Full wwPDB X-ray Structure Validation Report (i)

Oct 18, 2023 – 07:45 AM EDT

PDB ID	:	2EQ9
Title	:	Crystal structure of lipoamide dehydrogenase from thermus thermophilus HB8 with psbdb
Authors	:	Nakai, T.; Kamiya, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-03-30
Resolution	:	2.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

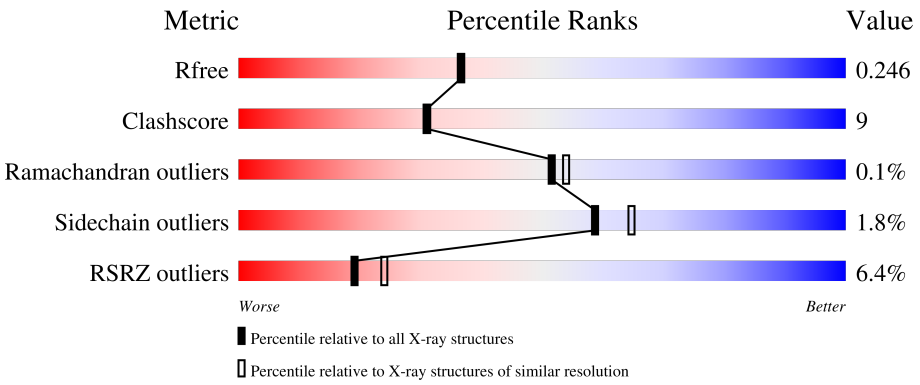
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.09 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	464	4% 81% 18% ••
1	B	464	% 83% 15% ••
1	D	464	2% 86% 12% ••
1	E	464	4% 84% 14% ••

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Mol	Chain	Length	Quality of chain
1	G	464	2% 83% 16%
1	H	464	2% 83% 16%
1	J	464	8% 79% 19%
1	K	464	13% 75% 23%
2	C	41	20% 76% 20%
2	F	41	63% 63% 34%
2	I	41	51% 66% 24% 7%
2	L	41	59% 61% 32% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 29827 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 Pyruvate dehydrogenase complex, dihydrolipoamide dehydrogenase E3 component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	460	3409	2170	596	634	9	0	0	0
1	B	460	3397	2162	594	632	9	0	0	0
1	D	460	3413	2173	597	634	9	0	0	0
1	E	460	3405	2167	595	634	9	0	0	0
1	G	460	3409	2170	596	634	9	0	0	0
1	H	460	3397	2162	594	632	9	0	0	0
1	J	460	3409	2170	596	634	9	0	0	0
1	K	460	3397	2162	594	632	9	0	0	0

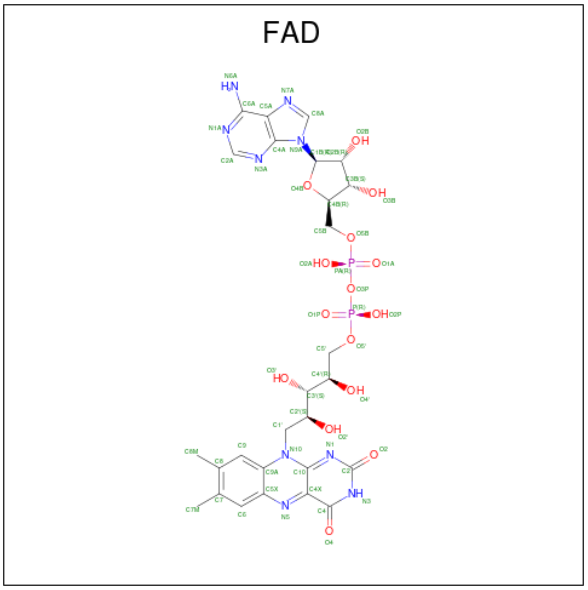
- Molecule 2 is a protein called Pyruvate dehydrogenase complex, dihydrolipoamide acetyltransferase E2 component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	40	290	184	53	52	1	0	0	0
2	F	40	290	184	53	52	1	0	0	0
2	I	40	290	184	53	52	1	0	0	0
2	L	40	290	184	53	52	1	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	129	MET	-	initiating methionine	UNP Q5SLR1
F	129	MET	-	initiating methionine	UNP Q5SLR1
I	129	MET	-	initiating methionine	UNP Q5SLR1
L	129	MET	-	initiating methionine	UNP Q5SLR1

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	53	27	9	15	2	0	0
3	B	1	53	27	9	15	2	0	0
3	D	1	53	27	9	15	2	0	0
3	E	1	53	27	9	15	2	0	0
3	G	1	53	27	9	15	2	0	0
3	H	1	53	27	9	15	2	0	0
3	J	1	53	27	9	15	2	0	0
3	K	1	53	27	9	15	2	0	0

- Molecule 4 is water.

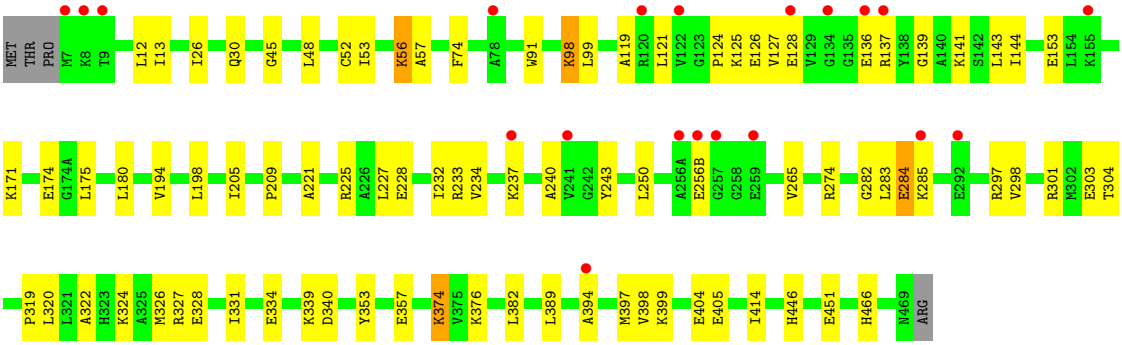
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	114	114	114	0	0
			Total	O		
4	B	138	138	138	0	0
			Total	O		
4	C	4	4	4	0	0
			Total	O		
4	D	158	158	158	0	0
			Total	O		
4	E	113	113	113	0	0
			Total	O		
4	F	6	6	6	0	0
			Total	O		
4	G	153	153	153	0	0
			Total	O		
4	H	145	145	145	0	0
			Total	O		
4	I	2	2	2	0	0
			Total	O		
4	J	117	117	117	0	0
			Total	O		
4	K	55	55	55	0	0
			Total	O		
4	L	2	2	2	0	0

3 Residue-property plots (i)

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

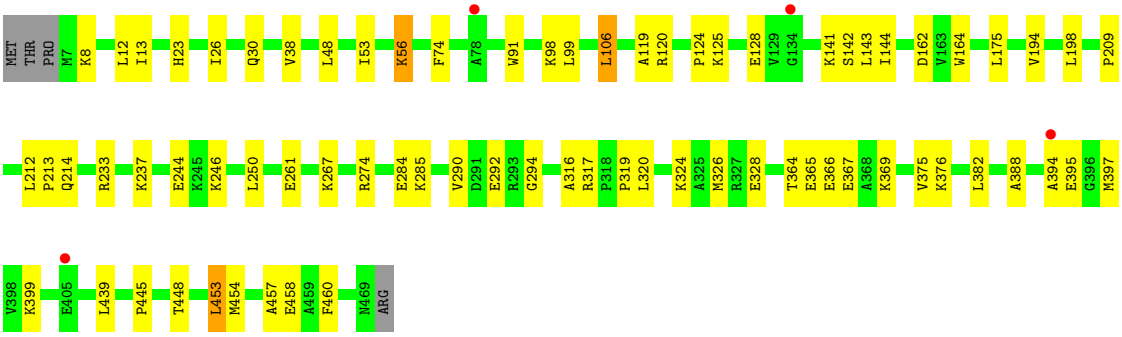
• Molecule 1: Pyruvate dehydrogenase complex, dihydrolipoamide dehydrogenase E3 component

Chain A:



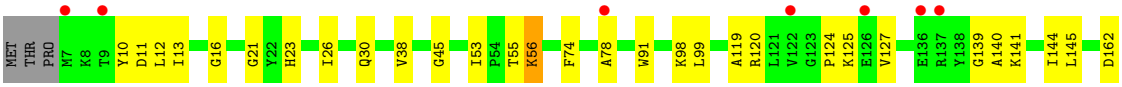
• Molecule 1: Pyruvate dehydrogenase complex, dihydrolipoamide dehydrogenase E3 component

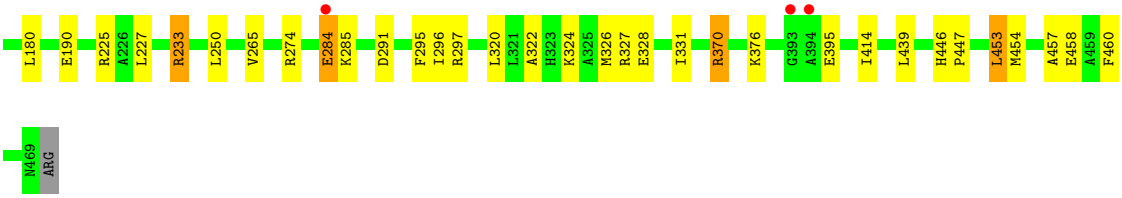
Chain B:



• Molecule 1: Pyruvate dehydrogenase complex, dihydrolipoamide dehydrogenase E3 component

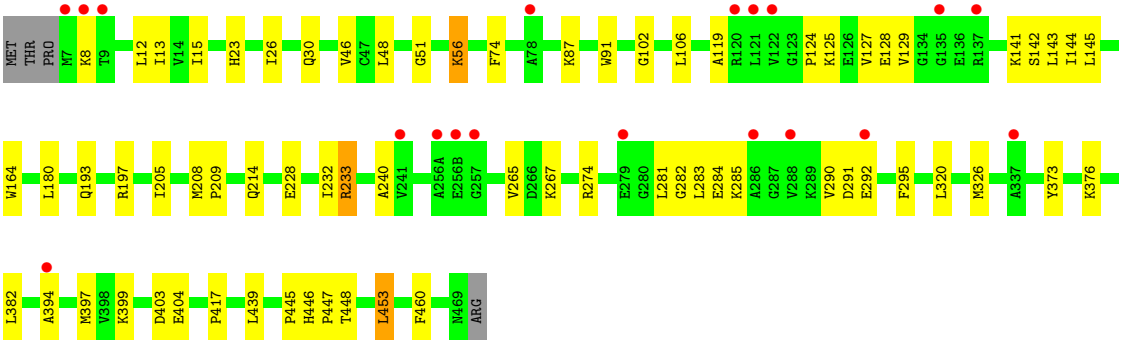
Chain D:





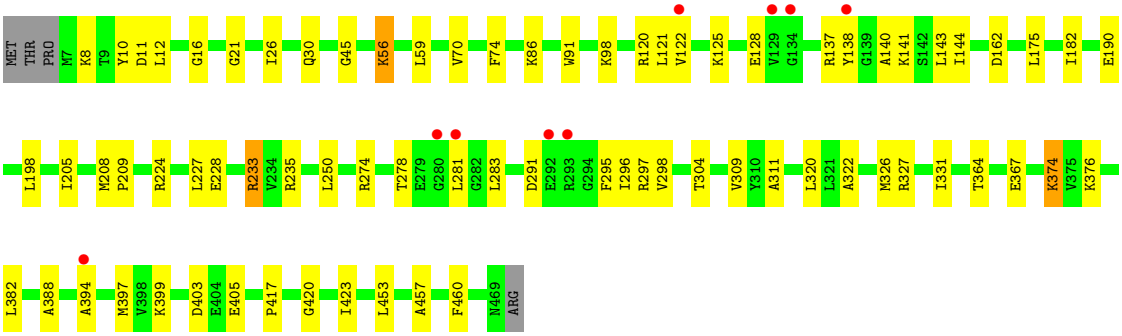
• Molecule 1: Pyruvate dehydrogenase complex, dihydrolipoamide dehydrogenase E3 component

Chain E:



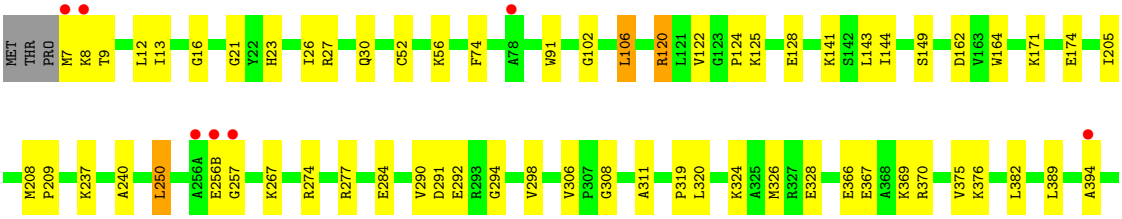
• Molecule 1: Pyruvate dehydrogenase complex, dihydrolipoamide dehydrogenase E3 component

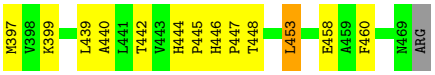
Chain G:



• Molecule 1: Pyruvate dehydrogenase complex, dihydrolipoamide dehydrogenase E3 component

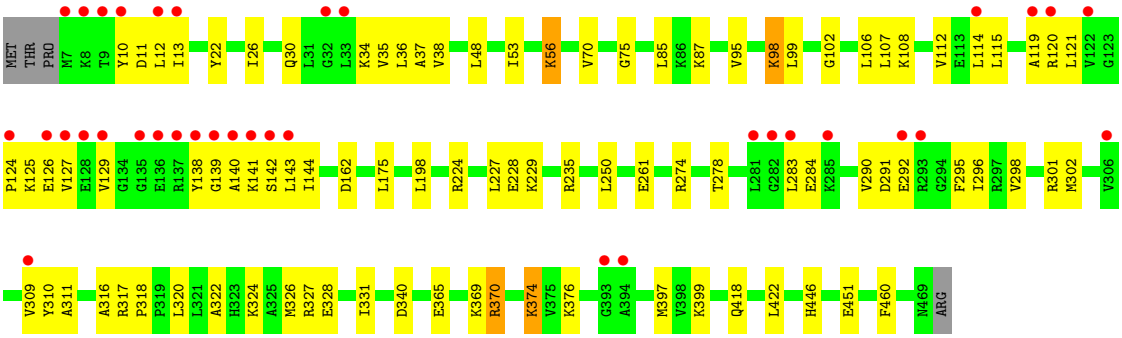
Chain H:





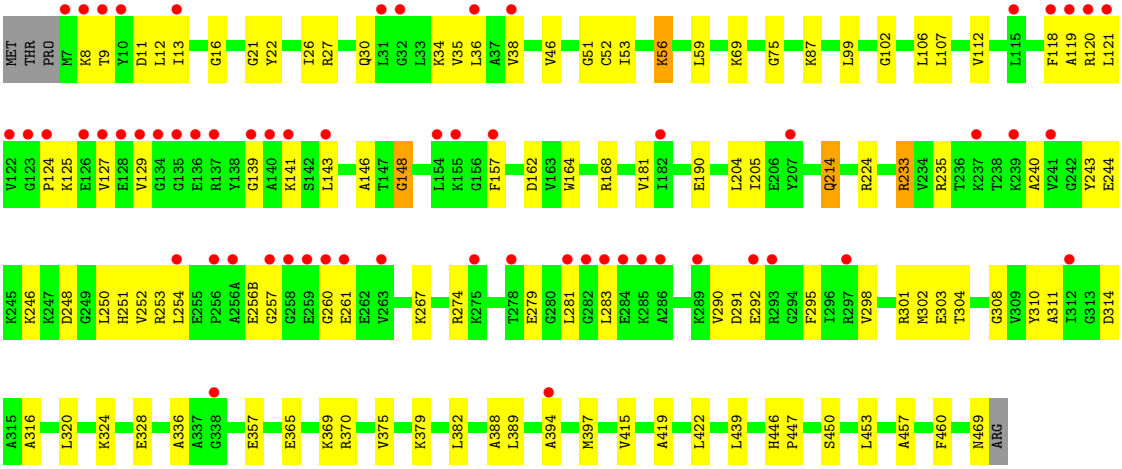
• Molecule 1: Pyruvate dehydrogenase complex, dihydrolipoamide dehydrogenase E3 component

Chain J:



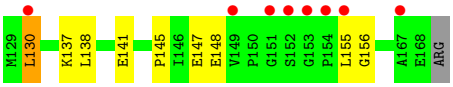
• Molecule 1: Pyruvate dehydrogenase complex, dihydrolipoamide dehydrogenase E3 component

Chain K:



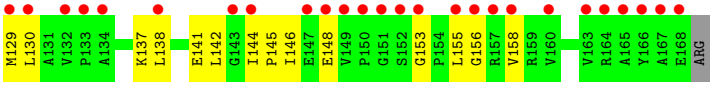
• Molecule 2: Pyruvate dehydrogenase complex, dihydrolipoamide acetyltransferase E2 component

Chain C:



