



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:07 AM UTC

PDB ID : 6I4Z / pdb_00006i4z
Title : Crystal structure of the disease-causing P453L mutant of the human dihydroliipoamide dehydrogenase
Authors : Szabo, E.; Wilk, P.; Torocsik, B.; Weiss, M.S.; Adam-Vizi, V.; Ambrus, A.
Deposited on : 2018-11-12
Resolution : 2.34 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:

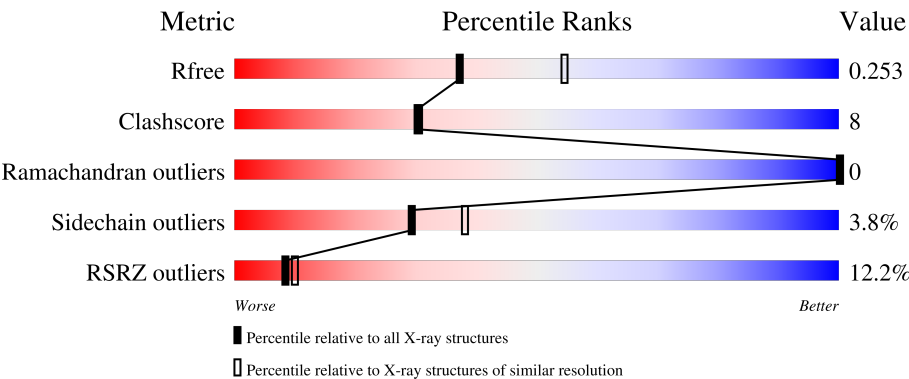
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	496	% 81%12%• 5%
1	B	496	16% 75%18%• 5%
1	C	496	2% 84%10%• 5%
1	D	496	21% 74%19%• 5%
1	E	496	15% 77%18%• 5%

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Mol	Chain	Length	Quality of chain
1	F	496	
1	G	496	
1	H	496	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	506	-	-	X	-
3	SO4	E	502	-	-	X	-
3	SO4	G	503	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 57894 atoms, of which 28801 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 Dihydrolipoyl dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	472	Total	C	H	N	O	S	0	1	0
			7087	2215	3573	607	673	19			
1	B	472	Total	C	H	N	O	S	0	1	0
			7086	2215	3572	607	673	19			
1	C	472	Total	C	H	N	O	S	0	0	0
			7075	2211	3567	607	671	19			
1	D	472	Total	C	H	N	O	S	0	0	0
			7075	2211	3567	607	671	19			
1	E	472	Total	C	H	N	O	S	0	1	0
			7086	2215	3572	607	673	19			
1	F	472	Total	C	H	N	O	S	0	0	0
			7075	2211	3567	607	671	19			
1	G	472	Total	C	H	N	O	S	0	0	0
			7076	2211	3568	607	671	19			
1	H	472	Total	C	H	N	O	S	0	0	0
			7075	2211	3567	607	671	19			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP P09622
A	-20	ALA	-	expression tag	UNP P09622
A	-19	SER	-	expression tag	UNP P09622
A	-18	TRP	-	expression tag	UNP P09622
A	-17	SER	-	expression tag	UNP P09622
A	-16	HIS	-	expression tag	UNP P09622
A	-15	PRO	-	expression tag	UNP P09622
A	-14	GLN	-	expression tag	UNP P09622
A	-13	PHE	-	expression tag	UNP P09622
A	-12	GLU	-	expression tag	UNP P09622
A	-11	LYS	-	expression tag	UNP P09622
A	-10	GLY	-	expression tag	UNP P09622
A	-9	ALA	-	expression tag	UNP P09622

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	LEU	-	expression tag	UNP P09622
A	-7	GLU	-	expression tag	UNP P09622
A	-6	VAL	-	expression tag	UNP P09622
A	-5	LEU	-	expression tag	UNP P09622
A	-4	PHE	-	expression tag	UNP P09622
A	-3	GLN	-	expression tag	UNP P09622
A	-2	GLY	-	expression tag	UNP P09622
A	-1	PRO	-	expression tag	UNP P09622
A	0	GLY	-	expression tag	UNP P09622
A	453	LEU	PRO	engineered mutation	UNP P09622
B	-21	MET	-	initiating methionine	UNP P09622
B	-20	ALA	-	expression tag	UNP P09622
B	-19	SER	-	expression tag	UNP P09622
B	-18	TRP	-	expression tag	UNP P09622
B	-17	SER	-	expression tag	UNP P09622
B	-16	HIS	-	expression tag	UNP P09622
B	-15	PRO	-	expression tag	UNP P09622
B	-14	GLN	-	expression tag	UNP P09622
B	-13	PHE	-	expression tag	UNP P09622
B	-12	GLU	-	expression tag	UNP P09622
B	-11	LYS	-	expression tag	UNP P09622
B	-10	GLY	-	expression tag	UNP P09622
B	-9	ALA	-	expression tag	UNP P09622
B	-8	LEU	-	expression tag	UNP P09622
B	-7	GLU	-	expression tag	UNP P09622
B	-6	VAL	-	expression tag	UNP P09622
B	-5	LEU	-	expression tag	UNP P09622
B	-4	PHE	-	expression tag	UNP P09622
B	-3	GLN	-	expression tag	UNP P09622
B	-2	GLY	-	expression tag	UNP P09622
B	-1	PRO	-	expression tag	UNP P09622
B	0	GLY	-	expression tag	UNP P09622
B	453	LEU	PRO	engineered mutation	UNP P09622
C	-21	MET	-	initiating methionine	UNP P09622
C	-20	ALA	-	expression tag	UNP P09622
C	-19	SER	-	expression tag	UNP P09622
C	-18	TRP	-	expression tag	UNP P09622
C	-17	SER	-	expression tag	UNP P09622
C	-16	HIS	-	expression tag	UNP P09622
C	-15	PRO	-	expression tag	UNP P09622
C	-14	GLN	-	expression tag	UNP P09622
C	-13	PHE	-	expression tag	UNP P09622

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	GLU	-	expression tag	UNP P09622
C	-11	LYS	-	expression tag	UNP P09622
C	-10	GLY	-	expression tag	UNP P09622
C	-9	ALA	-	expression tag	UNP P09622
C	-8	LEU	-	expression tag	UNP P09622
C	-7	GLU	-	expression tag	UNP P09622
C	-6	VAL	-	expression tag	UNP P09622
C	-5	LEU	-	expression tag	UNP P09622
C	-4	PHE	-	expression tag	UNP P09622
C	-3	GLN	-	expression tag	UNP P09622
C	-2	GLY	-	expression tag	UNP P09622
C	-1	PRO	-	expression tag	UNP P09622
C	0	GLY	-	expression tag	UNP P09622
C	453	LEU	PRO	engineered mutation	UNP P09622
D	-21	MET	-	initiating methionine	UNP P09622
D	-20	ALA	-	expression tag	UNP P09622
D	-19	SER	-	expression tag	UNP P09622
D	-18	TRP	-	expression tag	UNP P09622
D	-17	SER	-	expression tag	UNP P09622
D	-16	HIS	-	expression tag	UNP P09622
D	-15	PRO	-	expression tag	UNP P09622
D	-14	GLN	-	expression tag	UNP P09622
D	-13	PHE	-	expression tag	UNP P09622
D	-12	GLU	-	expression tag	UNP P09622
D	-11	LYS	-	expression tag	UNP P09622
D	-10	GLY	-	expression tag	UNP P09622
D	-9	ALA	-	expression tag	UNP P09622
D	-8	LEU	-	expression tag	UNP P09622
D	-7	GLU	-	expression tag	UNP P09622
D	-6	VAL	-	expression tag	UNP P09622
D	-5	LEU	-	expression tag	UNP P09622
D	-4	PHE	-	expression tag	UNP P09622
D	-3	GLN	-	expression tag	UNP P09622
D	-2	GLY	-	expression tag	UNP P09622
D	-1	PRO	-	expression tag	UNP P09622
D	0	GLY	-	expression tag	UNP P09622
D	453	LEU	PRO	engineered mutation	UNP P09622
E	-21	MET	-	initiating methionine	UNP P09622
E	-20	ALA	-	expression tag	UNP P09622
E	-19	SER	-	expression tag	UNP P09622
E	-18	TRP	-	expression tag	UNP P09622
E	-17	SER	-	expression tag	UNP P09622

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-16	HIS	-	expression tag	UNP P09622
E	-15	PRO	-	expression tag	UNP P09622
E	-14	GLN	-	expression tag	UNP P09622
E	-13	PHE	-	expression tag	UNP P09622
E	-12	GLU	-	expression tag	UNP P09622
E	-11	LYS	-	expression tag	UNP P09622
E	-10	GLY	-	expression tag	UNP P09622
E	-9	ALA	-	expression tag	UNP P09622
E	-8	LEU	-	expression tag	UNP P09622
E	-7	GLU	-	expression tag	UNP P09622
E	-6	VAL	-	expression tag	UNP P09622
E	-5	LEU	-	expression tag	UNP P09622
E	-4	PHE	-	expression tag	UNP P09622
E	-3	GLN	-	expression tag	UNP P09622
E	-2	GLY	-	expression tag	UNP P09622
E	-1	PRO	-	expression tag	UNP P09622
E	0	GLY	-	expression tag	UNP P09622
E	453	LEU	PRO	engineered mutation	UNP P09622
F	-21	MET	-	initiating methionine	UNP P09622
F	-20	ALA	-	expression tag	UNP P09622
F	-19	SER	-	expression tag	UNP P09622
F	-18	TRP	-	expression tag	UNP P09622
F	-17	SER	-	expression tag	UNP P09622
F	-16	HIS	-	expression tag	UNP P09622
F	-15	PRO	-	expression tag	UNP P09622
F	-14	GLN	-	expression tag	UNP P09622
F	-13	PHE	-	expression tag	UNP P09622
F	-12	GLU	-	expression tag	UNP P09622
F	-11	LYS	-	expression tag	UNP P09622
F	-10	GLY	-	expression tag	UNP P09622
F	-9	ALA	-	expression tag	UNP P09622
F	-8	LEU	-	expression tag	UNP P09622
F	-7	GLU	-	expression tag	UNP P09622
F	-6	VAL	-	expression tag	UNP P09622
F	-5	LEU	-	expression tag	UNP P09622
F	-4	PHE	-	expression tag	UNP P09622
F	-3	GLN	-	expression tag	UNP P09622
F	-2	GLY	-	expression tag	UNP P09622
F	-1	PRO	-	expression tag	UNP P09622
F	0	GLY	-	expression tag	UNP P09622
F	453	LEU	PRO	engineered mutation	UNP P09622
G	-21	MET	-	initiating methionine	UNP P09622

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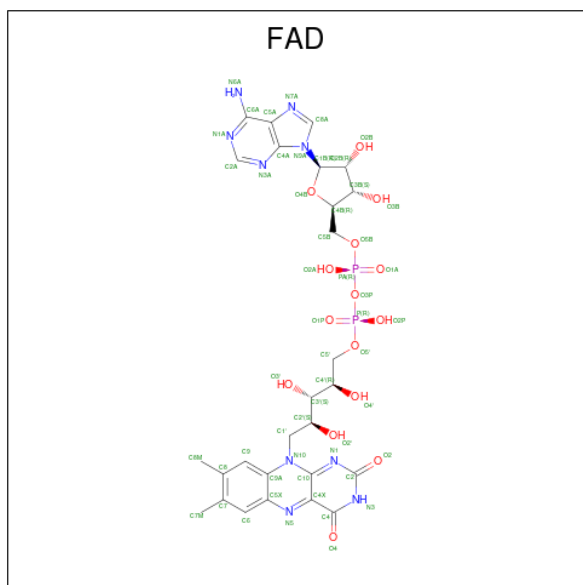
Chain	Residue	Modelled	Actual	Comment	Reference
G	-20	ALA	-	expression tag	UNP P09622
G	-19	SER	-	expression tag	UNP P09622
G	-18	TRP	-	expression tag	UNP P09622
G	-17	SER	-	expression tag	UNP P09622
G	-16	HIS	-	expression tag	UNP P09622
G	-15	PRO	-	expression tag	UNP P09622
G	-14	GLN	-	expression tag	UNP P09622
G	-13	PHE	-	expression tag	UNP P09622
G	-12	GLU	-	expression tag	UNP P09622
G	-11	LYS	-	expression tag	UNP P09622
G	-10	GLY	-	expression tag	UNP P09622
G	-9	ALA	-	expression tag	UNP P09622
G	-8	LEU	-	expression tag	UNP P09622
G	-7	GLU	-	expression tag	UNP P09622
G	-6	VAL	-	expression tag	UNP P09622
G	-5	LEU	-	expression tag	UNP P09622
G	-4	PHE	-	expression tag	UNP P09622
G	-3	GLN	-	expression tag	UNP P09622
G	-2	GLY	-	expression tag	UNP P09622
G	-1	PRO	-	expression tag	UNP P09622
G	0	GLY	-	expression tag	UNP P09622
G	453	LEU	PRO	engineered mutation	UNP P09622
H	-21	MET	-	initiating methionine	UNP P09622
H	-20	ALA	-	expression tag	UNP P09622
H	-19	SER	-	expression tag	UNP P09622
H	-18	TRP	-	expression tag	UNP P09622
H	-17	SER	-	expression tag	UNP P09622
H	-16	HIS	-	expression tag	UNP P09622
H	-15	PRO	-	expression tag	UNP P09622
H	-14	GLN	-	expression tag	UNP P09622
H	-13	PHE	-	expression tag	UNP P09622
H	-12	GLU	-	expression tag	UNP P09622
H	-11	LYS	-	expression tag	UNP P09622
H	-10	GLY	-	expression tag	UNP P09622
H	-9	ALA	-	expression tag	UNP P09622
H	-8	LEU	-	expression tag	UNP P09622
H	-7	GLU	-	expression tag	UNP P09622
H	-6	VAL	-	expression tag	UNP P09622
H	-5	LEU	-	expression tag	UNP P09622
H	-4	PHE	-	expression tag	UNP P09622
H	-3	GLN	-	expression tag	UNP P09622
H	-2	GLY	-	expression tag	UNP P09622

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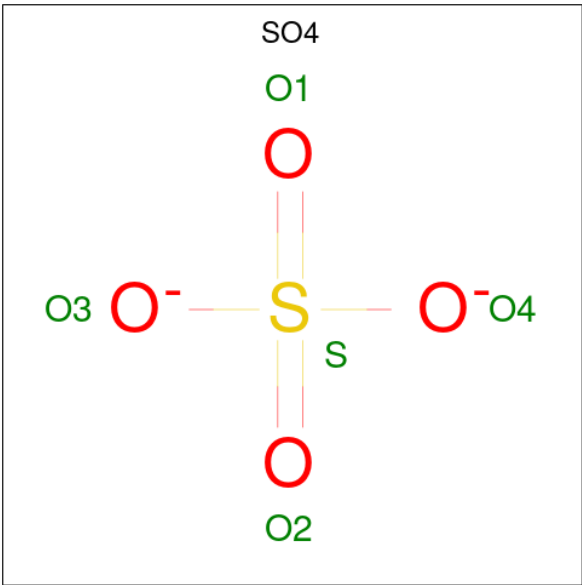
Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	PRO	-	expression tag	UNP P09622
H	0	GLY	-	expression tag	UNP P09622
H	453	LEU	PRO	engineered mutation	UNP P09622

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	B	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	C	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	D	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	E	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	F	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	G	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	H	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
3	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
3	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
3	B	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
3	B	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
3	C	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
3	C	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
3	C	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
3	D	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	124	Total	O	0	0
			124	124		
4	B	32	Total	O	0	0
			32	32		
4	C	120	Total	O	0	0
			120	120		
4	D	28	Total	O	0	0
			28	28		
4	E	41	Total	O	0	0
			41	41		
4	F	33	Total	O	0	0
			33	33		

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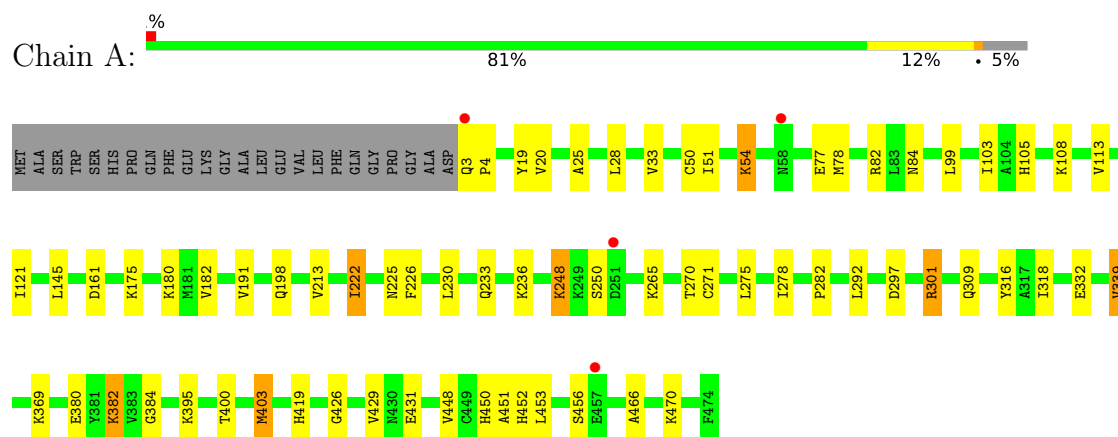
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	40	Total	O	0	0
			40	40		
4	H	34	Total	O	0	0
			34	34		

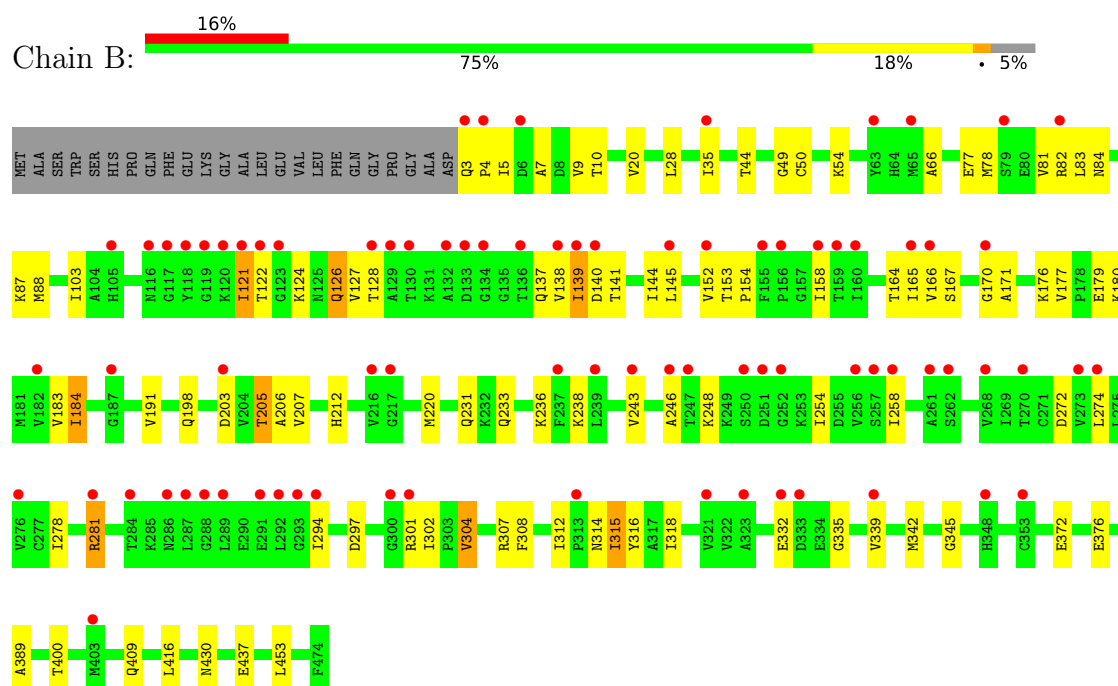
3 Residue-property plots [i](#)

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.

