

wwPDB X-ray Structure Validation Summary Report (i)

Jan 16, 2024 - 02:03 am GMT

PDB ID	:	6HUY
Title	:	HmdII from Desulfurobacterium thermolithotrophum reconstitued with Fe-
		guanylylpyridinol (FeGP) cofactor and co-crystallized with methenyl-tetrahy
		drofolate form A
Authors	:	Watanabe, T.; Wagner, T.; Huang, G.; Kahnt, J.; Ataka, K.; Ermler, U.;
		Shima, S.
Deposited on	:	2018-10-09
Resolution	:	2.25 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	:	4.02b-467
Mogul	:	1.8.4, CSD as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report		
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

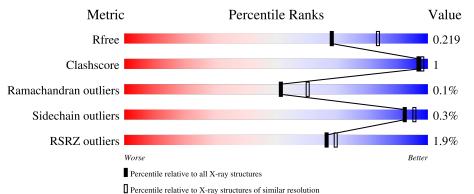


1 Overall quality at a glance (i)

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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
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	А	370	3% 	• 5%
1	С	370	93%	• 5%
2	В	370	.% 94%	• •
2	D	370	% • 95%	•••

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
4	GOL	D	401	-	-	-	Х
7	PG4	В	405	-	-	-	Х



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11842 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 Coenzyme F420-dependent N(5), N(10)-methenyltetrahydrom ethanopterin reductase-related protein.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	350	Total 2710	C 1737	1,	O 528	S 12	0	0	0
1	С	351		C 1742		O 529	S 12	0	0	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	358	LYS	-	expression tag	UNP F0S2B6
А	359	LEU	-	expression tag	UNP F0S2B6
А	360	ALA	-	expression tag	UNP F0S2B6
А	361	ALA	-	expression tag	UNP F0S2B6
А	362	ALA	-	expression tag	UNP F0S2B6
А	363	LEU	-	expression tag	UNP F0S2B6
A	364	GLU	-	expression tag	UNP F0S2B6
А	365	HIS	-	expression tag	UNP F0S2B6
A	366	HIS	-	expression tag	UNP F0S2B6
А	367	HIS	-	expression tag	UNP F0S2B6
А	368	HIS	-	expression tag	UNP F0S2B6
А	369	HIS	-	expression tag	UNP F0S2B6
А	370	HIS	-	expression tag	UNP F0S2B6
С	358	LYS	-	expression tag	UNP F0S2B6
С	359	LEU	-	expression tag	UNP F0S2B6
С	360	ALA	-	expression tag	UNP F0S2B6
С	361	ALA	-	expression tag	UNP F0S2B6
С	362	ALA	-	expression tag	UNP F0S2B6
С	363	LEU	-	expression tag	UNP F0S2B6
С	364	GLU	-	expression tag	UNP F0S2B6
С	365	HIS	-	expression tag	UNP F0S2B6
С	366	HIS	-	expression tag	UNP F0S2B6
С	367	HIS	-	expression tag	UNP F0S2B6
С	368	HIS	-	expression tag	UNP F0S2B6

There are 26 discrepancies between the modelled and reference sequences:



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Chain	Residue	Modelled	Actual	Comment	Reference
С	369	HIS	-	expression tag	UNP F0S2B6
С	370	HIS	-	expression tag	UNP F0S2B6

• Molecule 2 is a protein called Coenzyme F420-dependent N(5), N(10)-methenyltetrahydrom ethanopterin reductase-related protein.

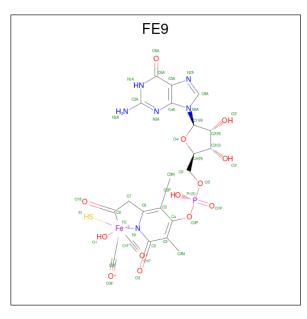
Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
0	D	357	Total	С	Ν	0	\mathbf{S}	0	1	0
	D	- 397	2776	1775	445	544	12	0	1	0
0	р	355	Total	С	Ν	0	S	0	1	0
	D	500	2760	1765	445	538	12	0	1	0

There are 26 discrepancies between the modelled and reference sequences:

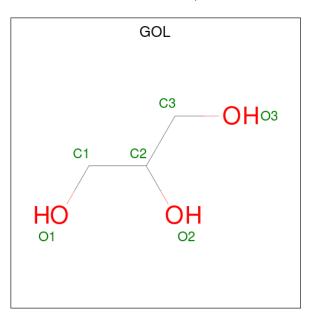
Chain	Residue	Modelled	Actual	Comment	Reference
В	358	LYS	-	expression tag	UNP F0S2B6
В	359	LEU	-	expression tag	UNP F0S2B6
В	360	ALA	-	expression tag	UNP F0S2B6
В	361	ALA	-	expression tag	UNP F0S2B6
В	362	ALA	-	expression tag	UNP F0S2B6
В	363	LEU	-	expression tag	UNP F0S2B6
В	364	GLU	-	expression tag	UNP F0S2B6
В	365	HIS	-	expression tag	UNP F0S2B6
В	366	HIS	-	expression tag	UNP F0S2B6
В	367	HIS	-	expression tag	UNP F0S2B6
В	368	HIS	-	expression tag	UNP F0S2B6
В	369	HIS	-	expression tag	UNP F0S2B6
В	370	HIS	-	expression tag	UNP F0S2B6
D	358	LYS	-	expression tag	UNP F0S2B6
D	359	LEU	-	expression tag	UNP F0S2B6
D	360	ALA	-	expression tag	UNP F0S2B6
D	361	ALA	-	expression tag	UNP F0S2B6
D	362	ALA	-	expression tag	UNP F0S2B6
D	363	LEU	-	expression tag	UNP F0S2B6
D	364	GLU	-	expression tag	UNP F0S2B6
D	365	HIS	-	expression tag	UNP F0S2B6
D	366	HIS	-	expression tag	UNP F0S2B6
D	367	HIS	-	expression tag	UNP F0S2B6
D	368	HIS	-	expression tag	UNP F0S2B6
D	369	HIS	-	expression tag	UNP F0S2B6
D	370	HIS	-	expression tag	UNP F0S2B6



 $\bullet \ \ Molecule \ 3 \ is \ iron-guanylyl \ pyridinol \ cofactor \ (three-letter \ code: \ FE9) \ (formula: \ C_{21}H_{23}FeN_6O_{13}PS).$



Mol	Chain	Residues		A	Aton	ıs			ZeroOcc	AltConf
2	٨	1	Total	С	Fe	Ν	Ο	Р	0	0
5	A	1	41	21	1	6	12	1	0	0
9	С	1	Total	С	Fe	Ν	Ο	Р	0	0
0		1	41	21	1	6	12	1	0	0



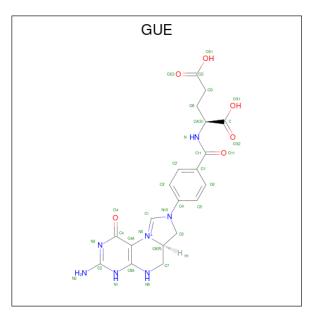
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0



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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total 6	${ m C} { m 3}$	O 3	0	0

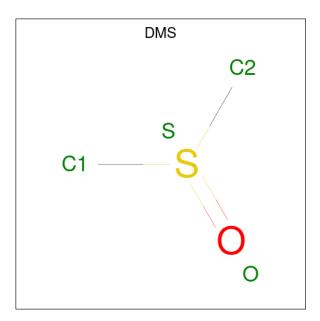
• Molecule 5 is 5,10-Methenyltetrahydrofolate (three-letter code: GUE) (formula: $C_{20}H_{22}N_7O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	Δ	1	Total	С	Ν	0	0	0
0	11	Ĩ	33	20	$\overline{7}$	6	0	0
5	В	1	Total	С	Ν	Ο	0	0
5	D	1	33	20	7	6	0	0
5	C	1	Total	С	Ν	Ο	0	0
5	U	1	33	20	7	6	0	0
5	л	1	Total	С	Ν	0	0	0
0	D	1	33	20	7	6	0	0

• Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).

