



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:28 PM UTC

PDB ID : 2EQ9 / pdb_00002eq9
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

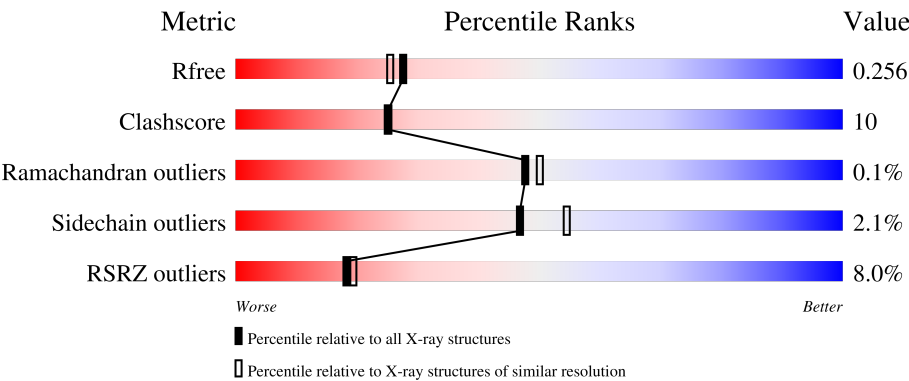
1 Overall quality at a glance i

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	464	4% 78% 20% ..
1	B	464	2% 82% 15% ..
1	D	464	4% 84% 14% ..
1	E	464	4% 82% 15% ..

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Mol	Chain	Length	Quality of chain
1	G	464	4% 81% 17% ..
1	H	464	2% 82% 16% ..
1	J	464	16% 77% 21% ..
1	K	464	18% 73% 25% ..
2	C	41	12% 73% 20% 5% .
2	F	41	49% 59% 37% ..
2	I	41	39% 66% 24% 7% .
2	L	41	44% 59% 32% 7% .

2 Entry composition

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

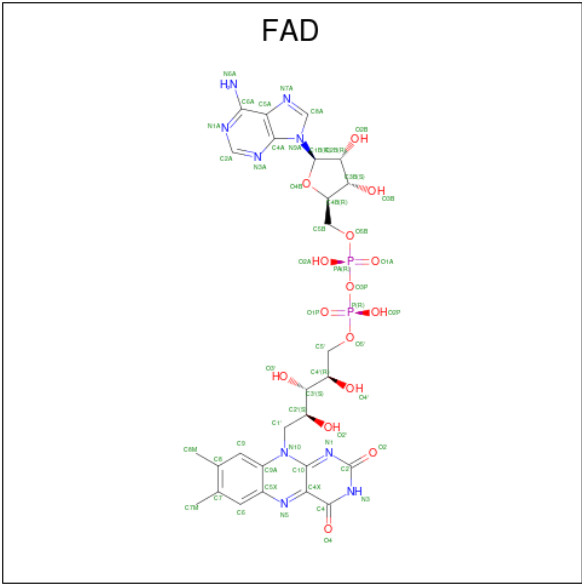
- Molecule 2 is a protein called Pyruvate dehydrogenase complex, dihydrolipoamide acetyltransferase E2 component.

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

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 (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

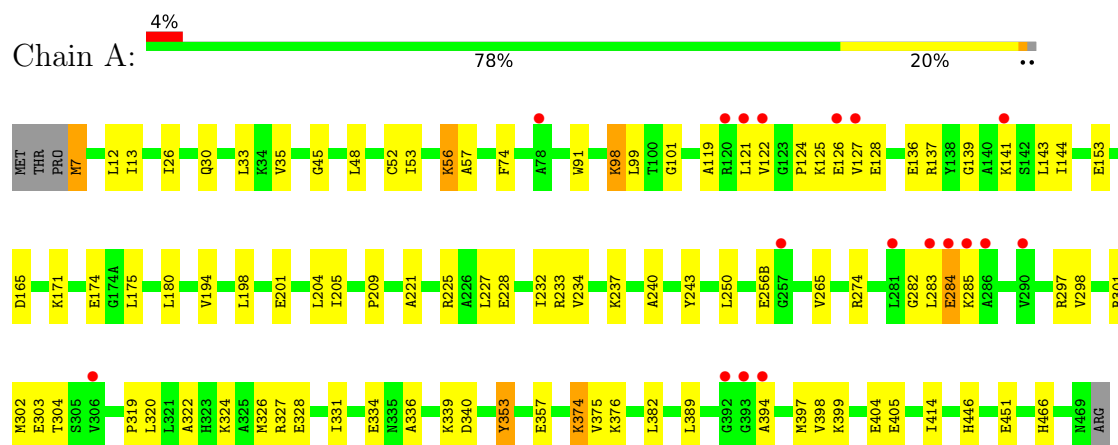
- Molecule 4 is water.

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

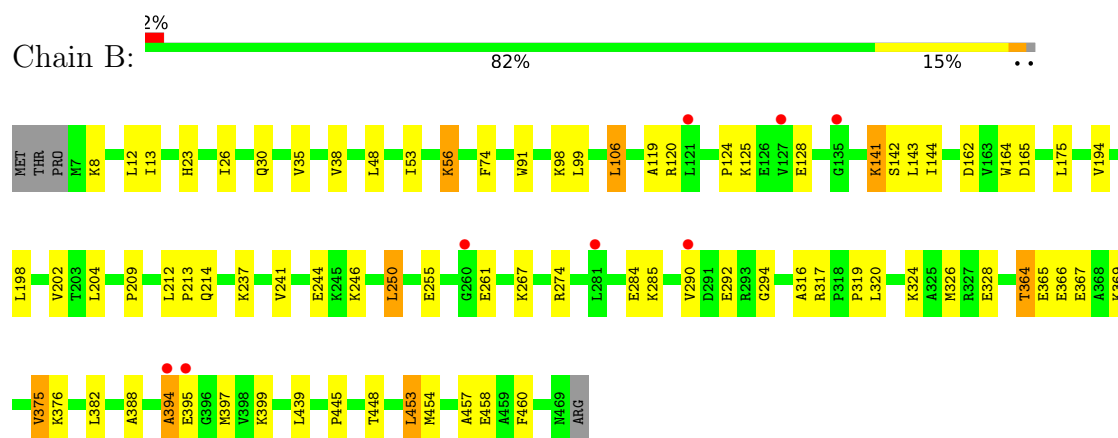
3 Residue-property plots [i](#)

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.

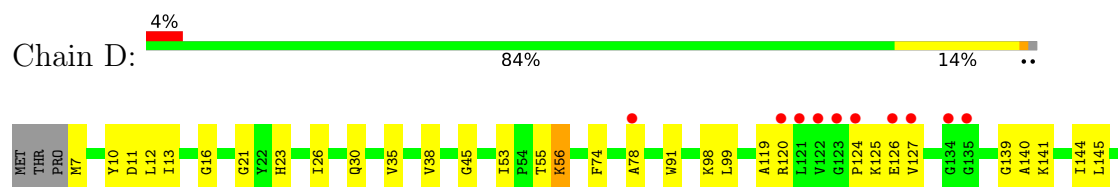
- Molecule 1: Pyruvate dehydrogenase complex, dihydrolipoamide dehydrogenase E3 component

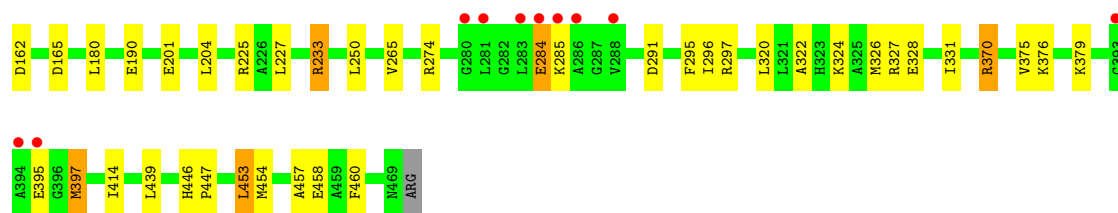


- Molecule 1: Pyruvate dehydrogenase complex, dihydrolipoamide dehydrogenase E3 component

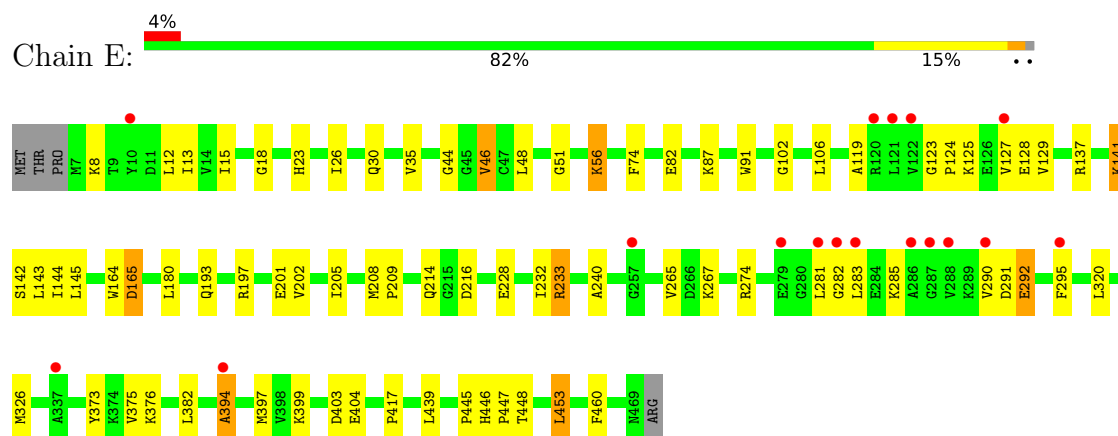


- Molecule 1: Pyruvate dehydrogenase complex, dihydrolipoamide dehydrogenase E3 component

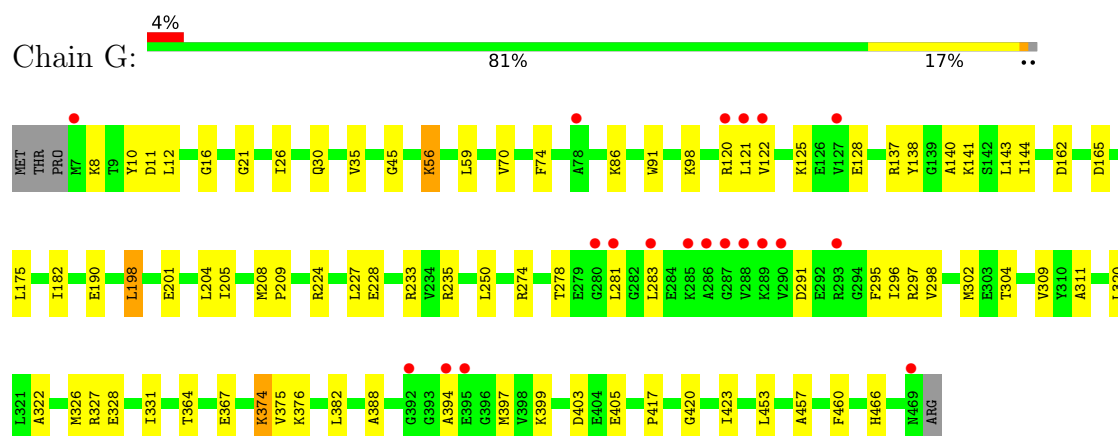




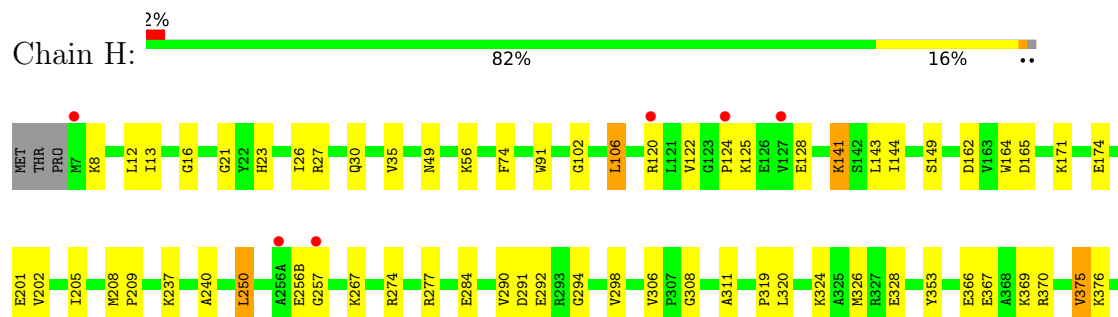
- Molecule 1: Pyruvate dehydrogenase complex, dihydrolipoamide dehydrogenase E3 component



