Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2022 – 10:15 PM EST

PDB ID	:	1FFV
Title	:	CARBON MONOXIDE DEHYDROGENASE FROM HYDROGENOPHAGA PSEUDOFLAVA
Authors	:	Haenzelmann, P.; Dobbek, H.; Gremer, L.; Huber, R.; Meyer, O.
Deposited on	:	2000-07-26
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 ⓘ 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 ⓘ) were used in the production of this report:

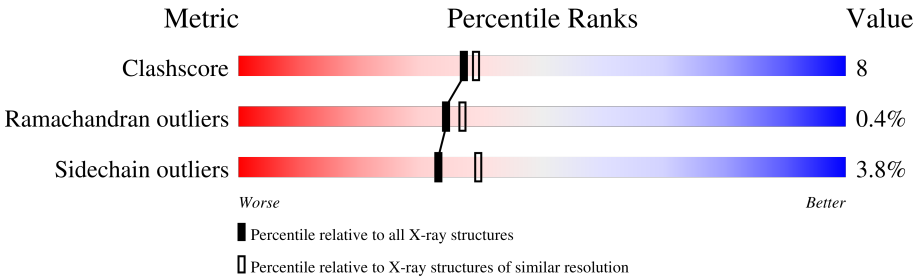
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
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	A	163	83% 10% • 5%
1	D	163	82% 13% • •
2	B	803	82% 16% ••
2	E	803	84% 14% ••
3	C	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	B	385	-	-	X	-
2	CSZ	E	385	-	-	X	-

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	A	155	Total	C	N	O	S	17	0	0
			1185	734	216	222	13			
1	D	156	Total	C	N	O	S	17	0	0
			1190	737	217	223	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	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						ZeroOcc	AltConf	Trace
2	B	797	Total	C	N	O	S	Se	50	0	0
			6087	3860	1056	1135	35	1			
2	E	797	Total	C	N	O	S	Se	39	0	0
			6087	3860	1056	1135	35	1			

There are 12 discrepancies between the modelled and reference sequences:

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

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

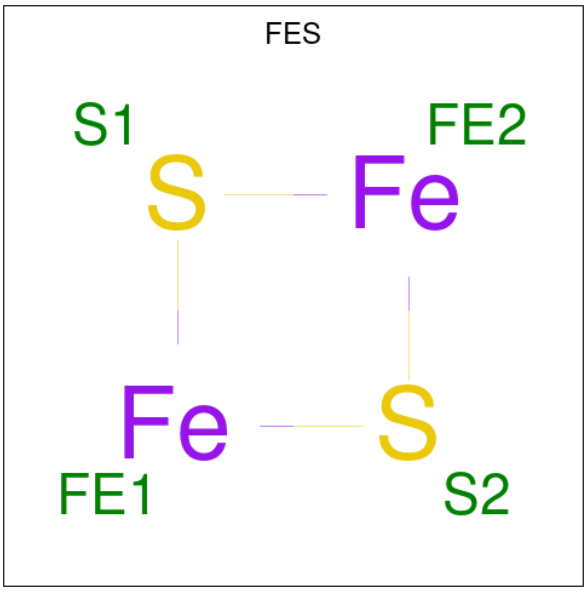
- Molecule 3 is a protein called CUTM, FLAVOPROTEIN OF CARBON MONOXIDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	287	Total	C	N	O	S	12	0	0
			2133	1343	384	394	12			
3	F	287	Total	C	N	O	S	6	0	0
			2141	1347	386	396	12			

There are 18 discrepancies between the modelled and reference sequences:

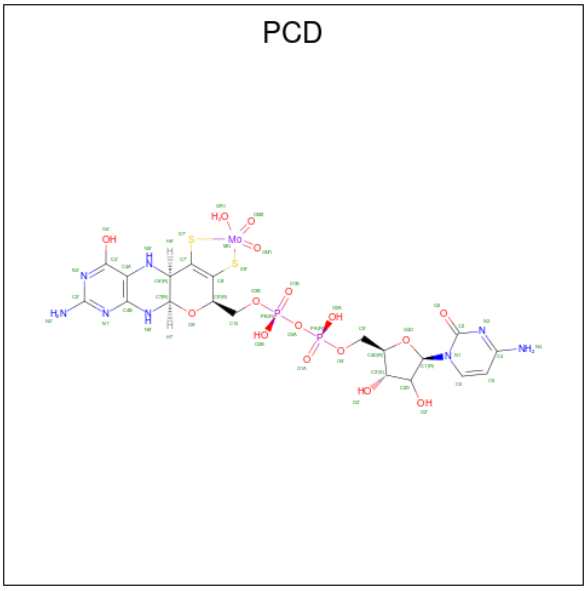
Chain	Residue	Modelled	Actual	Comment	Reference
C	120	ASP	HIS	conflict	UNP P19914
C	89	ALA	GLN	conflict	UNP P19914
C	119	GLY	ASN	conflict	UNP P19914
C	226	ALA	ARG	conflict	UNP P19914
C	228	ALA	GLY	conflict	UNP P19914
C	229	ALA	GLY	conflict	UNP P19914
C	230	GLU	ARG	conflict	UNP P19914
C	231	ALA	SER	conflict	UNP P19914
C	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: Fe_2S_2).



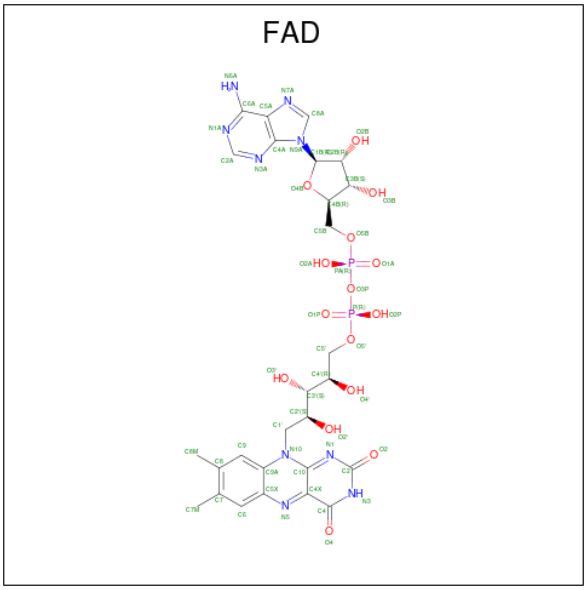
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 4 2 2	0	0
4	A	1	Total Fe S 4 2 2	0	0
4	D	1	Total Fe S 4 2 2	0	0
4	D	1	Total Fe S 4 2 2	0	0

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



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	B	1	Total	C	Mo	N	O	P	S	0	0
			48	19	1	8	16	2	2		
5	E	1	Total	C	Mo	N	O	P	S	0	0
			48	19	1	8	16	2	2		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
6	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	137	Total	O	0	0
			137	137		
7	B	490	Total	O	0	0
			490	490		
7	C	199	Total	O	0	0
			199	199		
7	D	147	Total	O	0	0
			147	147		
7	E	493	Total	O	0	0
			493	493		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	F	141	Total	O	0	0
			141	141		

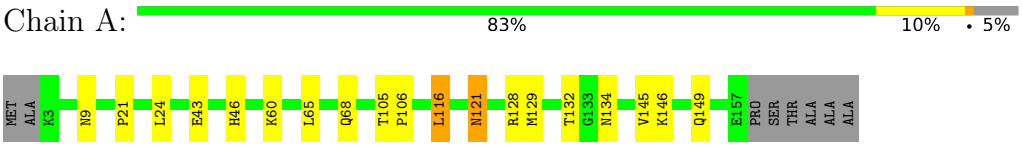
3 Residue-property plots (i)

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.