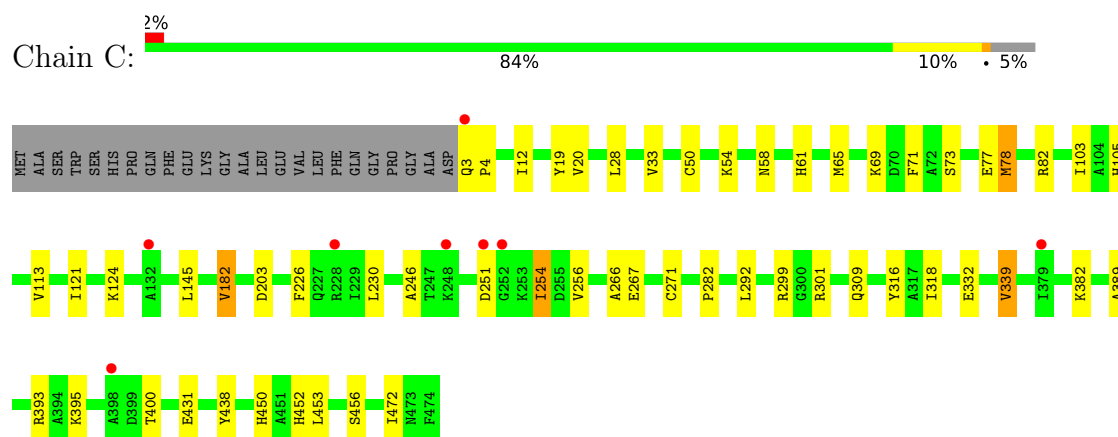
- Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial



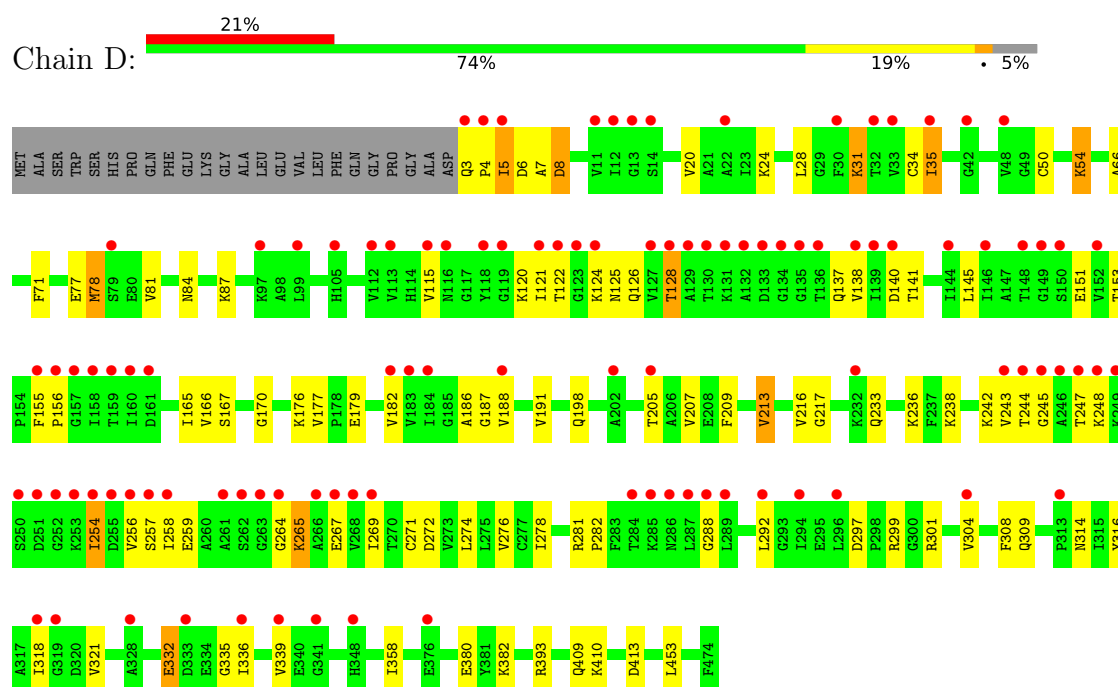
- Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial



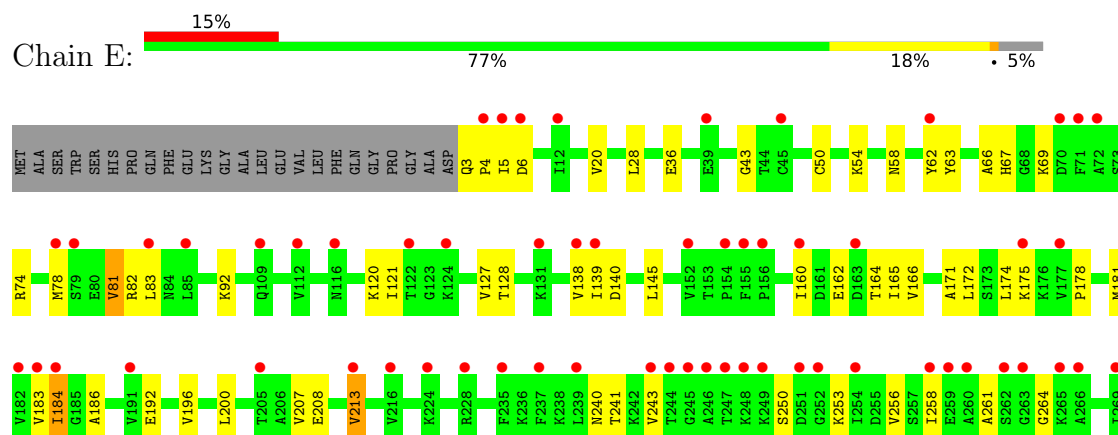
- Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

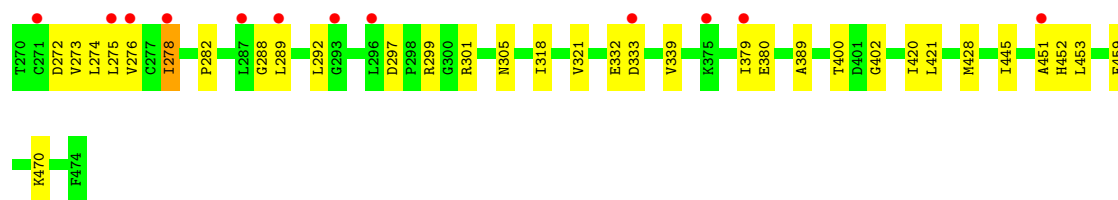


• Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial



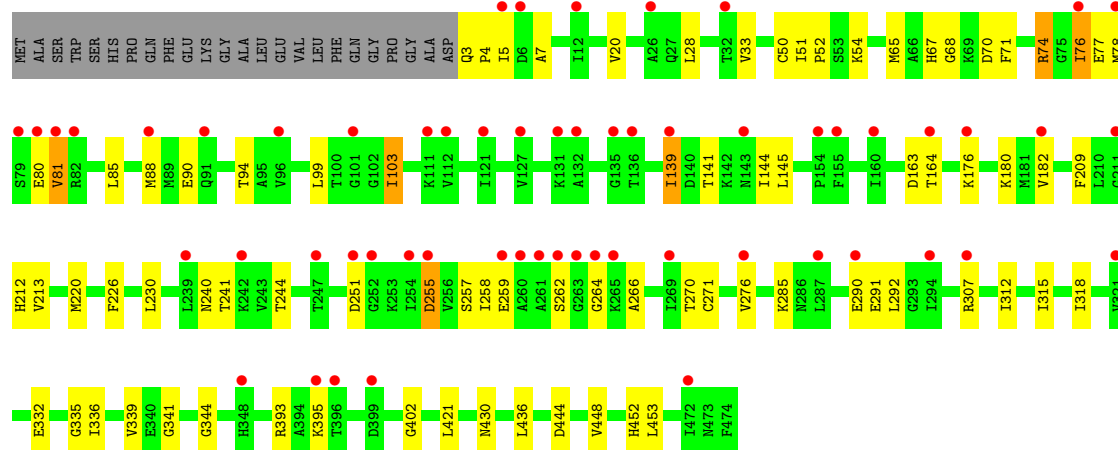
• Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial





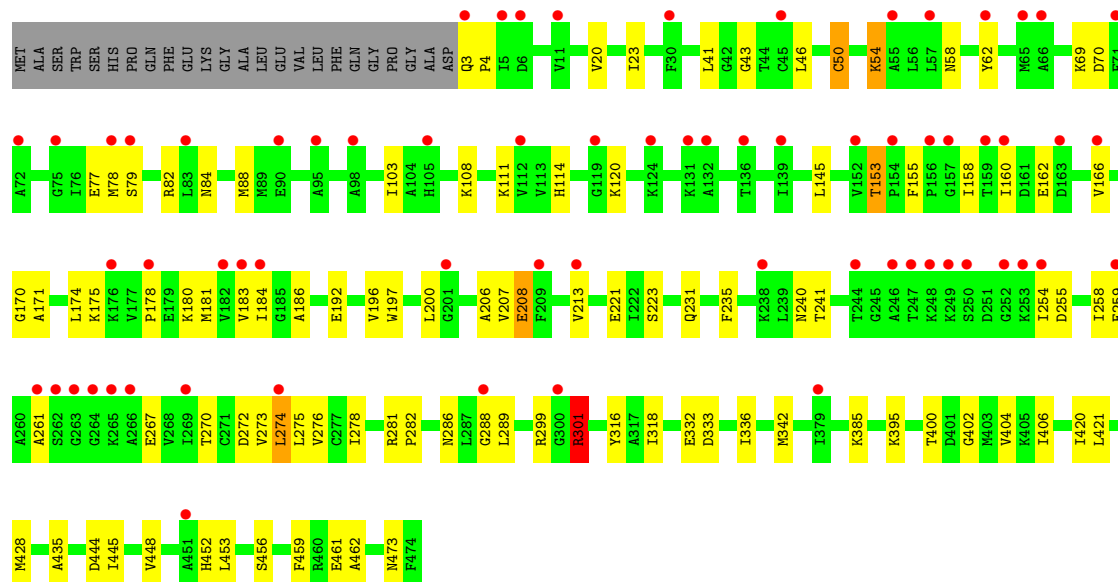
- Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

Chain F: 12% 79% 15% 5%



- Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

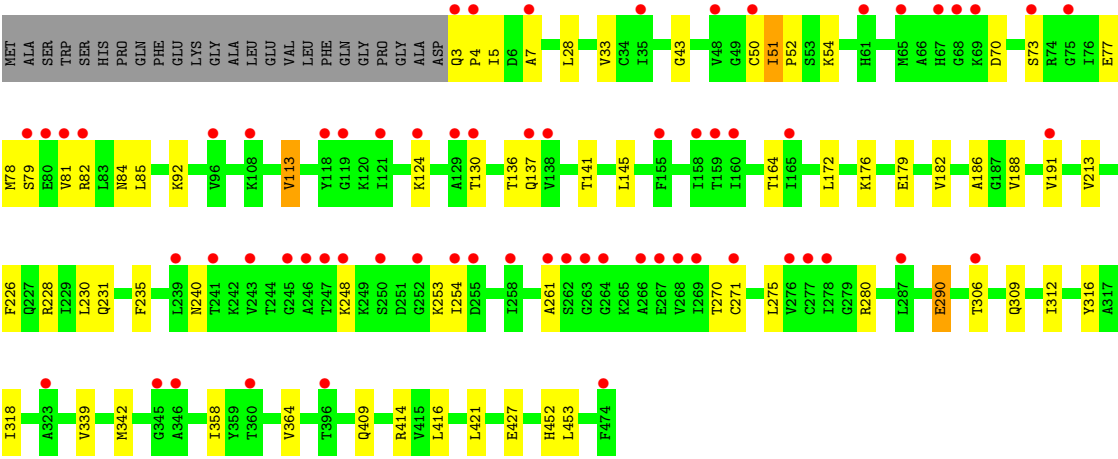
Chain G: 14% 75% 19% 5%



- Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

Chain H: 13% 81% 13% 5%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.56Å 123.39Å 158.41Å 105.95° 91.31° 90.00°	Depositor
Resolution (Å)	46.57 – 2.34 46.57 – 2.34	Depositor EDS
% Data completeness (in resolution range)	96.6 (46.57-2.34) 96.6 (46.57-2.34)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.34Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.227 , 0.249 0.231 , 0.253	Depositor DCC
R_{free} test set	2468 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.104 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	57894	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.56	0/3571	0.58	0/4821
1	B	0.55	2/3571 (0.1%)	0.57	2/4821 (0.0%)
1	C	0.58	0/3562	0.60	0/4809
1	D	0.49	0/3562	0.58	0/4809
1	E	0.42	0/3571	0.52	0/4821
1	F	0.48	2/3562 (0.1%)	0.53	2/4809 (0.0%)
1	G	0.46	0/3562	0.55	1/4809 (0.0%)
1	H	0.50	2/3562 (0.1%)	0.52	2/4809 (0.0%)
All	All	0.51	6/28523 (0.0%)	0.56	7/38508 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	281	ARG	CZ-NH2	-13.17	1.16	1.33
1	H	51	ILE	CA-CB	13.13	1.61	1.54
1	F	255	ASP	CG-OD1	-10.73	1.04	1.25
1	B	139	ILE	CG1-CD1	-8.88	1.17	1.51
1	F	139	ILE	CG1-CD1	-6.16	1.27	1.51
1	H	82	ARG	CZ-NH1	-5.29	1.25	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	281	ARG	NE-CZ-NH1	8.82	130.32	121.50
1	F	255	ASP	CB-CG-OD2	8.22	137.32	118.40
1	H	82	ARG	NE-CZ-NH2	7.81	126.23	119.20
1	B	281	ARG	NH1-CZ-NH2	-6.09	111.38	119.30
1	H	82	ARG	NE-CZ-NH1	-5.98	115.52	121.50
1	G	301	ARG	NE-CZ-NH2	-5.59	114.17	119.20
1	F	255	ASP	CB-CG-OD1	-5.40	105.98	118.40

