



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:24 PM GMT

PDB ID : 1FFU  
Title : CARBON MONOXIDE DEHYDROGENASE FROM HYDROGENOPHAGA PSEUDOFILAVA WHICH LACKS THE MO-PYRANOPTERIN MOIETY OF THE MOLYBDENUM COFACTOR  
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Deposited on : 2000-07-26  
Resolution : 2.35 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

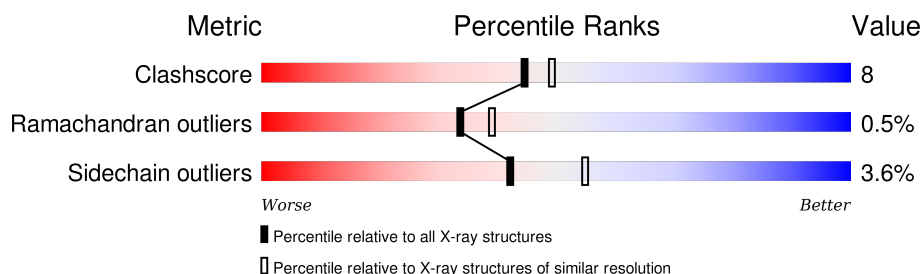
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	163	
1	D	163	
2	B	803	
2	E	803	
3	C	287	
3	F	287	

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
2	CSZ	B	385	-	-	X	-
2	CSZ	E	385	-	-	X	-
5	CDP	B	1920	X	-	-	-
5	CDP	E	1921	X	-	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20601 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	49	0	0
			6087	3860	1056	1135	35	1			
2	E	797	Total	C	N	O	S	Se	41	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	GB 4098682
B	385	CSZ	CYS	MODIFIED	GB 4098682

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Chain	Residue	Modelled	Actual	Comment	Reference
B	456	LEU	TRP	CONFLICT	GB 4098682
E	384	ARO	ARG	MODIFIED	GB 4098682
E	385	CSZ	CYS	MODIFIED	GB 4098682
E	456	LEU	TRP	CONFLICT	GB 4098682

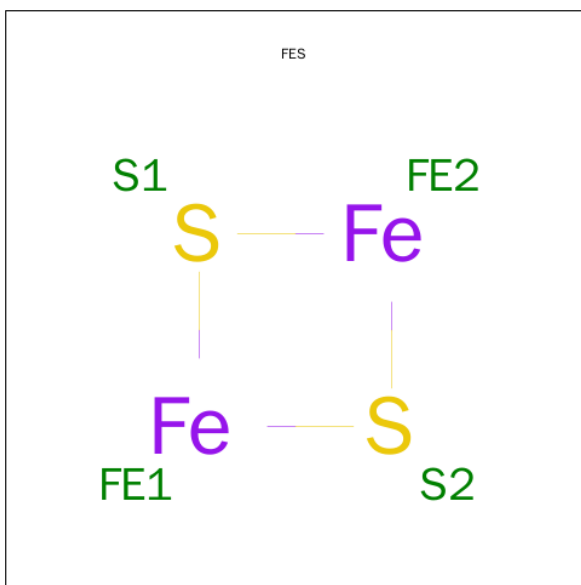
- Molecule 3 is a protein called CUTM, FLAVOPROTEIN OF CARBON MONOXIDE DE-HYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	287	Total	C	N	O	S	9	0	0
			2133	1343	384	394	12			
3	F	287	Total	C	N	O	S	6	0	0
			2133	1343	384	394	12			

There are 18 discrepancies between the modelled and reference sequences:

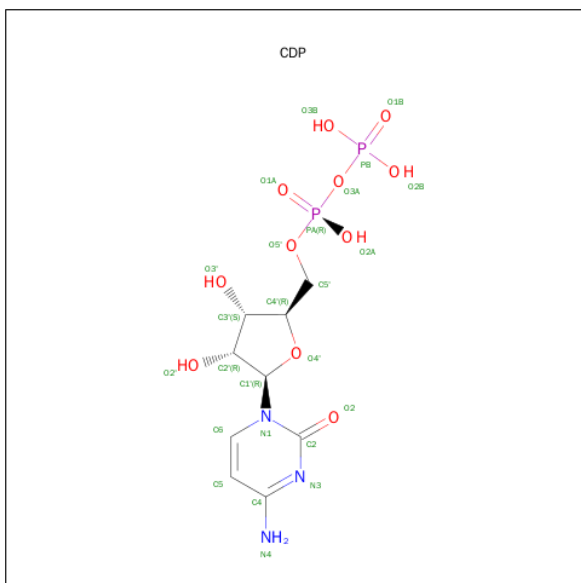
Chain	Residue	Modelled	Actual	Comment	Reference
C	120	ASP	HIS	CONFLICT	UNP P19914
C	177	ALA	GLN	CONFLICT	UNP P19914
C	207	GLY	ASN	CONFLICT	UNP P19914
C	226	ALA	ARG	CONFLICT	UNP P19914
C	228	ALA	GLY	CONFLICT	UNP P19914
C	229	ALA	GLY	CONFLICT	UNP P19914
C	230	GLU	ARG	CONFLICT	UNP P19914
C	231	ALA	SER	CONFLICT	UNP P19914
C	232	ALA	ARG	CONFLICT	UNP P19914
F	120	ASP	HIS	CONFLICT	UNP P19914
F	177	ALA	GLN	CONFLICT	UNP P19914
F	207	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<sub>2</sub>S<sub>2</sub>).



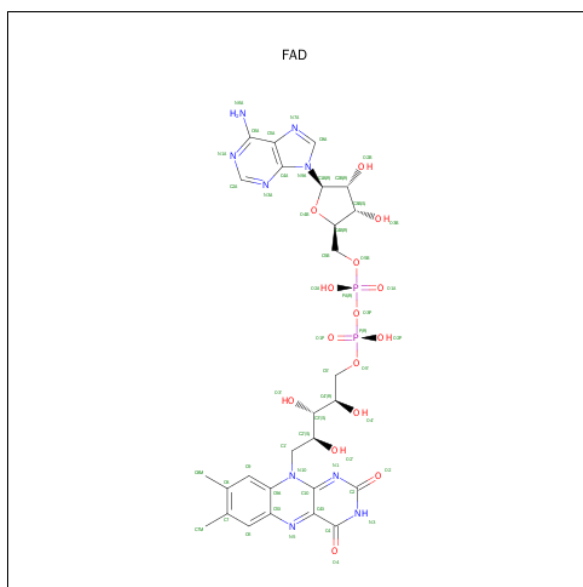
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	D	1	Total	Fe	S	0	0
			4	2	2		
4	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 5 is CYTIDINE-5'-DIPHOSPHATE (three-letter code: CDP) (formula:  $C_9H_{15}N_3O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
5	E	1	Total	C	N	O	P	0	0
			25	9	3	11	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	129	Total	O	0	0
			129	129		
7	B	498	Total	O	0	0
			498	498		
7	C	196	Total	O	0	0
			196	196		
7	D	147	Total	O	0	0
			147	147		
7	E	500	Total	O	0	0
			500	500		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	F	144	Total	O	0	0
			144	144		




### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.