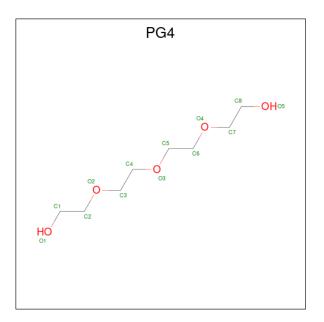




Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{O} & \text{S} \\ 4 & 2 & 1 & 1 \end{array}$	0	0
6	В	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{O} & \text{S} \\ 4 & 2 & 1 & 1 \end{array}$	0	0
6	В	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{O} & \text{S} \\ 4 & 2 & 1 & 1 \end{array}$	0	0
6	В	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{O} & \text{S} \\ 4 & 2 & 1 & 1 \end{array}$	0	0
6	С	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{O} & \text{S} \\ 4 & 2 & 1 & 1 \end{array}$	0	0
6	С	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{O} & \text{S} \\ 4 & 2 & 1 & 1 \end{array}$	0	0
6	D	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{O} & \text{S} \\ 4 & 2 & 1 & 1 \end{array}$	0	0
6	D	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{O} & \text{S} \\ 4 & 2 & 1 & 1 \end{array}$	0	0
6	D	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{O} & \text{S} \\ 4 & 2 & 1 & 1 \end{array}$	0	0

• Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).





Mo	Chain	Residues	Atoms		ZeroOcc	AltConf
7	В	1	TotalC85	O 3	0	0

• Molecule 8 is water.

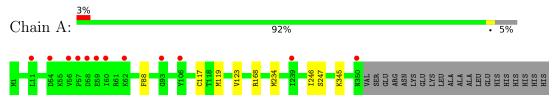
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	140	Total O 140 140	0	0
8	В	166	Total O 166 166	0	0
8	С	165	Total O 165 165	0	0
8	D	138	Total O 138 138	0	0



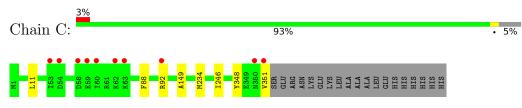
3 Residue-property plots (i)

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.

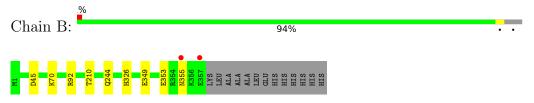
 \bullet Molecule 1: Coenzyme F420-dependent N(5),N(10)-methenyltetrahydromethan
opterin reductase-related protein



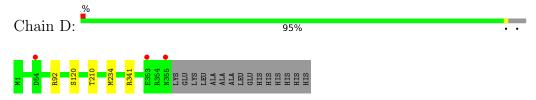
 \bullet Molecule 1: Coenzyme F420-dependent N(5),N(10)-methenyltetrahydromethan
opterin reductase-related protein



 \bullet Molecule 2: Coenzyme F420-dependent N(5),N(10)-methenyltetrahydromethan
opterin reductase-related protein



 \bullet Molecule 2: Coenzyme F420-dependent N(5),N(10)-methenyltetrahydromethan
opterin reductase-related protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	99.77Å 131.83Å 168.26Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.98 - 2.25	Depositor
Resolution (A)	47.83 - 2.25	EDS
% Data completeness	99.8 (24.98-2.25)	Depositor
(in resolution range)	99.8 (47.83-2.25)	EDS
R _{merge}	0.10	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.20 (at 2.24 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
D D.	0.187 , 0.212	Depositor
R, R_{free}	0.196 , 0.219	DCC
R_{free} test set	5121 reflections (4.85%)	wwPDB-VP
Wilson B-factor $(Å^2)$	42.3	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32 , 39.0	EDS
L-test for twinning ²	$ < L >=0.53, < L^2>=0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11842	wwPDB-VP
Average B, all atoms $(Å^2)$	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 52.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7779e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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: CSO, DMS, GOL, PG4, GUE, FE9

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.36	0/2759	0.51	0/3741	
1	С	0.36	0/2766	0.51	0/3751	
2	В	0.36	0/2820	0.49	0/3820	
2	D	0.37	0/2804	0.48	0/3799	
All	All	0.36	0/11149	0.50	0/15111	

