Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 04:51 PM JST

PDB ID	:	6LPI
Title	:	Crystal Structure of AHAS holo-enzyme
Authors	:	Zhang, Y.; Yang, X.; Xi, Z.; Shen, Y.
Deposited on	:	2020-01-10
Resolution	:	2.85 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:

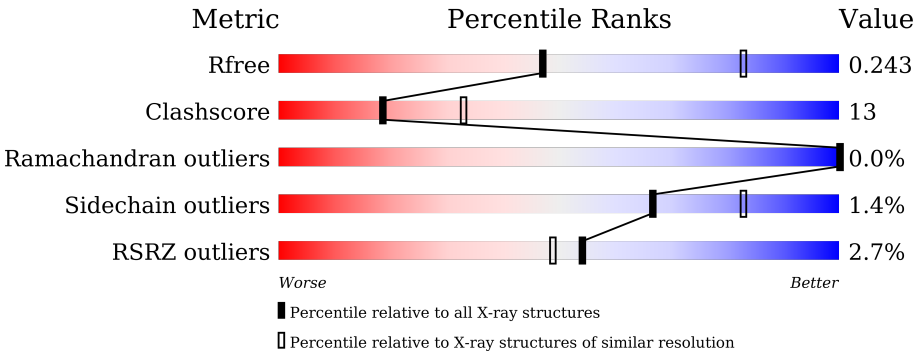
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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

Mol	Chain	Length	Quality of chain
1	E	127	62% 8% 30%
1	F	127	44% 25% 30%
1	G	127	43% 26% 31%
1	H	127	48% 21% 31%
2	A	562	66% 27% 6%
2	B	562	4% 70% 25%

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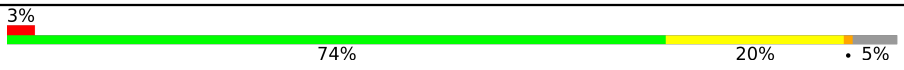
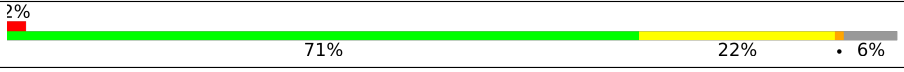
Mol	Chain	Length	Quality of chain
2	C	562	
2	D	562	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 18840 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 Acetolactate synthase isozyme 1 small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	89	Total	C	N	O	S	0	0	0
			689	440	117	127	5			
1	F	89	Total	C	N	O	S	0	0	0
			710	451	124	130	5			
1	G	88	Total	C	N	O	S	0	0	0
			691	441	118	127	5			
1	H	88	Total	C	N	O	S	0	0	0
			707	449	125	128	5			

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	PRO	-	expression tag	UNP P0ADF8
E	97	ALA	-	expression tag	UNP P0ADF8
E	98	SER	-	expression tag	UNP P0ADF8
E	99	THR	-	expression tag	UNP P0ADF8
E	100	ALA	-	expression tag	UNP P0ADF8
E	101	ALA	-	expression tag	UNP P0ADF8
E	102	THR	-	expression tag	UNP P0ADF8
E	103	SER	-	expression tag	UNP P0ADF8
E	104	ALA	-	expression tag	UNP P0ADF8
E	105	ALA	-	expression tag	UNP P0ADF8
E	106	ALA	-	expression tag	UNP P0ADF8
E	107	THR	-	expression tag	UNP P0ADF8
E	108	SER	-	expression tag	UNP P0ADF8
E	109	ALA	-	expression tag	UNP P0ADF8
E	110	ALA	-	expression tag	UNP P0ADF8
E	111	ALA	-	expression tag	UNP P0ADF8
E	112	THR	-	expression tag	UNP P0ADF8
E	113	SER	-	expression tag	UNP P0ADF8
E	114	ALA	-	expression tag	UNP P0ADF8
E	115	ALA	-	expression tag	UNP P0ADF8
E	116	ALA	-	expression tag	UNP P0ADF8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	117	THR	-	expression tag	UNP P0ADF8
E	118	SER	-	expression tag	UNP P0ADF8
E	119	ALA	-	expression tag	UNP P0ADF8
E	120	ALA	-	expression tag	UNP P0ADF8
E	121	ALA	-	expression tag	UNP P0ADF8
E	122	THR	-	expression tag	UNP P0ADF8
E	123	SER	-	expression tag	UNP P0ADF8
E	124	ALA	-	expression tag	UNP P0ADF8
E	125	ALA	-	expression tag	UNP P0ADF8
E	126	SER	-	expression tag	UNP P0ADF8
F	0	PRO	-	expression tag	UNP P0ADF8
F	97	ALA	-	expression tag	UNP P0ADF8
F	98	SER	-	expression tag	UNP P0ADF8
F	99	THR	-	expression tag	UNP P0ADF8
F	100	ALA	-	expression tag	UNP P0ADF8
F	101	ALA	-	expression tag	UNP P0ADF8
F	102	THR	-	expression tag	UNP P0ADF8
F	103	SER	-	expression tag	UNP P0ADF8
F	104	ALA	-	expression tag	UNP P0ADF8
F	105	ALA	-	expression tag	UNP P0ADF8
F	106	ALA	-	expression tag	UNP P0ADF8
F	107	THR	-	expression tag	UNP P0ADF8
F	108	SER	-	expression tag	UNP P0ADF8
F	109	ALA	-	expression tag	UNP P0ADF8
F	110	ALA	-	expression tag	UNP P0ADF8
F	111	ALA	-	expression tag	UNP P0ADF8
F	112	THR	-	expression tag	UNP P0ADF8
F	113	SER	-	expression tag	UNP P0ADF8
F	114	ALA	-	expression tag	UNP P0ADF8
F	115	ALA	-	expression tag	UNP P0ADF8
F	116	ALA	-	expression tag	UNP P0ADF8
F	117	THR	-	expression tag	UNP P0ADF8
F	118	SER	-	expression tag	UNP P0ADF8
F	119	ALA	-	expression tag	UNP P0ADF8
F	120	ALA	-	expression tag	UNP P0ADF8
F	121	ALA	-	expression tag	UNP P0ADF8
F	122	THR	-	expression tag	UNP P0ADF8
F	123	SER	-	expression tag	UNP P0ADF8
F	124	ALA	-	expression tag	UNP P0ADF8
F	125	ALA	-	expression tag	UNP P0ADF8
F	126	SER	-	expression tag	UNP P0ADF8
G	0	PRO	-	expression tag	UNP P0ADF8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	97	ALA	-	expression tag	UNP P0ADF8
G	98	SER	-	expression tag	UNP P0ADF8
G	99	THR	-	expression tag	UNP P0ADF8
G	100	ALA	-	expression tag	UNP P0ADF8
G	101	ALA	-	expression tag	UNP P0ADF8
G	102	THR	-	expression tag	UNP P0ADF8
G	103	SER	-	expression tag	UNP P0ADF8
G	104	ALA	-	expression tag	UNP P0ADF8
G	105	ALA	-	expression tag	UNP P0ADF8
G	106	ALA	-	expression tag	UNP P0ADF8
G	107	THR	-	expression tag	UNP P0ADF8
G	108	SER	-	expression tag	UNP P0ADF8
G	109	ALA	-	expression tag	UNP P0ADF8
G	110	ALA	-	expression tag	UNP P0ADF8
G	111	ALA	-	expression tag	UNP P0ADF8
G	112	THR	-	expression tag	UNP P0ADF8
G	113	SER	-	expression tag	UNP P0ADF8
G	114	ALA	-	expression tag	UNP P0ADF8
G	115	ALA	-	expression tag	UNP P0ADF8
G	116	ALA	-	expression tag	UNP P0ADF8
G	117	THR	-	expression tag	UNP P0ADF8
G	118	SER	-	expression tag	UNP P0ADF8
G	119	ALA	-	expression tag	UNP P0ADF8
G	120	ALA	-	expression tag	UNP P0ADF8
G	121	ALA	-	expression tag	UNP P0ADF8
G	122	THR	-	expression tag	UNP P0ADF8
G	123	SER	-	expression tag	UNP P0ADF8
G	124	ALA	-	expression tag	UNP P0ADF8
G	125	ALA	-	expression tag	UNP P0ADF8
G	126	SER	-	expression tag	UNP P0ADF8
H	0	PRO	-	expression tag	UNP P0ADF8
H	97	ALA	-	expression tag	UNP P0ADF8
H	98	SER	-	expression tag	UNP P0ADF8
H	99	THR	-	expression tag	UNP P0ADF8
H	100	ALA	-	expression tag	UNP P0ADF8
H	101	ALA	-	expression tag	UNP P0ADF8
H	102	THR	-	expression tag	UNP P0ADF8
H	103	SER	-	expression tag	UNP P0ADF8
H	104	ALA	-	expression tag	UNP P0ADF8
H	105	ALA	-	expression tag	UNP P0ADF8
H	106	ALA	-	expression tag	UNP P0ADF8
H	107	THR	-	expression tag	UNP P0ADF8