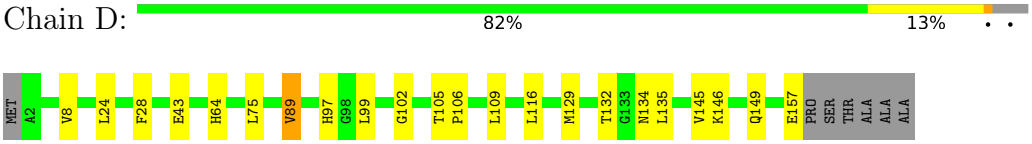
• Molecule 1: CUTS, IRON-SULFUR PROTEIN OF CARBON MONOXIDE DEHYDROGENASE

Chain A:



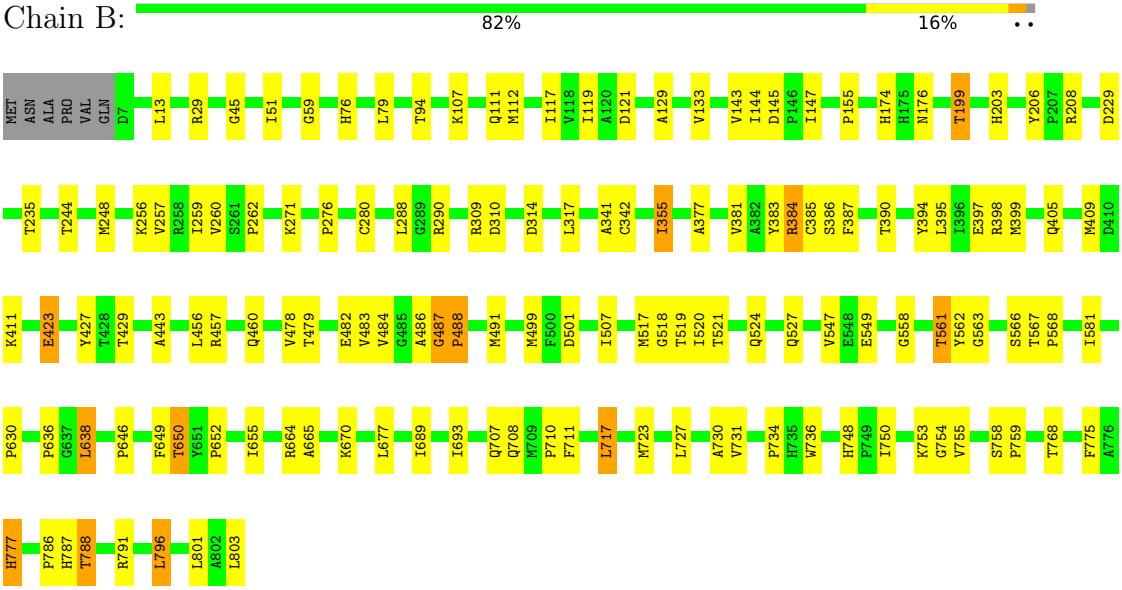
• Molecule 1: CUTS, IRON-SULFUR PROTEIN OF CARBON MONOXIDE DEHYDROGENASE

Chain D:



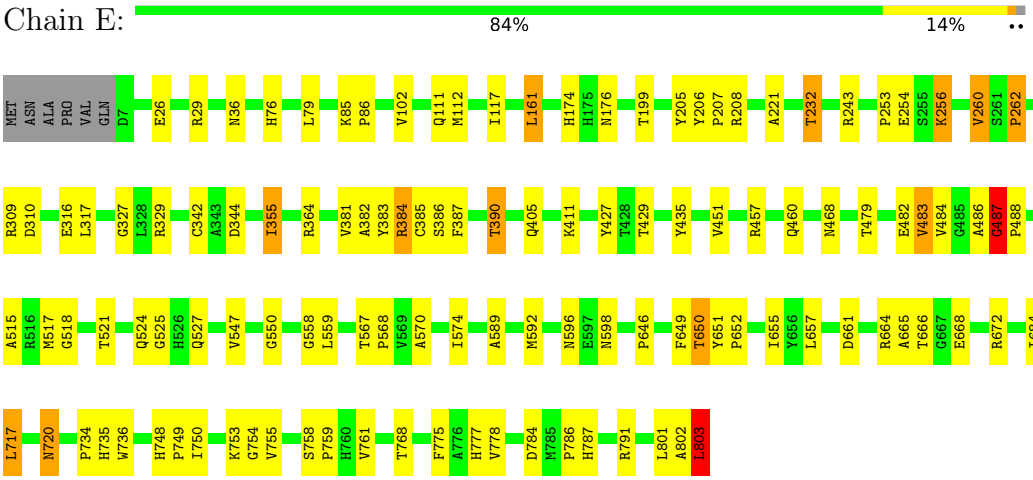
• Molecule 2: CUTL, MOLYBDOPROTEIN OF CARBON MONOXIDE DEHYDROGENASE

Chain B:



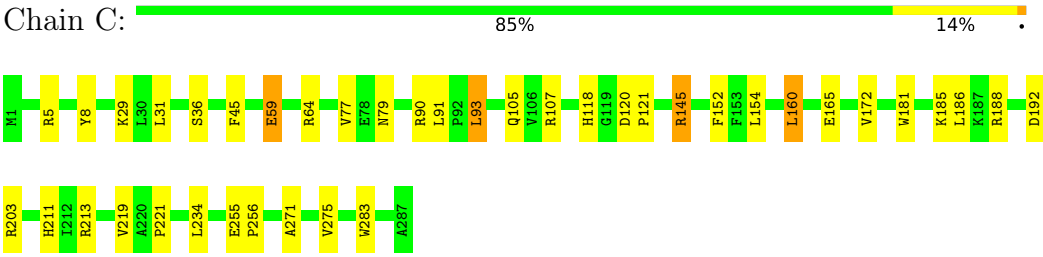
• Molecule 2: CUTL, MOLYBDOPROTEIN OF CARBON MONOXIDE DEHYDROGENASE

Chain E:



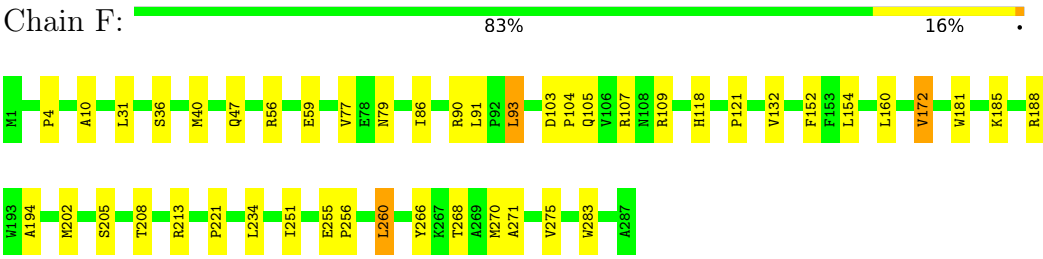
• Molecule 3: CUTM, FLAVOPROTEIN OF CARBON MONOXIDE DEHYDROGENASE

Chain C:



• Molecule 3: CUTM, FLAVOPROTEIN OF CARBON MONOXIDE DEHYDROGENASE

Chain F:



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 a, b, c, α, β, γ	86.37Å 193.79Å 218.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.25)	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

5.1 Standard geometry

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.36	0/1202	0.66	0/1619
1	D	0.37	0/1207	0.68	0/1626
2	B	0.36	0/6219	0.66	0/8465
2	E	0.36	0/6219	0.66	3/8465 (0.0%)
3	C	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	E	161	LEU	CA-CB-CG	6.25	129.67	115.30
2	E	803	LEU	CA-CB-CG	6.15	129.45	115.30
2	E	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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	6087	0	5990	105	0
2	E	6087	0	5990	90	0
3	C	2133	0	2162	29	0
3	F	2141	0	2173	34	0
4	A	8	0	0	0	0
4	D	8	0	0	0	0
5	B	48	0	21	6	0
5	E	48	0	21	4	0
6	C	53	0	27	6	0
6	F	53	0	27	6	0
7	A	137	0	0	1	0
7	B	490	0	0	15	0
7	C	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

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.