Note EDS was not executed.

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

Chain A: 




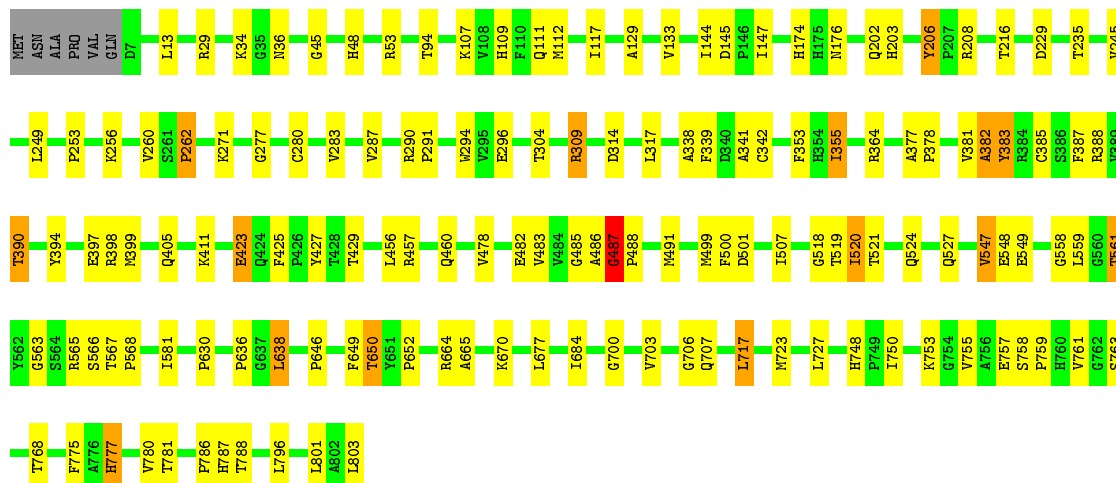
- Molecule 1: CUTS, IRON-SULFUR PROTEIN OF CARBON MONOXIDE DEHYDROGENASE

Chain D: 




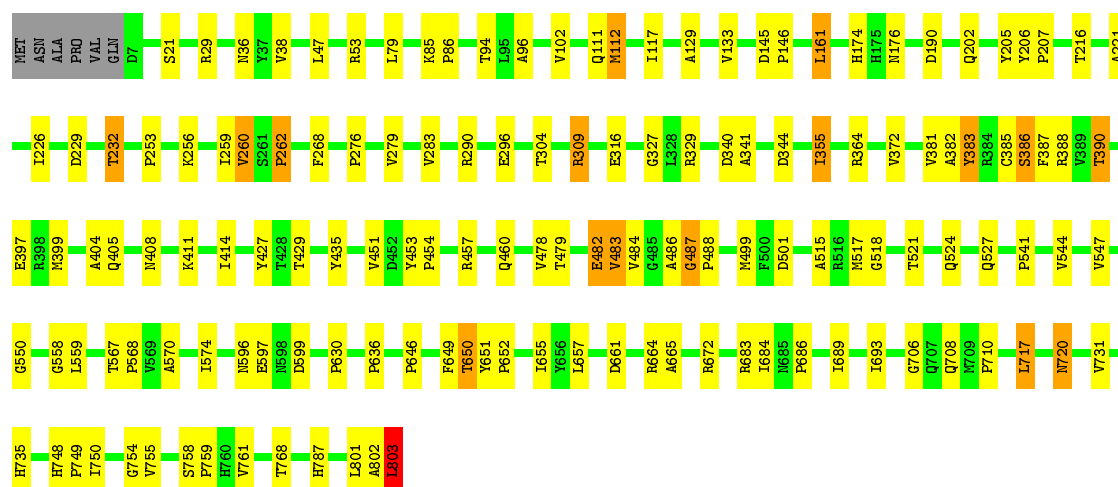
- Molecule 2: CUTL, MOLYBDOPROTEIN OF CARBON MONOXIDE DEHYDROGENASE

Chain B: 



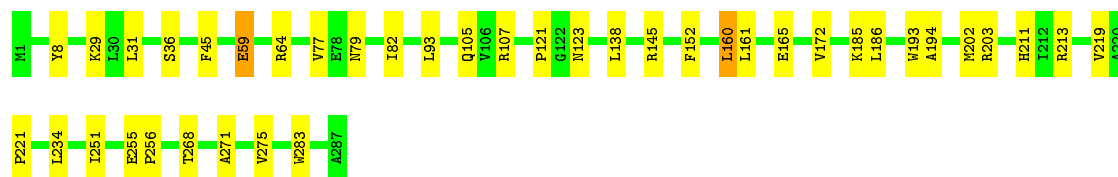
- Molecule 2: CUTL, MOLYBDOPROTEIN OF CARBON MONOXIDE DEHYDROGENASE

Chain E: 



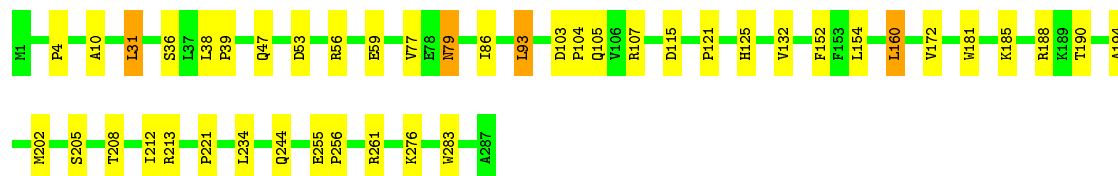
- Molecule 3: CUTM, FLAVOPROTEIN OF CARBON MONOXIDE DEHYDROGENASE

Chain C: 86% 13%



- Molecule 3: CUTM, FLAVOPROTEIN OF CARBON MONOXIDE DEHYDROGENASE

Chain F: 85% 14%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.23 Å   193.88 Å   218.29 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 2.35	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.35)	Depositor
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.208 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20601	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	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: ARO, CDP, FES, FAD, CSZ