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	3514	3573	3572	47	0
1	B	3514	3572	3572	76	0
1	C	3508	3567	3566	33	0
1	D	3508	3567	3566	104	0
1	E	3514	3572	3572	68	0
1	F	3508	3567	3566	56	0
1	G	3508	3568	3566	83	0
1	H	3508	3567	3566	45	0
2	A	53	31	31	0	0
2	B	53	31	31	1	0
2	C	53	31	31	1	0
2	D	53	31	31	1	0
2	E	53	31	31	2	0
2	F	53	31	31	0	0
2	G	53	31	31	1	0
2	H	53	31	31	4	0
3	A	25	0	0	2	0
3	B	10	0	0	0	0
3	C	30	0	0	2	0
3	D	20	0	0	0	0
3	E	15	0	0	4	0
3	F	10	0	0	1	0
3	G	15	0	0	2	0
3	H	10	0	0	1	0
4	A	124	0	0	1	0
4	B	32	0	0	3	0
4	C	120	0	0	1	0
4	D	28	0	0	2	0
4	E	41	0	0	3	0
4	F	33	0	0	3	0
4	G	40	0	0	0	0
4	H	34	0	0	1	0
All	All	29093	28801	28794	483	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (483) 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:F:259:GLU:HG2	1:F:266:ALA:HA	1.48	0.92
1:D:176:LYS:HD3	1:D:177:VAL:N	1.91	0.86
1:D:176:LYS:HD3	1:D:177:VAL:H	1.41	0.84
1:D:128:THR:HG22	1:D:138:VAL:HG22	1.63	0.80
1:E:164:THR:HG23	1:E:165:ILE:HD12	1.65	0.79
1:G:166:VAL:HG21	1:G:170:GLY:HA3	1.64	0.79
1:E:288:GLY:O	1:E:292:LEU:HD13	1.85	0.75
1:B:158:ILE:HD12	1:B:246:ALA:HB3	1.65	0.75
1:A:105:HIS:ND1	3:A:506:SO4:O3	2.20	0.75
1:G:184:ILE:HG22	1:G:278:ILE:HG23	1.68	0.74
1:G:162:GLU:HA	1:G:166:VAL:HG23	1.68	0.74
1:H:164:THR:OG1	1:H:248:LYS:NZ	2.21	0.73
1:C:266:ALA:HB2	4:C:644:HOH:O	1.87	0.73
1:G:178:PRO:HG3	1:G:181:MET:HE3	1.71	0.72
1:E:128:THR:HG22	1:E:138:VAL:HG22	1.71	0.72
1:G:288:GLY:N	3:G:503:SO4:O1	2.21	0.72
1:B:128:THR:HG22	1:B:138:VAL:HG23	1.71	0.72
1:D:8:ASP:OD1	1:D:8:ASP:N	2.21	0.72
1:F:5:ILE:HB	1:F:139:ILE:HD13	1.71	0.71
1:G:192:GLU:O	1:G:196:VAL:HG23	1.90	0.71
1:F:259:GLU:HG2	1:F:266:ALA:CA	2.21	0.71
1:G:120:LYS:HE2	1:G:286:ASN:O	1.89	0.70
1:C:105:HIS:ND1	3:C:506:SO4:O1	2.23	0.70
1:D:299:ARG:HH21	1:D:301:ARG:HH12	1.38	0.70
1:A:161:ASP:OD2	1:A:248:LYS:NZ	2.24	0.70
1:F:3:GLN:N	1:F:4:PRO:HD3	2.06	0.70
1:E:184:ILE:HG23	1:E:278:ILE:HG23	1.74	0.69
1:F:20:VAL:HG21	1:F:332:GLU:HG2	1.72	0.69
1:G:255:ASP:OD1	1:G:270:THR:HG22	1.92	0.69
1:A:395:LYS:HD2	1:A:400:THR:HG21	1.74	0.69
1:B:184:ILE:HD13	1:B:243:VAL:HG21	1.74	0.69
1:G:78:MET:HG2	1:H:81:VAL:HG12	1.75	0.68
1:D:121:ILE:CG2	1:D:292:LEU:HD21	2.23	0.68
1:G:108:LYS:O	1:G:111:LYS:HD3	1.93	0.68
1:G:153:THR:HG22	1:G:281:ARG:HG2	1.74	0.68
1:B:409:GLN:HG2	1:B:416:LEU:HD11	1.76	0.68
1:B:164:THR:HG23	1:B:254:ILE:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:ILE:C	1:D:258:ILE:HD12	2.20	0.67
1:E:186:ALA:HB1	1:E:213:VAL:HG22	1.75	0.67
1:E:288:GLY:N	3:E:502:SO4:O3	2.28	0.67
1:B:154:PRO:HD2	1:B:281:ARG:NH2	2.10	0.66
1:C:82:ARG:NH2	1:D:77:GLU:OE1	2.29	0.66
1:H:240:ASN:C	1:H:261:ALA:HB2	2.21	0.66
1:D:299:ARG:HE	1:D:301:ARG:NH2	1.94	0.65
1:A:3:GLN:N	1:A:4:PRO:HD3	2.12	0.65
1:G:79:SER:HG	1:H:79:SER:HG	1.43	0.65
1:H:92:LYS:NZ	1:H:172:LEU:O	2.28	0.65
1:B:121:ILE:HD12	1:B:144:ILE:CD1	2.26	0.65
1:F:290:GLU:HG3	3:F:503:SO4:S	2.37	0.64
1:B:5:ILE:HB	1:B:139:ILE:CD1	2.27	0.64
1:C:3:GLN:N	1:C:4:PRO:HD3	2.12	0.64
1:D:145:LEU:HD11	1:D:318:ILE:HG12	1.78	0.64
1:D:28:LEU:HD12	1:D:339:VAL:HG12	1.80	0.64
1:D:66:ALA:HB1	1:D:78:MET:HE3	1.80	0.64
1:E:20:VAL:HG21	1:E:332[B]:GLU:HG3	1.80	0.64
1:E:264:GLY:HA3	4:E:611:HOH:O	1.97	0.64
1:F:291:GLU:N	1:F:291:GLU:OE1	2.29	0.64
1:B:153:THR:OG1	1:B:281:ARG:HG3	1.97	0.63
1:D:3:GLN:N	1:D:4:PRO:HD3	2.13	0.63
1:A:77:GLU:OE1	1:B:82:ARG:NH1	2.32	0.63
1:A:403:MET:SD	1:A:403:MET:N	2.71	0.63
1:E:240:ASN:C	1:E:261:ALA:HB2	2.23	0.63
1:E:175:LYS:HD2	1:E:175:LYS:N	2.13	0.62
1:G:282:PRO:HG3	1:G:301:ARG:HG3	1.81	0.62
1:A:51:ILE:HG21	1:A:99:LEU:HD12	1.82	0.62
1:G:456:SER:N	1:H:427:GLU:OE1	2.32	0.62
1:G:54:LYS:CD	1:H:453:LEU:HD13	2.30	0.61
1:E:28:LEU:HD12	1:E:339:VAL:HG12	1.82	0.61
1:G:258:ILE:HD11	1:G:267:GLU:HG2	1.81	0.61
1:A:145:LEU:HD11	1:A:318:ILE:HG12	1.82	0.61
1:B:166:VAL:HG22	1:B:167:SER:O	2.00	0.61
1:C:124:LYS:NZ	3:C:507:SO4:O4	2.34	0.61
1:F:5:ILE:HB	1:F:139:ILE:CD1	2.30	0.61
1:A:28:LEU:HD12	1:A:339:VAL:HG13	1.82	0.61
1:D:297:ASP:OD1	1:D:301:ARG:N	2.32	0.61
1:C:73:SER:O	1:D:87:LYS:NZ	2.34	0.60
1:B:372:GLU:N	4:B:601:HOH:O	2.35	0.60
1:G:184:ILE:HG22	1:G:278:ILE:CG2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:LEU:CD2	1:D:276:VAL:HG13	2.32	0.60
1:G:274:LEU:HD23	1:G:275:LEU:N	2.16	0.60
1:B:3:GLN:N	1:B:4:PRO:CD	2.65	0.60
1:C:33:VAL:HG22	1:C:113:VAL:HB	1.83	0.60
1:H:28:LEU:HD12	1:H:339:VAL:HG12	1.84	0.60
1:F:436:LEU:HD23	4:F:616:HOH:O	2.01	0.59
1:D:35:ILE:HD12	1:D:115:VAL:HB	1.84	0.59
1:A:222:ILE:HD12	1:A:419:HIS:HB3	1.84	0.59
1:E:3:GLN:N	1:E:4:PRO:CD	2.65	0.59
1:B:28:LEU:HD12	1:B:339:VAL:HG12	1.83	0.59
1:B:307:ARG:NH2	1:B:345:GLY:O	2.33	0.59
1:D:20:VAL:HG21	1:D:332:GLU:HG2	1.85	0.59
1:E:74:ARG:O	1:F:88:MET:HG3	2.02	0.59
1:G:82:ARG:HG2	1:G:82:ARG:HH11	1.68	0.59
1:H:186:ALA:HB1	1:H:213:VAL:HG22	1.85	0.59
1:D:166:VAL:CG2	1:D:170:GLY:HA3	2.33	0.58
1:B:258:ILE:HD12	1:B:258:ILE:C	2.28	0.58
1:E:184:ILE:HG22	1:E:276:VAL:HA	1.84	0.58
1:F:244:THR:OG1	1:F:257:SER:OG	2.21	0.58
1:E:253:LYS:NZ	1:E:272:ASP:OD1	2.36	0.58
1:E:299:ARG:HH21	1:E:301:ARG:HH22	1.50	0.58
1:G:406:ILE:HD13	1:G:462:ALA:CB	2.34	0.58
1:D:244:THR:OG1	1:D:257:SER:OG	2.22	0.58
1:D:24:LYS:HB2	1:D:336:ILE:CD1	2.35	0.57
1:C:182:VAL:HG13	1:C:271:CYS:SG	2.44	0.57
1:C:251:ASP:OD1	1:C:251:ASP:O	2.22	0.57
1:E:165:ILE:HG23	1:E:274:LEU:HD22	1.85	0.57
1:B:126:GLN:NE2	1:B:140:ASP:OD1	2.33	0.57
1:H:452:HIS:O	1:H:453:LEU:HB2	2.04	0.57
1:E:164:THR:OG1	1:E:272:ASP:O	2.22	0.57
1:F:255:ASP:OD1	1:F:270:THR:HG22	2.03	0.57
1:D:122:THR:HG21	1:D:128:THR:HG23	1.87	0.57
1:D:153:THR:HG23	1:D:281:ARG:HD3	1.85	0.57
1:B:184:ILE:HG22	1:B:278:ILE:HG23	1.86	0.57
1:G:213:VAL:O	1:G:223:SER:OG	2.20	0.57
1:B:198:GLN:NE2	1:B:233:GLN:O	2.38	0.56
1:D:380:GLU:HG2	1:D:410:LYS:CE	2.35	0.56
1:B:3:GLN:O	1:B:137:GLN:NE2	2.31	0.56
1:G:171:ALA:HB2	1:G:275:LEU:HD13	1.88	0.56
1:G:420:ILE:HD13	1:G:428:MET:HB3	1.87	0.56
1:A:33:VAL:HG22	1:A:113:VAL:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:276:VAL:HG23	1:F:276:VAL:O	2.05	0.56
1:H:70:ASP:O	1:H:73:SER:OG	2.22	0.56
1:D:34:CYS:C	1:D:35:ILE:HD13	2.30	0.56
1:G:186:ALA:HB3	1:G:208:GLU:HG2	1.86	0.56
1:D:5:ILE:HG22	1:D:6:ASP:N	2.20	0.56
1:D:288:GLY:O	1:D:292:LEU:HD13	2.05	0.56
1:E:82:ARG:NH2	1:F:77:GLU:OE1	2.38	0.56
1:G:240:ASN:C	1:G:261:ALA:HB2	2.31	0.56
1:B:314:ASN:OD1	1:B:315:ILE:HD12	2.05	0.56
1:B:121:ILE:HD12	1:B:144:ILE:HD12	1.87	0.55
1:G:221:GLU:OE2	1:G:385:LYS:NZ	2.39	0.55
1:D:128:THR:HG22	1:D:138:VAL:CG2	2.34	0.55
1:G:3:GLN:N	1:G:4:PRO:HD3	2.21	0.55
1:H:290:GLU:N	3:H:503:SO4:O1	2.33	0.55
1:E:289:LEU:N	3:E:502:SO4:O3	2.40	0.55
1:F:5:ILE:HG21	1:F:33:VAL:HG21	1.88	0.55
1:D:245:GLY:N	1:D:257:SER:OG	2.40	0.55
1:A:282:PRO:HG3	1:A:301:ARG:HG3	1.88	0.54
1:B:212:HIS:ND1	1:B:220:MET:HE1	2.22	0.54
1:E:192:GLU:O	1:E:196:VAL:HG23	2.07	0.54
1:B:66:ALA:HB1	1:B:78:MET:CE	2.38	0.54
1:D:155:PHE:CD1	1:D:156:PRO:HD2	2.43	0.54
1:G:166:VAL:CG2	1:G:170:GLY:HA3	2.36	0.54
1:G:180:LYS:HD3	1:G:270:THR:O	2.08	0.54
1:H:130:THR:HG22	1:H:136:THR:HG22	1.89	0.54
1:B:180:LYS:HG2	1:B:203:ASP:HB3	1.89	0.54
1:H:226:PHE:CZ	1:H:230:LEU:HD11	2.43	0.54
1:A:470:LYS:NZ	4:A:603:HOH:O	2.40	0.54
1:F:99:LEU:O	1:F:103:ILE:HD13	2.08	0.54
1:D:304:VAL:CG1	1:D:308:PHE:HA	2.38	0.54
1:G:406:ILE:HD13	1:G:462:ALA:HB1	1.90	0.54
1:G:175:LYS:HD2	1:G:175:LYS:N	2.23	0.54
1:B:5:ILE:HB	1:B:139:ILE:HD13	1.89	0.53
1:B:372:GLU:CA	4:B:601:HOH:O	2.56	0.53
1:G:46:LEU:HD22	1:G:103:ILE:HD11	1.89	0.53
1:A:51:ILE:CG2	1:A:99:LEU:HD12	2.38	0.53
1:D:7:ALA:O	1:D:141:THR:HA	2.09	0.53
1:D:24:LYS:HG2	1:D:336:ILE:HG23	1.89	0.53
1:D:205:THR:HG22	1:D:236:LYS:CB	2.38	0.53
1:F:28:LEU:HD12	1:F:339:VAL:HG12	1.90	0.53
1:F:259:GLU:OE2	1:F:266:ALA:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:181:MET:HE1	1:G:197:TRP:CD1	2.43	0.53
1:G:20:VAL:HG21	1:G:332:GLU:HG2	1.90	0.53
1:F:212:HIS:ND1	1:F:220:MET:HE1	2.23	0.53
1:A:25:ALA:HB2	1:A:339:VAL:HG21	1.91	0.53
1:B:35:ILE:HG22	2:B:501:FAD:H2A	1.91	0.53
1:C:145:LEU:HD11	1:C:318:ILE:HG12	1.91	0.53
1:G:54:LYS:HD3	1:H:453:LEU:HD13	1.91	0.53
1:G:395:LYS:HD2	1:G:400:THR:HG21	1.91	0.53
1:E:184:ILE:HG21	1:E:276:VAL:HG13	1.91	0.53
1:E:380:GLU:HA	4:E:605:HOH:O	2.09	0.53
1:G:58:ASN:O	1:G:62:TYR:CD2	2.62	0.52
1:H:364:VAL:HG22	1:H:421:LEU:HD13	1.91	0.52
1:H:409:GLN:HG2	1:H:416:LEU:HD11	1.91	0.52
1:A:182:VAL:HG23	1:A:271:CYS:HB3	1.91	0.52
1:B:372:GLU:HA	4:B:601:HOH:O	2.08	0.52
1:B:297:ASP:OD1	1:B:301:ARG:N	2.36	0.52
1:D:3:GLN:N	1:D:4:PRO:CD	2.73	0.52
1:H:145:LEU:HD11	1:H:318:ILE:HG12	1.91	0.52
1:A:3:GLN:N	1:A:4:PRO:CD	2.73	0.52
1:B:294:ILE:HD11	1:B:312:ILE:HD13	1.92	0.52
1:E:178:PRO:HG3	1:E:181:MET:HE3	1.92	0.52
1:G:183:VAL:HG22	1:G:206:ALA:HA	1.91	0.52
1:G:452:HIS:ND1	1:G:453:LEU:HD23	2.24	0.52
1:F:145:LEU:HD11	1:F:318:ILE:HG12	1.92	0.52
1:D:299:ARG:HH21	1:D:301:ARG:NH1	2.07	0.51
1:H:414:ARG:HH21	1:H:416:LEU:HD23	1.75	0.51
1:B:318:ILE:HD13	1:B:335:GLY:HA2	1.91	0.51
1:D:166:VAL:HG21	1:D:170:GLY:HA3	1.92	0.51
1:E:299:ARG:NH2	1:E:301:ARG:HH22	2.07	0.51
1:G:461:GLU:OE2	1:G:473:ASN:ND2	2.42	0.51
1:F:68:GLY:HA3	4:F:604:HOH:O	2.10	0.51
1:D:242:LYS:HD2	1:D:243:VAL:H	1.75	0.51
1:E:288:GLY:CA	3:E:502:SO4:O3	2.57	0.51
1:G:174:LEU:HD11	1:G:273:VAL:HG11	1.92	0.51
1:D:54:LYS:HD3	1:D:54:LYS:N	2.25	0.51
1:G:58:ASN:CG	1:G:62:TYR:HE2	2.18	0.51
1:E:160:ILE:O	1:E:160:ILE:HG13	2.11	0.51
1:G:41:LEU:HD21	1:G:114:HIS:NE2	2.26	0.51
1:B:145:LEU:HD11	1:B:318:ILE:HG12	1.93	0.50
1:B:164:THR:CG2	1:B:254:ILE:HD11	2.42	0.50
1:F:3:GLN:N	1:F:4:PRO:CD	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ILE:HD12	1:B:144:ILE:HD13	1.93	0.50
1:G:241:THR:HG23	1:G:259:GLU:O	2.12	0.50
1:B:316:TYR:CD1	1:B:342:MET:HE2	2.46	0.50
1:E:186:ALA:N	1:E:208:GLU:OE1	2.40	0.50
1:H:85:LEU:HD23	1:H:176:LYS:HA	1.94	0.50
1:E:127:VAL:HB	1:E:139:ILE:CG2	2.42	0.50
1:E:321:VAL:HG22	1:E:321:VAL:O	2.12	0.50
1:E:6:ASP:OD1	1:E:140:ASP:HB2	2.11	0.50
1:B:166:VAL:HG21	1:B:171:ALA:N	2.26	0.50
1:G:258:ILE:HD12	1:G:258:ILE:C	2.37	0.50
1:B:7:ALA:O	1:B:141:THR:HA	2.12	0.49
1:E:184:ILE:O	1:E:184:ILE:CG2	2.60	0.49
1:D:205:THR:HG22	1:D:236:LYS:HB3	1.94	0.49
1:D:258:ILE:HD11	1:D:267:GLU:OE2	2.13	0.49
1:B:166:VAL:HG21	1:B:170:GLY:C	2.37	0.49
1:D:4:PRO:HB3	1:D:138:VAL:O	2.13	0.49
1:E:43:GLY:HA2	2:E:501:FAD:O3B	2.13	0.49
1:G:299:ARG:HH21	1:G:301:ARG:HH22	1.61	0.49
1:D:128:THR:CG2	1:D:138:VAL:HG22	2.39	0.49
1:E:66:ALA:HB2	1:F:71:PHE:HE2	1.78	0.49
1:E:69:LYS:O	1:E:69:LYS:HG3	2.12	0.49
1:H:51:ILE:HB	1:H:52:PRO:HD3	1.95	0.49
1:A:451:ALA:H	1:B:430:ASN:HD21	1.60	0.49
1:H:3:GLN:CG	1:H:4:PRO:HD3	2.43	0.49
1:D:120:LYS:NZ	4:D:601:HOH:O	2.24	0.49
1:D:304:VAL:HG12	1:D:308:PHE:HA	1.93	0.49
1:F:259:GLU:HB3	1:F:264:GLY:O	2.12	0.49
1:G:178:PRO:CG	1:G:181:MET:HE3	2.42	0.49
1:A:452:HIS:O	1:A:453:LEU:HB2	2.13	0.49
1:A:309:GLN:HG2	1:A:316:TYR:CE2	2.48	0.49
1:C:393:ARG:HD3	1:C:453:LEU:O	2.13	0.49
1:F:103:ILE:CD1	1:F:103:ILE:N	2.76	0.49
1:G:274:LEU:HD23	1:G:274:LEU:C	2.38	0.49
1:D:166:VAL:HG22	1:D:167:SER:O	2.12	0.49
1:E:58:ASN:O	1:E:62:TYR:CD2	2.65	0.49
1:F:5:ILE:HD12	1:F:139:ILE:HD11	1.95	0.49
1:G:186:ALA:H	1:G:208:GLU:HG2	1.78	0.49
1:C:61:HIS:NE2	1:C:65:MET:SD	2.86	0.48
1:C:246:ALA:HB1	1:C:254:ILE:HD13	1.94	0.48
1:D:54:LYS:HE3	2:D:501:FAD:O4	2.13	0.48
1:D:155:PHE:CZ	1:D:243:VAL:HB	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:ILE:HG23	1:D:274:LEU:HD22	1.95	0.48