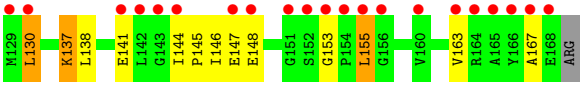
• Molecule 2: Pyruvate dehydrogenase complex, dihydrolipoamide acetyltransferase E2 component

Chain F:



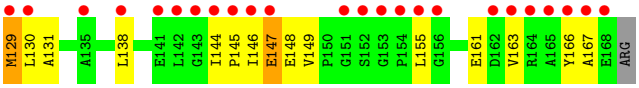
• Molecule 2: Pyruvate dehydrogenase complex, dihydrolipoamide acetyltransferase E2 component

Chain I:



• Molecule 2: Pyruvate dehydrogenase complex, dihydrolipoamide acetyltransferase E2 component

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	88.78Å 88.88Å 144.15Å 89.26° 87.01° 70.84°	Depositor
Resolution (Å)	43.62 – 2.09 43.62 – 2.09	Depositor EDS
% Data completeness (in resolution range)	96.6 (43.62-2.09) 96.7 (43.62-2.09)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.08Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.257 0.207 , 0.246	Depositor DCC
R_{free} test set	11948 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.059 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	29827	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.31	0/3464	0.61	0/4683
1	B	0.32	0/3452	0.61	0/4670
1	D	0.34	0/3468	0.62	0/4687
1	E	0.33	0/3460	0.61	0/4679
1	G	0.34	0/3464	0.62	0/4683
1	H	0.33	0/3452	0.61	1/4670 (0.0%)
1	J	0.31	0/3464	0.60	0/4683
1	K	0.29	0/3452	0.58	0/4670
2	C	0.26	0/294	0.60	1/399 (0.3%)
2	F	0.25	0/294	0.59	1/399 (0.3%)
2	I	0.28	0/294	0.56	0/399
2	L	0.26	0/294	0.57	0/399
All	All	0.32	0/28852	0.61	3/39021 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	156	GLY	N-CA-C	5.69	127.33	113.10
2	F	156	GLY	N-CA-C	5.51	126.86	113.10
1	H	52	CYS	CA-CB-SG	5.46	123.83	114.00

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	3409	0	3519	66	0
1	B	3397	0	3493	61	0
1	D	3413	0	3530	45	0
1	E	3405	0	3508	52	0
1	G	3409	0	3519	52	0
1	H	3397	0	3493	61	0
1	J	3409	0	3519	78	0
1	K	3397	0	3493	91	0
2	C	290	0	300	8	0
2	F	290	0	300	9	0
2	I	290	0	300	12	0
2	L	290	0	300	12	0
3	A	53	0	31	2	0
3	B	53	0	31	0	0
3	D	53	0	31	1	0
3	E	53	0	31	0	0
3	G	53	0	31	1	0
3	H	53	0	31	0	0
3	J	53	0	31	0	0
3	K	53	0	31	3	0
4	A	114	0	0	1	0
4	B	138	0	0	1	0
4	C	4	0	0	0	0
4	D	158	0	0	0	0
4	E	113	0	0	1	0
4	F	6	0	0	0	0
4	G	153	0	0	2	0
4	H	145	0	0	2	0
4	I	2	0	0	0	0
4	J	117	0	0	1	0
4	K	55	0	0	2	0
4	L	2	0	0	0	0
All	All	29827	0	29522	530	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 9.