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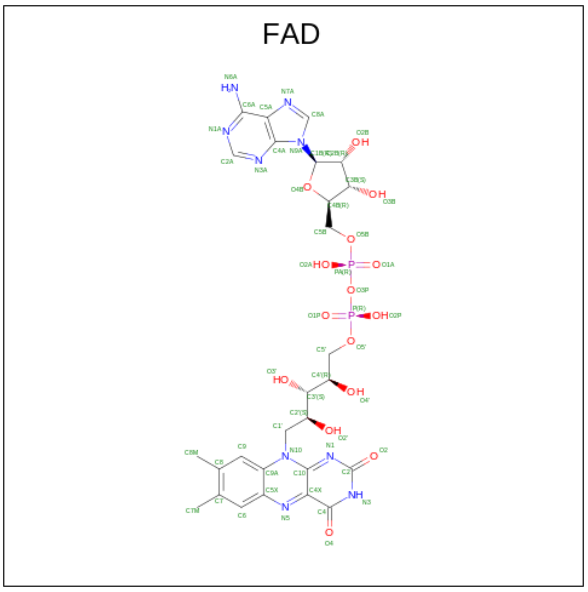
Chain	Residue	Modelled	Actual	Comment	Reference
H	108	SER	-	expression tag	UNP P0ADF8
H	109	ALA	-	expression tag	UNP P0ADF8
H	110	ALA	-	expression tag	UNP P0ADF8
H	111	ALA	-	expression tag	UNP P0ADF8
H	112	THR	-	expression tag	UNP P0ADF8
H	113	SER	-	expression tag	UNP P0ADF8
H	114	ALA	-	expression tag	UNP P0ADF8
H	115	ALA	-	expression tag	UNP P0ADF8
H	116	ALA	-	expression tag	UNP P0ADF8
H	117	THR	-	expression tag	UNP P0ADF8
H	118	SER	-	expression tag	UNP P0ADF8
H	119	ALA	-	expression tag	UNP P0ADF8
H	120	ALA	-	expression tag	UNP P0ADF8
H	121	ALA	-	expression tag	UNP P0ADF8
H	122	THR	-	expression tag	UNP P0ADF8
H	123	SER	-	expression tag	UNP P0ADF8
H	124	ALA	-	expression tag	UNP P0ADF8
H	125	ALA	-	expression tag	UNP P0ADF8
H	126	SER	-	expression tag	UNP P0ADF8

- Molecule 2 is a protein called Acetolactate synthase isozyme 1 large subunit.

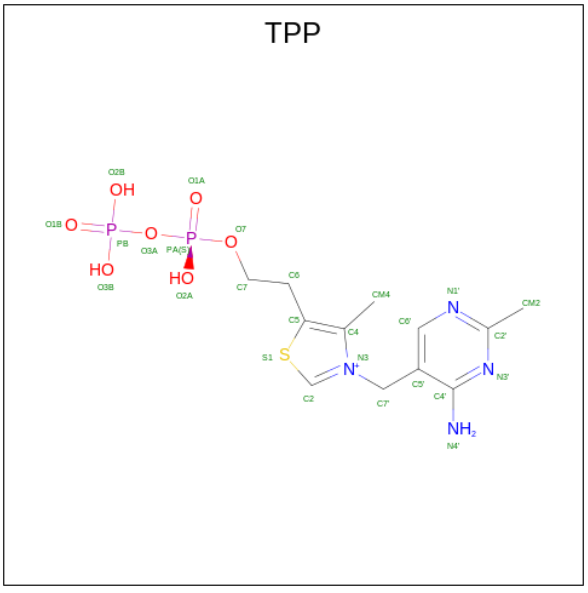
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	531	Total	C	N	O	S	0	0	0
			3971	2519	696	729	27			
2	B	539	Total	C	N	O	S	0	0	0
			3940	2500	677	736	27			
2	C	533	Total	C	N	O	S	0	0	0
			3918	2488	674	729	27			
2	D	529	Total	C	N	O	S	0	0	0
			3889	2467	678	719	25			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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	C	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		

- Molecule 4 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
4	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
4	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
4	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

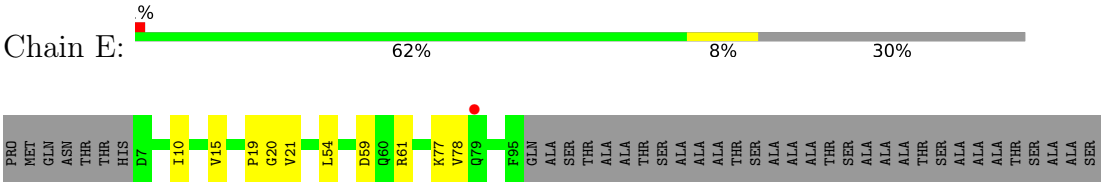
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	O	0	0
			1	1		
6	G	1	Total	O	0	0
			1	1		
6	C	1	Total	O	0	0
			1	1		
6	D	2	Total	O	0	0
			2	2		

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.

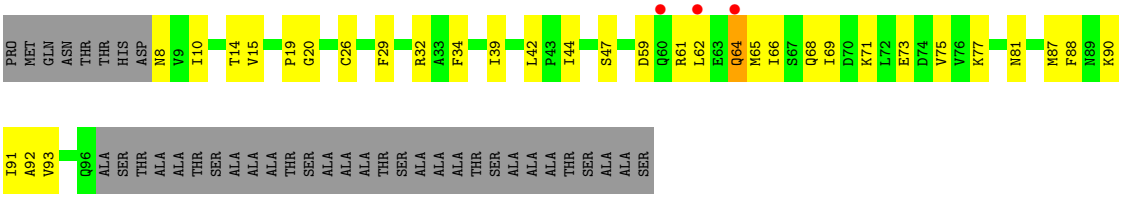
• Molecule 1: Acetolactate synthase isozyme 1 small subunit

Chain E:



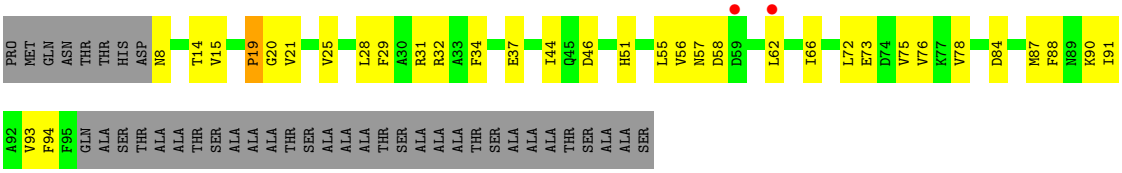
• Molecule 1: Acetolactate synthase isozyme 1 small subunit

Chain F:



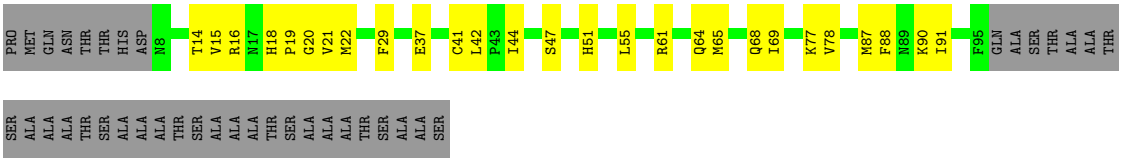
• Molecule 1: Acetolactate synthase isozyme 1 small subunit

Chain G:



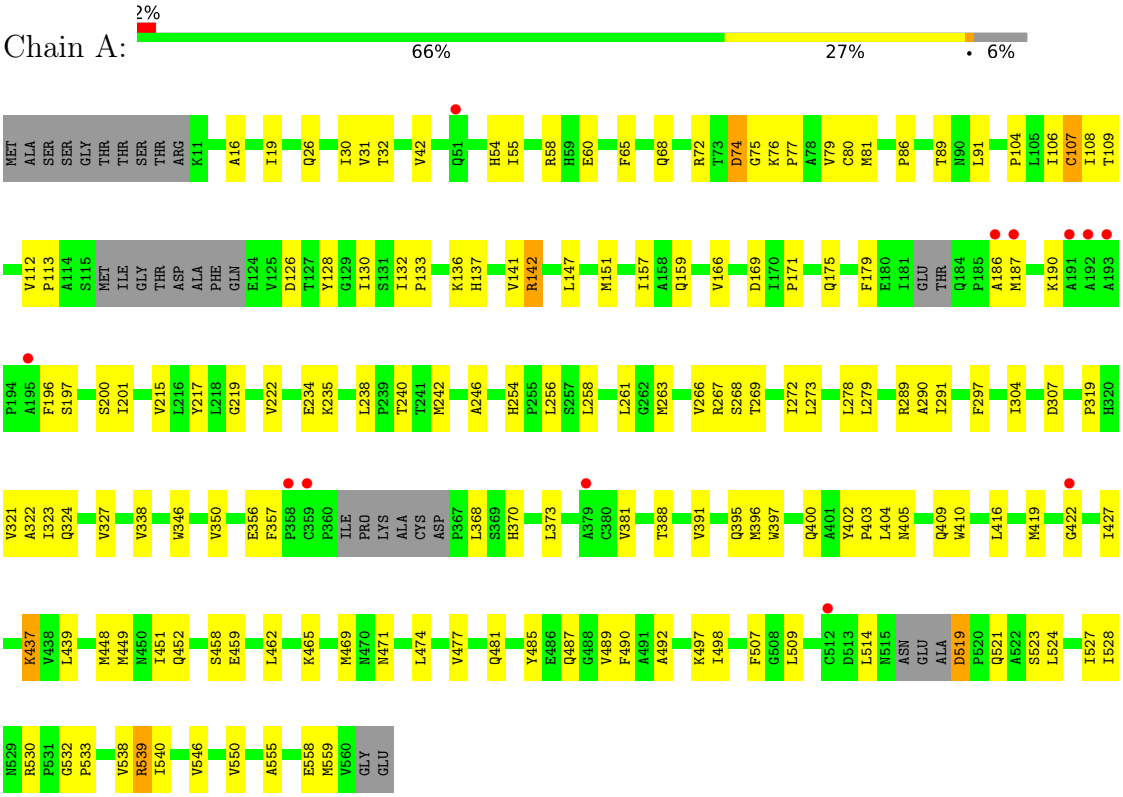
• Molecule 1: Acetolactate synthase isozyme 1 small subunit

Chain H:



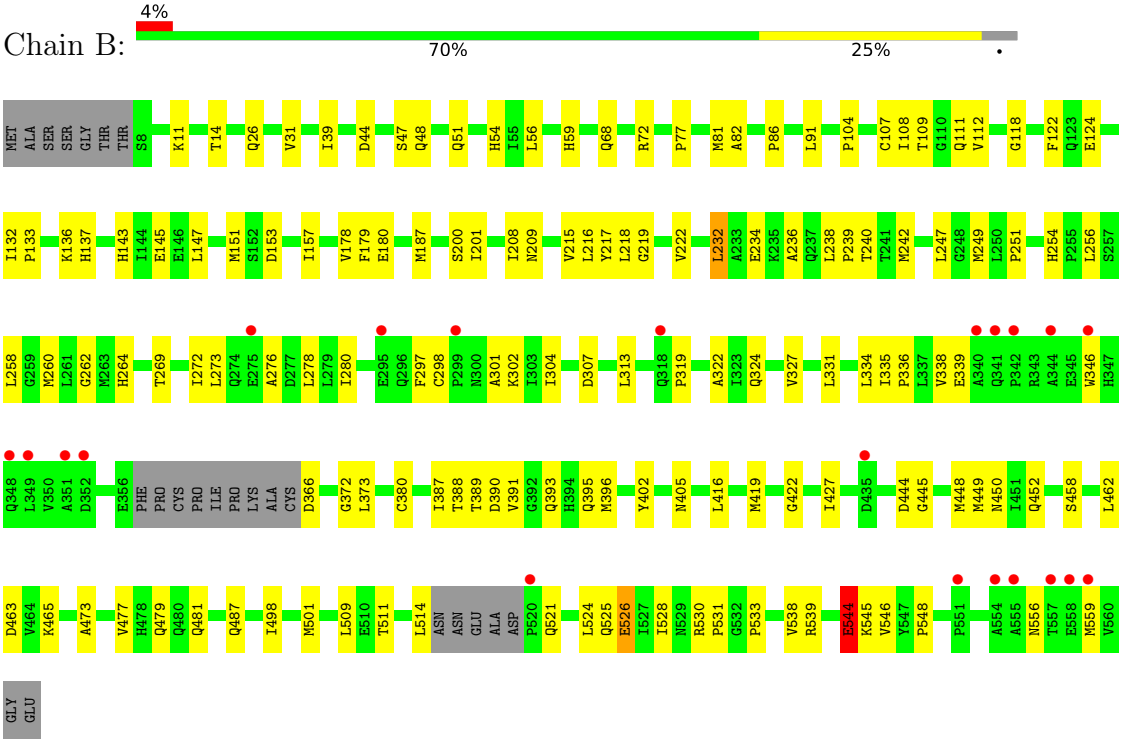
• Molecule 2: Acetolactate synthase isozyme 1 large subunit

Chain A:



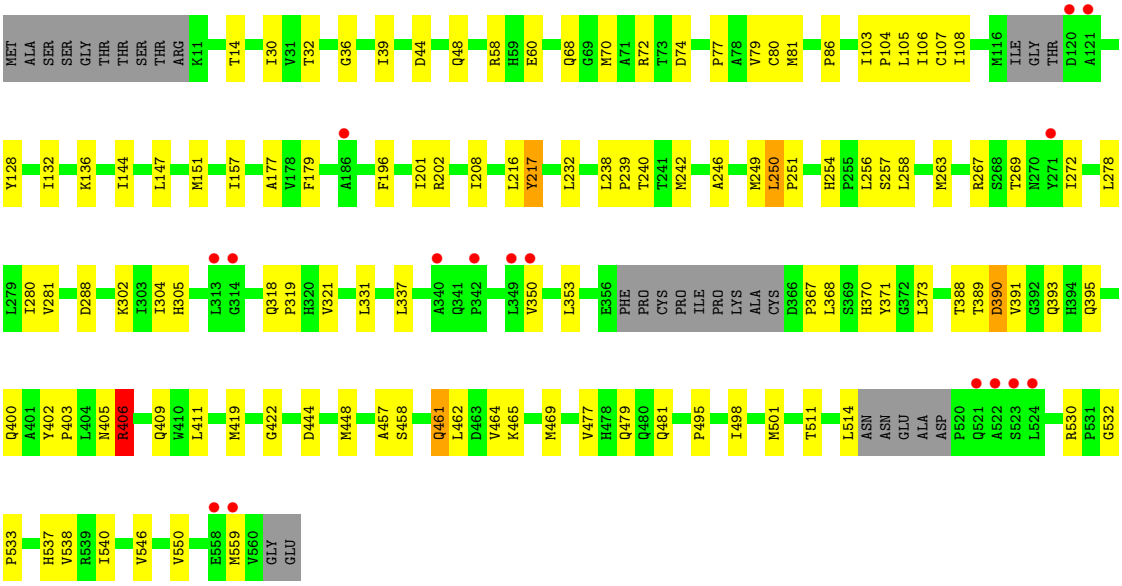
• Molecule 2: Acetolactate synthase isozyme 1 large subunit

