Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2023 – 06:13 AM EDT

PDB ID	:	3NIX
Title	:	Crystal structure of flavoprotein/dehydrogenase from Cytophaga hutchinsonii. Northeast Structural Genomics Consortium Target ChR43.
Authors	:	Vorobiev, S.; Su, M.; Seetharaman, J.; Sahdev, S.; Xiao, R.; Foote, E.L.; Ciccosanti, C.; Maglaqui, M.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2010-06-16
Resolution	:	2.60 Å(reported)

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

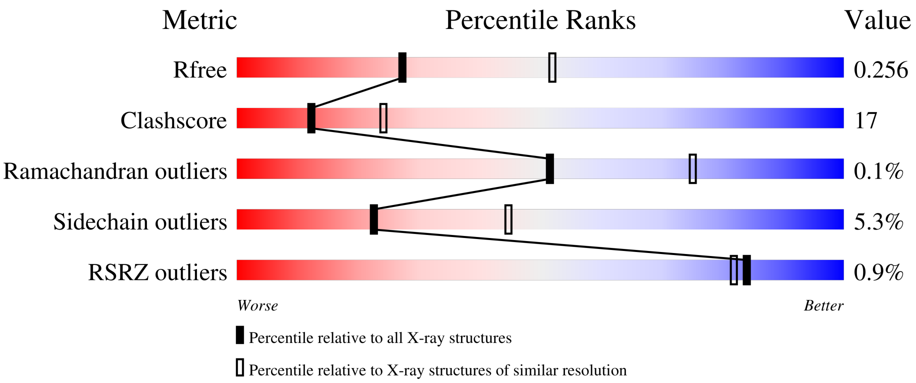
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

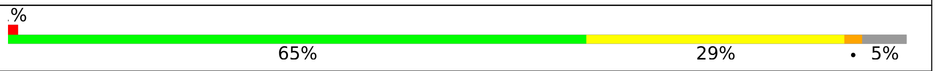
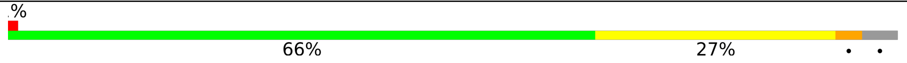
The reported resolution of this entry is 2.60 Å.

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))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	421	
1	B	421	
1	C	421	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

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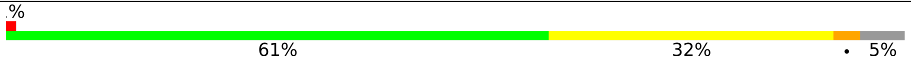
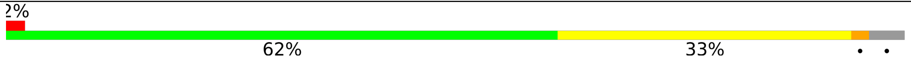
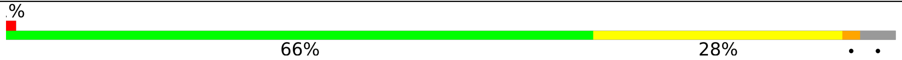
Mol	Chain	Length	Quality of chain
1	D	421	
1	E	421	
1	F	421	
1	G	421	
1	H	421	

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	FAD	F	506	X	-	-	-
2	FAD	G	507	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26852 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 Flavoprotein/dehydrogenase.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	407	Total C N O S Se 3210 2062 544 593 2 9	0	0	0
1	B	400	Total C N O S Se 3162 2032 537 582 2 9	0	0	0
1	C	405	Total C N O S Se 3185 2047 542 585 2 9	0	0	0
1	D	403	Total C N O S Se 3183 2046 541 585 2 9	0	0	0
1	E	406	Total C N O S Se 3212 2062 547 592 2 9	0	0	0
1	F	402	Total C N O S Se 3182 2045 540 586 2 9	0	0	0
1	G	406	Total C N O S Se 3204 2057 546 590 2 9	0	0	0
1	H	403	Total C N O S Se 3177 2041 540 585 2 9	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP Q11R94
A	414	LEU	-	expression tag	UNP Q11R94
A	415	GLU	-	expression tag	UNP Q11R94
A	416	HIS	-	expression tag	UNP Q11R94
A	417	HIS	-	expression tag	UNP Q11R94
A	418	HIS	-	expression tag	UNP Q11R94
A	419	HIS	-	expression tag	UNP Q11R94
A	420	HIS	-	expression tag	UNP Q11R94
A	421	HIS	-	expression tag	UNP Q11R94
B	1	MSE	-	initiating methionine	UNP Q11R94
B	414	LEU	-	expression tag	UNP Q11R94
B	415	GLU	-	expression tag	UNP Q11R94
B	416	HIS	-	expression tag	UNP Q11R94

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Chain	Residue	Modelled	Actual	Comment	Reference
B	417	HIS	-	expression tag	UNP Q11R94
B	418	HIS	-	expression tag	UNP Q11R94
B	419	HIS	-	expression tag	UNP Q11R94
B	420	HIS	-	expression tag	UNP Q11R94
B	421	HIS	-	expression tag	UNP Q11R94
C	1	MSE	-	initiating methionine	UNP Q11R94
C	414	LEU	-	expression tag	UNP Q11R94
C	415	GLU	-	expression tag	UNP Q11R94
C	416	HIS	-	expression tag	UNP Q11R94
C	417	HIS	-	expression tag	UNP Q11R94
C	418	HIS	-	expression tag	UNP Q11R94
C	419	HIS	-	expression tag	UNP Q11R94
C	420	HIS	-	expression tag	UNP Q11R94
C	421	HIS	-	expression tag	UNP Q11R94
D	1	MSE	-	initiating methionine	UNP Q11R94
D	414	LEU	-	expression tag	UNP Q11R94
D	415	GLU	-	expression tag	UNP Q11R94
D	416	HIS	-	expression tag	UNP Q11R94
D	417	HIS	-	expression tag	UNP Q11R94
D	418	HIS	-	expression tag	UNP Q11R94
D	419	HIS	-	expression tag	UNP Q11R94
D	420	HIS	-	expression tag	UNP Q11R94
D	421	HIS	-	expression tag	UNP Q11R94
E	1	MSE	-	initiating methionine	UNP Q11R94
E	414	LEU	-	expression tag	UNP Q11R94
E	415	GLU	-	expression tag	UNP Q11R94
E	416	HIS	-	expression tag	UNP Q11R94
E	417	HIS	-	expression tag	UNP Q11R94
E	418	HIS	-	expression tag	UNP Q11R94
E	419	HIS	-	expression tag	UNP Q11R94
E	420	HIS	-	expression tag	UNP Q11R94
E	421	HIS	-	expression tag	UNP Q11R94
F	1	MSE	-	initiating methionine	UNP Q11R94
F	414	LEU	-	expression tag	UNP Q11R94
F	415	GLU	-	expression tag	UNP Q11R94
F	416	HIS	-	expression tag	UNP Q11R94
F	417	HIS	-	expression tag	UNP Q11R94
F	418	HIS	-	expression tag	UNP Q11R94
F	419	HIS	-	expression tag	UNP Q11R94
F	420	HIS	-	expression tag	UNP Q11R94
F	421	HIS	-	expression tag	UNP Q11R94
G	1	MSE	-	initiating methionine	UNP Q11R94

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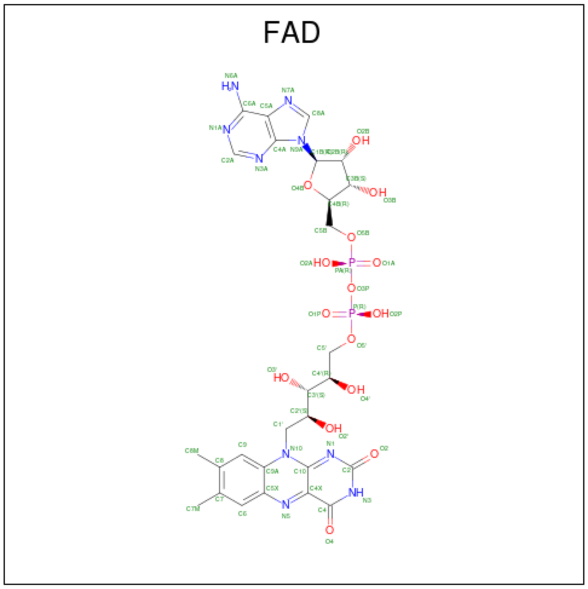
Chain	Residue	Modelled	Actual	Comment	Reference
G	414	LEU	-	expression tag	UNP Q11R94
G	415	GLU	-	expression tag	UNP Q11R94
G	416	HIS	-	expression tag	UNP Q11R94
G	417	HIS	-	expression tag	UNP Q11R94
G	418	HIS	-	expression tag	UNP Q11R94
G	419	HIS	-	expression tag	UNP Q11R94
G	420	HIS	-	expression tag	UNP Q11R94
G	421	HIS	-	expression tag	UNP Q11R94
H	1	MSE	-	initiating methionine	UNP Q11R94
H	414	LEU	-	expression tag	UNP Q11R94
H	415	GLU	-	expression tag	UNP Q11R94
H	416	HIS	-	expression tag	UNP Q11R94
H	417	HIS	-	expression tag	UNP Q11R94
H	418	HIS	-	expression tag	UNP Q11R94
H	419	HIS	-	expression tag	UNP Q11R94
H	420	HIS	-	expression tag	UNP Q11R94
H	421	HIS	-	expression tag	UNP Q11R94

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_{9}O_{15}P_{2}$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O P 53 27 9 15 2	0	0
2	D	1	Total C N O P 53 27 9 15 2	0	0
2	E	1	Total C N O P 53 27 9 15 2	0	0
2	F	1	Total C N O P 53 27 9 15 2	0	0
2	G	1	Total C N O P 53 27 9 15 2	0	0
2	H	1	Total C N O P 53 27 9 15 2	0	0

- Molecule 3 is water.

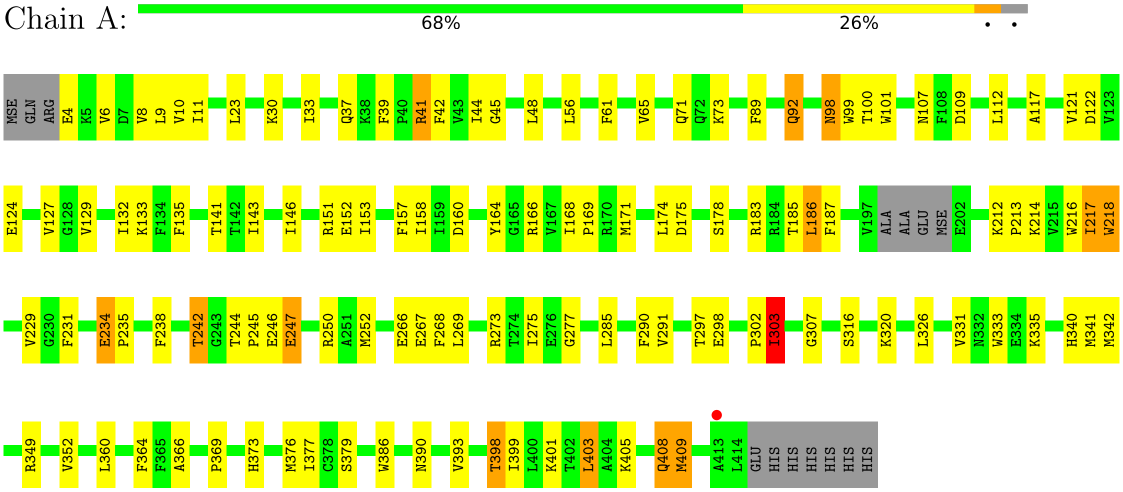
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	125	Total O 125 125	0	0
3	B	139	Total O 139 139	0	0
3	C	119	Total O 119 119	0	0
3	D	81	Total O 81 81	0	0
3	E	148	Total O 148 148	0	0
3	F	99	Total O 99 99	0	0
3	G	89	Total O 89 89	0	0
3	H	113	Total O 113 113	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

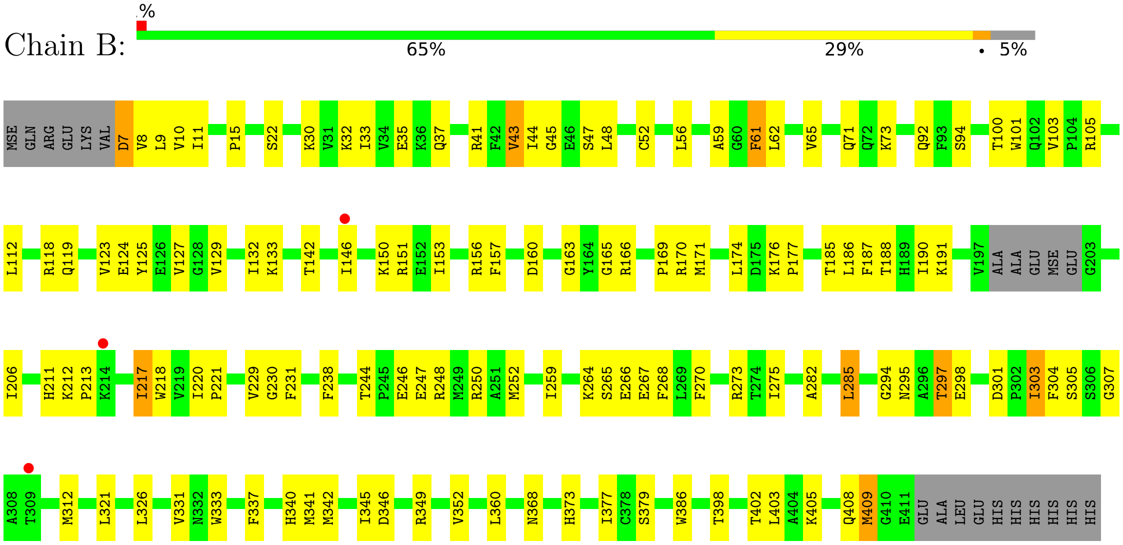
- Molecule 1: Flavoprotein/dehydrogenase

Chain A:



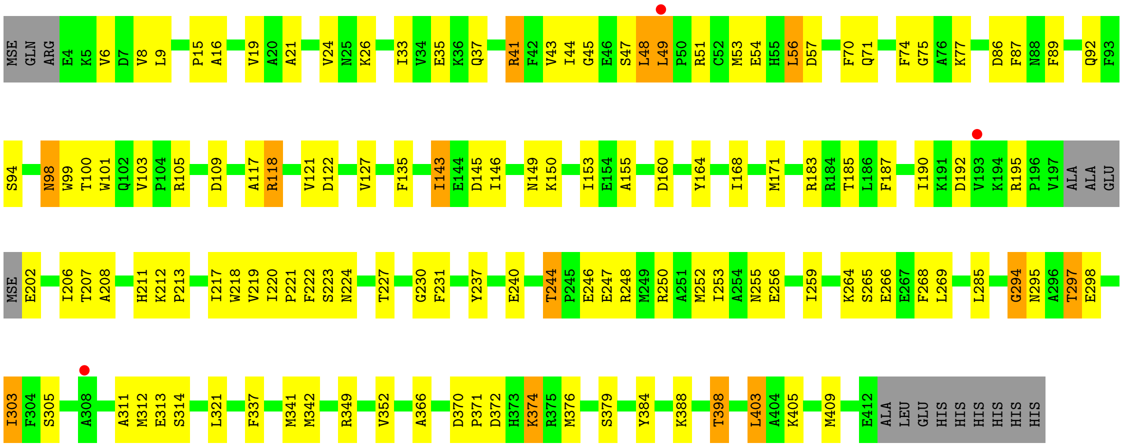
- Molecule 1: Flavoprotein/dehydrogenase

Chain B:



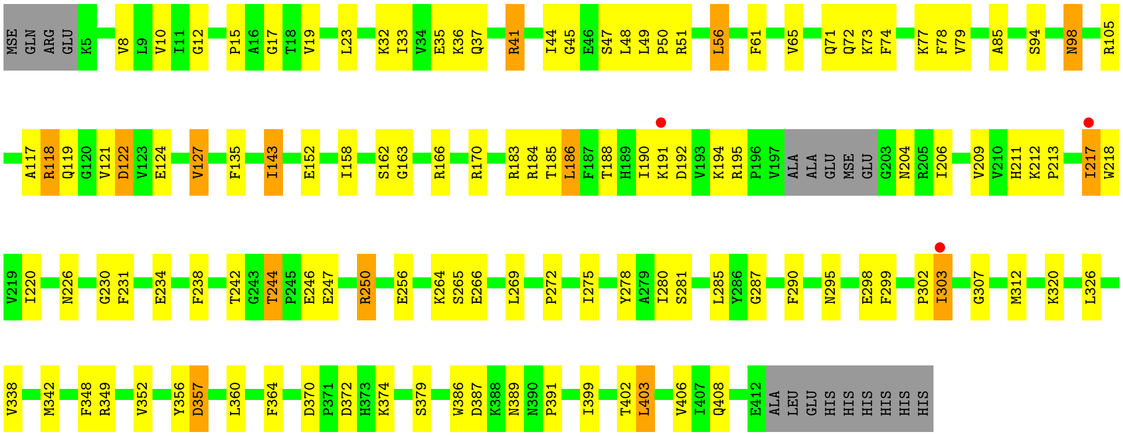
- Molecule 1: Flavoprotein/dehydrogenase

Chain C:



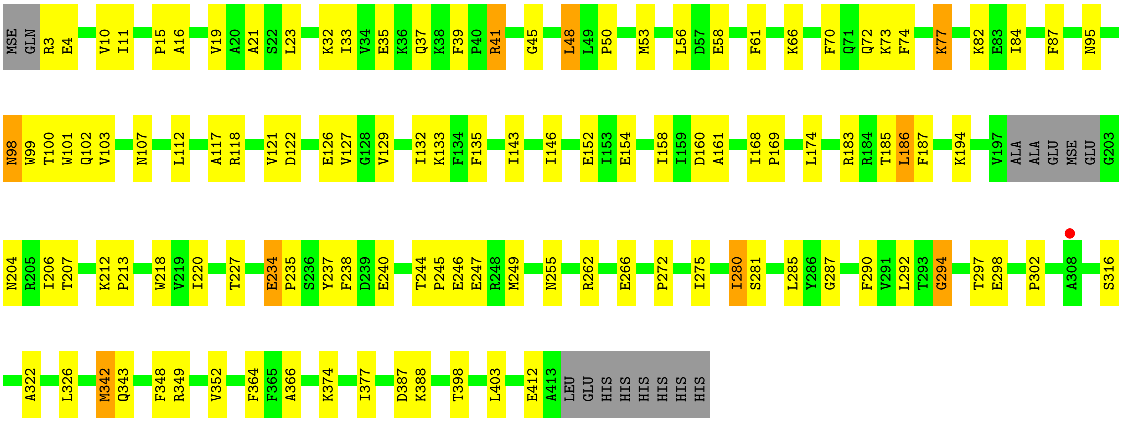
- Molecule 1: Flavoprotein/dehydrogenase

Chain D:



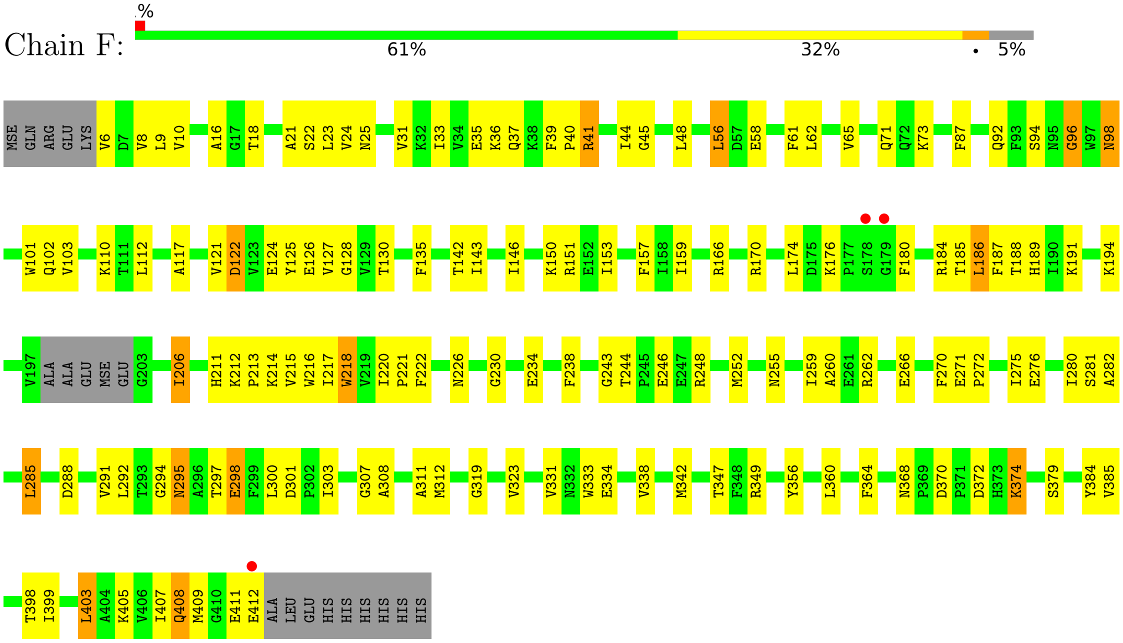
- Molecule 1: Flavoprotein/dehydrogenase

Chain E:



