

wwPDB X-ray Structure Validation Summary Report (i)

Dec 10, 2022 – 10:15 PM EST

PDB ID	:	1FFV						
Title	:	CARBON MONOXIDE DEHYDROGENASE FROM HY-						
		DROGENOPHAGA PSEUDOFLAVA						
Authors	:	laenzelmann, P.; Dobbek, H.; Gremer, L.; Huber, R.; Meyer, O.						
Deposited on	:	2000-07-26						
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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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.



Motria	Whole archive	Similar resolution
wietric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain	
1	А	163	83%	10% • 5%
1	D	163	82%	13% • •
2	В	803	82%	16% ••
2	Е	803	84%	14% ••
3	С	287	85%	14% •
3	F	287	83%	16% •

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 crite-



ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CSZ	В	385	-	-	Х	-
2	CSZ	Е	385	-	-	Х	-



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 20648 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 CUTS, IRON-SULFUR PROTEIN OF CARBON MONOXIDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	155	Total 1185	С 734	N 216	0 222	S 13	17	0	0
1	D	156	Total 1190	C 737	N 217	0 223	S 13	17	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	90	GLN	ARG	conflict	UNP P19915
D	90	GLN	ARG	conflict	UNP P19915

• Molecule 2 is a protein called CUTL, MOLYBDOPROTEIN OF CARBON MONOXIDE DEHYDROGENASE.

Mol	Chain	Residues		Atoms						AltConf	Trace
2	В	797	Total 6087	C 3860	N 1056	0 1135	S 35	Se 1	50	0	0
2	Е	797	Total 6087	C 3860	N 1056	0 1135	S 35	Se 1	39	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	19	GLY	ARG	conflict	GB 4098682
В	20	ALA	PRO	conflict	GB 4098682
В	21	SER	ARG	conflict	GB 4098682
В	22	ARG	ALA	conflict	GB 4098682
В	23	LEU	CYS	conflict	GB 4098682
В	24	ARG	ALA	conflict	GB 4098682
В	384	ARO	ARG	modified residue	GB 4098682
В	385	CSZ	CYS	modified residue	GB 4098682

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Chain Residue		Modelled	Actual	Comment	Reference
В	456	LEU	TRP	conflict	GB 4098682
Е	384	ARO	ARG	modified residue	GB 4098682
Ε	385	CSZ	CYS	modified residue	GB 4098682
Е	456	LEU	TRP	conflict	GB 4098682

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• Molecule 3 is a protein called CUTM, FLAVOPROTEIN OF CARBON MONOXIDE DE-HYDROGENASE.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
3 C	С	287	Total	С	Ν	Ο	\mathbf{S}	12	0	0
	U	201	2133	1343	384	394	12			
2	Б	287	Total	С	Ν	0	\mathbf{S}	6	0	0
0	Г	r 287	2141	1347	386	396	12			0

There are 18 discrepancies between the modelled and reference sequences:

Chain Residue		Modelled	Actual	Comment	Reference
С	120	ASP	HIS	conflict	UNP P19914
С	89	ALA	GLN	conflict	UNP P19914
С	119	GLY	ASN	conflict	UNP P19914
С	226	ALA	ARG	conflict	UNP P19914
С	228	ALA	GLY	conflict	UNP P19914
С	229	ALA	GLY	conflict	UNP P19914
С	230	GLU	ARG	conflict	UNP P19914
С	231	ALA	SER	conflict	UNP P19914
С	232	ALA	ARG	conflict	UNP P19914
F	120	ASP	HIS	conflict	UNP P19914
F	89	ALA	GLN	conflict	UNP P19914
F	119	GLY	ASN	conflict	UNP P19914
F	226	ALA	ARG	conflict	UNP P19914
F	228	ALA	GLY	conflict	UNP P19914
F	229	ALA	GLY	conflict	UNP P19914
F	230	GLU	ARG	conflict	UNP P19914
F	231	ALA	SER	conflict	UNP P19914
F	232	ALA	ARG	conflict	UNP P19914

• Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	TotalFeS422	0	0
4	А	1	TotalFeS422	0	0
4	D	1	TotalFeS422	0	0
4	D	1	Total Fe S 4 2 2	0	0

• Molecule 5 is (MOLYBDOPTERIN-CYTOSINE DINUCLEOTIDE-S,S)-DIOXO-AQUA-M OLYBDENUM(V) (three-letter code: PCD) (formula: $C_{19}H_{26}MoN_8O_{16}P_2S_2$).





Mol	Chain	Residues			Ato	ZeroOcc	AltConf				
Б	D	1	Total	С	Mo	Ν	Ο	Р	S	0	0
5 В		48	19	1	8	16	2	2	0	0	
5	F	1	Total	С	Mo	Ν	Ο	Р	S	0	0
5	Ľ	1	48	19	1	8	16	2	2	0	0

• Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	
6	C	1	Total	С	Ν	Ο	Р	0	0	
0	U	L	53	27	9	15	2	0		
6	Б	1	Total	С	Ν	Ο	Р	0	0	
0	Г	L	53	27	9	15	2	0		

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	137	Total O 137 137	0	0
7	В	490	Total O 490 490	0	0
7	С	199	Total O 199 199	0	0
7	D	147	Total O 147 147	0	0
7	Е	493	Total O 493 493	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	141	Total O 141 141	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. 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. 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.