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	0.34	0/1202	0.63	0/1619
1	D	0.34	0/1207	0.63	0/1626
2	B	0.34	0/6219	0.63	1/8465 (0.0%)
2	E	0.33	0/6219	0.63	2/8465 (0.0%)
3	C	0.32	0/2172	0.61	0/2947
3	F	0.31	0/2172	0.61	0/2947
All	All	0.33	0/19191	0.63	3/26069 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	803	LEU	CA-CB-CG	6.32	129.83	115.30
2	E	161	LEU	CA-CB-CG	6.24	129.66	115.30
2	B	487	GLY	N-CA-C	5.06	125.74	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	A	1185	0	1178	11	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	109	0
2	E	6087	0	5990	103	0
3	C	2133	0	2167	29	0
3	F	2133	0	2167	26	0
4	A	8	0	0	0	0
4	D	8	0	0	1	0
5	B	25	0	11	1	0
5	E	25	0	11	1	0
6	C	53	0	27	9	0
6	F	53	0	31	7	0
7	A	129	0	0	0	0
7	B	498	0	0	7	0
7	C	196	0	0	4	0
7	D	147	0	0	2	0
7	E	500	0	0	5	0
7	F	144	0	0	2	0
All	All	20601	0	18755	295	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 (295) 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)
2:B:381:VAL:HG13	2:B:385:CSZ:SE	2.03	1.09
2:B:385:CSZ:SE	2:B:388:ARG:H	1.91	1.03
2:E:385:CSZ:SE	2:E:388:ARG:H	2.03	0.90
2:E:381:VAL:HG13	2:E:385:CSZ:SE	2.24	0.87
2:E:253:PRO:HG2	2:E:256:LYS:HG3	1.59	0.84
2:E:29:ARG:HH22	2:E:527:GLN:HE22	1.26	0.82
2:E:748:HIS:HD2	2:E:750:ILE:H	1.29	0.80
2:B:253:PRO:HG2	2:B:256:LYS:HD3	1.64	0.80
3:C:203:ARG:HB2	3:C:211:HIS:HB3	1.64	0.78
2:B:29:ARG:HH22	2:B:527:GLN:HE22	1.31	0.78
6:C:1930:FAD:C5B	6:C:1930:FAD:H8A	2.14	0.78
2:E:457:ARG:HH11	2:E:460:GLN:HE22	1.29	0.77
6:C:1930:FAD:H51A	6:C:1930:FAD:H8A	1.65	0.77
2:B:581:ILE:HG23	2:B:638:LEU:HD22	1.67	0.76
2:E:174:HIS:HD2	2:E:176:ASN:H	1.31	0.76
6:F:1931:FAD:C5B	6:F:1931:FAD:H8A	2.17	0.75
2:B:520:ILE:H	2:B:561:THR:CG2	1.98	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:10:ALA:HB1	3:F:56:ARG:HD2	1.70	0.73
2:E:385:CSZ:SE	2:E:387:PHE:H	2.21	0.73
2:B:174:HIS:HD2	2:B:176:ASN:H	1.38	0.72
2:B:519:THR:HB	2:B:561:THR:HG22	1.71	0.71
2:E:427:TYR:HE2	2:E:429:THR:HG22	1.56	0.71
2:E:521:THR:HG21	7:E:2319:HOH:O	1.94	0.68
2:E:457:ARG:NH1	2:E:460:GLN:HE22	1.91	0.68
2:B:385:CSZ:SE	2:B:388:ARG:N	2.73	0.68
2:B:405:GLN:HE21	2:B:411:LYS:NZ	1.93	0.66
2:E:487:GLY:HA3	2:E:646:PRO:HG3	1.76	0.66
6:F:1931:FAD:H51A	6:F:1931:FAD:H8A	1.77	0.66
2:E:487:GLY:HA3	2:E:646:PRO:CG	2.26	0.66
3:F:185:LYS:HG3	3:F:194:ALA:HB2	1.78	0.66
2:E:457:ARG:HH11	2:E:460:GLN:NE2	1.94	0.66
1:D:146:LYS:HA	1:D:149:GLN:HE21	1.63	0.64
2:B:405:GLN:HE21	2:B:411:LYS:HZ1	1.46	0.63
2:B:174:HIS:CD2	2:B:176:ASN:H	2.16	0.63
2:E:221:ALA:HA	2:E:232:THR:HB	1.79	0.63
6:F:1931:FAD:H52A	6:F:1931:FAD:H8A	1.81	0.62
2:B:748:HIS:HD2	2:B:750:ILE:H	1.47	0.62
1:A:134:ASN:ND2	3:C:105:GLN:HE22	1.98	0.61
2:E:518:GLY:HA3	2:E:558:GLY:HA3	1.82	0.61
2:B:381:VAL:HG22	2:B:385:CSZ:SE	2.51	0.61
2:E:479:THR:HG22	2:E:655:ILE:HG13	1.83	0.61
2:E:385:CSZ:SE	2:E:387:PHE:N	2.83	0.61
3:C:36:SER:HB2	6:C:1930:FAD:H5'2	1.83	0.61
1:D:134:ASN:ND2	3:F:105:GLN:HE22	1.99	0.61
2:B:317:LEU:HD22	2:B:399:MET:HB3	1.83	0.61
2:E:427:TYR:CE2	2:E:429:THR:HG22	2.36	0.60
3:F:202:MET:HE1	3:F:283:TRP:HE3	1.65	0.60
1:D:134:ASN:HD21	3:F:105:GLN:HE22	1.49	0.60
2:B:665:ALA:HA	2:B:803:LEU:HD22	1.83	0.60
3:C:185:LYS:HG3	3:C:194:ALA:HB2	1.81	0.60
2:B:664:ARG:HA	2:B:796:LEU:HD21	1.84	0.60
2:B:521:THR:HG21	7:B:2272:HOH:O	2.01	0.60
2:B:229:ASP:HB2	2:B:256:LYS:O	2.01	0.60
2:E:487:GLY:HA2	2:E:499:MET:O	2.02	0.59
1:D:153:ARG:HD2	7:D:2045:HOH:O	2.02	0.59
3:C:77:VAL:HG13	3:C:107:ARG:O	2.01	0.59
2:E:390:THR:HG23	2:E:761:VAL:HG22	1.84	0.59