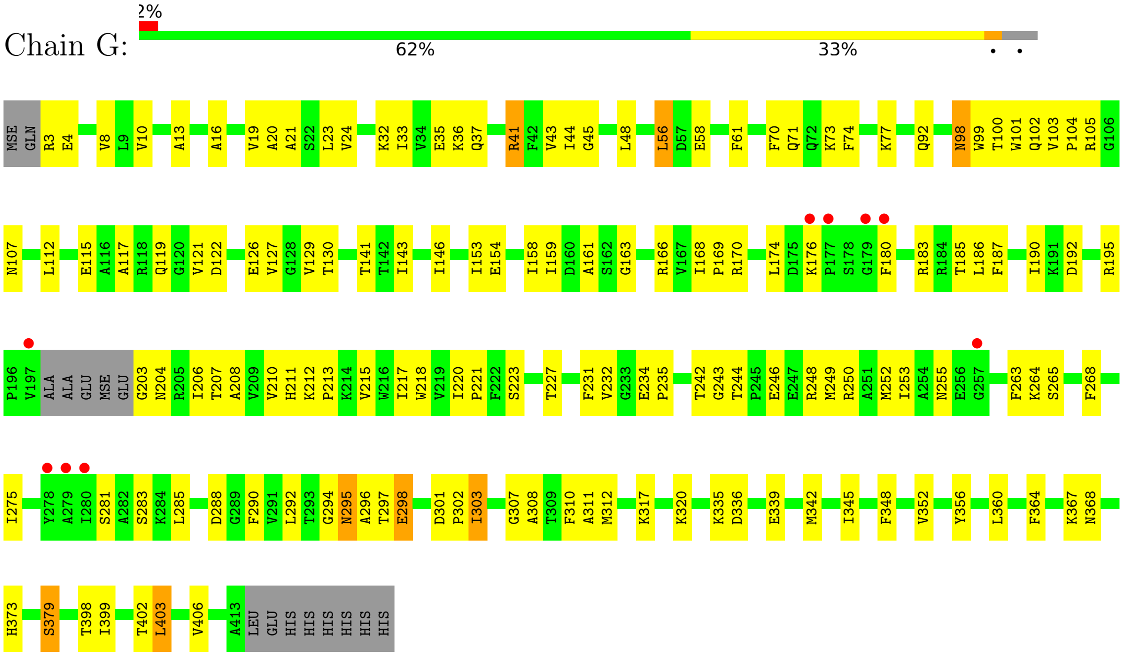
- Molecule 1: Flavoprotein/dehydrogenase

Chain F:



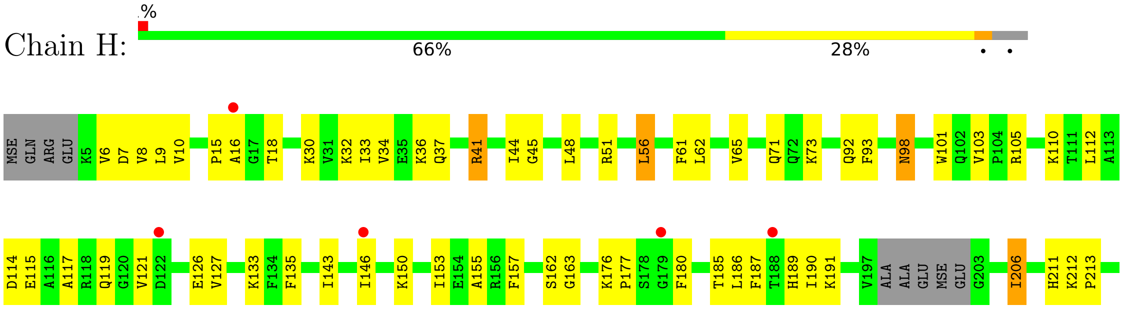
- Molecule 1: Flavoprotein/dehydrogenase

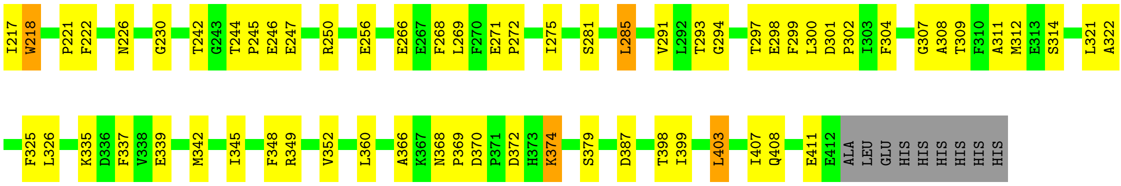
Chain G:



- Molecule 1: Flavoprotein/dehydrogenase

Chain H:




I217
W218
P221
F222
N226
G230
T242
G243
T244
P245
E246
E247
R250
E256
E266
E267
F268
L269
F270
E271
P272
I275
S281
L285
V291
L292
T293
G294
T297
E298
F299
L300
D301
P302
I303
F304
G307
A308
T309
F310
A311
M312
E313
S314
L321
A322
F325
L326
K335
D336
F337
V338
E339
M342
I345
F348
R349
V352
L360
A366
K367
N368
P369
D370
P371
D372
H373
K374
S379
D387
T398
I399
L403
I407
Q408
E411
E412
ALA
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.22Å 244.05Å 100.22Å 90.00° 104.10° 90.00°	Depositor
Resolution (Å)	29.33 – 2.60 29.73 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.33-2.60) 97.5 (29.73-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.08 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.6_289, REFMAC	Depositor
R, R_{free}	0.237 , 0.264 0.229 , 0.256	Depositor DCC
R_{free} test set	6026 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.8	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	26852	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.29 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3396e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.53	2/3281 (0.1%)	0.64	1/4415 (0.0%)
1	B	0.59	1/3233 (0.0%)	0.63	0/4349
1	C	0.53	1/3256 (0.0%)	0.62	0/4382
1	D	0.44	0/3254	0.59	0/4377
1	E	0.49	0/3283	0.64	0/4415
1	F	0.45	0/3253	0.59	1/4375 (0.0%)
1	G	0.46	0/3275	0.59	0/4406
1	H	0.50	0/3248	0.60	0/4370
All	All	0.50	4/26083 (0.0%)	0.61	2/35089 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	208	ALA	C-N	-5.91	1.20	1.34
1	A	247	GLU	CD-OE2	-5.64	1.19	1.25
1	B	61	PHE	CD2-CE2	-5.37	1.28	1.39
1	A	247	GLU	CD-OE1	-5.09	1.20	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	303	ILE	CB-CA-C	-5.52	100.55	111.60
1	F	96	GLY	N-CA-C	-5.36	99.69	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	3210	0	3125	109	0
1	B	3162	0	3084	111	0
1	C	3185	0	3096	111	0
1	D	3183	0	3108	104	0
1	E	3212	0	3136	91	0
1	F	3182	0	3110	120	0
1	G	3204	0	3121	124	0
1	H	3177	0	3090	101	0
2	A	53	0	28	4	0
2	B	53	0	29	5	0
2	C	53	0	29	3	0
2	D	53	0	29	8	0
2	E	53	0	29	5	0
2	F	53	0	28	6	0
2	G	53	0	29	13	0
2	H	53	0	29	10	0
3	A	125	0	0	12	0
3	B	139	0	0	7	0
3	C	119	0	0	5	0
3	D	81	0	0	6	0
3	E	148	0	0	15	0
3	F	99	0	0	14	0
3	G	89	0	0	9	0
3	H	113	0	0	5	0
All	All	26852	0	25100	865	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 17.

All (865) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:THR:HG22	1:C:298:GLU:H	1.12	1.11
1:D:41:ARG:HG2	1:D:41:ARG:HH11	0.88	1.02
1:B:297:THR:HG22	1:B:298:GLU:H	1.22	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:LEU:HG	3:D:1156:HOH:O	1.58	1.01
1:E:41:ARG:HG2	1:E:41:ARG:HH11	0.87	1.00
1:D:41:ARG:HG2	1:D:41:ARG:NH1	1.68	1.00
1:C:41:ARG:HH11	1:C:41:ARG:HG2	1.25	0.98
1:E:41:ARG:HG2	1:E:41:ARG:NH1	1.65	0.98
1:A:244:THR:HG22	1:A:247:GLU:HG3	1.43	0.97
1:D:41:ARG:HH11	1:D:41:ARG:CG	1.79	0.95
1:E:249:MSE:HE3	1:E:272:PRO:HB3	1.49	0.95
1:B:297:THR:HG22	1:B:298:GLU:N	1.80	0.94
1:C:206:ILE:HG13	1:C:220:ILE:HG12	1.50	0.94
1:G:127:VAL:CG1	1:G:143:ILE:HB	1.98	0.93
1:C:297:THR:HG22	1:C:298:GLU:N	1.83	0.93
1:F:127:VAL:HG12	1:F:143:ILE:HB	1.52	0.92
1:E:41:ARG:HH11	1:E:41:ARG:CG	1.80	0.92
1:C:94:SER:H	1:C:379:SER:HG	1.19	0.90
1:D:118:ARG:HH11	1:D:118:ARG:HG2	1.37	0.89
1:D:244:THR:HG22	1:D:247:GLU:HG3	1.54	0.89
1:E:186:LEU:HD13	1:E:249:MSE:HE2	1.56	0.88
1:F:127:VAL:HG11	1:F:143:ILE:HD12	1.56	0.88
1:E:11:ILE:HD13	1:E:129:VAL:HG21	1.55	0.87
1:B:7:ASP:HB3	1:B:30:LYS:O	1.74	0.87
1:G:19:VAL:HG21	1:G:312:MSE:HG2	1.57	0.85
1:H:45:GLY:HA2	2:H:508:FAD:C4X	2.06	0.85
1:A:244:THR:HG22	1:A:247:GLU:CG	2.06	0.85
1:A:89:PHE:HB3	3:A:1513:HOH:O	1.76	0.84
1:A:297:THR:HG22	1:A:298:GLU:N	1.92	0.84
1:E:82:LYS:HD3	3:E:782:HOH:O	1.76	0.84
1:A:390:ASN:HD22	1:A:393:VAL:HG23	1.39	0.84
1:F:303:ILE:HD11	1:F:356:TYR:CE2	2.13	0.83
1:C:41:ARG:HG2	1:C:41:ARG:NH1	1.88	0.83
1:F:45:GLY:HA2	2:F:506:FAD:C4X	2.09	0.83
1:C:244:THR:HG22	1:C:247:GLU:H	1.43	0.82
1:G:317:LYS:HG2	3:G:1282:HOH:O	1.80	0.82
1:B:8:VAL:HG23	1:B:326:LEU:HD11	1.61	0.82
1:G:45:GLY:HA2	2:G:507:FAD:C4X	2.10	0.81
1:C:98:ASN:HD22	1:C:99:TRP:N	1.78	0.80
1:C:297:THR:CG2	1:C:298:GLU:H	1.94	0.80
1:E:298:GLU:CD	1:E:349:ARG:HH22	1.83	0.80
1:C:211:HIS:O	1:C:212:LYS:HE2	1.81	0.80
1:B:15:PRO:HB3	1:B:312:MSE:HE3	1.64	0.80
1:G:307:GLY:HA3	2:G:507:FAD:H1'2	1.63	0.80