Chain B:



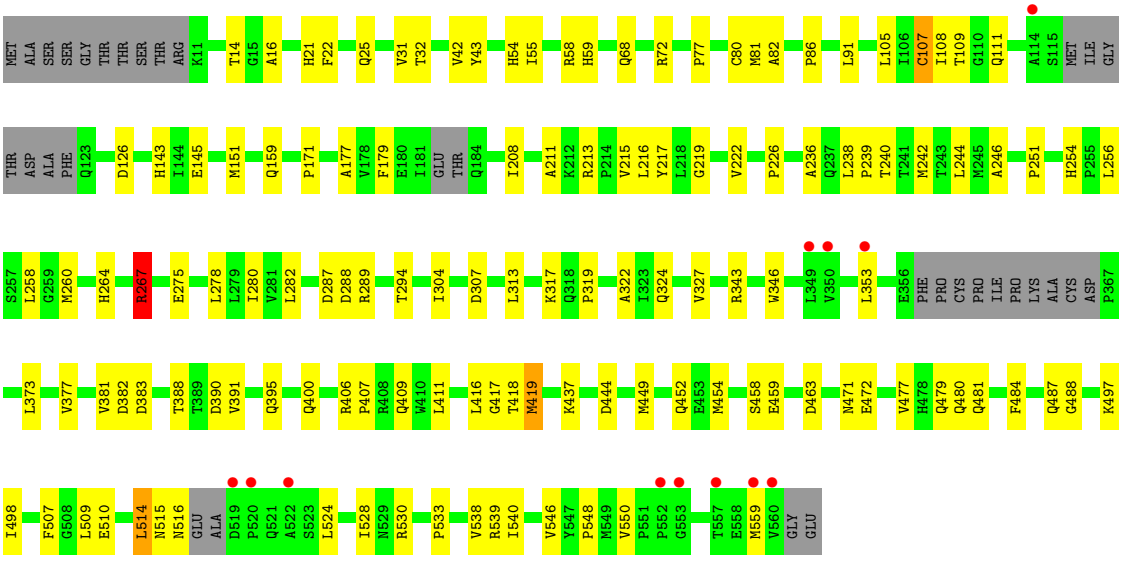
• Molecule 2: Acetolactate synthase isozyme 1 large subunit

Chain C:



• Molecule 2: Acetolactate synthase isozyme 1 large subunit

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	111.17Å 104.58Å 118.53Å 90.00° 105.68° 90.00°	Depositor
Resolution (Å)	35.93 – 2.85 35.93 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.2 (35.93-2.85) 95.9 (35.93-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.85Å)	Xtriage
Refinement program	PHENIX dev_2666	Depositor
R, R_{free}	0.167 , 0.243 0.167 , 0.243	Depositor DCC
R_{free} test set	2010 reflections (3.31%)	wwPDB-VP
Wilson B-factor (Å^2)	61.0	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 69.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18840	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TPP, 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	E	0.45	0/701	0.66	0/953
1	F	0.42	0/722	0.65	0/978
1	G	0.41	0/703	0.62	0/954
1	H	0.49	0/719	0.66	0/973
2	A	0.48	1/4049 (0.0%)	0.87	10/5508 (0.2%)
2	B	0.45	0/4017	0.72	4/5481 (0.1%)
2	C	0.43	0/3995	0.76	7/5448 (0.1%)
2	D	0.43	0/3965	0.69	5/5405 (0.1%)
All	All	0.45	1/18871 (0.0%)	0.75	26/25700 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1
2	B	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	356	GLU	CG-CD	5.61	1.60	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	530	ARG	NE-CZ-NH2	-24.21	108.20	120.30
2	A	530	ARG	NE-CZ-NH1	18.92	129.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	250	LEU	CB-CG-CD2	-17.72	80.88	111.00
2	C	406	ARG	CG-CD-NE	9.21	131.13	111.80
2	C	406	ARG	NE-CZ-NH1	8.79	124.69	120.30
2	A	279	LEU	CA-CB-CG	8.36	134.52	115.30
2	C	250	LEU	CB-CG-CD1	8.05	124.69	111.00
2	D	288	ASP	CB-CG-OD1	-7.39	111.64	118.30
2	A	530	ARG	CB-CG-CD	-7.28	92.67	111.60
2	A	437	LYS	CB-CG-CD	-7.08	93.19	111.60
2	C	74	ASP	CB-CG-OD2	-6.72	112.25	118.30
2	A	519	ASP	C-N-CD	-6.49	106.31	120.60
2	A	530	ARG	CD-NE-CZ	6.26	132.36	123.60
2	D	288	ASP	CB-CG-OD2	6.25	123.92	118.30
2	B	526	GLU	CG-CD-OE2	-6.11	106.08	118.30
2	C	288	ASP	CB-CG-OD2	5.69	123.42	118.30
2	B	544	GLU	CA-CB-CG	-5.57	101.16	113.40
2	B	56	LEU	CA-CB-CG	5.39	127.69	115.30
2	D	287	ASP	C-N-CA	-5.25	108.58	121.70
2	C	105	LEU	CA-CB-CG	5.21	127.28	115.30
2	A	530	ARG	CG-CD-NE	-5.17	100.94	111.80
2	B	232	LEU	CA-CB-CG	5.15	127.15	115.30
2	D	105	LEU	CA-CB-CG	5.09	127.00	115.30
2	A	519	ASP	C-N-CA	5.05	143.23	122.00
2	D	267	ARG	CG-CD-NE	-5.03	101.23	111.80
2	A	142	ARG	NE-CZ-NH1	-5.03	117.78	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	487	GLN	Peptide
2	B	526	GLU	Sidechain
1	G	46	ASP	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	689	0	670	7	0
1	F	710	0	708	23	0
1	G	691	0	683	23	0
1	H	707	0	711	26	0
2	A	3971	0	3978	118	0
2	B	3940	0	3875	129	0
2	C	3918	0	3862	100	0
2	D	3889	0	3834	95	0
3	A	53	0	31	2	0
3	B	53	0	31	1	0
3	C	53	0	31	0	0
3	D	53	0	31	3	0
4	A	26	0	16	7	0
4	B	26	0	16	1	0
4	C	26	0	16	4	0
4	D	26	0	16	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
6	F	1	0	0	1	0
6	G	1	0	0	0	0
All	All	18840	0	18509	491	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 13.