All (530) 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:B:388:ALA:HB1	1:B:394:ALA:HB2	1.39	1.04
1:D:233:ARG:HG2	1:D:233:ARG:HH11	1.24	1.00
1:J:11:ASP:HA	1:J:141:LYS:HD3	1.42	0.99
1:A:141:LYS:H	1:A:141:LYS:HD2	1.36	0.88
1:H:439:LEU:HD21	1:H:453:LEU:HD22	1.54	0.88
1:H:124:PRO:HB3	1:H:306:VAL:HG11	1.60	0.84
1:E:439:LEU:HD21	1:E:453:LEU:HD22	1.60	0.84
1:B:388:ALA:CB	1:B:394:ALA:HB2	2.08	0.83
1:J:38:VAL:HG11	1:J:119:ALA:HB2	1.59	0.82
1:G:141:LYS:H	1:G:141:LYS:HD2	1.44	0.82
1:H:367:GLU:HA	1:H:370:ARG:HH12	1.45	0.82
1:D:233:ARG:HH11	1:D:233:ARG:CG	1.93	0.81
1:D:370:ARG:HG2	1:D:370:ARG:HH11	1.46	0.79
1:H:125:LYS:HZ1	1:H:308:GLY:HA3	1.47	0.79
1:H:382:LEU:O	1:H:394:ALA:HB1	1.83	0.78
1:D:233:ARG:HG2	1:D:233:ARG:NH1	1.94	0.77
1:J:11:ASP:HB2	1:J:34:LYS:H	1.50	0.77
1:J:120:ARG:O	1:J:127:VAL:HG13	1.85	0.76
1:G:182:ILE:HG12	1:G:205:ILE:HD11	1.68	0.75
1:J:13:ILE:HG12	1:J:36:LEU:HB3	1.68	0.75
1:E:382:LEU:O	1:E:394:ALA:HB1	1.87	0.75
1:E:292:GLU:H	1:E:292:GLU:CD	1.90	0.75
1:D:11:ASP:HA	1:D:141:LYS:HD3	1.69	0.74
1:A:141:LYS:HD2	1:A:141:LYS:N	2.04	0.73
1:B:292:GLU:CD	1:B:292:GLU:H	1.92	0.72
1:B:439:LEU:HD21	1:B:453:LEU:HD22	1.72	0.72
1:E:124:PRO:HD3	1:G:120:ARG:HH22	1.54	0.72
1:G:141:LYS:HD2	1:G:141:LYS:N	2.04	0.71
1:K:205:ILE:HG22	1:K:235:ARG:HB2	1.74	0.70
1:A:301:ARG:HH12	1:A:340:ASP:HA	1.56	0.70
1:B:388:ALA:HB1	1:B:394:ALA:CB	2.21	0.70
1:B:382:LEU:HB3	1:B:394:ALA:HB1	1.74	0.69
1:J:302:MET:HE2	1:J:328:GLU:HB3	1.74	0.69
1:H:120:ARG:HG2	4:H:5511:HOH:O	1.91	0.69
1:G:70:VAL:HG23	4:G:4603:HOH:O	1.93	0.68
1:H:367:GLU:HA	1:H:370:ARG:NH1	2.07	0.68
1:D:291:ASP:OD2	1:D:295:PHE:HB2	1.94	0.68
1:A:283:LEU:C	1:A:285:LYS:H	1.96	0.67
1:J:121:LEU:HD22	1:J:283:LEU:HD23	1.76	0.67
1:K:439:LEU:HD21	1:K:453:LEU:HD22	1.77	0.67
1:K:38:VAL:HG11	1:K:119:ALA:HB2	1.74	0.67
1:D:370:ARG:HG2	1:D:370:ARG:NH1	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:PRO:HG2	1:B:448:THR:HG21	1.76	0.67
1:K:120:ARG:O	1:K:127:VAL:HG13	1.95	0.67
1:G:26:ILE:O	1:G:30:GLN:HG3	1.94	0.66
1:H:292:GLU:CD	1:H:292:GLU:H	1.98	0.66
1:K:205:ILE:HD11	1:K:240:ALA:HB2	1.77	0.66
1:K:253:ARG:NH1	1:K:260:GLY:HA3	2.11	0.66
1:G:11:ASP:HA	1:G:141:LYS:HD3	1.77	0.65
1:K:102:GLY:O	1:K:106:LEU:HD13	1.96	0.65
1:B:12:LEU:HD11	1:B:144:ILE:HG13	1.79	0.64
1:B:164:TRP:CE2	1:B:267:LYS:HG2	2.33	0.64
1:A:283:LEU:O	1:A:285:LYS:N	2.28	0.64
1:G:298:VAL:HG11	1:G:311:ALA:HB3	1.78	0.64
1:J:126:GLU:HA	1:J:138:TYR:O	1.98	0.64
1:G:298:VAL:CG1	1:G:311:ALA:HB3	2.28	0.64
1:B:395:GLU:O	1:B:395:GLU:HG2	1.98	0.63
1:K:26:ILE:O	1:K:30:GLN:HG3	1.98	0.63
1:A:374:LYS:HG3	1:A:405:GLU:OE2	1.99	0.63
1:K:52:CYS:O	1:K:56:LYS:HD2	1.99	0.63
1:G:327:ARG:O	1:G:331:ILE:HG12	1.99	0.62
1:B:175:LEU:HD21	1:B:198:LEU:HB3	1.81	0.62
1:A:194:VAL:O	1:A:198:LEU:HD13	2.00	0.62
1:J:10:TYR:O	1:J:140:ALA:HA	2.00	0.62
1:H:125:LYS:NZ	1:H:308:GLY:HA3	2.14	0.61
1:K:12:LEU:HB3	1:K:35:VAL:HG22	1.83	0.61
2:L:144:ILE:HD11	2:L:167:ALA:HB2	1.82	0.61
1:K:253:ARG:CZ	1:K:260:GLY:HA3	2.31	0.61
2:I:145:PRO:HG2	2:I:148:GLU:HB2	1.82	0.61
1:K:125:LYS:NZ	1:K:308:GLY:HA3	2.15	0.61
1:K:148:GLY:HA2	1:K:314:ASP:HB2	1.81	0.61
1:A:284:GLU:OE1	1:A:285:LYS:HE3	2.01	0.60
1:B:284:GLU:HG2	1:B:285:LYS:H	1.65	0.60
1:K:274:ARG:HB2	1:K:320:LEU:HD13	1.83	0.60
1:K:295:PHE:HB3	1:K:316:ALA:O	2.01	0.60
1:E:233:ARG:HG3	1:E:233:ARG:HH11	1.67	0.60
2:I:144:ILE:HD11	2:I:167:ALA:HB2	1.84	0.59
1:A:205:ILE:CD1	1:A:240:ALA:HB2	2.32	0.59
1:D:376:LYS:HE2	1:D:460:PHE:O	2.02	0.59
1:J:26:ILE:O	1:J:30:GLN:HG3	2.02	0.59
1:E:12:LEU:HD11	1:E:144:ILE:HG13	1.84	0.59
1:K:11:ASP:HB2	1:K:34:LYS:H	1.67	0.59
1:A:382:LEU:O	1:A:394:ALA:HB1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LYS:H	1:A:141:LYS:CD	2.13	0.59
1:K:107:LEU:O	1:K:112:VAL:HB	2.03	0.59
1:D:38:VAL:HG11	1:D:119:ALA:HB2	1.85	0.58
2:I:130:LEU:HD23	2:I:130:LEU:H	1.67	0.58
1:J:397:MET:HE2	1:J:399:LYS:HB2	1.83	0.58
2:C:147:GLU:CD	2:C:147:GLU:H	2.07	0.58
2:L:130:LEU:H	2:L:130:LEU:HD23	1.68	0.58
1:E:119:ALA:HB1	1:E:127:VAL:HG11	1.85	0.58
1:K:369:LYS:HG3	1:K:375:VAL:HG21	1.86	0.58
1:K:141:LYS:NZ	1:K:141:LYS:HB3	2.18	0.58
1:H:164:TRP:CZ2	1:H:267:LYS:HG2	2.39	0.57
1:K:292:GLU:CD	1:K:292:GLU:H	2.07	0.57
1:K:324:LYS:O	1:K:328:GLU:HG3	2.04	0.57
1:J:11:ASP:O	1:J:141:LYS:HB2	2.04	0.57
1:J:370:ARG:HH11	1:J:370:ARG:HG2	1.69	0.57
1:D:78:ALA:HB1	4:E:3529:HOH:O	2.03	0.57
1:J:298:VAL:HG11	1:J:311:ALA:HB3	1.86	0.57
1:J:119:ALA:HB1	1:J:127:VAL:HG11	1.87	0.57
1:G:56:LYS:N	1:G:56:LYS:HE3	2.20	0.57
1:H:164:TRP:CE2	1:H:267:LYS:HG2	2.39	0.57
1:B:246:LYS:HE3	1:K:370:ARG:O	2.05	0.56
1:H:205:ILE:CD1	1:H:240:ALA:HB2	2.35	0.56
1:B:162:ASP:HB3	1:B:250:LEU:HD21	1.88	0.56
1:G:122:VAL:HG11	1:G:137:ARG:NH1	2.21	0.56
2:C:130:LEU:HD23	2:C:130:LEU:H	1.71	0.56
1:K:164:TRP:CD1	1:K:168:ARG:HG2	2.41	0.56
1:E:397:MET:CE	1:E:399:LYS:HB2	2.35	0.56
1:G:162:ASP:HB3	1:G:250:LEU:HD11	1.87	0.56
1:J:124:PRO:O	1:J:125:LYS:HD3	2.06	0.56
1:K:125:LYS:HE2	1:K:125:LYS:HA	1.87	0.56
1:K:162:ASP:HB3	1:K:250:LEU:HD21	1.86	0.56
1:J:374:LYS:HE3	1:J:374:LYS:HA	1.88	0.55
1:K:250:LEU:HD12	1:K:250:LEU:N	2.21	0.55
1:B:164:TRP:CZ2	1:B:267:LYS:HG2	2.42	0.55
1:J:87:LYS:HG2	1:K:75:GLY:N	2.22	0.55
2:F:138:LEU:HD13	2:F:138:LEU:O	2.07	0.55
1:B:38:VAL:HG11	1:B:119:ALA:HB2	1.89	0.55
1:E:290:VAL:HG12	1:E:291:ASP:N	2.21	0.55
1:H:124:PRO:HB3	1:H:306:VAL:CG1	2.33	0.55
1:J:12:LEU:O	1:J:35:VAL:HA	2.07	0.55
1:J:322:ALA:O	1:J:326:MET:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:GLY:HA2	1:A:285:LYS:HD2	1.89	0.54
2:C:130:LEU:HD23	2:C:130:LEU:N	2.23	0.54
1:J:298:VAL:CG1	1:J:311:ALA:HB3	2.38	0.54
1:D:274:ARG:HB2	1:D:320:LEU:CD1	2.38	0.54
2:I:137:LYS:O	2:I:141:GLU:HG3	2.08	0.54
1:A:12:LEU:HD11	1:A:144:ILE:HG13	1.89	0.54
1:B:397:MET:CE	1:B:399:LYS:HB2	2.38	0.54
1:D:414:ILE:HD11	1:D:453:LEU:HD11	1.88	0.54
1:H:397:MET:CE	1:H:399:LYS:HB2	2.37	0.54
1:J:162:ASP:HB3	1:J:250:LEU:HD11	1.90	0.54
1:B:124:PRO:O	1:B:125:LYS:HE2	2.08	0.54
1:J:13:ILE:HB	1:J:143:LEU:CD2	2.38	0.54
1:D:297:ARG:HH11	1:D:297:ARG:HG3	1.73	0.54
2:I:146:ILE:HG23	2:I:147:GLU:N	2.23	0.54
1:B:23:HIS:CE1	1:B:326:MET:HG2	2.43	0.53
1:B:365:GLU:O	1:B:369:LYS:HG3	2.07	0.53
1:B:369:LYS:HG3	1:B:375:VAL:HG21	1.89	0.53
1:E:205:ILE:CD1	1:E:240:ALA:HB2	2.39	0.53
1:K:290:VAL:HG12	1:K:291:ASP:N	2.23	0.53
1:H:13:ILE:HB	1:H:143:LEU:CD2	2.38	0.53
1:A:175:LEU:HD11	1:A:198:LEU:HB3	1.89	0.53
1:G:397:MET:CE	1:G:399:LYS:HB2	2.38	0.53
1:E:23:HIS:CE1	1:E:326:MET:HG2	2.44	0.53
1:E:445:PRO:HG2	1:E:448:THR:HG21	1.90	0.53
1:G:8:LYS:HE2	1:G:138:TYR:CE2	2.44	0.53
1:J:327:ARG:O	1:J:331:ILE:HG12	2.08	0.53
1:A:322:ALA:O	1:A:326:MET:HG3	2.09	0.53
1:A:119:ALA:HB1	1:A:127:VAL:HG11	1.91	0.53
1:A:233:ARG:HA	1:A:233:ARG:HH21	1.74	0.53
1:J:290:VAL:HG12	1:J:296:ILE:HA	1.90	0.53
1:D:457:ALA:O	1:D:460:PHE:HB3	2.08	0.52
1:H:8:LYS:H	1:H:8:LYS:HD3	1.73	0.52
1:A:466:HIS:HA	1:B:106:LEU:HD21	1.90	0.52
1:B:125:LYS:HE2	1:B:125:LYS:HA	1.92	0.52
2:C:138:LEU:HD13	2:C:138:LEU:O	2.09	0.52
1:B:319:PRO:O	1:B:324:LYS:HD3	2.10	0.52
1:J:12:LEU:HD12	1:J:142:SER:O	2.10	0.52
1:K:303:GLU:HG3	1:K:310:TYR:CE2	2.44	0.52
1:A:221:ALA:HB1	1:A:225:ARG:NH2	2.24	0.52
1:H:205:ILE:HD11	1:H:240:ALA:HB2	1.90	0.52
1:K:12:LEU:O	1:K:35:VAL:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LYS:HD3	1:A:98:LYS:C	2.29	0.52
1:A:233:ARG:NH2	1:A:234:VAL:H	2.07	0.52
1:D:91:TRP:CD2	1:E:74:PHE:HB3	2.45	0.52
1:E:274:ARG:HB2	1:E:320:LEU:HD13	1.92	0.52
1:J:301:ARG:HH12	1:J:340:ASP:HA	1.74	0.52
1:K:298:VAL:HG11	1:K:311:ALA:HB3	1.92	0.52
1:H:122:VAL:HG12	1:H:122:VAL:O	2.10	0.52
1:J:10:TYR:CD2	1:J:34:LYS:HE2	2.45	0.52
1:J:365:GLU:O	1:J:369:LYS:HG3	2.09	0.52
1:E:26:ILE:O	1:E:30:GLN:HG3	2.10	0.51
1:H:26:ILE:O	1:H:30:GLN:HG3	2.10	0.51
1:G:291:ASP:OD2	1:G:295:PHE:HB2	2.11	0.51
1:H:8:LYS:HD3	1:H:8:LYS:N	2.25	0.51
1:J:12:LEU:HD11	1:J:144:ILE:HG13	1.92	0.51
1:J:284:GLU:H	1:J:284:GLU:CD	2.12	0.51
1:A:125:LYS:NZ	1:A:141:LYS:HA	2.25	0.51
1:K:46:VAL:O	1:K:51:GLY:N	2.43	0.51
1:G:141:LYS:H	1:G:141:LYS:CD	2.17	0.51
1:G:322:ALA:O	1:G:326:MET:HG3	2.11	0.51
2:C:137:LYS:O	2:C:141:GLU:HG3	2.10	0.51
1:K:8:LYS:HD3	1:K:8:LYS:N	2.24	0.51
1:B:209:PRO:HA	1:B:237:LYS:HG3	1.92	0.51
1:B:290:VAL:CG1	1:B:294:GLY:HA2	2.41	0.51
1:A:398:VAL:HG22	1:A:414:ILE:HG23	1.92	0.51
1:G:125:LYS:HB3	1:G:140:ALA:O	2.11	0.51
1:J:75:GLY:N	1:K:87:LYS:HG2	2.26	0.51
1:H:122:VAL:HG21	1:H:128:GLU:HB2	1.93	0.51
1:A:209:PRO:HA	1:A:237:LYS:HG2	1.93	0.50
1:J:397:MET:CE	1:J:399:LYS:HB2	2.40	0.50
1:K:59:LEU:HD11	1:K:190:GLU:HG2	1.92	0.50
1:K:303:GLU:HG3	1:K:310:TYR:CD2	2.47	0.50
1:H:298:VAL:CG1	1:H:311:ALA:HB3	2.41	0.50
1:G:397:MET:HE2	1:G:399:LYS:HB2	1.93	0.50
1:J:125:LYS:HD2	1:J:141:LYS:O	2.11	0.50
1:K:274:ARG:HB2	1:K:320:LEU:CD1	2.41	0.50
2:I:130:LEU:HD23	2:I:130:LEU:N	2.25	0.50
1:K:205:ILE:CD1	1:K:240:ALA:HB2	2.41	0.50
1:B:53:ILE:HG21	1:B:99:LEU:HD12	1.93	0.50
1:E:102:GLY:O	1:E:106:LEU:HD13	2.11	0.50
1:H:298:VAL:HG11	1:H:311:ALA:HB3	1.93	0.50
1:K:16:GLY:HA3	1:K:146:ALA:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:LYS:NZ	1:B:141:LYS:HB3	2.27	0.50
2:L:144:ILE:CD1	2:L:167:ALA:HB2	2.41	0.50
1:B:8:LYS:HD3	1:B:8:LYS:H	1.77	0.50
1:K:22:TYR:O	1:K:26:ILE:HG13	2.11	0.50
1:D:10:TYR:O	1:D:140:ALA:HA	2.12	0.49
1:E:376:LYS:HE2	1:E:460:PHE:O	2.11	0.49
1:H:439:LEU:HD21	1:H:453:LEU:CD2	2.35	0.49
1:J:85:LEU:HD11	1:J:175:LEU:HG	1.94	0.49
1:K:162:ASP:HA	1:K:267:LYS:CD	2.42	0.49
2:L:130:LEU:HD23	2:L:130:LEU:N	2.27	0.49
1:A:243:TYR:CE2	1:A:250:LEU:HD22	2.47	0.49
1:B:376:LYS:HE2	1:B:460:PHE:O	2.11	0.49
1:J:119:ALA:HA	1:J:129:VAL:HG22	1.94	0.49
1:J:318:PRO:HA	1:J:320:LEU:HD23	1.93	0.49
1:E:397:MET:HE2	1:E:399:LYS:HB2	1.94	0.49
2:F:142:LEU:O	2:F:144:ILE:HG13	2.13	0.49
2:I:138:LEU:HD12	2:I:163:VAL:HB	1.94	0.49
2:I:147:GLU:CD	2:I:147:GLU:H	2.15	0.49
1:K:16:GLY:O	1:K:21:GLY:HA3	2.13	0.49
1:K:224:ARG:HG2	1:K:224:ARG:HH11	1.78	0.49
1:A:283:LEU:C	1:A:285:LYS:N	2.64	0.49
1:G:98:LYS:HD3	1:H:389:LEU:HD21	1.93	0.49
1:D:327:ARG:O	1:D:331:ILE:HG12	2.13	0.49
1:E:205:ILE:HD11	1:E:240:ALA:HB2	1.93	0.49
1:K:248:ASP:CG	1:K:251:HIS:HE2	2.15	0.49
1:E:12:LEU:HD12	1:E:142:SER:O	2.12	0.49
1:K:164:TRP:CZ2	1:K:267:LYS:HG2	2.48	0.49
1:H:23:HIS:CE1	1:H:326:MET:HG2	2.47	0.49
1:H:319:PRO:O	1:H:324:LYS:HD3	2.12	0.49
1:J:125:LYS:O	1:J:139:GLY:HA2	2.13	0.49
1:D:324:LYS:O	1:D:328:GLU:HG3	2.13	0.49
1:H:162:ASP:HB3	1:H:250:LEU:HD21	1.94	0.49
1:A:319:PRO:O	1:A:324:LYS:HD3	2.13	0.48
1:E:164:TRP:CZ2	1:E:267:LYS:HG2	2.47	0.48
1:G:10:TYR:O	1:G:140:ALA:HA	2.13	0.48
1:K:38:VAL:HG12	3:K:7482:FAD:H2A	1.95	0.48
1:A:327:ARG:O	1:A:331:ILE:HG12	2.14	0.48
1:K:365:GLU:HG3	4:K:7516:HOH:O	2.13	0.48
1:D:56:LYS:N	1:D:56:LYS:HE3	2.27	0.48
1:A:301:ARG:NE	1:A:303:GLU:OE1	2.43	0.48
2:F:130:LEU:HD23	2:F:130:LEU:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:145:PRO:HG2	2:F:148:GLU:CG	2.44	0.48
1:J:115:LEU:HD23	1:J:129:VAL:HG21	1.96	0.48
1:K:35:VAL:HG12	1:K:36:LEU:N	2.29	0.48
1:D:370:ARG:O	1:K:246:LYS:HE3	2.13	0.48
1:H:102:GLY:O	1:H:106:LEU:HD22	2.13	0.48
1:D:26:ILE:O	1:D:30:GLN:HG3	2.13	0.48
1:H:13:ILE:HB	1:H:143:LEU:HD22	1.94	0.48
2:L:145:PRO:HG2	2:L:148:GLU:HB2	1.95	0.48
1:A:376:LYS:HD2	1:A:404:GLU:OE1	2.14	0.48
1:K:9:THR:HA	1:K:139:GLY:O	2.13	0.48
2:F:130:LEU:HD23	2:F:130:LEU:N	2.29	0.48
1:J:102:GLY:O	1:J:106:LEU:HG	2.14	0.48
1:J:370:ARG:HG2	1:J:370:ARG:NH1	2.28	0.48
1:A:297:ARG:O	1:A:304:THR:HA	2.14	0.47
1:B:364:THR:OG1	1:B:367:GLU:HG3	2.14	0.47
1:J:125:LYS:HB3	1:J:140:ALA:O	2.14	0.47
2:L:138:LEU:HD13	2:L:138:LEU:O	2.14	0.47
1:E:127:VAL:HG12	1:E:128:GLU:N	2.29	0.47
1:K:121:LEU:HD12	1:K:127:VAL:HG22	1.96	0.47
1:K:162:ASP:HA	1:K:267:LYS:HD2	1.96	0.47
1:J:121:LEU:CD2	1:J:283:LEU:HD23	2.42	0.47
2:L:146:ILE:HG23	2:L:147:GLU:N	2.30	0.47
1:A:324:LYS:O	1:A:328:GLU:HG3	2.13	0.47
2:L:138:LEU:HD12	2:L:163:VAL:HB	1.97	0.47
1:A:53:ILE:HG21	1:A:99:LEU:HD12	1.97	0.47
1:J:10:TYR:HA	1:J:34:LYS:HD3	1.96	0.47
1:B:8:LYS:HD3	1:B:8:LYS:N	2.29	0.47
1:H:376:LYS:HE2	1:H:460:PHE:O	2.14	0.47
1:A:45:GLY:HA2	3:A:8482:FAD:O3B	2.15	0.47
1:A:284:GLU:OE2	1:A:284:GLU:N	2.42	0.47
1:A:334:GLU:O	1:A:339:LYS:HB2	2.15	0.47
1:E:233:ARG:HG3	1:E:233:ARG:NH1	2.30	0.47
1:J:85:LEU:CD1	1:J:175:LEU:HG	2.45	0.47
1:J:301:ARG:HH11	1:J:301:ARG:HG2	1.79	0.47
1:K:281:LEU:HD23	1:K:283:LEU:HD21	1.95	0.47
1:K:301:ARG:HG2	1:K:301:ARG:HH11	1.79	0.47
1:K:457:ALA:O	1:K:460:PHE:HB3	2.14	0.47
1:D:370:ARG:HD3	1:K:244:GLU:OE1	2.15	0.47
1:K:379:LYS:HB3	1:K:397:MET:CE	2.45	0.47
1:J:98:LYS:HE3	1:J:98:LYS:O	2.15	0.47
1:E:281:LEU:HD23	1:E:283:LEU:HD21	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:69:LYS:HG3	4:K:7512:HOH:O	2.14	0.46
1:K:157:PHE:HZ	1:K:252:VAL:HG13	1.80	0.46
1:B:274:ARG:HB2	1:B:320:LEU:CD1	2.45	0.46
1:E:282:GLY:HA2	1:E:285:LYS:NZ	2.30	0.46
1:B:56:LYS:N	1:B:56:LYS:HE3	2.30	0.46
1:E:56:LYS:HE3	1:E:56:LYS:N	2.29	0.46
1:J:70:VAL:HG23	4:J:6538:HOH:O	2.13	0.46
1:J:143:LEU:O	1:J:309:VAL:HA	2.14	0.46
1:K:164:TRP:HB3	1:K:168:ARG:HB3	1.97	0.46
1:H:324:LYS:O	1:H:328:GLU:HG3	2.14	0.46
1:H:445:PRO:HG2	1:H:448:THR:HG21	1.97	0.46
1:J:12:LEU:HB3	1:J:35:VAL:HG22	1.97	0.46
1:A:171:LYS:HD3	1:A:174:GLU:OE2	2.16	0.46
1:E:46:VAL:O	1:E:51:GLY:N	2.48	0.46
1:E:124:PRO:O	1:E:125:LYS:HG3	2.16	0.46
1:J:324:LYS:HE2	1:J:328:GLU:OE2	2.16	0.46
1:K:310:TYR:CE1	1:K:336:ALA:HB2	2.51	0.46
1:D:297:ARG:HG3	1:D:297:ARG:NH1	2.30	0.46
1:E:382:LEU:CD1	1:E:417:PRO:HD2	2.45	0.46
1:H:274:ARG:HB2	1:H:320:LEU:CD1	2.46	0.46
1:H:370:ARG:HH11	1:H:370:ARG:HB3	1.81	0.46
1:J:175:LEU:CD1	1:J:198:LEU:HB3	2.45	0.46
1:A:91:TRP:CD2	1:B:74:PHE:HB3	2.51	0.46
1:E:13:ILE:HB	1:E:143:LEU:CD2	2.46	0.46
1:D:119:ALA:HB1	1:D:127:VAL:HG11	1.97	0.46
1:H:171:LYS:HD3	1:H:174:GLU:OE1	2.16	0.46
1:H:366:GLU:HG2	4:H:5553:HOH:O	2.16	0.46
1:J:30:GLN:NE2	1:K:469:ASN:ND2	2.64	0.46
1:K:357:GLU:HB2	1:K:419:ALA:HB3	1.97	0.46
1:H:369:LYS:HG3	1:H:375:VAL:HG21	1.98	0.45
1:E:8:LYS:HD3	1:E:8:LYS:N	2.31	0.45
1:K:256(B):GLU:HG2	1:K:257:GLY:N	2.31	0.45
1:E:291:ASP:OD2	1:E:295:PHE:HB2	2.16	0.45
1:B:124:PRO:C	1:B:125:LYS:HE2	2.37	0.45
1:B:324:LYS:O	1:B:328:GLU:HG3	2.17	0.45
2:C:145:PRO:HG2	2:C:148:GLU:HG3	1.97	0.45
1:H:290:VAL:HG11	1:H:294:GLY:HA2	1.98	0.45
1:J:11:ASP:HB2	1:J:34:LYS:N	2.27	0.45
2:C:145:PRO:HG2	2:C:148:GLU:CG	2.46	0.45
1:E:13:ILE:HB	1:E:143:LEU:HD23	1.98	0.45
1:K:290:VAL:CG1	1:K:291:ASP:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:149:VAL:HG22	2:L:166:TYR:CD2	2.52	0.45
1:A:121:LEU:HD22	1:A:283:LEU:HD23	1.98	0.45
1:G:382:LEU:CD1	1:G:417:PRO:HD2	2.47	0.45
2:I:138:LEU:C	2:I:138:LEU:HD13	2.36	0.45
1:B:13:ILE:HB	1:B:143:LEU:HD22	1.98	0.45
2:F:138:LEU:HD13	2:F:138:LEU:C	2.38	0.45
1:J:11:ASP:CB	1:J:34:LYS:H	2.26	0.45
1:K:214:GLN:HA	1:K:214:GLN:HE21	1.82	0.45
1:G:45:GLY:HA2	3:G:4482:FAD:O3B	2.17	0.45
1:G:91:TRP:CD2	1:H:74:PHE:HB3	2.53	0.44
1:H:290:VAL:CG1	1:H:294:GLY:HA2	2.47	0.44
1:J:22:TYR:O	1:J:26:ILE:HG13	2.17	0.44
1:J:141:LYS:HD2	1:J:141:LYS:N	2.32	0.44
1:A:153:GLU:HG3	4:A:8577:HOH:O	2.17	0.44
1:G:74:PHE:HB3	1:H:91:TRP:CD2	2.52	0.44
1:J:274:ARG:HB2	1:J:320:LEU:CD1	2.47	0.44
1:K:388:ALA:CB	1:K:394:ALA:HB2	2.46	0.44
1:A:125:LYS:HZ2	1:A:141:LYS:HA	1.82	0.44
1:B:175:LEU:HD21	1:B:198:LEU:CB	2.45	0.44
1:J:292:GLU:H	1:J:292:GLU:CD	2.21	0.44
1:D:23:HIS:CD2	1:D:326:MET:HB3	2.53	0.44
1:G:374:LYS:HG3	1:G:405:GLU:HG3	1.98	0.44
1:H:208:MET:HB3	1:H:209:PRO:CD	2.48	0.44
1:J:376:LYS:HE2	1:J:460:PHE:O	2.17	0.44
1:K:382:LEU:HD23	1:K:382:LEU:HA	1.84	0.44
1:D:446:HIS:HA	1:D:447:PRO:HA	1.81	0.44
1:K:250:LEU:N	1:K:250:LEU:CD1	2.81	0.44
1:D:125:LYS:O	1:D:139:GLY:HA2	2.17	0.44
2:F:145:PRO:HG2	2:F:148:GLU:HG3	1.99	0.44
1:G:16:GLY:O	1:G:21:GLY:HA3	2.18	0.44
1:H:16:GLY:O	1:H:21:GLY:HA3	2.17	0.44
1:J:107:LEU:O	1:J:112:VAL:HB	2.18	0.44
1:K:13:ILE:HG12	1:K:36:LEU:HB3	2.00	0.44
1:K:382:LEU:O	1:K:394:ALA:HB1	2.17	0.44
1:D:119:ALA:HB1	1:D:127:VAL:CG1	2.48	0.44
1:E:164:TRP:CE2	1:E:267:LYS:HG2	2.53	0.44
1:G:175:LEU:HD21	1:G:198:LEU:HD23	1.99	0.44
1:K:254:LEU:HB2	1:K:261:GLU:HG3	2.00	0.44
1:A:91:TRP:CG	1:B:74:PHE:HB3	2.53	0.44
1:D:454:MET:O	1:D:458:GLU:HG3	2.18	0.44
1:H:290:VAL:HG12	1:H:291:ASP:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:301:ARG:NH1	1:J:340:ASP:OD1	2.51	0.44
2:L:161:GLU:CD	2:L:161:GLU:H	2.20	0.44
1:A:397:MET:CE	1:A:399:LYS:HB2	2.48	0.44
1:B:214:GLN:HA	1:B:214:GLN:NE2	2.33	0.44
1:B:316:ALA:O	1:B:317:ARG:HB3	2.18	0.44
1:D:55:THR:HG21	1:D:190:GLU:OE1	2.17	0.44
1:G:224:ARG:O	1:G:228:GLU:HG3	2.17	0.44
1:B:125:LYS:HE2	1:B:125:LYS:CA	2.48	0.43
1:H:370:ARG:NH1	1:H:370:ARG:HB3	2.32	0.43
1:K:243:TYR:HB3	1:K:252:VAL:HG22	1.98	0.43
1:A:74:PHE:HB3	1:B:91:TRP:CD2	2.52	0.43
1:D:74:PHE:HB3	1:E:91:TRP:CD2	2.53	0.43
1:E:382:LEU:C	1:E:394:ALA:HB1	2.39	0.43
1:K:27:ARG:NE	1:K:30:GLN:OE1	2.41	0.43
1:E:180:LEU:HB2	1:E:265:VAL:HG11	2.00	0.43
1:E:214:GLN:HA	1:E:214:GLN:NE2	2.33	0.43
1:A:256(B):GLU:OE2	1:A:256(B):GLU:N	2.42	0.43
1:A:389:LEU:HD12	1:A:389:LEU:HA	1.90	0.43
1:B:244:GLU:OE1	1:K:370:ARG:HD3	2.18	0.43
1:B:395:GLU:N	1:B:395:GLU:OE1	2.51	0.43
1:G:297:ARG:HG3	1:G:297:ARG:HH11	1.84	0.43
1:G:382:LEU:O	1:G:394:ALA:HB1	2.18	0.43
1:H:12:LEU:HD21	1:H:144:ILE:HD12	2.01	0.43
1:H:256(B):GLU:HG2	1:H:257:GLY:N	2.33	0.43
2:I:153:GLY:O	2:I:155:LEU:N	2.52	0.43
1:A:228:GLU:HA	1:A:232:ILE:O	2.19	0.43
1:G:376:LYS:HB3	1:G:460:PHE:CE2	2.54	0.43
1:K:141:LYS:HB3	1:K:141:LYS:HZ2	1.82	0.43
1:K:415:VAL:HG13	1:K:415:VAL:O	2.18	0.43
1:B:13:ILE:HB	1:B:143:LEU:CD2	2.48	0.43
1:G:122:VAL:HG21	1:G:128:GLU:HB2	2.01	0.43
1:G:420:GLY:O	1:G:423:ILE:HG22	2.18	0.43
1:J:48:LEU:N	1:J:48:LEU:HD12	2.34	0.43
1:A:48:LEU:HD12	1:A:48:LEU:N	2.34	0.43
1:B:12:LEU:HD12	1:B:142:SER:O	2.19	0.43
1:E:15:ILE:HD12	1:E:145:LEU:CD2	2.49	0.43
1:E:376:LYS:HB2	1:E:404:GLU:HB3	2.01	0.43
1:G:59:LEU:HD11	1:G:190:GLU:HB3	2.01	0.43
1:J:141:LYS:HD2	1:J:141:LYS:H	1.84	0.43
1:K:233:ARG:CG	1:K:233:ARG:HH21	2.32	0.43
1:K:298:VAL:HG12	1:K:304:THR:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ILE:HG21	1:D:99:LEU:HD12	2.01	0.42
1:E:274:ARG:HB2	1:E:320:LEU:CD1	2.48	0.42
1:H:376:LYS:HB3	1:H:460:PHE:CE2	2.54	0.42
1:D:322:ALA:O	1:D:326:MET:HG3	2.19	0.42
1:J:53:ILE:HG21	1:J:99:LEU:HD12	2.01	0.42
1:J:56:LYS:HE3	1:J:56:LYS:N	2.34	0.42
1:J:446:HIS:HD1	1:J:451:GLU:CD	2.22	0.42
1:B:48:LEU:N	1:B:48:LEU:HD12	2.33	0.42
1:B:162:ASP:HA	1:B:267:LYS:HD2	2.01	0.42
1:B:454:MET:O	1:B:458:GLU:HG3	2.20	0.42
1:B:457:ALA:O	1:B:460:PHE:HB3	2.19	0.42
1:D:13:ILE:HG13	1:D:140:ALA:HB2	2.01	0.42
1:E:290:VAL:CG1	1:E:291:ASP:N	2.82	0.42
1:H:440:ALA:HB1	1:H:458:GLU:HG2	2.01	0.42
1:K:181:VAL:O	1:K:204:LEU:HA	2.19	0.42
1:E:87:LYS:HE2	1:E:87:LYS:HB2	1.90	0.42
1:J:95:VAL:HG13	1:K:389:LEU:HD23	2.01	0.42
1:A:298:VAL:HA	1:A:303:GLU:O	2.19	0.42
1:B:26:ILE:O	1:B:30:GLN:HG3	2.18	0.42
1:H:290:VAL:HG13	1:H:294:GLY:C	2.39	0.42
1:J:224:ARG:O	1:J:228:GLU:HG3	2.19	0.42
1:J:229:LYS:HE3	1:J:229:LYS:HB2	1.83	0.42
1:D:439:LEU:HD23	1:D:457:ALA:HB2	2.02	0.42
1:E:141:LYS:NZ	1:E:141:LYS:HB3	2.34	0.42
1:G:388:ALA:HB1	1:G:394:ALA:HA	2.00	0.42
1:K:164:TRP:CH2	1:K:267:LYS:HG2	2.54	0.42
1:A:137:ARG:HH11	1:A:137:ARG:HG3	1.84	0.42
1:A:274:ARG:HB2	1:A:320:LEU:CD1	2.49	0.42
1:A:446:HIS:HD1	1:A:451:GLU:CD	2.21	0.42
1:D:45:GLY:HA2	3:D:2482:FAD:O3B	2.20	0.42
1:G:121:LEU:HD11	1:G:143:LEU:HD13	2.02	0.42
1:G:278:THR:HG21	1:G:296:ILE:HG13	2.00	0.42
1:H:442:THR:HB	1:H:444:HIS:CE1	2.54	0.42
1:J:302:MET:O	1:J:310:TYR:HB3	2.20	0.42
1:K:302:MET:HE2	1:K:328:GLU:HB3	2.00	0.42
1:D:233:ARG:CG	1:D:233:ARG:NH1	2.63	0.42
2:F:146:ILE:HD11	2:F:158:VAL:HG11	2.02	0.42
1:K:53:ILE:HG21	1:K:99:LEU:HD12	2.02	0.42
2:L:138:LEU:HD13	2:L:138:LEU:C	2.40	0.42
1:A:13:ILE:HB	1:A:143:LEU:CD2	2.50	0.42
1:D:180:LEU:HB2	1:D:265:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:LEU:N	1:E:48:LEU:HD12	2.35	0.42
1:K:124:PRO:O	1:K:143:LEU:HD12	2.19	0.42
1:K:148:GLY:HA3	3:K:7482:FAD:O2A	2.19	0.42
1:A:52:CYS:O	1:A:56:LYS:HD2	2.20	0.41
1:A:57:ALA:HB1	1:A:91:TRP:CZ3	2.56	0.41
1:A:124:PRO:C	1:A:125:LYS:HG3	2.40	0.41
1:A:209:PRO:HA	1:A:237:LYS:CG	2.50	0.41
1:A:353:TYR:HA	1:A:357:GLU:HG2	2.02	0.41
1:D:16:GLY:O	1:D:21:GLY:HA3	2.20	0.41
1:D:162:ASP:HB3	1:D:250:LEU:HD11	2.02	0.41
1:E:208:MET:HB3	1:E:209:PRO:CD	2.50	0.41
1:H:205:ILE:O	1:H:205:ILE:HG13	2.19	0.41
1:H:209:PRO:HB3	1:H:237:LYS:HE2	2.01	0.41
1:H:397:MET:HE1	1:H:399:LYS:HB2	2.01	0.41
1:A:128:GLU:OE1	1:A:136:GLU:O	2.37	0.41
1:B:162:ASP:HA	1:B:267:LYS:CD	2.49	0.41
1:B:382:LEU:HD23	1:B:382:LEU:HA	1.86	0.41
1:D:225:ARG:HG2	1:D:225:ARG:HH11	1.85	0.41
2:F:137:LYS:O	2:F:141:GLU:HG3	2.19	0.41
1:H:125:LYS:NZ	1:H:141:LYS:O	2.45	0.41
1:K:87:LYS:HE2	1:K:87:LYS:HB2	1.81	0.41
1:K:235:ARG:HG3	1:K:235:ARG:HH11	1.85	0.41
1:D:12:LEU:HD11	1:D:144:ILE:HG13	2.02	0.41
1:E:119:ALA:HA	1:E:129:VAL:HG22	2.02	0.41
2:I:138:LEU:HD13	2:I:138:LEU:O	2.20	0.41
1:J:175:LEU:HD11	1:J:198:LEU:HB3	2.01	0.41
2:C:138:LEU:HD13	2:C:138:LEU:C	2.41	0.41
1:G:205:ILE:HG22	1:G:235:ARG:HB2	2.03	0.41
1:G:274:ARG:HB2	1:G:320:LEU:CD1	2.50	0.41
1:G:403:ASP:OD1	1:G:405:GLU:HB2	2.20	0.41
1:G:457:ALA:O	1:G:460:PHE:HB3	2.20	0.41
1:H:292:GLU:CD	1:H:292:GLU:N	2.71	0.41
2:L:129:MET:HE3	2:L:131:ALA:N	2.35	0.41
1:B:194:VAL:O	1:B:198:LEU:HG	2.20	0.41
1:H:446:HIS:HA	1:H:447:PRO:HA	1.81	0.41
1:J:37:ALA:O	1:J:114:LEU:HD12	2.19	0.41
1:G:208:MET:HB3	1:G:209:PRO:CD	2.51	0.41
1:G:364:THR:OG1	1:G:367:GLU:HG3	2.20	0.41
1:J:278:THR:HG21	1:J:296:ILE:HG13	2.01	0.41
1:K:118:PHE:O	1:K:129:VAL:HG13	2.20	0.41
1:A:389:LEU:HD21	1:B:98:LYS:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ARG:CG	1:B:128:GLU:HB3	2.51	0.41
1:E:446:HIS:HA	1:E:447:PRO:HA	1.86	0.41
1:H:7:MET:HE3	1:H:9:THR:HG22	2.03	0.41
1:J:235:ARG:HH22	1:J:261:GLU:CD	2.24	0.41
1:J:418:GLN:O	1:J:422:LEU:HG	2.21	0.41
1:A:137:ARG:HG3	1:A:137:ARG:NH1	2.36	0.41
1:D:124:PRO:O	1:D:125:LYS:HD3	2.21	0.41
1:D:145:LEU:HD12	1:D:296:ILE:HD13	2.02	0.41
1:K:446:HIS:HA	1:K:447:PRO:HA	1.90	0.41
1:A:126:GLU:HA	1:A:139:GLY:HA2	2.03	0.41
1:A:175:LEU:CD1	1:A:198:LEU:HB3	2.51	0.41
1:E:124:PRO:C	1:E:125:LYS:HG3	2.41	0.41
1:E:228:GLU:HA	1:E:232:ILE:O	2.21	0.41
1:G:12:LEU:HD11	1:G:144:ILE:HG13	2.02	0.41
1:G:86:LYS:HD2	1:G:86:LYS:HA	1.90	0.41
1:G:304:THR:HG23	1:G:309:VAL:O	2.21	0.41
1:H:149:SER:HA	1:H:277:ARG:HG3	2.03	0.41
1:B:274:ARG:HB2	1:B:320:LEU:HD13	2.02	0.41
1:H:27:ARG:NE	1:H:30:GLN:OE1	2.53	0.40
1:J:316:ALA:O	1:J:317:ARG:HB3	2.19	0.40
1:G:122:VAL:CG2	1:G:128:GLU:HB2	2.52	0.40
1:G:281:LEU:HB3	1:G:283:LEU:HG	2.04	0.40
1:J:291:ASP:OD2	1:J:295:PHE:HB2	2.21	0.40
1:B:366:GLU:HG2	4:B:1534:HOH:O	2.21	0.40
1:D:284:GLU:HG2	1:D:285:LYS:HG3	2.04	0.40
1:E:373:TYR:HD2	1:E:403:ASP:OD2	2.04	0.40
1:G:233:ARG:NH1	4:G:4581:HOH:O	2.47	0.40
2:I:144:ILE:CD1	2:I:167:ALA:HB2	2.49	0.40
1:K:422:LEU:HD22	1:K:450:SER:HA	2.02	0.40
1:A:180:LEU:HB2	1:A:265:VAL:HG11	2.04	0.40
1:E:193:GLN:O	1:E:197:ARG:HG3	2.22	0.40
1:A:26:ILE:O	1:A:30:GLN:HG3	2.21	0.40
1:A:127:VAL:HG12	1:A:128:GLU:N	2.37	0.40
3:A:8482:FAD:H9	3:A:8482:FAD:H1'1	1.89	0.40
1:B:212:LEU:N	1:B:213:PRO:CD	2.83	0.40
1:G:453:LEU:N	1:G:453:LEU:HD12	2.37	0.40
3:K:7482:FAD:H9	3:K:7482:FAD:H1'1	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	458/464 (99%)	443 (97%)	14 (3%)	1 (0%)	47	49
1	B	458/464 (99%)	444 (97%)	14 (3%)	0	100	100
1	D	458/464 (99%)	440 (96%)	17 (4%)	1 (0%)	47	49
1	E	458/464 (99%)	445 (97%)	13 (3%)	0	100	100
1	G	458/464 (99%)	449 (98%)	9 (2%)	0	100	100
1	H	458/464 (99%)	449 (98%)	9 (2%)	0	100	100
1	J	458/464 (99%)	434 (95%)	24 (5%)	0	100	100
1	K	458/464 (99%)	433 (94%)	23 (5%)	2 (0%)	34	32
2	C	38/41 (93%)	35 (92%)	3 (8%)	0	100	100
2	F	38/41 (93%)	34 (90%)	3 (8%)	1 (3%)	5	2
2	I	38/41 (93%)	35 (92%)	3 (8%)	0	100	100
2	L	38/41 (93%)	30 (79%)	8 (21%)	0	100	100
All	All	3816/3876 (98%)	3671 (96%)	140 (4%)	5 (0%)	51	54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	GLU
1	D	284	GLU
1	K	279	GLU
1	K	148	GLY
2	F	153	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	342/349 (98%)	338 (99%)	4 (1%)	71	77
1	B	339/349 (97%)	334 (98%)	5 (2%)	65	71
1	D	343/349 (98%)	335 (98%)	8 (2%)	50	55
1	E	341/349 (98%)	337 (99%)	4 (1%)	71	77
1	G	342/349 (98%)	338 (99%)	4 (1%)	71	77
1	H	339/349 (97%)	333 (98%)	6 (2%)	59	65
1	J	342/349 (98%)	336 (98%)	6 (2%)	59	65
1	K	339/349 (97%)	336 (99%)	3 (1%)	78	84
2	C	28/31 (90%)	26 (93%)	2 (7%)	14	11
2	F	28/31 (90%)	26 (93%)	2 (7%)	14	11
2	I	28/31 (90%)	25 (89%)	3 (11%)	6	3
2	L	28/31 (90%)	25 (89%)	3 (11%)	6	3
All	All	2839/2916 (97%)	2789 (98%)	50 (2%)	59	65