All (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
2:E:243:ARG:HD3	2:E:254:GLU:HG2	1.53	0.89
6:C:1922:FAD:H51A	6:C:1922:FAD:H8A	1.54	0.88
2:B:29:ARG:HH22	2:B:527:GLN:HE22	1.21	0.86
2:B:788:THR:HG22	2:B:791:ARG:H	1.40	0.86
6:F:1923:FAD:H8A	6:F:1923:FAD:H52A	1.55	0.86
2:E:457:ARG:HH11	2:E:460:GLN:HE22	1.25	0.84
2:B:520:ILE:H	2:B:561:THR:CG2	1.91	0.83
2:E:29:ARG:HH22	2:E:527:GLN:HE22	1.27	0.82
2:B:174:HIS:HD2	2:B:176:ASN:H	1.30	0.80
2:B:381:VAL:HG13	2:B:385:CSZ:SG	2.24	0.78
1:D:134:ASN:HD21	3:F:105:GLN:HE22	1.30	0.77
6:F:1923:FAD:H8A	6:F:1923:FAD:C5B	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:384:ARO:HD2	7:E:2188:HOH:O	1.87	0.75
6:C:1922:FAD:H8A	6:C:1922:FAD:C5B	2.17	0.73
2:B:385:CSZ:SE	7:B:2391:HOH:O	2.57	0.73
3:F:10:ALA:HB1	3:F:56:ARG:HD2	1.71	0.71
2:B:664:ARG:HD2	2:B:801:LEU:O	1.91	0.71
2:B:457:ARG:HH11	2:B:460:GLN:HE22	1.37	0.70
2:B:788:THR:HG21	7:B:2068:HOH:O	1.93	0.69
2:B:748:HIS:HD2	2:B:750:ILE:H	1.40	0.69
3:F:202:MET:HE2	3:F:283:TRP:HA	1.76	0.68
2:B:665:ALA:HA	2:B:803:LEU:HD22	1.75	0.68
2:B:174:HIS:CD2	2:B:176:ASN:H	2.13	0.67
2:B:519:THR:HB	2:B:561:THR:HG22	1.76	0.67
2:E:76:HIS:HD2	7:E:2381:HOH:O	1.77	0.67
5:B:1920:PCD:MO	5:B:1920:PCD:OM1	1.64	0.67
1:D:134:ASN:ND2	3:F:105:GLN:HE22	1.93	0.66
2:E:487:GLY:HA3	2:E:646:PRO:HG3	1.78	0.66
2:B:520:ILE:H	2:B:561:THR:HG23	1.60	0.66
2:E:479:THR:HG22	2:E:655:ILE:HG13	1.78	0.66
2:B:581:ILE:HG23	2:B:638:LEU:HD22	1.78	0.66
3:C:36:SER:HB2	6:C:1922:FAD:H5'2	1.77	0.66
2:B:199:THR:HG22	7:B:2227:HOH:O	1.95	0.65
2:E:484:VAL:HG23	2:E:650:THR:HG22	1.78	0.65
3:F:205:SER:O	3:F:208:THR:HG22	1.96	0.65
2:E:221:ALA:HA	2:E:232:THR:HB	1.78	0.65
2:E:720:ASN:HD22	2:E:720:ASN:H	1.44	0.65
2:E:253:PRO:HG2	2:E:256:LYS:HG3	1.78	0.65
2:E:381:VAL:HG13	2:E:385:CSZ:SG	2.36	0.65
3:F:202:MET:HE1	3:F:283:TRP:HE3	1.59	0.65
2:E:650:THR:HG21	2:E:754:GLY:H	1.63	0.64
2:E:748:HIS:HD2	2:E:750:ILE:H	1.46	0.64
2:E:664:ARG:HD2	2:E:801:LEU:O	1.97	0.64
2:B:487:GLY:HA3	2:B:646:PRO:HG3	1.80	0.64
3:C:45:PHE:HB3	7:C:2118:HOH:O	1.97	0.63
2:B:423:GLU:HG3	7:B:2366:HOH:O	1.99	0.62
2:E:174:HIS:CD2	2:E:176:ASN:H	2.09	0.62
3:C:59:GLU:HG3	7:C:1966:HOH:O	1.99	0.62
2:B:256:LYS:HE3	7:B:2354:HOH:O	1.98	0.62
7:D:1923:HOH:O	2:E:735:HIS:HD2	1.83	0.62
3:C:121:PRO:HG3	3:C:221:PRO:O	2.00	0.62
2:E:527:GLN:HA	2:E:547:VAL:HG22	1.81	0.61
2:B:405:GLN:HE21	2:B:411:LYS:NZ	1.97	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:243:ARG:CD	2:E:254:GLU:HG2	2.29	0.61
2:E:486:ALA:HA	2:E:649:PHE:CE2	2.35	0.61
3:F:121:PRO:HG3	3:F:221:PRO:O	2.00	0.61
2:B:487:GLY:HA2	2:B:499:MET:O	2.01	0.61
3:C:77:VAL:HG13	3:C:107:ARG:O	2.00	0.61
2:B:723:MET:HG3	7:B:2393:HOH:O	2.02	0.60
3:C:185:LYS:HG3	3:C:194:ALA:HB2	1.82	0.60
2:E:487:GLY:HA3	2:E:646:PRO:CG	2.31	0.60
2:B:342:CYS:SG	2:B:381:VAL:HG23	2.42	0.60
1:A:121:ASN:H	1:A:121:ASN:HD22	1.49	0.60
2:B:45:GLY:O	2:B:290:ARG:HD2	2.02	0.60
2:B:518:GLY:HA3	2:B:558:GLY:HA3	1.83	0.60
2:E:666:THR:OG1	2:E:668:GLU:HG2	2.02	0.59
2:E:483:VAL:HG13	2:E:651:TYR:CE2	2.37	0.59
3:F:36:SER:HB2	6:F:1923:FAD:H5'2	1.84	0.59
2:B:650:THR:HG21	2:B:754:GLY:H	1.67	0.59
2:E:720:ASN:H	2:E:720:ASN:ND2	2.00	0.58
2:B:723:MET:HE1	3:C:193:TRP:CZ3	2.38	0.58
3:C:79:ASN:HD21	3:C:107:ARG:HE	1.50	0.58
2:B:748:HIS:CD2	2:B:750:ILE:H	2.21	0.58
6:C:1922:FAD:H51A	6:C:1922:FAD:C8A	2.31	0.57
2:E:457:ARG:HH11	2:E:460:GLN:NE2	2.01	0.57
3:C:255:GLU:HG2	7:C:1969:HOH:O	2.04	0.56
3:C:202:MET:CE	3:C:283:TRP:HE3	2.19	0.56
2:B:486:ALA:HA	2:B:649:PHE:CE2	2.40	0.56
3:C:29:LYS:HD3	7:C:2024:HOH:O	2.06	0.56
3:C:93:LEU:HG	3:C:181:TRP:HB2	1.88	0.56
1:A:121:ASN:HD22	1:A:121:ASN:N	2.03	0.56
2:E:748:HIS:CD2	2:E:750:ILE:H	2.24	0.55
2:B:487:GLY:HA3	2:B:646:PRO:CG	2.36	0.55
3:F:59:GLU:HB3	7:F:2038:HOH:O	2.05	0.55
3:F:93:LEU:HG	3:F:181:TRP:HB2	1.87	0.55
1:D:89:VAL:HG13	1:D:109:LEU:HD22	1.89	0.55
2:B:317:LEU:HD22	2:B:399:MET:HB3	1.89	0.55
2:B:650:THR:HG23	2:B:753:LYS:HB3	1.87	0.55
2:B:385:CSZ:SE	5:B:1920:PCD:OR1	2.75	0.54
3:C:145:ARG:HD3	3:C:165:GLU:OE2	2.07	0.54
3:F:86:ILE:HG13	7:F:2062:HOH:O	2.07	0.54
3:F:185:LYS:HG3	3:F:194:ALA:HB2	1.90	0.54
3:F:79:ASN:HD21	3:F:107:ARG:HE	1.56	0.54
2:E:518:GLY:HA3	2:E:558:GLY:HA3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:457:ARG:NH1	2:E:460:GLN:HE22	2.00	0.53
2:E:486:ALA:HA	2:E:649:PHE:HE2	1.71	0.53
2:E:717:LEU:HD13	2:E:720:ASN:HB3	1.90	0.53
3:F:77:VAL:HG13	3:F:107:ARG:O	2.08	0.53
2:E:786:PRO:O	2:E:791:ARG:HD3	2.08	0.53
2:B:768:THR:OG1	2:B:787:HIS:HE1	1.92	0.53
1:D:129:MET:CE	3:F:190:THR:HG21	2.38	0.52
2:E:589:ALA:HA	2:E:592:MET:HE2	1.90	0.52
2:B:111:GLN:O	2:B:112:MET:HB2	2.09	0.52
2:B:527:GLN:HA	2:B:547:VAL:HG22	1.91	0.52
2:E:381:VAL:HG13	2:E:385:CSZ:SE	2.60	0.52
2:E:661:ASP:OD2	2:E:672:ARG:HD3	2.09	0.52
2:E:355:ILE:HG13	2:E:483:VAL:CG2	2.39	0.51
2:E:427:TYR:HE2	2:E:429:THR:HG22	1.75	0.51
2:E:405:GLN:HE21	2:E:411:LYS:NZ	2.08	0.51
3:F:255:GLU:N	3:F:256:PRO:HD3	2.26	0.51
1:A:146:LYS:HA	1:A:149:GLN:HE21	1.75	0.51
1:D:146:LYS:HA	1:D:149:GLN:HE21	1.76	0.51
2:B:405:GLN:HE21	2:B:411:LYS:HZ1	1.59	0.51
2:B:208:ARG:NH2	2:B:377:ALA:O	2.44	0.50
2:B:398:ARG:HD2	7:B:2102:HOH:O	2.12	0.50
1:A:21:PRO:HB3	3:C:8:TYR:HB2	1.93	0.50
2:B:521:THR:HG21	7:B:2266:HOH:O	2.12	0.50
2:B:384:ARO:HG	5:B:1920:PCD:S7'	2.52	0.50
2:E:111:GLN:HE22	2:E:717:LEU:H	1.59	0.50
2:B:59:GLY:O	2:B:107:LYS:HB2	2.12	0.50
3:C:202:MET:HE2	3:C:283:TRP:HE3	1.75	0.50
1:D:129:MET:HE3	3:F:190:THR:HG21	1.93	0.49
1:A:121:ASN:H	1:A:121:ASN:ND2	2.10	0.49
3:C:79:ASN:ND2	3:C:107:ARG:HE	2.11	0.49
2:E:720:ASN:HD22	2:E:720:ASN:N	2.05	0.49
3:F:79:ASN:ND2	3:F:107:ARG:HE	2.10	0.49
2:B:723:MET:HE1	3:C:193:TRP:CH2	2.48	0.49
2:B:94:THR:HB	2:B:341:ALA:HA	1.94	0.48
2:B:143:VAL:CG2	2:B:155:PRO:HG2	2.43	0.48
2:B:562:TYR:HA	7:B:2389:HOH:O	2.12	0.48
3:F:154:LEU:HD21	3:F:160:LEU:HD13	1.95	0.48
2:B:670:LYS:HE2	7:B:2396:HOH:O	2.13	0.48
2:B:427:TYR:HE2	2:B:429:THR:HG22	1.77	0.48
2:B:562:TYR:CA	7:B:2389:HOH:O	2.61	0.48
1:A:129:MET:HA	1:A:132:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:HIS:HD2	7:F:1945:HOH:O	1.96	0.48
2:E:787:HIS:HD2	7:E:2131:HOH:O	1.97	0.48
3:F:202:MET:CE	3:F:283:TRP:HE3	2.25	0.48
2:E:385:CSZ:SE	7:E:2367:HOH:O	2.82	0.48
2:E:517:MET:SD	2:E:517:MET:N	2.87	0.48
2:E:36:ASN:O	2:E:262:PRO:HB2	2.14	0.48
2:E:650:THR:HG23	2:E:652:PRO:HD3	1.96	0.48
2:E:768:THR:HA	2:E:787:HIS:CE1	2.49	0.48
2:E:111:GLN:NE2	2:E:717:LEU:H	2.12	0.47
2:E:208:ARG:HD2	2:E:310:ASP:OD2	2.14	0.47
3:F:103:ASP:HB2	3:F:104:PRO:CD	2.44	0.47