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

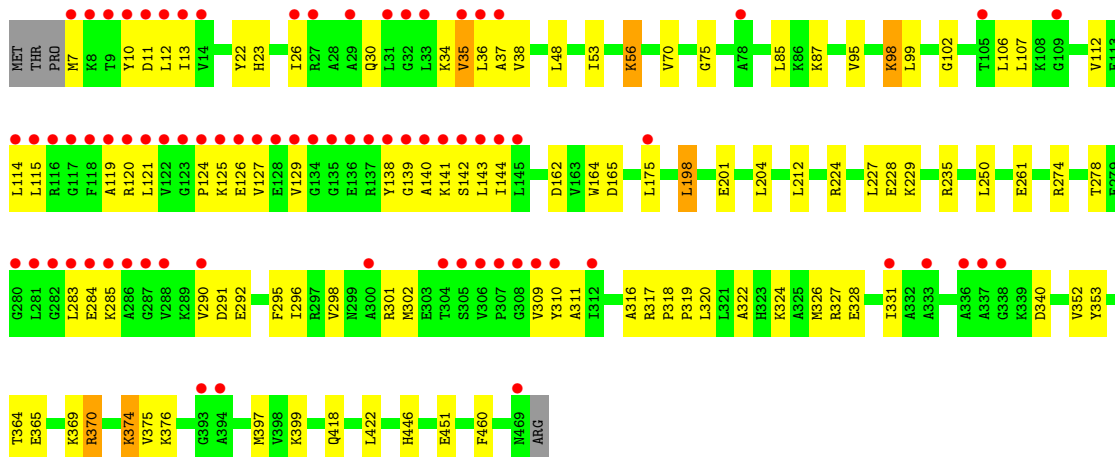
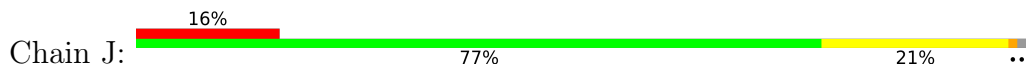


- Molecule 1: Pyruvate dehydrogenase complex, dihydrolipoamide dehydrogenase E3 component

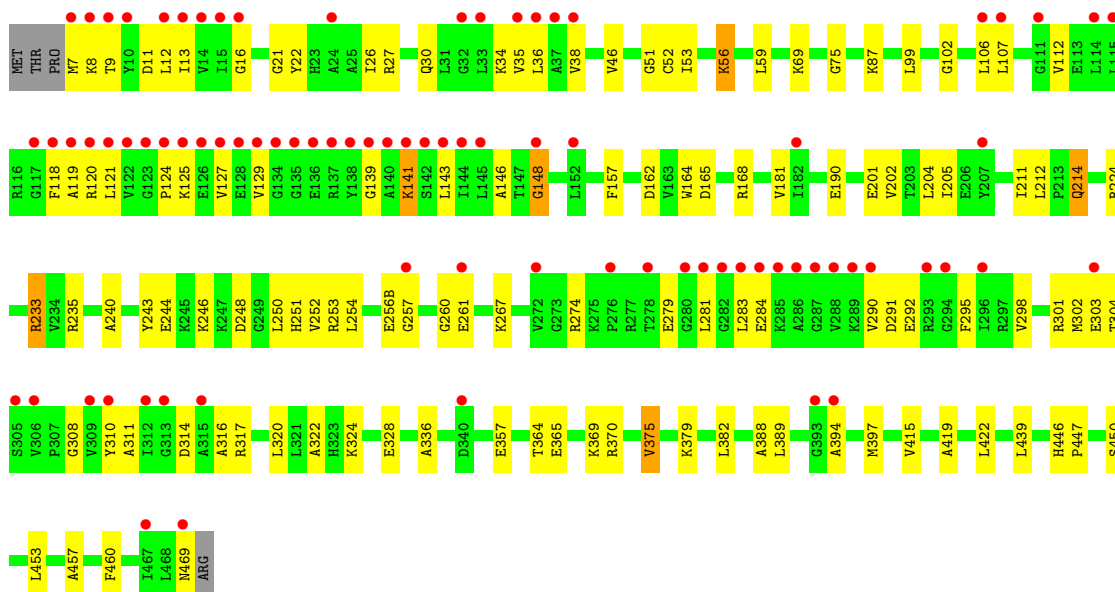




- Molecule 1: Pyruvate dehydrogenase complex, dihydrolipoamide dehydrogenase E3 component



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



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

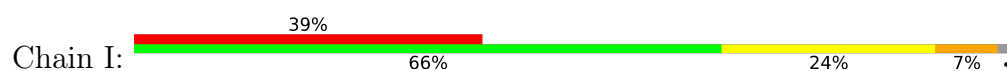




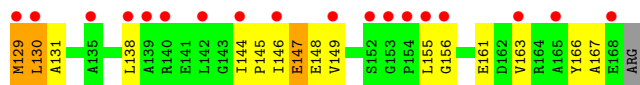
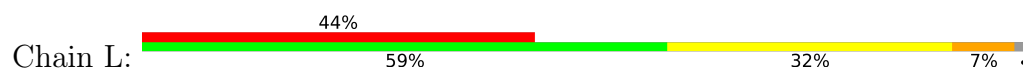
- Molecule 2: Pyruvate dehydrogenase complex, dihydrolipoamide acetyltransferase E2 component



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



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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.08Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.257 0.216 , 0.256	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 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.39	0/3464	0.91	8/4683 (0.2%)
1	B	0.39	0/3452	0.91	6/4670 (0.1%)
1	D	0.42	0/3468	0.91	4/4687 (0.1%)
1	E	0.41	0/3460	0.92	9/4679 (0.2%)
1	G	0.42	0/3464	0.91	5/4683 (0.1%)
1	H	0.41	0/3452	0.91	7/4670 (0.1%)
1	J	0.39	0/3464	0.93	11/4683 (0.2%)
1	K	0.36	0/3452	0.90	7/4670 (0.1%)
2	C	0.37	0/294	0.97	1/399 (0.3%)
2	F	0.35	0/294	0.91	1/399 (0.3%)
2	I	0.38	0/294	0.92	1/399 (0.3%)
2	L	0.35	0/294	0.93	1/399 (0.3%)
All	All	0.40	0/28852	0.91	61/39021 (0.2%)

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	156	GLY	N-CA-C	9.00	127.33	115.36
2	F	156	GLY	N-CA-C	8.11	126.86	115.43
1	H	375	VAL	N-CA-C	7.54	119.31	109.58
1	A	375	VAL	N-CA-C	7.48	119.38	109.21
1	A	35	VAL	N-CA-C	7.22	118.88	108.48
1	B	35	VAL	N-CA-C	7.20	118.97	108.53
1	D	35	VAL	N-CA-C	7.13	118.75	108.48
1	A	122	VAL	N-CA-C	-7.09	106.58	113.53
1	B	165	ASP	N-CA-C	-6.89	100.00	110.14
1	H	35	VAL	N-CA-C	6.87	118.49	108.53
1	G	35	VAL	N-CA-C	6.83	118.44	108.53
1	J	201	GLU	N-CA-C	-6.79	99.46	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	35	VAL	N-CA-C	6.79	118.37	108.53
2	L	156	GLY	N-CA-C	6.64	123.55	114.92
1	G	201	GLU	N-CA-C	-6.50	99.92	110.20
1	J	165	ASP	N-CA-C	-6.48	100.61	110.14
1	G	165	ASP	N-CA-C	-6.41	100.72	110.14
1	B	394	ALA	N-CA-C	6.37	118.79	108.41
1	J	375	VAL	N-CA-C	6.33	117.91	109.37
1	A	165	ASP	N-CA-C	-6.22	101.25	110.46
1	K	317	ARG	N-CA-C	6.16	113.67	108.13
1	D	201	GLU	N-CA-C	-6.15	100.49	110.20
1	E	202	VAL	N-CA-C	6.04	116.82	108.12
1	E	394	ALA	N-CA-C	6.00	118.90	107.75
1	E	46	VAL	N-CA-C	5.98	116.16	110.42
1	K	202	VAL	N-CA-C	5.97	117.36	108.46
1	J	23	HIS	N-CA-C	-5.88	104.27	112.45
1	K	364	THR	N-CA-C	-5.83	103.01	110.53
1	E	375	VAL	N-CA-C	5.80	117.10	109.21
1	H	165	ASP	N-CA-C	-5.75	101.68	110.14
1	H	353	TYR	N-CA-C	5.75	119.07	112.97
1	K	201	GLU	N-CA-C	-5.72	100.35	109.96
1	D	375	VAL	N-CA-C	5.69	117.82	109.63
1	B	375	VAL	N-CA-C	5.67	117.80	109.63
1	A	201	GLU	N-CA-C	-5.62	101.32	110.20
1	A	101	GLY	N-CA-C	-5.60	105.61	112.77
1	E	165	ASP	N-CA-C	-5.56	101.97	110.14
1	A	336	ALA	N-CA-C	-5.55	105.38	111.82
1	K	375	VAL	N-CA-C	5.47	117.51	109.63
1	K	322	ALA	N-CA-C	5.42	116.99	111.14
1	A	353	TYR	N-CA-C	5.39	118.68	112.97
1	J	35	VAL	N-CA-C	5.39	117.14	108.85
1	J	164	TRP	N-CA-C	5.37	118.47	110.52
1	E	216	ASP	CA-C-N	5.37	125.01	119.05
1	E	216	ASP	C-N-CA	5.37	125.01	119.05
1	B	364	THR	N-CA-C	-5.34	103.64	110.53
1	J	364	THR	N-CA-C	-5.33	103.66	110.53
1	G	466	HIS	N-CA-C	5.32	119.64	113.20
1	G	375	VAL	N-CA-C	5.25	117.19	109.63
1	B	202	VAL	N-CA-C	5.25	115.67	108.12
2	I	146	ILE	N-CA-C	5.24	115.86	110.36
1	H	201	GLU	N-CA-C	-5.22	100.79	109.46
1	J	353	TYR	N-CA-C	5.21	118.50	112.97
1	K	165	ASP	N-CA-C	-5.18	101.80	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	165	ASP	N-CA-C	-5.18	102.53	110.14
1	H	49	ASN	N-CA-C	5.17	119.48	112.04
1	E	201	GLU	N-CA-C	-5.09	101.01	109.46
1	J	212	LEU	CA-C-N	5.04	125.32	119.47
1	J	212	LEU	C-N-CA	5.04	125.32	119.47
1	H	202	VAL	N-CA-C	5.04	115.37	108.12
1	J	352	VAL	N-CA-C	-5.00	100.45	107.75

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	3409	0	3519	70	0
1	B	3397	0	3493	65	0
1	D	3413	0	3530	50	0
1	E	3405	0	3508	58	0
1	G	3409	0	3519	55	0
1	H	3397	0	3493	64	0
1	J	3409	0	3519	82	0
1	K	3397	0	3493	95	0
2	C	290	0	300	9	0
2	F	290	0	300	10	0
2	I	290	0	300	13	0
2	L	290	0	300	14	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	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	566	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 10.