1:D:6:ASP:OD1	1:D:6:ASP:O	2.32	0.48
1:D:207:VAL:HG22	1:D:238:LYS:HB2	1.94	0.48
1:E:20:VAL:HG11	1:E:332[B]:GLU:HG3	1.96	0.48
1:D:217:GLY:HA3	4:D:612:HOH:O	2.14	0.48
1:D:258:ILE:HD11	1:D:267:GLU:CD	2.38	0.48
1:G:88:MET:HE1	1:G:200:LEU:HD11	1.95	0.48
1:G:155:PHE:CD1	1:G:158:ILE:CD1	2.97	0.48
1:C:28:LEU:HD12	1:C:339:VAL:CG1	2.44	0.48
1:A:452:HIS:NE2	1:B:332[A]:GLU:OE2	2.47	0.48
1:G:3:GLN:N	1:G:4:PRO:CD	2.77	0.48
1:F:241:THR:HG21	1:F:258:ILE:HD12	1.96	0.48
1:H:3:GLN:N	1:H:4:PRO:CD	2.77	0.48
1:C:71:PHE:HD2	1:C:78:MET:HE1	1.79	0.48
1:F:258:ILE:O	1:F:259:GLU:HG3	2.14	0.48
1:G:186:ALA:HB3	1:G:208:GLU:CG	2.44	0.48
1:G:445:ILE:HG21	1:G:459:PHE:CE2	2.49	0.47
1:D:5:ILE:HG22	1:D:6:ASP:H	1.79	0.47
1:E:5:ILE:O	1:E:139:ILE:HD12	2.14	0.47
1:H:309:GLN:HG2	1:H:316:TYR:CE2	2.49	0.47
1:E:121:ILE:HG21	1:E:292:LEU:HD21	1.97	0.47
1:D:380:GLU:HG2	1:D:410:LYS:HE3	1.96	0.47
1:F:67:HIS:HA	1:F:81:VAL:HG21	1.97	0.47
1:F:144:ILE:HB	1:F:315:ILE:HG12	1.96	0.47
1:G:207:VAL:HG13	1:G:241:THR:HB	1.97	0.47
1:A:222:ILE:CD1	1:A:419:HIS:HB3	2.44	0.47
1:C:20:VAL:HG21	1:C:332:GLU:HG3	1.97	0.47
1:D:198:GLN:NE2	1:D:233:GLN:O	2.47	0.47
1:B:176:LYS:HG3	1:B:177:VAL:N	2.29	0.47
1:C:254:ILE:HD11	1:C:256:VAL:HG22	1.97	0.47
1:E:83:LEU:HD22	1:E:200:LEU:HD22	1.96	0.47
1:E:183:VAL:HG13	1:E:275:LEU:HD23	1.96	0.47
1:H:186:ALA:CB	1:H:213:VAL:HG22	2.45	0.47
1:D:121:ILE:HG21	1:D:292:LEU:HD21	1.95	0.47
1:D:265:LYS:CD	1:D:265:LYS:N	2.78	0.47
1:F:318:ILE:HD13	1:F:335:GLY:HA2	1.97	0.47
1:H:280:ARG:HD2	2:H:501:FAD:HM82	1.96	0.47
1:B:166:VAL:CG2	1:B:170:GLY:HA3	2.45	0.47
1:D:245:GLY:O	1:D:257:SER:OG	2.32	0.47
1:D:137:GLN:HA	1:D:137:GLN:NE2	2.30	0.46
1:E:127:VAL:O	1:E:139:ILE:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:254:ILE:O	1:G:270:THR:HA	2.15	0.46
1:F:258:ILE:C	1:F:259:GLU:HG3	2.39	0.46
1:H:253:LYS:HD3	1:H:270:THR:HG21	1.97	0.46
1:B:83:LEU:CD1	1:B:88:MET:HE3	2.45	0.46
1:B:183:VAL:CG2	1:B:206:ALA:HA	2.46	0.46
1:C:69:LYS:O	1:C:69:LYS:HG2	2.15	0.46
1:G:46:LEU:HD22	1:G:103:ILE:CD1	2.44	0.46
1:H:188:VAL:HG13	1:H:358:ILE:HG12	1.97	0.46
1:B:165:ILE:HG23	1:B:274:LEU:HD23	1.97	0.46
1:C:77:GLU:OE2	1:D:84:ASN:ND2	2.42	0.46
1:G:145:LEU:HD11	1:G:318:ILE:HG12	1.98	0.46
1:H:191:VAL:HG21	1:H:213:VAL:CG1	2.45	0.46
1:A:448:VAL:HG22	1:B:437:GLU:HG2	1.97	0.46
1:D:121:ILE:HG22	1:D:292:LEU:HD21	1.97	0.46
1:E:171:ALA:HB2	1:E:275:LEU:HD13	1.97	0.46
1:F:90:GLU:OE2	1:F:94:THR:OG1	2.33	0.46
1:D:24:LYS:CG	1:D:336:ILE:HD12	2.46	0.46
1:C:452:HIS:O	1:C:453:LEU:HB2	2.16	0.46
1:D:259:GLU:HB2	1:D:264:GLY:O	2.15	0.46
1:G:289:LEU:N	3:G:503:SO4:O1	2.47	0.46
1:D:122:THR:HG21	1:D:128:THR:CG2	2.45	0.46
1:H:33:VAL:HG22	1:H:113:VAL:CG2	2.46	0.46
1:B:304:VAL:CG1	1:B:308:PHE:HA	2.46	0.45
1:C:3:GLN:N	1:C:4:PRO:CD	2.78	0.45
1:D:126:GLN:OE1	1:D:140:ASP:OD1	2.34	0.45
1:F:51:ILE:HB	1:F:52:PRO:HD3	1.98	0.45
1:E:139:ILE:HG23	1:E:139:ILE:O	2.16	0.45
1:E:282:PRO:HG3	1:E:301:ARG:HG3	1.98	0.45
1:E:445:ILE:HG21	1:E:459:PHE:CE2	2.52	0.45
1:F:307:ARG:HH21	1:F:341:GLY:C	2.24	0.45
1:A:77:GLU:OE1	1:B:82:ARG:NH2	2.48	0.45
1:C:121:ILE:HG21	1:C:292:LEU:HD11	1.98	0.45
1:E:36:GLU:OE2	2:E:501:FAD:O2B	2.25	0.45
1:B:158:ILE:HD11	1:B:246:ALA:N	2.32	0.45
1:E:420:ILE:HD13	1:E:428:MET:HB3	1.98	0.45
1:F:226:PHE:CZ	1:F:230:LEU:HD11	2.51	0.45
1:G:46:LEU:CD2	1:G:103:ILE:HD11	2.46	0.45
1:G:153:THR:HG22	1:G:281:ARG:CG	2.45	0.45
1:B:166:VAL:HG23	1:B:170:GLY:HA3	1.99	0.45
1:D:245:GLY:C	1:D:257:SER:HG	2.24	0.45
1:D:166:VAL:HG21	1:D:170:GLY:C	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:GLY:O	1:D:191:VAL:HG23	2.17	0.45
1:F:251:ASP:OD1	1:F:251:ASP:O	2.34	0.45
1:D:165:ILE:HG12	1:D:254:ILE:HD13	1.98	0.45
1:B:207:VAL:HG22	1:B:238:LYS:HB2	1.98	0.45
1:D:122:THR:HG23	1:D:128:THR:OG1	2.17	0.45
1:E:452:HIS:O	1:E:453:LEU:HB2	2.15	0.45
1:A:431:GLU:OE2	1:A:450:HIS:HE1	1.99	0.44
1:A:175:LYS:N	1:A:175:LYS:HD2	2.33	0.44
1:A:20:VAL:HG11	1:A:332[B]:GLU:HG3	1.98	0.44
1:A:84:ASN:ND2	1:B:77:GLU:OE2	2.45	0.44
1:A:180:LYS:NZ	1:A:270:THR:O	2.46	0.44
1:B:158:ILE:HD11	1:B:246:ALA:H	1.82	0.44
1:E:452:HIS:ND1	1:E:453:LEU:HD23	2.32	0.44
1:F:292:LEU:HB3	1:F:312:ILE:HD11	1.99	0.44
1:A:25:ALA:HB2	1:A:339:VAL:CG2	2.48	0.44
1:E:174:LEU:HD11	1:E:273:VAL:HG11	1.99	0.44
1:A:451:ALA:H	1:B:430:ASN:ND2	2.15	0.44
1:D:166:VAL:HG21	1:D:170:GLY:CA	2.48	0.44
1:D:243:VAL:HG22	1:D:258:ILE:HG22	2.00	0.44
1:D:256:VAL:HB	1:D:269:ILE:HG13	1.98	0.44
1:D:122:THR:CG2	1:D:128:THR:HG23	2.48	0.44
1:F:452:HIS:ND1	1:F:453:LEU:HD23	2.32	0.44
1:H:7:ALA:O	1:H:141:THR:HA	2.18	0.44
1:H:231:GLN:HA	1:H:235:PHE:O	2.18	0.44
1:D:186:ALA:HB1	1:D:213:VAL:HG22	2.00	0.43
1:F:180:LYS:NZ	4:F:603:HOH:O	2.49	0.43
1:G:82:ARG:HB2	1:H:77:GLU:HB2	2.00	0.43
1:B:205:THR:HG23	1:B:236:LYS:HB2	2.00	0.43
1:B:304:VAL:HG12	1:B:308:PHE:HA	2.00	0.43
1:D:182:VAL:HG23	1:D:271:CYS:HB3	2.00	0.43
1:E:145:LEU:HD11	1:E:318:ILE:HG12	1.99	0.43
1:F:70:ASP:OD1	1:F:74:ARG:NH2	2.51	0.43
1:F:182:VAL:HG23	1:F:271:CYS:HB3	1.99	0.43
1:F:444:ASP:O	1:F:448:VAL:HG23	2.19	0.43
1:G:69:LYS:O	1:G:70:ASP:C	2.61	0.43
1:A:77:GLU:HB3	1:B:82:ARG:NH2	2.34	0.43
1:E:451:ALA:H	1:F:430:ASN:HD21	1.65	0.43
1:A:225:ASN:N	1:A:225:ASN:HD22	2.17	0.43
1:D:265:LYS:H	1:D:265:LYS:HD3	1.83	0.43
1:E:299:ARG:NH2	3:E:503:SO4:O1	2.50	0.43
1:F:163:ASP:OD1	1:F:164:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:78:MET:SD	1:H:78:MET:SD	3.16	0.43
1:B:158:ILE:CD1	1:B:246:ALA:HB3	2.43	0.43
1:B:304:VAL:CG1	1:B:308:PHE:C	2.92	0.43
1:D:137:GLN:OE1	1:D:138:VAL:O	2.36	0.43
1:D:205:THR:HG22	1:D:236:LYS:HB2	2.00	0.43
1:D:265:LYS:CD	1:D:265:LYS:H	2.32	0.43
1:E:120:LYS:HG2	1:E:121:ILE:N	2.33	0.43
1:E:389:ALA:HA	1:E:400:THR:HB	2.00	0.43
1:H:5:ILE:HD12	1:H:137:GLN:NE2	2.33	0.43
1:B:44:THR:O	1:B:49:GLY:N	2.52	0.43
1:D:125:ASN:OD1	1:D:314:ASN:ND2	2.51	0.43
1:E:63:TYR:HB2	1:F:76:ILE:HD13	2.01	0.43
1:G:166:VAL:HG21	1:G:170:GLY:CA	2.41	0.43
1:D:124:LYS:HD2	1:D:124:LYS:N	2.34	0.43
1:D:321:VAL:O	1:D:321:VAL:HG22	2.19	0.43
1:B:312:ILE:HG22	1:B:314:ASN:OD1	2.19	0.43
1:G:406:ILE:HD13	1:G:462:ALA:HB3	2.01	0.43
1:A:382:LYS:CE	1:A:466:ALA:O	2.67	0.42
1:C:71:PHE:CD2	1:C:78:MET:HE1	2.54	0.42
1:D:209:PHE:CD1	1:D:209:PHE:C	2.96	0.42
1:A:384:GLY:HA3	1:A:466:ALA:HB2	2.01	0.42
1:D:304:VAL:CG1	1:D:308:PHE:C	2.92	0.42
1:F:85:LEU:HD23	1:F:176:LYS:HA	2.01	0.42
1:G:77:GLU:OE1	1:H:84:ASN:ND2	2.39	0.42
1:D:274:LEU:C	1:D:274:LEU:HD23	2.44	0.42
1:E:402:GLY:HA3	1:E:421:LEU:O	2.18	0.42
1:G:50:CYS:HB3	1:H:453:LEU:HD12	2.00	0.42
1:G:406:ILE:N	1:G:406:ILE:HD12	2.34	0.42
1:A:19:TYR:CE1	1:A:103:ILE:HD12	2.55	0.42
1:D:71:PHE:CD2	1:D:78:MET:HE1	2.54	0.42
1:G:452:HIS:O	1:G:453:LEU:HB2	2.19	0.42
1:G:274:LEU:C	1:G:274:LEU:CD2	2.93	0.42
1:A:426:GLY:O	1:A:429:VAL:HG12	2.18	0.42
1:C:472:ILE:HG21	1:D:20:VAL:HG22	2.02	0.42
1:D:188:VAL:HG23	1:D:358:ILE:HG12	2.00	0.42
1:E:207:VAL:HG23	1:E:241:THR:HB	2.02	0.42
1:H:43:GLY:HA2	2:H:501:FAD:O3B	2.19	0.42
1:D:179:GLU:HB2	1:D:272:ASP:OD2	2.19	0.42
1:E:4:PRO:HA	1:E:138:VAL:O	2.20	0.42
1:E:67:HIS:HA	1:E:81:VAL:HG21	2.02	0.42
1:F:7:ALA:O	1:F:141:THR:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:VAL:CG1	1:F:336:ILE:HD11	2.50	0.42
1:A:382:LYS:HE3	1:A:466:ALA:O	2.19	0.42
1:B:302:ILE:O	1:B:304:VAL:HG23	2.20	0.42
1:D:247:THR:HG22	1:D:248:LYS:N	2.35	0.42
1:F:209:PHE:O	1:F:240:ASN:HA	2.20	0.42
1:B:144:ILE:HB	1:B:315:ILE:HG13	2.02	0.41
1:D:24:LYS:HB2	1:D:336:ILE:HD12	2.00	0.41
1:E:184:ILE:HD11	1:E:243:VAL:HG21	2.02	0.41
1:D:282:PRO:HB3	1:D:321:VAL:HA	2.01	0.41
1:D:382:LYS:NZ	1:D:413:ASP:OD1	2.50	0.41
1:C:452:HIS:ND1	1:C:453:LEU:HD23	2.36	0.41
1:D:393:ARG:HD3	1:D:453:LEU:O	2.19	0.41
1:F:259:GLU:CD	1:F:266:ALA:HB2	2.44	0.41
1:A:121:ILE:HG21	1:A:292:LEU:HD11	2.02	0.41
1:D:125:ASN:HB3	1:D:141:THR:O	2.20	0.41
1:G:186:ALA:CB	1:G:208:GLU:HG2	2.51	0.41
1:G:299:ARG:NH2	1:G:301:ARG:HH22	2.18	0.41
1:H:124:LYS:HZ2	1:H:312:ILE:HG22	1.85	0.41
1:B:183:VAL:HG23	1:B:206:ALA:HA	2.02	0.41
1:D:258:ILE:CD1	1:D:267:GLU:HG2	2.51	0.41
1:G:435:ALA:HB1	1:G:445:ILE:HD11	2.02	0.41
1:A:54:LYS:HG2	1:B:453:LEU:HD13	2.02	0.41
1:B:122:THR:OG1	1:B:128:THR:HG23	2.21	0.41
1:B:164:THR:HG21	1:B:248:LYS:HD2	2.03	0.41
1:B:318:ILE:HD13	1:B:335:GLY:CA	2.50	0.41
1:D:5:ILE:CG2	1:D:6:ASP:N	2.81	0.41
1:G:84:ASN:HB2	1:H:77:GLU:OE2	2.20	0.41
1:H:33:VAL:HG22	1:H:113:VAL:HG22	2.02	0.41
1:H:182:VAL:HG23	1:H:271:CYS:HB3	2.02	0.41
1:A:250:SER:OG	1:F:344:GLY:O	2.24	0.41
1:C:431:GLU:OE2	1:C:450:HIS:HE1	2.04	0.41
1:F:80:GLU:O	1:F:80:GLU:HG3	2.21	0.41
1:F:402:GLY:HA3	1:F:421:LEU:O	2.21	0.41
1:F:452:HIS:O	1:F:453:LEU:HB2	2.19	0.41
1:C:472:ILE:HD12	1:D:20:VAL:HG13	2.03	0.41
1:D:5:ILE:CG2	1:D:6:ASP:H	2.33	0.41
1:D:8:ASP:OD1	1:D:31:LYS:CB	2.69	0.41
1:E:92:LYS:NZ	1:E:172:LEU:O	2.39	0.41
1:E:256:VAL:HG22	1:E:274:LEU:HD12	2.02	0.41
1:E:297:ASP:OD1	1:E:297:ASP:C	2.64	0.41
1:A:198:GLN:NE2	1:A:233:GLN:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:PHE:CZ	1:A:230:LEU:HD11	2.56	0.41
1:A:297:ASP:OD1	1:A:297:ASP:C	2.64	0.41
1:B:179:GLU:HB3	1:B:272:ASP:OD2	2.21	0.41
1:F:393:ARG:HD3	1:F:453:LEU:O	2.20	0.41
1:G:231:GLN:HA	1:G:235:PHE:O	2.21	0.41
1:G:402:GLY:HA3	1:G:421:LEU:O	2.20	0.41
1:G:444:ASP:O	1:G:448:VAL:HG23	2.21	0.41
2:H:501:FAD:HM82	4:H:607:HOH:O	2.20	0.41
1:A:51:ILE:HD12	1:A:99:LEU:CD1	2.51	0.41
1:A:77:GLU:OE2	1:B:84:ASN:ND2	2.39	0.41
1:B:10:THR:HG21	1:B:127:VAL:HG21	2.02	0.41
2:C:501:FAD:H9	2:C:501:FAD:H1'1	1.88	0.41
1:H:409:GLN:HG2	1:H:416:LEU:HD21	2.02	0.41
1:B:389:ALA:HA	1:B:400:THR:HB	2.03	0.40
1:C:19:TYR:CE1	1:C:103:ILE:HD12	2.56	0.40
1:C:226:PHE:CZ	1:C:230:LEU:HD11	2.56	0.40
1:D:318:ILE:HD13	1:D:335:GLY:HA2	2.03	0.40
1:E:160:ILE:HG23	4:E:608:HOH:O	2.21	0.40
1:G:153:THR:OG1	1:G:278:ILE:CD1	2.69	0.40
1:H:164:THR:HB	1:H:254:ILE:HD11	2.02	0.40
1:C:282:PRO:HG3	1:C:301:ARG:HG3	2.03	0.40
1:E:5:ILE:HG22	1:E:6:ASP:N	2.36	0.40
1:G:43:GLY:HA2	2:G:501:FAD:O3B	2.21	0.40
1:G:160:ILE:HG23	1:G:166:VAL:HA	2.02	0.40
1:B:20:VAL:HG21	1:B:332[B]:GLU:HG3	2.03	0.40
1:C:389:ALA:HA	1:C:400:THR:HB	2.03	0.40
1:G:316:TYR:CD1	1:G:342:MET:HE2	2.56	0.40
1:G:404:VAL:HG12	1:G:406:ILE:CD1	2.51	0.40
1:H:316:TYR:CD1	1:H:342:MET:HE2	2.56	0.40
2:H:501:FAD:HM73	2:H:501:FAD:HM81	1.92	0.40
1:A:108:LYS:NZ	3:A:506:SO4:O1	2.37	0.40
1:B:10:THR:HB	1:B:141:THR:HG21	2.04	0.40
1:C:309:GLN:HG2	1:C:316:TYR:CE2	2.56	0.40
1:D:309:GLN:HG2	1:D:316:TYR:CE2	2.57	0.40
1:B:205:THR:CG2	1:B:236:LYS:HB2	2.51	0.40
1:C:438:TYR:O	1:E:305:ASN:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	471/496 (95%)	464 (98%)	7 (2%)	0	100	100
1	B	471/496 (95%)	464 (98%)	7 (2%)	0	100	100
1	C	470/496 (95%)	461 (98%)	9 (2%)	0	100	100
1	D	470/496 (95%)	459 (98%)	11 (2%)	0	100	100
1	E	471/496 (95%)	459 (98%)	12 (2%)	0	100	100
1	F	470/496 (95%)	461 (98%)	9 (2%)	0	100	100
1	G	470/496 (95%)	459 (98%)	11 (2%)	0	100	100
1	H	470/496 (95%)	458 (97%)	12 (3%)	0	100	100
All	All	3763/3968 (95%)	3685 (98%)	78 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	373/390 (96%)	354 (95%)	19 (5%)	21	26
1	B	373/390 (96%)	356 (95%)	17 (5%)	24	31
1	C	372/390 (95%)	358 (96%)	14 (4%)	29	38
1	D	372/390 (95%)	355 (95%)	17 (5%)	24	31
1	E	373/390 (96%)	359 (96%)	14 (4%)	29	38
1	F	372/390 (95%)	360 (97%)	12 (3%)	34	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	372/390 (95%)	361 (97%)	11 (3%)	36	47
1	H	372/390 (95%)	364 (98%)	8 (2%)	45	58
All	All	2979/3120 (96%)	2867 (96%)	112 (4%)	29	38