2:E:707:GLN:O	2:E:786:PRO:HG3	2.15	0.47
2:B:443:ALA:HB3	2:B:655:ILE:HD12	1.96	0.47
2:E:26:GLU:OE2	2:E:525:GLY:HA2	2.14	0.47
2:E:487:GLY:HA2	2:E:499:MET:O	2.14	0.47
2:E:567:THR:HB	2:E:568:PRO:HD3	1.96	0.47
2:B:707:GLN:O	2:B:786:PRO:HG3	2.15	0.47
2:E:268:PHE:HA	5:E:1921:PCD:S7'	2.54	0.47
2:B:519:THR:HB	2:B:561:THR:CG2	2.44	0.47
1:A:145:VAL:O	1:A:149:GLN:HG3	2.15	0.47
2:B:507:ILE:HD13	2:B:581:ILE:HD13	1.98	0.46
6:C:1922:FAD:C5B	6:C:1922:FAD:C8A	2.91	0.46
2:E:327:GLY:HA2	2:E:364:ARG:O	2.15	0.46
2:B:563:GLY:N	5:B:1920:PCD:OM2	2.38	0.46
1:D:8:VAL:HG11	1:D:28:PHE:CE2	2.50	0.46
2:B:484:VAL:HG23	2:B:650:THR:HG22	1.98	0.46
3:C:90:ARG:O	3:C:91:LEU:HD23	2.15	0.46
2:B:386:SER:O	2:B:387:PHE:HB2	2.16	0.46
2:B:397:GLU:HG3	2:B:478:VAL:HG13	1.98	0.46
1:D:102:GLY:HA2	1:D:105:THR:OG1	2.16	0.46
2:E:596:ASN:HD22	2:E:598:ASN:H	1.64	0.46
2:B:76:HIS:HE1	2:B:121:ASP:OD1	1.98	0.46
2:B:677:LEU:C	2:B:677:LEU:HD23	2.36	0.46
2:B:775:PHE:CZ	2:B:796:LEU:HD13	2.51	0.45
7:A:2015:HOH:O	3:C:5:ARG:HG2	2.16	0.45
2:B:395:LEU:O	2:B:399:MET:HG2	2.16	0.45
2:E:316:GLU:OE2	2:E:329:ARG:HD2	2.16	0.45
1:A:65:LEU:HB2	1:A:68:GLN:HG3	1.98	0.45
2:B:355:ILE:HG13	2:B:483:VAL:HG11	1.99	0.45
2:B:443:ALA:CB	2:B:655:ILE:HD12	2.46	0.45
2:B:199:THR:HB	7:B:2279:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:768:THR:HA	2:B:787:HIS:CE1	2.51	0.45
2:E:429:THR:CG2	2:E:435:TYR:CE1	2.99	0.45
2:E:451:VAL:HG21	2:E:657:LEU:HD13	1.99	0.45
2:B:758:SER:N	2:B:759:PRO:HD2	2.32	0.45
1:A:121:ASN:N	1:A:121:ASN:ND2	2.64	0.45
2:E:390:THR:HG23	2:E:761:VAL:HG22	1.98	0.45
2:E:499:MET:HA	2:E:559:LEU:HG	1.97	0.45
6:F:1923:FAD:H2B	6:F:1923:FAD:H51A	1.79	0.45
1:A:116:LEU:HA	1:A:116:LEU:HD12	1.81	0.44
2:E:355:ILE:HG13	2:E:483:VAL:HG21	1.99	0.44
2:E:521:THR:HG21	7:E:2314:HOH:O	2.17	0.44
2:E:484:VAL:CG2	2:E:650:THR:HG22	2.47	0.44
6:F:1923:FAD:H52A	6:F:1923:FAD:C8A	2.38	0.44
3:C:154:LEU:HD21	3:C:160:LEU:HD13	1.99	0.44
1:D:89:VAL:HG13	1:D:109:LEU:CD2	2.47	0.44
2:B:244:THR:O	2:B:248:MET:HG2	2.17	0.44
2:E:344:ASP:HB2	7:E:2210:HOH:O	2.16	0.44
2:E:382:ALA:N	2:E:385:CSZ:SE	3.01	0.44
2:B:129:ALA:O	2:B:133:VAL:HG23	2.17	0.44
3:C:152:PHE:HA	3:C:160:LEU:HD22	1.99	0.44
2:E:775:PHE:O	2:E:778:VAL:HG22	2.18	0.44
2:B:788:THR:HG23	7:B:2040:HOH:O	2.18	0.44
2:E:570:ALA:O	2:E:574:ILE:HG13	2.17	0.44
2:B:507:ILE:CD1	2:B:581:ILE:HD13	2.47	0.44
3:F:91:LEU:HD21	3:F:172:VAL:HG22	2.00	0.44
2:E:85:LYS:HB2	2:E:86:PRO:HD3	1.99	0.43
2:B:517:MET:SD	2:B:517:MET:N	2.91	0.43
2:B:630:PRO:HG3	2:B:636:PRO:HG3	1.99	0.43
3:C:188:ARG:HD3	3:C:192:ASP:OD2	2.18	0.43
2:E:429:THR:HG21	2:E:435:TYR:CE1	2.53	0.43
3:F:266:TYR:O	3:F:270:MET:HG2	2.18	0.43
2:E:385:CSZ:SE	5:E:1921:PCD:OR1	2.86	0.43
2:B:487:GLY:O	2:B:488:PRO:C	2.56	0.43
2:B:519:THR:O	2:B:549:GLU:HB3	2.18	0.43
1:D:105:THR:HB	1:D:106:PRO:HD3	1.99	0.43
2:E:734:PRO:HG2	2:E:736:TRP:CH2	2.54	0.43
3:F:4:PRO:HG3	3:F:47:GLN:HG2	2.00	0.43
3:F:59:GLU:HG2	7:F:2039:HOH:O	2.18	0.43
1:A:132:THR:HG22	2:B:731:VAL:HG23	2.01	0.43
2:B:79:LEU:HD12	2:B:117:ILE:HD11	2.01	0.43
2:B:483:VAL:O	2:B:483:VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:734:PRO:HG2	2:B:736:TRP:CH2	2.53	0.43
3:F:251:ILE:HG23	3:F:268:THR:CG2	2.48	0.43
1:A:134:ASN:ND2	3:C:105:GLN:HE22	2.17	0.42
1:A:105:THR:HB	1:A:106:PRO:HD3	2.01	0.42
2:B:423:GLU:HG3	2:B:423:GLU:H	1.58	0.42
2:E:758:SER:N	2:E:759:PRO:HD2	2.34	0.42
6:F:1923:FAD:C5B	6:F:1923:FAD:C8A	2.92	0.42
2:B:235:THR:HB	2:B:271:LYS:HD3	2.00	0.42
3:C:255:GLU:N	3:C:256:PRO:HD3	2.35	0.42
1:D:129:MET:HE1	7:F:2030:HOH:O	2.19	0.42
2:E:111:GLN:O	2:E:112:MET:HB2	2.20	0.42
2:E:768:THR:OG1	2:E:787:HIS:HE1	2.01	0.42
3:F:152:PHE:HA	3:F:160:LEU:HD22	2.01	0.42
1:A:46:HIS:HE1	2:B:723:MET:HE3	1.85	0.42
2:B:567:THR:HB	2:B:568:PRO:HD3	2.01	0.42
2:E:386:SER:O	2:E:387:PHE:HB2	2.19	0.42
2:E:665:ALA:HA	2:E:803:LEU:HB3	2.01	0.42
3:F:271:ALA:O	3:F:275:VAL:HG23	2.19	0.42
2:E:427:TYR:CE2	2:E:429:THR:HG22	2.54	0.42
2:B:394:TYR:O	2:B:398:ARG:HG2	2.20	0.42
2:B:727:LEU:HD23	2:B:727:LEU:HA	1.84	0.42
2:E:515:ALA:O	2:E:547:VAL:HA	2.20	0.42
2:E:748:HIS:HA	2:E:749:PRO:HD3	1.97	0.42
2:B:385:CSZ:SE	2:B:385:CSZ:N	3.03	0.42
2:B:650:THR:CG2	2:B:753:LYS:HB3	2.50	0.42
2:E:102:VAL:HA	2:E:276:PRO:HB3	2.01	0.42
2:E:381:VAL:CG1	2:E:385:CSZ:SE	3.18	0.42
2:B:479:THR:HG22	2:B:655:ILE:HG12	2.01	0.41
2:E:260:VAL:HA	2:E:550:GLY:O	2.20	0.41
2:B:257:VAL:HG12	2:B:259:ILE:CD1	2.50	0.41
2:B:708:GLN:HG3	2:B:710:PRO:HD3	2.03	0.41
1:D:97:HIS:HA	7:D:1911:HOH:O	2.19	0.41
3:C:271:ALA:O	3:C:275:VAL:HG23	2.20	0.41
2:B:427:TYR:CE2	2:B:429:THR:HG22	2.55	0.41
2:E:784:ASP:O	2:E:791:ARG:NH1	2.54	0.41
2:B:208:ARG:HD2	2:B:310:ASP:OD2	2.21	0.41
2:E:684:ILE:HB	5:E:1921:PCD:O2	2.21	0.41
1:A:60:LYS:HG3	3:C:105:GLN:HB3	2.03	0.41
2:B:409:MET:HB2	2:B:409:MET:HE2	1.81	0.41
2:B:561:THR:HB	2:B:566:SER:OG	2.21	0.41
3:C:219:VAL:HG11	3:C:271:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:GLU:HB3	7:D:1940:HOH:O	2.21	0.41
2:B:117:ILE:HD13	2:B:280:CYS:HB3	2.03	0.41
1:D:145:VAL:O	1:D:149:GLN:HG3	2.21	0.41
2:E:527:GLN:HA	2:E:547:VAL:CG2	2.48	0.41
2:B:145:ASP:OD2	2:B:147:ILE:HB	2.21	0.41
2:B:650:THR:HG23	2:B:652:PRO:HD3	2.02	0.41
2:B:689:ILE:O	2:B:693:ILE:HG12	2.20	0.41
2:B:777:HIS:H	2:B:777:HIS:CD2	2.38	0.41
6:C:1922:FAD:N1	6:C:1922:FAD:O2'	2.49	0.41
1:D:129:MET:CE	1:D:132:THR:HG21	2.51	0.41
2:E:355:ILE:HG13	2:E:483:VAL:HG22	2.02	0.41
3:F:260:LEU:HD13	3:F:260:LEU:HA	1.91	0.41
2:B:119:ILE:HG21	2:B:288:LEU:CD1	2.51	0.40
2:E:205:TYR:O	2:E:207:PRO:HD3	2.21	0.40
2:E:650:THR:HG23	2:E:753:LYS:HB3	2.03	0.40
3:F:188:ARG:HD3	3:F:192:ASP:OD2	2.21	0.40
2:B:229:ASP:HB2	2:B:256:LYS:O	2.22	0.40
3:F:40:MET:HE1	3:F:118:HIS:HE1	1.86	0.40
3:F:90:ARG:HA	3:F:90:ARG:HD3	1.93	0.40
3:F:103:ASP:HB2	3:F:104:PRO:HD2	2.03	0.40
2:B:457:ARG:NH1	2:B:460:GLN:HE22	2.11	0.40
3:C:118:HIS:CD2	3:C:120:ASP:HB2	2.57	0.40
3:F:59:GLU:HG2	7:F:1982:HOH:O	2.20	0.40
2:B:51:ILE:HG12	2:B:117:ILE:HG22	2.04	0.40
2:B:203:HIS:HD2	2:B:314:ASP:OD1	2.04	0.40
2:B:711:PHE:CE2	2:B:717:LEU:HG	2.57	0.40
2:E:802:ALA:O	2:E:803:LEU:HD13	2.21	0.40
1:A:128:ARG:HD3	2:B:730:ALA:O	2.21	0.40
2:E:79:LEU:HD12	2:E:117:ILE:HD11	2.03	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	153/163 (94%)	149 (97%)	4 (3%)	0	100	100
1	D	154/163 (94%)	149 (97%)	5 (3%)	0	100	100
2	B	793/803 (99%)	763 (96%)	26 (3%)	4 (0%)	29	29
2	E	793/803 (99%)	765 (96%)	23 (3%)	5 (1%)	25	25
3	C	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