All (566) 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:E:292:GLU:H	1:E:292:GLU:CD	1.90	0.80
1:H:125:LYS:HZ1	1:H:308:GLY:HA3	1.47	0.79
1:D:370:ARG:HG2	1:D:370:ARG:HH11	1.46	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:B:292:GLU:CD	1:B:292:GLU:H	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:302:MET:HE2	1:J:328:GLU:HB3	1.71	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:A:283:LEU:C	1:A:285:LYS:H	1.96	0.72
1:G:141:LYS:HD2	1:G:141:LYS:N	2.04	0.71
1:H:292:GLU:CD	1:H:292:GLU:H	1.98	0.71
1:J:397:MET:HE2	1:J:399:LYS:HB2	1.74	0.70
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:K:302:MET:HE2	1:K:328:GLU:HB3	1.74	0.69
1:B:382:LEU:HB3	1:B:394:ALA:HB1	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:H:397:MET:HE2	1:H:399:LYS:HB2	1.76	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
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:J:7:MET:HE2	1:J:126:GLU:OE2	1.95	0.66
1:G:26:ILE:O	1:G:30:GLN:HG3	1.94	0.66
1:K:205:ILE:HD11	1:K:240:ALA:HB2	1.77	0.66
1:G:397:MET:HE2	1:G:399:LYS: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
2:L:129:MET:HE3	2:L:131:ALA:N	2.12	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:K:379:LYS:HD3	1:K:397:MET:HE1	1.78	0.64
1:D:7:MET:HE2	1:D:126:GLU:OE2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:147:GLU:CD	2:C:147:GLU:H	2.07	0.63
1:K:52:CYS:O	1:K:56:LYS:HD2	1.99	0.63
1:A:302:MET:HE2	1:A:328:GLU:HB3	1.81	0.62
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:K:292:GLU:CD	1:K:292:GLU:H	2.07	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
2:L:129:MET:HE2	2:L:129:MET:O	2.00	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:L:129:MET:HE3	2:L:131:ALA:H	1.66	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
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:A:397:MET:HE2	1:A:399:LYS:HB2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:164:TRP:CZ2	1:H:267:LYS:HG2	2.39	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:J:284:GLU:H	1:J:284:GLU:CD	2.12	0.57
1:B:246:LYS:HE3	1:K:370:ARG:O	2.05	0.56
1:A:98:LYS:HD3	1:A:98:LYS:C	2.29	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:G:302:MET:HE2	1:G:328:GLU:HB3	1.88	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
1:E:397:MET:HE2	1:E:399:LYS:HB2	1.88	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
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
2:I:147:GLU:CD	2:I:147:GLU:H	2.15	0.54
1:A:12:LEU:HD11	1:A:144:ILE:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:125:LYS:HZ2	1:A:141:LYS:HA	1.73	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:K:248:ASP:CG	1:K:251:HIS:HE2	2.15	0.54
1:D:297:ARG:HH11	1:D:297:ARG:HG3	1.73	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
2:I:146:ILE:HG23	2:I:147:GLU:N	2.23	0.53
1:E:205:ILE:CD1	1:E:240:ALA:HB2	2.39	0.53
1:B:397:MET:HE2	1:B:399:LYS:HB2	1.90	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: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:G:397:MET:CE	1:G:399:LYS:HB2	2.38	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
1:K:7:MET:HE3	1:K:9:THR:HG22	1.92	0.52
1:A:233:ARG:NH2	1:A:234:VAL:H	2.07	0.52
1:A:283:LEU:C	1:A:285:LYS:N	2.64	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:125:LYS:NZ	1:A:141:LYS:HA	2.25	0.51
1:D:379:LYS:HD3	1:D:397:MET:HE1	1.92	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: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: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:J:397:MET:CE	1:J:399:LYS:HB2	2.40	0.50
1:K:16:GLY:HA3	1:K:146:ALA:O	2.11	0.50
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
2:I:138:LEU:C	2:I:138:LEU:HD13	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:LYS:HD3	1:B:8:LYS:H	1.77	0.50
1:H:23:HIS:CE1	1:H:326:MET:HE3	2.46	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
2:F:138:LEU:HD13	2:F:138:LEU:C	2.38	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:B:124:PRO:C	1:B:125:LYS:HE2	2.37	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
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: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:J:292:GLU:H	1:J:292:GLU:CD	2.21	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:G:326:MET:HE1	1:H:446:HIS:CE1	2.48	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
2:F:145:PRO:HG2	2:F:148:GLU:CG	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:161:GLU:CD	2:L:161:GLU:H	2.20	0.48
1:E:382:LEU:C	1:E:394:ALA:HB1	2.39	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
2:L:138:LEU:HD13	2:L:138:LEU:C	2.40	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:J:446:HIS:HD1	1:J:451:GLU:CD	2.22	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:H:290:VAL:HG13	1:H:294:GLY:C	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:446:HIS:HD1	1:A:451:GLU:CD	2.21	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
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:A:124:PRO:C	1:A:125:LYS:HG3	2.40	0.46
1:H:292:GLU:CD	1:H:292:GLU:N	2.71	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
2:C:138:LEU:HD13	2:C:138:LEU:C	2.41	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:J:235:ARG:HH22	1:J:261:GLU:CD	2.24	0.46
1:K:324:LYS:HZ3	1:K:328:GLU:CD	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:256(B):GLU:HG2	1:K:257:GLY:N	2.31	0.45
1:E:124:PRO:C	1:E:125:LYS:HG3	2.41	0.45
1:E:291:ASP:OD2	1:E:295:PHE:HB2	2.16	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
1:B:204:LEU:C	1:B:204:LEU:HD23	2.41	0.45
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:E:292:GLU:CD	1:E:292:GLU:N	2.69	0.45
1:G:382:LEU:CD1	1:G:417:PRO:HD2	2.47	0.45
1:B:13:ILE:HB	1:B:143:LEU:HD22	1.98	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:G:204:LEU:C	1:G:204:LEU:HD23	2.43	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:B:175:LEU:HD21	1:B:198:LEU:CB	2.45	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:379:LYS:HB3	1:D:397:MET:HE3	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:I:153:GLY:C	2:I:155:LEU:N	2.76	0.44
1:J:301:ARG:NH1	1:J:340:ASP:OD1	2.51	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:J:204:LEU:HD23	1:J:204:LEU:C	2.43	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: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:A:204:LEU:C	1:A:204:LEU:HD23	2.42	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
4:G:4555:HOH:O	1:H:326:MET:HE1	2.17	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
1:J:318:PRO:HA	1:J:319:PRO:C	2.44	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:B:13:ILE:HB	1:B:143:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:7:MET:HE2	1:A:126:GLU:OE2	2.19	0.42
1:D:53:ILE:HG21	1:D:99:LEU:HD12	2.01	0.42
1:D:204:LEU:C	1:D:204:LEU:HD23	2.44	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: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:E:165:ASP:OD1	1:E:165:ASP:C	2.61	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: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:K:415:VAL:O	1:K:415:VAL:HG13	2.18	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:J:283:LEU:C	1:J:285:LYS:N	2.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ARG:HB2	1:A:320:LEU:CD1	2.49	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: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
2:F:147:GLU:H	2:F:147:GLU:CD	2.27	0.42
1:K:53:ILE:HG21	1:K:99:LEU:HD12	2.02	0.42
1:A:13:ILE:HB	1:A:143:LEU:CD2	2.50	0.42
1:B:241:VAL:HG21	1:B:255:GLU:CD	2.45	0.42
1:D:180:LEU:HB2	1:D:265:VAL:HG11	2.02	0.42
1:E:48:LEU:N	1:E:48:LEU:HD12	2.35	0.42
1:H:256(B):GLU:H	1:H:256(B):GLU:CD	2.28	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: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: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
1:E:123:GLY:C	1:E:125:LYS:H	2.27	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
1:A:397:MET:CE	1:A:399:LYS:HB2	2.48	0.41
1:D:326:MET:HE1	1:E:446:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:194:VAL:O	1:B:198:LEU:HG	2.20	0.41
2:C:161:GLU:CD	2:C:161:GLU:H	2.28	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
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: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:128:GLU:CD	1:E:137:ARG:HE	2.29	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:K:211:ILE:O	1:K:212:LEU:C	2.64	0.41
1:B:274:ARG:HB2	1:B:320:LEU:HD13	2.02	0.41
1:B:290:VAL:HG13	1:B:294:GLY:C	2.46	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:18:GLY:HA2	1:E:44:GLY:C	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	43	44
1	B	458/464 (99%)	444 (97%)	14 (3%)	0	100	100
1	D	458/464 (99%)	440 (96%)	17 (4%)	1 (0%)	43	44
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%)	30	28
2	C	38/41 (93%)	35 (92%)	3 (8%)	0	100	100
2	F	38/41 (93%)	34 (90%)	3 (8%)	1 (3%)	4	1
2	I	38/41 (93%)	35 (92%)	3 (8%)	0	100	100
2	L	38/41 (93%)	30 (79%)	8 (21%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3816/3876 (98%)	3671 (96%)	140 (4%)	5 (0%)	48	50

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 ⓘ

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%)	336 (98%)	6 (2%)	51	60
1	B	339/349 (97%)	333 (98%)	6 (2%)	51	60
1	D	343/349 (98%)	334 (97%)	9 (3%)	40	46
1	E	341/349 (98%)	335 (98%)	6 (2%)	51	60
1	G	342/349 (98%)	338 (99%)	4 (1%)	63	72
1	H	339/349 (97%)	333 (98%)	6 (2%)	51	60
1	J	342/349 (98%)	336 (98%)	6 (2%)	51	60
1	K	339/349 (97%)	334 (98%)	5 (2%)	57	65
2	C	28/31 (90%)	25 (89%)	3 (11%)	6	4
2	F	28/31 (90%)	24 (86%)	4 (14%)	3	1
2	I	28/31 (90%)	26 (93%)	2 (7%)	13	11
2	L	28/31 (90%)	24 (86%)	4 (14%)	3	1
All	All	2839/2916 (97%)	2778 (98%)	61 (2%)	47	54

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	MET
1	A	33	LEU
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	141	LYS
1	B	250	LEU
1	B	261	GLU
1	B	453	LEU
2	C	130	LEU
2	C	147	GLU
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	397	MET
1	D	453	LEU
1	E	56	LYS
1	E	82	GLU
1	E	141	LYS
1	E	233	ARG
1	E	292	GLU
1	E	453	LEU
2	F	129	MET
2	F	147	GLU
2	F	155	LEU
2	F	161	GLU
1	G	56	LYS
1	G	198	LEU
1	G	227	LEU
1	G	374	LYS
1	H	56	LYS
1	H	106	LEU
1	H	141	LYS
1	H	250	LEU
1	H	284	GLU

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Mol	Chain	Res	Type
1	H	453	LEU
2	I	130	LEU
2	I	155	LEU
1	J	56	LYS
1	J	98	LYS
1	J	198	LEU
1	J	227	LEU
1	J	370	ARG
1	J	374	LYS
1	K	56	LYS
1	K	141	LYS
1	K	214	GLN
1	K	233	ARG
1	K	284	GLU
2	L	129	MET
2	L	130	LEU
2	L	147	GLU
2	L	155	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	GLN
1	B	214	GLN
1	B	418	GLN
1	D	418	GLN
1	E	214	GLN
1	E	418	GLN
1	H	214	GLN
1	H	418	GLN
1	J	23	HIS
1	J	30	GLN
1	J	110	ASN
1	K	23	HIS
1	K	214	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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	A	8482	-	58,58,58	2.18	17 (29%)	85,89,89	1.16	6 (7%)
3	FAD	G	4482	-	58,58,58	2.18	18 (31%)	85,89,89	1.20	6 (7%)
3	FAD	J	6482	-	58,58,58	2.22	18 (31%)	85,89,89	1.19	7 (8%)
3	FAD	K	7482	-	58,58,58	2.10	19 (32%)	85,89,89	1.14	6 (7%)
3	FAD	E	3482	-	58,58,58	2.04	15 (25%)	85,89,89	1.19	9 (10%)
3	FAD	H	5482	-	58,58,58	2.12	19 (32%)	85,89,89	1.17	6 (7%)
3	FAD	B	1482	-	58,58,58	2.13	15 (25%)	85,89,89	1.19	7 (8%)
3	FAD	D	2482	-	58,58,58	2.15	16 (27%)	85,89,89	1.21	10 (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	A	8482	-	-	1/34/50/50	0/6/6/6
3	FAD	G	4482	-	-	3/34/50/50	0/6/6/6
3	FAD	J	6482	-	-	1/34/50/50	0/6/6/6
3	FAD	K	7482	-	-	3/34/50/50	0/6/6/6
3	FAD	E	3482	-	-	1/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	H	5482	-	-	2/34/50/50	0/6/6/6
3	FAD	B	1482	-	-	2/34/50/50	0/6/6/6
3	FAD	D	2482	-	-	3/34/50/50	0/6/6/6