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:F:22:SER:HB2	3:F:866:HOH:O	1.81	0.80
1:A:98:ASN:HA	3:A:1513:HOH:O	1.81	0.79
1:A:244:THR:CG2	1:A:247:GLU:HG3	2.11	0.79
1:C:253:ILE:HG23	1:C:259:ILE:HD12	1.62	0.79
1:C:48:LEU:O	1:C:100:THR:HG21	1.82	0.79
1:C:98:ASN:HD22	1:C:98:ASN:C	1.86	0.79
1:E:66:LYS:HG2	3:E:1120:HOH:O	1.82	0.78
1:B:297:THR:CG2	1:B:298:GLU:N	2.48	0.77
1:G:246:GLU:O	1:G:250:ARG:HG3	1.83	0.77
1:D:212:LYS:HB3	1:D:213:PRO:HD2	1.64	0.77
1:D:45:GLY:HA2	2:D:504:FAD:C4X	2.15	0.77
1:G:373:HIS:CE1	1:G:403:LEU:HD11	2.20	0.76
1:A:244:THR:HG21	3:B:1514:HOH:O	1.86	0.76
1:C:41:ARG:HH11	1:C:41:ARG:CG	1.98	0.76
1:C:77:LYS:HE2	1:C:86:ASP:OD1	1.86	0.76
1:E:186:LEU:C	1:E:249:MSE:HE1	2.07	0.75
1:E:84:ILE:HG23	3:E:1586:HOH:O	1.87	0.75
1:C:297:THR:CG2	1:C:298:GLU:N	2.49	0.74
1:D:118:ARG:HG2	1:D:118:ARG:NH1	1.99	0.74
1:C:127:VAL:HG13	1:C:143:ILE:HB	1.66	0.74
1:C:45:GLY:HA2	2:C:503:FAD:C4X	2.18	0.73
1:D:185:THR:HG22	1:D:275:ILE:O	1.88	0.73
1:E:297:THR:HG22	1:E:298:GLU:N	2.01	0.73
1:G:23:LEU:HD21	1:G:58:GLU:HG2	1.69	0.73
1:H:98:ASN:HD22	1:H:98:ASN:H	1.36	0.73
1:E:249:MSE:CE	1:E:272:PRO:HB3	2.17	0.73
1:F:307:GLY:HA3	2:F:506:FAD:H1'2	1.69	0.73
1:A:169:PRO:HA	1:A:174:LEU:HB2	1.71	0.72
1:E:152:GLU:OE2	1:H:133:LYS:HE3	1.89	0.72
1:F:301:ASP:OD2	1:F:303:ILE:HG13	1.89	0.72
1:A:45:GLY:HA2	2:A:501:FAD:C4X	2.19	0.72
1:C:127:VAL:HG11	1:C:143:ILE:HD12	1.72	0.72
1:A:390:ASN:ND2	1:A:393:VAL:HG23	2.05	0.71
1:A:127:VAL:HG13	1:A:143:ILE:HB	1.72	0.71
1:H:127:VAL:HG13	1:H:143:ILE:HB	1.71	0.71
1:H:176:LYS:HG2	1:H:281:SER:HB3	1.71	0.71
1:C:298:GLU:OE2	1:C:349:ARG:NH2	2.24	0.71
1:E:16:ALA:HB3	3:E:751:HOH:O	1.91	0.71
1:E:169:PRO:HA	1:E:174:LEU:HB2	1.72	0.71
1:G:244:THR:HG22	1:G:246:GLU:H	1.55	0.71
1:F:297:THR:HG22	1:F:298:GLU:N	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:GLY:HA2	2:E:505:FAD:C4X	2.20	0.71
1:D:127:VAL:HG13	1:D:143:ILE:HB	1.72	0.70
1:E:298:GLU:OE2	1:E:349:ARG:NH2	2.24	0.70
1:G:211:HIS:O	1:G:212:LYS:HD3	1.91	0.70
1:C:41:ARG:HG2	1:C:41:ARG:O	1.92	0.70
1:G:21:ALA:CB	1:G:33:ILE:HD11	2.22	0.70
1:A:408:GLN:HE21	1:A:409:MSE:HE2	1.56	0.70
1:E:160:ASP:HB2	1:E:168:ILE:HD12	1.73	0.69
1:D:348:PHE:O	1:D:352:VAL:HG23	1.91	0.69
1:C:77:LYS:HZ2	1:C:202:GLU:N	1.91	0.69
1:B:273:ARG:HD3	3:B:1539:HOH:O	1.92	0.69
1:D:94:SER:H	1:D:379:SER:HG	1.40	0.69
1:E:237:TYR:O	1:E:240:GLU:HG2	1.93	0.69
1:G:105:ARG:HH12	2:G:507:FAD:H4’	1.57	0.68
1:A:107:ASN:HB3	3:A:831:HOH:O	1.92	0.68
1:D:278:TYR:CD1	1:D:299:PHE:HE2	2.11	0.68
1:H:115:GLU:O	1:H:119:GLN:HG3	1.94	0.68
1:G:303:ILE:HD11	1:G:356:TYR:CE2	2.28	0.68
1:A:212:LYS:HB3	1:A:213:PRO:HD2	1.74	0.68
1:C:87:PHE:CE2	1:C:374:LYS:HG3	2.28	0.68
1:H:297:THR:HG22	1:H:298:GLU:N	2.07	0.68
1:A:39:PHE:CE1	1:A:41:ARG:HD3	2.28	0.68
1:E:245:PRO:HD3	3:E:739:HOH:O	1.94	0.68
1:F:281:SER:OG	1:F:298:GLU:HG3	1.93	0.68
1:A:39:PHE:HE1	1:A:41:ARG:HD3	1.59	0.67
1:A:92:GLN:HB2	1:A:379:SER:OG	1.94	0.67
1:G:212:LYS:HB2	1:G:215:VAL:HB	1.76	0.67
1:H:342:MSE:HA	1:H:342:MSE:HE2	1.74	0.67
1:B:206:ILE:HG13	1:B:220:ILE:HG12	1.77	0.67
1:F:248:ARG:O	1:F:252:MSE:HG3	1.93	0.67
1:B:94:SER:H	1:B:379:SER:HG	1.42	0.66
1:E:135:PHE:HD2	1:H:135:PHE:CD2	2.13	0.66
1:A:127:VAL:HG11	1:A:143:ILE:HD12	1.76	0.66
1:B:92:GLN:HB2	1:B:379:SER:OG	1.96	0.66
1:G:250:ARG:HG2	1:G:268:PHE:CZ	2.31	0.66
1:A:250:ARG:NH2	1:A:266:GLU:O	2.29	0.65
1:G:174:LEU:O	1:G:283:SER:N	2.20	0.65
1:G:285:LEU:HG	1:G:297:THR:HG23	1.77	0.65
1:G:127:VAL:HG11	1:G:143:ILE:HD12	1.79	0.65
1:A:132:ILE:H	1:A:171:MSE:SE	2.30	0.65
1:C:48:LEU:CD1	1:C:48:LEU:N	2.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:ALA:HB2	1:G:33:ILE:HD11	1.79	0.65
1:G:35:GLU:OE1	2:G:507:FAD:H1B	1.97	0.65
1:C:246:GLU:O	1:C:250:ARG:HG3	1.97	0.65
1:H:71:GLN:HG2	1:H:221:PRO:O	1.97	0.65
1:A:303:ILE:CD1	1:A:352:VAL:HG22	2.27	0.64
1:F:92:GLN:NE2	1:F:379:SER:HA	2.13	0.64
1:F:374:LYS:HE2	3:F:825:HOH:O	1.97	0.64
1:B:45:GLY:HA2	2:B:502:FAD:C4X	2.28	0.64
1:D:23:LEU:HD13	1:D:320:LYS:HG3	1.79	0.64
1:H:185:THR:HG22	1:H:275:ILE:O	1.98	0.64
1:D:98:ASN:C	1:D:98:ASN:HD22	2.00	0.64
1:C:48:LEU:N	1:C:48:LEU:HD12	2.12	0.64
1:G:23:LEU:HD13	1:G:320:LYS:HG3	1.79	0.63
1:E:342:MSE:N	1:E:342:MSE:HE2	2.13	0.63
1:H:37:GLN:NE2	1:H:41:ARG:HG3	2.14	0.63
1:F:73:LYS:HE3	1:F:206:ILE:HG22	1.79	0.63
1:A:244:THR:HG23	1:A:247:GLU:H	1.64	0.62
1:D:12:GLY:O	1:D:17:GLY:HA3	1.99	0.62
1:F:127:VAL:CG1	1:F:143:ILE:HB	2.25	0.62
1:A:231:PHE:CD2	1:A:252:MSE:HE2	2.33	0.62
1:C:41:ARG:NH2	1:C:109:ASP:OD2	2.25	0.62
1:C:342:MSE:N	1:C:342:MSE:HE2	2.15	0.62
1:B:303:ILE:HD12	1:B:352:VAL:HG22	1.80	0.62
1:G:74:PHE:HD2	1:G:204:ASN:HD22	1.47	0.62
1:D:74:PHE:HD2	1:D:204:ASN:HD22	1.48	0.62
1:E:23:LEU:HD21	1:E:58:GLU:HG2	1.81	0.62
1:F:23:LEU:HD21	1:F:58:GLU:HG2	1.82	0.61
1:G:73:LYS:HE3	1:G:206:ILE:HG22	1.81	0.61
1:E:187:PHE:N	1:E:249:MSE:HE1	2.14	0.61
1:H:126:GLU:OE1	1:H:146:ILE:HD11	2.00	0.61
1:E:135:PHE:CD2	1:H:135:PHE:CD2	2.88	0.61
1:B:185:THR:HG22	1:B:275:ILE:O	2.01	0.61
1:C:47:SER:C	1:C:48:LEU:HD12	2.21	0.61
1:A:185:THR:HG22	1:A:275:ILE:O	2.01	0.60
1:A:242:THR:OG1	1:B:340:HIS:ND1	2.26	0.60
1:F:87:PHE:CE2	1:F:374:LYS:HD2	2.37	0.60
1:F:211:HIS:O	1:F:212:LYS:HD3	2.02	0.60
1:F:166:ARG:HB2	1:F:170:ARG:HG3	1.82	0.60
1:B:246:GLU:OE2	1:B:250:ARG:NH1	2.34	0.60
1:C:74:PHE:CE1	1:C:99:TRP:HB2	2.36	0.60
1:C:211:HIS:CE1	1:C:256:GLU:HB2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ILE:H	1:B:171:MSE:SE	2.34	0.60
1:G:163:GLY:HA3	2:G:507:FAD:O1A	2.01	0.60
1:H:180:PHE:HE2	1:H:300:LEU:HD22	1.66	0.60
1:E:98:ASN:HD22	1:E:99:TRP:N	1.98	0.60
1:G:294:GLY:HA2	1:G:311:ALA:HA	1.83	0.60
1:F:61:PHE:CD2	1:F:112:LEU:HG	2.36	0.59
1:B:142:THR:HG21	1:B:150:LYS:HD2	1.84	0.59
1:D:298:GLU:OE2	1:D:349:ARG:NH2	2.34	0.59
1:E:41:ARG:HG2	1:E:41:ARG:O	2.02	0.59
1:F:6:VAL:N	3:F:641:HOH:O	2.34	0.59
1:G:16:ALA:HB3	1:G:161:ALA:HB1	1.84	0.59
1:G:117:ALA:HA	1:G:121:VAL:O	2.03	0.59
1:A:246:GLU:OE2	1:A:250:ARG:NH1	2.35	0.59
1:A:405:LYS:HE3	1:A:409:MSE:HE3	1.83	0.59
1:B:373:HIS:O	1:B:377:ILE:HG13	2.01	0.59
1:H:56:LEU:HD13	1:H:312:MSE:SE	2.53	0.59
1:C:56:LEU:HD13	1:C:312:MSE:SE	2.53	0.59
1:F:212:LYS:HB3	1:F:213:PRO:HD2	1.84	0.59
1:F:399:ILE:O	1:F:403:LEU:HB2	2.02	0.59
1:F:399:ILE:HG12	1:F:403:LEU:HD22	1.84	0.59
1:D:32:LYS:NZ	1:D:124:GLU:OE1	2.36	0.59
1:F:285:LEU:HA	1:F:292:LEU:HD12	1.84	0.59
1:F:347:THR:HG21	1:F:385:VAL:HG12	1.85	0.59
1:G:192:ASP:CG	1:G:195:ARG:HB2	2.23	0.59
1:A:245:PRO:HD3	3:A:1596:HOH:O	2.02	0.58
1:B:342:MSE:HE2	1:B:342:MSE:N	2.18	0.58
1:E:212:LYS:HB3	1:E:213:PRO:HD2	1.84	0.58
1:F:130:THR:HG22	1:F:142:THR:O	2.03	0.58
1:A:216:TRP:CH2	1:A:303:ILE:HA	2.37	0.58
1:E:16:ALA:HB3	1:E:161:ALA:HB1	1.85	0.58
1:A:303:ILE:HD12	1:A:352:VAL:HG22	1.86	0.58
1:F:71:GLN:HG2	1:F:221:PRO:O	2.04	0.58
1:A:408:GLN:NE2	1:A:409:MSE:HE2	2.18	0.58
1:C:71:GLN:HG2	1:C:221:PRO:O	2.03	0.58
1:E:127:VAL:HG13	1:E:143:ILE:HB	1.84	0.58
1:E:204:ASN:ND2	3:E:1559:HOH:O	2.34	0.58
1:B:43:VAL:HG12	1:B:105:ARG:CB	2.34	0.58
1:D:218:TRP:CD1	1:D:220:ILE:HD12	2.38	0.58
1:C:49:LEU:CD1	1:C:49:LEU:N	2.66	0.58
1:C:220:ILE:O	1:C:227:THR:HG23	2.03	0.58
1:B:250:ARG:NH2	1:B:266:GLU:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:ARG:NH1	1:D:41:ARG:CG	2.49	0.58
1:F:96:GLY:HA3	1:F:384:TYR:CZ	2.39	0.58
1:D:44:ILE:HG13	1:D:45:GLY:N	2.18	0.57
1:E:206:ILE:HG21	3:E:689:HOH:O	2.04	0.57
1:F:117:ALA:HA	1:F:121:VAL:O	2.04	0.57
1:B:244:THR:HG23	1:B:247:GLU:H	1.69	0.57
1:A:231:PHE:CG	1:A:252:MSE:HE2	2.39	0.57
1:B:9:LEU:HD13	1:B:153:ILE:HG21	1.86	0.57
1:B:211:HIS:O	1:B:212:LYS:HD2	2.05	0.57
1:D:303:ILE:HD11	1:D:352:VAL:HG13	1.87	0.57
1:E:4:GLU:OE1	1:E:32:LYS:HE3	2.04	0.57
1:B:285:LEU:HD21	1:B:342:MSE:HE3	1.86	0.57
1:A:298:GLU:OE1	1:A:349:ARG:NH2	2.36	0.57
1:C:405:LYS:HE3	1:C:409:MSE:HE1	1.84	0.57
1:E:117:ALA:HA	1:E:121:VAL:O	2.05	0.57
1:G:183:ARG:NH1	3:G:1511:HOH:O	2.37	0.57
1:G:48:LEU:HB2	1:G:101:TRP:O	2.05	0.57
1:C:250:ARG:NH2	1:C:266:GLU:O	2.38	0.57
1:G:104:PRO:HB2	1:G:107:ASN:ND2	2.20	0.57
1:H:244:THR:HG22	1:H:247:GLU:HB2	1.87	0.57
1:D:399:ILE:O	1:D:403:LEU:HB2	2.04	0.56
1:G:399:ILE:O	1:G:403:LEU:HB2	2.04	0.56
1:B:65:VAL:HG11	1:B:101:TRP:CZ3	2.40	0.56
1:B:398:THR:HG22	3:B:1471:HOH:O	2.05	0.56
1:C:303:ILE:C	1:C:305:SER:H	2.09	0.56
1:C:398:THR:CG2	3:C:1003:HOH:O	2.52	0.56
1:D:280:ILE:HG13	1:D:281:SER:N	2.20	0.56
1:A:117:ALA:HA	1:A:121:VAL:O	2.05	0.56
1:F:285:LEU:HD21	1:F:342:MSE:HE3	1.86	0.56
1:G:10:VAL:HB	1:G:33:ILE:HG12	1.87	0.56
1:A:307:GLY:HA3	2:A:501:FAD:H1'2	1.88	0.56
1:C:49:LEU:N	1:C:49:LEU:HD12	2.20	0.56
1:A:41:ARG:NH1	2:A:501:FAD:O3B	2.39	0.56
1:C:98:ASN:C	1:C:98:ASN:ND2	2.59	0.56
1:G:402:THR:O	1:G:406:VAL:HG23	2.05	0.56
1:H:7:ASP:HB2	1:H:30:LYS:O	2.05	0.56
1:B:43:VAL:HG12	1:B:105:ARG:HB3	1.87	0.56
1:B:321:LEU:CD1	1:B:337:PHE:HB2	2.35	0.56
1:C:372:ASP:O	1:C:376:MSE:HG3	2.06	0.56
1:G:244:THR:HG22	1:G:246:GLU:N	2.20	0.56
1:B:8:VAL:CG2	1:B:326:LEU:HD11	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:308:ALA:N	2:F:506:FAD:O2	2.37	0.55
1:E:183:ARG:NH1	3:E:794:HOH:O	2.40	0.55
1:G:37:GLN:OE1	1:G:41:ARG:HD2	2.05	0.55
1:H:189:HIS:CE1	1:H:222:PHE:HE2	2.24	0.55
1:F:185:THR:HG22	1:F:275:ILE:O	2.06	0.55
1:H:98:ASN:HD22	1:H:98:ASN:N	1.99	0.55
1:B:212:LYS:HB3	1:B:213:PRO:HD2	1.87	0.55
1:C:212:LYS:HB3	1:C:213:PRO:HD2	1.87	0.55
1:D:183:ARG:NH1	3:D:608:HOH:O	2.34	0.55
1:A:285:LEU:HD21	1:A:342:MSE:HE3	1.87	0.55
1:C:127:VAL:CG1	1:C:143:ILE:HD12	2.36	0.55
1:H:44:ILE:HG13	1:H:45:GLY:H	1.71	0.55
1:H:93:PHE:H	1:H:379:SER:HG	1.55	0.55
1:C:41:ARG:NH1	1:C:41:ARG:O	2.39	0.55
1:D:79:VAL:HB	1:D:209:VAL:HG22	1.89	0.55
1:B:37:GLN:HG3	3:B:1504:HOH:O	2.05	0.55
1:F:408:GLN:NE2	1:F:412:GLU:OE1	2.39	0.55
1:A:41:ARG:NH2	1:A:109:ASP:OD2	2.39	0.55
1:B:47:SER:HB2	1:B:220:ILE:HD13	1.89	0.55
1:B:231:PHE:CD2	1:B:252:MSE:HE2	2.42	0.55
1:E:135:PHE:CD2	1:H:135:PHE:HD2	2.25	0.55
1:A:6:VAL:HG12	1:A:30:LYS:HE2	1.88	0.54
1:A:61:PHE:CD2	1:A:112:LEU:HG	2.42	0.54
1:A:297:THR:HG22	1:A:298:GLU:H	1.69	0.54
1:H:387:ASP:HB2	3:H:1580:HOH:O	2.06	0.54
1:B:7:ASP:CB	1:B:30:LYS:O	2.51	0.54
1:E:366:ALA:HA	3:E:802:HOH:O	2.07	0.54
1:F:45:GLY:HA2	2:F:506:FAD:N5	2.21	0.54
1:A:133:LYS:HE3	1:D:152:GLU:OE2	2.06	0.54
1:G:127:VAL:HG12	1:G:143:ILE:HB	1.86	0.54
1:A:399:ILE:O	1:A:403:LEU:HB2	2.08	0.54
1:A:303:ILE:HD11	1:A:352:VAL:HG13	1.90	0.54
1:B:321:LEU:HD22	1:B:331:VAL:HG13	1.89	0.54
1:D:206:ILE:HG13	1:D:220:ILE:HG12	1.90	0.54
1:A:399:ILE:CG1	1:A:403:LEU:HD23	2.37	0.54
1:C:15:PRO:O	1:C:19:VAL:HG23	2.07	0.54
1:H:73:LYS:HE3	1:H:206:ILE:HG22	1.88	0.54
1:C:48:LEU:O	1:C:100:THR:CG2	2.54	0.54
1:B:340:HIS:CE1	1:B:386:TRP:CD1	2.96	0.54
1:E:280:ILE:HG13	1:E:281:SER:N	2.22	0.54
1:G:360:LEU:HD11	1:G:364:PHE:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:VAL:HG11	1:A:333:TRP:CE2	2.43	0.53
1:C:8:VAL:HG21	1:C:24:VAL:HG11	1.88	0.53
1:F:44:ILE:HD13	1:F:187:PHE:CE1	2.44	0.53
1:F:370:ASP:C	1:F:370:ASP:OD1	2.46	0.53
1:H:244:THR:HG23	1:H:247:GLU:H	1.72	0.53
1:A:244:THR:CG2	1:A:247:GLU:H	2.21	0.53
1:D:278:TYR:CD1	1:D:299:PHE:CE2	2.94	0.53
1:E:194:LYS:HD2	1:E:262:ARG:HA	1.90	0.53
1:A:399:ILE:HG13	1:A:403:LEU:HD23	1.90	0.53
1:B:71:GLN:HG2	1:B:221:PRO:O	2.08	0.53
1:A:135:PHE:CD2	1:D:135:PHE:HD2	2.27	0.53
1:D:302:PRO:HB3	2:D:504:FAD:C6	2.38	0.53
1:H:307:GLY:HA3	2:H:508:FAD:H1'2	1.90	0.53
1:C:294:GLY:O	1:C:297:THR:HB	2.08	0.53
1:D:73:LYS:HE3	1:D:206:ILE:HG22	1.90	0.53
1:F:9:LEU:HD13	1:F:153:ILE:HG21	1.91	0.53
1:H:250:ARG:NH2	1:H:266:GLU:O	2.42	0.53
1:B:11:ILE:HD13	1:B:129:VAL:HG21	1.91	0.53
1:B:340:HIS:CE1	1:B:386:TRP:NE1	2.77	0.53
1:E:98:ASN:ND2	1:E:99:TRP:HD1	2.07	0.53
1:G:185:THR:CG2	1:G:275:ILE:HB	2.38	0.53
1:B:59:ALA:HB2	3:B:874:HOH:O	2.07	0.52
1:D:44:ILE:HG13	1:D:45:GLY:H	1.75	0.52
1:G:41:ARG:NH1	1:G:41:ARG:HG2	2.24	0.52
1:G:61:PHE:CD2	1:G:112:LEU:HG	2.43	0.52
1:D:360:LEU:HD11	1:D:364:PHE:CE1	2.44	0.52
1:F:103:VAL:O	1:F:103:VAL:HG23	2.09	0.52
1:H:157:PHE:HE2	1:H:291:VAL:HG12	1.73	0.52
1:G:98:ASN:HD22	1:G:98:ASN:H	1.57	0.52
1:A:160:ASP:OD1	1:A:160:ASP:C	2.47	0.52
1:B:124:GLU:OE2	1:B:151:ARG:NH2	2.40	0.52
1:B:238:PHE:CE2	1:B:252:MSE:HE1	2.44	0.52
1:B:405:LYS:HE3	1:B:409:MSE:HE3	1.91	0.52
1:C:183:ARG:NH1	3:C:736:HOH:O	2.43	0.52
1:D:303:ILE:CD1	1:D:352:VAL:HG13	2.38	0.52
1:E:37:GLN:OE1	1:E:41:ARG:HD2	2.09	0.52
1:D:72:GLN:HB2	3:D:982:HOH:O	2.08	0.52
1:F:185:THR:CG2	1:F:275:ILE:HB	2.40	0.52
1:G:248:ARG:O	1:G:252:MSE:HG3	2.10	0.52
1:B:217:ILE:HG13	1:B:218:TRP:N	2.20	0.52
1:D:163:GLY:HA3	2:D:504:FAD:O3P	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:VAL:HG11	1:E:143:ILE:HD12	1.92	0.52
1:F:280:ILE:HD11	3:F:951:HOH:O	2.09	0.52
1:H:117:ALA:HA	1:H:121:VAL:O	2.08	0.52
1:C:237:TYR:O	1:C:240:GLU:HB2	2.10	0.52
1:D:250:ARG:NH2	1:D:266:GLU:O	2.43	0.52
1:E:185:THR:HG22	1:E:275:ILE:O	2.10	0.52
1:E:244:THR:OG1	1:E:247:GLU:HG3	2.09	0.52
1:F:331:VAL:HG11	1:F:333:TRP:CE2	2.45	0.52
1:G:36:LYS:O	1:G:126:GLU:HA	2.09	0.52
1:D:8:VAL:CG2	1:D:326:LEU:HD11	2.40	0.52
1:A:9:LEU:HD13	1:A:153:ILE:HG21	1.92	0.52
1:A:408:GLN:NE2	1:A:409:MSE:CE	2.72	0.52
1:D:19:VAL:HG21	1:D:312:MSE:HG2	1.92	0.52
1:D:158:ILE:O	1:D:290:PHE:HA	2.10	0.51
1:G:180:PHE:HB3	1:G:183:ARG:HH22	1.73	0.51
1:D:117:ALA:HA	1:D:121:VAL:O	2.09	0.51
1:H:45:GLY:HA2	2:H:508:FAD:N5	2.25	0.51
1:B:273:ARG:HB3	3:B:1539:HOH:O	2.10	0.51
1:B:294:GLY:O	1:B:297:THR:HB	2.10	0.51
1:C:9:LEU:HD13	1:C:153:ILE:HG21	1.91	0.51
1:C:217:ILE:HA	1:C:230:GLY:O	2.10	0.51
1:H:6:VAL:O	1:H:155:ALA:HA	2.10	0.51
1:H:244:THR:OG1	1:H:245:PRO:HD2	2.10	0.51
1:B:15:PRO:HB3	1:B:312:MSE:CE	2.38	0.51
1:D:191:LYS:HA	1:D:226:ASN:HD22	1.76	0.51
1:F:405:LYS:HE2	1:F:409:MSE:HE2	1.93	0.51
1:G:3:ARG:N	3:G:683:HOH:O	2.44	0.51
1:C:53:MSE:O	1:C:57:ASP:HB2	2.11	0.51
1:C:145:ASP:OD2	1:C:149:ASN:HB2	2.11	0.51
1:C:303:ILE:HD11	1:C:352:VAL:HG13	1.93	0.51
1:F:218:TRP:CD1	1:F:220:ILE:HD12	2.45	0.51
1:G:70:PHE:CG	1:G:103:VAL:HG12	2.45	0.51
1:G:190:ILE:HG21	1:G:263:PHE:CD1	2.45	0.51
1:G:243:GLY:O	1:G:248:ARG:HD3	2.11	0.51
1:C:264:LYS:O	1:C:265:SER:HB2	2.10	0.51
1:G:399:ILE:HG12	1:G:403:LEU:HD23	1.92	0.51
1:H:92:GLN:HB2	1:H:379:SER:HG	1.76	0.51
1:A:124:GLU:OE2	1:A:151:ARG:NH2	2.44	0.51
1:C:117:ALA:HA	1:C:121:VAL:O	2.11	0.51
1:C:222:PHE:HB2	1:C:224:ASN:OD1	2.11	0.51
1:G:107:ASN:ND2	3:G:1038:HOH:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:368:ASN:HA	3:H:952:HOH:O	2.10	0.51
1:B:346:ASP:OD1	1:B:349:ARG:NH1	2.44	0.50
1:C:47:SER:HB2	1:C:220:ILE:HD13	1.93	0.50
1:F:16:ALA:HB2	1:F:311:ALA:HB1	1.93	0.50
1:G:301:ASP:HB2	3:G:1511:HOH:O	2.11	0.50
1:H:298:GLU:OE2	1:H:349:ARG:NH2	2.42	0.50
1:D:61:PHE:O	1:D:65:VAL:HG23	2.11	0.50
1:E:343:GLN:OE1	1:E:388:LYS:HE2	2.11	0.50
1:G:56:LEU:HD13	1:G:312:MSE:SE	2.62	0.50
1:C:118:ARG:HH11	1:C:118:ARG:HB3	1.76	0.50
1:H:246:GLU:HA	1:H:272:PRO:HG2	1.93	0.50
1:A:175:ASP:HB2	3:A:966:HOH:O	2.12	0.50
1:B:307:GLY:HA3	2:B:502:FAD:H1'2	1.92	0.50
1:A:127:VAL:CG1	1:A:143:ILE:HD12	2.41	0.50
1:B:73:LYS:N	1:B:100:THR:O	2.37	0.50
1:D:246:GLU:OE2	1:D:250:ARG:NH1	2.45	0.50
1:F:44:ILE:HG13	1:F:45:GLY:H	1.76	0.50
1:G:310:PHE:CZ	1:G:345:ILE:HD13	2.45	0.50
1:A:8:VAL:CG2	1:A:326:LEU:HD11	2.41	0.50
1:F:94:SER:H	1:F:379:SER:HG	1.59	0.50
1:F:334:GLU:HA	3:F:1565:HOH:O	2.10	0.50
1:H:92:GLN:HB2	1:H:379:SER:OG	2.11	0.50
1:A:8:VAL:HG23	1:A:326:LEU:HD11	1.93	0.50
1:C:48:LEU:CD1	1:C:103:VAL:HG22	2.42	0.50
1:C:75:GLY:HA2	1:C:89:PHE:CE2	2.47	0.50
1:E:23:LEU:HD21	1:E:58:GLU:CG	2.42	0.50
1:E:387:ASP:HB3	3:E:847:HOH:O	2.10	0.50
1:G:211:HIS:CD2	1:G:212:LYS:HG2	2.47	0.50
1:D:307:GLY:HA3	2:D:504:FAD:O3'	2.11	0.50
1:E:15:PRO:O	1:E:19:VAL:HG23	2.11	0.50
1:F:214:LYS:HE3	1:F:234:GLU:HG3	1.93	0.50
1:H:301:ASP:CG	1:H:302:PRO:HD2	2.33	0.50
1:G:295:ASN:N	1:G:295:ASN:HD22	2.10	0.49
1:B:132:ILE:N	1:B:171:MSE:SE	2.95	0.49
1:B:188:THR:HA	1:B:270:PHE:CE2	2.48	0.49
1:D:118:ARG:HH11	1:D:118:ARG:CG	2.12	0.49
1:F:176:LYS:HE3	1:G:223:SER:HB2	1.94	0.49
1:G:92:GLN:NE2	1:G:379:SER:HA	2.27	0.49
1:H:366:ALA:O	1:H:369:PRO:HD3	2.12	0.49
1:A:216:TRP:CZ2	1:A:303:ILE:HA	2.48	0.49
1:G:190:ILE:HG21	1:G:263:PHE:HD1	1.78	0.49