2:B:394:TYR:O	2:B:398:ARG:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:507:ILE:HD13	2:B:581:ILE:HD13	1.85	0.59
2:E:650:THR:HG21	2:E:754:GLY:H	1.68	0.59
2:E:720:ASN:H	2:E:720:ASN:HD22	1.51	0.58
2:B:561:THR:HB	2:B:566:SER:OG	2.03	0.58
2:B:664:ARG:HD2	2:B:801:LEU:O	2.03	0.58
2:B:457:ARG:HH11	2:B:460:GLN:HE22	1.48	0.58
2:B:45:GLY:O	2:B:290:ARG:HD2	2.02	0.58
2:E:111:GLN:NE2	2:E:717:LEU:H	2.01	0.58
3:F:4:PRO:HG3	3:F:47:GLN:HG2	1.85	0.58
2:E:405:GLN:HE21	2:E:411:LYS:NZ	2.01	0.58
1:A:134:ASN:HD21	3:C:105:GLN:HE22	1.52	0.57
2:B:723:MET:HE1	3:C:193:TRP:CZ3	2.39	0.57
3:C:255:GLU:HG2	7:C:1977:HOH:O	2.03	0.57
2:B:487:GLY:HA2	2:B:499:MET:O	2.04	0.57
2:B:487:GLY:HA3	2:B:646:PRO:HG3	1.86	0.57
2:E:486:ALA:HA	2:E:649:PHE:CE2	2.40	0.56
3:F:255:GLU:N	3:F:256:PRO:HD3	2.21	0.56
2:E:385:CSZ:SE	2:E:388:ARG:N	2.84	0.56
2:B:748:HIS:CD2	2:B:750:ILE:H	2.22	0.56
3:C:79:ASN:HD22	3:C:82:ILE:HD12	1.71	0.56
6:C:1930:FAD:H52A	6:C:1930:FAD:H8A	1.87	0.55
2:E:232:THR:HG23	2:E:259:ILE:HD13	1.87	0.55
2:E:451:VAL:HG21	2:E:657:LEU:HD13	1.89	0.55
1:D:89:VAL:HG12	1:D:109:LEU:HD22	1.89	0.55
2:B:758:SER:N	2:B:759:PRO:HD2	2.22	0.55
2:E:190:ASP:HA	2:E:329:ARG:HH21	1.72	0.54
3:F:154:LEU:HD21	3:F:160:LEU:HD13	1.89	0.54
3:F:152:PHE:HA	3:F:160:LEU:HD22	1.90	0.54
2:B:342:CYS:SG	2:B:381:VAL:HG23	2.48	0.54
2:B:527:GLN:HA	2:B:547:VAL:HG22	1.89	0.54
2:B:518:GLY:HA3	2:B:558:GLY:HA3	1.89	0.54
2:B:381:VAL:CG1	2:B:385:CSZ:SE	2.93	0.54
3:F:121:PRO:HG3	3:F:221:PRO:O	2.07	0.54
3:F:93:LEU:HG	3:F:181:TRP:HB2	1.90	0.54
3:C:121:PRO:HG3	3:C:221:PRO:O	2.06	0.54
2:B:339:PHE:O	2:B:378:PRO:HB3	2.08	0.53
2:B:111:GLN:O	2:B:112:MET:HB2	2.08	0.53
2:E:720:ASN:H	2:E:720:ASN:ND2	2.06	0.53
2:E:597:GLU:C	2:E:599:ASP:H	2.11	0.53
3:C:202:MET:CE	3:C:283:TRP:HE3	2.22	0.53
2:E:499:MET:HA	2:E:559:LEU:HG	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:567:THR:HB	2:E:568:PRO:HD3	1.90	0.53
2:E:664:ARG:HD2	2:E:801:LEU:O	2.09	0.53
3:C:202:MET:HE1	3:C:283:TRP:HE3	1.73	0.52
2:E:102:VAL:HA	2:E:276:PRO:HB3	1.89	0.52
2:B:398:ARG:HD2	7:B:2107:HOH:O	2.09	0.52
1:D:132:THR:HG21	3:F:190:THR:HG21	1.91	0.52
2:E:21:SER:OG	2:E:686:PRO:HG2	2.10	0.52
3:F:36:SER:HB2	6:F:1931:FAD:H5'2	1.92	0.52
2:B:397:GLU:HG3	2:B:478:VAL:HG13	1.92	0.52
1:A:87:HIS:ND1	1:A:89:VAL:HG22	2.25	0.52
2:B:390:THR:HG23	2:B:761:VAL:HG22	1.91	0.52
2:B:700:GLY:HA3	2:B:763:SER:OG	2.10	0.52
2:B:519:THR:HB	2:B:561:THR:CG2	2.40	0.52
2:E:205:TYR:O	2:E:207:PRO:HD3	2.11	0.51
3:C:123:ASN:ND2	3:C:193:TRP:HE1	2.08	0.51
2:E:53:ARG:NH1	2:E:304:THR:HG21	2.25	0.51
2:B:777:HIS:CD2	2:B:777:HIS:H	2.28	0.51
2:E:630:PRO:HG3	2:E:636:PRO:HG3	1.93	0.51
2:E:385:CSZ:SE	2:E:387:PHE:CA	3.09	0.51
3:C:45:PHE:HB3	7:C:2123:HOH:O	2.10	0.51
2:E:758:SER:N	2:E:759:PRO:HD2	2.25	0.51
2:B:563:GLY:HA2	2:B:757:GLU:OE1	2.11	0.51
1:A:146:LYS:HA	1:A:149:GLN:HE21	1.75	0.50
2:E:382:ALA:O	2:E:385:CSZ:SG	2.69	0.50
2:E:229:ASP:HB2	2:E:256:LYS:O	2.11	0.50
2:B:487:GLY:HA3	2:B:646:PRO:CG	2.42	0.50
2:E:174:HIS:CD2	2:E:176:ASN:H	2.21	0.50
3:F:59:GLU:HB3	7:F:2049:HOH:O	2.11	0.50
2:E:768:THR:OG1	2:E:787:HIS:HE1	1.94	0.50
2:E:483:VAL:HG13	2:E:651:TYR:CE2	2.46	0.50
2:E:661:ASP:OD2	2:E:672:ARG:HD3	2.11	0.50
2:E:527:GLN:HA	2:E:547:VAL:HG22	1.92	0.50
1:D:123:THR:O	1:D:127:ILE:HG13	2.12	0.49
2:B:107:LYS:HE3	2:B:109:HIS:NE2	2.27	0.49
2:B:385:CSZ:SE	2:B:387:PHE:HA	2.62	0.49
3:C:29:LYS:HD3	7:C:2032:HOH:O	2.12	0.49
3:C:79:ASN:HD21	3:C:107:ARG:HE	1.60	0.49
2:B:486:ALA:HA	2:B:649:PHE:CE2	2.48	0.48
2:E:111:GLN:HE22	2:E:717:LEU:H	1.59	0.48
6:C:1930:FAD:C8A	6:C:1930:FAD:C5B	2.90	0.48