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LYS
1	A	98	LYS
1	A	227	LEU
1	A	374	LYS
1	B	56	LYS
1	B	106	LEU
1	B	233	ARG
1	B	261	GLU
1	B	453	LEU
2	C	130	LEU
2	C	155	LEU
1	D	56	LYS
1	D	98	LYS
1	D	120	ARG
1	D	227	LEU
1	D	233	ARG
1	D	370	ARG
1	D	395	GLU
1	D	453	LEU

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Mol	Chain	Res	Type
1	E	56	LYS
1	E	233	ARG
1	E	284	GLU
1	E	453	LEU
2	F	129	MET
2	F	155	LEU
1	G	56	LYS
1	G	227	LEU
1	G	233	ARG
1	G	374	LYS
1	H	56	LYS
1	H	106	LEU
1	H	120	ARG
1	H	250	LEU
1	H	284	GLU
1	H	453	LEU
2	I	130	LEU
2	I	137	LYS
2	I	155	LEU
1	J	56	LYS
1	J	98	LYS
1	J	108	LYS
1	J	227	LEU
1	J	370	ARG
1	J	374	LYS
1	K	56	LYS
1	K	214	GLN
1	K	233	ARG
2	L	129	MET
2	L	147	GLU
2	L	155	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	214	GLN
1	B	418	GLN
1	D	418	GLN
1	E	214	GLN
1	E	418	GLN
1	G	418	GLN
1	H	214	GLN