Note EDS was not executed.

• Molecule 1: CUTS, IRON-SULFUR PROTEIN OF CARBON MONOXIDE DEHYDROGENASE



 \bullet Molecule 2: CUTL, MOLYBDOPROTEIN OF CARBON MONOXIDE DEHYDROGENASE





• Molecule 3: CUTM, FLAVOPROTEIN OF CARBON MONOXIDE DEHYDROGENASE

Cl	nai	n	C:											859	%												1	.4%)	•				
M1	R5	Y8	K29	L30 L31	836	r 45	E59	R64	E78 N79		R90 1.91	P92	L93	0105	V106	R107	H118	G119	D120 P121	R145	F152	F153 L154	T 160	E165	V172	W181	K185	L186	K187 R188		W193	A194	M202	
R203	H211	1212 R213	V219	A220 P221	L234	E255 P256	A271	1075	W283	A287																								

• Molecule 3: CUTM, FLAVOPROTEIN OF CARBON MONOXIDE DEHYDROGENASE



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source		
Space group	P 21 21 21	Depositor		
Cell constants	86.37Å 193.79Å 218.75Å	Depositor		
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor		
Resolution (Å)	20.00 - 2.25	Depositor		
% Data completeness	(Not available) $(20.00-2.25)$	Depositor		
(in resolution range)	(100 available) (20.00 2.29)	Depositor		
R_{merge}	0.08	Depositor		
R _{sym}	(Not available)	Depositor		
Refinement program	CNS	Depositor		
R, R_{free}	0.209 , 0.237	Depositor		
Estimated twinning fraction	No twinning to report.	Xtriage		
Total number of atoms	20648	wwPDB-VP		
Average B, all atoms $(Å^2)$	32.0	wwPDB-VP		



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: CSZ, FES, FAD, PCD, ARO

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	Chain	Bond	lengths	Bo	ond angles
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.36	0/1202	0.66	0/1619
1	D	0.37	0/1207	0.68	0/1626
2	В	0.36	0/6219	0.66	0/8465
2	Е	0.36	0/6219	0.66	3/8465~(0.0%)
3	С	0.35	0/2172	0.63	0/2947
3	F	0.33	0/2180	0.63	0/2958
All	All	0.36	0/19199	0.66	3/26080~(0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Е	161	LEU	CA-CB-CG	6.25	129.67	115.30
2	Е	803	LEU	CA-CB-CG	6.15	129.45	115.30
2	Е	487	GLY	N-CA-C	5.20	126.11	113.10

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	1185	0	1178	16	0
1	D	1190	0	1183	16	0

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1	F	F	V

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	6087	0	5990	105	0
2	Е	6087	0	5990	90	0
3	С	2133	0	2162	29	0
3	F	2141	0	2173	34	0
4	А	8	0	0	0	0
4	D	8	0	0	0	0
5	В	48	0	21	6	0
5	Ε	48	0	21	4	0
6	С	53	0	27	6	0
6	F	53	0	27	6	0
7	А	137	0	0	1	0
7	В	490	0	0	15	0
7	С	199	0	0	4	0
7	D	147	0	0	3	0
7	E	493	0	0	7	0
7	F	141	0	0	6	0
All	All	20648	0	18772	292	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 8.

The worst 5 of 292 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)
5:B:1920:PCD:S8'	7:B:2389:HOH:O	1.96	1.24
5:E:1921:PCD:H7	7:E:2188:HOH:O	1.62	0.98
5:B:1920:PCD:H102	7:B:2389:HOH:O	1.68	0.93
3:C:203:ARG:HB2	3:C:211:HIS:HB3	1.52	0.91
2:E:174:HIS:HD2	2:E:176:ASN:H	1.20	0.89

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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	153/163~(94%)	149~(97%)	4(3%)	0	100 100
1	D	154/163~(94%)	149~(97%)	5(3%)	0	100 100
2	В	793/803~(99%)	763~(96%)	26~(3%)	4 (0%)	29 29
2	Ε	793/803~(99%)	765~(96%)	23~(3%)	5(1%)	25 25
3	С	285/287~(99%)	277~(97%)	8(3%)	0	100 100
3	F	285/287~(99%)	275~(96%)	10 (4%)	0	100 100
All	All	2463/2506~(98%)	2378 (96%)	76(3%)	9~(0%)	34 37

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	487	GLY
2	Е	487	GLY
2	В	488	PRO
2	Е	262	PRO
2	В	262	PRO

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	Perce	ntiles
1	А	128/132~(97%)	123~(96%)	5(4%)	32	38
1	D	128/132~(97%)	121 (94%)	7~(6%)	21	21
2	В	634/639~(99%)	611 (96%)	23~(4%)	35	42
2	Ε	634/639~(99%)	612~(96%)	22~(4%)	36	43
3	С	212/214~(99%)	202~(95%)	10~(5%)	26	29
3	F	214/214~(100%)	206~(96%)	8 (4%)	34	40
All	All	1950/1970~(99%)	1875 (96%)	75 (4%)	33	39

 $5~{\rm of}~75$ residues with a non-rotameric side chain are listed below:



Mol	Chain	Res	Type
2	Ε	468	ASN
3	F	172	VAL
2	Е	483	VAL
2	Е	777	HIS
2	В	717	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	134	ASN
2	Е	301	ASN
3	F	88	GLN
1	D	149	GLN
2	Е	174	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

4 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).