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	6482	FAD	P-O3P	-10.59	1.48	1.59
3	G	4482	FAD	P-O3P	-10.10	1.48	1.59
3	A	8482	FAD	P-O3P	-10.08	1.48	1.59
3	B	1482	FAD	P-O3P	-10.04	1.48	1.59
3	D	2482	FAD	P-O3P	-9.67	1.49	1.59
3	H	5482	FAD	P-O3P	-9.28	1.49	1.59
3	K	7482	FAD	P-O3P	-9.07	1.49	1.59
3	E	3482	FAD	P-O3P	-8.78	1.50	1.59
3	E	3482	FAD	PA-O2A	-4.40	1.34	1.55
3	H	5482	FAD	C1'-C2'	4.35	1.58	1.52
3	H	5482	FAD	PA-O2A	-4.26	1.35	1.55
3	A	8482	FAD	PA-O2A	-4.24	1.35	1.55
3	G	4482	FAD	PA-O2A	-4.16	1.36	1.55
3	B	1482	FAD	PA-O2A	-4.13	1.36	1.55
3	K	7482	FAD	PA-O2A	-4.11	1.36	1.55
3	E	3482	FAD	O5'-C5'	4.09	1.60	1.44
3	A	8482	FAD	O5'-C5'	4.07	1.60	1.44
3	J	6482	FAD	PA-O2A	-4.05	1.36	1.55
3	H	5482	FAD	O5'-C5'	4.03	1.59	1.44
3	D	2482	FAD	C1'-C2'	4.00	1.58	1.52
3	K	7482	FAD	O5'-C5'	3.99	1.59	1.44
3	G	4482	FAD	O5'-C5'	3.91	1.59	1.44
3	D	2482	FAD	PA-O2A	-3.90	1.37	1.55
3	G	4482	FAD	C1'-C2'	3.88	1.58	1.52
3	B	1482	FAD	O5'-C5'	3.86	1.59	1.44
3	J	6482	FAD	C1'-C2'	3.86	1.58	1.52
3	A	8482	FAD	C1'-C2'	3.78	1.57	1.52
3	D	2482	FAD	O5'-C5'	3.77	1.58	1.44
3	E	3482	FAD	C1'-C2'	3.72	1.57	1.52
3	J	6482	FAD	P-O2P	-3.64	1.38	1.55
3	J	6482	FAD	O5'-C5'	3.61	1.58	1.44
3	D	2482	FAD	P-O2P	-3.57	1.38	1.55
3	A	8482	FAD	P-O2P	-3.51	1.39	1.55
3	K	7482	FAD	P-O2P	-3.46	1.39	1.55
3	G	4482	FAD	P-O2P	-3.45	1.39	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1482	FAD	P-O2P	-3.42	1.39	1.55
3	H	5482	FAD	P-O2P	-3.37	1.39	1.55
3	E	3482	FAD	P-O2P	-3.30	1.40	1.55
3	K	7482	FAD	O4B-C1B	3.23	1.49	1.42
3	H	5482	FAD	C4X-N5	2.96	1.37	1.30
3	A	8482	FAD	C8-C7	2.94	1.48	1.40
3	J	6482	FAD	O2-C2	-2.91	1.18	1.24
3	H	5482	FAD	O2-C2	-2.90	1.18	1.24
3	K	7482	FAD	C4X-N5	2.89	1.37	1.30
3	B	1482	FAD	C1'-C2'	2.89	1.56	1.52
3	B	1482	FAD	C8-C7	2.88	1.47	1.40
3	G	4482	FAD	C8-C7	2.86	1.47	1.40
3	K	7482	FAD	C8-C7	2.86	1.47	1.40
3	A	8482	FAD	O4B-C1B	2.86	1.48	1.42
3	E	3482	FAD	C8-C7	2.80	1.47	1.40
3	D	2482	FAD	O2-C2	-2.80	1.18	1.24
3	D	2482	FAD	C8-C7	2.79	1.47	1.40
3	K	7482	FAD	C9A-C5X	2.74	1.45	1.41
3	J	6482	FAD	C9A-C5X	2.74	1.45	1.41
3	B	1482	FAD	O4B-C1B	2.71	1.48	1.42
3	E	3482	FAD	C4A-N3A	2.71	1.39	1.34
3	J	6482	FAD	O4B-C1B	2.67	1.48	1.42
3	H	5482	FAD	C8-C7	2.66	1.47	1.40
3	J	6482	FAD	C4X-N5	2.66	1.36	1.30
3	K	7482	FAD	O2-C2	-2.65	1.19	1.24
3	D	2482	FAD	C5A-C6A	2.65	1.48	1.41
3	G	4482	FAD	C4X-N5	2.65	1.36	1.30
3	G	4482	FAD	C5A-C6A	2.64	1.48	1.41
3	J	6482	FAD	C8-C7	2.61	1.47	1.40
3	D	2482	FAD	C9A-C5X	2.60	1.45	1.41
3	A	8482	FAD	C5A-C6A	2.55	1.48	1.41
3	K	7482	FAD	C1'-C2'	2.55	1.56	1.52
3	A	8482	FAD	C4A-N3A	2.55	1.39	1.34
3	B	1482	FAD	C4X-N5	2.55	1.36	1.30
3	A	8482	FAD	O2-C2	-2.53	1.19	1.24
3	J	6482	FAD	C4A-N3A	2.53	1.39	1.34
3	G	4482	FAD	C4A-N3A	2.52	1.39	1.34
3	H	5482	FAD	C5A-C6A	2.52	1.48	1.41
3	H	5482	FAD	C9A-C5X	2.52	1.45	1.41
3	D	2482	FAD	C4A-N3A	2.51	1.39	1.34
3	B	1482	FAD	C5A-C6A	2.51	1.48	1.41
3	G	4482	FAD	O2-C2	-2.48	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	8482	FAD	C4X-N5	2.48	1.36	1.30
3	D	2482	FAD	C4X-N5	2.46	1.36	1.30
3	K	7482	FAD	C5A-C6A	2.45	1.47	1.41
3	G	4482	FAD	C9A-N10	2.45	1.45	1.41
3	E	3482	FAD	C4X-N5	2.45	1.36	1.30
3	E	3482	FAD	O4B-C1B	2.44	1.47	1.42
3	B	1482	FAD	C9A-N10	2.44	1.45	1.41
3	J	6482	FAD	C5A-C6A	2.40	1.47	1.41
3	G	4482	FAD	O4B-C1B	2.38	1.47	1.42
3	E	3482	FAD	C9A-C5X	2.35	1.45	1.41
3	H	5482	FAD	O4B-C1B	2.35	1.47	1.42
3	K	7482	FAD	C4A-N3A	2.35	1.38	1.34
3	D	2482	FAD	C6-C5X	2.34	1.43	1.40
3	K	7482	FAD	C2-N3	2.33	1.44	1.39
3	B	1482	FAD	C4A-N3A	2.32	1.38	1.34
3	B	1482	FAD	C2-N3	2.31	1.44	1.39
3	D	2482	FAD	O4B-C1B	2.31	1.47	1.42
3	A	8482	FAD	C9A-N10	2.31	1.45	1.41
3	H	5482	FAD	C9A-N10	2.31	1.45	1.41
3	B	1482	FAD	O2-C2	-2.28	1.19	1.24
3	G	4482	FAD	C9A-C5X	2.28	1.44	1.41
3	E	3482	FAD	C5A-C6A	2.28	1.47	1.41
3	J	6482	FAD	C10-N1	2.27	1.37	1.33
3	B	1482	FAD	C10-N1	2.27	1.37	1.33
3	H	5482	FAD	C4A-N3A	2.25	1.38	1.34
3	E	3482	FAD	C6-C5X	2.24	1.43	1.40
3	E	3482	FAD	C2-N3	2.23	1.43	1.39
3	A	8482	FAD	C5A-C4A	2.23	1.43	1.39
3	A	8482	FAD	C6-C5X	2.22	1.43	1.40
3	J	6482	FAD	P-O5'	-2.22	1.50	1.59
3	J	6482	FAD	C2-N3	2.21	1.43	1.39
3	G	4482	FAD	C10-N1	2.21	1.37	1.33
3	D	2482	FAD	P-O5'	-2.20	1.50	1.59
3	J	6482	FAD	C5A-C4A	2.20	1.43	1.39
3	K	7482	FAD	C10-N1	2.20	1.37	1.33
3	K	7482	FAD	C6-C5X	2.19	1.43	1.40
3	D	2482	FAD	C2-N3	2.18	1.43	1.39
3	G	4482	FAD	C2A-N1A	2.18	1.37	1.33
3	G	4482	FAD	C2-N3	2.17	1.43	1.39
3	H	5482	FAD	P-O5'	-2.17	1.50	1.59
3	A	8482	FAD	C9A-C5X	2.17	1.44	1.41
3	H	5482	FAD	C2A-N1A	2.15	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2482	FAD	C2A-N1A	2.13	1.37	1.33
3	E	3482	FAD	C9A-N10	2.13	1.44	1.41
3	H	5482	FAD	C10-N1	2.13	1.37	1.33
3	J	6482	FAD	C9A-N10	2.10	1.44	1.41
3	E	3482	FAD	O2-C2	-2.09	1.20	1.24
3	J	6482	FAD	C2A-N1A	2.08	1.37	1.33
3	K	7482	FAD	C9A-N10	2.07	1.44	1.41
3	B	1482	FAD	C9A-C5X	2.06	1.44	1.41
3	H	5482	FAD	C6-C5X	2.05	1.43	1.40
3	G	4482	FAD	O4'-C4'	2.05	1.47	1.43
3	A	8482	FAD	P-O5'	-2.02	1.51	1.59
3	H	5482	FAD	C5A-C4A	2.02	1.42	1.39
3	K	7482	FAD	P-O5'	-2.02	1.51	1.59
3	K	7482	FAD	C2A-N1A	2.02	1.37	1.33
3	H	5482	FAD	C2-N3	2.02	1.43	1.39
3	G	4482	FAD	C5A-C4A	2.02	1.42	1.39
3	A	8482	FAD	C2A-N1A	2.01	1.37	1.33
3	K	7482	FAD	C5A-C4A	2.00	1.42	1.39

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	5482	FAD	O4B-C1B-N9A	-4.21	100.00	108.09
3	A	8482	FAD	O4B-C1B-N9A	-3.86	100.69	108.09
3	B	1482	FAD	O4B-C1B-N9A	-3.78	100.82	108.09
3	D	2482	FAD	O4B-C1B-N9A	-3.78	100.83	108.09
3	E	3482	FAD	O4B-C1B-N9A	-3.65	101.08	108.09
3	G	4482	FAD	O4B-C1B-N9A	-3.47	101.43	108.09
3	J	6482	FAD	O4B-C1B-N9A	-3.44	101.47	108.09
3	K	7482	FAD	O4B-C1B-N9A	-3.17	102.01	108.09
3	J	6482	FAD	O5B-PA-O1A	-3.08	96.73	108.94
3	B	1482	FAD	O5B-PA-O1A	-2.97	97.16	108.94
3	K	7482	FAD	O5B-PA-O1A	-2.95	97.25	108.94
3	D	2482	FAD	O5B-PA-O1A	-2.90	97.45	108.94
3	G	4482	FAD	O5B-PA-O1A	-2.85	97.64	108.94
3	E	3482	FAD	O5B-PA-O1A	-2.71	98.19	108.94
3	J	6482	FAD	C2A-N1A-C6A	2.67	123.12	118.73
3	J	6482	FAD	C5'-C4'-C3'	-2.63	107.26	112.22
3	A	8482	FAD	C2A-N1A-C6A	2.61	123.02	118.73
3	H	5482	FAD	O5B-PA-O1A	-2.60	98.65	108.94
3	G	4482	FAD	C2A-N1A-C6A	2.58	122.96	118.73
3	D	2482	FAD	C5'-C4'-C3'	-2.58	107.36	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	5482	FAD	C2A-N1A-C6A	2.57	122.95	118.73
3	E	3482	FAD	C5'-C4'-C3'	-2.56	107.39	112.22
3	E	3482	FAD	C2A-N1A-C6A	2.56	122.93	118.73
3	D	2482	FAD	C4-N3-C2	-2.52	121.17	125.64
3	A	8482	FAD	O5B-PA-O1A	-2.51	98.97	108.94
3	D	2482	FAD	O4B-C1B-C2B	-2.43	101.42	106.62
3	B	1482	FAD	C5X-C9A-N10	-2.42	115.78	117.97
3	K	7482	FAD	C2A-N1A-C6A	2.41	122.69	118.73
3	G	4482	FAD	C5'-C4'-C3'	-2.40	107.70	112.22
3	G	4482	FAD	C4-N3-C2	-2.40	121.39	125.64
3	J	6482	FAD	C4-N3-C2	-2.39	121.40	125.64
3	B	1482	FAD	C2A-N1A-C6A	2.31	122.52	118.73
3	B	1482	FAD	C5'-C4'-C3'	-2.29	107.90	112.22
3	A	8482	FAD	C4-N3-C2	-2.28	121.59	125.64
3	D	2482	FAD	C2A-N1A-C6A	2.26	122.44	118.73
3	H	5482	FAD	C4-N3-C2	-2.25	121.64	125.64
3	A	8482	FAD	C5'-C4'-C3'	-2.24	107.99	112.22
3	B	1482	FAD	C4-N3-C2	-2.23	121.69	125.64
3	D	2482	FAD	O2A-PA-O3P	2.22	113.27	107.27
3	E	3482	FAD	C4-N3-C2	-2.21	121.72	125.64
3	H	5482	FAD	C2B-C1B-N9A	2.21	118.79	113.30
3	K	7482	FAD	C5'-C4'-C3'	-2.21	108.06	112.22
3	K	7482	FAD	C4-N3-C2	-2.16	121.81	125.64
3	D	2482	FAD	C5X-C9A-N10	-2.15	116.03	117.97
3	K	7482	FAD	C4X-C10-N10	2.13	119.53	116.48
3	G	4482	FAD	C5X-C9A-N10	-2.13	116.04	117.97
3	D	2482	FAD	C4X-C10-N10	2.13	119.53	116.48
3	H	5482	FAD	C4X-C10-N10	2.13	119.53	116.48
3	J	6482	FAD	C5X-C9A-N10	-2.11	116.06	117.97
3	A	8482	FAD	C2B-C1B-N9A	2.11	118.54	113.30
3	E	3482	FAD	C2B-C1B-N9A	2.10	118.52	113.30
3	E	3482	FAD	C4X-C10-N10	2.09	119.48	116.48
3	J	6482	FAD	C4X-C10-N10	2.09	119.47	116.48
3	E	3482	FAD	O4B-C1B-C2B	-2.08	102.16	106.62
3	E	3482	FAD	C5X-C9A-N10	-2.04	116.12	117.97
3	D	2482	FAD	C2B-C1B-N9A	2.04	118.36	113.30
3	B	1482	FAD	O2A-PA-O3P	2.02	112.73	107.27

There are no chirality outliers.