All (491) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:PHE:CD1	2:D:151:MET:HE2	1.61	1.32
2:B:544:GLU:HG3	2:B:545:LYS:H	1.06	1.09
2:C:406:ARG:CD	2:C:409:GLN:HB2	1.83	1.08
2:C:406:ARG:HD2	2:C:409:GLN:HB2	1.34	1.06
2:D:22:PHE:CE1	2:D:151:MET:HE2	1.99	0.96
2:C:242:MET:HE2	2:C:246:ALA:O	1.65	0.95
2:B:544:GLU:HG3	2:B:545:LYS:N	1.74	0.93
2:A:254:HIS:HD2	2:A:256:LEU:H	1.16	0.93
2:D:22:PHE:CD1	2:D:151:MET:CE	2.52	0.92
2:A:437:LYS:NZ	2:A:528:ILE:O	2.04	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:76:LYS:HG3	2:A:77:PRO:HD2	1.55	0.88
2:A:481:GLN:HE22	2:A:490:PHE:H	1.22	0.86
2:A:291:ILE:HD12	2:A:297:PHE:CE2	2.13	0.84
2:B:111:GLN:HE21	2:B:112:VAL:H	1.22	0.83
2:C:318:GLN:HG3	2:C:319:PRO:HD2	1.60	0.83
2:B:44:ASP:O	2:B:47:SER:HB3	1.80	0.81
2:C:406:ARG:HD3	2:C:409:GLN:HB2	1.63	0.79
2:C:479:GLN:HE22	2:C:546:VAL:H	1.31	0.77
2:D:239:PRO:HB2	2:D:258:LEU:HD11	1.67	0.76
2:B:48:GLN:OE1	2:D:487:GLN:NE2	2.18	0.76
2:D:68:GLN:OE1	2:D:72:ARG:NH1	2.18	0.76
1:E:19:PRO:HG2	2:A:142:ARG:NH1	2.00	0.75
2:C:68:GLN:OE1	2:C:72:ARG:NH1	2.19	0.75
2:A:437:LYS:NZ	2:A:465:LYS:HE2	2.00	0.75
2:B:479:GLN:HE22	2:B:546:VAL:H	1.31	0.75
2:B:242:MET:HE2	2:B:247:LEU:HA	1.69	0.74
1:G:31:ARG:HH11	1:G:32:ARG:HH21	1.34	0.74
2:B:448:MET:HG3	2:D:452:GLN:HB2	1.70	0.73
2:A:58:ARG:HG2	2:C:448:MET:HG2	1.71	0.72
2:C:136:LYS:HD3	2:C:157:ILE:HG22	1.70	0.72
2:D:437:LYS:NZ	2:D:528:ILE:O	2.20	0.72
2:C:465:LYS:NZ	2:C:532:GLY:O	2.22	0.71
1:H:16:ARG:O	1:H:21:VAL:HG21	1.90	0.71
2:A:481:GLN:NE2	2:A:490:PHE:H	1.89	0.71
2:C:242:MET:HE2	2:C:249:MET:HB2	1.72	0.70
2:B:416:LEU:HG	2:D:86:PRO:HG3	1.74	0.70
2:D:43:TYR:HE2	2:D:54:HIS:CE1	2.09	0.70
2:A:258:LEU:O	2:A:269:THR:HG21	1.91	0.70
1:F:42:LEU:HD11	1:H:88:PHE:HB3	1.74	0.70
2:D:307:ASP:OD2	3:D:601:FAD:O3B	2.08	0.70
2:C:389:THR:HG22	2:C:390:ASP:O	1.92	0.70
2:C:196:PHE:CD1	2:C:201:ILE:HD11	2.27	0.69
2:C:242:MET:CE	2:C:249:MET:HB2	2.22	0.69
2:A:452:GLN:HB2	2:C:448:MET:HG3	1.74	0.69
2:C:318:GLN:HG3	2:C:319:PRO:CD	2.22	0.69
2:B:143:HIS:HB3	2:B:145:GLU:OE1	1.92	0.69
2:D:514:LEU:HD11	2:D:539:ARG:H	1.58	0.69
2:B:450:ASN:HD22	2:B:452:GLN:HE22	1.40	0.68
2:D:550:VAL:HG22	2:D:559:MET:HG2	1.75	0.68
2:B:278:LEU:HD11	2:B:304:ILE:HG13	1.76	0.68
2:A:487:GLN:HE21	2:C:48:GLN:NE2	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:44:ILE:HD11	1:H:51:HIS:CD2	2.30	0.67
2:B:251:PRO:HG2	2:B:254:HIS:HB2	1.76	0.67
1:E:59:ASP:HB3	1:E:61:ARG:H	1.60	0.67
4:A:602:TPP:N1'	2:C:60:GLU:OE1	2.28	0.67
1:H:64:GLN:OE1	1:H:68:GLN:NE2	2.28	0.66
2:D:58:ARG:NH1	2:D:459:GLU:OE2	2.29	0.66
2:A:509:LEU:HD22	2:A:533:PRO:HB2	1.77	0.66
2:C:208:ILE:HG12	2:C:280:ILE:HD13	1.79	0.65
2:A:514:LEU:HD12	2:A:538:VAL:HG22	1.79	0.65
2:D:216:LEU:HB3	2:D:240:THR:HG22	1.79	0.65
2:B:393:GLN:HE21	2:B:479:GLN:HE21	1.44	0.65
2:D:294:THR:O	2:D:317:LYS:NZ	2.30	0.65
2:B:548:PRO:HB2	2:B:559:MET:HB3	1.79	0.65
2:B:254:HIS:HE1	2:B:256:LEU:HD12	1.63	0.64
2:C:389:THR:HG21	2:C:395:GLN:HG3	1.78	0.64
2:A:514:LEU:O	2:A:539:ARG:NH2	2.29	0.64
2:B:458:SER:HA	2:B:533:PRO:HG3	1.81	0.63
2:D:480:GLN:HG2	2:D:484:PHE:HD2	1.62	0.63
2:D:373:LEU:HD22	2:D:538:VAL:HG21	1.80	0.62
2:A:254:HIS:CD2	2:A:256:LEU:H	2.07	0.62
2:B:201:ILE:HD12	2:B:201:ILE:N	2.15	0.62
2:A:477:VAL:O	2:A:481:GLN:HG3	2.00	0.62
1:F:73:GLU:HG3	2:B:157:ILE:HD13	1.81	0.62
2:B:216:LEU:HB3	2:B:240:THR:HG22	1.81	0.62
1:H:37:GLU:HB2	1:H:55:LEU:HD23	1.82	0.62
2:B:68:GLN:OE1	2:B:72:ARG:NH1	2.33	0.61
2:D:480:GLN:HG2	2:D:484:PHE:CD2	2.35	0.61
2:B:86:PRO:HG3	2:D:416:LEU:HG	1.82	0.61
2:B:81:MET:HA	2:B:108:ILE:O	2.01	0.60
2:C:501:MET:HG3	2:C:511:THR:HB	1.84	0.60
1:G:94:PHE:HA	1:H:90:LYS:HD3	1.84	0.60
2:C:457:ALA:HA	2:C:462:LEU:HD12	1.83	0.60
2:A:197:SER:OG	2:A:200:SER:OG	2.17	0.59
2:A:215:VAL:HG21	2:A:273:LEU:HD23	1.84	0.59
2:B:389:THR:HG21	2:B:395:GLN:HA	1.84	0.59
2:D:22:PHE:CE1	2:D:151:MET:CE	2.82	0.59
2:A:416:LEU:HG	2:C:86:PRO:HG3	1.83	0.59
2:B:514:LEU:HD12	2:B:538:VAL:HG22	1.83	0.59
2:C:201:ILE:HD12	2:C:201:ILE:H	1.66	0.59
2:C:479:GLN:NE2	2:C:546:VAL:H	1.98	0.59
2:A:196:PHE:CD1	2:A:201:ILE:HD11	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:29:PHE:CZ	1:H:69:ILE:HD11	2.37	0.59
2:D:267:ARG:NH1	2:D:559:MET:HB2	2.18	0.59