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Mol	Chain	Res	Type
1	H	418	GLN
1	J	23	HIS
1	J	30	GLN
1	K	214	GLN
1	K	418	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
3	FAD	H	5482	-	53,58,58	1.86	16 (30%)	68,89,89	1.21	7 (10%)
3	FAD	J	6482	-	53,58,58	1.86	16 (30%)	68,89,89	1.27	10 (14%)
3	FAD	G	4482	-	53,58,58	1.84	17 (32%)	68,89,89	1.26	8 (11%)
3	FAD	A	8482	-	53,58,58	1.87	14 (26%)	68,89,89	1.22	7 (10%)
3	FAD	D	2482	-	53,58,58	1.84	15 (28%)	68,89,89	1.26	9 (13%)
3	FAD	B	1482	-	53,58,58	1.82	14 (26%)	68,89,89	1.23	8 (11%)
3	FAD	K	7482	-	53,58,58	1.89	16 (30%)	68,89,89	1.21	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FAD	E	3482	-	53,58,58	1.82	15 (28%)	68,89,89	1.24	8 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	H	5482	-	-	2/30/50/50	0/6/6/6
3	FAD	J	6482	-	-	2/30/50/50	0/6/6/6
3	FAD	G	4482	-	-	3/30/50/50	0/6/6/6
3	FAD	A	8482	-	-	2/30/50/50	0/6/6/6
3	FAD	D	2482	-	-	2/30/50/50	0/6/6/6
3	FAD	B	1482	-	-	2/30/50/50	0/6/6/6
3	FAD	K	7482	-	-	3/30/50/50	0/6/6/6
3	FAD	E	3482	-	-	2/30/50/50	0/6/6/6

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	7482	FAD	O4B-C1B	6.00	1.49	1.41
3	A	8482	FAD	O4B-C1B	5.40	1.48	1.41
3	B	1482	FAD	O4B-C1B	5.15	1.48	1.41
3	J	6482	FAD	O4B-C1B	5.09	1.48	1.41
3	E	3482	FAD	O4B-C1B	4.71	1.47	1.41
3	G	4482	FAD	O4B-C1B	4.60	1.47	1.41
3	H	5482	FAD	O4B-C1B	4.55	1.47	1.41
3	D	2482	FAD	O4B-C1B	4.49	1.47	1.41
3	E	3482	FAD	PA-O2A	-4.34	1.34	1.55
3	H	5482	FAD	C1'-C2'	4.29	1.58	1.52
3	H	5482	FAD	PA-O2A	-4.20	1.35	1.55
3	A	8482	FAD	PA-O2A	-4.18	1.35	1.55
3	G	4482	FAD	PA-O2A	-4.10	1.36	1.55
3	B	1482	FAD	PA-O2A	-4.07	1.36	1.55
3	K	7482	FAD	PA-O2A	-4.06	1.36	1.55
3	J	6482	FAD	PA-O2A	-3.99	1.36	1.55
3	E	3482	FAD	O5'-C5'	3.98	1.60	1.44
3	A	8482	FAD	O5'-C5'	3.96	1.60	1.44
3	D	2482	FAD	C1'-C2'	3.95	1.58	1.52
3	H	5482	FAD	O5'-C5'	3.92	1.59	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	7482	FAD	O5'-C5'	3.89	1.59	1.44
3	D	2482	FAD	PA-O2A	-3.85	1.37	1.55
3	G	4482	FAD	C1'-C2'	3.83	1.58	1.52
3	J	6482	FAD	C1'-C2'	3.81	1.58	1.52
3	G	4482	FAD	O5'-C5'	3.81	1.59	1.44
3	B	1482	FAD	O5'-C5'	3.76	1.59	1.44
3	A	8482	FAD	C1'-C2'	3.73	1.57	1.52
3	E	3482	FAD	C1'-C2'	3.67	1.57	1.52
3	D	2482	FAD	O5'-C5'	3.67	1.58	1.44
3	J	6482	FAD	P-O2P	-3.59	1.38	1.55
3	D	2482	FAD	P-O2P	-3.52	1.38	1.55
3	J	6482	FAD	O5'-C5'	3.51	1.58	1.44
3	A	8482	FAD	P-O2P	-3.46	1.39	1.55
3	K	7482	FAD	P-O2P	-3.41	1.39	1.55
3	G	4482	FAD	P-O2P	-3.40	1.39	1.55
3	B	1482	FAD	P-O2P	-3.37	1.39	1.55
3	H	5482	FAD	P-O2P	-3.32	1.39	1.55
3	H	5482	FAD	C4X-N5	3.29	1.37	1.30
3	E	3482	FAD	P-O2P	-3.25	1.40	1.55
3	K	7482	FAD	C4X-N5	3.22	1.37	1.30
3	J	6482	FAD	O2-C2	-3.05	1.18	1.24
3	H	5482	FAD	O2-C2	-3.04	1.18	1.24
3	J	6482	FAD	C4X-N5	2.96	1.36	1.30
3	G	4482	FAD	C4X-N5	2.95	1.36	1.30
3	D	2482	FAD	O2-C2	-2.93	1.18	1.24
3	A	8482	FAD	C8-C7	2.86	1.48	1.40
3	B	1482	FAD	C1'-C2'	2.85	1.56	1.52
3	H	5482	FAD	C2B-C1B	-2.85	1.49	1.53
3	B	1482	FAD	C4X-N5	2.84	1.36	1.30
3	B	1482	FAD	C8-C7	2.80	1.47	1.40
3	G	4482	FAD	C8-C7	2.78	1.47	1.40
3	K	7482	FAD	C8-C7	2.78	1.47	1.40
3	E	3482	FAD	C4A-N3A	2.78	1.39	1.35
3	K	7482	FAD	O2-C2	-2.78	1.19	1.24
3	A	8482	FAD	C4X-N5	2.76	1.36	1.30
3	D	2482	FAD	C4X-N5	2.74	1.36	1.30
3	E	3482	FAD	C4X-N5	2.73	1.36	1.30
3	E	3482	FAD	C8-C7	2.72	1.47	1.40
3	D	2482	FAD	C8-C7	2.71	1.47	1.40
3	A	8482	FAD	O2-C2	-2.65	1.19	1.24
3	K	7482	FAD	C9A-C5X	2.64	1.45	1.41
3	J	6482	FAD	C9A-C5X	2.64	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	4482	FAD	O2-C2	-2.59	1.19	1.24
3	H	5482	FAD	C8-C7	2.58	1.47	1.40
3	A	8482	FAD	C4A-N3A	2.56	1.39	1.35
3	E	3482	FAD	C2B-C1B	-2.56	1.49	1.53
3	K	7482	FAD	C2A-N3A	2.55	1.36	1.32
3	J	6482	FAD	C8-C7	2.53	1.47	1.40
3	A	8482	FAD	C2B-C1B	-2.53	1.49	1.53
3	J	6482	FAD	C4A-N3A	2.53	1.39	1.35
3	G	4482	FAD	C4A-N3A	2.53	1.39	1.35
3	K	7482	FAD	C1'-C2'	2.52	1.56	1.52
3	D	2482	FAD	C9A-C5X	2.51	1.45	1.41
3	D	2482	FAD	C4A-N3A	2.50	1.39	1.35
3	D	2482	FAD	C2A-N3A	2.49	1.36	1.32
3	H	5482	FAD	C9A-C5X	2.43	1.45	1.41
3	G	4482	FAD	C9A-N10	2.42	1.45	1.41
3	B	1482	FAD	C9A-N10	2.42	1.45	1.41
3	B	1482	FAD	C2A-N3A	2.38	1.35	1.32
3	B	1482	FAD	O2-C2	-2.38	1.19	1.24
3	G	4482	FAD	C2A-N3A	2.34	1.35	1.32
3	B	1482	FAD	C2B-C1B	-2.33	1.50	1.53
3	G	4482	FAD	C2B-C1B	-2.30	1.50	1.53
3	K	7482	FAD	C2B-C1B	-2.29	1.50	1.53
3	A	8482	FAD	C9A-N10	2.28	1.45	1.41
3	H	5482	FAD	C9A-N10	2.28	1.45	1.41
3	K	7482	FAD	C4A-N3A	2.28	1.38	1.35
3	J	6482	FAD	C2B-C1B	-2.28	1.50	1.53
3	E	3482	FAD	C9A-C5X	2.27	1.45	1.41
3	D	2482	FAD	C6-C5X	2.27	1.43	1.40
3	B	1482	FAD	C4A-N3A	2.25	1.38	1.35
3	J	6482	FAD	C10-N1	2.25	1.37	1.33
3	B	1482	FAD	C10-N1	2.25	1.37	1.33
3	A	8482	FAD	C2A-N3A	2.24	1.35	1.32
3	G	4482	FAD	C9A-C5X	2.20	1.44	1.41
3	J	6482	FAD	C2A-N3A	2.19	1.35	1.32
3	G	4482	FAD	C10-N1	2.18	1.37	1.33
3	K	7482	FAD	C2-N3	2.18	1.44	1.39
3	K	7482	FAD	C10-N1	2.18	1.37	1.33
3	E	3482	FAD	C6-C5X	2.18	1.43	1.40
3	E	3482	FAD	O2-C2	-2.17	1.20	1.24
3	B	1482	FAD	C2-N3	2.16	1.44	1.39
3	A	8482	FAD	C6-C5X	2.16	1.43	1.40
3	H	5482	FAD	C4A-N3A	2.15	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	6482	FAD	P-O5'	-2.13	1.50	1.59
3	K	7482	FAD	C6-C5X	2.13	1.43	1.40
3	H	5482	FAD	C2A-N3A	2.12	1.35	1.32
3	E	3482	FAD	C2A-N3A	2.12	1.35	1.32
3	D	2482	FAD	P-O5'	-2.11	1.50	1.59
3	E	3482	FAD	C9A-N10	2.11	1.44	1.41
3	H	5482	FAD	C10-N1	2.10	1.37	1.33
3	A	8482	FAD	C9A-C5X	2.10	1.44	1.41
3	G	4482	FAD	C2A-N1A	2.10	1.37	1.33
3	E	3482	FAD	C2-N3	2.09	1.43	1.39
3	J	6482	FAD	C9A-N10	2.08	1.44	1.41
3	H	5482	FAD	P-O5'	-2.08	1.50	1.59
3	H	5482	FAD	C2A-N1A	2.07	1.37	1.33
3	J	6482	FAD	C2-N3	2.07	1.43	1.39
3	D	2482	FAD	C2A-N1A	2.05	1.37	1.33
3	K	7482	FAD	C9A-N10	2.05	1.44	1.41
3	D	2482	FAD	C2-N3	2.04	1.43	1.39
3	G	4482	FAD	C2-N3	2.03	1.43	1.39
3	G	4482	FAD	O4'-C4'	2.02	1.47	1.43

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2482	FAD	O4B-C1B-C2B	-3.77	101.42	106.93
3	E	3482	FAD	O4B-C1B-C2B	-3.26	102.16	106.93
3	J	6482	FAD	O5B-PA-O1A	-3.16	96.73	109.07
3	B	1482	FAD	O4B-C1B-C2B	-3.11	102.38	106.93
3	B	1482	FAD	O5B-PA-O1A	-3.05	97.16	109.07
3	K	7482	FAD	O5B-PA-O1A	-3.02	97.25	109.07
3	D	2482	FAD	O5B-PA-O1A	-2.97	97.45	109.07
3	A	8482	FAD	O4B-C1B-C2B	-2.93	102.65	106.93
3	G	4482	FAD	O5B-PA-O1A	-2.92	97.64	109.07
3	G	4482	FAD	O4B-C1B-C2B	-2.89	102.70	106.93
3	E	3482	FAD	O5B-PA-O1A	-2.78	98.19	109.07
3	H	5482	FAD	C5A-C6A-N6A	2.69	124.43	120.35
3	H	5482	FAD	O5B-PA-O1A	-2.67	98.65	109.07
3	A	8482	FAD	O5B-PA-O1A	-2.58	98.97	109.07
3	J	6482	FAD	C5'-C4'-C3'	-2.56	107.26	112.20
3	A	8482	FAD	C5A-C6A-N6A	2.55	124.23	120.35
3	J	6482	FAD	C2A-N1A-C6A	2.55	123.12	118.75
3	H	5482	FAD	O4B-C1B-C2B	-2.52	103.24	106.93
3	D	2482	FAD	C5'-C4'-C3'	-2.51	107.36	112.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	3482	FAD	C5'-C4'-C3'	-2.49	107.39	112.20
3	K	7482	FAD	O4B-C1B-C2B	-2.49	103.28	106.93
3	A	8482	FAD	C2A-N1A-C6A	2.49	123.02	118.75
3	H	5482	FAD	C5A-C6A-N1A	-2.47	114.75	120.35
3	G	4482	FAD	C2A-N1A-C6A	2.46	122.96	118.75
3	H	5482	FAD	C2A-N1A-C6A	2.45	122.95	118.75
3	E	3482	FAD	C2A-N1A-C6A	2.44	122.93	118.75
3	G	4482	FAD	C5A-C6A-N6A	2.44	124.06	120.35
3	A	8482	FAD	C5A-C6A-N1A	-2.42	114.87	120.35
3	D	2482	FAD	C4-N3-C2	-2.42	121.17	125.64
3	J	6482	FAD	C5A-C6A-N1A	-2.41	114.88	120.35
3	J	6482	FAD	O4B-C1B-C2B	-2.41	103.40	106.93
3	G	4482	FAD	C5A-C6A-N1A	-2.41	114.90	120.35
3	B	1482	FAD	C5A-C6A-N1A	-2.34	115.05	120.35
3	G	4482	FAD	C5'-C4'-C3'	-2.33	107.70	112.20
3	E	3482	FAD	C5A-C6A-N1A	-2.33	115.07	120.35
3	K	7482	FAD	C5A-C6A-N1A	-2.31	115.11	120.35
3	G	4482	FAD	C4-N3-C2	-2.30	121.39	125.64
3	K	7482	FAD	C2A-N1A-C6A	2.30	122.69	118.75
3	J	6482	FAD	C4-N3-C2	-2.30	121.40	125.64
3	D	2482	FAD	C5A-C6A-N1A	-2.29	115.16	120.35
3	D	2482	FAD	C5A-C6A-N6A	2.28	123.81	120.35
3	J	6482	FAD	C5A-C6A-N6A	2.27	123.81	120.35
3	K	7482	FAD	C5A-C6A-N6A	2.27	123.80	120.35
3	E	3482	FAD	C5A-C6A-N6A	2.24	123.76	120.35
3	B	1482	FAD	C5'-C4'-C3'	-2.23	107.90	112.20
3	B	1482	FAD	C5A-C6A-N6A	2.21	123.71	120.35
3	B	1482	FAD	C2A-N1A-C6A	2.20	122.52	118.75
3	A	8482	FAD	C4-N3-C2	-2.19	121.59	125.64
3	A	8482	FAD	C5'-C4'-C3'	-2.18	107.99	112.20
3	H	5482	FAD	C4-N3-C2	-2.16	121.64	125.64
3	D	2482	FAD	C2A-N1A-C6A	2.16	122.44	118.75
3	K	7482	FAD	C5'-C4'-C3'	-2.15	108.06	112.20
3	B	1482	FAD	C4-N3-C2	-2.14	121.69	125.64
3	E	3482	FAD	C4-N3-C2	-2.12	121.72	125.64
3	J	6482	FAD	C4A-C5A-N7A	2.11	111.60	109.40
3	B	1482	FAD	C5X-C9A-N10	-2.10	115.78	117.95
3	K	7482	FAD	C4X-C10-N10	2.09	119.53	116.48
3	D	2482	FAD	C4X-C10-N10	2.08	119.53	116.48
3	H	5482	FAD	C4X-C10-N10	2.08	119.53	116.48
3	K	7482	FAD	C4-N3-C2	-2.08	121.81	125.64
3	D	2482	FAD	C10-N1-C2	2.06	121.02	116.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	3482	FAD	C4X-C10-N10	2.05	119.48	116.48
3	J	6482	FAD	C4X-C10-N10	2.04	119.47	116.48
3	G	4482	FAD	C10-N1-C2	2.04	120.98	116.90
3	J	6482	FAD	C10-N1-C2	2.01	120.92	116.90

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	8482	FAD	PA-O3P-P-O5'
3	B	1482	FAD	PA-O3P-P-O5'
3	D	2482	FAD	PA-O3P-P-O5'
3	E	3482	FAD	PA-O3P-P-O5'
3	G	4482	FAD	PA-O3P-P-O5'
3	H	5482	FAD	PA-O3P-P-O5'
3	J	6482	FAD	PA-O3P-P-O5'
3	K	7482	FAD	PA-O3P-P-O5'
3	G	4482	FAD	O4B-C4B-C5B-O5B
3	G	4482	FAD	P-O3P-PA-O1A
3	D	2482	FAD	O4B-C4B-C5B-O5B
3	B	1482	FAD	O4B-C4B-C5B-O5B
3	H	5482	FAD	O4B-C4B-C5B-O5B
3	E	3482	FAD	O4B-C4B-C5B-O5B
3	K	7482	FAD	O4B-C4B-C5B-O5B
3	K	7482	FAD	P-O3P-PA-O1A
3	A	8482	FAD	O4B-C4B-C5B-O5B
3	J	6482	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