2:B:520:ILE:H	2:B:561:THR:HG23	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:GLN:NE2	2:B:781:THR:OG1	2.45	0.48
3:C:161:LEU:HD21	6:C:1930:FAD:H2A	1.96	0.48
2:E:748:HIS:CD2	2:E:750:ILE:H	2.19	0.48
2:B:567:THR:HB	2:B:568:PRO:HD3	1.95	0.48
2:B:216:THR:HB	2:B:296:GLU:HG3	1.95	0.48
3:C:255:GLU:N	3:C:256:PRO:HD3	2.29	0.48
2:B:355:ILE:HG13	2:B:483:VAL:HG11	1.96	0.48
2:B:670:LYS:HE2	7:B:2404:HOH:O	2.13	0.48
3:C:271:ALA:O	3:C:275:VAL:HG23	2.14	0.48
2:B:423:GLU:HG3	2:B:423:GLU:H	1.46	0.48
2:E:344:ASP:HB2	7:E:2214:HOH:O	2.13	0.47
2:B:727:LEU:HD23	2:B:727:LEU:HA	1.78	0.47
1:D:60:LYS:HD3	4:D:1910:FES:S1	2.54	0.47
2:E:36:ASN:O	2:E:262:PRO:HB2	2.14	0.47
2:E:596:ASN:O	2:E:599:ASP:HB2	2.14	0.47
2:E:482:GLU:HB2	2:E:652:PRO:HG2	1.97	0.47
2:B:507:ILE:CD1	2:B:581:ILE:HD13	2.44	0.47
2:E:85:LYS:HB2	2:E:86:PRO:HD3	1.96	0.47
3:C:161:LEU:HD21	6:C:1930:FAD:C2A	2.45	0.47
2:E:355:ILE:HG13	2:E:483:VAL:CG2	2.45	0.47
3:C:145:ARG:HD3	3:C:165:GLU:OE2	2.14	0.47
2:B:385:CSZ:SE	2:B:387:PHE:CA	3.13	0.47
2:B:94:THR:HB	2:B:341:ALA:HA	1.97	0.47
2:E:260:VAL:HA	2:E:550:GLY:O	2.15	0.47
1:D:129:MET:HA	1:D:132:THR:HG23	1.97	0.47
2:E:385:CSZ:SE	2:E:387:PHE:HA	2.65	0.46
3:F:79:ASN:ND2	3:F:107:ARG:HE	2.13	0.46
2:E:515:ALA:O	2:E:547:VAL:HA	2.15	0.46
2:E:517:MET:SD	2:E:517:MET:N	2.88	0.46
2:E:96:ALA:HB3	2:E:340:ASP:O	2.14	0.46
2:E:47:LEU:HG	2:E:290:ARG:HD2	1.97	0.46
2:B:381:VAL:O	2:B:382:ALA:HB2	2.16	0.46
2:B:145:ASP:OD2	2:B:147:ILE:HB	2.15	0.46
3:F:188:ARG:HD2	3:F:261:ARG:HG2	1.98	0.46
3:F:38:LEU:HB2	3:F:39:PRO:HD3	1.96	0.46
2:B:53:ARG:NH1	2:B:304:THR:HG21	2.30	0.46
3:C:59:GLU:HG3	7:C:1974:HOH:O	2.15	0.46
2:B:290:ARG:HB2	2:B:291:PRO:CD	2.45	0.45
2:E:355:ILE:HG13	2:E:483:VAL:HG21	1.98	0.45
2:B:483:VAL:HG13	2:B:483:VAL:O	2.16	0.45
2:B:309:ARG:NH2	2:B:383:TYR:HB3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:650:THR:HG23	2:B:753:LYS:HB3	1.98	0.45
2:B:630:PRO:HG3	2:B:636:PRO:HG3	1.98	0.45
6:C:1930:FAD:C8A	6:C:1930:FAD:H51A	2.42	0.45
2:E:316:GLU:OE2	2:E:329:ARG:HD2	2.17	0.45
2:B:208:ARG:NH2	2:B:377:ALA:O	2.50	0.45
2:B:216:THR:HB	2:B:296:GLU:CG	2.47	0.45
2:E:453:TYR:N	2:E:454:PRO:HD2	2.32	0.45
2:B:527:GLN:HA	2:B:547:VAL:CG2	2.47	0.45
1:A:60:LYS:HE3	3:C:105:GLN:HB2	1.99	0.45
2:B:117:ILE:HD13	2:B:280:CYS:HB3	1.99	0.45
3:F:86:ILE:HG13	7:F:2073:HOH:O	2.16	0.45
3:C:152:PHE:HA	3:C:160:LEU:HD22	1.99	0.44
2:E:787:HIS:HD2	7:E:2133:HOH:O	2.00	0.44
2:B:581:ILE:HG23	2:B:638:LEU:CD2	2.41	0.44
2:B:723:MET:HG3	7:B:2400:HOH:O	2.17	0.44
3:F:115:ASP:OD2	3:F:125:HIS:HB2	2.17	0.44
2:E:404:ALA:HB2	2:E:414:ILE:HG21	1.99	0.44
2:B:703:VAL:HA	2:B:707:GLN:HB2	1.99	0.44
1:A:21:PRO:HB3	3:C:8:TYR:HB2	1.98	0.44
2:E:720:ASN:N	2:E:720:ASN:HD22	2.10	0.44
2:E:129:ALA:O	2:E:133:VAL:HG23	2.18	0.44
2:B:768:THR:OG1	2:B:787:HIS:HE1	2.00	0.44
1:A:116:LEU:HD12	1:A:116:LEU:HA	1.78	0.44
2:E:279:VAL:O	2:E:283:VAL:HG23	2.17	0.44
2:B:111:GLN:NE2	2:B:717:LEU:H	2.16	0.44
3:F:205:SER:O	3:F:208:THR:HG22	2.18	0.44
1:D:102:GLY:HA2	1:D:105:THR:OG1	2.18	0.44
2:B:385:CSZ:SE	2:B:387:PHE:H	2.50	0.44
2:E:768:THR:HA	2:E:787:HIS:CE1	2.52	0.44
3:F:79:ASN:HD22	3:F:79:ASN:HA	1.69	0.43
1:D:47:CYS:O	1:D:134:ASN:HA	2.18	0.43
3:F:31:LEU:HB3	3:F:53:ASP:HA	2.01	0.43
2:E:802:ALA:HB3	7:E:2367:HOH:O	2.18	0.43
2:B:129:ALA:O	2:B:133:VAL:HG23	2.18	0.43
2:E:484:VAL:HG22	2:E:650:THR:HG22	2.00	0.43
2:B:650:THR:HG23	2:B:652:PRO:HD3	1.98	0.43
3:F:103:ASP:HB2	3:F:104:PRO:CD	2.49	0.43
2:B:34:LYS:HG3	2:E:226:ILE:HD13	2.01	0.43
2:E:229:ASP:HB3	2:E:256:LYS:HB3	2.00	0.43
2:B:768:THR:HA	2:B:787:HIS:CE1	2.54	0.43