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	487	GLY
2	E	487	GLY
2	B	488	PRO
2	E	262	PRO
2	B	262	PRO
2	E	488	PRO
2	B	755	VAL
2	E	755	VAL
2	E	706	GLY

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	128/132 (97%)	123 (96%)	5 (4%)	32	38
1	D	128/132 (97%)	121 (94%)	7 (6%)	21	21
2	B	634/639 (99%)	611 (96%)	23 (4%)	35	42
2	E	634/639 (99%)	612 (96%)	22 (4%)	36	43
3	C	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

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	24	LEU
1	A	43	GLU
1	A	116	LEU
1	A	121	ASN
2	B	13	LEU
2	B	144	ILE
2	B	199	THR
2	B	206	TYR
2	B	260	VAL
2	B	276	PRO
2	B	309	ARG
2	B	355	ILE
2	B	383	TYR
2	B	390	THR
2	B	423	GLU
2	B	456	LEU
2	B	482	GLU
2	B	491	MET
2	B	501	ASP
2	B	524	GLN
2	B	561	THR
2	B	638	LEU
2	B	650	THR
2	B	717	LEU
2	B	777	HIS
2	B	788	THR
2	B	796	LEU
3	C	31	LEU
3	C	59	GLU
3	C	64	ARG
3	C	93	LEU
3	C	145	ARG
3	C	160	LEU
3	C	172	VAL
3	C	186	LEU
3	C	213	ARG
3	C	234	LEU
1	D	24	LEU
1	D	43	GLU
1	D	75	LEU
1	D	89	VAL