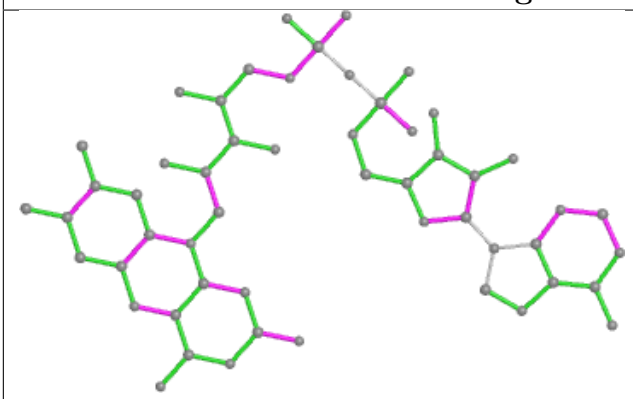
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	4482	FAD	1	0
3	A	8482	FAD	2	0
3	D	2482	FAD	1	0
3	K	7482	FAD	3	0

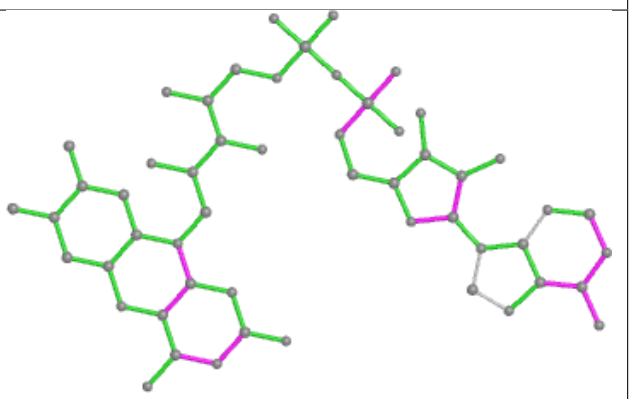
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

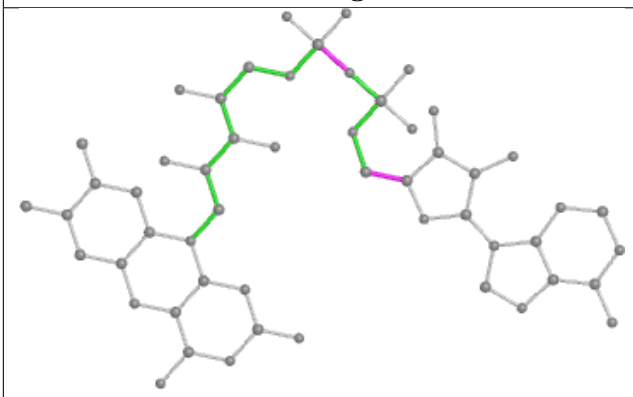
Ligand FAD H 5482



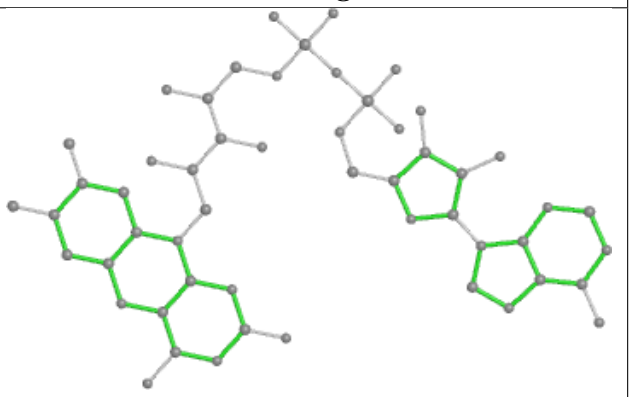
Bond lengths



Bond angles

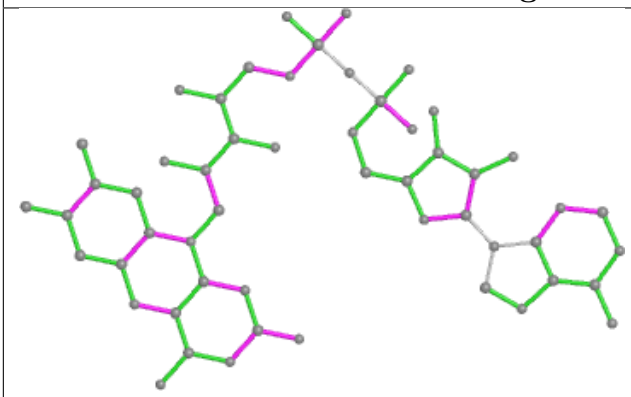


Torsions

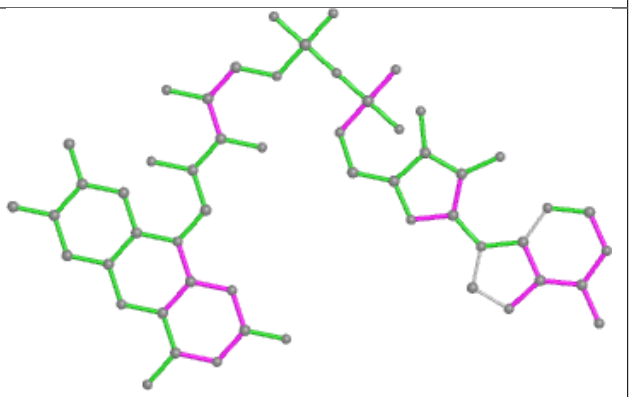


Rings

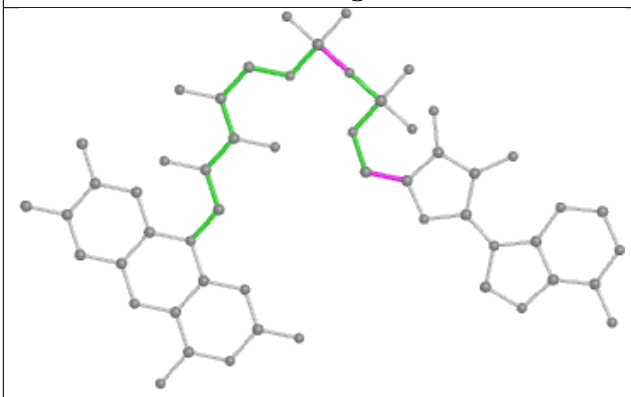
Ligand FAD J 6482



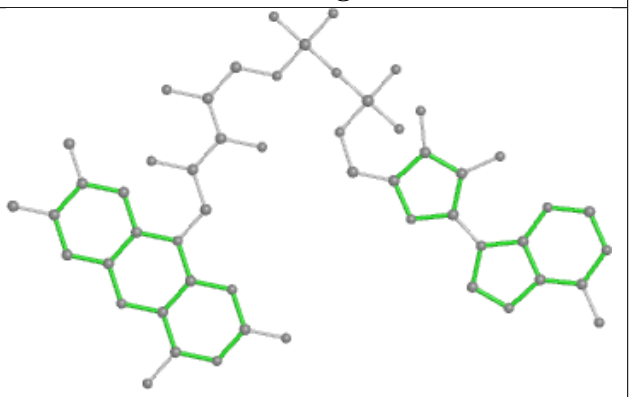
Bond lengths



Bond angles

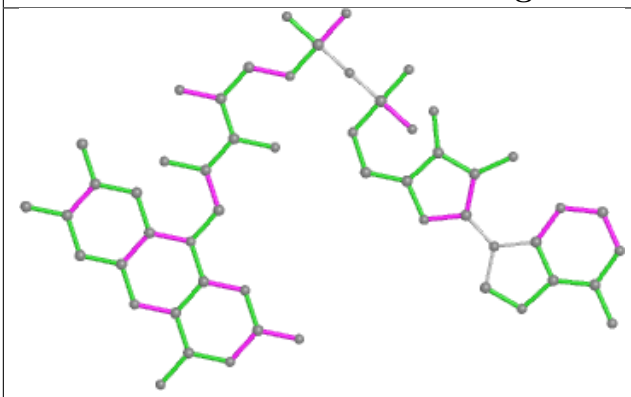


Torsions

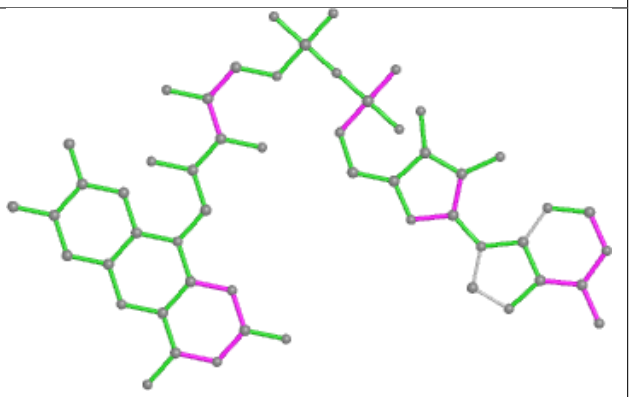


Rings

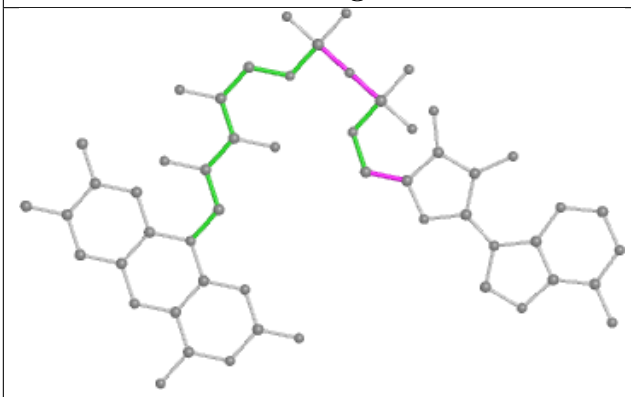
Ligand FAD G 4482



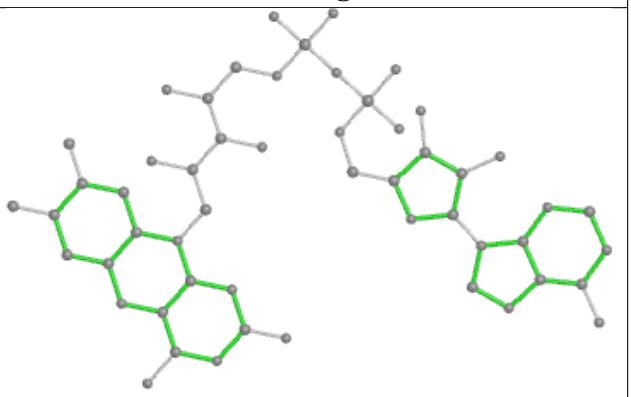
Bond lengths



Bond angles

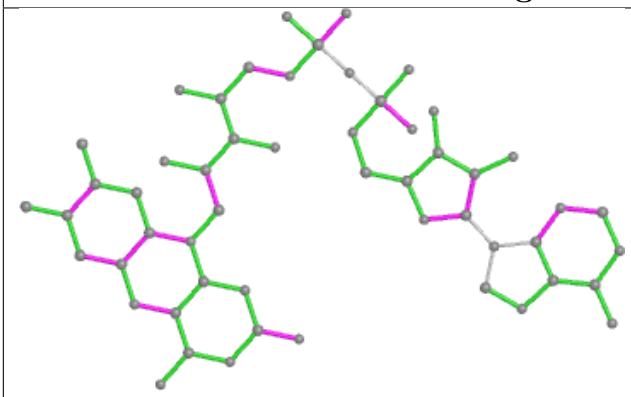


Torsions

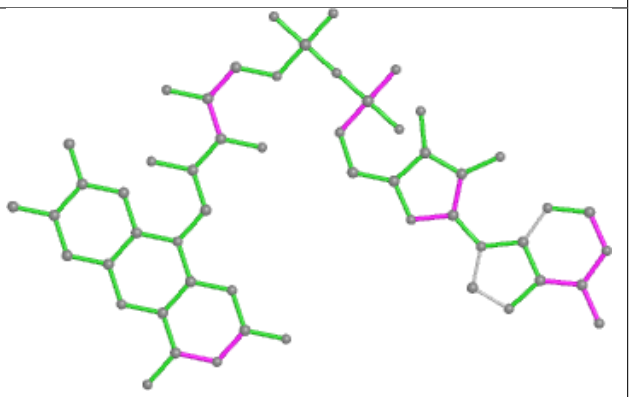


Rings

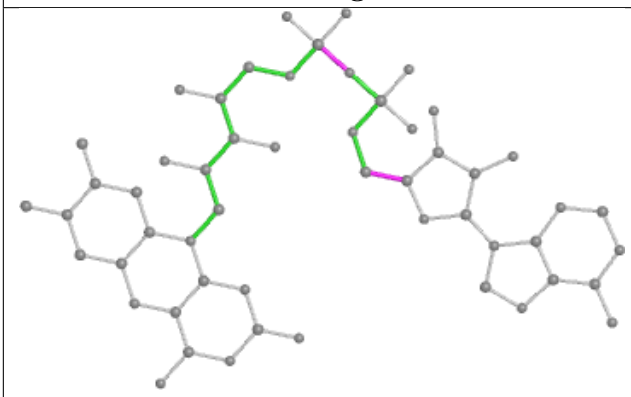
Ligand FAD A 8482



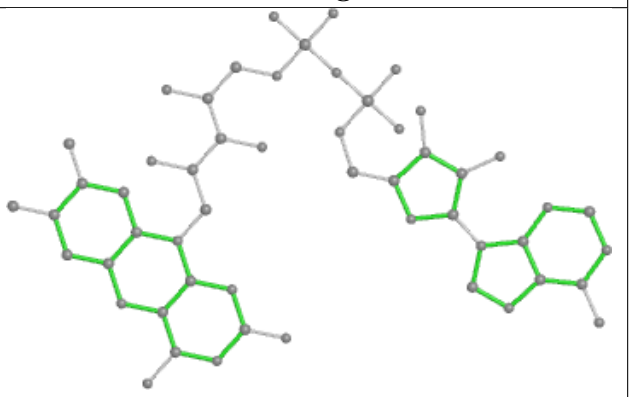
Bond lengths



Bond angles

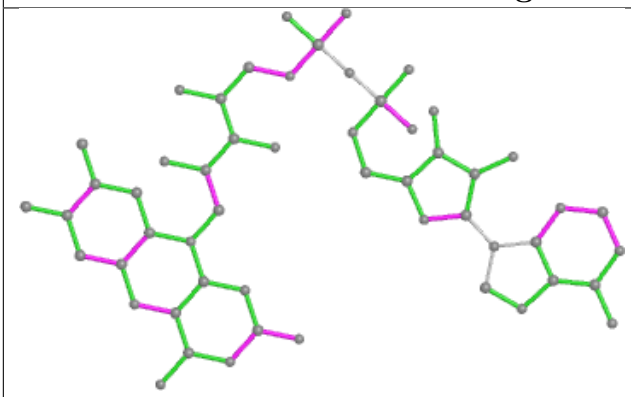


Torsions



Rings

Ligand FAD D 2482



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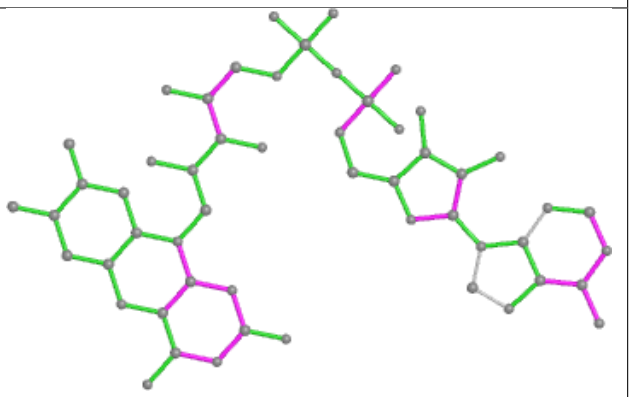
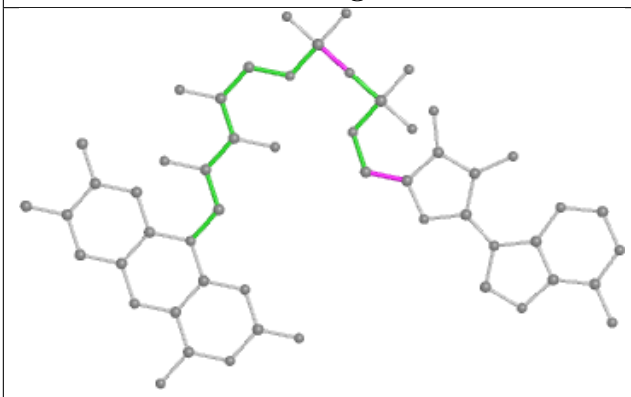
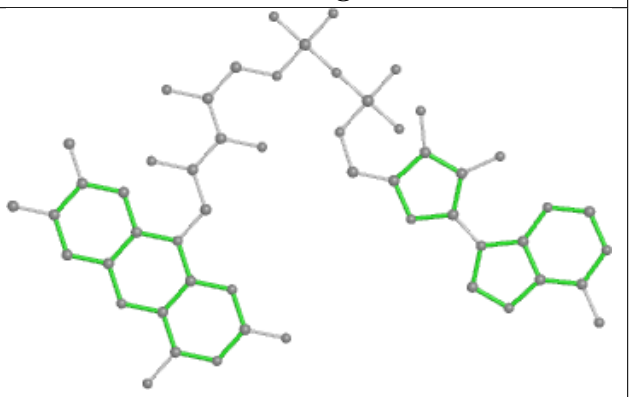