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:H:217:ILE:HA	1:H:230:GLY:O	2.12	0.49
1:A:238:PHE:CE2	1:A:252:MSE:HE1	2.47	0.49
1:F:319:GLY:O	1:F:323:VAL:HG23	2.12	0.49
1:G:302:PRO:HB3	2:G:507:FAD:C6	2.42	0.49
1:A:73:LYS:N	1:A:100:THR:O	2.37	0.49
1:B:301:ASP:OD2	1:B:303:ILE:HG13	2.12	0.49
1:B:331:VAL:HG11	1:B:333:TRP:CE2	2.48	0.49
1:D:264:LYS:O	1:D:265:SER:HB2	2.12	0.49
1:F:266:GLU:HA	1:F:266:GLU:OE1	2.12	0.49
1:A:11:ILE:HD13	1:A:129:VAL:HG21	1.93	0.49
1:C:244:THR:HG22	1:C:247:GLU:HG3	1.94	0.49
1:E:73:LYS:HG3	1:E:102:GLN:NE2	2.28	0.49
1:E:107:ASN:HB3	3:E:1288:HOH:O	2.12	0.49
1:F:370:ASP:OD1	1:F:372:ASP:N	2.43	0.49
1:G:13:ALA:HB2	1:G:35:GLU:HB2	1.94	0.49
1:E:53:MSE:HE1	1:E:101:TRP:CH2	2.47	0.49
1:G:41:ARG:HG2	1:G:41:ARG:HH11	1.77	0.49
1:C:211:HIS:HE1	1:C:255:ASN:O	1.96	0.49
1:D:15:PRO:CD	1:D:105:ARG:HH21	2.26	0.49
1:F:186:LEU:HD21	3:F:1482:HOH:O	2.12	0.49
1:G:127:VAL:HG11	1:G:143:ILE:HB	1.88	0.49
1:G:168:ILE:HB	1:G:169:PRO:HD3	1.94	0.49
1:A:44:ILE:HD13	1:A:187:PHE:CE1	2.48	0.48
1:B:303:ILE:HD11	1:B:352:VAL:HG13	1.95	0.48
1:F:212:LYS:HB2	1:F:215:VAL:HB	1.95	0.48
1:G:104:PRO:HB2	1:G:107:ASN:HD22	1.77	0.48
1:H:308:ALA:HB3	2:H:508:FAD:O2	2.13	0.48
1:A:302:PRO:HB3	2:A:501:FAD:C6	2.43	0.48
1:B:22:SER:OG	1:B:119:GLN:NE2	2.47	0.48
1:C:127:VAL:HG13	1:C:143:ILE:CB	2.39	0.48
1:E:297:THR:HG22	1:E:298:GLU:H	1.74	0.48
1:G:308:ALA:N	2:G:507:FAD:O2	2.46	0.48
1:A:341:MSE:C	1:A:342:MSE:HE2	2.33	0.48
1:B:44:ILE:HD13	1:B:187:PHE:CE1	2.49	0.48
1:G:212:LYS:HB3	1:G:213:PRO:HD2	1.95	0.48
1:B:35:GLU:OE1	1:B:37:GLN:N	2.45	0.48
1:C:220:ILE:C	1:C:227:THR:HG23	2.34	0.48
1:F:102:GLN:HG2	1:F:220:ILE:HG23	1.95	0.48
1:F:214:LYS:HE3	1:F:234:GLU:CG	2.44	0.48
1:F:338:VAL:CG2	3:F:1565:HOH:O	2.62	0.48
1:C:388:LYS:HB2	3:E:1199:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:GLY:HA3	2:D:504:FAD:H1'2	1.95	0.48
1:F:36:LYS:HE3	1:F:128:GLY:HA3	1.95	0.48
1:B:217:ILE:HD13	1:B:259:ILE:HD13	1.95	0.48
1:D:166:ARG:HB2	1:D:170:ARG:HG3	1.95	0.48
1:E:98:ASN:HD22	1:E:98:ASN:C	2.17	0.48
1:H:370:ASP:OD1	1:H:372:ASP:N	2.47	0.48
1:H:246:GLU:OE2	1:H:250:ARG:NH1	2.47	0.48
1:E:285:LEU:HA	1:E:292:LEU:HD12	1.95	0.48
1:G:166:ARG:HB2	1:G:170:ARG:HG3	1.94	0.48
1:H:9:LEU:HD13	1:H:153:ILE:HG21	1.94	0.48
1:B:218:TRP:CD1	1:B:220:ILE:HG13	2.49	0.47
2:C:503:FAD:H9	2:C:503:FAD:H1'1	1.64	0.47
1:F:399:ILE:CG1	1:F:403:LEU:HD22	2.44	0.47
1:F:407:ILE:O	1:F:411:GLU:HG3	2.14	0.47
1:H:8:VAL:CG2	1:H:326:LEU:HD11	2.45	0.47
1:B:92:GLN:HE21	1:B:379:SER:HG	1.62	0.47
1:D:162:SER:O	1:D:163:GLY:C	2.53	0.47
1:A:65:VAL:HG11	1:A:101:TRP:CZ3	2.49	0.47
1:D:15:PRO:HD3	1:D:105:ARG:HH21	1.80	0.47
1:E:21:ALA:CB	1:E:33:ILE:HD11	2.45	0.47
1:E:302:PRO:HB3	2:E:505:FAD:C6	2.44	0.47
1:F:41:ARG:O	1:F:41:ARG:HD3	2.15	0.47
1:B:8:VAL:HG22	1:B:157:PHE:HB3	1.97	0.47
1:B:41:ARG:HD2	1:B:41:ARG:O	2.15	0.47
1:E:322:ALA:O	1:E:326:LEU:HG	2.15	0.47
1:F:102:GLN:HE22	1:F:221:PRO:HD2	1.79	0.47
1:F:103:VAL:O	1:F:103:VAL:CG2	2.63	0.47
1:G:44:ILE:HG13	1:G:45:GLY:H	1.79	0.47
1:H:321:LEU:CD1	1:H:337:PHE:HB2	2.45	0.47
1:C:21:ALA:CB	1:C:33:ILE:HD11	2.45	0.47
1:C:44:ILE:HD13	1:C:187:PHE:CE1	2.50	0.47
1:C:366:ALA:HA	3:C:1317:HOH:O	2.14	0.47
1:F:65:VAL:HG11	1:F:101:TRP:CZ3	2.49	0.47
1:F:96:GLY:HA3	1:F:384:TYR:CE1	2.49	0.47
1:F:102:GLN:NE2	1:F:221:PRO:HD2	2.29	0.47
1:A:214:LYS:HE3	1:A:234:GLU:HG3	1.96	0.47
1:D:32:LYS:HG3	1:D:122:ASP:OD2	2.14	0.47
1:G:185:THR:HB	1:G:232:VAL:HG22	1.97	0.47
1:B:35:GLU:OE1	2:B:502:FAD:O2B	2.33	0.47
1:D:287:GLY:HA3	1:D:290:PHE:CE1	2.50	0.47
1:E:70:PHE:CG	1:E:103:VAL:HG12	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:308:ALA:H	2:F:506:FAD:C2	2.28	0.47
1:G:234:GLU:HA	1:G:235:PRO:HD2	1.75	0.47
1:B:174:LEU:O	1:B:282:ALA:HA	2.15	0.46
1:B:218:TRP:HD1	1:B:220:ILE:HG13	1.80	0.46
1:D:402:THR:O	1:D:406:VAL:HG23	2.15	0.46
1:F:333:TRP:C	3:F:1565:HOH:O	2.53	0.46
1:G:8:VAL:HG21	1:G:24:VAL:HG11	1.97	0.46
1:G:176:LYS:O	1:G:281:SER:N	2.39	0.46
1:H:302:PRO:HB3	2:H:508:FAD:C6	2.46	0.46
1:D:56:LEU:HD12	1:D:56:LEU:HA	1.84	0.46
1:D:342:MSE:HE2	1:D:342:MSE:HA	1.97	0.46
1:H:45:GLY:HA2	2:H:508:FAD:C10	2.44	0.46
1:A:10:VAL:O	1:A:33:ILE:HA	2.15	0.46
1:C:185:THR:HA	1:C:231:PHE:O	2.15	0.46
1:D:194:LYS:O	1:D:195:ARG:C	2.54	0.46
1:F:338:VAL:HG23	3:F:1565:HOH:O	2.16	0.46
1:G:3:ARG:HD3	1:G:154:GLU:HB2	1.98	0.46
1:G:45:GLY:HA2	2:G:507:FAD:C10	2.45	0.46
1:G:73:LYS:HG3	1:G:102:GLN:NE2	2.30	0.46
1:H:44:ILE:HD13	1:H:187:PHE:CE1	2.50	0.46
1:H:399:ILE:O	1:H:403:LEU:HB2	2.15	0.46
1:A:244:THR:HG22	1:A:247:GLU:CB	2.46	0.46
1:C:35:GLU:OE1	2:C:503:FAD:O2B	2.31	0.46
1:D:188:THR:HG23	1:D:190:ILE:HG13	1.97	0.46
1:E:220:ILE:O	1:E:227:THR:HG23	2.15	0.46
1:D:56:LEU:HD13	1:D:312:MSE:SE	2.66	0.46
1:G:168:ILE:N	1:G:169:PRO:CD	2.78	0.46
1:G:169:PRO:HA	1:G:174:LEU:HB2	1.98	0.46
1:H:44:ILE:HG13	1:H:45:GLY:N	2.31	0.46
1:A:4:GLU:N	3:A:1060:HOH:O	2.48	0.46
1:F:37:GLN:CD	1:F:41:ARG:HG3	2.36	0.46
1:F:188:THR:HA	1:F:270:PHE:CE2	2.50	0.46
1:F:194:LYS:HD3	1:F:262:ARG:O	2.16	0.46
1:H:37:GLN:CD	1:H:41:ARG:HG3	2.36	0.46
1:H:226:ASN:ND2	1:H:269:LEU:HD21	2.30	0.46
1:A:376:MSE:HB3	1:A:390:ASN:OD1	2.16	0.46
1:B:132:ILE:HG13	1:B:171:MSE:SE	2.66	0.46
1:D:47:SER:CB	1:D:206:ILE:HD12	2.46	0.46
1:D:211:HIS:HD1	1:D:256:GLU:HB2	1.81	0.46
1:D:8:VAL:HG23	1:D:326:LEU:HD11	1.98	0.46
1:H:163:GLY:HA3	2:H:508:FAD:O3P	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:PRO:HA	1:B:174:LEU:HB2	1.97	0.46
1:C:248:ARG:O	1:C:252:MSE:HG3	2.16	0.46
1:H:342:MSE:HE2	1:H:345:ILE:HB	1.98	0.46
1:B:341:MSE:O	1:B:345:ILE:HG12	2.15	0.46
1:C:127:VAL:HG12	1:C:127:VAL:O	2.15	0.46
1:G:208:ALA:HA	1:G:217:ILE:O	2.15	0.46
1:A:373:HIS:O	1:A:377:ILE:HG13	2.16	0.45
1:B:176:LYS:O	1:B:177:PRO:C	2.54	0.45
1:D:389:ASN:O	1:D:391:PRO:HD3	2.16	0.45
1:E:72:GLN:HB3	1:E:74:PHE:CE1	2.50	0.45
1:E:302:PRO:HB3	2:E:505:FAD:C5X	2.47	0.45
1:F:189:HIS:CE1	1:F:222:PHE:HE2	2.34	0.45
1:G:100:THR:OG1	1:G:101:TRP:N	2.49	0.45
1:H:61:PHE:O	1:H:65:VAL:HG23	2.15	0.45
1:H:212:LYS:HB3	1:H:213:PRO:HD2	1.98	0.45
1:D:73:LYS:HE3	1:D:206:ILE:CG2	2.46	0.45
1:F:98:ASN:H	1:F:98:ASN:HD22	1.64	0.45
1:F:174:LEU:O	1:F:282:ALA:HA	2.16	0.45
1:H:299:PHE:CE1	2:H:508:FAD:H1'1	2.51	0.45
1:B:127:VAL:HG23	1:B:127:VAL:O	2.16	0.45
1:C:51:ARG:HH21	1:C:313:GLU:CD	2.18	0.45
1:C:37:GLN:OE1	1:C:41:ARG:HD2	2.17	0.45
1:D:23:LEU:HD11	1:D:320:LYS:HE3	1.99	0.45
1:D:127:VAL:HG11	1:D:143:ILE:HD13	1.98	0.45
1:H:51:ARG:HB3	1:H:309:THR:HG21	1.98	0.45
1:B:165:GLY:O	1:B:170:ARG:HD2	2.16	0.45
1:B:341:MSE:C	1:B:342:MSE:HE2	2.36	0.45
1:G:45:GLY:HA2	2:G:507:FAD:N5	2.30	0.45
1:B:217:ILE:CD1	1:B:259:ILE:HD13	2.45	0.45
1:C:6:VAL:O	1:C:155:ALA:HA	2.17	0.45
1:C:164:TYR:CE1	1:C:295:ASN:ND2	2.84	0.45
1:G:77:LYS:HD2	1:G:207:THR:HG23	1.98	0.45
1:H:65:VAL:HG11	1:H:101:TRP:CZ3	2.51	0.45
1:A:132:ILE:N	1:A:171:MSE:SE	3.00	0.45
1:A:141:THR:O	1:A:152:GLU:HA	2.16	0.45
1:B:244:THR:HG22	1:B:247:GLU:HB2	1.98	0.45
1:B:303:ILE:C	1:B:305:SER:H	2.19	0.45
1:C:8:VAL:CG2	1:C:24:VAL:HG11	2.46	0.45
1:C:54:GLU:OE2	1:C:384:TYR:HE1	2.00	0.45
1:C:74:PHE:CD1	1:C:99:TRP:HB2	2.52	0.45
1:F:360:LEU:HD11	1:F:364:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:220:ILE:O	1:G:227:THR:HG23	2.17	0.45
1:H:36:LYS:O	1:H:126:GLU:HA	2.16	0.45
1:D:280:ILE:HG13	1:D:281:SER:H	1.81	0.45
1:D:338:VAL:O	1:D:342:MSE:HG2	2.17	0.45
1:F:294:GLY:HA2	1:F:311:ALA:HA	1.98	0.45
1:G:335:LYS:HG2	1:G:336:ASP:OD1	2.17	0.45
1:E:158:ILE:O	1:E:290:PHE:HA	2.17	0.45
1:F:180:PHE:CZ	1:F:349:ARG:HG3	2.52	0.45
1:F:281:SER:CB	1:F:298:GLU:HG3	2.46	0.45
1:H:294:GLY:HA2	1:H:311:ALA:HA	1.97	0.45
1:H:335:LYS:O	1:H:339:GLU:HB2	2.16	0.45
1:A:342:MSE:HE2	1:A:342:MSE:N	2.32	0.45
1:B:264:LYS:O	1:B:265:SER:HB2	2.17	0.45
1:C:218:TRP:CE2	1:C:230:GLY:HA3	2.52	0.45
1:F:36:LYS:O	1:F:126:GLU:HA	2.17	0.45
1:F:122:ASP:HB2	3:F:1059:HOH:O	2.17	0.45
1:G:166:ARG:HD2	1:G:296:ALA:HA	1.98	0.45
1:B:244:THR:CG2	1:B:247:GLU:H	2.30	0.44
1:D:186:LEU:HD23	1:D:186:LEU:HA	1.87	0.44
1:F:125:TYR:O	1:F:127:VAL:HG23	2.17	0.44
1:F:246:GLU:HA	1:F:272:PRO:HG2	1.99	0.44
1:G:41:ARG:HH11	1:G:41:ARG:CG	2.29	0.44
1:E:207:THR:HG21	3:E:1033:HOH:O	2.16	0.44
1:G:105:ARG:NH1	2:G:507:FAD:H4'	2.29	0.44
1:H:143:ILE:O	1:H:150:LYS:HA	2.18	0.44
1:H:285:LEU:HD11	1:H:297:THR:HG23	1.99	0.44
1:B:267:GLU:HG2	1:B:268:PHE:N	2.32	0.44
1:E:73:LYS:O	1:E:74:PHE:HD1	2.00	0.44
1:F:271:GLU:O	1:F:272:PRO:C	2.55	0.44
1:H:293:THR:HB	1:H:314:SER:OG	2.17	0.44
1:A:218:TRP:CD1	1:A:218:TRP:C	2.91	0.44
1:C:266:GLU:OE1	1:C:266:GLU:HA	2.17	0.44
1:E:348:PHE:O	1:E:352:VAL:HG23	2.17	0.44
1:G:44:ILE:HD13	1:G:187:PHE:CE1	2.52	0.44
1:G:348:PHE:O	1:G:352:VAL:HG23	2.18	0.44
1:H:162:SER:O	1:H:163:GLY:C	2.54	0.44
1:C:54:GLU:OE2	1:C:384:TYR:CE1	2.70	0.44
1:C:75:GLY:HA2	1:C:89:PHE:CD2	2.52	0.44
1:D:98:ASN:C	1:D:98:ASN:ND2	2.70	0.44
1:F:294:GLY:O	1:F:297:THR:HB	2.18	0.44
1:H:110:LYS:NZ	1:H:114:ASP:OD2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ILE:O	1:A:290:PHE:HA	2.18	0.44
1:D:10:VAL:HB	1:D:33:ILE:HG12	1.99	0.44
1:E:234:GLU:HA	1:E:235:PRO:HD2	1.88	0.44
1:A:234:GLU:HA	1:A:235:PRO:HD2	1.88	0.44
1:E:126:GLU:HB3	1:E:146:ILE:HG12	1.98	0.44
1:F:157:PHE:HE2	1:F:291:VAL:HG12	1.83	0.44
1:F:244:THR:O	1:F:248:ARG:HG3	2.17	0.44
1:H:10:VAL:HB	1:H:33:ILE:HG12	2.00	0.44
1:H:191:LYS:HA	1:H:226:ASN:HD22	1.83	0.44
1:B:100:THR:HG23	1:B:101:TRP:N	2.33	0.44
1:B:285:LEU:CD2	1:B:342:MSE:HE3	2.48	0.44
1:E:61:PHE:CD2	1:E:112:LEU:HG	2.53	0.44
1:F:21:ALA:CB	1:F:33:ILE:HD11	2.48	0.44
1:F:180:PHE:HE2	1:F:300:LEU:HD22	1.83	0.44
1:A:267:GLU:HG2	1:A:268:PHE:N	2.31	0.44
1:B:41:ARG:HD2	1:B:41:ARG:C	2.38	0.44
1:B:190:ILE:HD12	1:B:229:VAL:HG21	2.00	0.44
1:B:244:THR:HG22	1:B:247:GLU:CG	2.48	0.44
1:F:56:LEU:HD13	1:F:312:MSE:SE	2.68	0.44
1:F:243:GLY:O	1:F:248:ARG:HD3	2.17	0.44
1:H:32:LYS:HZ2	1:H:34:VAL:HG12	1.82	0.44
1:D:49:LEU:O	1:D:50:PRO:C	2.56	0.43
1:E:87:PHE:CE2	1:E:374:LYS:HG3	2.53	0.43
1:F:288:ASP:N	3:F:1590:HOH:O	2.49	0.43
1:G:163:GLY:HA3	2:G:507:FAD:PA	2.58	0.43
1:G:250:ARG:HG2	1:G:268:PHE:HZ	1.81	0.43
1:G:288:ASP:HA	3:G:797:HOH:O	2.18	0.43
1:H:211:HIS:CE1	1:H:256:GLU:HB2	2.53	0.43
1:A:183:ARG:NH2	3:A:850:HOH:O	2.51	0.43
1:A:212:LYS:HB3	1:A:213:PRO:CD	2.44	0.43
1:D:47:SER:OG	1:D:206:ILE:HD12	2.18	0.43
1:E:246:GLU:HA	1:E:272:PRO:HG2	1.99	0.43
1:E:287:GLY:HA3	1:E:290:PHE:CE1	2.52	0.43
1:E:364:PHE:HE1	1:E:377:ILE:HG21	1.83	0.43
1:H:16:ALA:N	3:H:1273:HOH:O	2.50	0.43
1:F:295:ASN:N	1:F:295:ASN:HD22	2.16	0.43
1:G:264:LYS:O	1:G:265:SER:HB2	2.18	0.43
1:G:310:PHE:CE2	1:G:345:ILE:HD13	2.53	0.43
1:A:10:VAL:HB	1:A:33:ILE:HG12	2.01	0.43
1:A:23:LEU:HD13	1:A:320:LYS:HG3	2.01	0.43
1:B:32:LYS:HE3	3:B:1383:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:ASP:OD1	1:C:371:PRO:HD2	2.18	0.43
1:D:163:GLY:HA3	2:D:504:FAD:PA	2.58	0.43
1:F:259:ILE:O	1:F:260:ALA:C	2.57	0.43
1:G:185:THR:HA	1:G:231:PHE:O	2.18	0.43
1:G:367:LYS:HG2	1:G:368:ASN:ND2	2.34	0.43
1:A:373:HIS:CE1	1:A:403:LEU:HD11	2.53	0.43
1:A:398:THR:HG22	3:A:1553:HOH:O	2.18	0.43
1:C:16:ALA:HB2	1:C:311:ALA:HB1	1.99	0.43
1:C:26:LYS:HD3	3:C:1417:HOH:O	2.19	0.43
2:E:505:FAD:H1'1	2:E:505:FAD:H9	1.73	0.43
1:G:19:VAL:CG2	1:G:312:MSE:HG2	2.38	0.43
1:G:285:LEU:HA	1:G:292:LEU:HD12	2.00	0.43
1:H:374:LYS:HE2	3:H:1322:HOH:O	2.17	0.43
1:B:166:ARG:HD2	1:B:295:ASN:O	2.19	0.43
1:B:408:GLN:NE2	1:B:409:MSE:HE2	2.34	0.43
1:C:92:GLN:HB2	1:C:379:SER:OG	2.18	0.43
1:C:135:PHE:CD2	1:F:135:PHE:CD2	3.06	0.43
1:D:23:LEU:CD1	1:D:320:LYS:HE3	2.48	0.43
1:F:65:VAL:HG11	1:F:101:TRP:CE3	2.53	0.43
1:G:339:GLU:CD	3:G:738:HOH:O	2.57	0.43
1:A:37:GLN:NE2	3:A:1537:HOH:O	2.51	0.43
1:E:23:LEU:HD12	1:E:316:SER:HA	2.01	0.43
1:G:73:LYS:HE3	1:G:206:ILE:CG2	2.47	0.43
1:G:297:THR:HB	1:G:298:GLU:H	1.67	0.43
1:B:303:ILE:HG13	1:B:303:ILE:H	1.59	0.43
1:D:217:ILE:HA	1:D:230:GLY:O	2.17	0.43
1:E:294:GLY:HA3	2:E:505:FAD:O1P	2.19	0.43
1:F:10:VAL:O	1:F:33:ILE:HA	2.19	0.43
1:H:15:PRO:CD	1:H:105:ARG:HH21	2.31	0.43
1:H:304:PHE:HZ	1:H:360:LEU:HD23	1.83	0.43
1:B:408:GLN:NE2	1:B:409:MSE:CE	2.81	0.43
1:C:207:THR:HB	1:C:219:VAL:HB	2.01	0.43
1:C:398:THR:HG22	3:C:1003:HOH:O	2.15	0.43
1:E:48:LEU:CD1	1:E:103:VAL:HG22	2.48	0.43
1:E:100:THR:OG1	1:E:101:TRP:N	2.51	0.43
1:E:218:TRP:CD1	1:E:218:TRP:C	2.93	0.43
1:F:39:PHE:HA	1:F:40:PRO:C	2.39	0.43
1:F:216:TRP:CH2	1:F:303:ILE:HA	2.53	0.43
1:H:246:GLU:CG	1:H:250:ARG:HH11	2.32	0.43
1:C:190:ILE:HG12	1:C:268:PHE:CE1	2.54	0.42
1:D:37:GLN:OE1	1:D:41:ARG:HD2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:LEU:HB2	1:D:238:PHE:HE2	1.84	0.42
1:G:35:GLU:HA	2:G:507:FAD:N3A	2.34	0.42
1:D:41:ARG:HG2	1:D:41:ARG:O	2.19	0.42
1:D:303:ILE:H	1:D:303:ILE:HG13	1.55	0.42
1:D:357:ASP:C	1:D:357:ASP:OD1	2.58	0.42
1:H:127:VAL:HG11	1:H:143:ILE:HD12	2.01	0.42
1:B:9:LEU:HD13	1:B:153:ILE:HD13	2.01	0.42
1:B:211:HIS:O	1:B:212:LYS:CD	2.66	0.42
1:B:248:ARG:O	1:B:252:MSE:HG3	2.19	0.42
1:D:35:GLU:OE1	2:D:504:FAD:H1B	2.19	0.42
1:D:246:GLU:HA	1:D:272:PRO:HG2	2.00	0.42
1:F:25:ASN:HB3	3:F:895:HOH:O	2.19	0.42
1:G:168:ILE:N	1:G:169:PRO:HD2	2.34	0.42
1:H:150:LYS:NZ	3:H:929:HOH:O	2.44	0.42
1:H:190:ILE:HG12	1:H:268:PHE:CD1	2.54	0.42
1:D:85:ALA:HB2	1:D:364:PHE:O	2.18	0.42
1:E:77:LYS:HD2	3:E:1586:HOH:O	2.19	0.42
1:E:266:GLU:OE1	1:E:266:GLU:HA	2.20	0.42
1:G:129:VAL:HG13	1:G:141:THR:HG23	2.01	0.42
1:G:249:MSE:HG3	1:G:253:ILE:CD1	2.49	0.42
1:A:186:LEU:HD23	1:A:186:LEU:HA	1.73	0.42
1:A:277:GLY:HA2	3:A:719:HOH:O	2.20	0.42
1:A:340:HIS:CE1	1:A:386:TRP:NE1	2.88	0.42
1:D:36:LYS:HA	1:D:127:VAL:O	2.19	0.42
1:D:184:ARG:HD2	1:D:238:PHE:CG	2.54	0.42
1:D:212:LYS:HB3	1:D:213:PRO:CD	2.42	0.42
1:E:127:VAL:CG1	1:E:143:ILE:HG21	2.49	0.42
1:B:10:VAL:O	1:B:33:ILE:HA	2.19	0.42
1:D:77:LYS:HG2	1:D:78:PHE:N	2.34	0.42
1:D:119:GLN:NE2	3:D:1045:HOH:O	2.52	0.42
1:F:24:VAL:HG11	1:F:31:VAL:HB	2.01	0.42
1:A:217:ILE:HD12	1:A:229:VAL:HG13	2.01	0.42
1:B:103:VAL:O	1:B:103:VAL:HG23	2.20	0.42
1:F:44:ILE:HD13	1:F:187:PHE:CZ	2.55	0.42
1:F:217:ILE:HA	1:F:230:GLY:O	2.19	0.42
1:G:20:ALA:HB1	1:G:159:ILE:HD13	2.01	0.42
1:G:285:LEU:CD2	1:G:342:MSE:HE2	2.49	0.42
1:H:56:LEU:HD11	1:H:112:LEU:HD21	2.02	0.42
1:B:10:VAL:HB	1:B:33:ILE:HG12	2.02	0.42
1:B:156:ARG:NH1	1:B:326:LEU:HD22	2.35	0.42
1:B:217:ILE:HD12	1:B:229:VAL:HG13	2.02	0.42