2:B:258:LEU:HB3	2:B:269:THR:HG21	1.85	0.58
2:B:319:PRO:HG2	2:B:322:ALA:HB2	1.85	0.58
2:D:479:GLN:HE22	2:D:546:VAL:H	1.50	0.58
2:A:263:MET:HE1	2:A:289:ARG:HE	1.67	0.58
2:B:444:ASP:OD2	2:B:473:ALA:N	2.32	0.58
2:C:196:PHE:CE1	2:C:201:ILE:HD11	2.39	0.58
2:B:136:LYS:HE2	2:B:157:ILE:HG22	1.86	0.58
1:H:44:ILE:O	1:H:47:SER:HB3	2.04	0.58
2:C:278:LEU:HA	2:C:302:LYS:O	2.04	0.58
2:A:291:ILE:HD12	2:A:297:PHE:CZ	2.39	0.58
2:C:251:PRO:HA	2:C:405:ASN:HA	1.86	0.58
2:B:219:GLY:O	2:B:222:VAL:HG22	2.04	0.57
2:C:537:HIS:HD2	2:C:538:VAL:N	2.01	0.57
2:B:509:LEU:HG	2:B:533:PRO:HB2	1.86	0.57
2:A:159:GLN:HG3	2:A:190:LYS:HG2	1.86	0.57
2:B:307:ASP:O	2:B:324:GLN:HA	2.04	0.57
2:B:215:VAL:HG11	2:B:273:LEU:HD23	1.85	0.57
2:B:242:MET:HE3	2:B:249:MET:HB2	1.87	0.57
2:A:30:ILE:HG23	2:A:55:ILE:HD13	1.85	0.57
2:A:388:THR:HG21	2:A:422:GLY:O	2.05	0.57
2:D:16:ALA:HB1	2:D:42:VAL:HA	1.87	0.57
2:A:381:VAL:HG11	2:A:439:LEU:HD11	1.87	0.57
2:C:251:PRO:HG2	2:C:254:HIS:HB2	1.85	0.56
2:C:267:ARG:HA	2:C:559:MET:CE	2.35	0.56
2:D:406:ARG:HG3	2:D:409:GLN:HB2	1.87	0.56
2:A:272:ILE:HD13	2:A:350:VAL:HG13	1.86	0.56
2:C:464:VAL:O	2:C:533:PRO:HA	2.05	0.56
2:B:477:VAL:O	2:B:481:GLN:HG3	2.05	0.56
2:C:79:VAL:HA	2:C:106:ILE:O	2.05	0.56
2:D:509:LEU:HG	2:D:533:PRO:HB2	1.88	0.56
2:A:524:LEU:O	2:A:528:ILE:HD12	2.06	0.56
2:B:44:ASP:O	2:B:47:SER:CB	2.53	0.56
2:A:196:PHE:HD1	2:A:201:ILE:HD11	1.70	0.56
2:B:264:HIS:ND1	2:B:396:MET:HG3	2.21	0.56
4:A:602:TPP:HN42	4:A:602:TPP:H2	1.71	0.56
2:B:479:GLN:NE2	2:B:546:VAL:H	2.03	0.55
2:C:68:GLN:HG2	2:C:72:ARG:HD2	1.88	0.55
2:B:48:GLN:OE1	2:D:487:GLN:HG2	2.05	0.55
2:B:444:ASP:OD1	4:B:602:TPP:O2A	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:471:ASN:ND2	4:A:602:TPP:O3B	2.40	0.55
2:C:242:MET:HE1	2:C:250:LEU:H	1.72	0.55
2:A:16:ALA:HB1	2:A:42:VAL:HA	1.88	0.55
2:C:242:MET:CE	2:C:250:LEU:H	2.19	0.55
2:C:250:LEU:HD21	2:C:257:SER:HB2	1.89	0.55
2:B:269:THR:HA	2:B:272:ILE:HB	1.87	0.55
2:C:136:LYS:HD3	2:C:157:ILE:CG2	2.37	0.55
2:B:251:PRO:HB3	2:B:405:ASN:HB3	1.88	0.54
1:G:8:ASN:HA	1:G:57:ASN:HA	1.89	0.54
2:C:370:HIS:HB3	2:C:540:ILE:HD13	1.90	0.54
4:C:602:TPP:HN42	4:C:602:TPP:C2	2.21	0.54
2:B:236:ALA:HB3	2:B:238:LEU:HG	1.88	0.54
1:H:18:HIS:O	1:H:21:VAL:HG23	2.08	0.54
2:D:390:ASP:O	2:D:395:GLN:HB2	2.08	0.54
2:C:128:TYR:O	2:C:132:ILE:HG13	2.08	0.54
2:A:319:PRO:HG2	2:A:322:ALA:HB2	1.90	0.54
2:B:335:ILE:O	2:B:338:VAL:HG12	2.07	0.54
4:C:602:TPP:HN42	4:C:602:TPP:H2	1.73	0.53
1:G:84:ASP:O	1:G:87:MET:HB2	2.09	0.53
2:D:313:LEU:HD22	2:D:322:ALA:HB1	1.90	0.53
2:B:147:LEU:O	2:B:151:MET:HG3	2.08	0.53
2:B:200:SER:OG	2:B:201:ILE:HD12	2.08	0.53
1:G:90:LYS:O	1:G:93:VAL:HG22	2.09	0.53
4:A:602:TPP:HN42	4:A:602:TPP:C2	2.22	0.53
2:B:122:PHE:CB	2:D:289:ARG:HD2	2.39	0.53
2:C:514:LEU:HD12	2:C:538:VAL:HG12	1.90	0.53
1:F:29:PHE:CD2	1:F:34:PHE:HB2	2.44	0.53
2:B:111:GLN:HE21	2:B:112:VAL:N	2.01	0.53
2:C:196:PHE:HD1	2:C:201:ILE:HD11	1.72	0.53
2:B:319:PRO:CG	2:B:322:ALA:HB2	2.40	0.52
2:B:201:ILE:HG23	2:B:334:LEU:HD13	1.90	0.52
2:B:278:LEU:HA	2:B:302:LYS:O	2.09	0.52
2:D:215:VAL:HG23	2:D:239:PRO:O	2.10	0.52
2:A:327:VAL:HG23	3:A:601:FAD:N1A	2.24	0.52
2:A:497:LYS:O	2:A:498:ILE:HD13	2.09	0.52
2:B:242:MET:HE2	2:B:247:LEU:CA	2.40	0.52
2:B:262:GLY:HA2	2:B:556:ASN:ND2	2.25	0.52
2:A:234:GLU:OE1	2:A:254:HIS:HE1	1.92	0.52
2:B:201:ILE:N	2:B:201:ILE:CD1	2.73	0.52
2:C:250:LEU:CD2	2:C:257:SER:HB2	2.39	0.52
2:D:211:ALA:O	2:D:343:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:391:VAL:HA	2:B:395:GLN:OE1	2.10	0.52
1:F:39:ILE:HG12	1:H:41:CYS:HB3	1.91	0.51
2:A:550:VAL:HG22	2:A:559:MET:HG2	1.92	0.51
1:G:87:MET:O	1:G:91:ILE:HG23	2.10	0.51
2:A:291:ILE:HD12	2:A:297:PHE:CD2	2.44	0.51
2:A:469:MET:HB3	2:A:540:ILE:HD12	1.92	0.51
2:C:217:TYR:HB3	2:C:281:VAL:HG12	1.90	0.51
2:A:373:LEU:HD22	2:A:538:VAL:HG21	1.91	0.51
1:F:32:ARG:NH2	1:F:64:GLN:HE22	2.08	0.51
2:D:236:ALA:HB3	2:D:238:LEU:HG	1.93	0.51
2:C:77:PRO:HA	2:C:104:PRO:O	2.11	0.51
2:C:81:MET:HA	2:C:108:ILE:O	2.10	0.51
2:C:272:ILE:HD13	2:C:350:VAL:HG13	1.92	0.51
2:D:43:TYR:CE2	2:D:54:HIS:CE1	2.94	0.51
2:C:250:LEU:HD21	2:C:254:HIS:HB3	1.92	0.51
2:C:254:HIS:HE1	2:C:256:LEU:HD12	1.75	0.51