All (16) torsion outliers are listed below:

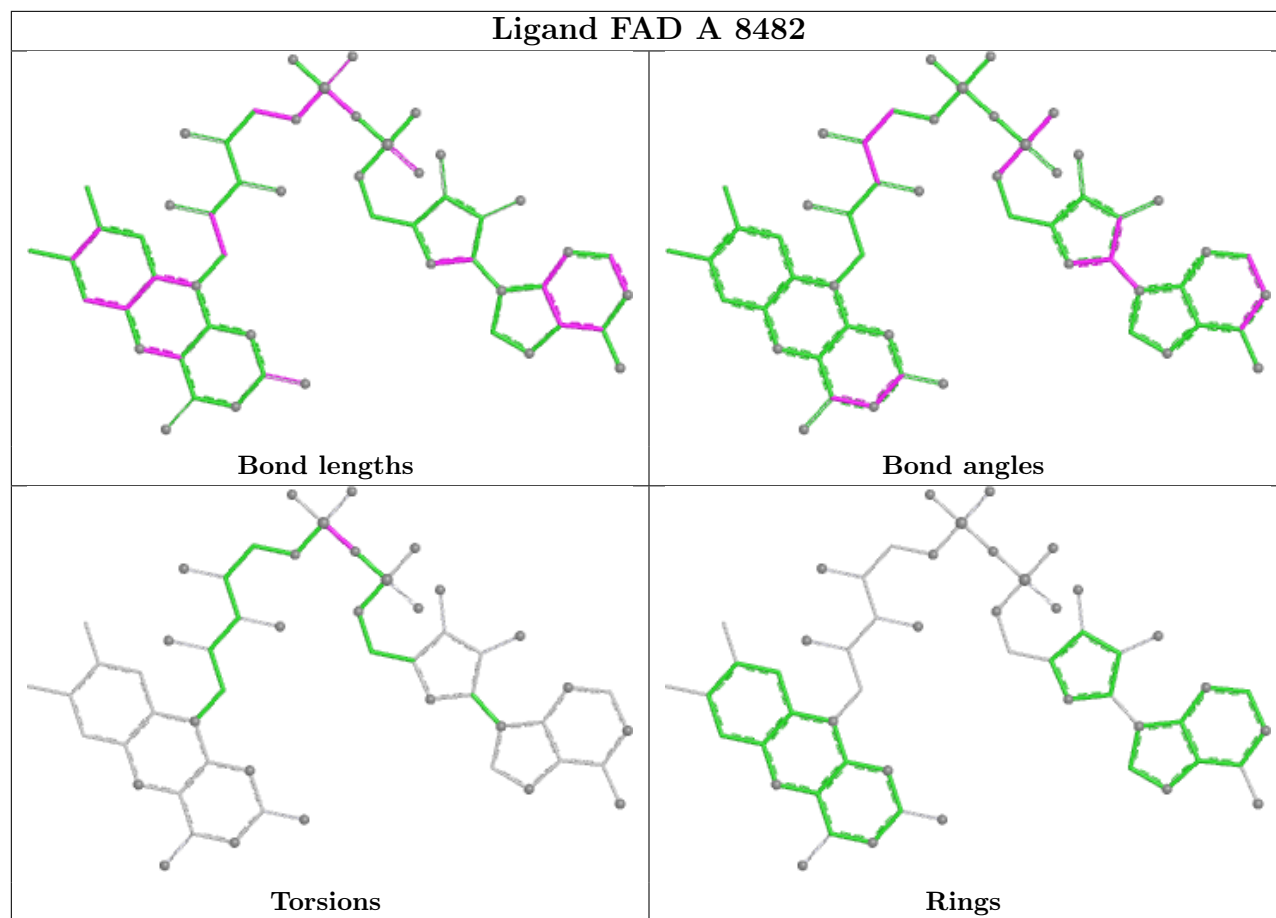
Mol	Chain	Res	Type	Atoms
3	A	8482	FAD	PA-O3P-P-O5'
3	B	1482	FAD	PA-O3P-P-O5'
3	D	2482	FAD	PA-O3P-P-O5'
3	E	3482	FAD	PA-O3P-P-O5'
3	G	4482	FAD	PA-O3P-P-O5'
3	H	5482	FAD	PA-O3P-P-O5'
3	J	6482	FAD	PA-O3P-P-O5'
3	K	7482	FAD	PA-O3P-P-O5'
3	G	4482	FAD	P-O3P-PA-O1A
3	G	4482	FAD	O4B-C4B-C5B-O5B
3	K	7482	FAD	P-O3P-PA-O1A
3	D	2482	FAD	O4B-C4B-C5B-O5B
3	D	2482	FAD	P-O3P-PA-O2A
3	K	7482	FAD	P-O3P-PA-O2A
3	B	1482	FAD	O4B-C4B-C5B-O5B
3	H	5482	FAD	O4B-C4B-C5B-O5B

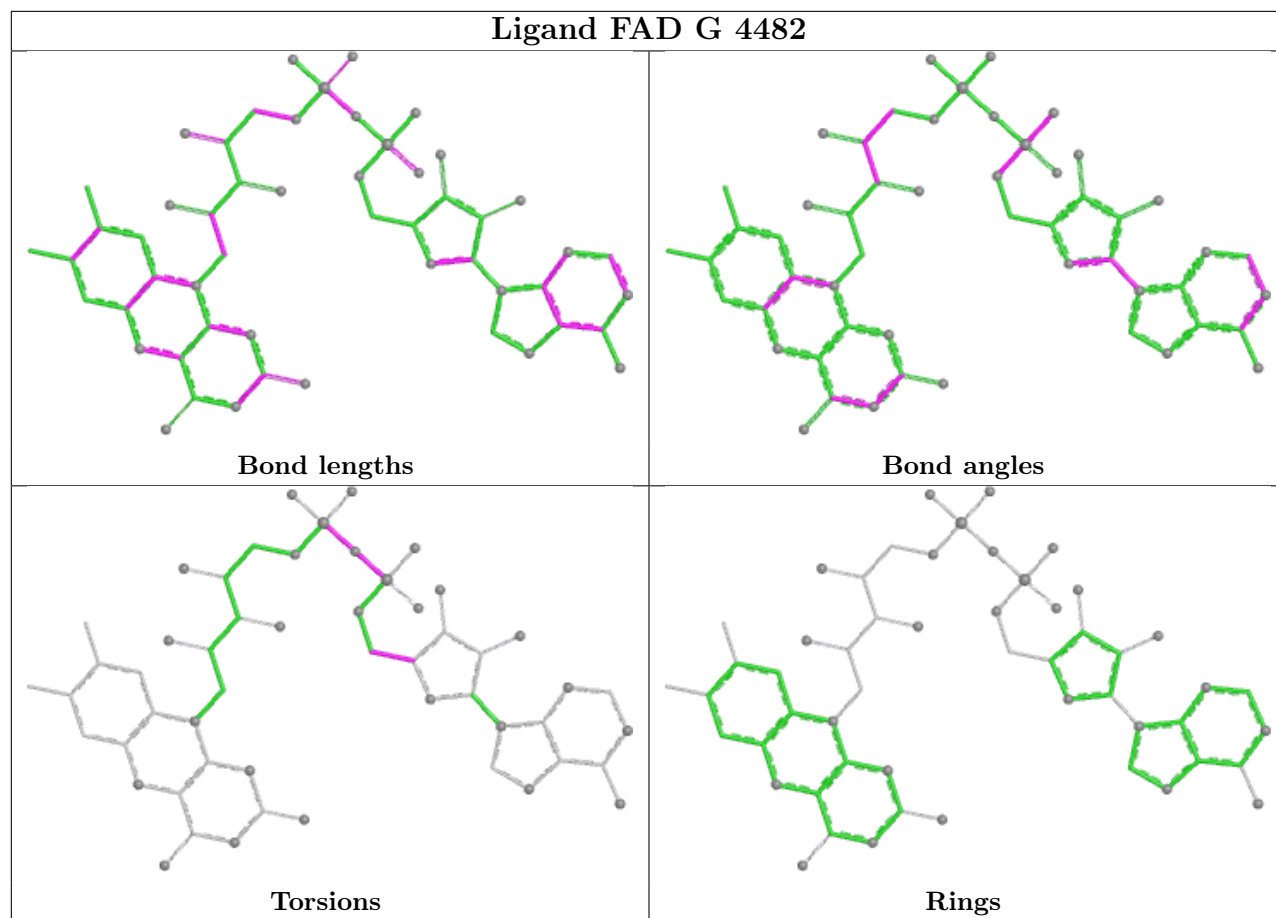
There are no ring outliers.

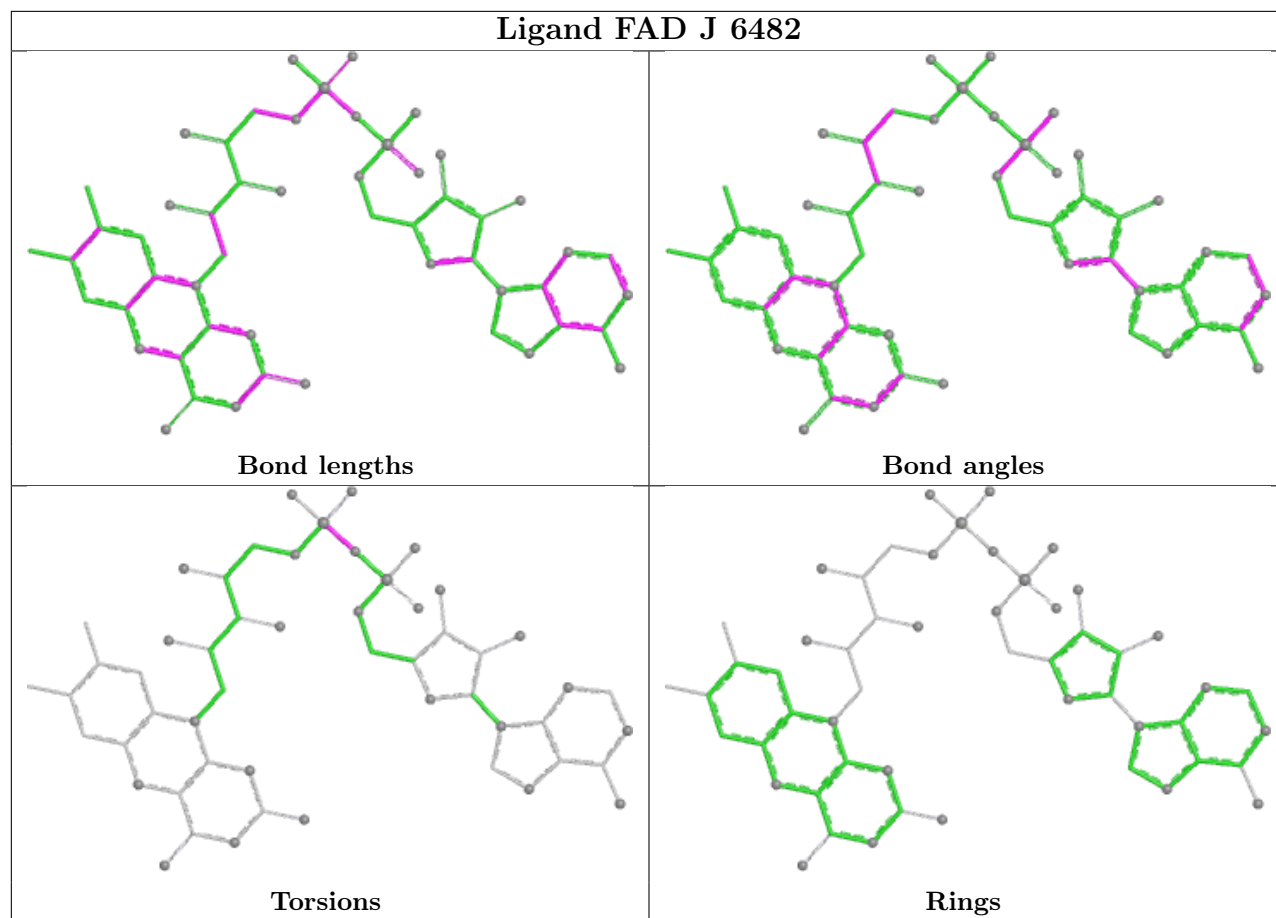
4 monomers are involved in 7 short contacts:

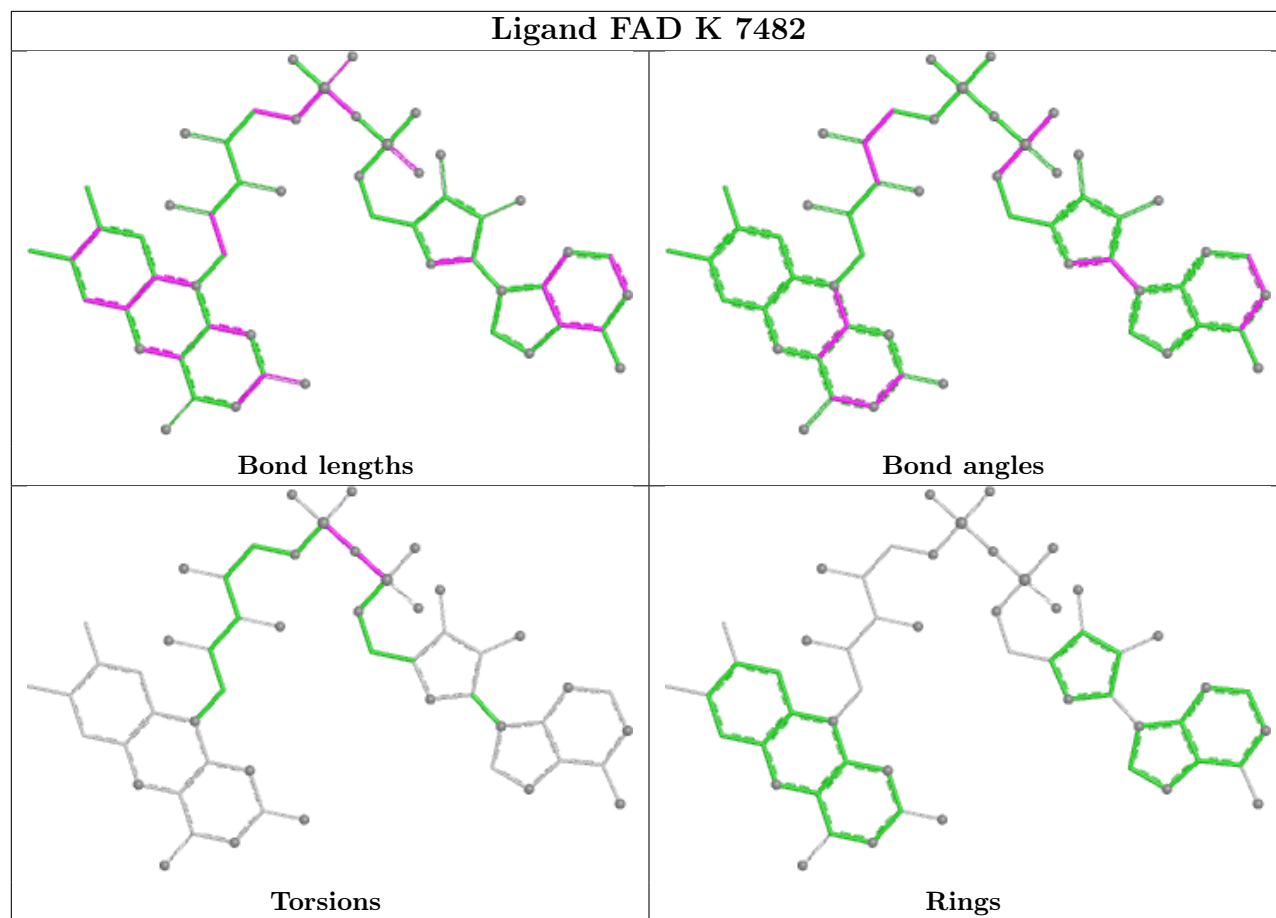
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	8482	FAD	2	0
3	G	4482	FAD	1	0
3	K	7482	FAD	3	0
3	D	2482	FAD	1	0