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:E:16:ALA:CB	1:E:161:ALA:HB1	2.48	0.42
1:H:16:ALA:HB2	1:H:311:ALA:HB1	2.01	0.42
1:H:41:ARG:O	1:H:41:ARG:HD3	2.20	0.42
1:H:271:GLU:O	1:H:272:PRO:C	2.58	0.42
1:A:164:TYR:O	1:A:166:ARG:HG2	2.19	0.42
1:B:71:GLN:HE21	1:B:71:GLN:HB2	1.64	0.42
1:B:270:PHE:CE2	1:B:273:ARG:NH1	2.88	0.42
1:B:285:LEU:HD21	1:B:342:MSE:CE	2.49	0.42
1:D:226:ASN:ND2	1:D:269:LEU:HD21	2.35	0.42
2:D:504:FAD:H1'1	2:D:504:FAD:H9	1.78	0.42
1:F:92:GLN:HE21	1:F:379:SER:HA	1.82	0.42
1:F:110:LYS:HG3	3:F:1451:HOH:O	2.20	0.42
1:F:186:LEU:HB2	1:F:238:PHE:HE2	1.85	0.42
1:G:127:VAL:HG13	1:G:143:ILE:HB	1.94	0.42
1:G:158:ILE:O	1:G:290:PHE:HA	2.20	0.42
1:H:285:LEU:HD12	1:H:285:LEU:HA	1.69	0.42
1:A:269:LEU:HD13	1:A:269:LEU:HA	1.89	0.42
1:C:70:PHE:CG	1:C:103:VAL:HG12	2.55	0.42
1:F:142:THR:HG21	1:F:150:LYS:HD3	2.02	0.42
1:F:191:LYS:HA	1:F:226:ASN:HD22	1.85	0.42
1:G:32:LYS:HD3	1:G:153:ILE:HD13	2.02	0.42
1:G:36:LYS:HA	1:G:127:VAL:O	2.20	0.42
2:G:507:FAD:H1'1	2:G:507:FAD:H9	1.69	0.42
1:H:15:PRO:HD2	2:H:508:FAD:O2P	2.20	0.42
1:B:123:VAL:HG11	1:B:125:TYR:CZ	2.55	0.41
1:C:403:LEU:HD22	1:C:403:LEU:HA	1.71	0.41
1:E:186:LEU:HB2	1:E:238:PHE:HE2	1.85	0.41
1:E:186:LEU:HD22	1:E:249:MSE:CE	2.50	0.41
1:F:280:ILE:O	1:F:298:GLU:HG2	2.20	0.41
1:H:15:PRO:HD3	1:H:105:ARG:HH21	1.85	0.41
1:A:23:LEU:HD12	1:A:316:SER:HA	2.02	0.41
1:A:168:ILE:HB	1:A:169:PRO:HD3	2.01	0.41
1:A:297:THR:CG2	1:A:298:GLU:N	2.64	0.41
1:A:335:LYS:HB2	1:A:335:LYS:HE2	1.82	0.41
1:C:53:MSE:HE1	1:C:101:TRP:CH2	2.55	0.41
1:C:246:GLU:OE2	1:C:250:ARG:NH1	2.53	0.41
1:D:51:ARG:HD3	1:D:386:TRP:HZ3	1.86	0.41
1:E:132:ILE:O	1:E:133:LYS:HD2	2.19	0.41
1:F:124:GLU:OE2	1:F:151:ARG:NH2	2.45	0.41
1:G:73:LYS:HG3	1:G:102:GLN:HE21	1.85	0.41
1:G:98:ASN:HD22	1:G:98:ASN:N	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:266:GLU:OE1	1:H:266:GLU:HA	2.20	0.41
1:A:135:PHE:CD2	1:D:135:PHE:CD2	3.07	0.41
1:A:242:THR:HG1	1:B:386:TRP:HD1	1.68	0.41
1:A:360:LEU:HD11	1:A:364:PHE:CE1	2.56	0.41
1:C:337:PHE:O	1:C:341:MSE:HG2	2.20	0.41
1:A:401:LYS:HG3	3:A:647:HOH:O	2.19	0.41
1:B:45:GLY:HA2	2:B:502:FAD:C10	2.51	0.41
1:B:163:GLY:HA3	2:B:502:FAD:O3P	2.20	0.41
1:C:71:GLN:HB2	1:C:223:SER:N	2.34	0.41
1:G:127:VAL:HG11	1:G:143:ILE:CD1	2.49	0.41
1:H:98:ASN:N	1:H:98:ASN:ND2	2.67	0.41
1:H:126:GLU:CD	1:H:146:ILE:HD11	2.41	0.41
1:A:42:PHE:CD2	1:A:42:PHE:C	2.93	0.41
1:A:98:ASN:ND2	1:A:99:TRP:HD1	2.18	0.41
1:A:168:ILE:N	1:A:169:PRO:CD	2.83	0.41
1:C:160:ASP:OD2	1:C:168:ILE:HB	2.21	0.41
1:E:35:GLU:HG2	1:E:39:PHE:CE1	2.54	0.41
1:E:127:VAL:CG1	1:E:143:ILE:HD12	2.51	0.41
1:A:157:PHE:HE2	1:A:291:VAL:HG12	1.86	0.41
1:A:366:ALA:O	1:A:369:PRO:HD3	2.21	0.41
1:C:321:LEU:CD1	1:C:337:PHE:HB2	2.51	0.41
1:D:266:GLU:HA	1:D:266:GLU:OE1	2.20	0.41
1:E:3:ARG:HD3	1:E:154:GLU:OE1	2.19	0.41
1:E:220:ILE:C	1:E:227:THR:HG23	2.41	0.41
1:F:184:ARG:HG3	1:F:276:GLU:CD	2.40	0.41
1:G:71:GLN:HG2	1:G:221:PRO:O	2.21	0.41
1:G:115:GLU:O	1:G:119:GLN:HG3	2.20	0.41
1:G:176:LYS:O	1:G:281:SER:HB3	2.20	0.41
1:G:220:ILE:C	1:G:227:THR:HG23	2.41	0.41
1:H:103:VAL:O	1:H:103:VAL:HG23	2.21	0.41
1:H:176:LYS:HA	1:H:177:PRO:HD3	1.93	0.41
1:H:348:PHE:O	1:H:352:VAL:HG23	2.21	0.41
1:B:160:ASP:C	1:B:160:ASP:OD1	2.59	0.41
1:C:43:VAL:HG12	1:C:105:ARG:HB3	2.03	0.41
1:C:303:ILE:H	1:C:303:ILE:HG13	1.58	0.41
1:D:192:ASP:CG	1:D:195:ARG:HB2	2.41	0.41
1:H:185:THR:CG2	1:H:275:ILE:HB	2.50	0.41
1:H:218:TRP:CD1	1:H:218:TRP:C	2.93	0.41
1:H:250:ARG:HG3	1:H:268:PHE:CZ	2.56	0.41
1:A:218:TRP:O	1:A:229:VAL:HA	2.20	0.41
1:C:21:ALA:HB2	1:C:33:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:ASN:ND2	3:D:973:HOH:O	2.54	0.41
1:D:303:ILE:HD11	1:D:356:TYR:CE2	2.56	0.41
1:D:387:ASP:HB2	3:D:983:HOH:O	2.21	0.41
1:F:403:LEU:O	1:F:407:ILE:HG13	2.20	0.41
1:H:191:LYS:HB2	1:H:191:LYS:HE3	1.93	0.41
1:B:191:LYS:HB2	1:B:191:LYS:HE3	1.48	0.41
1:C:48:LEU:HD11	1:C:103:VAL:HG22	2.03	0.41
1:C:244:THR:HB	1:C:247:GLU:OE1	2.21	0.41
1:D:217:ILE:HG21	1:D:231:PHE:CZ	2.56	0.41
1:D:370:ASP:OD1	1:D:372:ASP:HB2	2.20	0.41
1:F:98:ASN:HD22	1:F:98:ASN:N	2.19	0.41
1:F:126:GLU:HB3	1:F:146:ILE:HG12	2.03	0.41
1:G:119:GLN:NE2	3:G:1001:HOH:O	2.52	0.41
1:G:203:GLY:N	3:G:1544:HOH:O	2.54	0.41
1:B:217:ILE:HA	1:B:230:GLY:O	2.21	0.41
1:B:304:PHE:HZ	1:B:360:LEU:CD2	2.34	0.41
1:C:171:MSE:HE3	1:C:171:MSE:HB2	1.99	0.41
1:F:56:LEU:HB3	1:F:62:LEU:HG	2.02	0.41
1:F:403:LEU:HA	1:F:403:LEU:HD12	1.72	0.41
1:G:98:ASN:ND2	1:G:99:TRP:HD1	2.19	0.41
2:H:508:FAD:H1'1	2:H:508:FAD:H9	1.83	0.41
1:C:150:LYS:HB2	1:C:150:LYS:HE3	1.89	0.40
1:D:184:ARG:HG2	1:D:185:THR:N	2.36	0.40
1:E:10:VAL:HB	1:E:33:ILE:HG12	2.03	0.40
1:E:234:GLU:HB2	3:E:1582:HOH:O	2.21	0.40
1:G:4:GLU:H	1:G:4:GLU:HG2	1.74	0.40
1:H:407:ILE:O	1:H:411:GLU:HG3	2.21	0.40
1:A:157:PHE:CE2	1:A:291:VAL:HG12	2.57	0.40
1:C:192:ASP:OD2	1:C:195:ARG:HB2	2.21	0.40
1:F:8:VAL:HG11	1:F:159:ILE:HD12	2.04	0.40
1:F:191:LYS:HB2	1:F:191:LYS:HE3	1.82	0.40
1:F:368:ASN:HA	3:F:1329:HOH:O	2.20	0.40
1:G:285:LEU:HG	1:G:297:THR:CG2	2.46	0.40
1:H:322:ALA:O	1:H:325:PHE:HB3	2.21	0.40
1:A:273:ARG:HD2	3:A:1558:HOH:O	2.20	0.40
1:B:303:ILE:CD1	1:B:352:VAL:HG22	2.50	0.40
1:H:127:VAL:HG11	1:H:143:ILE:CD1	2.50	0.40
1:A:98:ASN:C	1:A:98:ASN:HD22	2.24	0.40
1:B:61:PHE:CD2	1:B:112:LEU:HG	2.56	0.40
1:G:303:ILE:HD11	1:G:356:TYR:CZ	2.56	0.40
1:C:269:LEU:N	1:C:269:LEU:HD22	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:GLU:OE2	2:F:506:FAD:H1B	2.21	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	403/421 (96%)	380 (94%)	22 (6%)	1 (0%)	47	71
1	B	396/421 (94%)	377 (95%)	19 (5%)	0	100	100
1	C	401/421 (95%)	380 (95%)	20 (5%)	1 (0%)	47	71
1	D	399/421 (95%)	378 (95%)	21 (5%)	0	100	100
1	E	402/421 (96%)	387 (96%)	14 (4%)	1 (0%)	47	71
1	F	398/421 (94%)	380 (96%)	18 (4%)	0	100	100
1	G	402/421 (96%)	377 (94%)	24 (6%)	1 (0%)	47	71
1	H	399/421 (95%)	381 (96%)	18 (4%)	0	100	100
All	All	3200/3368 (95%)	3040 (95%)	156 (5%)	4 (0%)	51	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	294	GLY
1	G	210	VAL
1	A	303	ILE
1	E	294	GLY

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	336/340 (99%)	317 (94%)	19 (6%)	20	41
1	B	332/340 (98%)	314 (95%)	18 (5%)	22	44
1	C	332/340 (98%)	315 (95%)	17 (5%)	24	46
1	D	334/340 (98%)	313 (94%)	21 (6%)	18	36
1	E	337/340 (99%)	320 (95%)	17 (5%)	24	47
1	F	335/340 (98%)	318 (95%)	17 (5%)	24	46
1	G	335/340 (98%)	318 (95%)	17 (5%)	24	46
1	H	332/340 (98%)	317 (96%)	15 (4%)	27	52
All	All	2673/2720 (98%)	2532 (95%)	141 (5%)	22	45

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	48	LEU
1	A	56	LEU
1	A	71	GLN
1	A	92	GLN
1	A	98	ASN
1	A	122	ASP
1	A	146	ILE
1	A	178	SER
1	A	186	LEU
1	A	217	ILE
1	A	218	TRP
1	A	234	GLU
1	A	242	THR
1	A	303	ILE
1	A	398	THR
1	A	403	LEU
1	A	408	GLN
1	A	409	MSE

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Mol	Chain	Res	Type
1	B	7	ASP
1	B	43	VAL
1	B	48	LEU
1	B	52	CYS
1	B	56	LEU
1	B	62	LEU
1	B	118	ARG
1	B	133	LYS
1	B	146	ILE
1	B	186	LEU
1	B	217	ILE
1	B	285	LEU
1	B	297	THR
1	B	303	ILE
1	B	368	ASN
1	B	402	THR
1	B	403	LEU
1	B	409	MSE
1	C	41	ARG
1	C	48	LEU
1	C	49	LEU
1	C	56	LEU
1	C	98	ASN
1	C	118	ARG
1	C	122	ASP
1	C	143	ILE
1	C	146	ILE
1	C	244	THR
1	C	285	LEU
1	C	297	THR
1	C	303	ILE
1	C	314	SER
1	C	374	LYS
1	C	398	THR
1	C	403	LEU
1	D	41	ARG
1	D	48	LEU
1	D	56	LEU
1	D	71	GLN
1	D	98	ASN
1	D	118	ARG
1	D	122	ASP

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Mol	Chain	Res	Type
1	D	127	VAL
1	D	143	ILE
1	D	186	LEU
1	D	217	ILE
1	D	234	GLU
1	D	242	THR
1	D	244	THR
1	D	250	ARG
1	D	285	LEU
1	D	303	ILE
1	D	357	ASP
1	D	374	LYS
1	D	403	LEU
1	D	408	GLN
1	E	41	ARG
1	E	48	LEU
1	E	50	PRO
1	E	56	LEU
1	E	77	LYS
1	E	95	ASN
1	E	98	ASN
1	E	118	ARG
1	E	122	ASP
1	E	186	LEU
1	E	234	GLU
1	E	255	ASN
1	E	280	ILE
1	E	342	MSE
1	E	398	THR
1	E	403	LEU
1	E	412	GLU
1	F	18	THR
1	F	41	ARG
1	F	48	LEU
1	F	56	LEU
1	F	98	ASN
1	F	122	ASP
1	F	186	LEU
1	F	206	ILE
1	F	218	TRP
1	F	255	ASN
1	F	285	LEU

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Mol	Chain	Res	Type
1	F	295	ASN
1	F	298	GLU
1	F	374	LYS
1	F	398	THR
1	F	403	LEU
1	F	408	GLN
1	G	41	ARG
1	G	43	VAL
1	G	56	LEU
1	G	98	ASN
1	G	122	ASP
1	G	130	THR
1	G	146	ILE
1	G	186	LEU
1	G	218	TRP
1	G	242	THR
1	G	255	ASN
1	G	295	ASN
1	G	298	GLU
1	G	303	ILE
1	G	379	SER
1	G	398	THR
1	G	403	LEU
1	H	18	THR
1	H	41	ARG
1	H	48	LEU
1	H	56	LEU
1	H	62	LEU
1	H	98	ASN
1	H	186	LEU
1	H	206	ILE
1	H	218	TRP
1	H	242	THR
1	H	285	LEU
1	H	374	LYS
1	H	398	THR
1	H	403	LEU
1	H	408	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	71	GLN
1	A	92	GLN
1	A	98	ASN
1	A	119	GLN
1	A	226	ASN
1	A	390	ASN
1	A	408	GLN
1	B	71	GLN
1	B	92	GLN
1	B	119	GLN
1	B	389	ASN
1	B	408	GLN
1	C	71	GLN
1	C	92	GLN
1	C	98	ASN
1	C	119	GLN
1	D	68	GLN
1	D	71	GLN
1	D	92	GLN
1	D	98	ASN
1	D	119	GLN
1	D	226	ASN
1	D	295	ASN
1	D	408	GLN
1	E	71	GLN
1	E	72	GLN
1	E	92	GLN
1	E	98	ASN
1	E	119	GLN
1	E	226	ASN
1	E	255	ASN
1	E	324	GLN
1	E	408	GLN
1	F	25	ASN
1	F	37	GLN
1	F	71	GLN
1	F	92	GLN
1	F	98	ASN
1	F	102	GLN
1	F	119	GLN
1	F	149	ASN
1	F	226	ASN

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Mol	Chain	Res	Type
1	F	295	ASN
1	F	324	GLN
1	G	25	ASN
1	G	71	GLN
1	G	92	GLN
1	G	98	ASN
1	G	107	ASN
1	G	119	GLN
1	G	226	ASN
1	G	295	ASN
1	G	324	GLN
1	G	368	ASN
1	G	373	HIS
1	G	397	ASN
1	H	37	GLN
1	H	71	GLN
1	H	92	GLN
1	H	98	ASN
1	H	119	GLN
1	H	226	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
2	FAD	H	508	-	53,58,58	2.60	15 (28%)	68,89,89	1.63	17 (25%)
2	FAD	E	505	-	53,58,58	2.55	14 (26%)	68,89,89	1.66	17 (25%)
2	FAD	A	501	-	53,58,58	2.57	14 (26%)	68,89,89	1.83	21 (30%)
2	FAD	D	504	-	53,58,58	2.59	16 (30%)	68,89,89	1.71	18 (26%)
2	FAD	F	506	-	53,58,58	2.57	12 (22%)	68,89,89	1.73	17 (25%)
2	FAD	B	502	-	53,58,58	2.66	11 (20%)	68,89,89	1.70	21 (30%)
2	FAD	C	503	-	53,58,58	2.70	14 (26%)	68,89,89	1.71	18 (26%)
2	FAD	G	507	-	53,58,58	2.58	13 (24%)	68,89,89	1.96	21 (30%)

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	FAD	H	508	-	-	4/30/50/50	0/6/6/6
2	FAD	A	501	-	-	6/30/50/50	0/6/6/6
2	FAD	E	505	-	-	8/30/50/50	0/6/6/6
2	FAD	D	504	-	-	7/30/50/50	0/6/6/6
2	FAD	F	506	-	1/1/9/9	5/30/50/50	0/6/6/6
2	FAD	B	502	-	-	6/30/50/50	0/6/6/6
2	FAD	C	503	-	-	6/30/50/50	0/6/6/6
2	FAD	G	507	-	1/1/9/9	10/30/50/50	0/6/6/6