2:D:388:THR:HA	2:D:411:LEU:O	2.11	0.51
2:A:132:ILE:HB	2:A:133:PRO:HD3	1.93	0.51
1:F:59:ASP:HB3	1:F:61:ARG:H	1.76	0.51
2:D:477:VAL:O	2:D:481:GLN:HG3	2.11	0.51
2:B:501:MET:HG3	2:B:511:THR:HB	1.93	0.50
2:D:143:HIS:HB3	2:D:145:GLU:OE1	2.10	0.50
2:A:200:SER:CB	2:A:323:ILE:HD11	2.41	0.50
2:A:391:VAL:HA	2:A:395:GLN:OE1	2.11	0.50
1:F:73:GLU:HB2	2:B:137:HIS:CD2	2.47	0.50
2:C:269:THR:HA	2:C:272:ILE:HB	1.92	0.50
1:E:77:LYS:HG2	1:E:78:VAL:N	2.26	0.50
2:A:215:VAL:HG21	2:A:273:LEU:CD2	2.40	0.50
2:B:313:LEU:HD11	2:B:324:GLN:HB2	1.92	0.50
2:B:450:ASN:ND2	2:B:452:GLN:HE22	2.07	0.50
1:E:19:PRO:HG2	2:A:142:ARG:HH11	1.76	0.50
2:A:481:GLN:NE2	2:A:489:VAL:HA	2.26	0.50
1:G:55:LEU:HB2	1:G:88:PHE:CD2	2.47	0.50
2:A:68:GLN:O	2:A:72:ARG:HG3	2.11	0.50
2:D:515:ASN:HA	2:D:516:ASN:C	2.32	0.50
2:A:77:PRO:HA	2:A:104:PRO:O	2.12	0.50
2:A:79:VAL:HA	2:A:106:ILE:O	2.12	0.50
1:F:87:MET:O	1:F:91:ILE:HG23	2.12	0.50
2:A:449:MET:CE	4:A:602:TPP:HM23	2.42	0.50
2:D:254:HIS:HE1	2:D:256:LEU:HD12	1.77	0.50
2:A:519:ASP:N	2:A:523:SER:H	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:HIS:CE1	2:B:256:LEU:HD12	2.45	0.49
2:D:226:PRO:HB3	2:D:407:PRO:HG3	1.94	0.49
2:A:112:VAL:HG22	2:A:113:PRO:HD2	1.93	0.49
2:A:370:HIS:HB3	2:A:540:ILE:HD13	1.94	0.49
1:G:44:ILE:HD11	1:G:51:HIS:ND1	2.27	0.49
2:C:217:TYR:O	2:C:281:VAL:HA	2.12	0.49
2:C:393:GLN:NE2	2:C:479:GLN:HE21	2.10	0.49
2:A:448:MET:HE3	2:C:58:ARG:HD2	1.95	0.49
2:C:267:ARG:HA	2:C:559:MET:HE1	1.94	0.49
2:B:238:LEU:O	2:B:240:THR:HG23	2.13	0.49
2:B:388:THR:HG21	2:B:422:GLY:O	2.11	0.49
2:B:393:GLN:HE21	2:B:479:GLN:NE2	2.10	0.49
2:B:393:GLN:NE2	2:B:479:GLN:HE21	2.09	0.49
1:G:31:ARG:HD2	1:G:32:ARG:NH2	2.27	0.49
2:A:524:LEU:O	2:A:527:ILE:HG22	2.12	0.49
2:B:390:ASP:O	2:B:395:GLN:HB2	2.12	0.49
2:B:242:MET:HE3	2:B:249:MET:N	2.26	0.49
2:C:14:THR:HA	2:C:177:ALA:O	2.13	0.49
2:D:497:LYS:O	2:D:498:ILE:HD12	2.12	0.49
2:B:59:HIS:HA	2:D:449:MET:CE	2.43	0.49
2:B:216:LEU:HD21	2:B:218:LEU:HD21	1.95	0.49
2:A:514:LEU:HD12	2:A:538:VAL:CG2	2.42	0.48
1:F:91:ILE:HD12	1:H:91:ILE:HD12	1.95	0.48
2:D:54:HIS:CD2	2:D:55:ILE:N	2.82	0.48
1:F:90:LYS:O	1:F:93:VAL:HG22	2.13	0.48
2:D:68:GLN:O	2:D:72:ARG:HG3	2.13	0.48
2:D:208:ILE:HG12	2:D:280:ILE:HD13	1.95	0.48
2:A:126:ASP:O	2:A:130:ILE:HG13	2.13	0.48
2:B:14:THR:HG22	2:B:178:VAL:HG22	1.95	0.48
2:B:91:LEU:HD13	2:B:107:CYS:SG	2.53	0.48
2:A:60:GLU:OE2	4:C:602:TPP:N1'	2.45	0.48
2:C:373:LEU:HD22	2:C:538:VAL:HG11	1.95	0.48
2:D:278:LEU:HD11	2:D:304:ILE:HG13	1.95	0.48
2:D:216:LEU:O	2:D:240:THR:HA	2.14	0.48
2:B:242:MET:HE3	2:B:249:MET:H	1.78	0.48
2:B:232:LEU:HD12	2:B:331:LEU:HD22	1.96	0.47
2:C:278:LEU:HD11	2:C:304:ILE:HG13	1.96	0.47
2:B:514:LEU:HD12	2:B:538:VAL:CG2	2.44	0.47
2:C:444:ASP:N	2:C:444:ASP:OD1	2.46	0.47
2:C:537:HIS:CD2	2:C:538:VAL:N	2.81	0.47
2:A:200:SER:HB3	2:A:323:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:261:LEU:H	2:A:261:LEU:HD23	1.79	0.47
2:B:31:VAL:O	2:B:54:HIS:HA	2.14	0.47
2:B:234:GLU:OE2	2:B:254:HIS:NE2	2.43	0.47
1:H:14:THR:OG1	1:H:77:LYS:HE3	2.14	0.47
2:B:465:LYS:HE3	2:B:528:ILE:O	2.14	0.47
2:D:307:ASP:O	2:D:324:GLN:HA	2.15	0.47
2:A:136:LYS:HD3	2:A:157:ILE:CG2	2.44	0.47
2:C:144:ILE:HD12	2:C:177:ALA:HB3	1.96	0.47
1:E:19:PRO:HA	1:E:20:GLY:HA2	1.61	0.47
2:A:242:MET:HB3	2:A:246:ALA:HB3	1.95	0.47
1:F:44:ILE:HB	1:F:47:SER:HB3	1.96	0.47
2:B:145:GLU:CD	2:B:145:GLU:H	2.18	0.47
2:D:275:GLU:HG3	2:D:353:LEU:HD11	1.96	0.47
1:H:16:ARG:CZ	1:H:16:ARG:HB2	2.45	0.47
1:H:29:PHE:HZ	1:H:69:ILE:HD11	1.79	0.47
2:A:404:LEU:HD22	2:A:410:TRP:HB2	1.96	0.47
2:B:247:LEU:HD11	2:B:260:MET:CE	2.45	0.46
2:C:232:LEU:HD12	2:C:331:LEU:HD22	1.97	0.46
2:C:267:ARG:HA	2:C:559:MET:HE3	1.97	0.46
2:C:391:VAL:HA	2:C:395:GLN:OE1	2.15	0.46
2:D:244:LEU:HD12	2:D:260:MET:HE1	1.97	0.46
2:A:487:GLN:OE1	2:A:487:GLN:N	2.48	0.46
2:A:268:SER:HB3	2:A:357:PHE:CB	2.46	0.46
2:A:458:SER:HA	2:A:533:PRO:HG3	1.96	0.46
1:F:39:ILE:HD11	1:H:22:MET:CE	2.45	0.46
1:G:31:ARG:HH11	1:G:32:ARG:NH2	2.08	0.46
2:B:525:GLN:OE1	2:B:525:GLN:O	2.33	0.46
1:G:8:ASN:HA	1:G:56:VAL:O	2.16	0.46
2:C:147:LEU:O	2:C:151:MET:HG3	2.15	0.46
1:G:19:PRO:HA	1:G:20:GLY:HA2	1.50	0.46
2:C:208:ILE:HG12	2:C:280:ILE:CD1	2.45	0.46