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	А	2710	0	2770	9	0
1	С	2717	0	2778	7	0
2	В	2776	0	2834	5	0
2	D	2760	0	2822	3	0
3	А	41	0	20	2	0
3	С	41	0	20	1	0
4	А	6	0	8	0	0
4	D	6	0	8	0	0
5	А	33	0	0	0	0



Mol	Chain	Non-H		H(added)	Clashes	Symm-Clashes
5	В	33	0	0	0	0
5	С	33	0	0	0	0
5	D	33	0	0	0	0
6	В	16	0	24	0	0
6	С	8	0	12	0	0
6	D	12	0	18	0	0
7	В	8	0	9	0	0
8	А	140	0	0	1	0
8	В	166	0	0	2	0
8	С	165	0	0	1	0
8	D	138	0	0	2	0
All	All	11842	0	11323	20	0

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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 1.

The worst 5 of 20 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:92:ARG:NH1	2:D:234:MET:SD	2.57	0.77
2:B:326:HIS:ND1	8:B:501:HOH:O	2.22	0.72
1:C:92:ARG:HG2	1:C:348:TYR:O	2.01	0.60
2:B:45:ASP:OD1	2:B:70:LYS:NZ	2.25	0.60
1:A:88:PHE:CD1	3:A:401:FE9:H11	2.38	0.58

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	А	348/370~(94%)	336~(97%)	12 (3%)	0	100 100	



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percer	ntiles
1	С	349/370~(94%)	338~(97%)	10 (3%)	1 (0%)	41	46
2	В	355/370~(96%)	343~(97%)	11 (3%)	1 (0%)	41	46
2	D	353/370~(95%)	344 (98%)	9 (2%)	0	100	100
All	All	1405/1480~(95%)	1361 (97%)	42 (3%)	2(0%)	51	60

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All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type		
2	В	355	ASN		
1	С	149	ALA		

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	А	301/318~(95%)	300 (100%)	1 (0%)		92	95	
1	С	302/318~(95%)	302 (100%)	0		100	100	
2	В	308/317~(97%)	307~(100%)	1 (0%)		92	95	
2	D	306/317~(96%)	304 (99%)	2(1%)		84	90	
All	All	1217/1270~(96%)	1213 (100%)	4 (0%)		92	95	

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	168	ARG
2	B 92		ARG
2	D	92	ARG
2	D	120	SER

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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	Dec	Res Link Bond lengths			В	Bond ang	gles	
	туре	Chain	Res		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	CSO	D	117	2	3,6,7	0.86	0	$0,\!6,\!8$	-	-
2	CSO	В	117	2	3,6,7	0.75	0	$0,\!6,\!8$	-	-

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	CSO	D	117	2	-	0/1/5/7	-
2	CSO	В	117	2	-	0/1/5/7	-

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.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.



5.6 Ligand geometry (i)

18 ligands are modelled in this entry.

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	Bo	ond leng	ths	В	ond ang	les
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
6	DMS	В	401	-	3,3,3	0.49	0	3, 3, 3	0.57	0
3	FE9	А	401	-	34,45,47	1.41	4 (11%)	37,71,80	1.23	4 (10%)
6	DMS	С	402	-	3,3,3	0.45	0	3,3,3	0.70	0
5	GUE	С	404	-	33,36,36	1.90	6 (18%)	$38,\!52,\!52$	1.44	3 (7%)
3	FE9	С	401	1	34,45,47	1.45	3 (8%)	37,71,80	1.22	6 (16%)
6	DMS	D	403	-	3,3,3	0.46	0	3,3,3	0.66	0
6	DMS	D	402	-	3,3,3	0.48	0	3,3,3	0.62	0
5	GUE	В	406	-	33,36,36	1.73	6 (18%)	$38,\!52,\!52$	1.46	4 (10%)
4	GOL	D	401	-	$5,\!5,\!5$	0.29	0	$5,\!5,\!5$	0.36	0
6	DMS	С	403	-	3,3,3	0.48	0	3,3,3	0.72	0
6	DMS	В	404	-	3,3,3	0.51	0	3,3,3	0.66	0
5	GUE	D	405	-	33,36,36	1.83	6 (18%)	$38,\!52,\!52$	1.68	3 (7%)
4	GOL	А	402	-	$5,\!5,\!5$	0.49	0	$5,\!5,\!5$	0.40	0
6	DMS	D	404	-	3,3,3	0.51	0	3, 3, 3	0.63	0
7	PG4	В	405	-	7,7,12	0.62	0	6,6,11	0.12	0
5	GUE	А	403	-	33,36,36	1.85	6 (18%)	$38,\!52,\!52$	1.42	3 (7%)
6	DMS	В	402	-	3,3,3	0.49	0	3,3,3	0.56	0
6	DMS	В	403	-	3,3,3	0.51	0	$3,\!3,\!3$	0.60	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
3	FE9	А	401	-	-	1/9/53/65	0/5/5/5
5	GUE	С	404	-	-	4/21/42/42	0/4/4/4
3	FE9	С	401	1	-	1/9/53/65	0/5/5/5
5	GUE	В	406	-	-	4/21/42/42	0/4/4/4
4	GOL	D	401	-	-	0/4/4/4	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GUE	D	405	-	-	3/21/42/42	0/4/4/4
4	GOL	А	402	-	-	2/4/4/4	-
7	PG4	В	405	-	-	4/5/5/10	-
5	GUE	А	403	-	-	2/21/42/42	0/4/4/4