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	CYS
1	A	54	LYS
1	A	78	MET
1	A	82	ARG
1	A	191	VAL
1	A	213	VAL
1	A	222	ILE
1	A	236	LYS
1	A	248	LYS
1	A	265	LYS
1	A	275	LEU
1	A	278	ILE
1	A	301	ARG
1	A	339	VAL
1	A	369	LYS
1	A	380	GLU
1	A	382	LYS
1	A	403	MET
1	A	456	SER
1	B	9	VAL
1	B	50	CYS
1	B	54	LYS
1	B	81	VAL
1	B	87	LYS
1	B	103	ILE
1	B	121	ILE
1	B	124	LYS
1	B	126	GLN
1	B	152	VAL
1	B	184	ILE
1	B	191	VAL
1	B	205	THR
1	B	231	GLN
1	B	304	VAL

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Mol	Chain	Res	Type
1	B	315	ILE
1	B	376	GLU
1	C	12	ILE
1	C	50	CYS
1	C	54	LYS
1	C	58	ASN
1	C	78	MET
1	C	182	VAL
1	C	203	ASP
1	C	254	ILE
1	C	267	GLU
1	C	299	ARG
1	C	339	VAL
1	C	382	LYS
1	C	395	LYS
1	C	456	SER
1	D	5	ILE
1	D	8	ASP
1	D	31	LYS
1	D	35	ILE
1	D	50	CYS
1	D	54	LYS
1	D	78	MET
1	D	81	VAL
1	D	128	THR
1	D	151	GLU
1	D	213	VAL
1	D	216	VAL
1	D	254	ILE
1	D	265	LYS
1	D	278	ILE
1	D	332	GLU
1	D	409	GLN
1	E	50	CYS
1	E	54	LYS
1	E	78	MET
1	E	81	VAL
1	E	162	GLU
1	E	166	VAL
1	E	184	ILE
1	E	213	VAL
1	E	250	SER

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Mol	Chain	Res	Type
1	E	258	ILE
1	E	278	ILE
1	E	333	ASP
1	E	379	ILE
1	E	470	LYS
1	F	50	CYS
1	F	54	LYS
1	F	65	MET
1	F	74	ARG
1	F	76	ILE
1	F	78	MET
1	F	81	VAL
1	F	103	ILE
1	F	213	VAL
1	F	262	SER
1	F	285	LYS
1	F	395	LYS
1	G	23	ILE
1	G	50	CYS
1	G	54	LYS
1	G	153	THR
1	G	208	GLU
1	G	272	ASP
1	G	274	LEU
1	G	276	VAL
1	G	301	ARG
1	G	333	ASP
1	G	336	ILE
1	H	50	CYS
1	H	54	LYS
1	H	113	VAL
1	H	179	GLU
1	H	228	ARG
1	H	275	LEU
1	H	290	GLU
1	H	306	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	116	ASN

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Mol	Chain	Res	Type
1	A	143	ASN
1	A	240	ASN
1	A	286	ASN
1	A	348	HIS
1	B	110	ASN
1	B	227	GLN
1	B	231	GLN
1	B	430	ASN
1	C	3	GLN
1	C	110	ASN
1	C	143	ASN
1	C	231	GLN
1	C	348	HIS
1	D	109	GLN
1	D	240	ASN
1	D	352	ASN
1	E	137	GLN
1	E	143	ASN
1	E	240	ASN
1	F	3	GLN
1	F	126	GLN
1	F	137	GLN
1	F	231	GLN
1	F	240	ASN
1	F	397	ASN
1	G	47	ASN
1	G	126	GLN
1	G	143	ASN
1	G	233	GLN
1	G	240	ASN
1	H	38	ASN
1	H	125	ASN
1	H	137	GLN
1	H	143	ASN
1	H	240	ASN
1	H	352	ASN

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](#)

35 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	SO4	H	503	-	4,4,4	0.14	0	6,6,6	0.21	0
3	SO4	C	504	-	4,4,4	0.28	0	6,6,6	0.13	0
3	SO4	B	502	-	4,4,4	0.20	0	6,6,6	0.12	0
3	SO4	H	502	-	4,4,4	0.22	0	6,6,6	0.10	0
3	SO4	G	503	-	4,4,4	0.24	0	6,6,6	0.10	0
3	SO4	A	504	-	4,4,4	0.31	0	6,6,6	0.09	0
3	SO4	D	504	-	4,4,4	0.31	0	6,6,6	0.10	0
3	SO4	C	503	-	4,4,4	0.20	0	6,6,6	0.12	0
3	SO4	C	507	-	4,4,4	0.29	0	6,6,6	0.15	0
3	SO4	G	504	-	4,4,4	0.29	0	6,6,6	0.19	0
2	FAD	C	501	-	58,58,58	0.64	1 (1%)	85,89,89	0.55	0
3	SO4	E	502	-	4,4,4	0.25	0	6,6,6	0.13	0
3	SO4	C	505	-	4,4,4	0.17	0	6,6,6	0.10	0
3	SO4	E	504	-	4,4,4	0.33	0	6,6,6	0.11	0
3	SO4	C	506	-	4,4,4	0.43	0	6,6,6	0.28	0
2	FAD	G	501	-	58,58,58	0.47	1 (1%)	85,89,89	0.48	1 (1%)
2	FAD	A	501	-	58,58,58	0.46	0	85,89,89	0.42	0
2	FAD	F	501	-	58,58,58	0.44	0	85,89,89	0.41	0
2	FAD	D	501	-	58,58,58	0.48	0	85,89,89	0.42	0
3	SO4	F	503	-	4,4,4	0.74	0	6,6,6	1.29	0
3	SO4	C	502	-	4,4,4	0.35	0	6,6,6	0.29	0
3	SO4	D	503	-	4,4,4	0.22	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	G	502	-	4,4,4	0.25	0	6,6,6	0.21	0
2	FAD	E	501	-	58,58,58	0.44	0	85,89,89	0.44	0
3	SO4	A	505	-	4,4,4	0.28	0	6,6,6	0.16	0
2	FAD	B	501	-	58,58,58	0.74	1 (1%)	85,89,89	0.40	0
3	SO4	A	506	-	4,4,4	0.26	0	6,6,6	0.13	0
3	SO4	A	503	-	4,4,4	0.31	0	6,6,6	0.16	0
3	SO4	E	503	-	4,4,4	0.26	0	6,6,6	0.19	0
3	SO4	D	505	-	4,4,4	0.25	0	6,6,6	0.18	0
3	SO4	B	503	-	4,4,4	0.30	0	6,6,6	0.17	0
3	SO4	A	502	-	4,4,4	0.23	0	6,6,6	0.35	0
2	FAD	H	501	-	58,58,58	0.62	3 (5%)	85,89,89	0.44	1 (1%)
3	SO4	F	502	-	4,4,4	0.24	0	6,6,6	0.19	0
3	SO4	D	502	-	4,4,4	0.24	0	6,6,6	0.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	E	501	-	-	3/34/50/50	0/6/6/6
2	FAD	B	501	-	-	2/34/50/50	0/6/6/6
2	FAD	G	501	-	-	3/34/50/50	0/6/6/6
2	FAD	A	501	-	-	2/34/50/50	0/6/6/6
2	FAD	F	501	-	-	2/34/50/50	0/6/6/6
2	FAD	D	501	-	-	2/34/50/50	0/6/6/6
2	FAD	C	501	-	-	2/34/50/50	0/6/6/6
2	FAD	H	501	-	-	3/34/50/50	0/6/6/6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FAD	P-O3P	4.72	1.64	1.59
2	C	501	FAD	P-O3P	2.89	1.62	1.59
2	H	501	FAD	P-O3P	2.64	1.62	1.59
2	H	501	FAD	P-O2P	-2.12	1.45	1.55
2	H	501	FAD	C1'-C2'	2.01	1.55	1.52
2	G	501	FAD	P-O3P	2.01	1.61	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	501	FAD	C4'-C3'-C2'	-2.69	109.09	113.57
2	H	501	FAD	C4'-C3'-C2'	2.15	117.14	113.57

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	501	FAD	C5'-O5'-P-O1P
2	G	501	FAD	O4B-C4B-C5B-O5B
2	G	501	FAD	C3B-C4B-C5B-O5B
2	G	501	FAD	O4'-C4'-C5'-O5'
2	E	501	FAD	O4B-C4B-C5B-O5B
2	E	501	FAD	C3B-C4B-C5B-O5B
2	B	501	FAD	O4B-C4B-C5B-O5B
2	H	501	FAD	O4B-C4B-C5B-O5B
2	H	501	FAD	C3B-C4B-C5B-O5B
2	B	501	FAD	C3B-C4B-C5B-O5B
2	A	501	FAD	PA-O3P-P-O5'
2	C	501	FAD	PA-O3P-P-O5'
2	E	501	FAD	PA-O3P-P-O5'
2	F	501	FAD	O4B-C4B-C5B-O5B
2	C	501	FAD	O4B-C4B-C5B-O5B
2	D	501	FAD	O4B-C4B-C5B-O5B
2	D	501	FAD	C2B-C1B-N9A-C8A
2	A	501	FAD	O4B-C4B-C5B-O5B
2	F	501	FAD	C3B-C4B-C5B-O5B

There are no ring outliers.

14 monomers are involved in 22 short contacts:

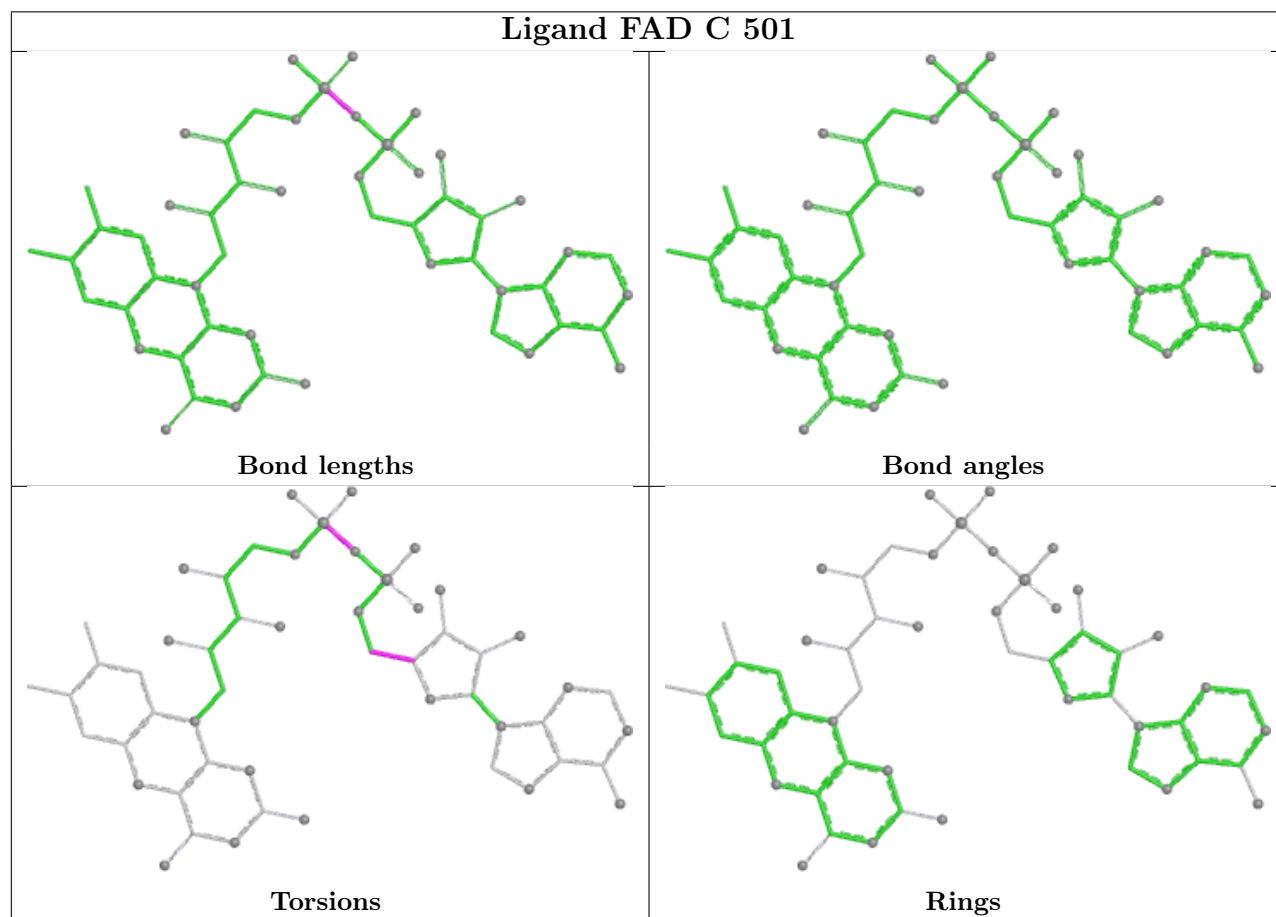
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	503	SO4	1	0
3	G	503	SO4	2	0
3	C	507	SO4	1	0
2	C	501	FAD	1	0
3	E	502	SO4	3	0
3	C	506	SO4	1	0
2	G	501	FAD	1	0
2	D	501	FAD	1	0
3	F	503	SO4	1	0
2	E	501	FAD	2	0
2	B	501	FAD	1	0