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	503	FAD	O4-C4	12.14	1.46	1.23
2	B	502	FAD	O4-C4	11.88	1.46	1.23
2	E	505	FAD	O4-C4	11.80	1.46	1.23
2	D	504	FAD	O4-C4	11.74	1.45	1.23
2	G	507	FAD	O4-C4	11.61	1.45	1.23
2	F	506	FAD	O4-C4	11.56	1.45	1.23
2	H	508	FAD	O4-C4	11.37	1.45	1.23
2	A	501	FAD	O4-C4	11.11	1.44	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	503	FAD	O2-C2	7.13	1.37	1.24
2	B	502	FAD	O2-C2	6.98	1.37	1.24
2	G	507	FAD	O2'-C2'	-6.83	1.28	1.43
2	F	506	FAD	O2'-C2'	-6.82	1.28	1.43
2	D	504	FAD	O2'-C2'	-6.78	1.29	1.43
2	C	503	FAD	O2'-C2'	-6.78	1.29	1.43
2	B	502	FAD	O2'-C2'	-6.69	1.29	1.43
2	H	508	FAD	O2-C2	6.64	1.36	1.24
2	D	504	FAD	O2-C2	6.54	1.36	1.24
2	E	505	FAD	O2'-C2'	-6.47	1.29	1.43
2	H	508	FAD	O2'-C2'	-6.38	1.29	1.43
2	E	505	FAD	O2-C2	6.36	1.36	1.24
2	A	501	FAD	O2'-C2'	-6.23	1.30	1.43
2	G	507	FAD	O2-C2	6.23	1.35	1.24
2	F	506	FAD	O2-C2	6.18	1.35	1.24
2	A	501	FAD	O2-C2	5.71	1.34	1.24
2	H	508	FAD	C2B-C1B	-5.13	1.46	1.53
2	C	503	FAD	C2B-C1B	-5.10	1.46	1.53
2	B	502	FAD	C2B-C1B	-4.83	1.46	1.53
2	A	501	FAD	C2B-C1B	-4.74	1.46	1.53
2	H	508	FAD	C2B-C3B	-4.62	1.40	1.53
2	E	505	FAD	C2B-C1B	-4.50	1.46	1.53
2	F	506	FAD	C2B-C3B	-4.48	1.41	1.53
2	F	506	FAD	C2B-C1B	-4.27	1.47	1.53
2	G	507	FAD	C2B-C3B	-4.11	1.42	1.53
2	A	501	FAD	C2B-C3B	-3.93	1.42	1.53
2	B	502	FAD	C2B-C3B	-3.93	1.42	1.53
2	C	503	FAD	C2B-C3B	-3.92	1.42	1.53
2	D	504	FAD	C2B-C1B	-3.89	1.47	1.53
2	C	503	FAD	C9A-N10	-3.84	1.34	1.41
2	D	504	FAD	C2B-C3B	-3.67	1.43	1.53
2	B	502	FAD	O3'-C3'	-3.62	1.34	1.43
2	A	501	FAD	O4'-C4'	-3.61	1.35	1.43
2	E	505	FAD	C2B-C3B	-3.60	1.43	1.53
2	G	507	FAD	O3'-C3'	-3.55	1.34	1.43
2	G	507	FAD	C2B-C1B	-3.50	1.48	1.53
2	A	501	FAD	O3'-C3'	-3.42	1.34	1.43
2	F	506	FAD	O3'-C3'	-3.30	1.35	1.43
2	G	507	FAD	C9A-N10	-3.29	1.35	1.41
2	H	508	FAD	C9A-N10	-3.27	1.35	1.41
2	H	508	FAD	O3'-C3'	-3.26	1.35	1.43
2	B	502	FAD	C9A-N10	-3.20	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	504	FAD	C9A-N10	-3.15	1.35	1.41
2	D	504	FAD	O3'-C3'	-3.14	1.35	1.43
2	E	505	FAD	O4'-C4'	-3.01	1.37	1.43
2	E	505	FAD	C9A-N10	-3.01	1.35	1.41
2	G	507	FAD	C3B-C4B	-2.96	1.45	1.53
2	A	501	FAD	C3B-C4B	-2.94	1.45	1.53
2	G	507	FAD	C2A-N3A	2.85	1.36	1.32
2	C	503	FAD	O3'-C3'	-2.81	1.36	1.43
2	A	501	FAD	C2-N3	-2.81	1.32	1.39
2	F	506	FAD	C9A-N10	-2.80	1.36	1.41
2	H	508	FAD	O4'-C4'	-2.77	1.37	1.43
2	D	504	FAD	C3B-C4B	-2.77	1.45	1.53
2	D	504	FAD	O4'-C4'	-2.74	1.37	1.43
2	F	506	FAD	O4'-C4'	-2.73	1.37	1.43
2	F	506	FAD	O4B-C4B	-2.71	1.38	1.45
2	A	501	FAD	C9A-N10	-2.71	1.36	1.41
2	H	508	FAD	C3B-C4B	-2.69	1.46	1.53
2	E	505	FAD	O3'-C3'	-2.66	1.36	1.43
2	G	507	FAD	O4B-C4B	-2.65	1.39	1.45
2	B	502	FAD	O4'-C4'	-2.64	1.37	1.43
2	H	508	FAD	O4B-C4B	-2.64	1.39	1.45
2	E	505	FAD	C4X-N5	2.64	1.35	1.30
2	B	502	FAD	C3B-C4B	-2.63	1.46	1.53
2	F	506	FAD	C3B-C4B	-2.62	1.46	1.53
2	E	505	FAD	C2-N3	-2.61	1.33	1.39
2	A	501	FAD	C4-N3	-2.60	1.34	1.38
2	C	503	FAD	C3B-C4B	-2.59	1.46	1.53
2	A	501	FAD	O4B-C4B	-2.59	1.39	1.45
2	B	502	FAD	O4B-C4B	-2.57	1.39	1.45
2	C	503	FAD	O4B-C4B	-2.55	1.39	1.45
2	C	503	FAD	O4'-C4'	-2.52	1.38	1.43
2	C	503	FAD	C5'-C4'	-2.41	1.48	1.51
2	F	506	FAD	C5X-N5	-2.36	1.34	1.39
2	D	504	FAD	C4X-N5	2.36	1.35	1.30
2	A	501	FAD	C4X-N5	2.33	1.35	1.30
2	D	504	FAD	O4B-C4B	-2.31	1.39	1.45
2	E	505	FAD	C3B-C4B	-2.30	1.47	1.53
2	G	507	FAD	C5X-N5	-2.27	1.35	1.39
2	H	508	FAD	C8M-C8	2.27	1.55	1.51
2	B	502	FAD	C5X-N5	-2.26	1.35	1.39
2	G	507	FAD	C4X-N5	2.26	1.35	1.30
2	C	503	FAD	C2-N3	-2.24	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	504	FAD	C5X-N5	-2.22	1.35	1.39
2	A	501	FAD	C5X-N5	-2.22	1.35	1.39
2	H	508	FAD	C5X-N5	-2.22	1.35	1.39
2	H	508	FAD	C4X-N5	2.21	1.35	1.30
2	C	503	FAD	C4X-N5	2.16	1.35	1.30
2	C	503	FAD	C5X-N5	-2.15	1.35	1.39
2	E	505	FAD	C5X-N5	-2.13	1.35	1.39
2	G	507	FAD	C2'-C3'	-2.13	1.49	1.53
2	D	504	FAD	C2A-N3A	2.13	1.35	1.32
2	D	504	FAD	C8M-C8	2.08	1.55	1.51
2	D	504	FAD	C4-N3	-2.07	1.35	1.38
2	D	504	FAD	C2'-C3'	-2.06	1.49	1.53
2	E	505	FAD	C4-N3	-2.03	1.35	1.38
2	H	508	FAD	C2-N3	-2.03	1.34	1.39
2	H	508	FAD	C4-N3	-2.03	1.35	1.38
2	E	505	FAD	O4B-C4B	-2.02	1.40	1.45
2	F	506	FAD	C4-N3	-2.01	1.35	1.38

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	503	FAD	N3A-C2A-N1A	-5.04	120.80	128.68
2	G	507	FAD	O2'-C2'-C3'	4.75	120.65	109.10
2	F	506	FAD	O2'-C2'-C3'	4.59	120.25	109.10
2	D	504	FAD	O2'-C2'-C3'	4.47	119.97	109.10
2	F	506	FAD	C1'-C2'-C3'	4.38	122.03	109.79
2	G	507	FAD	C5'-C4'-C3'	-4.37	103.77	112.20
2	H	508	FAD	O2'-C2'-C3'	4.25	119.44	109.10
2	E	505	FAD	N3A-C2A-N1A	-4.18	122.15	128.68
2	D	504	FAD	N3A-C2A-N1A	-4.17	122.16	128.68
2	B	502	FAD	N3A-C2A-N1A	-4.06	122.34	128.68
2	G	507	FAD	O2'-C2'-C1'	4.02	119.51	109.80
2	G	507	FAD	C4-N3-C2	-3.99	118.28	125.64
2	D	504	FAD	O2'-C2'-C1'	3.93	119.30	109.80
2	H	508	FAD	N3A-C2A-N1A	-3.91	122.57	128.68
2	E	505	FAD	O2'-C2'-C3'	3.85	118.47	109.10
2	A	501	FAD	C4-N3-C2	-3.84	118.55	125.64
2	C	503	FAD	C1'-C2'-C3'	3.82	120.46	109.79
2	B	502	FAD	C1'-C2'-C3'	3.73	120.21	109.79
2	F	506	FAD	N3A-C2A-N1A	-3.69	122.92	128.68
2	F	506	FAD	C4-N3-C2	-3.68	118.84	125.64
2	A	501	FAD	O5'-C5'-C4'	3.66	119.13	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	N3A-C2A-N1A	-3.65	122.97	128.68
2	G	507	FAD	O4-C4-C4X	-3.61	117.02	126.60
2	G	507	FAD	N3A-C2A-N1A	-3.60	123.06	128.68
2	A	501	FAD	C4-C4X-N5	3.57	123.32	118.23
2	A	501	FAD	C5'-C4'-C3'	-3.54	105.36	112.20
2	B	502	FAD	O5'-C5'-C4'	3.48	118.65	109.36
2	C	503	FAD	O2'-C2'-C3'	3.45	117.48	109.10
2	A	501	FAD	O2'-C2'-C3'	3.44	117.46	109.10
2	D	504	FAD	C4-N3-C2	-3.43	119.30	125.64
2	B	502	FAD	C4-N3-C2	-3.38	119.39	125.64
2	A	501	FAD	C1'-C2'-C3'	3.30	119.02	109.79
2	A	501	FAD	C4X-C10-N10	3.30	121.30	116.48
2	E	505	FAD	C4-C4X-N5	3.22	122.82	118.23
2	G	507	FAD	C4A-C5A-N7A	-3.21	106.06	109.40
2	G	507	FAD	C5X-C9A-N10	3.21	121.27	117.95
2	F	506	FAD	O5'-C5'-C4'	3.19	117.87	109.36
2	C	503	FAD	C4-C4X-N5	3.18	122.76	118.23
2	D	504	FAD	C3B-C2B-C1B	3.17	105.75	100.98
2	B	502	FAD	O2'-C2'-C3'	3.17	116.80	109.10
2	E	505	FAD	C1'-C2'-C3'	3.15	118.60	109.79
2	E	505	FAD	O2'-C2'-C1'	3.14	117.38	109.80
2	G	507	FAD	C3B-C2B-C1B	3.12	105.68	100.98
2	H	508	FAD	C4-C4X-N5	3.12	122.67	118.23
2	A	501	FAD	C4X-C4-N3	3.11	121.08	113.19
2	G	507	FAD	C1'-C2'-C3'	3.02	118.22	109.79
2	G	507	FAD	O2-C2-N1	-3.01	116.83	121.83
2	A	501	FAD	C10-C4X-N5	-2.99	118.52	124.86
2	G	507	FAD	P-O3P-PA	-2.98	122.60	132.83
2	H	508	FAD	C1'-C2'-C3'	2.96	118.07	109.79
2	F	506	FAD	O2'-C2'-C1'	2.96	116.95	109.80
2	H	508	FAD	C4-N3-C2	-2.95	120.19	125.64
2	G	507	FAD	C4X-C4-N3	2.93	120.62	113.19
2	A	501	FAD	O4'-C4'-C3'	2.90	116.15	109.10
2	E	505	FAD	C9A-C5X-N5	-2.87	119.31	122.43
2	G	507	FAD	C4X-C10-N1	-2.85	118.11	124.73
2	B	502	FAD	C5'-C4'-C3'	-2.85	106.71	112.20
2	B	502	FAD	C4X-C10-N10	2.84	120.64	116.48
2	B	502	FAD	C4-C4X-N5	2.83	122.26	118.23
2	B	502	FAD	O2'-C2'-C1'	2.81	116.60	109.80
2	F	506	FAD	C4X-C10-N1	-2.81	118.20	124.73
2	G	507	FAD	O4'-C4'-C3'	2.81	115.94	109.10
2	E	505	FAD	C4X-C10-N1	-2.81	118.22	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	508	FAD	C1B-N9A-C4A	-2.79	121.75	126.64
2	H	508	FAD	O2'-C2'-C1'	2.78	116.53	109.80
2	D	504	FAD	C4X-C4-N3	2.77	120.21	113.19
2	E	505	FAD	C4-N3-C2	-2.73	120.60	125.64
2	E	505	FAD	C4X-C4-N3	2.72	120.11	113.19
2	C	503	FAD	C9A-C5X-N5	-2.72	119.48	122.43
2	A	501	FAD	C4X-C10-N1	-2.71	118.43	124.73
2	C	503	FAD	C4-N3-C2	-2.69	120.68	125.64
2	F	506	FAD	P-O3P-PA	-2.68	123.63	132.83
2	G	507	FAD	O5'-C5'-C4'	2.67	116.50	109.36
2	C	503	FAD	O4-C4-C4X	-2.67	119.51	126.60
2	C	503	FAD	C4X-C4-N3	2.66	119.94	113.19
2	E	505	FAD	C10-C4X-N5	-2.65	119.23	124.86
2	D	504	FAD	C4-C4X-N5	2.64	122.00	118.23
2	C	503	FAD	C10-C4X-N5	-2.64	119.26	124.86
2	F	506	FAD	C4X-C10-N10	2.64	120.33	116.48
2	A	501	FAD	O3B-C3B-C4B	-2.63	103.44	111.05
2	H	508	FAD	C4X-C4-N3	2.63	119.86	113.19
2	H	508	FAD	C4X-C10-N10	2.60	120.29	116.48
2	B	502	FAD	O4-C4-C4X	-2.59	119.74	126.60
2	F	506	FAD	C4X-C4-N3	2.59	119.75	113.19
2	B	502	FAD	C4X-C4-N3	2.58	119.73	113.19
2	C	503	FAD	C4X-C10-N1	-2.57	118.76	124.73
2	B	502	FAD	C10-C4X-N5	-2.56	119.43	124.86
2	C	503	FAD	C1B-N9A-C4A	-2.55	122.16	126.64
2	A	501	FAD	C5B-C4B-C3B	-2.53	105.69	115.18
2	G	507	FAD	C9-C9A-N10	-2.52	118.43	121.84
2	D	504	FAD	C5X-C9A-N10	2.52	120.56	117.95
2	H	508	FAD	C10-C4X-N5	-2.49	119.57	124.86
2	A	501	FAD	O4'-C4'-C5'	-2.48	104.35	109.92
2	D	504	FAD	C5'-C4'-C3'	-2.47	107.44	112.20
2	D	504	FAD	C9A-C5X-N5	-2.46	119.75	122.43
2	D	504	FAD	O4-C4-C4X	-2.46	120.06	126.60
2	H	508	FAD	P-O3P-PA	-2.46	124.38	132.83
2	D	504	FAD	C4X-C10-N1	-2.46	119.03	124.73
2	A	501	FAD	C4A-C5A-N7A	-2.45	106.85	109.40
2	F	506	FAD	C10-C4X-N5	-2.44	119.68	124.86
2	H	508	FAD	C3B-C2B-C1B	2.43	104.63	100.98
2	D	504	FAD	C10-C4X-N5	-2.43	119.70	124.86
2	B	502	FAD	C3B-C2B-C1B	2.43	104.63	100.98
2	C	503	FAD	C3B-C2B-C1B	2.42	104.62	100.98
2	B	502	FAD	C9A-C5X-N5	-2.41	119.82	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	506	FAD	O4-C4-C4X	-2.36	120.35	126.60
2	E	505	FAD	C3B-C2B-C1B	2.36	104.52	100.98
2	D	504	FAD	O5'-C5'-C4'	2.35	115.64	109.36
2	D	504	FAD	C4X-C10-N10	2.34	119.90	116.48
2	E	505	FAD	C10-N1-C2	2.33	121.57	116.90
2	C	503	FAD	O2'-C2'-C1'	2.32	115.42	109.80
2	H	508	FAD	O5'-C5'-C4'	2.32	115.56	109.36
2	F	506	FAD	N3-C2-N1	2.32	123.93	119.38
2	C	503	FAD	C10-N1-C2	2.32	121.53	116.90
2	G	507	FAD	C9A-C5X-N5	-2.31	119.92	122.43
2	E	505	FAD	O5'-C5'-C4'	2.29	115.48	109.36
2	E	505	FAD	O4'-C4'-C3'	2.29	114.67	109.10
2	A	501	FAD	O2'-C2'-C1'	2.29	115.33	109.80
2	D	504	FAD	O2-C2-N1	-2.28	118.05	121.83
2	G	507	FAD	C4X-C10-N10	2.28	119.81	116.48
2	B	502	FAD	O2-C2-N1	-2.27	118.06	121.83
2	E	505	FAD	C5X-C9A-N10	2.26	120.29	117.95
2	D	504	FAD	P-O3P-PA	-2.24	125.14	132.83
2	B	502	FAD	C5X-C9A-N10	2.23	120.26	117.95
2	B	502	FAD	C1B-N9A-C4A	-2.22	122.74	126.64
2	F	506	FAD	O4B-C4B-C3B	2.22	109.51	105.11
2	H	508	FAD	C9A-C5X-N5	-2.21	120.03	122.43
2	G	507	FAD	O4B-C1B-C2B	-2.18	103.73	106.93
2	A	501	FAD	C9A-C5X-N5	-2.18	120.06	122.43
2	C	503	FAD	O4'-C4'-C3'	2.17	114.39	109.10
2	C	503	FAD	O4'-C4'-C5'	-2.17	105.03	109.92
2	B	502	FAD	C4X-C10-N1	-2.13	119.79	124.73
2	A	501	FAD	O4B-C4B-C3B	2.13	109.33	105.11
2	H	508	FAD	O4B-C4B-C3B	2.13	109.32	105.11
2	C	503	FAD	C5X-C9A-N10	2.12	120.14	117.95
2	E	505	FAD	C4X-C10-N10	2.11	119.56	116.48
2	H	508	FAD	C4X-C10-N1	-2.10	119.86	124.73
2	B	502	FAD	O4B-C4B-C3B	2.10	109.27	105.11
2	B	502	FAD	O4'-C4'-C3'	2.10	114.19	109.10
2	F	506	FAD	C3B-C2B-C1B	2.08	104.11	100.98
2	B	502	FAD	C4A-C5A-N7A	-2.07	107.24	109.40
2	G	507	FAD	C10-C4X-N5	-2.06	120.49	124.86
2	A	501	FAD	O4-C4-N3	-2.04	116.20	120.12
2	D	504	FAD	O3B-C3B-C4B	-2.04	105.15	111.05
2	A	501	FAD	C4'-C3'-C2'	2.03	117.58	113.36
2	C	503	FAD	C4X-C10-N10	2.03	119.44	116.48
2	E	505	FAD	O4-C4-C4X	-2.02	121.23	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	506	FAD	C5'-C4'-C3'	-2.01	108.32	112.20
2	H	508	FAD	C5X-C9A-N10	2.01	120.03	117.95
2	F	506	FAD	O2-C2-N1	-2.00	118.51	121.83

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	506	FAD	C2'
2	G	507	FAD	C2'

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	C1'-C2'-C3'-C4'
2	A	501	FAD	PA-O3P-P-O5'
2	B	502	FAD	C1'-C2'-C3'-O3'
2	B	502	FAD	C1'-C2'-C3'-C4'
2	B	502	FAD	PA-O3P-P-O5'
2	C	503	FAD	C1'-C2'-C3'-C4'
2	D	504	FAD	C1'-C2'-C3'-C4'
2	D	504	FAD	PA-O3P-P-O5'
2	E	505	FAD	C5B-O5B-PA-O1A
2	E	505	FAD	O4B-C4B-C5B-O5B
2	E	505	FAD	C1'-C2'-C3'-O3'
2	E	505	FAD	C1'-C2'-C3'-C4'
2	F	506	FAD	N10-C1'-C2'-O2'
2	F	506	FAD	PA-O3P-P-O5'
2	G	507	FAD	N10-C1'-C2'-C3'
2	G	507	FAD	C1'-C2'-C3'-C4'
2	G	507	FAD	O4'-C4'-C5'-O5'
2	G	507	FAD	C5'-O5'-P-O1P
2	H	508	FAD	C1'-C2'-C3'-O3'
2	H	508	FAD	C1'-C2'-C3'-C4'
2	F	506	FAD	O2'-C2'-C3'-O3'
2	F	506	FAD	O2'-C2'-C3'-C4'
2	G	507	FAD	C3'-C4'-C5'-O5'
2	C	503	FAD	P-O3P-PA-O1A
2	B	502	FAD	O4B-C4B-C5B-O5B
2	C	503	FAD	PA-O3P-P-O5'
2	E	505	FAD	PA-O3P-P-O5'
2	G	507	FAD	PA-O3P-P-O5'
2	E	505	FAD	C5B-O5B-PA-O3P

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Mol	Chain	Res	Type	Atoms
2	G	507	FAD	C5'-O5'-P-O3P
2	E	505	FAD	P-O3P-PA-O1A
2	D	504	FAD	C5'-O5'-P-O2P
2	G	507	FAD	C5'-O5'-P-O2P
2	A	501	FAD	C1'-C2'-C3'-O3'
2	C	503	FAD	C1'-C2'-C3'-O3'
2	D	504	FAD	C1'-C2'-C3'-O3'
2	G	507	FAD	C1'-C2'-C3'-O3'
2	E	505	FAD	P-O3P-PA-O2A
2	H	508	FAD	P-O3P-PA-O1A
2	A	501	FAD	P-O3P-PA-O1A
2	B	502	FAD	P-O3P-PA-O1A
2	C	503	FAD	P-O3P-PA-O2A
2	D	504	FAD	P-O3P-PA-O1A
2	D	504	FAD	O4'-C4'-C5'-O5'
2	G	507	FAD	O4B-C4B-C5B-O5B
2	H	508	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	O4B-C4B-C5B-O5B
2	C	503	FAD	O4B-C4B-C5B-O5B
2	D	504	FAD	O4B-C4B-C5B-O5B
2	F	506	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	C5B-O5B-PA-O1A
2	B	502	FAD	C5B-O5B-PA-O1A

There are no ring outliers.