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The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
5	А	403	GUE	C1-N5	-6.15	1.26	1.33
5	С	404	GUE	C1-N5	-6.11	1.26	1.33
5	D	405	GUE	C1-N5	-5.80	1.26	1.33
5	В	406	GUE	C1-N5	-5.44	1.27	1.33
5	С	404	GUE	C8A-N8	4.88	1.36	1.32

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
5	D	405	GUE	C6-C9-N10	-7.21	99.00	102.82
5	В	406	GUE	C6-C9-N10	-5.97	99.66	102.82
5	С	404	GUE	C6-C9-N10	-5.96	99.67	102.82
5	А	403	GUE	C6-C9-N10	-5.65	99.83	102.82
3	А	401	FE9	O2-C2-N1	-3.42	116.81	124.11

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	402	GOL	C1-C2-C3-O3
5	В	406	GUE	N-CA-CB-CG
7	В	405	PG4	O2-C3-C4-O3
5	В	406	GUE	C-CA-CB-CG
4	А	402	GOL	O2-C2-C3-O3

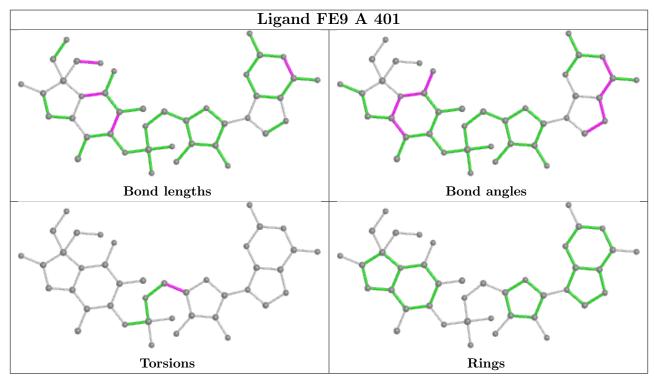
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	401	FE9	2	0
3	С	401	FE9	1	0