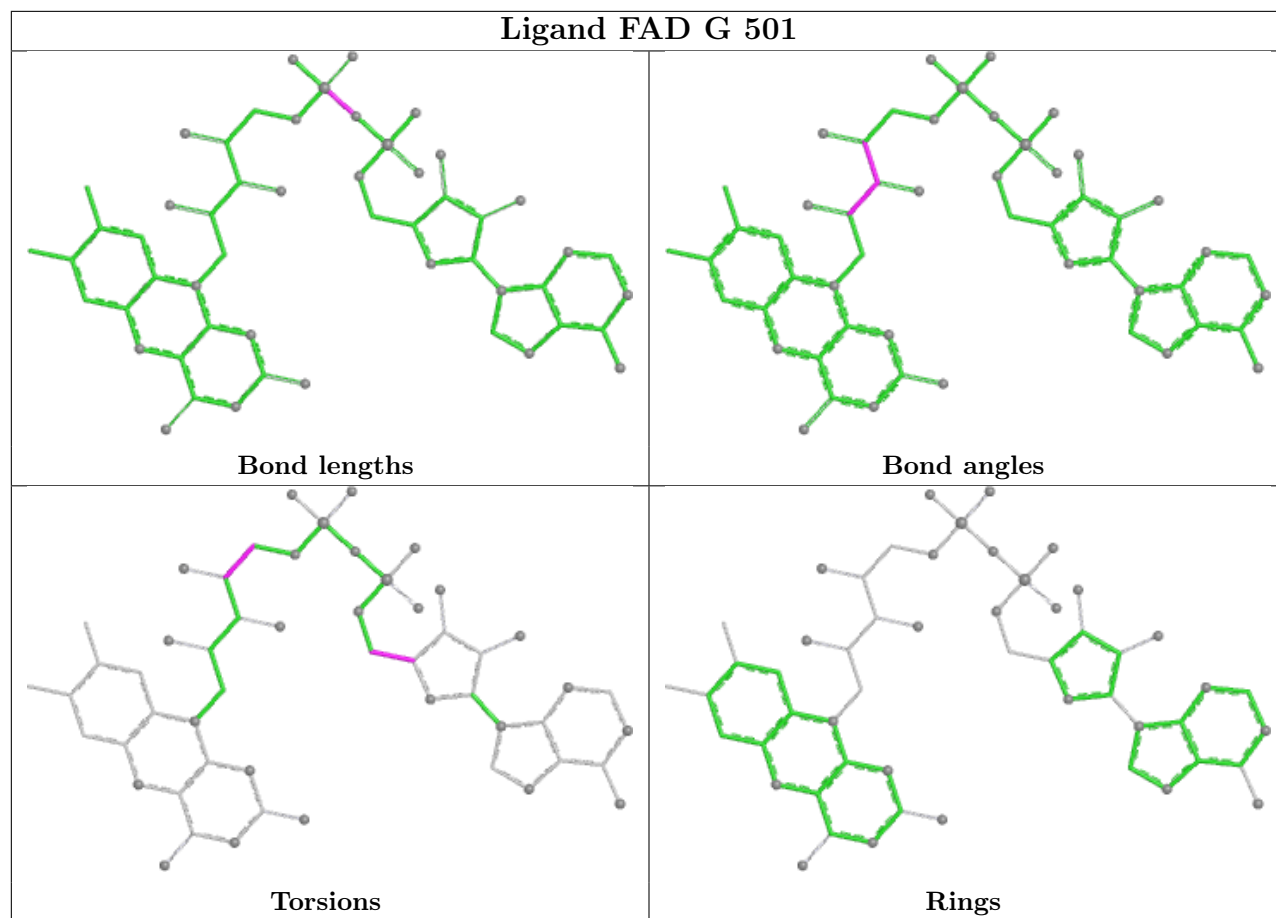
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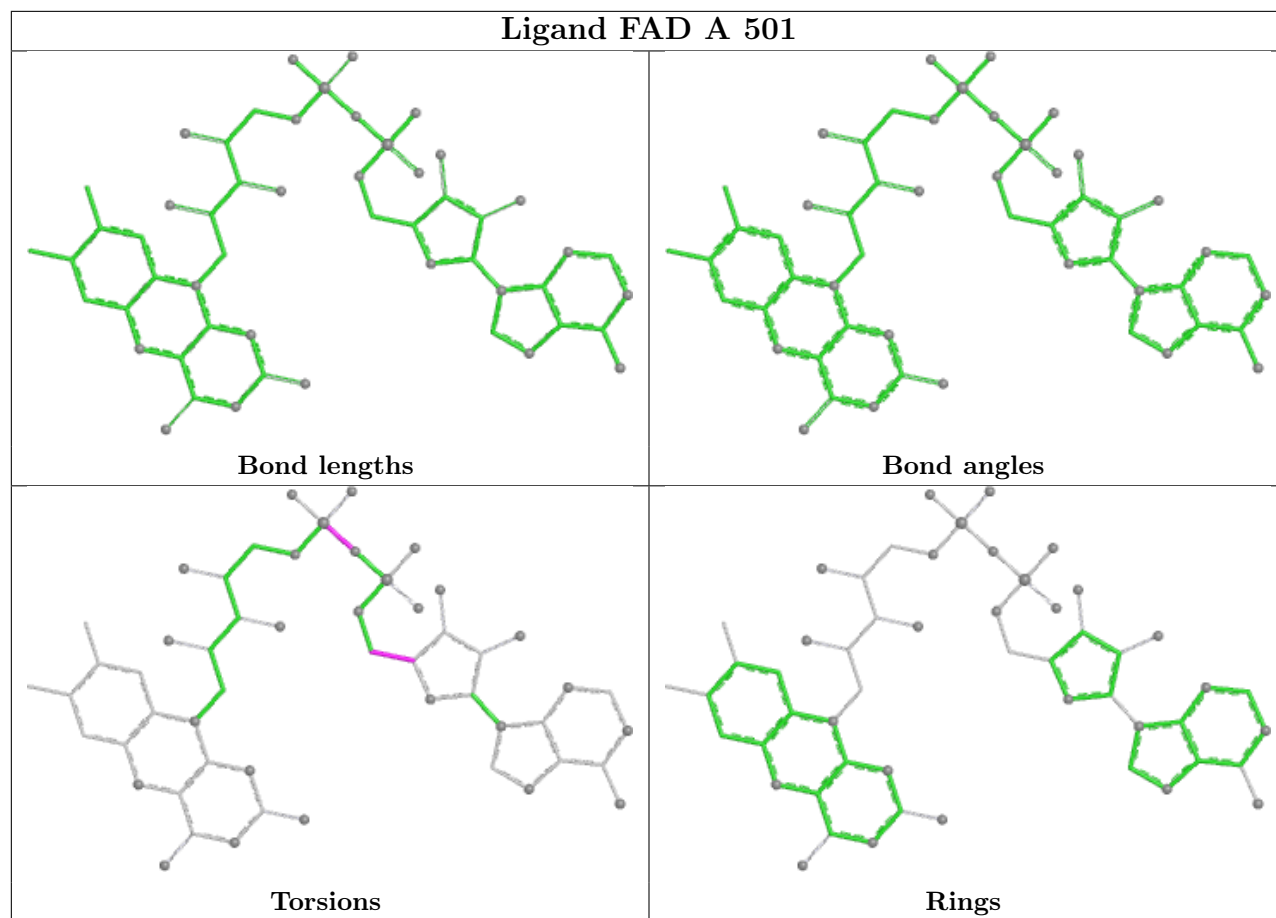
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	506	SO4	2	0
3	E	503	SO4	1	0
2	H	501	FAD	4	0

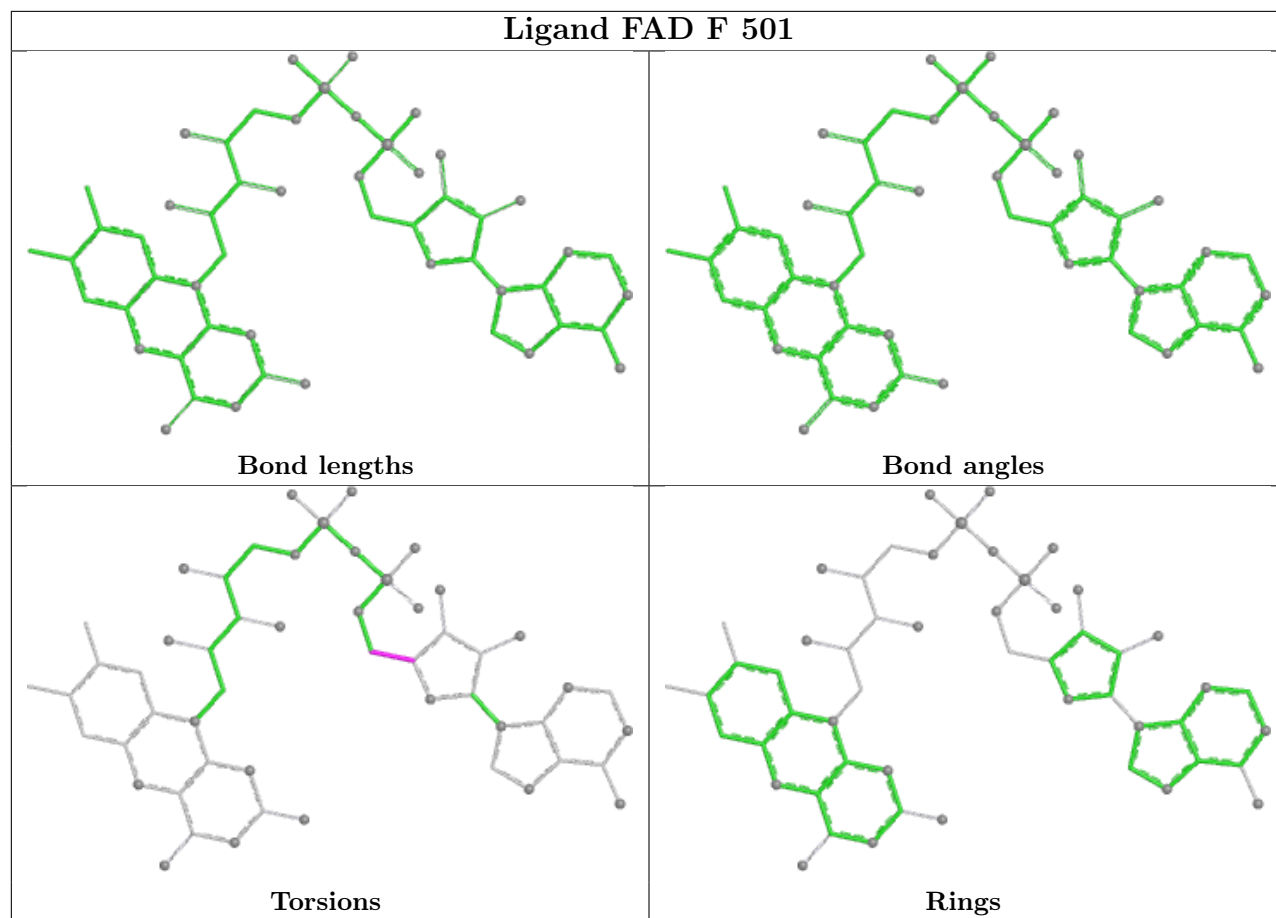
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

