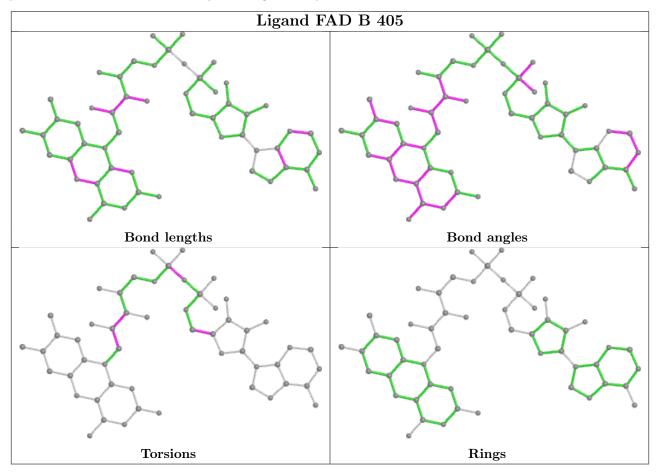
1 monomer is involved in 4 short contacts:

Mol	Chain	Res Type		Clashes	Symm-Clashes	
10	В	403	KEN	4	0	

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 then 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.



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, 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	$\langle RSRZ \rangle$	$\# RSRZ {>}2$	$\mathbf{OWAB}(\mathbf{A}^2)$	Q<0.9
1	G	231/275~(84%)	-0.78	1 (0%) 92 93	14, 19, 34, 56	0
2	А	385/405~(95%)	-0.85	0 100 100	13, 17, 30, 43	0
3	В	$280/281 \ (99\%)$	-0.69	0 100 100	16, 24, 40, 57	0
All	All	896/961~(93%)	-0.78	1 (0%) 95 95	13, 20, 36, 57	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	G	45	ALA	3.3	

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 monosaccharides 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, 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.

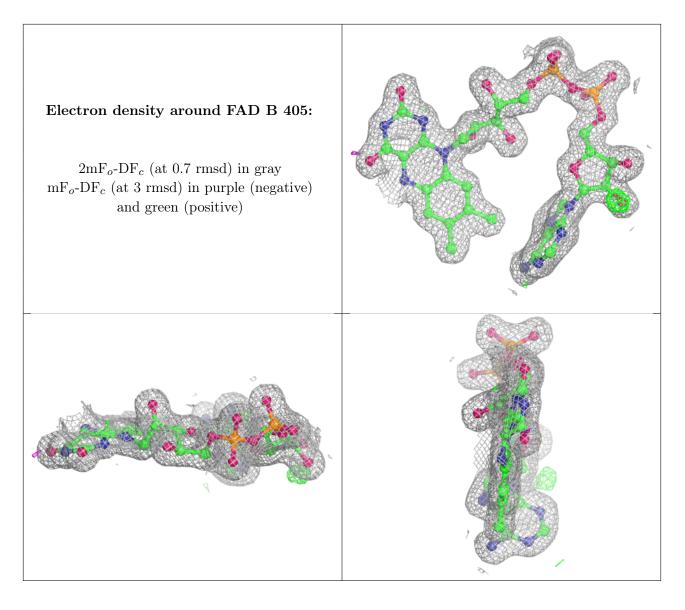
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
10	KEN	В	403	4/4	0.73	0.17	30,39,43,45	0
5	DTZ	G	304[B]	1/3	0.82	0.09	53,53,53,53	1



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	DTZ	G	304[A]	2/3	0.82	0.09	54,54,54,60	2
6	UNL	G	305	5/-	0.96	0.12	$25,\!51,\!54,\!54$	0
7	MG	В	402	1/1	0.98	0.14	$37,\!37,\!37,\!37$	0
11	UNK	В	404	4/-	0.98	0.05	$21,\!21,\!22,\!22$	0
12	FAD	В	405	53/53	0.98	0.05	17,20,24,29	0
7	MG	А	503	1/1	0.99	0.06	$12,\!12,\!12,\!12$	0
7	MG	А	504	1/1	0.99	0.07	36, 36, 36, 36	0
4	SF4	G	301	8/8	1.00	0.07	$15,\!16,\!16,\!17$	0
4	SF4	G	302	8/8	1.00	0.07	$13,\!15,\!16,\!16$	0
8	NFU	А	502	8/8	1.00	0.08	$12,\!14,\!15,\!19$	0
9	CL	А	505	1/1	1.00	0.04	20,20,20,20	0
4	SF4	G	303	8/8	1.00	0.07	$15,\!16,\!17,\!17$	0
7	MG	А	501	1/1	1.00	0.07	20,20,20,20	0
4	SF4	В	401	8/8	1.00	0.07	$17,\!18,\!19,\!19$	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.