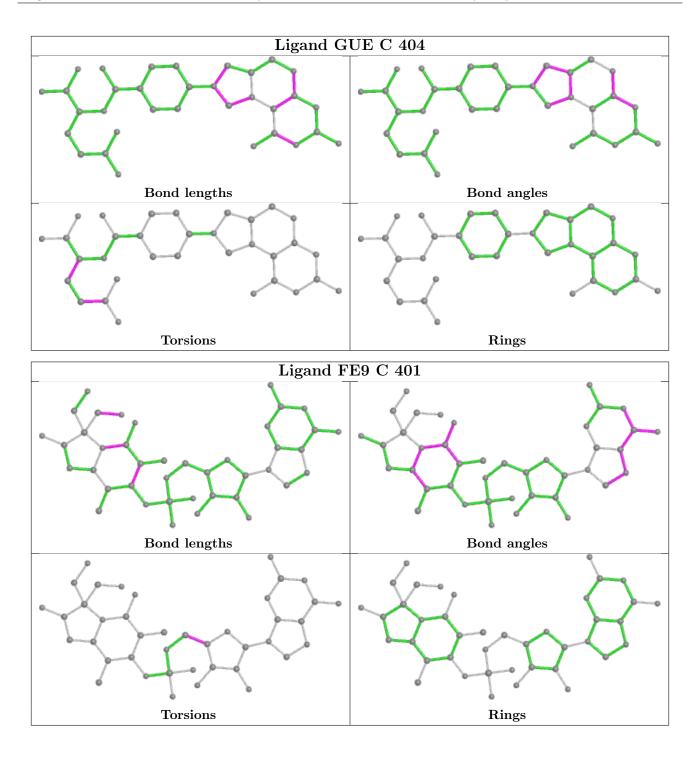


The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

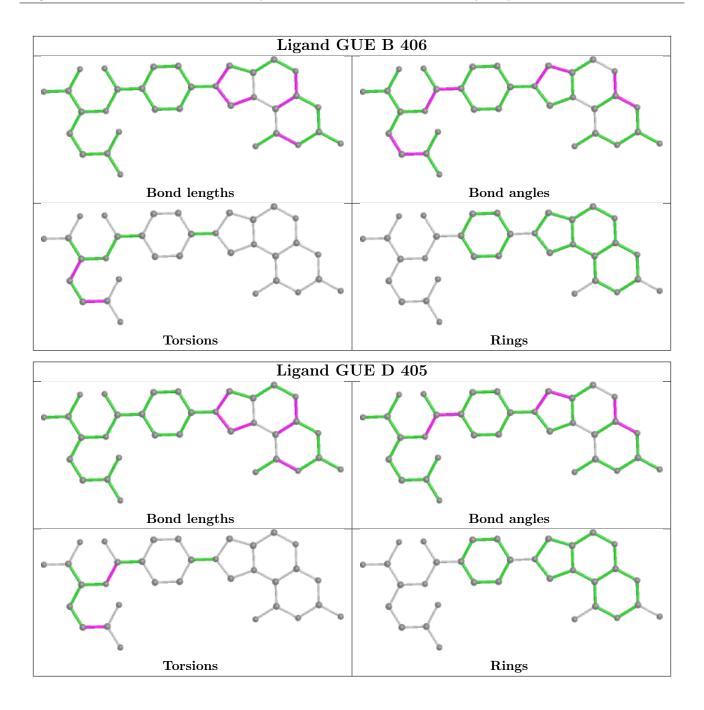




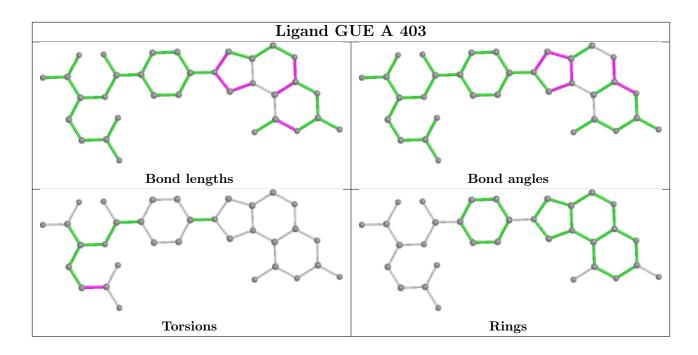












5.7 Other polymers (i)

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	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	350/370~(94%)	-0.10	12 (3%) 45 47	34, 56, 87, 128	0
1	С	351/370~(94%)	-0.12	10 (2%) 53 55	32, 51, 81, 113	0
2	В	356/370~(96%)	-0.23	2 (0%) 89 89	33, 51, 80, 123	0
2	D	354/370~(95%)	-0.21	3 (0%) 86 87	31, 52, 81, 102	0
All	All	1411/1480~(95%)	-0.17	27 (1%) 66 69	31, 52, 84, 128	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
2	В	357	GLU	5.3
2	В	355	ASN	4.4
1	С	351	VAL	4.3
1	С	60	ILE	3.8
1	А	59	GLU	3.6