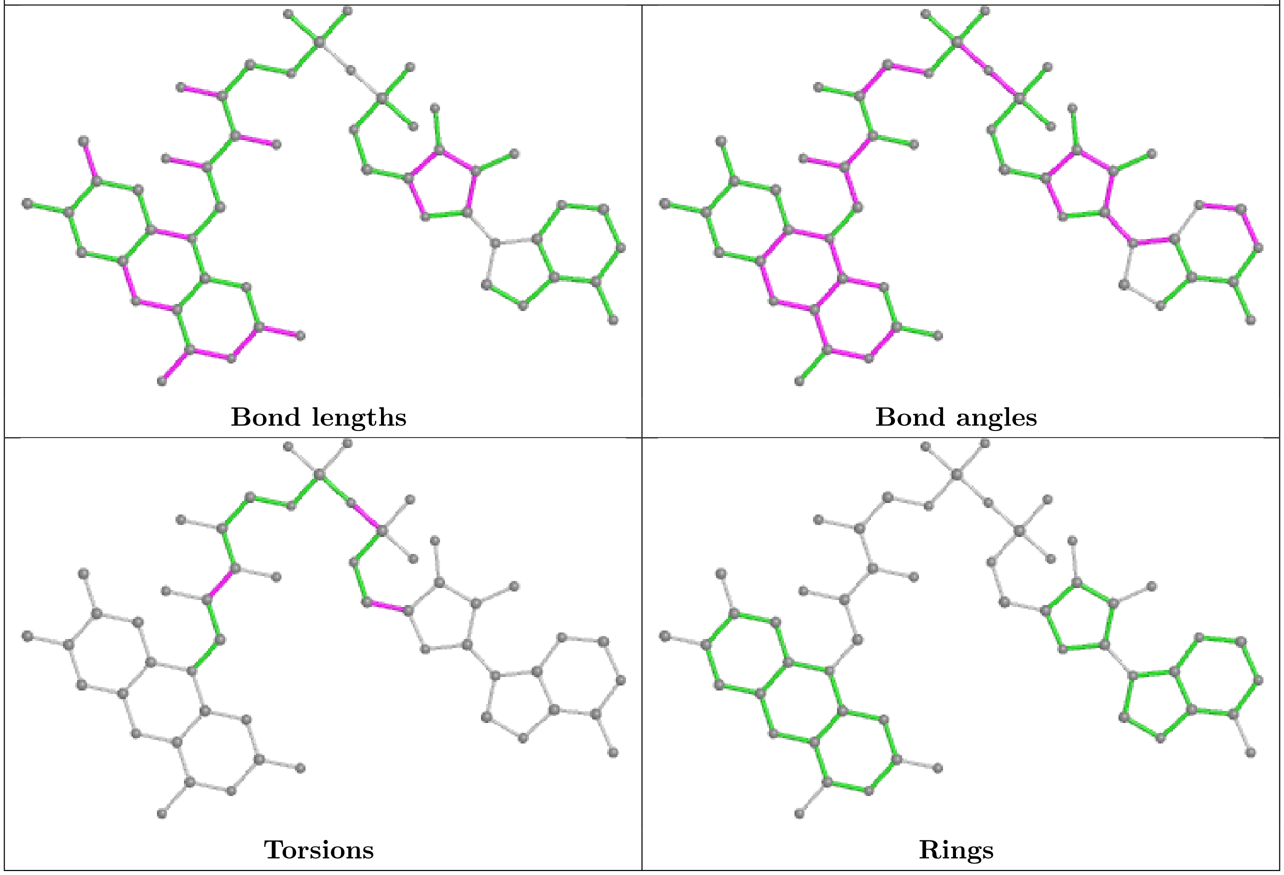
8 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	508	FAD	10	0
2	E	505	FAD	5	0
2	A	501	FAD	4	0
2	D	504	FAD	8	0
2	F	506	FAD	6	0
2	B	502	FAD	5	0
2	C	503	FAD	3	0
2	G	507	FAD	13	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 H 508