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Mol	Chain	Res	Type
1	D	99	LEU
1	D	116	LEU
1	D	135	LEU
2	E	161	LEU
2	E	199	THR
2	E	206	TYR
2	E	232	THR
2	E	256	LYS
2	E	260	VAL
2	E	309	ARG
2	E	317	LEU
2	E	342	CYS
2	E	355	ILE
2	E	383	TYR
2	E	390	THR
2	E	468	ASN
2	E	482	GLU
2	E	483	VAL
2	E	501	ASP
2	E	524	GLN
2	E	650	THR
2	E	717	LEU
2	E	720	ASN
2	E	777	HIS
2	E	803	LEU
3	F	31	LEU
3	F	93	LEU
3	F	109	ARG
3	F	132	VAL
3	F	172	VAL
3	F	213	ARG
3	F	234	LEU
3	F	260	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	34	ASN
1	A	121	ASN
1	A	134	ASN
1	A	149	GLN

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Mol	Chain	Res	Type
2	B	48	HIS
2	B	76	HIS
2	B	174	HIS
2	B	202	GLN
2	B	203	HIS
2	B	270	ASN
2	B	301	ASN
2	B	405	GLN
2	B	460	GLN
2	B	527	GLN
2	B	546	GLN
2	B	708	GLN
2	B	716	ASN
2	B	748	HIS
2	B	777	HIS
2	B	787	HIS
3	C	55	ASN
3	C	79	ASN
3	C	88	GLN
3	C	108	ASN
3	C	123	ASN
1	D	34	ASN
1	D	64	HIS
1	D	134	ASN
1	D	149	GLN
2	E	76	HIS
2	E	111	GLN
2	E	174	HIS
2	E	202	GLN
2	E	270	ASN
2	E	301	ASN
2	E	405	GLN
2	E	460	GLN
2	E	527	GLN
2	E	546	GLN
2	E	596	ASN
2	E	708	GLN
2	E	720	ASN
2	E	735	HIS
2	E	748	HIS
2	E	777	HIS
2	E	787	HIS

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Mol	Chain	Res	Type
3	F	55	ASN
3	F	79	ASN
3	F	88	GLN
3	F	108	ASN
3	F	123	ASN
3	F	142	ASN
3	F	244	GLN

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					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	B	385	2	3,6,7	0.67	0	0,6,8	-	-
2	CSZ	E	385	2	3,6,7	0.61	0	0,6,8	-	-
2	ARO	B	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	E	384	2	-	2/10/11/13	-
2	CSZ	B	385	2	-	0/0/5/7	-
2	CSZ	E	385	2	-	0/0/5/7	-
2	ARO	B	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	B	384	ARO	OH-CG	-5.85	1.25	1.43
2	E	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	E	384	ARO	OH-CG-CB	3.25	116.54	109.18
2	B	384	ARO	OH-CG-CB	2.46	114.76	109.18
2	E	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	B	384	ARO	NE-CD-CG-CB
2	B	384	ARO	NE-CD-CG-OH
2	E	384	ARO	NE-CD-CG-OH
2	E	384	ARO	NE-CD-CG-CB
2	B	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	E	384	ARO	1	0
2	B	385	CSZ	4	0
2	E	385	CSZ	6	0
2	B	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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	FES	A	1907	1	0,4,4	-	-	-		
4	FES	A	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	B	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	C	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	E	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	A	1907	1	-	-	0/1/1/1
4	FES	A	1908	1	-	-	0/1/1/1
6	FAD	F	1923	-	-	10/30/50/50	0/6/6/6
5	PCD	B	1920	-	-	3/20/78/78	0/6/6/6
4	FES	D	1909	1	-	-	0/1/1/1
6	FAD	C	1922	-	-	11/30/50/50	0/6/6/6
4	FES	D	1910	1	-	-	0/1/1/1
5	PCD	E	1921	-	-	3/20/78/78	0/6/6/6

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1922	FAD	O4B-C1B	6.80	1.50	1.41
6	F	1923	FAD	O4B-C1B	6.63	1.50	1.41
6	F	1923	FAD	C1'-C2'	6.42	1.61	1.52
5	B	1920	PCD	C6-N1	5.63	1.42	1.35
5	E	1921	PCD	C6-N1	5.55	1.42	1.35
6	C	1922	FAD	C1'-C2'	5.47	1.60	1.52
6	F	1923	FAD	O5'-C5'	4.37	1.61	1.44
6	C	1922	FAD	O5'-C5'	4.36	1.61	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1922	FAD	PA-O2A	-4.11	1.36	1.55
6	F	1923	FAD	PA-O2A	-3.83	1.37	1.55
5	E	1921	PCD	C6-C5	-3.58	1.30	1.38
6	C	1922	FAD	P-O2P	-3.50	1.38	1.55
5	B	1920	PCD	C6-C5	-3.38	1.30	1.38
6	F	1923	FAD	P-O2P	-3.27	1.40	1.55
5	B	1920	PCD	C10-C9'	-3.21	1.47	1.52
5	E	1921	PCD	C10-C9'	-3.07	1.47	1.52
5	B	1920	PCD	C6'-N5'	2.99	1.49	1.45
5	E	1921	PCD	C7-C6'	-2.91	1.51	1.53
6	C	1922	FAD	O2-C2	-2.82	1.19	1.24
5	E	1921	PCD	C6'-N5'	2.70	1.49	1.45
5	E	1921	PCD	O9'-C9'	2.52	1.47	1.43
5	B	1920	PCD	C7-C6'	-2.52	1.51	1.53
5	E	1921	PCD	PB-O2B	-2.48	1.43	1.55
6	C	1922	FAD	C2B-C1B	-2.40	1.50	1.53
6	F	1923	FAD	O2-C2	-2.40	1.19	1.24
6	F	1923	FAD	PA-O5B	-2.40	1.49	1.59
5	B	1920	PCD	C2'-N1'	-2.39	1.31	1.35
6	F	1923	FAD	C6-C7	-2.36	1.36	1.39
6	C	1922	FAD	PA-O5B	-2.36	1.49	1.59
5	E	1921	PCD	C2'-N1'	-2.36	1.31	1.35
5	B	1920	PCD	PB-O2B	-2.29	1.44	1.55
6	C	1922	FAD	C6-C7	-2.28	1.36	1.39
5	E	1921	PCD	C4'-N3'	2.11	1.41	1.36
5	B	1920	PCD	O3'-C3'	2.05	1.47	1.43
5	B	1920	PCD	C4-N3	2.03	1.38	1.35