6.2 Non-standard residues in protein, DNA, RNA chains (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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q < 0.9
2	CSO	В	117	7/8	0.97	0.18	$46,\!46,\!56,\!57$	0
2	CSO	D	117	7/8	0.97	0.18	50,51,63,64	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



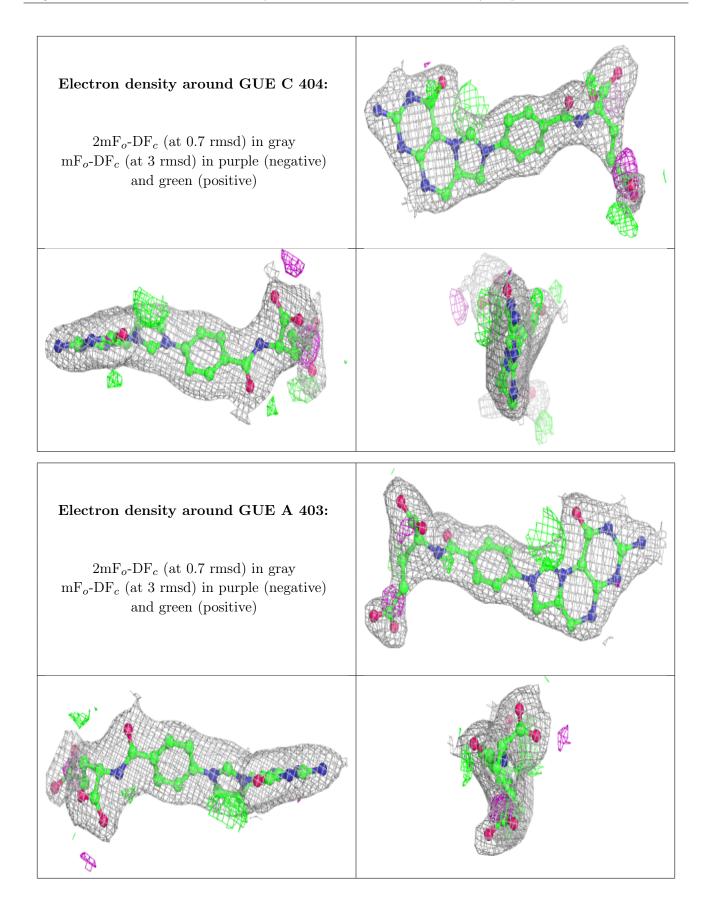
6.4 Ligands (i)

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.