2:B:548:GLU:HB3	7:B:2244:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:ASN:O	2:B:262:PRO:HB2	2.18	0.43
1:D:114:ARG:O	1:D:118:GLU:HG3	2.18	0.43
6:F:1931:FAD:N1	6:F:1931:FAD:O2'	2.49	0.43
2:E:405:GLN:HE21	2:E:411:LYS:HZ1	1.67	0.43
2:B:235:THR:HB	2:B:271:LYS:HD3	1.99	0.43
3:C:251:ILE:HG23	3:C:268:THR:CG2	2.48	0.43
2:B:245:VAL:O	2:B:249:LEU:HG	2.18	0.43
2:E:216:THR:HB	2:E:296:GLU:HG3	2.01	0.43
2:E:689:ILE:O	2:E:693:ILE:HG12	2.18	0.43
2:E:748:HIS:HA	2:E:749:PRO:HD3	1.96	0.43
3:C:79:ASN:ND2	3:C:107:ARG:HE	2.17	0.43
2:E:541:PRO:HG2	2:E:544:VAL:HG22	2.01	0.43
1:D:132:THR:HG22	2:E:731:VAL:HG23	2.00	0.42
2:B:500:PHE:O	2:B:559:LEU:HD23	2.18	0.42
2:B:283:VAL:O	2:B:287:VAL:HG23	2.19	0.42
2:E:38:VAL:HG23	7:E:1927:HOH:O	2.18	0.42
1:A:11:ASN:OD1	1:A:75:LEU:HD23	2.20	0.42
7:D:1924:HOH:O	2:E:735:HIS:HD2	2.02	0.42
3:F:244:GLN:HE22	3:F:276:LYS:NZ	2.16	0.42
2:B:519:THR:O	2:B:549:GLU:HB3	2.18	0.42
2:E:570:ALA:O	2:E:574:ILE:HG13	2.19	0.42
2:B:353:PHE:C	2:B:355:ILE:H	2.23	0.42
2:B:34:LYS:HG3	2:E:226:ILE:CD1	2.50	0.42
1:A:124:GLU:HG3	1:A:145:VAL:HG11	2.02	0.42
2:E:684:ILE:HB	5:E:1921:CDP:O2	2.20	0.42
1:D:89:VAL:HG12	1:D:109:LEU:CD2	2.50	0.42
1:D:53:ASP:HB3	1:D:75:LEU:HB2	2.00	0.42
3:F:103:ASP:HB2	3:F:104:PRO:HD2	2.00	0.42
2:E:527:GLN:HA	2:E:547:VAL:CG2	2.50	0.42
2:B:499:MET:HA	2:B:559:LEU:HG	2.01	0.41
2:B:427:TYR:HE2	2:B:429:THR:HG22	1.84	0.41
6:F:1931:FAD:H9	6:F:1931:FAD:H1'2	1.88	0.41
3:C:219:VAL:HG11	3:C:271:ALA:HB2	2.02	0.41
1:D:105:THR:HB	1:D:106:PRO:HD3	2.02	0.41
6:F:1931:FAD:C5B	6:F:1931:FAD:C8A	2.94	0.41
2:E:79:LEU:HD12	2:E:117:ILE:HD11	2.02	0.41
3:F:212:ILE:HG12	3:F:213:ARG:N	2.36	0.41
2:B:206:TYR:CE1	2:B:309:ARG:HG3	2.55	0.41
2:B:786:PRO:HB2	2:B:788:THR:HG23	2.02	0.41
2:E:94:THR:HB	2:E:341:ALA:HA	2.02	0.41
2:E:435:TYR:HD1	2:E:435:TYR:N	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:NH1	1:A:137:ARG:O	2.53	0.41
2:B:203:HIS:HD2	2:B:314:ASP:OD1	2.03	0.41
2:E:386:SER:O	2:E:387:PHE:HB2	2.21	0.41
2:B:48:HIS:HD2	7:B:2063:HOH:O	2.03	0.41
2:B:677:LEU:C	2:B:677:LEU:HD23	2.41	0.41
2:E:268:PHE:O	2:E:383:TYR:N	2.54	0.41
2:B:425:PHE:HA	2:B:427:TYR:N	2.35	0.41
2:E:665:ALA:HA	2:E:803:LEU:HB3	2.02	0.41
2:B:684:ILE:HB	5:B:1920:CDP:O2	2.21	0.41
6:C:1930:FAD:HO2'	6:C:1930:FAD:C10	2.32	0.41
3:C:138:LEU:HD22	3:C:161:LEU:HD13	2.02	0.41
2:B:109:HIS:HB3	2:B:338:ALA:HB1	2.03	0.41
2:B:355:ILE:HG13	2:B:483:VAL:CG1	2.50	0.41
2:B:650:THR:CG2	2:B:652:PRO:HD3	2.51	0.41
2:E:145:ASP:HA	2:E:146:PRO:HD3	1.96	0.41
2:B:390:THR:HG22	2:B:761:VAL:HA	2.01	0.41
2:E:802:ALA:O	2:E:803:LEU:HD13	2.21	0.41
2:E:435:TYR:CD1	2:E:435:TYR:N	2.88	0.41
2:B:507:ILE:N	2:B:507:ILE:HD12	2.37	0.40
2:E:397:GLU:HG3	2:E:478:VAL:HG13	2.03	0.40
2:B:277:GLY:HA3	2:B:294:TRP:CZ3	2.57	0.40
2:E:202:GLN:HB3	2:E:399:MET:SD	2.60	0.40
2:B:457:ARG:HH11	2:B:460:GLN:NE2	2.18	0.40
2:B:787:HIS:HD2	7:B:2119:HOH:O	2.04	0.40
2:E:327:GLY:HA2	2:E:364:ARG:O	2.21	0.40
2:B:707:GLN:O	2:B:786:PRO:HG3	2.21	0.40
2:E:708:GLN:HG3	2:E:710:PRO:HD3	2.04	0.40
2:E:381:VAL:HG22	2:E:385:CSZ:SE	2.71	0.40
2:E:111:GLN:O	2:E:112:MET:HB2	2.22	0.40
1:A:129:MET:HA	1:A:132:THR:HG23	2.04	0.40
2:B:485:GLY:HA2	2:B:565:ARG:HA	2.03	0.40
2:B:775:PHE:HB3	2:B:780:VAL:HG21	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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%)	150 (98%)	3 (2%)	0	100	100
1	D	154/163 (94%)	149 (97%)	5 (3%)	0	100	100
2	B	793/803 (99%)	759 (96%)	27 (3%)	7 (1%)	21	22
2	E	793/803 (99%)	758 (96%)	29 (4%)	6 (1%)	24	26
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%)	2368 (96%)	82 (3%)	13 (0%)	34	39