Mal	Turne	Chain	Dec	Tink	B	ond leng	gths	E	Bond ang	gles
	Type	Unain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	ARO	E	384	2	9,11,12	1.50	1 (11%)	7,13,15	1.63	2 (28%)
2	CSZ	В	385	2	3,6,7	0.67	0	0,6,8	-	-
2	CSZ	Е	385	2	3,6,7	0.61	0	0,6,8	-	-
2	ARO	В	384	2	9,11,12	1.99	1 (11%)	$7,\!13,\!15$	1.18	1 (14%)

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	ARO	Е	384	2	-	2/10/11/13	-
2	CSZ	В	385	2	-	0/0/5/7	-
2	CSZ	Ε	385	2	-	0/0/5/7	-
2	ARO	В	384	2	-	3/10/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	384	ARO	OH-CG	-5.85	1.25	1.43
2	Е	384	ARO	OH-CG	-4.31	1.30	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Ε	384	ARO	OH-CG-CB	3.25	116.54	109.18
2	В	384	ARO	OH-CG-CB	2.46	114.76	109.18
2	Е	384	ARO	OH-CG-CD	2.18	116.77	109.32

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	384	ARO	NE-CD-CG-CB
2	В	384	ARO	NE-CD-CG-OH
2	Е	384	ARO	NE-CD-CG-OH
2	Е	384	ARO	NE-CD-CG-CB
2	В	384	ARO	CA-CB-CG-CD

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Е	384	ARO	1	0
2	В	385	CSZ	4	0
2	Е	385	CSZ	6	0
2	В	384	ARO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.



5.6 Ligand geometry (i)

8 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).

Mal	Tuno	Chain	Res	Tink	Bo	ond leng	ths	Bond angles		
WIOI	туре	Unam			Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FES	А	1907	1	0,4,4	-	-	-		
4	FES	А	1908	1	0,4,4	-	-	-		
6	FAD	F	1923	-	53,58,58	1.93	8 (15%)	68,89,89	4.93	17 (25%)
5	PCD	В	1920	-	36,53,53	1.79	9 (25%)	41,86,86	1.56	9 (21%)
4	FES	D	1909	1	0,4,4	-	-	-		
6	FAD	С	1922	-	53,58,58	1.92	9 (16%)	68,89,89	4.78	17 (25%)
4	FES	D	1910	1	0,4,4	-	-	-		
5	PCD	Е	1921	-	36,53,53	1.84	9 (25%)	41,86,86	1.65	8 (19%)

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	FES	А	1907	1	-	-	0/1/1/1
4	FES	А	1908	1	-	-	0/1/1/1
6	FAD	F	1923	-	-	10/30/50/50	0/6/6/6
5	PCD	В	1920	-	-	3/20/78/78	0/6/6/6
4	FES	D	1909	1	-	-	0/1/1/1
6	FAD	С	1922	-	-	11/30/50/50	0/6/6/6
4	FES	D	1910	1	-	-	0/1/1/1
5	PCD	Е	1921	-	-	3/20/78/78	0/6/6/6

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
6	С	1922	FAD	O4B-C1B	6.80	1.50	1.41
6	F	1923	FAD	O4B-C1B	6.63	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
6	F	1923	FAD	C1'-C2'	6.42	1.61	1.52
5	В	1920	PCD	C6-N1	5.63	1.42	1.35
5	Ε	1921	PCD	C6-N1	5.55	1.42	1.35

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The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	F	1923	FAD	O3'-C3'-C2'	-17.77	65.88	108.81
6	С	1922	FAD	O3'-C3'-C2'	-17.76	65.90	108.81
6	F	1923	FAD	O4'-C4'-C3'	-17.73	66.00	109.10
6	С	1922	FAD	O4'-C4'-C3'	-17.46	66.65	109.10
6	F	1923	FAD	O4'-C4'-C5'	-14.44	77.46	109.92

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	В	1920	PCD	C10-O3B-PB-O1B
5	Е	1921	PCD	C2D-C1'-N1-C6
5	Е	1921	PCD	O4D-C1'-N1-C6
6	С	1922	FAD	C1'-C2'-C3'-O3'
6	С	1922	FAD	O2'-C2'-C3'-C4'

There are no ring outliers.

4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	1923	FAD	6	0
5	В	1920	PCD	6	0
6	С	1922	FAD	6	0
5	Е	1921	PCD	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)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