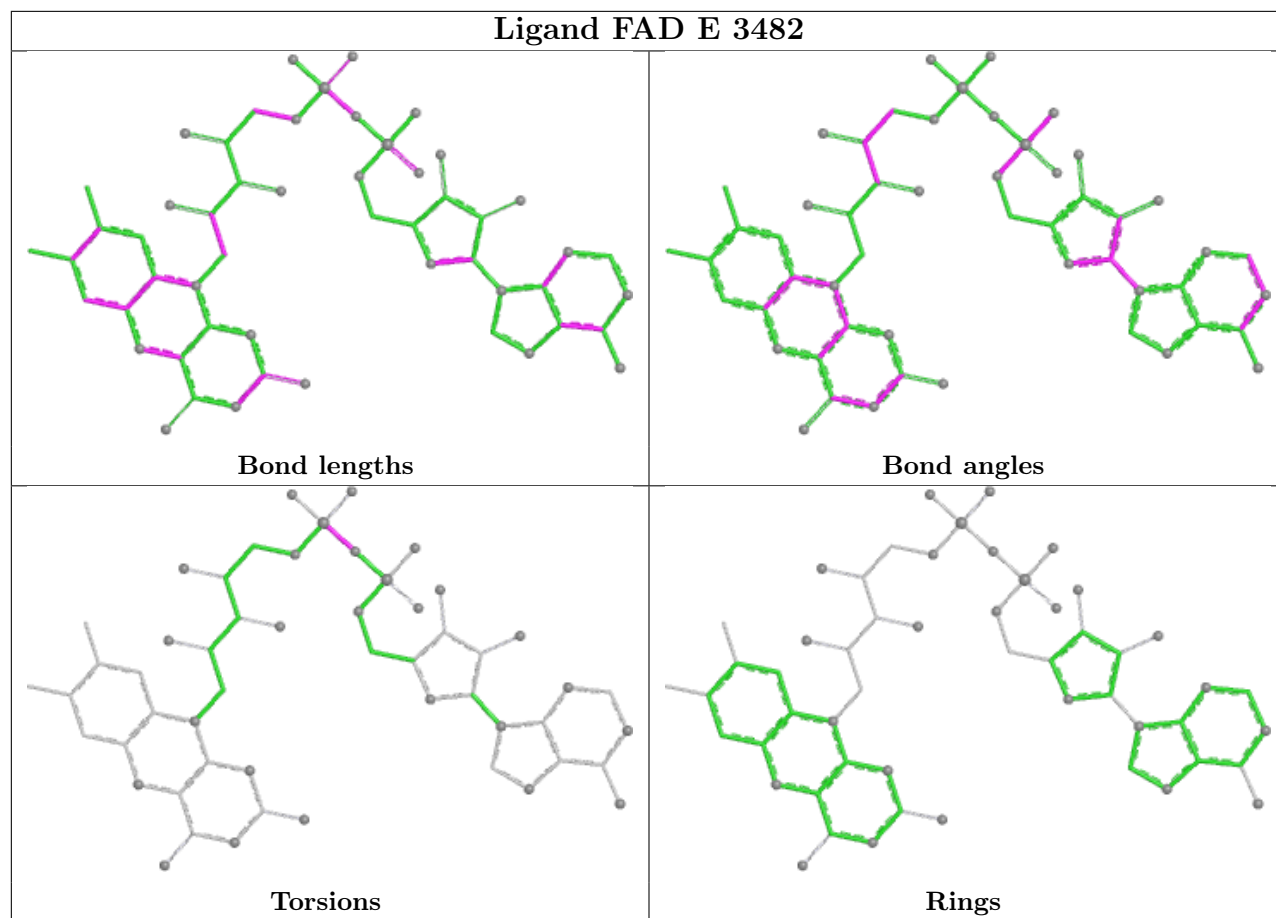
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