Bond angles

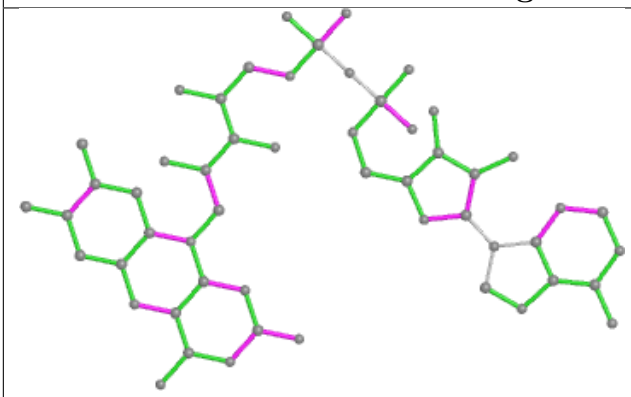


Torsions



Rings

Ligand FAD B 1482



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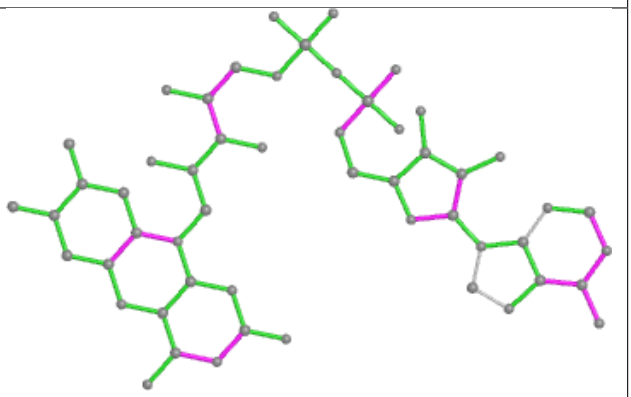
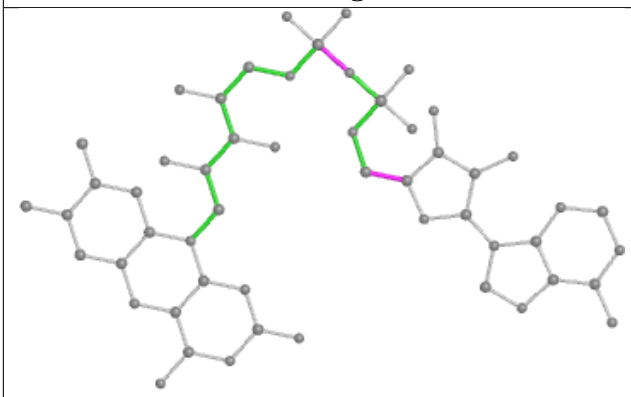
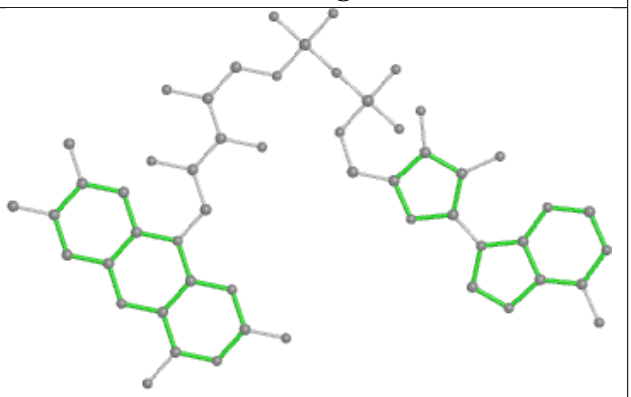


Bond angles

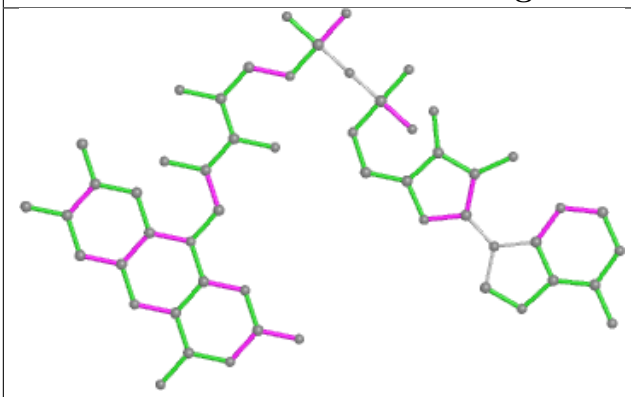


Torsions



Rings

Ligand FAD K 7482



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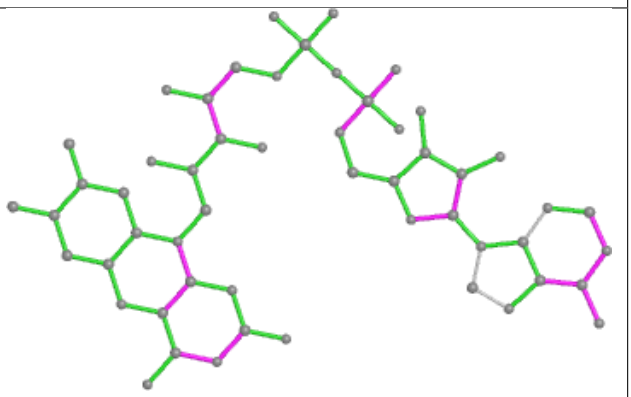
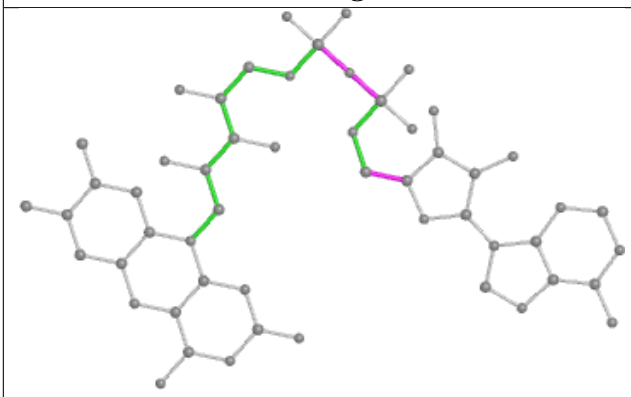


Bond angles



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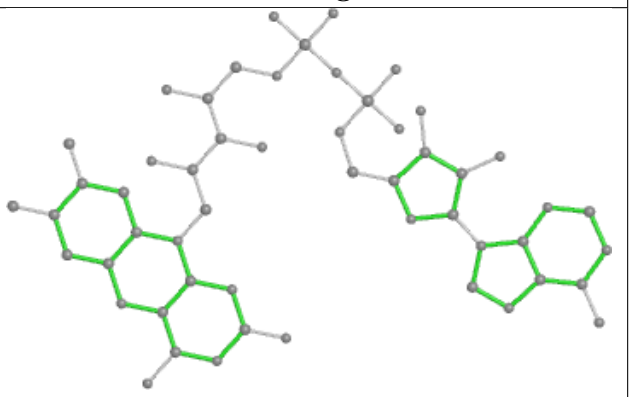
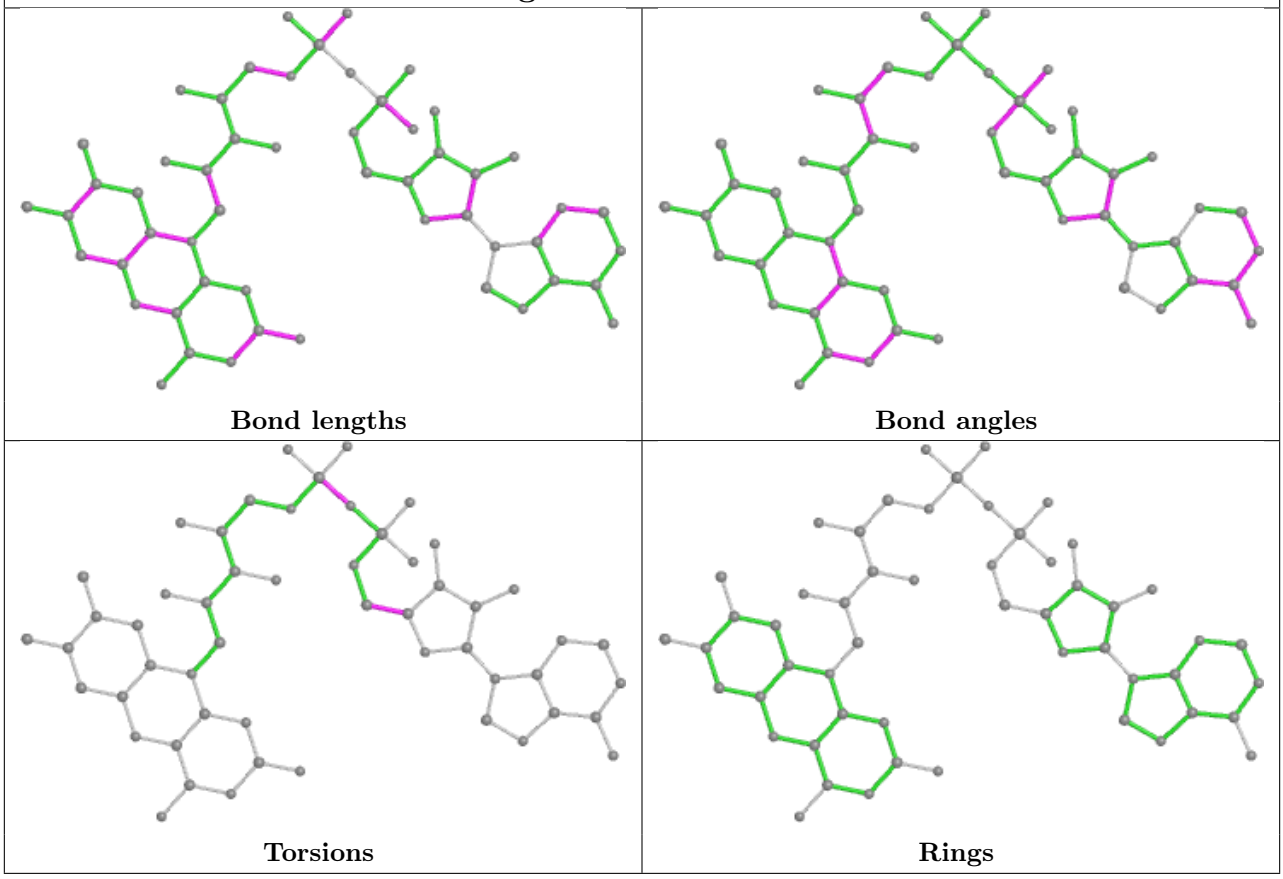


Rings

Ligand FAD E 3482



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	460/464 (99%)	0.11	20 (4%)	35	41	25, 38, 63, 79	0
1	B	460/464 (99%)	-0.09	4 (0%)	84	86	24, 38, 55, 69	0
1	D	460/464 (99%)	-0.06	10 (2%)	62	66	23, 34, 62, 80	0
1	E	460/464 (99%)	0.10	19 (4%)	37	43	22, 38, 70, 85	0
1	G	460/464 (99%)	-0.06	9 (1%)	65	69	24, 36, 61, 76	0
1	H	460/464 (99%)	-0.09	7 (1%)	73	77	24, 35, 55, 73	0
1	J	460/464 (99%)	0.25	36 (7%)	13	17	24, 40, 77, 99	0
1	K	460/464 (99%)	0.65	61 (13%)	3	4	26, 49, 87, 101	0
2	C	40/41 (97%)	0.94	8 (20%)	1	1	33, 55, 74, 76	0
2	F	40/41 (97%)	2.86	26 (65%)	0	0	54, 74, 86, 90	0
2	I	40/41 (97%)	2.69	21 (52%)	0	0	45, 76, 90, 91	0
2	L	40/41 (97%)	2.45	24 (60%)	0	0	47, 77, 87, 88	0
All	All	3840/3876 (99%)	0.19	245 (6%)	19	24	22, 38, 73, 101	0

All (245) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	155	LEU	15.1
2	I	129	MET	8.9
2	F	155	LEU	7.9
1	K	120	ARG	6.8
2	I	130	LEU	6.8
1	K	137	ARG	6.6
2	L	142	LEU	6.5
1	K	293	ARG	6.3
1	J	122	VAL	6.2
2	F	129	MET	6.2
2	L	155	LEU	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	394	ALA	5.7
2	F	165	ALA	5.6
1	A	257	GLY	5.6
2	F	163	VAL	5.5
1	K	136	GLU	5.4
2	C	155	LEU	5.3
1	K	127	VAL	5.3
1	K	135	GLY	5.3
2	I	166	TYR	5.3
1	K	123	GLY	5.2
2	F	168	GLU	5.1
1	E	7	MET	4.9
1	E	394	ALA	4.9
2	F	166	TYR	4.9
2	L	166	TYR	4.9
2	L	129	MET	4.9
1	K	7	MET	4.9
2	I	142	LEU	4.8
1	H	394	ALA	4.8
2	F	144	ILE	4.7
2	F	167	ALA	4.7
1	K	121	LEU	4.7
1	J	8	LYS	4.6
1	K	254	LEU	4.6
1	J	7	MET	4.5
1	E	122	VAL	4.4
2	I	143	GLY	4.4
2	L	165	ALA	4.3
1	A	122	VAL	4.3
1	J	9	THR	4.3
1	H	257	GLY	4.2
2	L	153	GLY	4.2
1	E	257	GLY	4.2
1	K	122	VAL	4.1
1	K	257	GLY	4.0
1	K	260	GLY	4.0
1	D	284	GLU	4.0
1	K	119	ALA	4.0
2	F	143	GLY	4.0
1	K	10	TYR	3.9
2	C	154	PRO	3.9
1	K	281	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
2	F	138	LEU	3.9
1	J	285	LYS	3.9
1	A	7	MET	3.9
1	K	13	ILE	3.8
2	L	130	LEU	3.8
1	G	394	ALA	3.8
2	L	143	GLY	3.8
2	L	154	PRO	3.8
2	I	167	ALA	3.8
1	K	8	LYS	3.7
1	J	120	ARG	3.7
1	E	9	THR	3.7
2	F	153	GLY	3.6
1	K	207	TYR	3.6
1	K	126	GLU	3.6
1	A	394	ALA	3.6
2	F	156	GLY	3.6
1	J	10	TYR	3.6
2	I	153	GLY	3.6
2	L	144	ILE	3.6
1	K	38	VAL	3.6
1	K	32	GLY	3.5
1	K	155	LYS	3.5
1	D	7	MET	3.5
1	E	286	ALA	3.4
1	K	259	GLU	3.4
1	E	337	ALA	3.4
2	F	149	VAL	3.4
1	K	134	GLY	3.4
1	J	13	ILE	3.4
1	K	141	LYS	3.3
1	A	9	THR	3.3
1	J	12	LEU	3.3
2	C	151	GLY	3.3
2	F	130	LEU	3.3
1	J	136	GLU	3.2
1	J	282	GLY	3.2
1	J	139	GLY	3.2
1	K	282	GLY	3.2
2	F	160	VAL	3.2
1	K	286	ALA	3.2
2	L	167	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
2	L	151	GLY	3.2
1	J	283	LEU	3.2
1	E	241	VAL	3.2
2	C	130	LEU	3.2
2	I	160	VAL	3.2
1	K	256(A)	ALA	3.1
2	L	163	VAL	3.1
2	I	144	ILE	3.1
1	K	289	LYS	3.1
1	K	283	LEU	3.1
2	F	164	ARG	3.1
2	L	152	SER	3.0
1	A	259	GLU	3.0
1	J	394	ALA	3.0
1	K	143	LEU	3.0
2	F	132	VAL	3.0
2	F	151	GLY	3.0
1	J	124	PRO	3.0
1	K	241	VAL	3.0
1	K	9	THR	3.0
1	E	121	LEU	3.0
2	I	163	VAL	2.9
2	I	141	GLU	2.9
2	L	156	GLY	2.9
1	J	126	GLU	2.9
1	E	256(A)	ALA	2.9
2	I	168	GLU	2.9
2	L	141	GLU	2.9
1	J	138	TYR	2.9
1	A	134	GLY	2.9
1	J	393	GLY	2.9
2	L	164	ARG	2.9
1	B	78	ALA	2.9
2	F	147	GLU	2.9
1	E	120	ARG	2.9
1	H	256(B)	GLU	2.9
1	H	256(A)	ALA	2.9
1	J	281	LEU	2.9
2	F	134	ALA	2.8
2	I	154	PRO	2.8
1	J	128	GLU	2.8
1	J	127	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	135	GLY	2.8
1	D	78	ALA	2.8
1	E	8	LYS	2.8
2	I	165	ALA	2.8
1	D	126	GLU	2.8
1	K	292	GLU	2.8
2	I	164	ARG	2.8
2	I	148	GLU	2.7
1	A	136	GLU	2.7
2	L	138	LEU	2.7
1	B	134	GLY	2.7
1	K	140	ALA	2.7
2	L	135	ALA	2.7
1	K	263	VAL	2.7
2	C	152	SER	2.7
1	J	135	GLY	2.7
1	D	136	GLU	2.7
1	K	261	GLU	2.7
1	E	256(B)	GLU	2.6
1	E	292	GLU	2.6
1	G	134	GLY	2.6
1	K	258	GLY	2.6
1	K	128	GLU	2.6
1	E	288	VAL	2.6
1	A	137	ARG	2.6
1	A	292	GLU	2.6
1	H	7	MET	2.6
1	K	124	PRO	2.6
1	G	292	GLU	2.6
1	A	155	LYS	2.6
1	K	338	GLY	2.6
1	E	137	ARG	2.5
1	J	137	ARG	2.5
1	D	9	THR	2.5
1	J	32	GLY	2.5
1	J	293	ARG	2.5
1	K	239	LYS	2.5
1	H	8	LYS	2.5
2	I	152	SER	2.5
1	A	256(A)	ALA	2.5
1	J	141	LYS	2.5
1	K	284	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	297	ARG	2.5
2	I	156	GLY	2.5
2	F	158	VAL	2.5
2	F	133	PRO	2.5
1	G	293	ARG	2.5
1	A	78	ALA	2.5
1	K	129	VAL	2.4
2	F	148	GLU	2.4
2	L	146	ILE	2.4
1	H	78	ALA	2.4
1	K	115	LEU	2.4
1	A	128	GLU	2.4
1	A	256(B)	GLU	2.4
2	I	147	GLU	2.4
2	F	150	PRO	2.4
1	J	114	LEU	2.4
1	J	309	VAL	2.4
1	D	394	ALA	2.4
1	E	279	GLU	2.4
1	K	312	ILE	2.4
1	J	306	VAL	2.4
1	K	256	PRO	2.4
2	L	168	GLU	2.4
1	D	137	ARG	2.4
1	K	182	ILE	2.4
1	K	118	PHE	2.3
1	A	285	LYS	2.3
1	D	122	VAL	2.3
1	K	154	LEU	2.3
1	G	280	GLY	2.3
1	J	292	GLU	2.3
1	A	241	VAL	2.3
1	G	281	LEU	2.2
1	K	285	LYS	2.2
1	J	119	ALA	2.2
1	A	120	ARG	2.2
2	C	153	GLY	2.2
1	K	394	ALA	2.2
2	C	167	ALA	2.2
1	G	122	VAL	2.1
1	K	237	LYS	2.1
2	L	162	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	157	ARG	2.1
1	J	33	LEU	2.1
2	I	151	GLY	2.1
1	G	138	TYR	2.1
1	A	237	LYS	2.1
1	K	278	THR	2.1
1	J	143	LEU	2.1
1	J	142	SER	2.1
1	K	36	LEU	2.1
1	J	140	ALA	2.1
1	D	393	GLY	2.1
1	E	78	ALA	2.0
1	G	129	VAL	2.0
1	J	129	VAL	2.0
2	F	152	SER	2.0
1	K	275	LYS	2.0
2	L	145	PRO	2.0
1	K	139	GLY	2.0
1	K	157	PHE	2.0
1	B	405	GLU	2.0
2	L	147	GLU	2.0
1	K	31	LEU	2.0
1	A	8	LYS	2.0
2	C	149	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