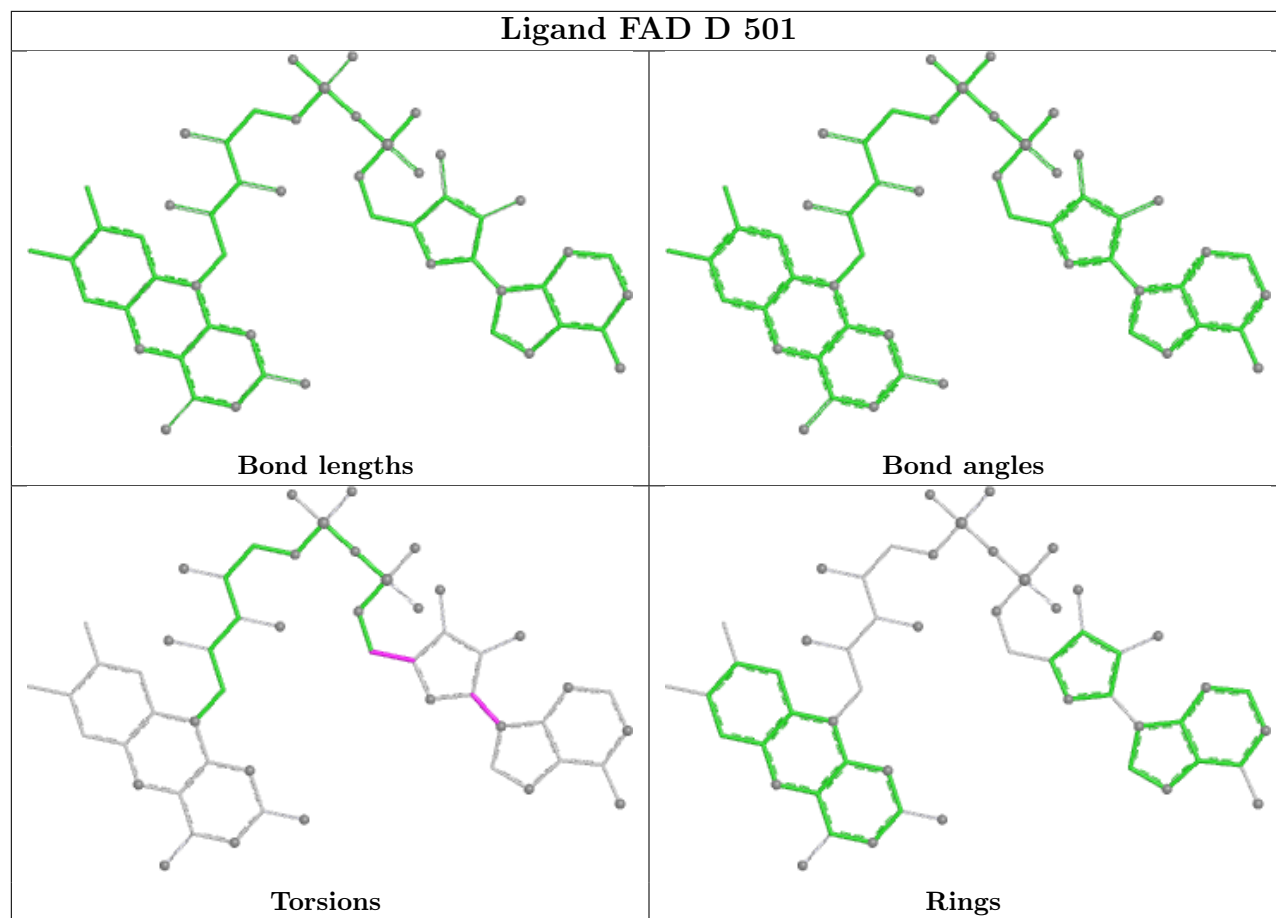




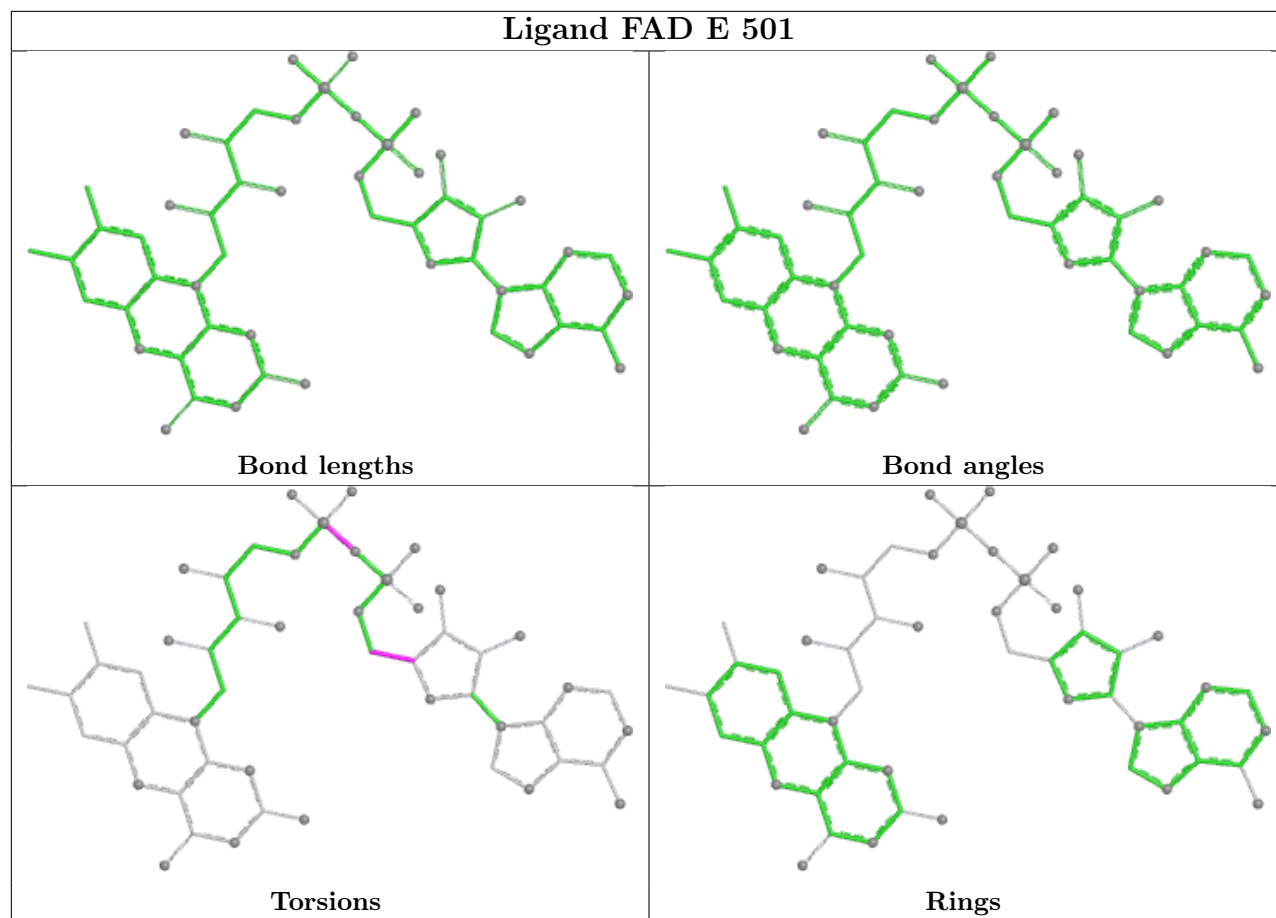


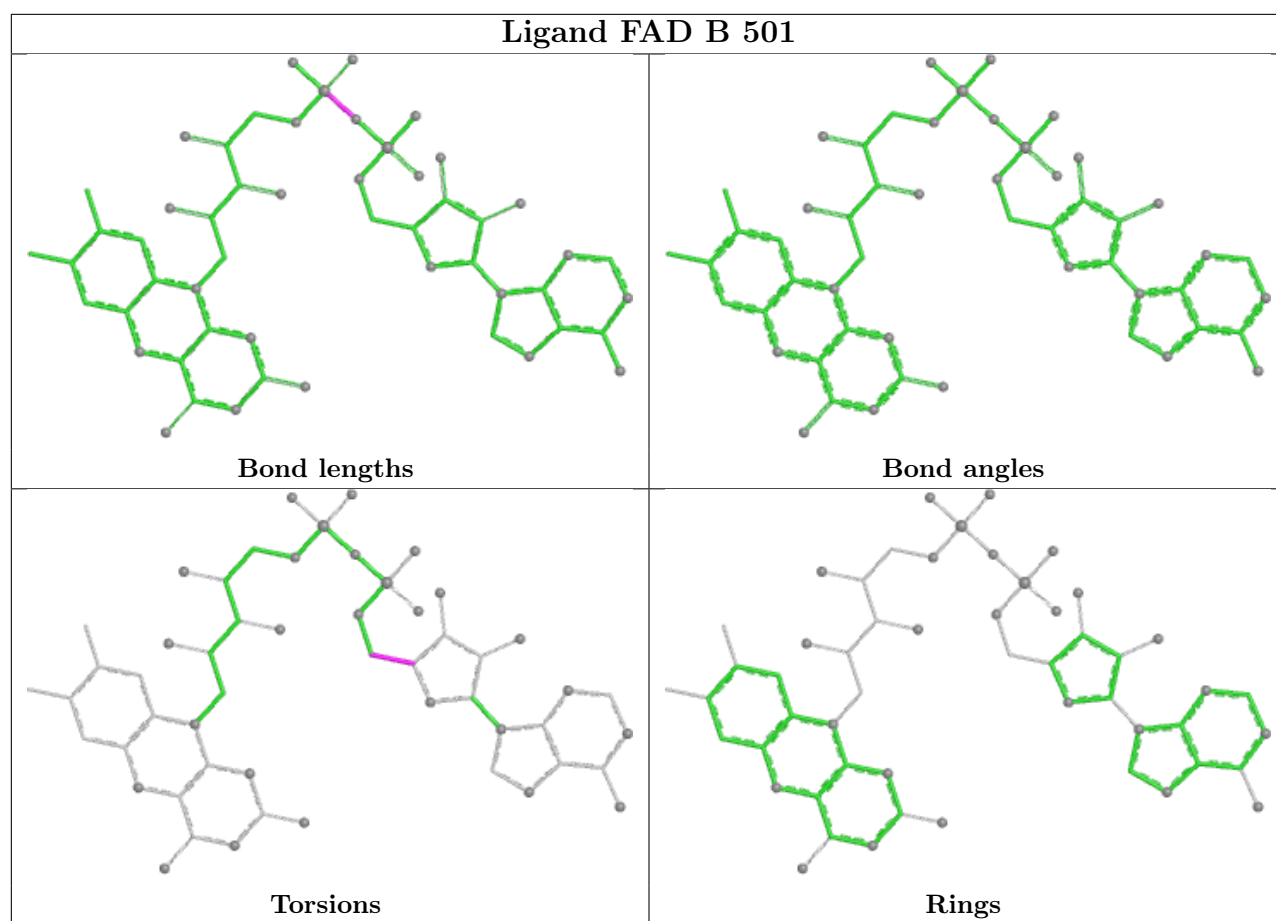
Ligand FAD F 501

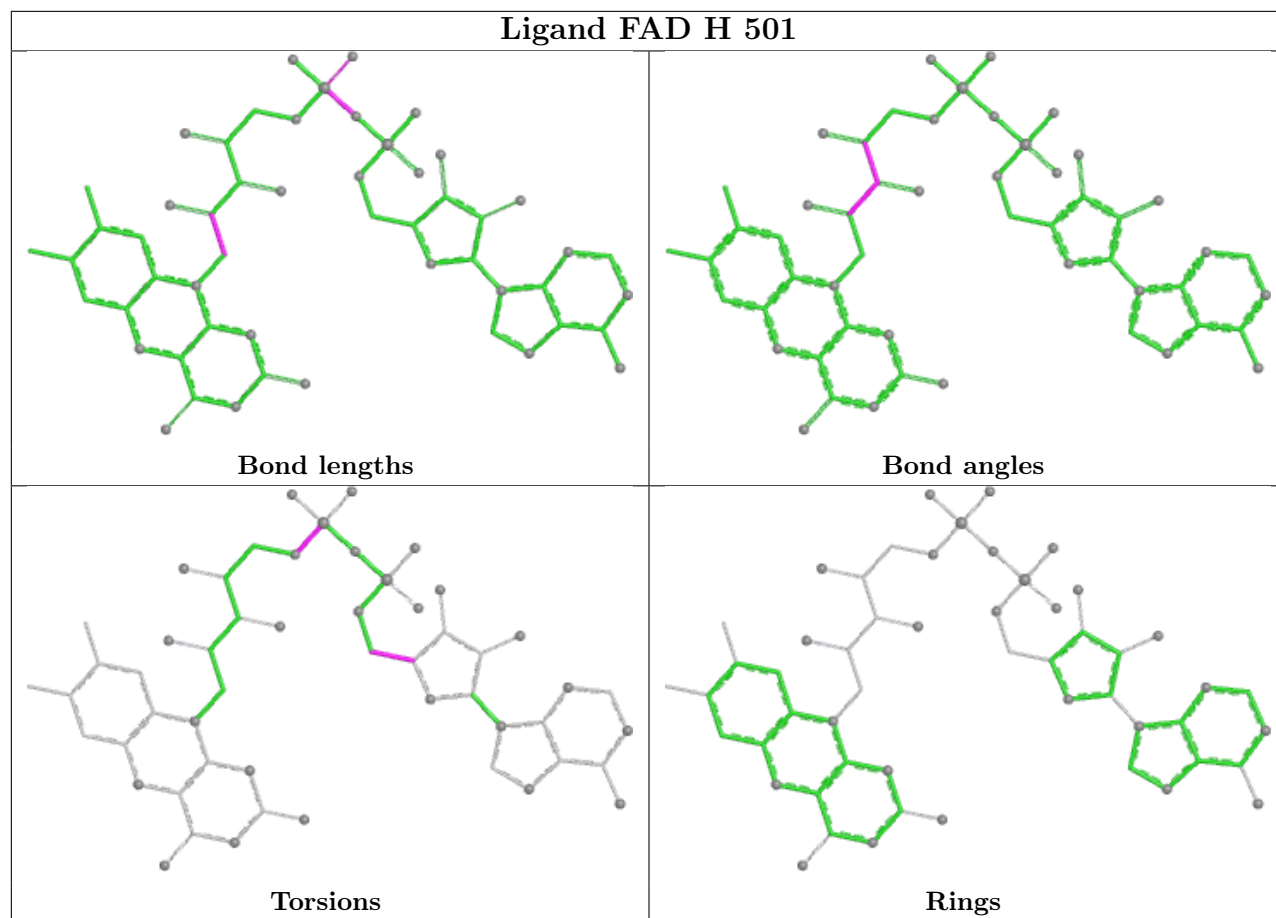




Ligand FAD E 501







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	472/496 (95%)	0.20	4 (0%) 82 85	23, 39, 66, 94	1 (0%)
1	B	472/496 (95%)	1.13	81 (17%) 4 4	31, 70, 111, 142	1 (0%)
1	C	472/496 (95%)	0.30	8 (1%) 69 73	25, 40, 67, 89	0
1	D	472/496 (95%)	1.26	105 (22%) 2 2	31, 73, 119, 150	0
1	E	472/496 (95%)	1.16	72 (15%) 5 6	33, 68, 105, 137	1 (0%)
1	F	472/496 (95%)	1.14	58 (12%) 8 9	40, 67, 104, 133	0
1	G	472/496 (95%)	1.12	67 (14%) 6 7	35, 67, 109, 138	0
1	H	472/496 (95%)	1.10	65 (13%) 6 7	34, 65, 106, 141	0
All	All	3776/3968 (95%)	0.93	460 (12%) 8 10	23, 62, 107, 150	3 (0%)

All (460) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	288	GLY	5.5
1	E	160	ILE	5.2
1	D	130	THR	5.1
1	B	119	GLY	5.0
1	G	264	GLY	4.8
1	D	247	THR	4.5
1	D	157	GLY	4.4
1	D	246	ALA	4.4
1	F	96	VAL	4.4
1	H	4	PRO	4.3
1	D	263	GLY	4.3
1	G	246	ALA	4.3
1	B	287	LEU	4.2
1	B	300	GLY	4.0
1	D	5	ILE	4.0
1	B	247	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	159	THR	4.0
1	B	332[A]	GLU	4.0
1	D	156	PRO	3.9
1	D	268	VAL	3.9
1	G	62	TYR	3.9
1	F	287	LEU	3.9
1	E	79	SER	3.8
1	D	136	THR	3.8
1	G	183	VAL	3.8
1	D	139	ILE	3.7
1	E	252	GLY	3.7
1	B	129	ALA	3.7
1	F	5	ILE	3.7
1	D	292	LEU	3.7
1	H	264	GLY	3.7
1	E	259	GLU	3.7
1	H	155	PHE	3.7
1	F	132	ALA	3.7
1	D	288	GLY	3.6
1	B	138	VAL	3.6
1	B	136	THR	3.6
1	D	122	THR	3.6
1	H	67	HIS	3.6
1	F	247	THR	3.6
1	G	154	PRO	3.6
1	D	30	PHE	3.5
1	E	62	TYR	3.5
1	D	245	GLY	3.5
1	E	247	THR	3.5
1	H	278	ILE	3.5
1	D	161	ASP	3.5
1	C	228	ARG	3.5
1	D	287	LEU	3.4
1	G	266	ALA	3.4
1	D	134	GLY	3.4
1	G	252	GLY	3.4
1	B	348	HIS	3.4
1	D	188	VAL	3.4
1	G	213	VAL	3.4
1	H	323	ALA	3.4
1	D	182	VAL	3.3
1	D	250	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	243	VAL	3.3
1	D	4	PRO	3.3
1	F	348	HIS	3.3
1	B	294	ILE	3.3
1	D	336	ILE	3.3
1	H	243	VAL	3.3
1	G	78	MET	3.3
1	H	245	GLY	3.3
1	D	160	ILE	3.3
1	F	121	ILE	3.3
1	F	176	LYS	3.3
1	D	252	GLY	3.2
1	E	263	GLY	3.2
1	D	296	LEU	3.2
1	G	79	SER	3.2
1	B	301	ARG	3.2
1	H	75	GLY	3.2
1	E	184	ILE	3.2
1	D	244	THR	3.2
1	B	243	VAL	3.2
1	D	243	VAL	3.2
1	G	156	PRO	3.2
1	G	254	ILE	3.2
1	D	266	ALA	3.2
1	D	289	LEU	3.2
1	D	123	GLY	3.1
1	D	12	ILE	3.1
1	H	247	THR	3.1
1	E	213	VAL	3.1
1	D	121	ILE	3.1
1	G	139	ILE	3.1
1	B	270	THR	3.1
1	E	156	PRO	3.1
1	B	121	ILE	3.1
1	D	158	ILE	3.1
1	F	12	ILE	3.1
1	G	262	SER	3.1
1	F	263	GLY	3.1
1	H	137	GLN	3.1
1	F	261	ALA	3.1
1	G	66	ALA	3.1
1	F	321	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	117	GLY	3.0
1	D	119	GLY	3.0
1	D	333	ASP	3.0
1	D	183	VAL	3.0
1	E	139	ILE	3.0
1	F	160	ILE	3.0
1	G	238	LYS	3.0
1	B	116	ASN	3.0
1	C	251	ASP	3.0
1	H	119	GLY	3.0
1	G	209	PHE	3.0
1	B	313	PRO	3.0
1	E	260	ALA	3.0
1	H	271	CYS	3.0
1	D	48	VAL	3.0
1	D	257	SER	3.0
1	D	262	SER	3.0
1	H	73	SER	3.0
1	H	79	SER	3.0
1	F	264	GLY	3.0
1	H	246	ALA	3.0
1	D	205	THR	3.0
1	H	82	ARG	3.0
1	D	255	ASP	3.0
1	B	246	ALA	2.9
1	F	276	VAL	2.9
1	H	254	ILE	2.9
1	B	130	THR	2.9
1	F	136	THR	2.9
1	B	286	ASN	2.9
1	E	237	PHE	2.9
1	H	124	LYS	2.9
1	D	32	THR	2.9
1	G	163	ASP	2.9
1	E	271	CYS	2.9
1	E	254	ILE	2.9
1	H	306	THR	2.9
1	F	79	SER	2.9
1	E	249	LYS	2.9
1	E	182	VAL	2.9
1	E	39	GLU	2.9
1	E	70	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	252	GLY	2.8
1	E	216	VAL	2.8
1	B	158	ILE	2.8
1	D	35	ILE	2.8
1	G	184	ILE	2.8
1	H	269	ILE	2.8
1	B	120	LYS	2.8
1	H	263	GLY	2.8
1	B	274	LEU	2.8
1	H	287	LEU	2.8
1	D	267	GLU	2.8
1	D	294	ILE	2.8
1	H	262	SER	2.8
1	D	33	VAL	2.8
1	B	3	GLN	2.8
1	E	293	GLY	2.8
1	D	132	ALA	2.8
1	F	269	ILE	2.7
1	F	396	THR	2.7
1	F	262	SER	2.7
1	H	277	CYS	2.7
1	H	96	VAL	2.7
1	B	159	THR	2.7
1	B	284	THR	2.7
1	D	184	ILE	2.7
1	D	124	LYS	2.7
1	F	131	LYS	2.7
1	F	239	LEU	2.7
1	D	202	ALA	2.7
1	D	348	HIS	2.7
1	B	276	VAL	2.7
1	D	138	VAL	2.7
1	D	286	ASN	2.7
1	D	105	HIS	2.7
1	A	58	ASN	2.7
1	H	138	VAL	2.7
1	G	159	THR	2.7
1	H	248	LYS	2.7
1	B	79	SER	2.7
1	E	262	SER	2.7
1	B	281	ARG	2.7
1	E	83	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	3	GLN	2.6
1	H	3	GLN	2.6
1	G	124	LYS	2.6
1	F	259	GLU	2.6
1	B	160	ILE	2.6
1	B	217	GLY	2.6
1	B	258	ILE	2.6
1	D	42	GLY	2.6
1	D	14	SER	2.6
1	G	250	SER	2.6
1	B	145	LEU	2.6
1	G	71	PHE	2.6
1	B	82	ARG	2.6
1	D	256	VAL	2.6
1	E	183	VAL	2.6
1	G	157	GLY	2.6
1	B	262	SER	2.6
1	C	379	ILE	2.6
1	H	258	ILE	2.6
1	G	259	GLU	2.6
1	F	255	ASP	2.6
1	B	182	VAL	2.6
1	G	136	THR	2.6
1	G	201	GLY	2.6
1	G	3	GLN	2.6
1	G	90	GLU	2.6
1	G	72	ALA	2.6
1	G	98	ALA	2.6
1	E	258	ILE	2.6
1	E	72	ALA	2.5
1	E	246	ALA	2.5
1	D	116	ASN	2.5
1	F	6	ASP	2.5
1	F	78	MET	2.5
1	H	68	GLY	2.5
1	B	256	VAL	2.5
1	D	253	LYS	2.5
1	G	105	HIS	2.5
1	G	249	LYS	2.5
1	B	118	TYR	2.5
1	E	85	LEU	2.5
1	B	133	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	140	ASP	2.5
1	G	132	ALA	2.5
1	D	264	GLY	2.5
1	E	71	PHE	2.5
1	F	76	ILE	2.5
1	D	232	LYS	2.5
1	D	328	ALA	2.5
1	E	6	ASP	2.5
1	H	130	THR	2.5
1	E	235	PHE	2.5
1	G	30	PHE	2.5
1	G	166	VAL	2.5
1	H	121	ILE	2.5
1	B	239	LEU	2.5
1	H	65	MET	2.5
1	D	248	LYS	2.5
1	G	248	LYS	2.5
1	G	75	GLY	2.5
1	G	263	GLY	2.5
1	D	128	THR	2.4
1	F	307	ARG	2.4
1	B	250	SER	2.4
1	B	152	VAL	2.4
1	D	144	ILE	2.4
1	E	177	VAL	2.4
1	F	127	VAL	2.4
1	F	294	ILE	2.4
1	B	292	LEU	2.4
1	E	131	LYS	2.4
1	D	3	GLN	2.4
1	D	313	PRO	2.4
1	E	266	ALA	2.4
1	D	376	GLU	2.4
1	B	321	VAL	2.4
1	D	112	VAL	2.4
1	F	139	ILE	2.4
1	F	254	ILE	2.4
1	H	48	VAL	2.4
1	F	242	LYS	2.4
1	F	88	MET	2.4
1	H	239	LEU	2.4
1	E	109	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	252	GLY	2.4
1	G	451	ALA	2.4
1	H	129	ALA	2.4
1	B	353	CYS	2.4
1	E	248	LYS	2.4
1	D	127	VAL	2.4
1	E	152	VAL	2.4
1	E	191	VAL	2.4
1	E	269	ILE	2.4
1	G	131	LYS	2.4
1	F	112	VAL	2.4
1	F	182	VAL	2.4
1	H	160	ILE	2.4
1	B	403	MET	2.4
1	B	289	LEU	2.4
1	B	251	ASP	2.4
1	F	260	ALA	2.4
1	G	55	ALA	2.4
1	H	250	SER	2.4
1	H	165	ILE	2.4
1	E	239	LEU	2.4
1	G	83	LEU	2.4
1	B	105	HIS	2.4
1	B	333	ASP	2.3
1	G	6	ASP	2.3
1	D	135	GLY	2.3
1	E	224	LYS	2.3
1	E	265	LYS	2.3
1	F	164	THR	2.3
1	B	257	SER	2.3
1	B	339	VAL	2.3
1	D	146	ILE	2.3
1	E	12	ILE	2.3
1	G	57	LEU	2.3
1	F	80	GLU	2.3
1	E	163	ASP	2.3
1	D	249	LYS	2.3
1	G	176	LYS	2.3
1	B	134	GLY	2.3
1	E	245	GLY	2.3
1	B	132	ALA	2.3
1	G	5	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	61	HIS	2.3
1	B	291	GLU	2.3
1	D	11	VAL	2.3
1	F	155	PHE	2.3
1	H	268	VAL	2.3
1	B	203	ASP	2.3
1	E	116	ASN	2.3
1	B	4	PRO	2.3
1	B	123	GLY	2.3
1	F	211	GLY	2.3
1	G	247	THR	2.3
1	F	82	ARG	2.3
1	D	269	ILE	2.3
1	B	155	PHE	2.3
1	D	339	VAL	2.3
1	E	155	PHE	2.3
1	E	375	LYS	2.3
1	H	108	LYS	2.3
1	F	251	ASP	2.3
1	E	154	PRO	2.3
1	B	293	GLY	2.3
1	G	288	GLY	2.3
1	D	118	TYR	2.3
1	E	205	THR	2.3
1	F	290	GLU	2.3
1	B	35	ILE	2.3
1	F	111	LYS	2.3
1	F	265	LYS	2.3
1	B	216	VAL	2.3
1	B	273	VAL	2.3
1	D	113	VAL	2.3
1	H	81	VAL	2.3
1	H	276	VAL	2.3
1	E	45	CYS	2.2
1	G	300	GLY	2.2
1	A	457	GLU	2.2
1	B	323	ALA	2.2
1	H	261	ALA	2.2
1	B	122	THR	2.2
1	D	79	SER	2.2
1	D	155	PHE	2.2
1	D	304	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	182	VAL	2.2
1	F	154	PRO	2.2
1	E	124	LYS	2.2
1	B	165	ILE	2.2
1	D	254	ILE	2.2
1	E	278	ILE	2.2
1	E	296	LEU	2.2
1	E	112	VAL	2.2
1	D	251	ASP	2.2
1	B	65	MET	2.2
1	B	252	GLY	2.2
1	D	341	GLY	2.2
1	D	285	LYS	2.2
1	D	150	SER	2.2
1	E	244	THR	2.2
1	G	261	ALA	2.2
1	B	6	ASP	2.2
1	E	251	ASP	2.2
1	E	333	ASP	2.2
1	F	143	ASN	2.2
1	F	399	ASP	2.2
1	G	11	VAL	2.2
1	G	152	VAL	2.2
1	B	156	PRO	2.2
1	D	97	LYS	2.2
1	D	149	GLY	2.2
1	D	129	ALA	2.2
1	F	32	THR	2.2
1	E	228	ARG	2.1
1	B	139	ILE	2.1
1	H	35	ILE	2.1
1	B	166	VAL	2.1
1	B	268	VAL	2.1
1	D	152	VAL	2.1
1	F	81	VAL	2.1
1	C	248	LYS	2.1
1	E	175	LYS	2.1
1	G	253	LYS	2.1
1	B	187	GLY	2.1
1	F	101	GLY	2.1
1	B	261	ALA	2.1
1	C	132	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	244	THR	2.1
1	H	266	ALA	2.1
1	H	346	ALA	2.1
1	H	360	THR	2.1
1	B	63	TYR	2.1
1	F	472	ILE	2.1
1	G	65	MET	2.1
1	H	80	GLU	2.1
1	H	267	GLU	2.1
1	D	115	VAL	2.1
1	A	3	GLN	2.1
1	E	4	PRO	2.1
1	F	252	GLY	2.1
1	G	119	GLY	2.1
1	H	345	GLY	2.1
1	B	128	THR	2.1
1	H	241	THR	2.1
1	D	140	ASP	2.1
1	D	258	ILE	2.1
1	E	379	ILE	2.1
1	G	274	LEU	2.1
1	G	379	ILE	2.1
1	H	255	ASP	2.1
1	G	112	VAL	2.1
1	H	474	PHE	2.1
1	F	135	GLY	2.1
1	D	284	THR	2.1
1	E	122	THR	2.1
1	E	451	ALA	2.1
1	F	395	LYS	2.1
1	E	78	MET	2.1
1	E	289	LEU	2.1
1	A	251	ASP	2.1
1	G	178	PRO	2.1
1	E	138	VAL	2.1
1	E	276	VAL	2.1
1	H	191	VAL	2.1
1	B	170	GLY	2.1
1	D	13	GLY	2.1
1	G	265	LYS	2.0
1	H	69	LYS	2.0
1	H	159	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	398	ALA	2.0
1	H	7	ALA	2.0
1	H	50	CYS	2.0
1	F	91	GLN	2.0
1	D	99	LEU	2.0
1	D	133	ASP	2.0
1	E	275	LEU	2.0
1	D	318	ILE	2.0
1	G	269	ILE	2.0
1	H	118	TYR	2.0
1	D	319	GLY	2.0
1	B	237	PHE	2.0
1	D	148	THR	2.0
1	H	396	THR	2.0
1	D	22	ALA	2.0
1	D	261	ALA	2.0
1	F	26	ALA	2.0
1	G	95	ALA	2.0
1	G	45	CYS	2.0
1	E	287	LEU	2.0
1	E	5	ILE	2.0
1	G	160	ILE	2.0
1	H	158	ILE	2.0
1	D	131	LYS	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](#)