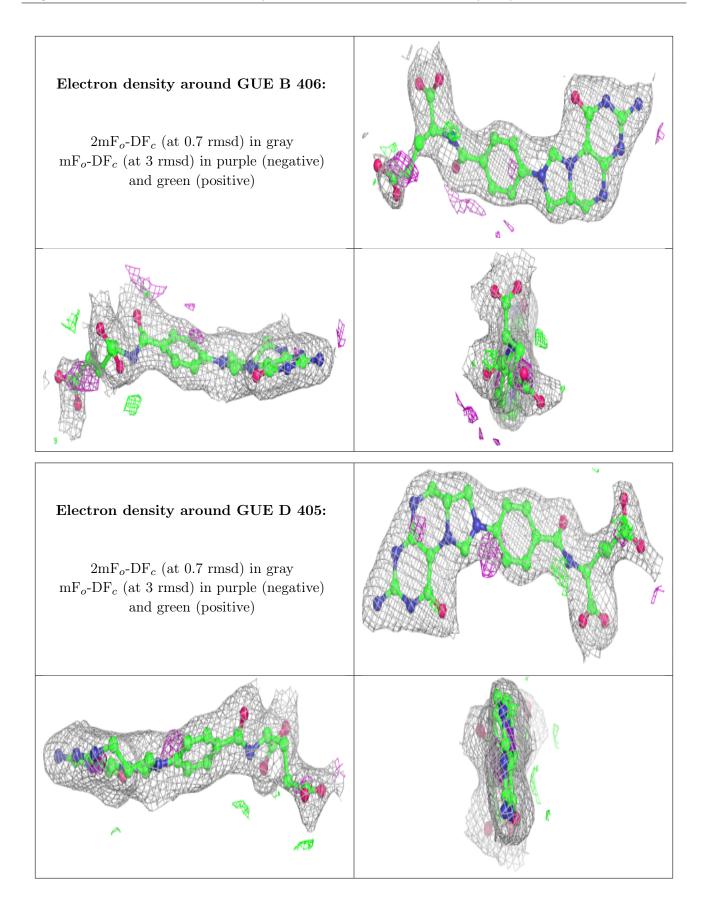
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} extsf{-}\mathbf{factors}(\mathbf{A}^2)$	Q<0.9
4	GOL	D	401	6/6	0.61	0.54	82,83,85,86	0
7	PG4	В	405	8/13	0.63	0.42	71,74,74,75	0
6	DMS	В	404	4/4	0.65	0.34	127,128,128,128	0
4	GOL	А	402	6/6	0.87	0.29	57,61,62,64	0
6	DMS	В	402	4/4	0.88	0.30	91,92,92,92	0
6	DMS	С	403	4/4	0.90	0.16	93,93,93,94	0
6	DMS	В	403	4/4	0.92	0.14	92,93,93,94	0
5	GUE	С	404	33/33	0.93	0.13	40,47,79,80	0
6	DMS	D	404	4/4	0.93	0.13	95,96,96,96	0
5	GUE	А	403	33/33	0.93	0.12	$43,\!55,\!76,\!77$	0
5	GUE	В	406	33/33	0.94	0.14	45,55,80,82	0
5	GUE	D	405	33/33	0.94	0.14	42,51,74,75	0
6	DMS	В	401	4/4	0.94	0.12	85,85,86,86	0
6	DMS	D	402	4/4	0.95	0.14	75,76,77,77	0
6	DMS	D	403	4/4	0.95	0.14	81,82,83,83	0
6	DMS	С	402	4/4	0.97	0.07	72,72,72,73	0
3	FE9	А	401	41/43	0.97	0.10	48,55,62,65	0
3	FE9	С	401	41/43	0.97	0.10	47,55,59,59	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.

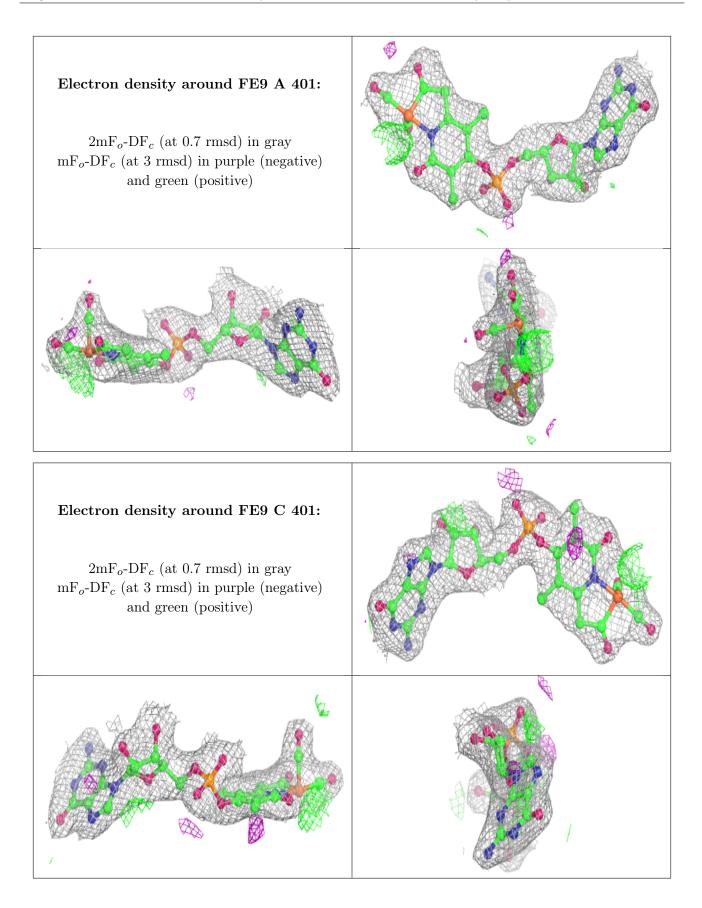














6.5 Other polymers (i)

There are no such residues in this entry.