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	382	ALA
2	B	487	GLY
2	E	487	GLY
2	E	488	PRO
2	B	262	PRO
2	B	488	PRO
2	E	262	PRO
2	B	706	GLY
2	E	706	GLY
2	E	309	ARG
2	B	520	ILE
2	E	755	VAL
2	B	755	VAL

### 5.3.2 Protein sidechains ⓘ

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%)	125 (98%)	3 (2%)	58	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	128/132 (97%)	120 (94%)	8 (6%)	22	25
2	B	634/639 (99%)	613 (97%)	21 (3%)	45	58
2	E	634/639 (99%)	613 (97%)	21 (3%)	45	58
3	C	212/212 (100%)	203 (96%)	9 (4%)	36	46
3	F	212/212 (100%)	204 (96%)	8 (4%)	40	52
All	All	1948/1966 (99%)	1878 (96%)	70 (4%)	42	55

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	75	LEU
1	A	116	LEU
2	B	13	LEU
2	B	144	ILE
2	B	206	TYR
2	B	260	VAL
2	B	309	ARG
2	B	355	ILE
2	B	364	ARG
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	547	VAL
2	B	561	THR
2	B	638	LEU
2	B	650	THR
2	B	717	LEU
2	B	777	HIS
3	C	31	LEU
3	C	59	GLU
3	C	64	ARG
3	C	93	LEU
3	C	160	LEU
3	C	172	VAL

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Mol	Chain	Res	Type
3	C	186	LEU
3	C	213	ARG
3	C	234	LEU
1	D	24	LEU
1	D	43	GLU
1	D	67	VAL
1	D	75	LEU
1	D	99	LEU
1	D	116	LEU
1	D	135	LEU
1	D	145	VAL
2	E	112	MET
2	E	161	LEU
2	E	206	TYR
2	E	232	THR
2	E	260	VAL
2	E	309	ARG
2	E	355	ILE
2	E	372	VAL
2	E	383	TYR
2	E	386	SER
2	E	390	THR
2	E	408	ASN
2	E	482	GLU
2	E	483	VAL
2	E	501	ASP
2	E	524	GLN
2	E	650	THR
2	E	683	ARG
2	E	717	LEU
2	E	720	ASN
2	E	803	LEU
3	F	31	LEU
3	F	77	VAL
3	F	79	ASN
3	F	93	LEU
3	F	132	VAL
3	F	160	LEU
3	F	172	VAL
3	F	234	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	34	ASN
1	A	134	ASN
1	A	149	GLN
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	625	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	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

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Mol	Chain	Res	Type
2	E	748	HIS
2	E	787	HIS
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 ⓘ

There are no RNA molecules in this entry.

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

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	B	384	2	7,11,12	1.69	1 (14%)	4,13,15	1.75	2 (50%)
2	CSZ	B	385	2	3,6,7	0.58	0	1,6,8	2.20	1 (100%)
2	ARO	E	384	2	7,11,12	2.27	1 (14%)	4,13,15	1.92	2 (50%)
2	CSZ	E	385	2	3,6,7	0.62	0	1,6,8	2.05	1 (100%)

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	B	384	2	-	0/7/11/13	0/0/0/0
2	CSZ	B	385	2	-	0/0/5/7	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ARO	E	384	2	-	0/7/11/13	0/0/0/0
2	CSZ	E	385	2	-	0/0/5/7	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	384	ARO	OH-CG	-5.89	1.25	1.43
2	B	384	ARO	OH-CG	-4.30	1.30	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	384	ARO	O-C-CA	-2.22	119.70	125.49
2	B	385	CSZ	O-C-CA	-2.20	119.77	125.49
2	E	385	CSZ	O-C-CA	-2.05	120.14	125.49
2	B	384	ARO	OH-CG-CD	2.01	116.17	109.18
2	B	384	ARO	OH-CG-CB	2.19	114.28	109.15
2	E	384	ARO	OH-CG-CB	2.59	115.20	109.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	385	CSZ	8	0
2	E	385	CSZ	9	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	0.00	-	0,4,4	0.00	-
4	FES	A	1908	1	0,4,4	0.00	-	0,4,4	0.00	-
5	CDP	B	1920	-	19,26,26	1.56	3 (15%)	27,40,40	3.82	14 (51%)
6	FAD	C	1930	-	48,58,58	1.94	9 (18%)	54,89,89	4.71	16 (29%)
4	FES	D	1909	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FES	D	1910	1	0,4,4	0.00	-	0,4,4	0.00	-
5	CDP	E	1921	-	19,26,26	1.59	2 (10%)	27,40,40	3.83	14 (51%)
6	FAD	F	1931	-	48,58,58	1.92	8 (16%)	54,89,89	4.83	14 (25%)

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	-	0/0/4/4	0/1/1/1
4	FES	A	1908	1	-	0/0/4/4	0/1/1/1
5	CDP	B	1920	-	1/1/6/6	0/12/32/32	0/2/2/2
6	FAD	C	1930	-	-	0/30/50/50	0/6/6/6
4	FES	D	1909	1	-	0/0/4/4	0/1/1/1
4	FES	D	1910	1	-	0/0/4/4	0/1/1/1
5	CDP	E	1921	-	1/1/6/6	0/12/32/32	0/2/2/2
6	FAD	F	1931	-	-	0/30/50/50	0/6/6/6