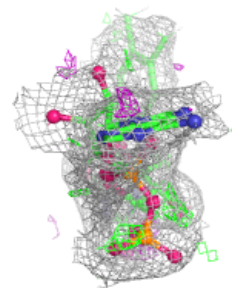
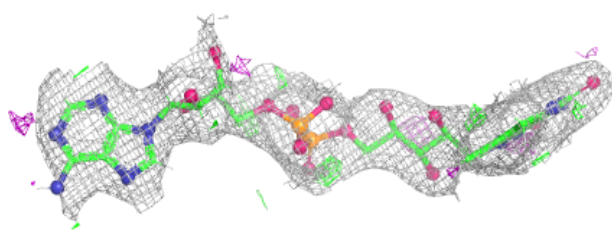
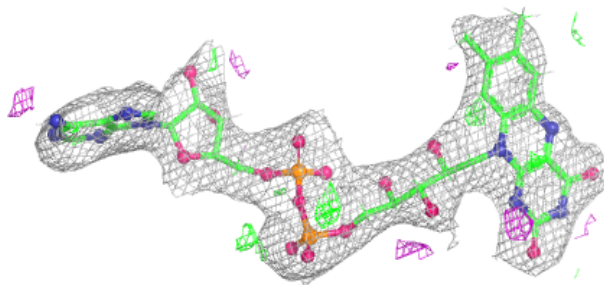
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	G	504	5/5	0.51	0.15	94,94,96,96	0
3	SO4	C	506	5/5	0.68	0.20	56,63,70,70	0
3	SO4	B	502	5/5	0.68	0.15	97,98,98,100	0
3	SO4	G	503	5/5	0.69	0.14	90,105,107,108	0
3	SO4	A	506	5/5	0.71	0.14	75,88,90,90	0
3	SO4	F	503	5/5	0.71	0.14	50,53,57,57	5
3	SO4	G	502	5/5	0.72	0.15	89,89,92,93	0
3	SO4	D	504	5/5	0.73	0.15	82,83,85,85	0
3	SO4	E	503	5/5	0.73	0.14	105,105,106,108	0
3	SO4	E	504	5/5	0.74	0.11	84,84,86,87	0
3	SO4	D	505	5/5	0.76	0.15	51,53,56,57	5
3	SO4	E	502	5/5	0.76	0.12	80,97,99,99	0
3	SO4	D	502	5/5	0.77	0.13	100,100,101,101	0
3	SO4	B	503	5/5	0.79	0.12	96,97,98,99	0
3	SO4	C	502	5/5	0.81	0.16	66,66,67,67	0
3	SO4	C	507	5/5	0.81	0.14	41,42,44,46	5
3	SO4	A	505	5/5	0.82	0.13	80,82,83,83	0
3	SO4	F	502	5/5	0.82	0.12	83,84,84,85	0
3	SO4	D	503	5/5	0.82	0.10	98,98,98,99	0
3	SO4	H	502	5/5	0.86	0.10	90,91,93,93	0
3	SO4	C	504	5/5	0.87	0.13	82,82,84,84	0
2	FAD	D	501	53/53	0.88	0.13	42,64,81,84	0
3	SO4	C	503	5/5	0.88	0.14	74,75,76,77	0
2	FAD	B	501	53/53	0.89	0.12	42,58,74,78	0
2	FAD	H	501	53/53	0.90	0.11	39,55,67,71	0
3	SO4	H	503	5/5	0.90	0.10	49,53,55,60	5
3	SO4	A	503	5/5	0.91	0.11	64,64,65,67	0
2	FAD	F	501	53/53	0.91	0.10	36,54,68,76	0
2	FAD	E	501	53/53	0.91	0.12	28,56,84,88	0
2	FAD	G	501	53/53	0.92	0.10	29,53,66,68	0
3	SO4	A	504	5/5	0.93	0.08	65,67,70,72	0
3	SO4	C	505	5/5	0.93	0.09	73,74,76,78	0
3	SO4	A	502	5/5	0.95	0.09	47,48,49,51	0
2	FAD	C	501	53/53	0.95	0.08	17,26,36,38	0
2	FAD	A	501	53/53	0.95	0.08	15,26,34,40	0

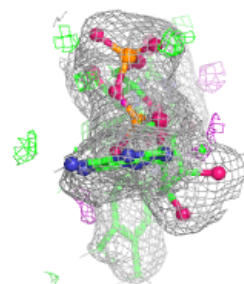
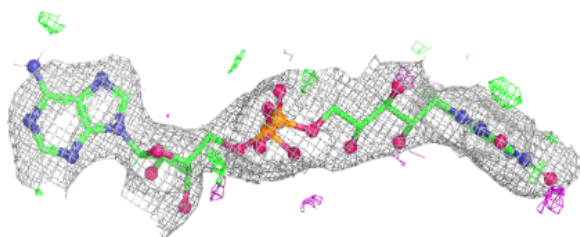
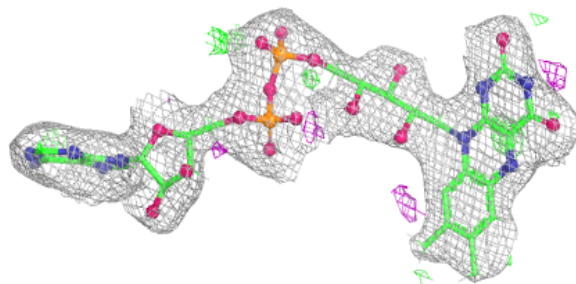
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD D 501:

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

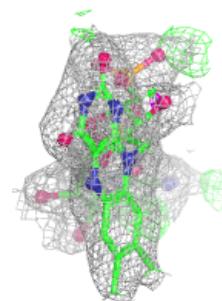
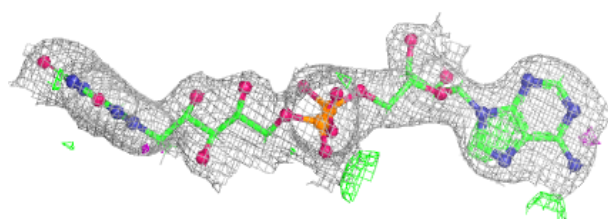
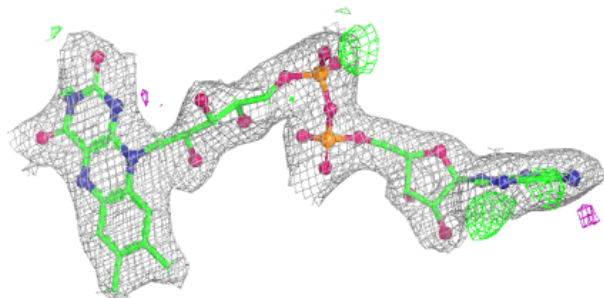
**Electron density around FAD B 501:**

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

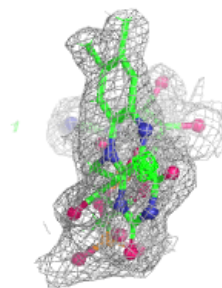
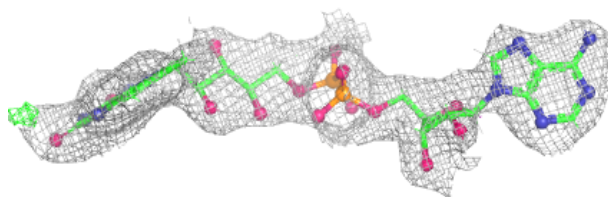
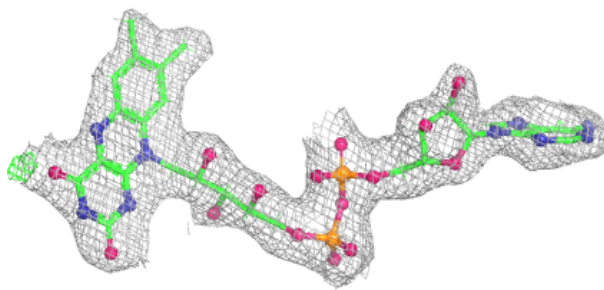


Electron density around FAD H 501:

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

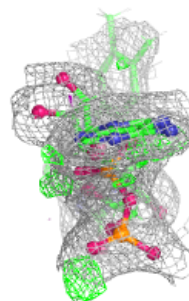
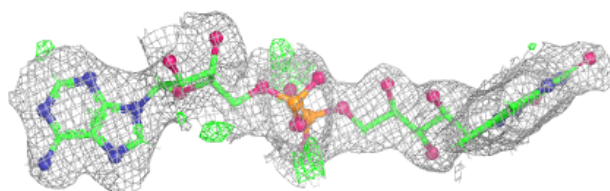
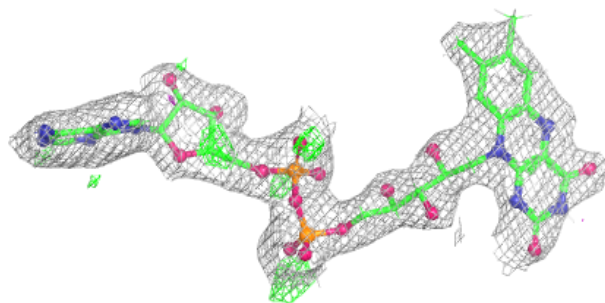
**Electron density around FAD F 501:**

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

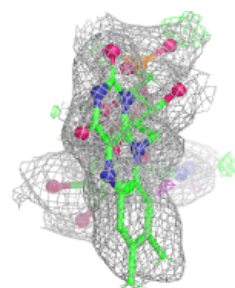
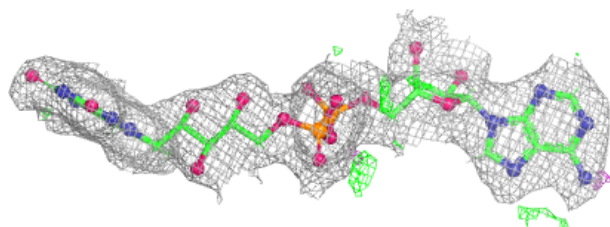
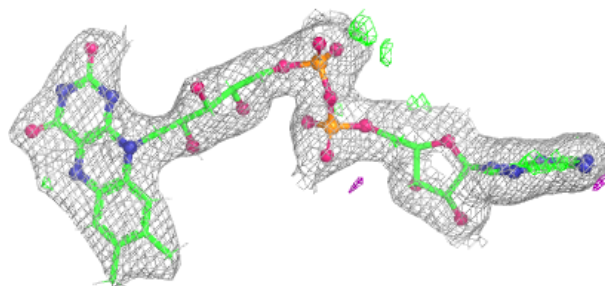


Electron density around FAD E 501:

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

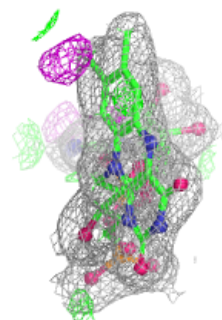
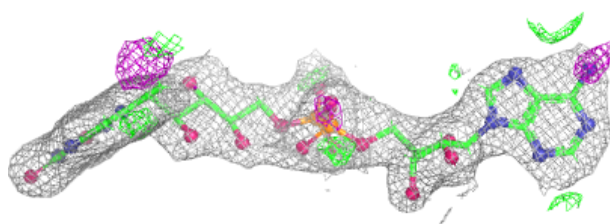
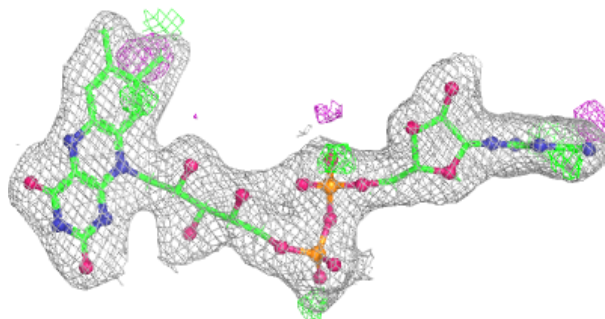
**Electron density around FAD G 501:**

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

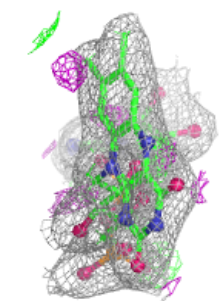
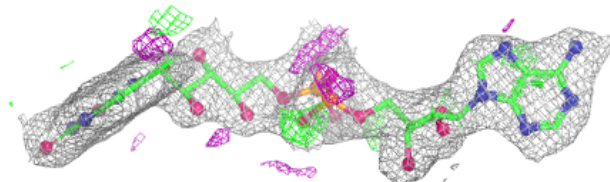
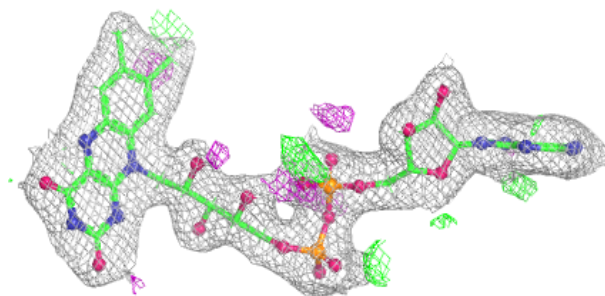


Electron density around FAD C 501:

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

**Electron density around FAD A 501:**

$2mF_o-DF_c$ (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.