All (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	C	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	C	1922	FAD	O4'-C4'-C3'	-17.46	66.65	109.10
6	F	1923	FAD	O4'-C4'-C5'	-14.44	77.46	109.92
6	C	1922	FAD	O5'-C5'-C4'	-14.14	71.61	109.36
6	F	1923	FAD	O5'-C5'-C4'	-13.89	72.28	109.36
6	C	1922	FAD	O4'-C4'-C5'	-13.26	80.11	109.92
6	F	1923	FAD	O3'-C3'-C4'	-12.83	77.81	108.81
6	F	1923	FAD	C1'-C2'-C3'	-12.35	75.27	109.79
6	C	1922	FAD	O3'-C3'-C4'	-11.30	81.52	108.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1922	FAD	O2'-C2'-C1'	-10.13	85.31	109.80
6	F	1923	FAD	O2'-C2'-C3'	9.76	132.83	109.10
6	C	1922	FAD	C1'-C2'-C3'	-9.54	83.12	109.79
6	C	1922	FAD	O2'-C2'-C3'	8.03	128.62	109.10
6	C	1922	FAD	C5'-C4'-C3'	7.57	126.84	112.20
6	F	1923	FAD	O2'-C2'-C1'	-7.13	92.56	109.80
6	F	1923	FAD	C5'-C4'-C3'	6.84	125.41	112.20
5	E	1921	PCD	O9'-C7-N8'	4.84	113.54	108.57
5	B	1920	PCD	C8'-C7'-S7'	3.73	122.27	120.15
6	C	1922	FAD	C4'-C3'-C2'	3.63	120.91	113.36
5	E	1921	PCD	C8'-C7'-S7'	3.44	122.10	120.15
5	E	1921	PCD	N3'-C2'-N1'	-3.39	120.10	125.42
5	B	1920	PCD	O9'-C7-N8'	3.30	111.96	108.57
5	B	1920	PCD	N3'-C2'-N1'	-3.29	120.25	125.42
6	F	1923	FAD	C4'-C3'-C2'	3.16	119.94	113.36
5	E	1921	PCD	N2'-C2'-N1'	2.86	121.70	117.25
5	B	1920	PCD	N2'-C2'-N1'	2.76	121.55	117.25
6	F	1923	FAD	C5A-C6A-N6A	2.74	124.52	120.35
6	C	1922	FAD	C5A-C6A-N6A	2.70	124.46	120.35
6	F	1923	FAD	C2B-C3B-C4B	-2.70	97.39	102.64
6	C	1922	FAD	C5A-C6A-N1A	-2.67	114.30	120.35
6	F	1923	FAD	C5A-C6A-N1A	-2.65	114.34	120.35
6	C	1922	FAD	C2A-N1A-C6A	2.59	123.19	118.75
5	E	1921	PCD	C4A-C4'-N3'	-2.43	117.11	124.01
5	B	1920	PCD	C4A-C4'-N3'	-2.41	117.17	124.01
5	B	1920	PCD	C4A-C4B-N8'	2.40	120.33	118.13
6	F	1923	FAD	C2A-N1A-C6A	2.40	122.85	118.75
5	B	1920	PCD	C4B-N8'-C7	-2.37	119.03	123.67
5	E	1921	PCD	C2'-N3'-C4'	2.36	122.37	116.43
6	F	1923	FAD	C4X-C10-N10	2.34	119.90	116.48
5	E	1921	PCD	C4B-N8'-C7	-2.33	119.11	123.67
5	E	1921	PCD	C4A-C4B-N8'	2.33	120.26	118.13
6	F	1923	FAD	O4B-C4B-C3B	-2.33	100.50	105.11
5	B	1920	PCD	C2'-N3'-C4'	2.33	122.30	116.43
6	F	1923	FAD	C4-N3-C2	-2.31	121.38	125.64
6	C	1922	FAD	C4X-C10-N10	2.29	119.83	116.48
6	C	1922	FAD	C4-N3-C2	-2.28	121.42	125.64
5	B	1920	PCD	O9'-C7-C6'	-2.10	107.56	108.96
6	C	1922	FAD	O4B-C4B-C3B	-2.10	100.95	105.11
6	C	1922	FAD	P-O3P-PA	2.01	139.73	132.83

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1920	PCD	C10-O3B-PB-O1B
5	E	1921	PCD	C2D-C1'-N1-C6
5	E	1921	PCD	O4D-C1'-N1-C6
6	C	1922	FAD	C1'-C2'-C3'-O3'
6	C	1922	FAD	O2'-C2'-C3'-C4'
6	C	1922	FAD	C2'-C3'-C4'-O4'
6	C	1922	FAD	O4'-C4'-C5'-O5'
6	F	1923	FAD	O4B-C4B-C5B-O5B
6	F	1923	FAD	C1'-C2'-C3'-O3'
6	F	1923	FAD	O2'-C2'-C3'-C4'
6	F	1923	FAD	C2'-C3'-C4'-O4'
6	F	1923	FAD	O4'-C4'-C5'-O5'
6	F	1923	FAD	C3B-C4B-C5B-O5B
6	C	1922	FAD	O3'-C3'-C4'-C5'
6	F	1923	FAD	O3'-C3'-C4'-C5'
6	F	1923	FAD	O2'-C2'-C3'-O3'
5	B	1920	PCD	C5'-O5'-PA-O3A
5	B	1920	PCD	C10-O3B-PB-O3A
6	C	1922	FAD	P-O3P-PA-O2A
6	F	1923	FAD	P-O3P-PA-O2A
6	F	1923	FAD	C4'-C5'-O5'-P
6	C	1922	FAD	O2'-C2'-C3'-O3'
6	C	1922	FAD	P-O3P-PA-O1A
6	C	1922	FAD	C3B-C4B-C5B-O5B
5	E	1921	PCD	C10-O3B-PB-O3A
6	C	1922	FAD	C4'-C5'-O5'-P
6	C	1922	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

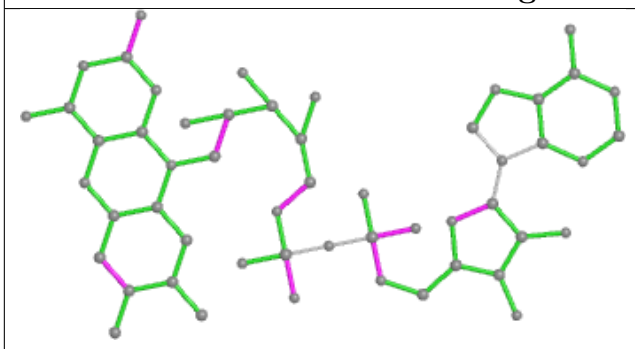
4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	1923	FAD	6	0
5	B	1920	PCD	6	0
6	C	1922	FAD	6	0
5	E	1921	PCD	4	0

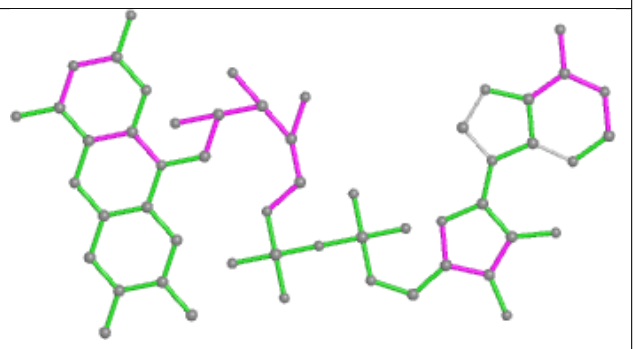
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