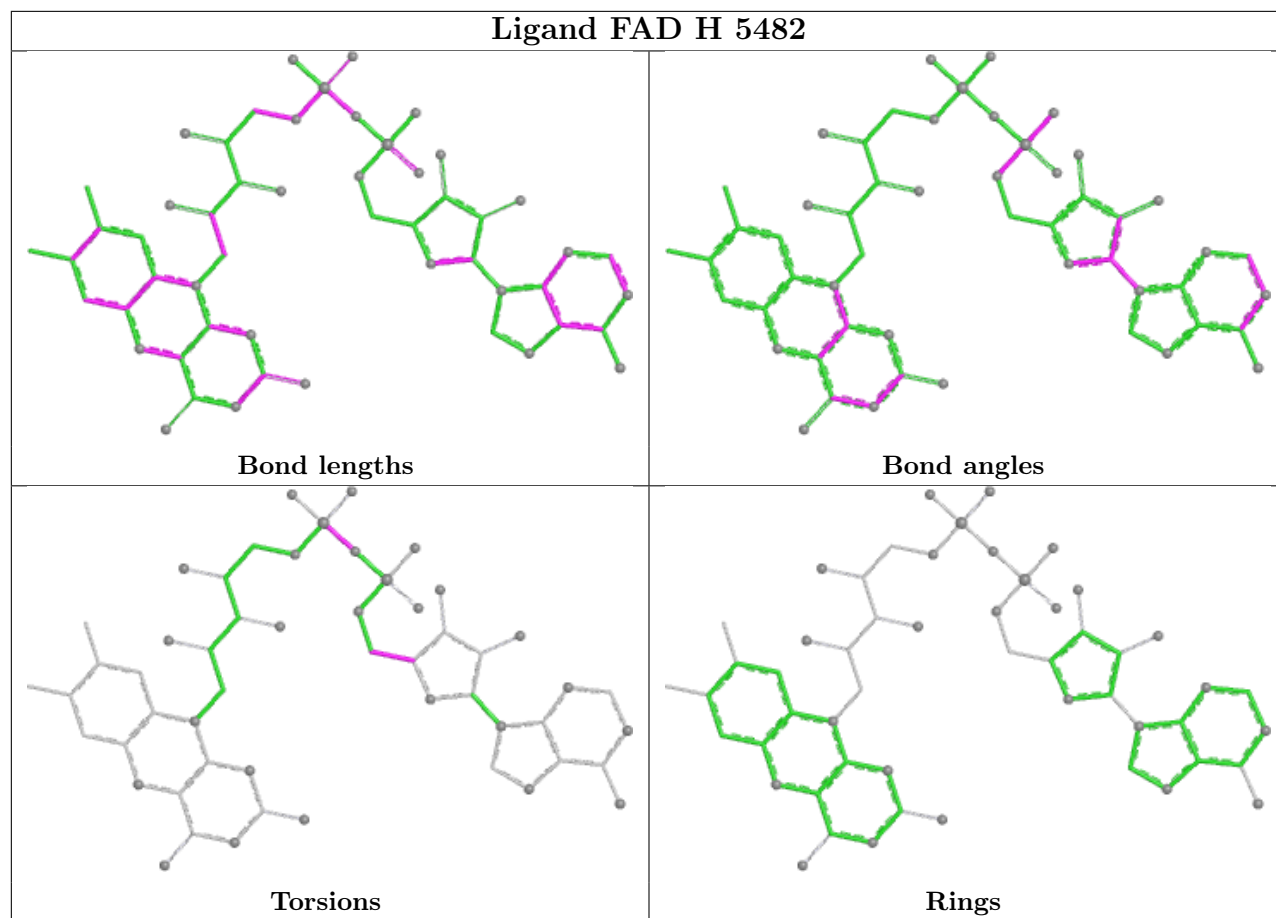


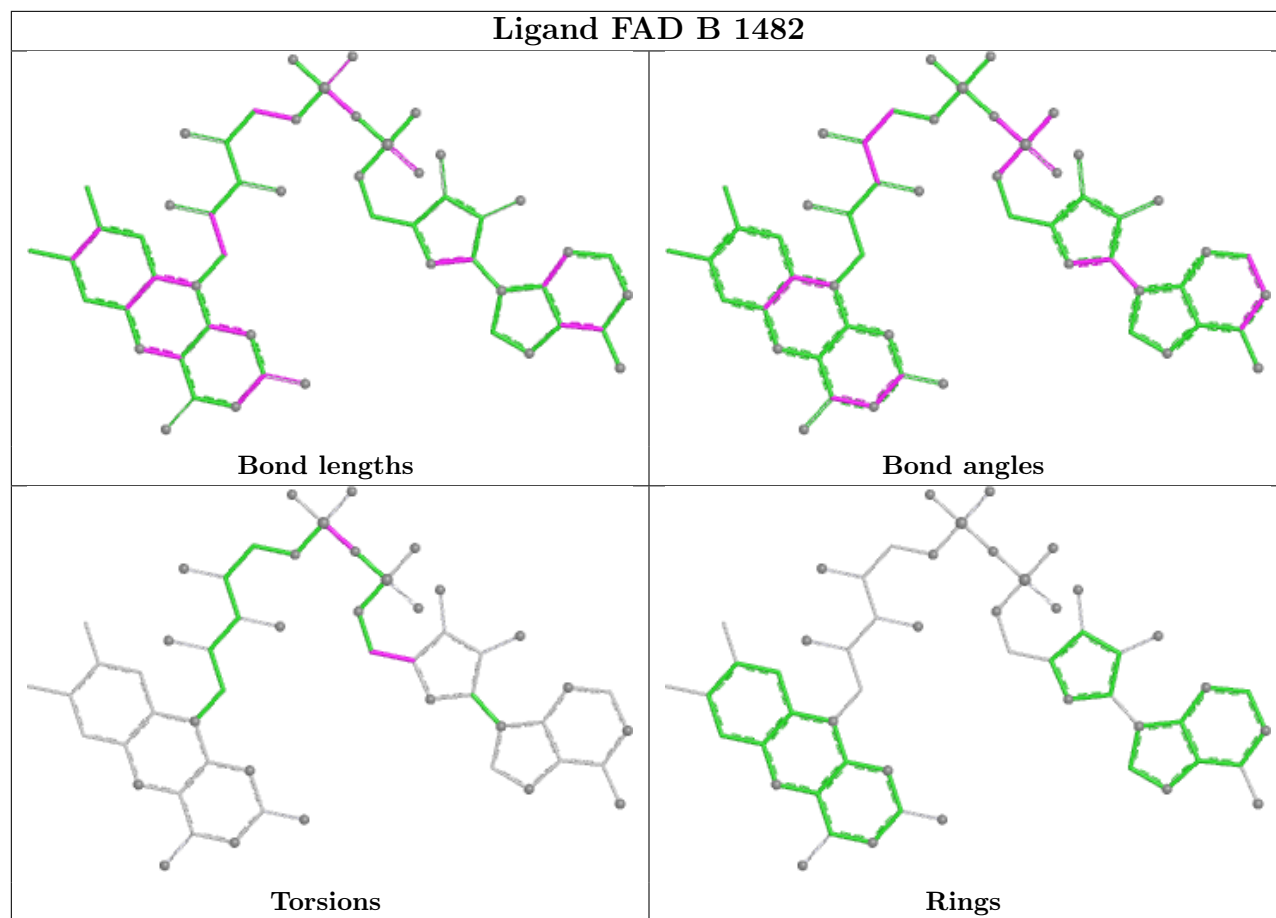


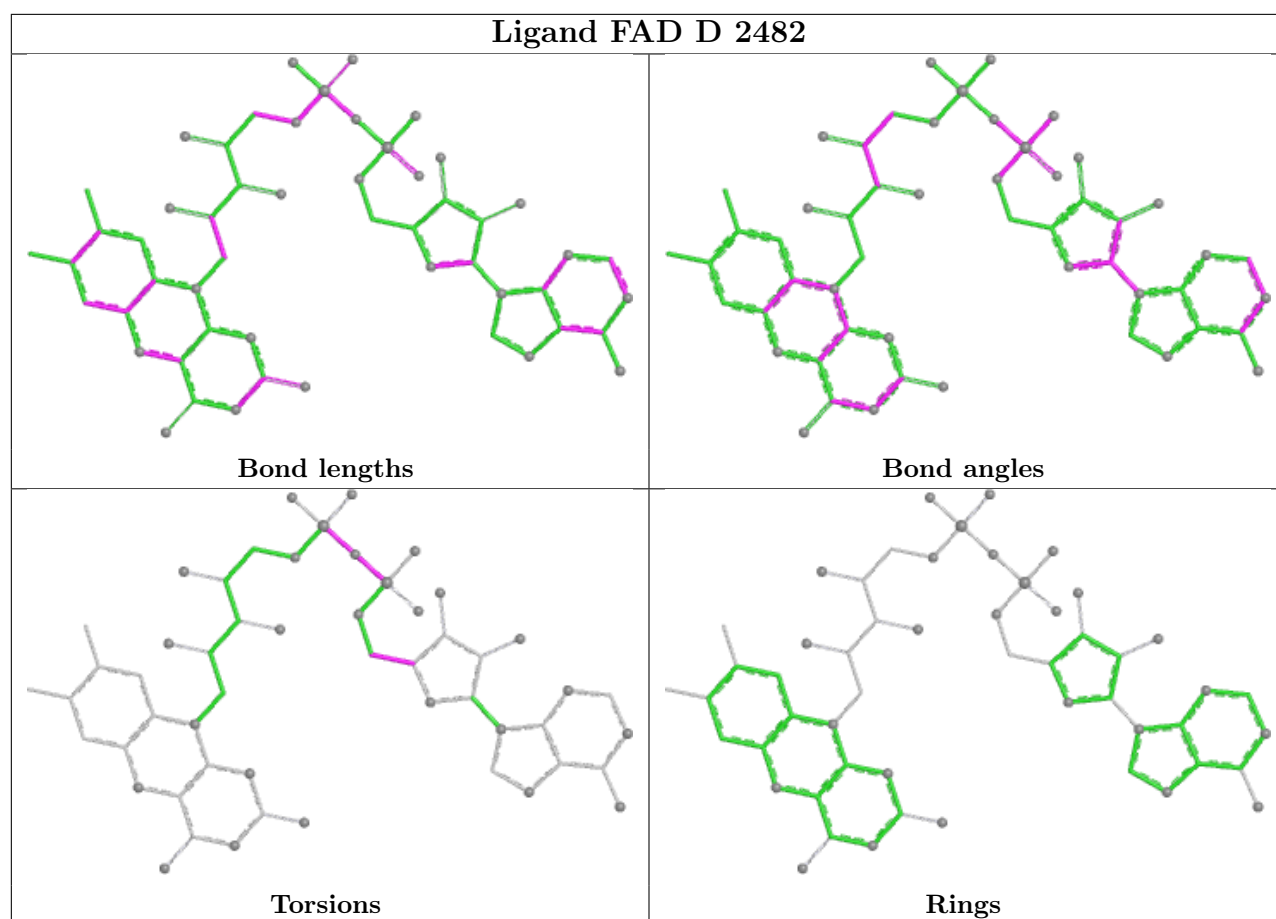












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	460/464 (99%)	0.25	18 (3%) 43 45	25, 38, 63, 79	0
1	B	460/464 (99%)	0.15	8 (1%) 69 71	24, 38, 55, 69	0
1	D	460/464 (99%)	0.11	20 (4%) 40 41	23, 34, 62, 80	0
1	E	460/464 (99%)	0.22	17 (3%) 45 47	22, 38, 70, 85	0
1	G	460/464 (99%)	0.17	20 (4%) 40 41	24, 36, 61, 76	0
1	H	460/464 (99%)	0.10	8 (1%) 69 71	24, 35, 55, 73	0
1	J	460/464 (99%)	0.69	76 (16%) 4 4	24, 40, 77, 99	0
1	K	460/464 (99%)	1.05	82 (17%) 4 4	26, 49, 87, 101	0
2	C	40/41 (97%)	0.99	5 (12%) 8 8	33, 55, 74, 76	0
2	F	40/41 (97%)	2.06	20 (50%) 0 0	54, 74, 86, 90	0
2	I	40/41 (97%)	1.92	16 (40%) 1 1	45, 76, 90, 91	0
2	L	40/41 (97%)	1.86	18 (45%) 0 1	47, 77, 87, 88	0
All	All	3840/3876 (99%)	0.40	308 (8%) 18 19	22, 38, 73, 101	0

All (308) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	394	ALA	8.3
2	I	155	LEU	7.6
1	E	394	ALA	6.8
1	J	127	VAL	6.5
1	B	394	ALA	6.5
1	K	127	VAL	6.2
1	J	139	GLY	6.0
1	K	283	LEU	5.8
1	K	286	ALA	5.5
1	J	12	LEU	5.3
1	J	122	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	J	124	PRO	5.2
1	J	13	ILE	5.2
1	A	394	ALA	5.1
1	J	140	ALA	5.1
1	K	124	PRO	5.1
2	L	155	LEU	5.1
1	J	119	ALA	5.0
1	J	283	LEU	5.0
2	L	142	LEU	5.0
1	J	10	TYR	5.0
1	K	119	ALA	5.0
1	E	286	ALA	4.8
1	E	122	VAL	4.8
1	K	121	LEU	4.8
1	J	32	GLY	4.8
1	J	142	SER	4.8
1	K	281	LEU	4.7
2	F	155	LEU	4.7
2	I	129	MET	4.7
2	F	163	VAL	4.6
1	J	129	VAL	4.5
1	J	134	GLY	4.5
1	K	312	ILE	4.4
1	J	138	TYR	4.4
1	G	394	ALA	4.4
1	K	10	TYR	4.3
2	I	154	PRO	4.3
1	K	38	VAL	4.3
1	K	135	GLY	4.2
1	K	285	LYS	4.2
1	K	296	ILE	4.2
1	K	15	ILE	4.2
1	A	122	VAL	4.2
1	A	286	ALA	4.1
1	J	114	LEU	4.1
1	J	286	ALA	4.1
1	K	118	PHE	4.1
1	J	306	VAL	4.1
1	J	126	GLU	4.0
2	I	153	GLY	4.0
1	J	394	ALA	3.9
1	K	129	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
2	C	155	LEU	3.9
1	E	288	VAL	3.8
1	K	288	VAL	3.8
1	K	122	VAL	3.8
1	K	138	TYR	3.8
1	G	281	LEU	3.8
1	D	394	ALA	3.7
1	K	289	LYS	3.7
1	E	257	GLY	3.7
1	K	142	SER	3.7
1	J	120	ARG	3.7
1	J	282	GLY	3.7
1	J	393	GLY	3.7
1	D	122	VAL	3.6
1	J	35	VAL	3.6
1	K	120	ARG	3.6
1	K	293	ARG	3.6
1	K	290	VAL	3.6
1	K	394	ALA	3.6
1	J	9	THR	3.6
1	J	33	LEU	3.6
1	J	281	LEU	3.6
1	G	122	VAL	3.5
1	J	309	VAL	3.5
2	F	168	GLU	3.5
2	F	154	PRO	3.5
1	D	121	LEU	3.5
1	E	121	LEU	3.5
1	E	287	GLY	3.5
1	J	121	LEU	3.5
1	H	124	PRO	3.4
1	K	123	GLY	3.4
1	J	143	LEU	3.4
2	I	163	VAL	3.4
2	C	154	PRO	3.4
1	E	120	ARG	3.4
1	K	140	ALA	3.4
1	A	285	LYS	3.4
1	K	143	LEU	3.4
2	L	138	LEU	3.4
1	H	257	GLY	3.4
1	J	280	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	K	134	GLY	3.3
1	K	13	ILE	3.3
1	K	115	LEU	3.3
2	I	156	GLY	3.3
1	K	287	GLY	3.3
1	B	135	GLY	3.2
2	C	153	GLY	3.2
1	J	288	VAL	3.2
1	D	124	PRO	3.2
1	K	137	ARG	3.2
1	K	144	ILE	3.2
2	F	144	ILE	3.2
2	F	153	GLY	3.2
2	F	156	GLY	3.2
1	K	136	GLU	3.2
1	J	285	LYS	3.2
1	E	290	VAL	3.1
1	E	337	ALA	3.1
1	K	37	ALA	3.1
1	J	128	GLU	3.1
2	L	154	PRO	3.1
1	E	283	LEU	3.1
1	B	260	GLY	3.1
1	J	304	THR	3.1
1	D	78	ALA	3.1
2	L	129	MET	3.1
1	K	126	GLU	3.0
1	G	121	LEU	3.0
1	K	36	LEU	3.0
1	J	305	SER	3.0
1	K	9	THR	3.0
1	D	284	GLU	3.0
1	J	118	PHE	3.0
2	I	168	GLU	3.0
1	K	310	TYR	3.0
1	D	281	LEU	3.0
1	K	32	GLY	3.0
2	F	146	ILE	3.0
1	G	127	VAL	2.9
1	J	117	GLY	2.9
1	J	287	GLY	2.9
1	K	278	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	78	ALA	2.9
2	L	135	ALA	2.9
1	J	8	LYS	2.9
1	J	36	LEU	2.9
1	K	272	VAL	2.9
1	G	120	ARG	2.9
1	D	126	GLU	2.9
1	B	127	VAL	2.9
1	K	257	GLY	2.9
2	I	130	LEU	2.8
1	K	14	VAL	2.8
1	A	120	ARG	2.8
1	K	12	LEU	2.8
1	K	33	LEU	2.8
1	J	469	ASN	2.8
2	L	156	GLY	2.8
2	L	146	ILE	2.8
1	K	282	GLY	2.8
1	K	393	GLY	2.8
1	K	8	LYS	2.8
1	J	26	ILE	2.8
1	J	144	ILE	2.8
1	J	336	ALA	2.7
1	J	7	MET	2.7
1	J	135	GLY	2.7
2	C	150	PRO	2.7
1	D	123	GLY	2.7
1	J	338	GLY	2.7
1	K	117	GLY	2.7
2	F	133	PRO	2.7
1	K	35	VAL	2.7
1	K	467	ILE	2.7
2	L	149	VAL	2.7
1	G	280	GLY	2.7
1	J	137	ARG	2.7
1	K	111	GLY	2.7
1	K	280	GLY	2.7
2	L	140	ARG	2.7
1	D	127	VAL	2.6
1	K	309	VAL	2.6
1	D	134	GLY	2.6
1	J	123	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	L	153	GLY	2.6
2	C	168	GLU	2.6
1	K	7	MET	2.6
1	A	392	GLY	2.6
1	G	287	GLY	2.6
1	B	290	VAL	2.6
2	F	158	VAL	2.6
2	I	144	ILE	2.6
2	I	142	LEU	2.6
1	J	331	ILE	2.5
2	I	160	VAL	2.5
2	L	163	VAL	2.5
1	J	310	TYR	2.5
1	K	125	LYS	2.5
1	K	141	LYS	2.5
1	K	469	ASN	2.5
1	A	281	LEU	2.5
1	K	128	GLU	2.5
1	A	284	GLU	2.5
1	J	29	ALA	2.5
1	J	37	ALA	2.5
1	K	305	SER	2.5
1	K	16	GLY	2.5
1	J	27	ARG	2.5
1	J	116	ARG	2.5
1	J	312	ILE	2.5
2	L	144	ILE	2.5
1	K	284	GLU	2.5
2	L	152	SER	2.5
1	J	300	ALA	2.5
2	F	134	ALA	2.5
2	I	150	PRO	2.5
2	F	138	LEU	2.5
1	E	127	VAL	2.4
1	K	340	ASP	2.4
1	E	281	LEU	2.4
1	K	152	LEU	2.4
1	D	393	GLY	2.4
1	E	295	PHE	2.4
1	H	393	GLY	2.4
2	I	146	ILE	2.4
1	D	286	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	289	LYS	2.4
1	J	31	LEU	2.4
1	J	136	GLU	2.4
1	H	256(A)	ALA	2.4
1	G	283	LEU	2.4
1	A	306	VAL	2.4
1	K	207	TYR	2.3
1	G	78	ALA	2.3
2	L	168	GLU	2.3
1	B	121	LEU	2.3
1	D	283	LEU	2.3
1	J	145	LEU	2.3
1	D	135	GLY	2.3
1	J	308	GLY	2.3
1	K	139	GLY	2.3
1	K	145	LEU	2.3
1	K	294	GLY	2.3
1	H	120	ARG	2.3
2	F	129	MET	2.3
1	J	284	GLU	2.3
1	J	333	ALA	2.3
1	A	257	GLY	2.3
1	K	106	LEU	2.3
1	K	107	LEU	2.3
2	F	152	SER	2.3
2	I	152	SER	2.3
1	G	469	ASN	2.3
1	G	286	ALA	2.3
2	I	165	ALA	2.3
1	A	393	GLY	2.3
1	A	121	LEU	2.3
1	J	115	LEU	2.3
1	A	126	GLU	2.2
1	D	288	VAL	2.2
1	K	306	VAL	2.2
1	J	125	LYS	2.2
1	J	141	LYS	2.2
1	J	109	GLY	2.2
1	K	24	ALA	2.2
1	K	148	GLY	2.2
1	K	303	GLU	2.2
1	G	392	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	78	ALA	2.2
1	K	315	ALA	2.2
1	A	283	LEU	2.2
2	F	130	LEU	2.2
1	J	11	ASP	2.2
1	A	290	VAL	2.2
1	G	288	VAL	2.2
1	J	14	VAL	2.2
2	F	160	VAL	2.2
1	D	280	GLY	2.2
1	G	395	GLU	2.2
1	K	114	LEU	2.2
2	F	140	ARG	2.2
1	K	276	PRO	2.1
1	B	395	GLU	2.1
1	E	282	GLY	2.1
2	L	139	ALA	2.1
1	D	120	ARG	2.1
1	J	175	LEU	2.1
1	A	141	LYS	2.1
1	G	285	LYS	2.1
1	J	307	PRO	2.1
1	K	182	ILE	2.1
1	D	285	LYS	2.1
1	D	395	GLU	2.1
1	E	279	GLU	2.1
1	J	105	THR	2.1
1	G	293	ARG	2.1
1	K	313	GLY	2.1
1	A	127	VAL	2.1
1	H	127	VAL	2.1
1	J	290	VAL	2.1
1	J	337	ALA	2.1
2	L	165	ALA	2.1
1	E	10	TYR	2.1
2	F	145	PRO	2.1
2	I	145	PRO	2.1
2	F	132	VAL	2.1
1	H	7	MET	2.0
1	K	261	GLU	2.0
2	F	142	LEU	2.0
2	L	130	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	290	VAL	2.0
1	G	7	MET	2.0
1	B	281	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