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1930	FAD	PA-O2A	-4.42	1.36	1.54
6	F	1931	FAD	PA-O2A	-4.27	1.36	1.54
6	C	1930	FAD	C10-N10	-3.47	1.35	1.39
6	C	1930	FAD	P-O2P	-3.47	1.40	1.54
6	F	1931	FAD	C10-N10	-3.46	1.35	1.39
6	F	1931	FAD	P-O2P	-3.40	1.40	1.54
6	C	1930	FAD	PA-O5B	-2.04	1.49	1.59
6	F	1931	FAD	PA-O5B	-2.01	1.49	1.59
5	B	1920	CDP	PA-O1A	2.01	1.58	1.51
5	E	1921	CDP	PA-O1A	2.06	1.58	1.51
5	B	1920	CDP	PB-O1B	2.17	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1930	FAD	C4-C4X	2.45	1.46	1.41
6	F	1931	FAD	C4X-C10	2.76	1.46	1.41
6	C	1930	FAD	C4X-C10	2.81	1.46	1.41
6	F	1931	FAD	C9A-N10	3.04	1.43	1.38
6	C	1930	FAD	C9A-N10	3.71	1.43	1.38
6	C	1930	FAD	O5'-C5'	4.07	1.61	1.44
6	F	1931	FAD	O5'-C5'	4.09	1.61	1.44
5	B	1920	CDP	C5-C4	4.22	1.50	1.40
5	E	1921	CDP	C5-C4	4.53	1.51	1.40
6	C	1930	FAD	O4B-C1B	6.94	1.50	1.41
6	F	1931	FAD	O4B-C1B	7.43	1.50	1.41

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1930	FAD	O4'-C4'-C3'	-17.01	66.25	109.02
6	C	1930	FAD	O3'-C3'-C2'	-16.19	67.95	108.75
6	F	1931	FAD	O4'-C4'-C3'	-15.96	68.88	109.02
6	F	1931	FAD	O3'-C3'-C2'	-15.35	70.06	108.75
6	F	1931	FAD	O4'-C4'-C5'	-13.65	80.46	110.19
6	F	1931	FAD	O3'-C3'-C4'	-12.08	78.30	108.75
6	C	1930	FAD	O4'-C4'-C5'	-11.79	84.51	110.19
6	F	1931	FAD	C1'-C2'-C3'	-11.33	77.42	109.82
6	C	1930	FAD	C1'-C2'-C3'	-9.82	81.73	109.82
6	C	1930	FAD	O3'-C3'-C4'	-9.47	84.88	108.75
6	C	1930	FAD	O2'-C2'-C1'	-9.29	87.13	109.94
6	F	1931	FAD	O2'-C2'-C1'	-7.96	90.39	109.94
5	E	1921	CDP	O3'-C3'-C2'	-6.61	90.33	111.83
5	B	1920	CDP	O3'-C3'-C2'	-6.54	90.57	111.83
5	E	1921	CDP	C2'-C3'-C4'	-6.24	89.78	102.61
5	B	1920	CDP	C2'-C3'-C4'	-6.12	90.04	102.61
5	E	1921	CDP	C5-C4-N3	-6.01	114.23	121.80
5	B	1920	CDP	C5-C4-N3	-5.96	114.28	121.80
6	C	1930	FAD	C4X-C4-N3	-4.94	116.83	123.59
6	F	1931	FAD	C4X-C4-N3	-4.86	116.95	123.59
6	C	1930	FAD	C4B-O4B-C1B	-3.91	105.42	109.72
6	F	1931	FAD	C4B-O4B-C1B	-3.77	105.58	109.72
5	B	1920	CDP	O5'-C5'-C4'	-3.74	95.34	109.12
5	E	1921	CDP	O5'-C5'-C4'	-3.67	95.60	109.12
6	C	1930	FAD	N3A-C2A-N1A	-3.02	126.58	128.89
6	F	1931	FAD	O4B-C1B-N9A	-2.78	102.28	108.10
6	F	1931	FAD	N3A-C2A-N1A	-2.76	126.78	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1920	CDP	O2B-PB-O3A	-2.49	93.77	105.09
5	B	1920	CDP	O3B-PB-O3A	-2.46	93.92	105.09
6	C	1930	FAD	O4B-C1B-N9A	-2.44	102.98	108.10
5	E	1921	CDP	O2B-PB-O3A	-2.42	94.10	105.09
5	E	1921	CDP	O3B-PB-O3A	-2.33	94.54	105.09
6	C	1930	FAD	C4-C4X-C10	-2.10	118.60	119.94
6	C	1930	FAD	O2A-PA-O3P	2.01	114.21	105.09
5	E	1921	CDP	O2'-C2'-C3'	2.08	118.59	111.83
5	B	1920	CDP	O2'-C2'-C3'	2.09	118.63	111.83
6	F	1931	FAD	O2A-PA-O3P	2.11	114.66	105.09
6	C	1930	FAD	C2A-N1A-C6A	2.33	122.94	118.77
6	F	1931	FAD	C2A-N1A-C6A	2.39	123.03	118.77
6	C	1930	FAD	P-O3P-PA	2.61	140.05	132.73
5	E	1921	CDP	N4-C4-N3	3.46	122.81	116.50
5	E	1921	CDP	O3A-PA-O5'	3.58	112.44	102.94
5	B	1920	CDP	O3A-PA-O5'	3.80	113.02	102.94
5	B	1920	CDP	O4'-C4'-C3'	3.96	113.12	105.15
5	B	1920	CDP	N4-C4-N3	4.11	123.99	116.50
5	E	1921	CDP	O4'-C4'-C3'	4.11	113.43	105.15
5	B	1920	CDP	O4'-C1'-N1	6.28	121.32	108.08
5	B	1920	CDP	C2-N3-C4	6.34	124.56	115.61
5	E	1921	CDP	C2-N3-C4	6.39	124.63	115.61
5	E	1921	CDP	O4'-C1'-N1	6.83	122.48	108.08
5	E	1921	CDP	O2B-PB-O1B	7.00	133.13	110.58
6	C	1930	FAD	C4-N3-C2	7.03	121.32	115.25
6	F	1931	FAD	C4-N3-C2	7.03	121.33	115.25
5	B	1920	CDP	O2B-PB-O1B	7.10	133.44	110.58
5	E	1921	CDP	C4'-O4'-C1'	7.15	117.58	109.72
5	B	1920	CDP	C4'-O4'-C1'	7.34	117.79	109.72
6	C	1930	FAD	O2'-C2'-C3'	7.95	129.01	109.02
6	F	1931	FAD	O2'-C2'-C3'	8.94	131.50	109.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	E	1921	CDP	C2'
5	B	1920	CDP	C2'

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1920	CDP	1	0
6	C	1930	FAD	9	0
4	D	1910	FES	1	0
5	E	1921	CDP	1	0
6	F	1931	FAD	7	0

## 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.