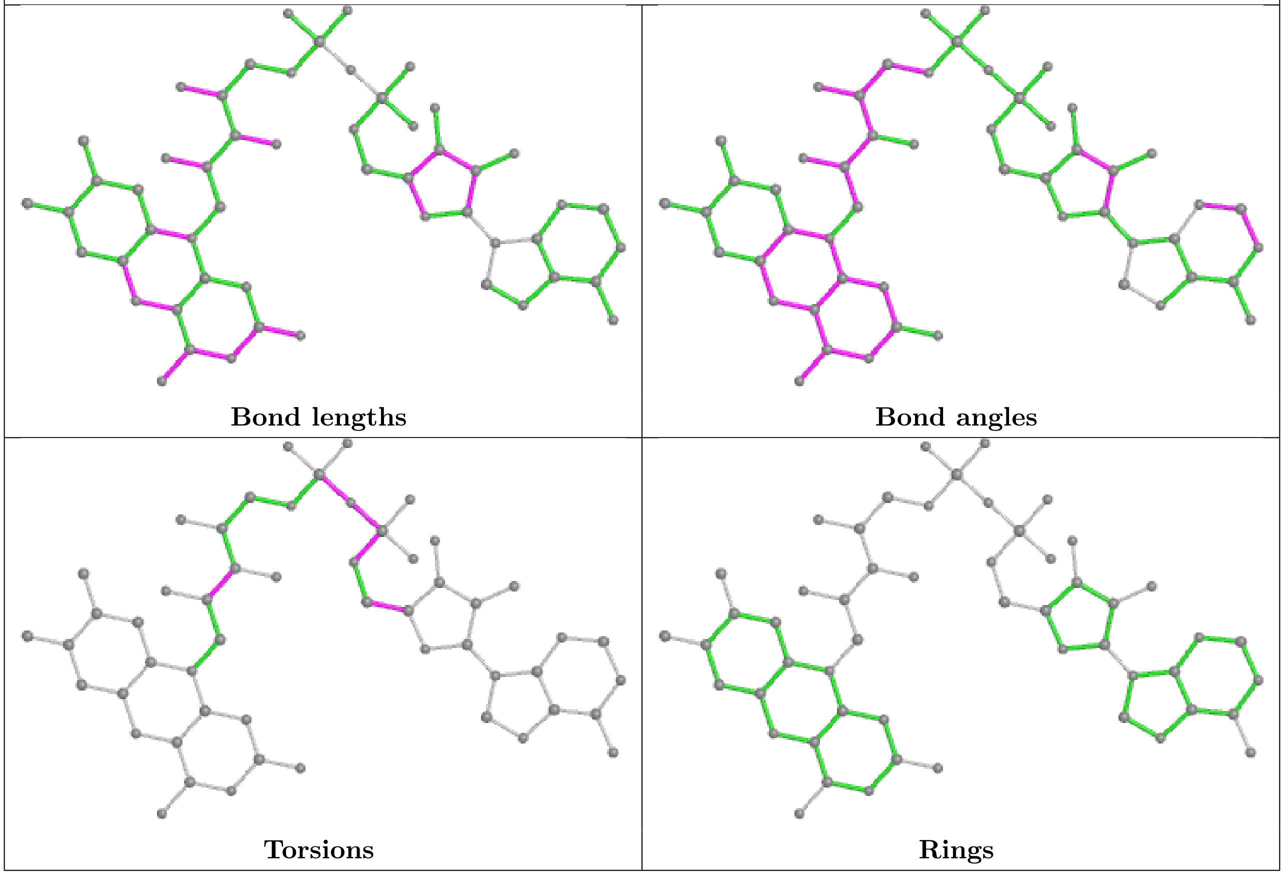
Bond lengths

Bond angles

Torsions

Rings

Ligand FAD E 505



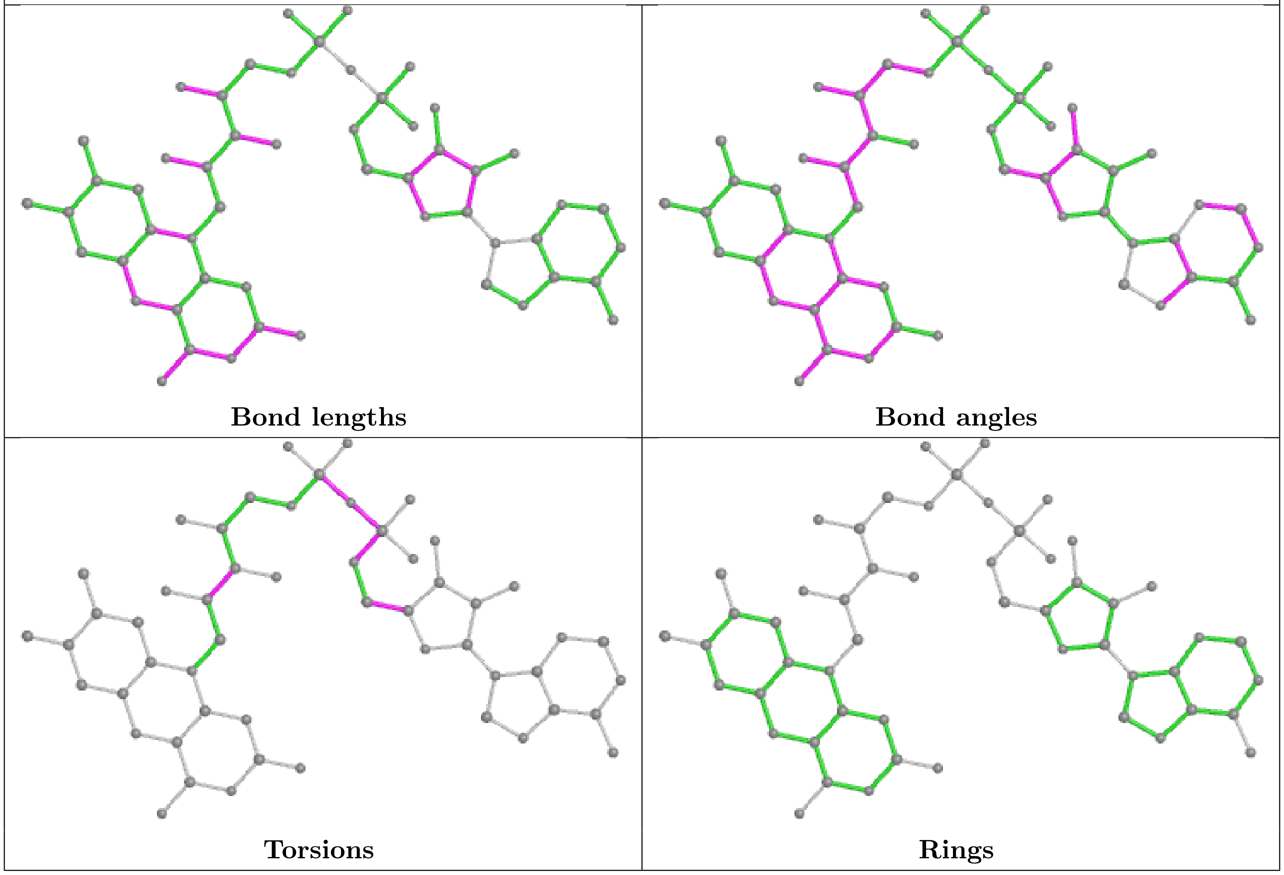
Bond lengths

Bond angles

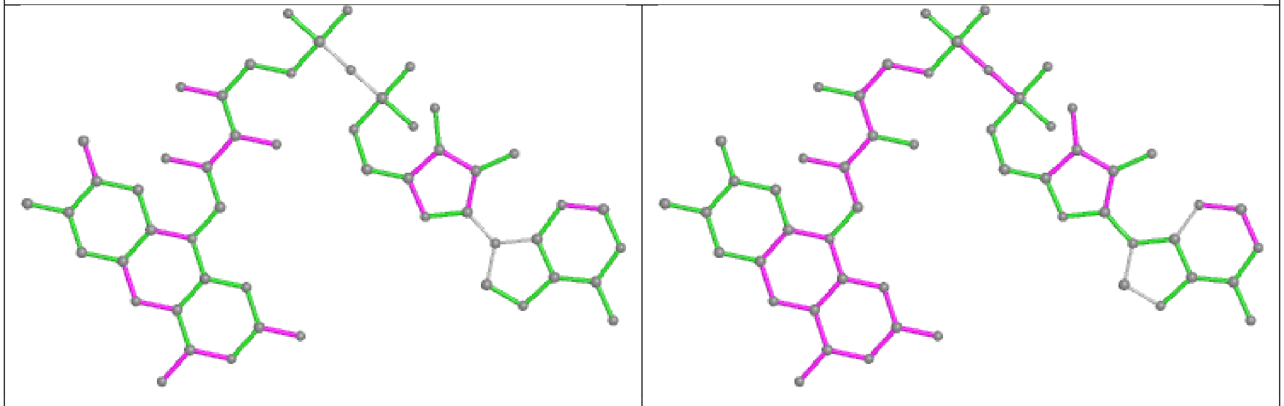
Torsions

Rings

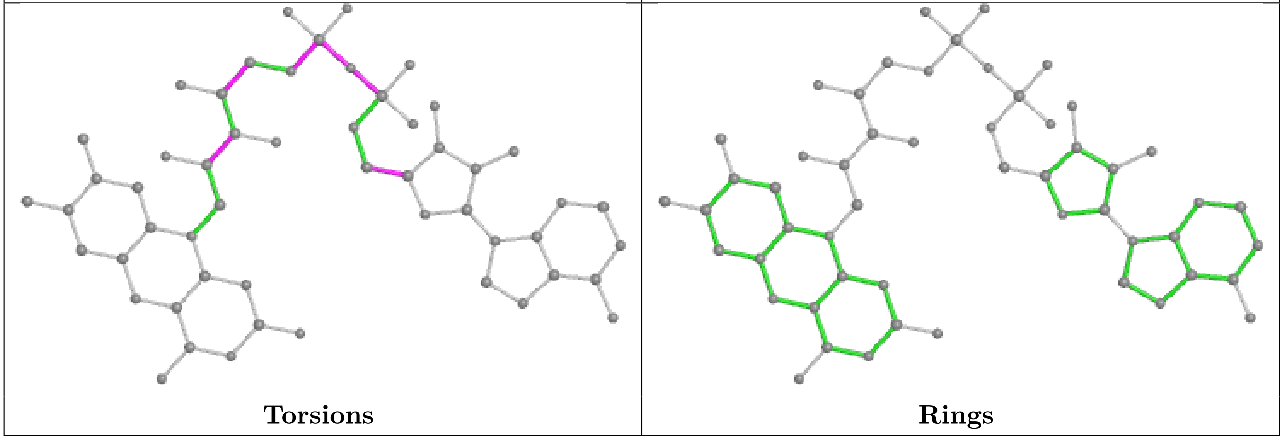
Ligand FAD A 501



Ligand FAD D 504

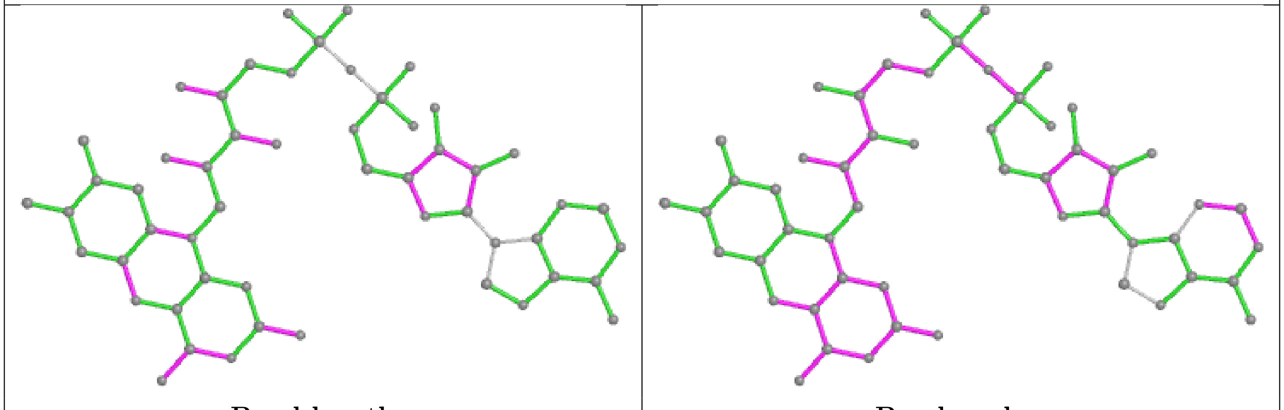


Bond lengths **Bond angles**



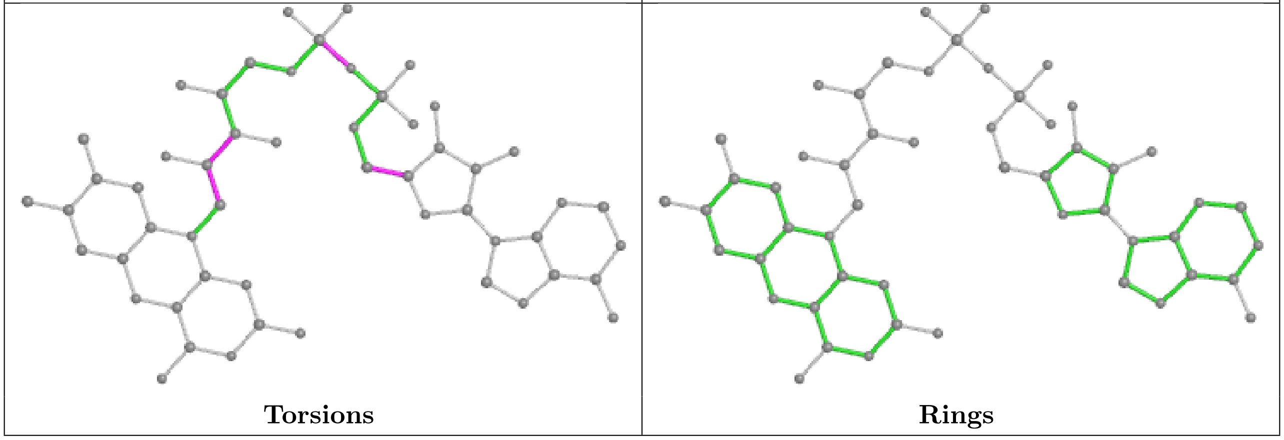
Torsions **Rings**

Ligand FAD F 506



Bond lengths

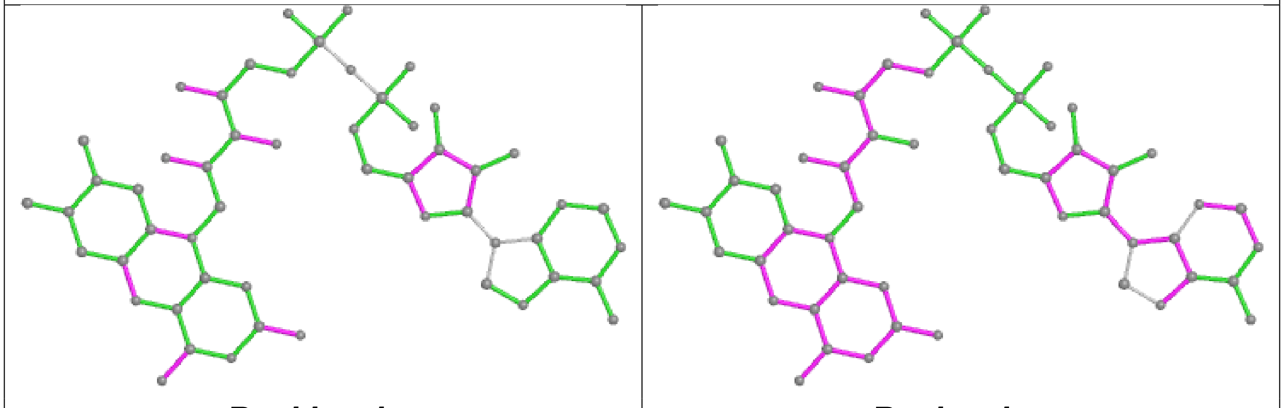
Bond angles



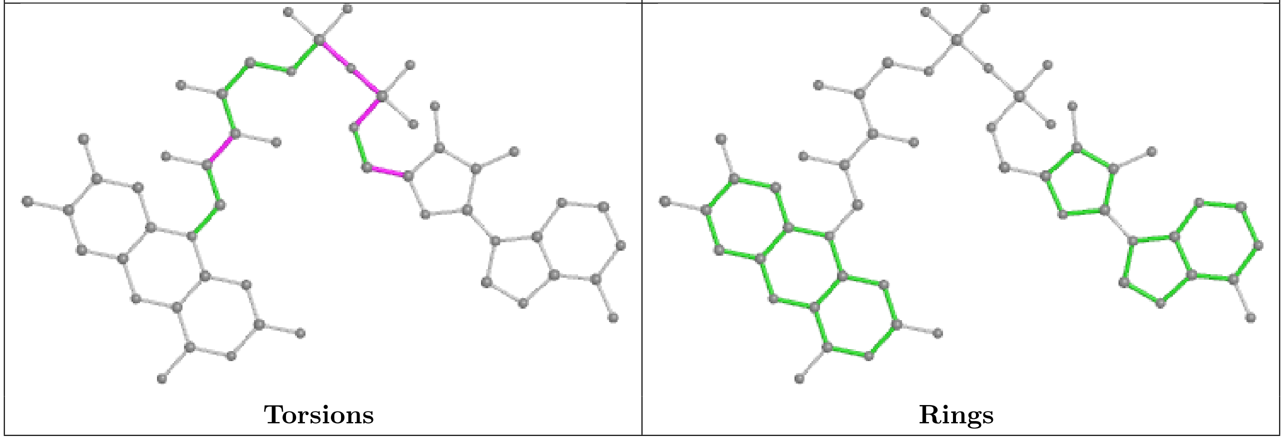
Torsions

Rings

Ligand FAD B 502

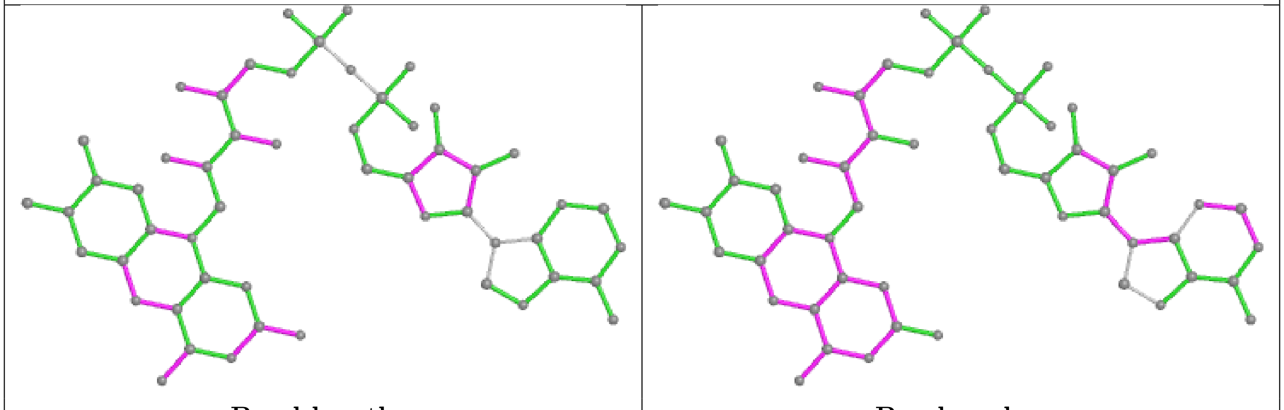


Bond lengths **Bond angles**

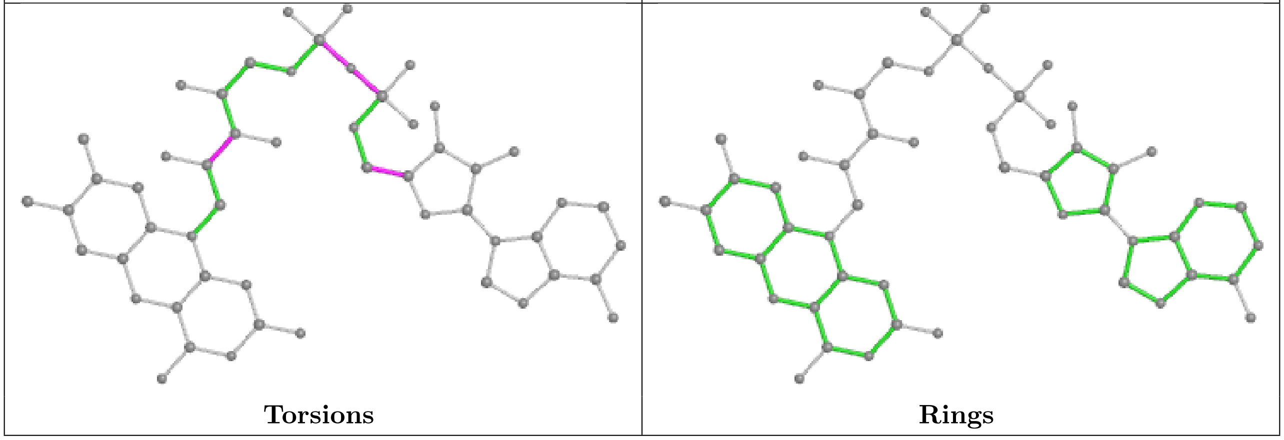


Torsions **Rings**

Ligand FAD C 503

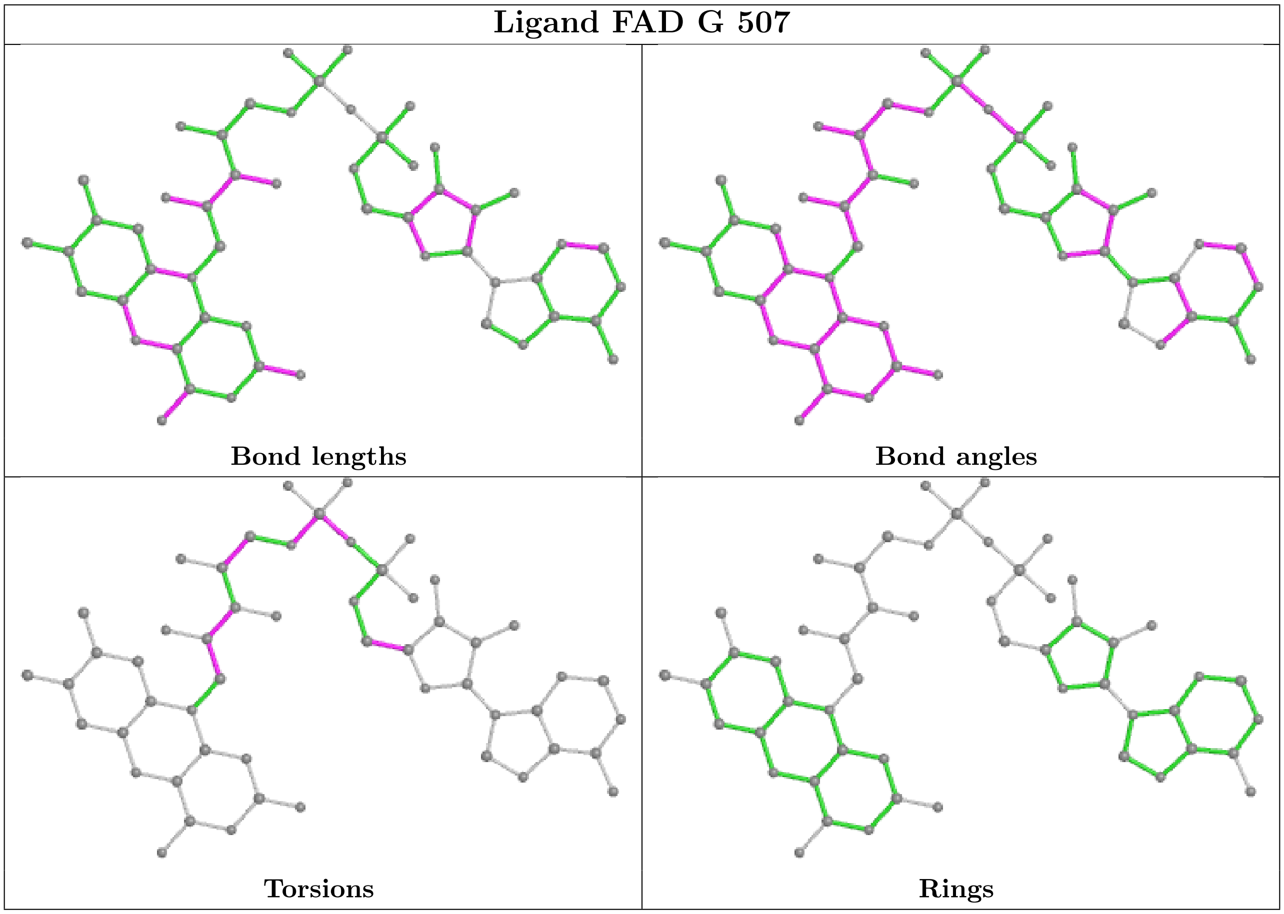


Bond lengths Bond angles



Torsions Rings

Ligand FAD G 507



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	398/421 (94%)	-0.31	1 (0%)	94	93	10, 26, 48, 62	0
1	B	391/421 (92%)	-0.26	3 (0%)	86	84	14, 29, 50, 65	0
1	C	396/421 (94%)	-0.23	3 (0%)	86	84	13, 29, 50, 66	0
1	D	394/421 (93%)	-0.26	3 (0%)	86	84	12, 31, 51, 71	0
1	E	397/421 (94%)	-0.26	1 (0%)	94	93	11, 26, 46, 64	0
1	F	393/421 (93%)	-0.18	3 (0%)	86	84	16, 31, 52, 71	0
1	G	397/421 (94%)	-0.10	9 (2%)	60	54	15, 33, 63, 78	0
1	H	394/421 (93%)	-0.18	5 (1%)	77	73	18, 33, 51, 65	0
All	All	3160/3368 (93%)	-0.22	28 (0%)	84	82	10, 30, 52, 78	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	179	GLY	5.2
1	G	278	TYR	4.8
1	G	179	GLY	4.4
1	G	177	PRO	3.5
1	G	280	ILE	3.5
1	G	180	PHE	3.2
1	G	279	ALA	2.9
1	H	179	GLY	2.9
1	A	413	ALA	2.7
1	C	49	LEU	2.7
1	F	178	SER	2.7
1	G	197	VAL	2.6
1	H	188	THR	2.6
1	B	214	LYS	2.6
1	G	176	LYS	2.4
1	H	122	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	308	ALA	2.3
1	H	16	ALA	2.3
1	D	217	ILE	2.3
1	D	191	LYS	2.2
1	E	308	ALA	2.2
1	F	412	GLU	2.2
1	B	146	ILE	2.1
1	H	146	ILE	2.1
1	G	257	GLY	2.1
1	C	193	VAL	2.1
1	D	303	ILE	2.0
1	B	309	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

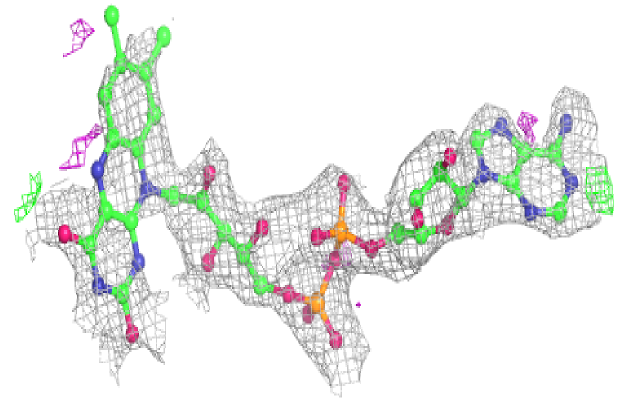
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled '$Q< 0.9$' lists the number of atoms with occupancy less than 0.9.

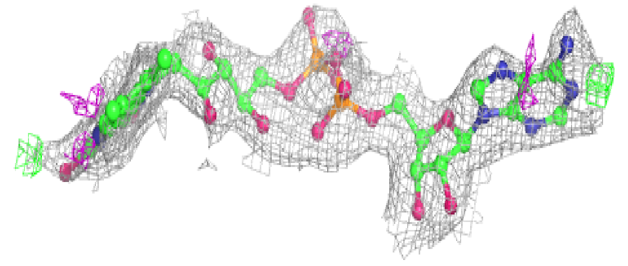
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	FAD	G	507	53/53	0.87	0.23	31,50,64,82	0
2	FAD	F	506	53/53	0.92	0.16	16,33,51,85	0
2	FAD	D	504	53/53	0.93	0.16	14,29,42,54	0
2	FAD	C	503	53/53	0.94	0.16	6,20,36,48	0
2	FAD	E	505	53/53	0.94	0.16	7,23,34,39	0
2	FAD	H	508	53/53	0.94	0.17	12,28,38,48	0
2	FAD	B	502	53/53	0.95	0.16	3,18,35,63	0
2	FAD	A	501	53/53	0.96	0.13	5,19,30,48	0

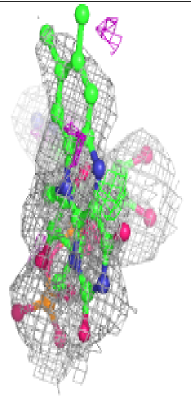
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD G 507:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

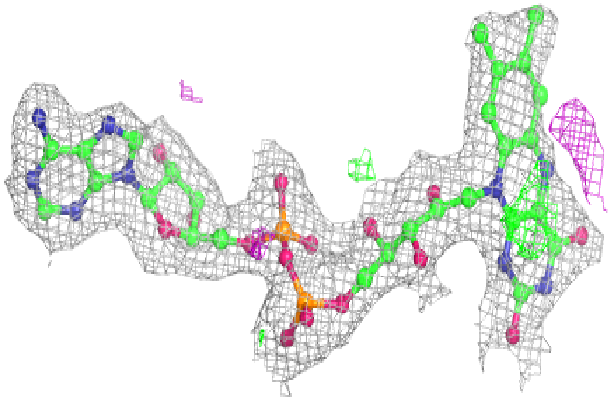


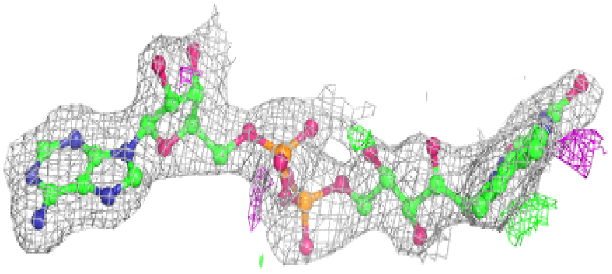


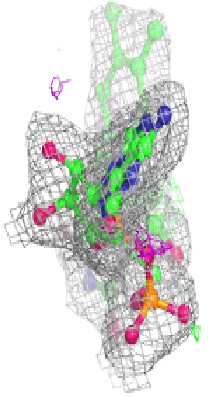


Electron density around FAD F 506:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

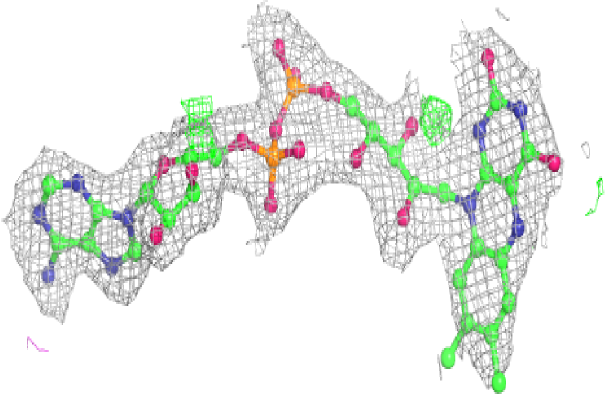


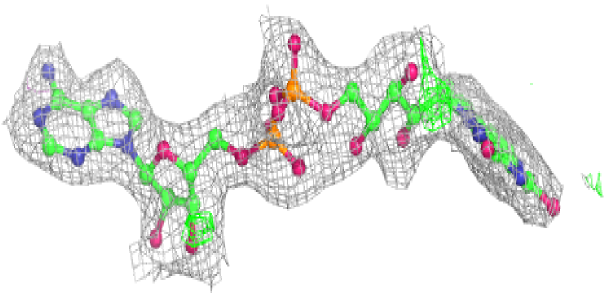


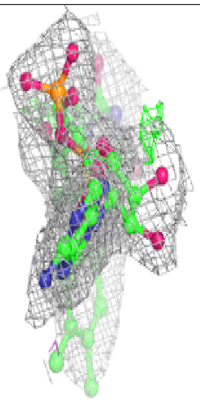


Electron density around FAD D 504:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

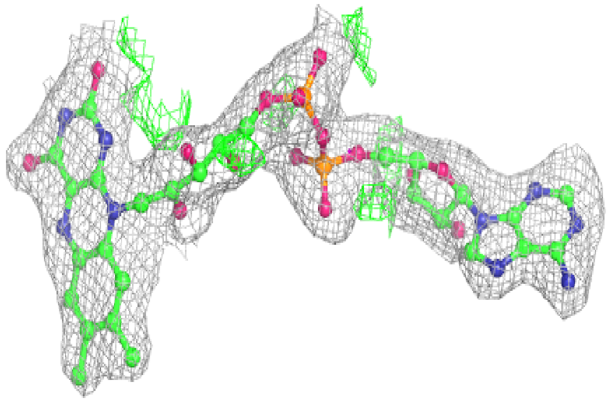


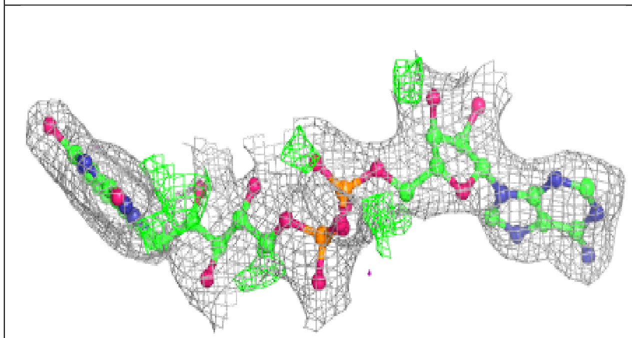


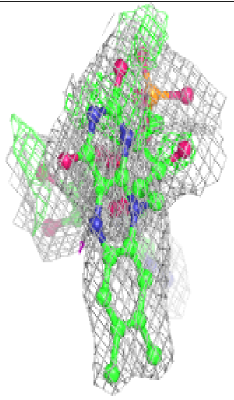


Electron density around FAD C 503:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

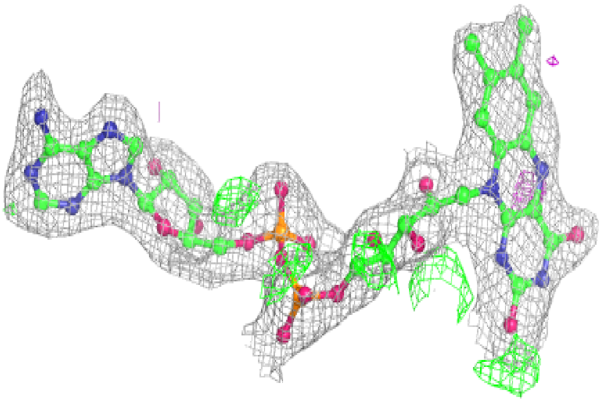


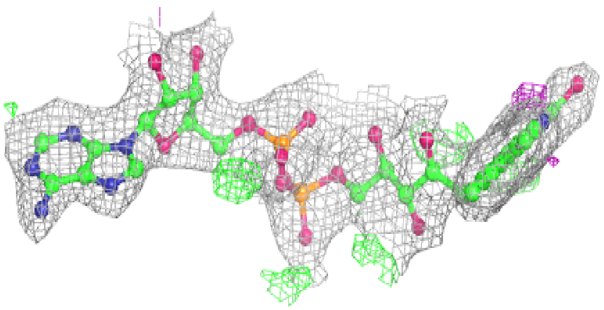


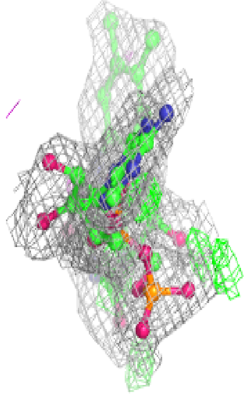


Electron density around FAD E 505:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

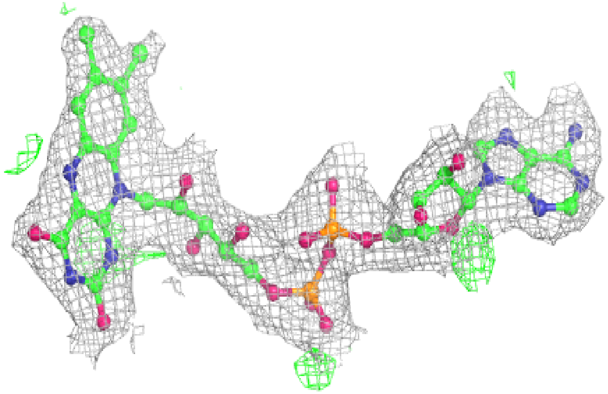


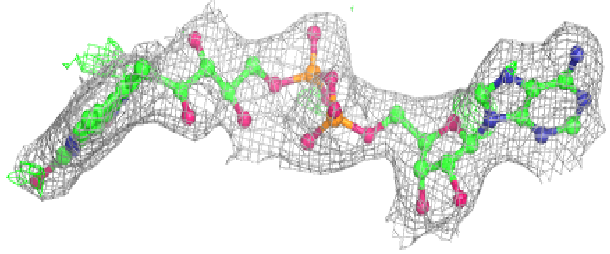


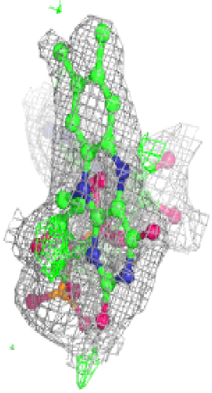


Electron density around FAD H 508:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

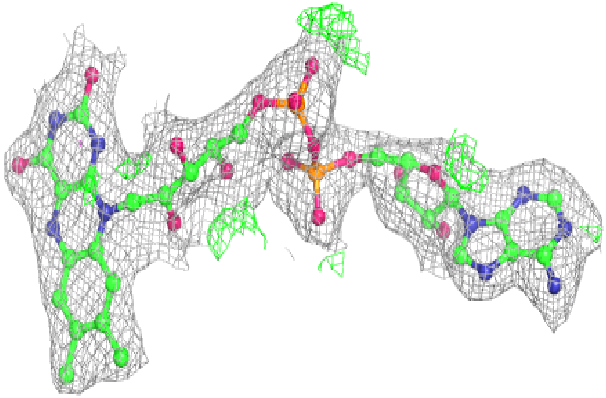


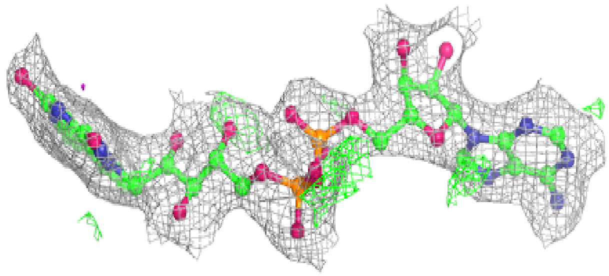


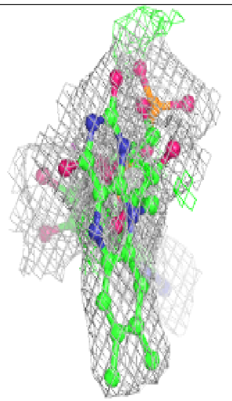


Electron density around FAD B 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around FAD A 501:

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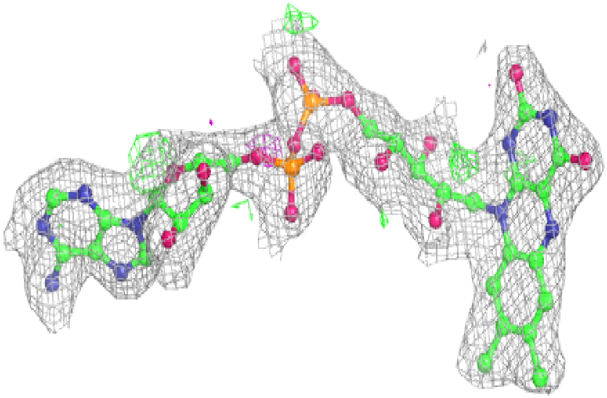
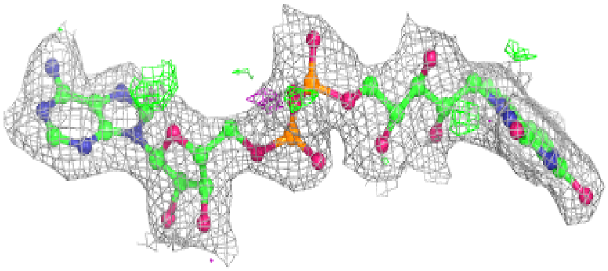
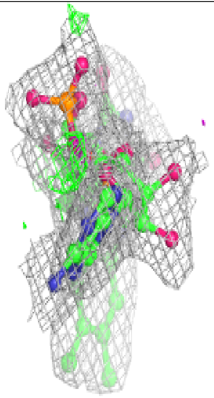
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers ⓘ

There are no such residues in this entry.