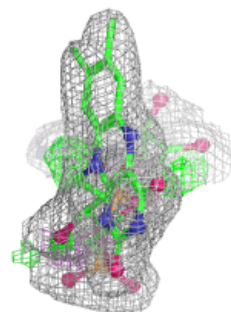
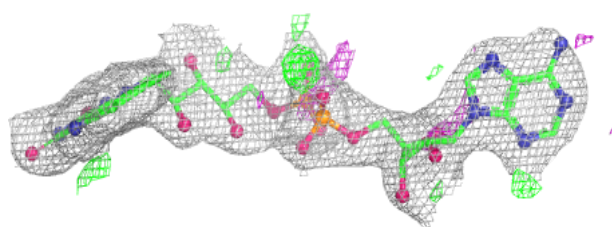
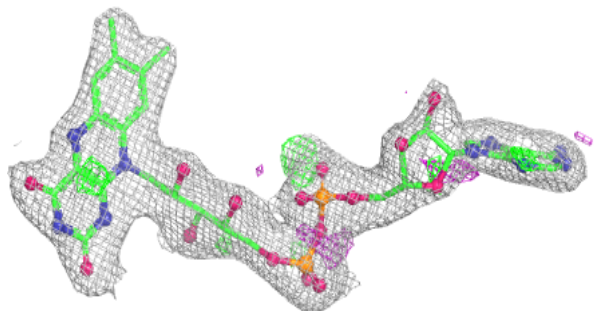
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FAD	K	7482	53/53	0.91	0.10	40,45,56,56	0
3	FAD	J	6482	53/53	0.94	0.07	30,34,40,41	0
3	FAD	G	4482	53/53	0.95	0.07	29,34,42,44	0
3	FAD	A	8482	53/53	0.96	0.07	28,34,40,41	0
3	FAD	H	5482	53/53	0.96	0.07	25,29,32,33	0
3	FAD	B	1482	53/53	0.96	0.07	33,37,43,44	0
3	FAD	E	3482	53/53	0.96	0.07	31,36,43,43	0
3	FAD	D	2482	53/53	0.97	0.06	26,30,40,41	0

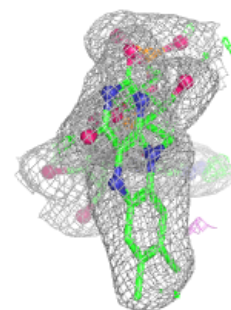
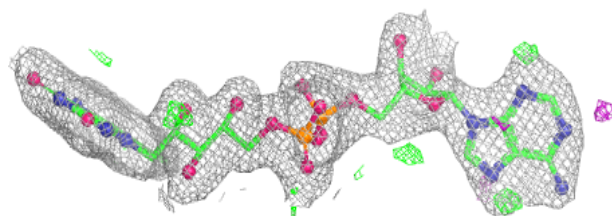
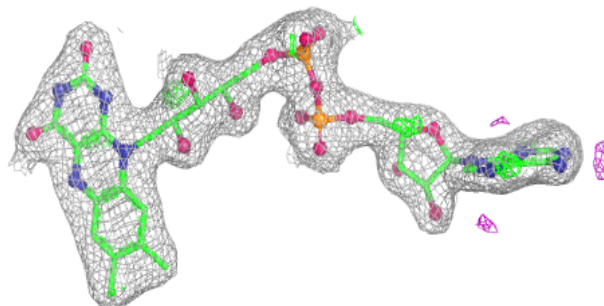
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

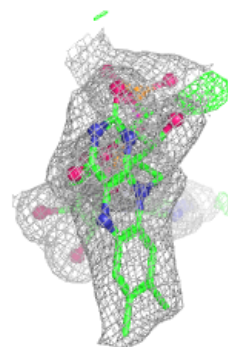
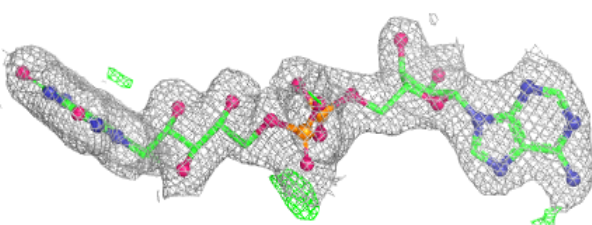
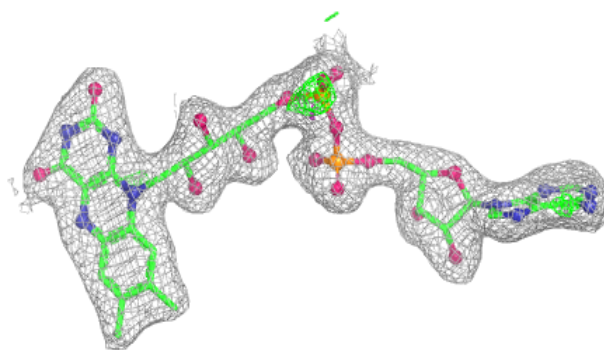
**Electron density around FAD J 6482:**

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

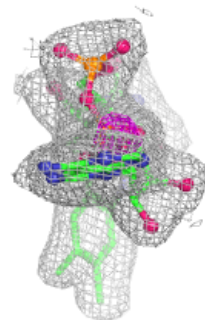
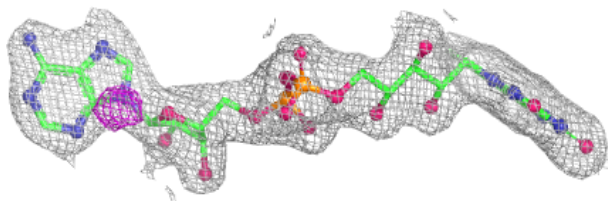
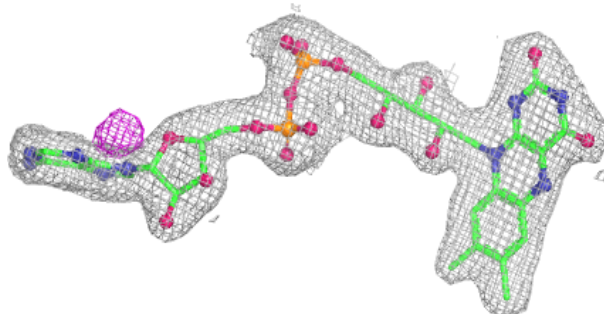


Electron density around FAD G 4482:

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

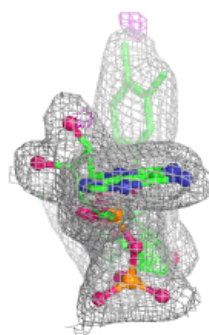
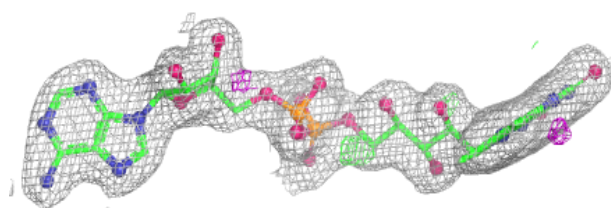
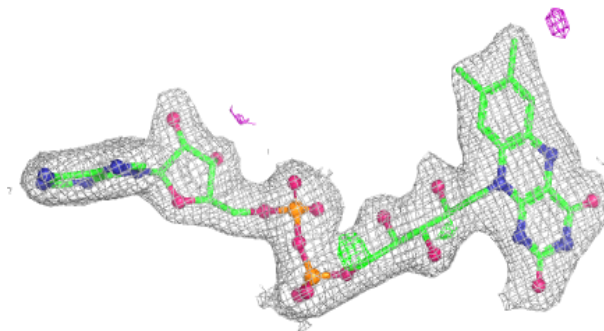
**Electron density around FAD A 8482:**

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

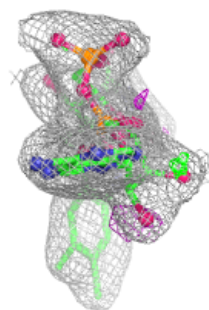
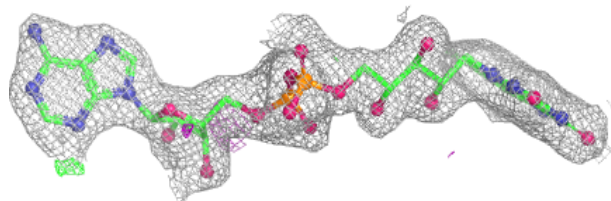
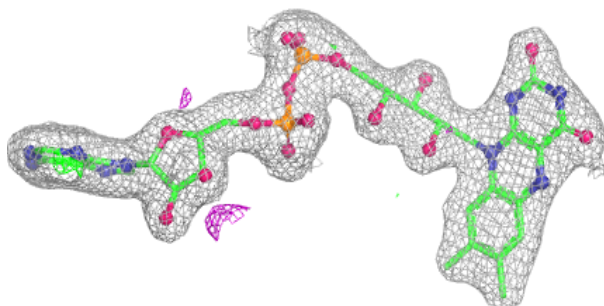


Electron density around FAD H 5482:

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

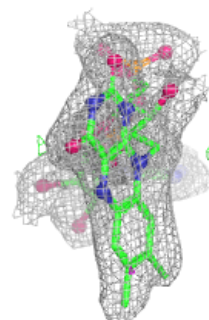
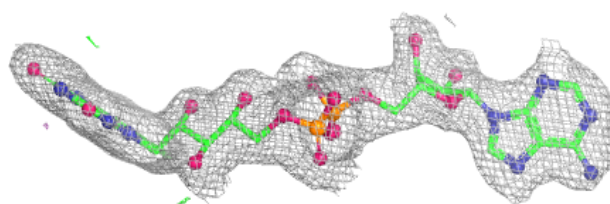
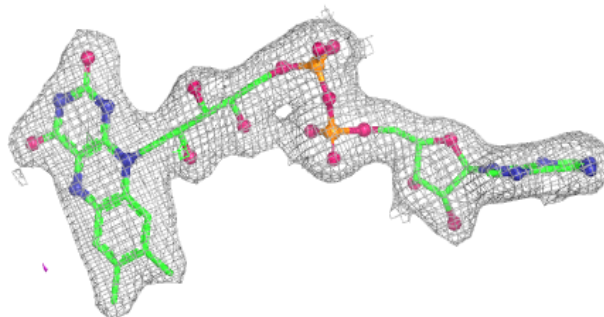
**Electron density around FAD B 1482:**

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

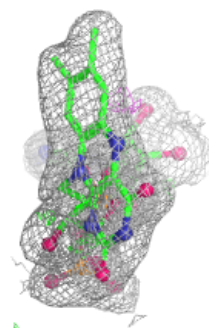
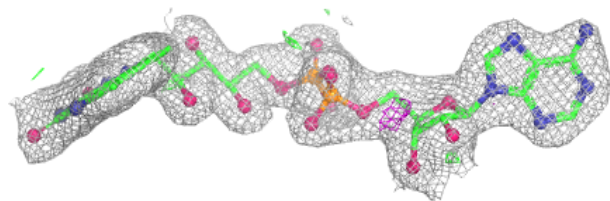
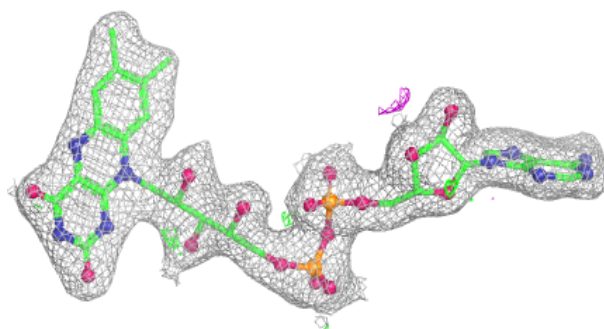


Electron density around FAD E 3482:

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

**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)



6.5 Other polymers ⓘ

There are no such residues in this entry.