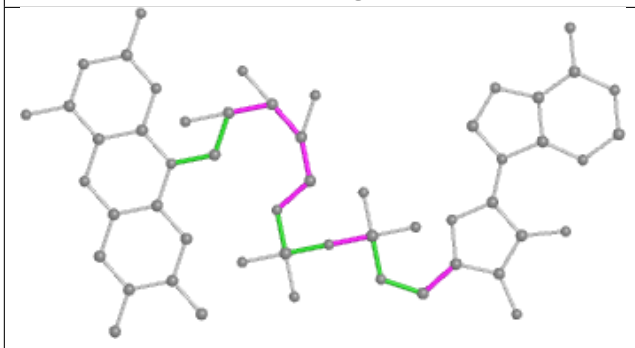
Ligand FAD F 1923



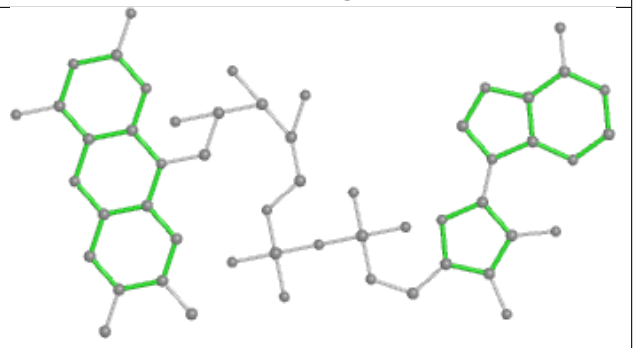
Bond lengths



Bond angles

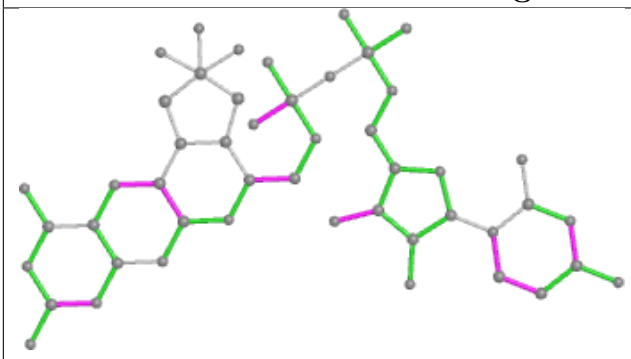


Torsions

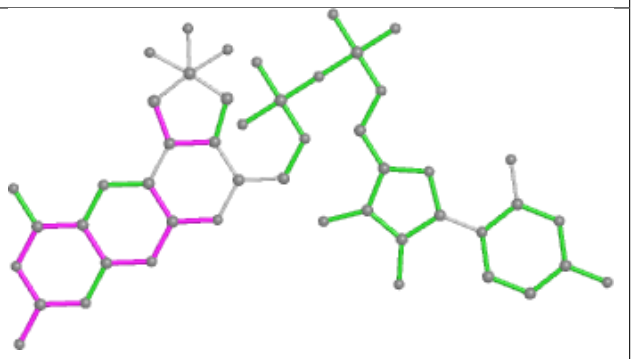


Rings

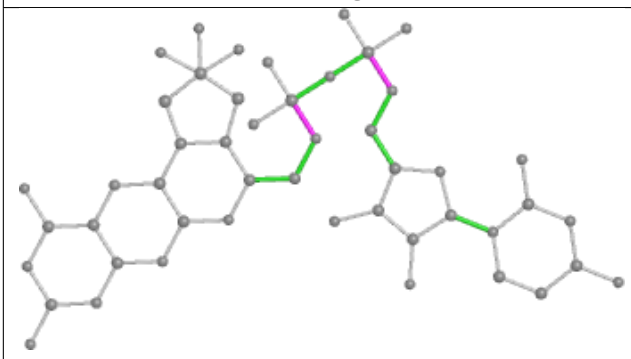
Ligand PCD B 1920



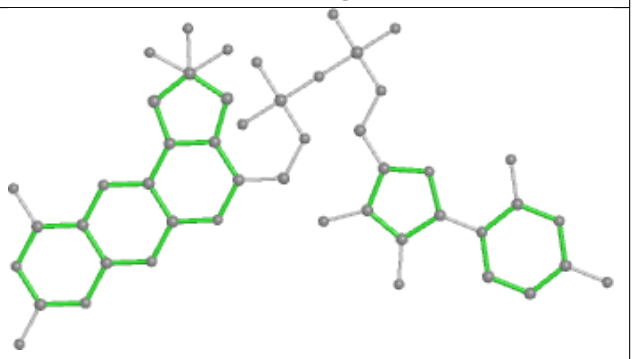
Bond lengths



Bond angles

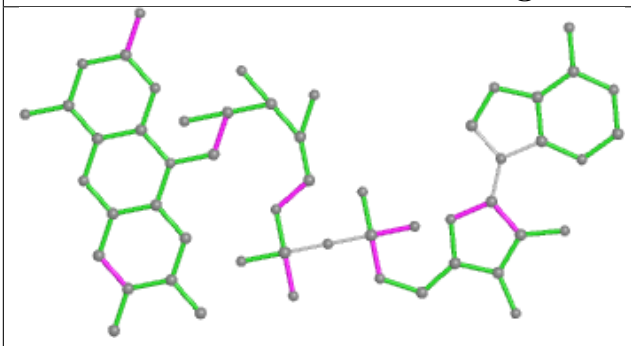


Torsions

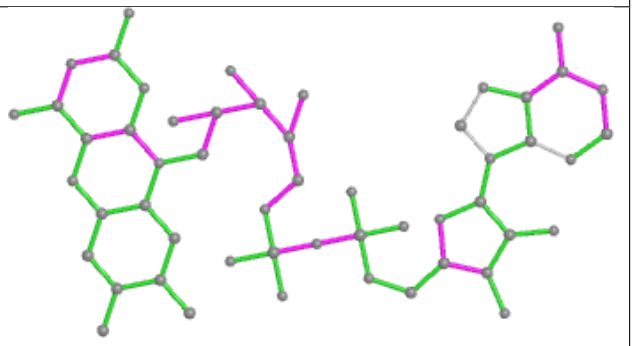


Rings

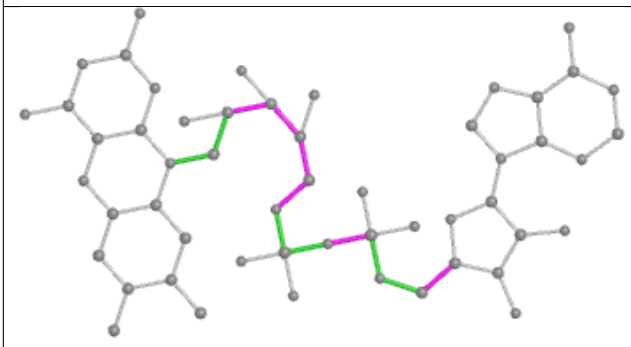
Ligand FAD C 1922



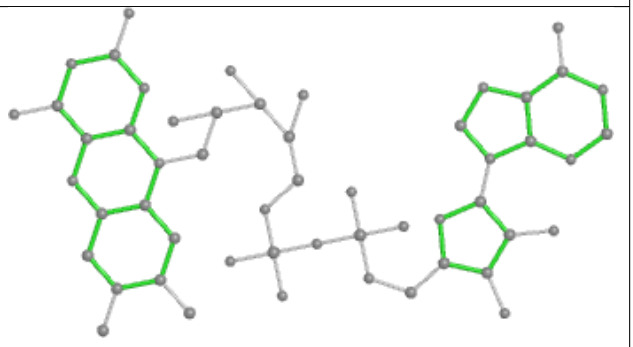
Bond lengths



Bond angles

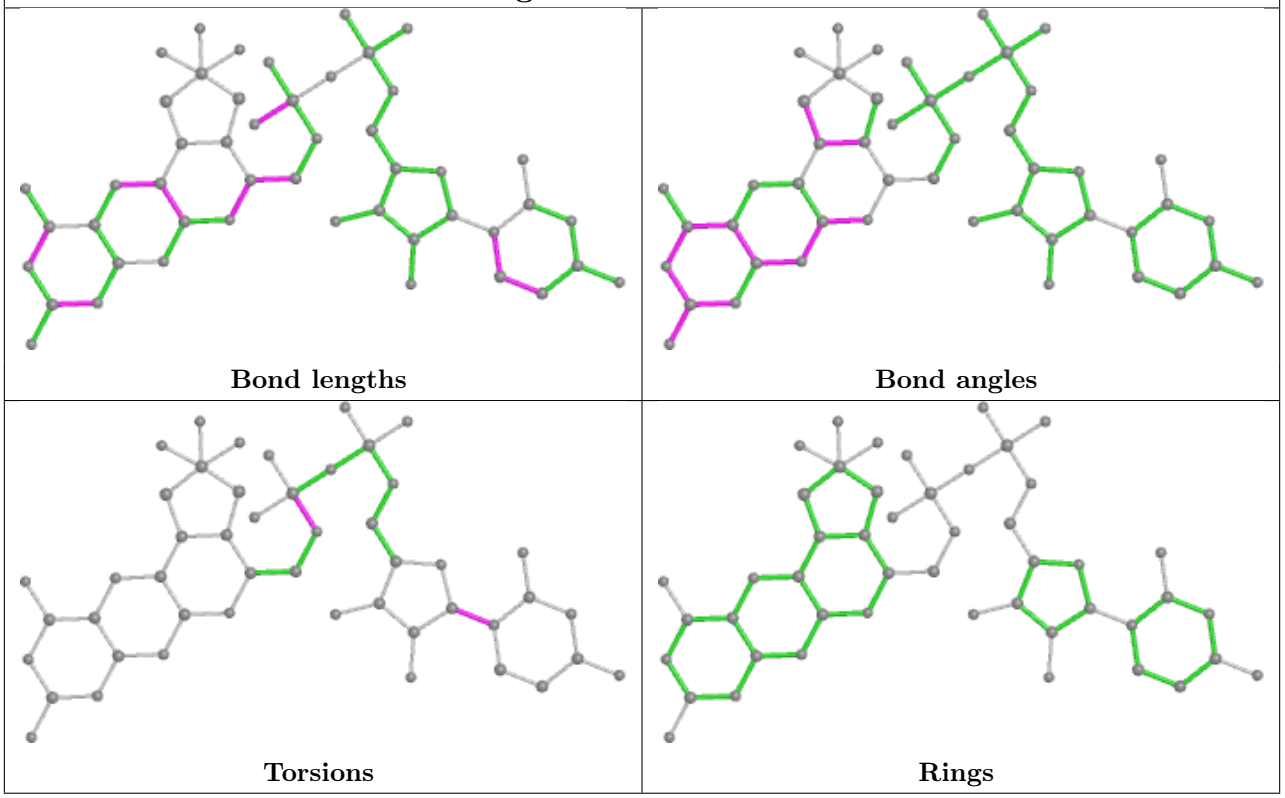


Torsions



Rings

Ligand PCD E 1921



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.