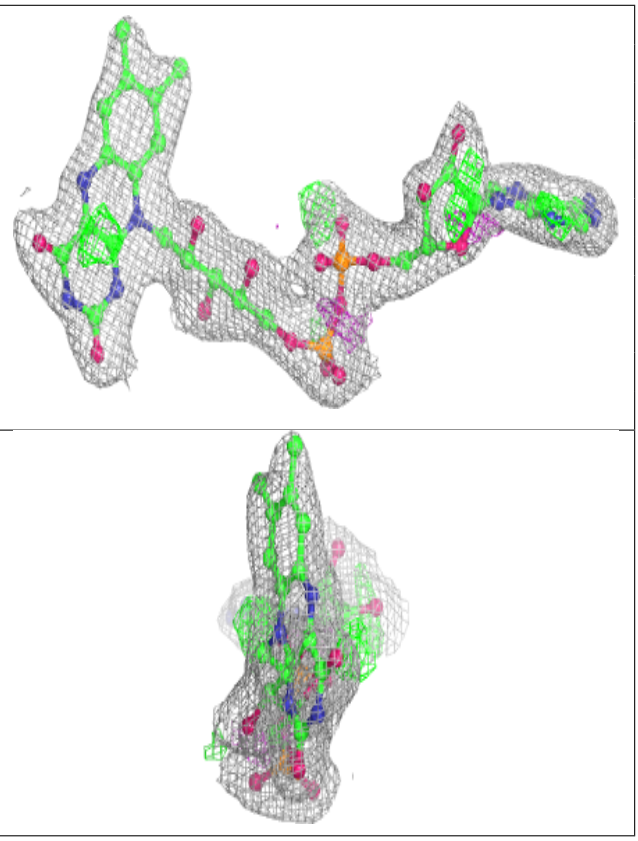
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FAD	K	7482	53/53	0.93	0.13	40,45,56,56	0
3	FAD	J	6482	53/53	0.95	0.11	30,34,40,41	0
3	FAD	B	1482	53/53	0.96	0.11	33,37,43,44	0
3	FAD	G	4482	53/53	0.96	0.10	29,34,42,44	0
3	FAD	A	8482	53/53	0.97	0.12	28,34,40,41	0
3	FAD	H	5482	53/53	0.97	0.13	25,29,32,33	0
3	FAD	D	2482	53/53	0.97	0.11	26,30,40,41	0
3	FAD	E	3482	53/53	0.97	0.13	31,36,43,43	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.

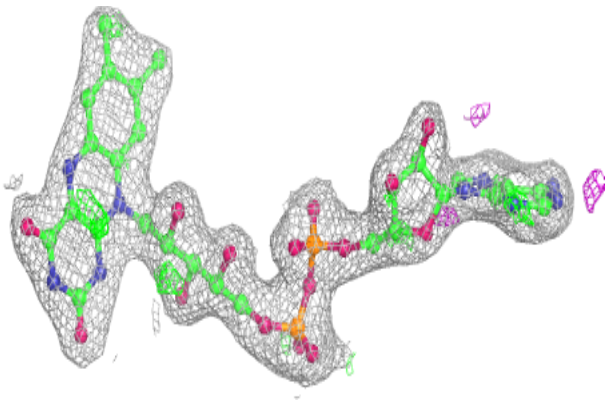
Electron density around FAD K 7482:

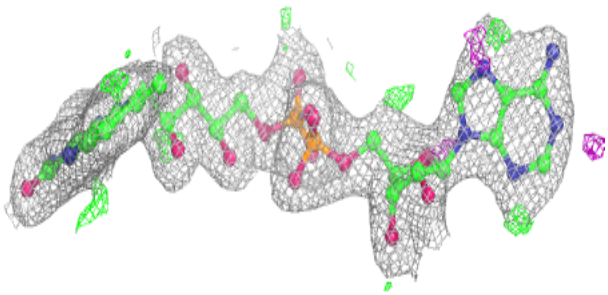
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

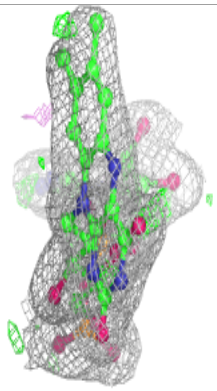


Electron density around FAD J 6482:

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

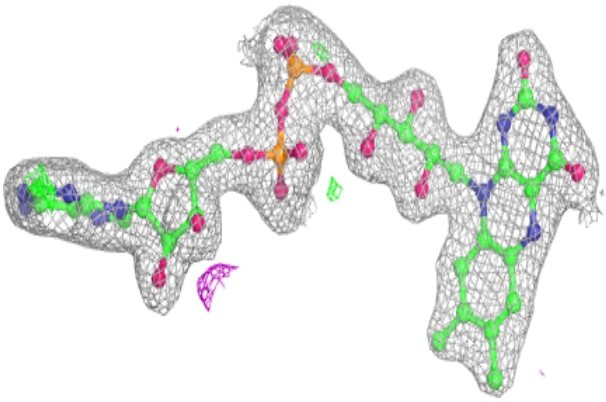


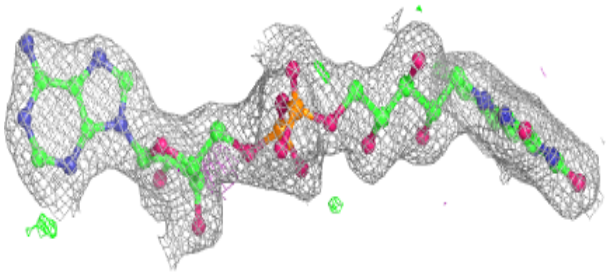


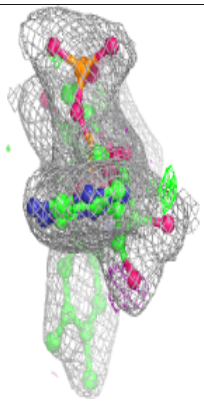


Electron density around FAD B 1482:

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

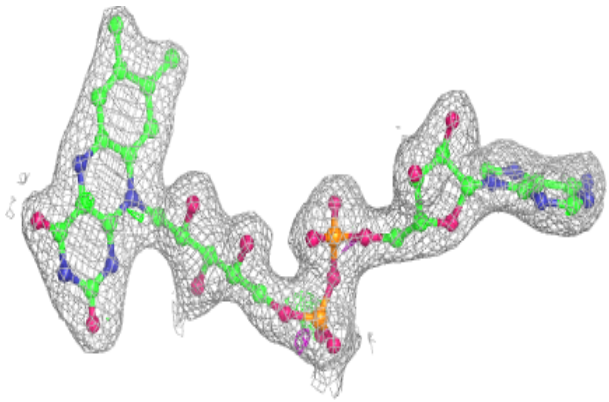


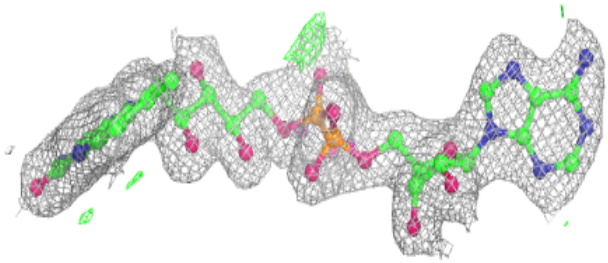


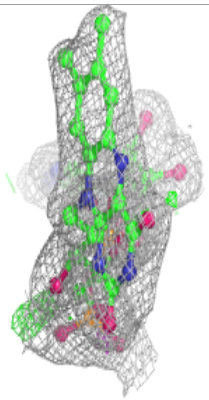


Electron density around FAD G 4482:

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

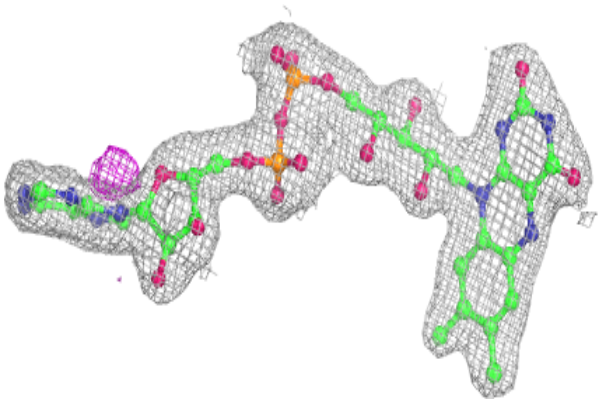


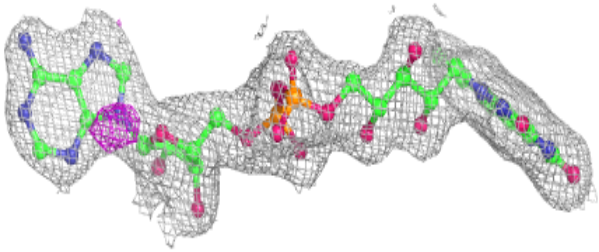


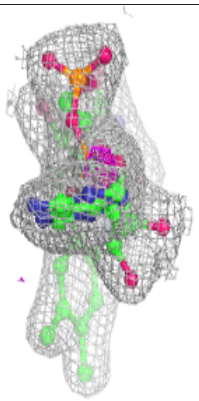


Electron density around FAD A 8482:

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

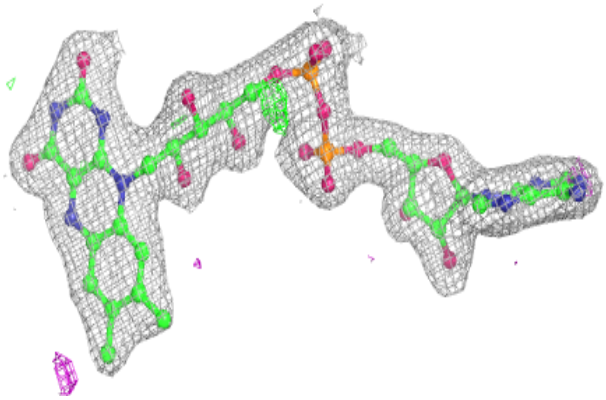


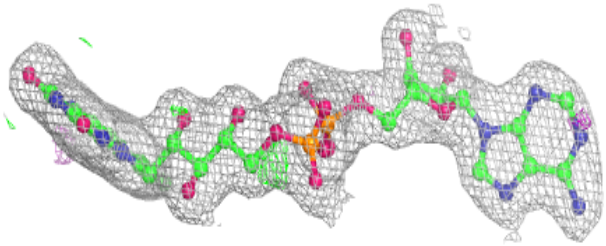


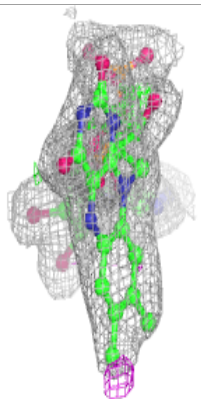


Electron density around FAD H 5482:

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

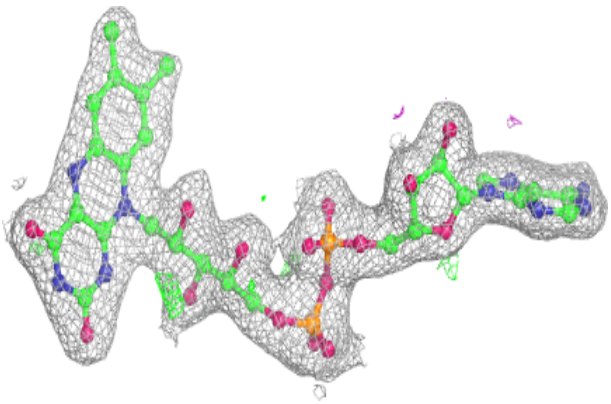


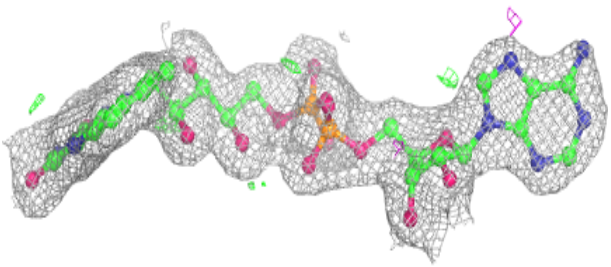


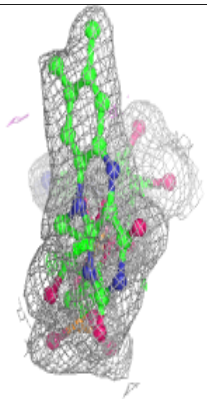


Electron density around FAD D 2482:

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

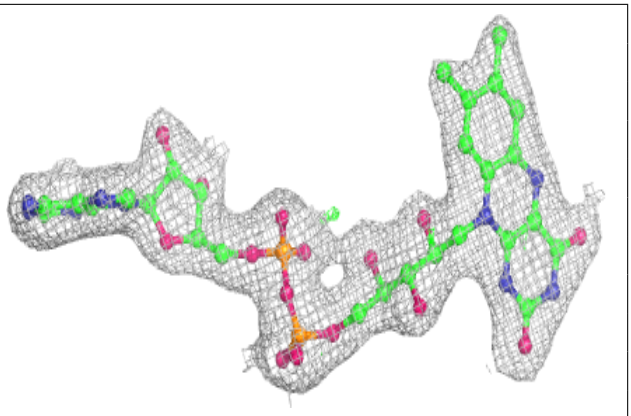


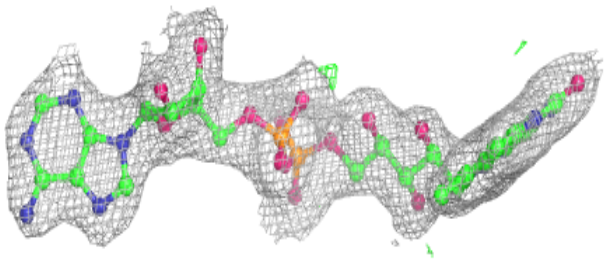


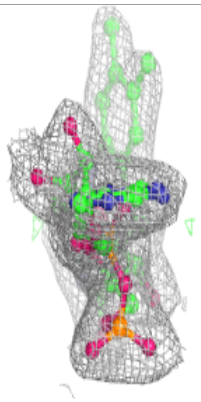


Electron density around FAD E 3482:

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







6.5 Other polymers (i)

There are no such residues in this entry.