2:C:304:ILE:HG23	2:C:321:VAL:HB	1.97	0.46
2:A:219:GLY:O	2:A:222:VAL:HG22	2.16	0.46
2:A:474:LEU:HD22	4:A:602:TPP:HM41	1.98	0.46
2:B:82:ALA:O	2:B:109:THR:HA	2.15	0.46
1:G:37:GLU:HB2	1:G:55:LEU:HD23	1.97	0.46
2:C:242:MET:CE	2:C:246:ALA:O	2.51	0.46
2:B:209:ASN:HD21	2:B:339:GLU:N	2.14	0.46
2:C:202:ARG:HE	2:C:337:LEU:HD11	1.81	0.46
2:A:26:GLN:NE2	2:A:187:MET:HA	2.31	0.45
2:A:32:THR:O	2:A:80:CYS:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:42:VAL:HG23	2:A:175:GLN:OE1	2.15	0.45
2:D:216:LEU:HD11	2:D:282:LEU:CD1	2.46	0.45
2:A:448:MET:HA	2:A:451:ILE:HB	1.99	0.45
2:B:463:ASP:OD1	2:B:531:PRO:HA	2.16	0.45
2:D:437:LYS:HE2	2:D:463:ASP:OD1	2.17	0.45
2:A:26:GLN:NE2	2:A:186:ALA:O	2.49	0.45
1:G:58:ASP:OD1	1:G:62:LEU:HD22	2.15	0.45
1:G:73:GLU:HG3	2:C:157:ILE:HD13	1.98	0.45
2:C:390:ASP:OD2	2:C:422:GLY:HA3	2.16	0.45
2:A:74:ASP:OD1	2:A:75:GLY:N	2.50	0.45
2:A:396:MET:O	2:A:400:GLN:HG3	2.17	0.45
1:G:29:PHE:CD2	1:G:34:PHE:HB2	2.51	0.45
1:H:77:LYS:HG2	1:H:78:VAL:N	2.31	0.45
2:A:514:LEU:H	2:A:514:LEU:HG	1.59	0.45
2:A:474:LEU:HD12	2:A:492:ALA:HA	1.97	0.45
2:D:208:ILE:HG12	2:D:280:ILE:CD1	2.47	0.45
2:D:219:GLY:O	2:D:222:VAL:HG22	2.16	0.45
2:C:406:ARG:HD3	2:C:409:GLN:CB	2.38	0.45
2:B:419:MET:HB2	2:B:449:MET:SD	2.57	0.45
1:G:66:ILE:HG23	1:G:78:VAL:HG11	1.99	0.45
2:D:377:VAL:HG22	2:D:524:LEU:HD21	1.99	0.45
2:A:397:TRP:NE1	2:A:546:VAL:HG22	2.32	0.45
2:A:405:ASN:H	2:A:409:GLN:HE22	1.65	0.45
2:B:132:ILE:HB	2:B:133:PRO:HD3	1.99	0.45
2:B:239:PRO:HB2	2:B:258:LEU:HD11	1.98	0.45
2:B:59:HIS:HA	2:D:449:MET:HE3	1.98	0.44
2:B:242:MET:CE	2:B:249:MET:H	2.30	0.44
2:D:264:HIS:O	2:D:400:GLN:NE2	2.49	0.44
2:A:307:ASP:O	2:A:324:GLN:HA	2.17	0.44
1:F:8:ASN:N	6:F:201:HOH:O	2.50	0.44
1:G:15:VAL:HG12	1:G:75:VAL:HA	1.98	0.44
2:D:327:VAL:HG23	3:D:601:FAD:H2A	1.98	0.44
2:D:383:ASP:O	2:D:406:ARG:HD3	2.17	0.44
2:D:54:HIS:HD2	2:D:55:ILE:N	2.16	0.44
2:C:469:MET:HB3	2:C:540:ILE:HD12	1.98	0.44
2:A:291:ILE:CD1	2:A:297:PHE:CE2	2.95	0.44
2:B:238:LEU:HD13	2:B:280:ILE:HD12	2.00	0.44
2:C:68:GLN:HG3	2:C:103:ILE:HG21	1.99	0.44
2:D:14:THR:HA	2:D:177:ALA:O	2.17	0.44
2:A:267:ARG:HG3	2:A:559:MET:CE	2.47	0.44
2:A:507:PHE:HA	2:C:498:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:92:ALA:HB2	1:H:42:LEU:CD1	2.48	0.44
2:B:208:ILE:HG12	2:B:280:ILE:CD1	2.48	0.44
2:D:21:HIS:O	2:D:25:GLN:HG2	2.17	0.44
2:A:304:ILE:HG23	2:A:321:VAL:HB	1.99	0.44
2:A:449:MET:HE3	4:A:602:TPP:HM23	2.00	0.44
2:A:86:PRO:HA	2:A:89:THR:OG1	2.18	0.44
2:C:239:PRO:HB2	2:C:258:LEU:HD11	1.99	0.44
2:B:242:MET:O	2:B:260:MET:HA	2.18	0.43
2:C:367:PRO:C	2:C:368:LEU:HD23	2.38	0.43
2:D:91:LEU:HD13	2:D:107:CYS:SG	2.58	0.43
2:D:548:PRO:HG2	2:D:559:MET:HE2	2.00	0.43
2:A:19:ILE:HA	2:A:151:MET:CE	2.48	0.43
2:A:91:LEU:HD13	2:A:107:CYS:SG	2.57	0.43
2:B:366:ASP:O	2:B:372:GLY:HA3	2.18	0.43
2:C:538:VAL:HG23	2:C:540:ILE:HG13	1.99	0.43
1:F:15:VAL:HG12	1:F:75:VAL:HG22	2.00	0.43
2:C:242:MET:HB3	2:C:246:ALA:HB3	2.00	0.43
2:A:263:MET:CE	2:A:289:ARG:HG2	2.49	0.43
2:B:77:PRO:HA	2:B:104:PRO:O	2.18	0.43
2:B:136:LYS:HE2	2:B:157:ILE:CG2	2.48	0.43
2:A:346:TRP:O	2:A:350:VAL:HG23	2.18	0.43
2:B:521:GLN:HA	2:B:521:GLN:OE1	2.17	0.43
2:C:147:LEU:HD23	2:C:147:LEU:HA	1.77	0.43
2:C:242:MET:HE3	2:C:250:LEU:N	2.33	0.43
2:D:481:GLN:O	2:D:488:GLY:HA2	2.19	0.43
2:B:133:PRO:HB2	2:D:126:ASP:HB3	2.00	0.43
1:G:21:VAL:O	1:G:25:VAL:HG23	2.19	0.43
2:B:11:LYS:O	2:B:180:GLU:HA	2.19	0.43
1:G:14:THR:O	1:G:76:VAL:N	2.49	0.43
2:A:405:ASN:H	2:A:409:GLN:NE2	2.17	0.43
2:C:388:THR:HA	2:C:411:LEU:O	2.18	0.43
2:D:458:SER:HA	2:D:533:PRO:HG3	2.00	0.43
2:D:471:ASN:HA	2:D:540:ILE:O	2.18	0.43
1:F:88:PHE:HD2	1:H:42:LEU:HD21	1.84	0.43
2:B:465:LYS:NZ	2:B:530:ARG:O	2.39	0.43
2:B:544:GLU:CG	2:B:545:LYS:N	2.62	0.43
1:F:26:CYS:SG	1:H:22:MET:HB3	2.59	0.42
2:B:215:VAL:HG11	2:B:273:LEU:CD2	2.49	0.42
2:C:402:TYR:CD1	2:C:403:PRO:HD2	2.54	0.42
2:D:381:VAL:HG22	2:D:382:ASP:H	1.83	0.42
1:F:19:PRO:HA	1:F:20:GLY:HA2	1.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:GLY:N	2:B:124:GLU:OE1	2.42	0.42
2:B:297:PHE:HA	2:B:298:CYS:HA	1.71	0.42
2:D:444:ASP:OD1	2:D:471:ASN:OD1	2.38	0.42
2:A:527:ILE:HD12	2:A:527:ILE:HA	1.83	0.42
2:C:72:ARG:HD2	2:C:72:ARG:HH11	1.72	0.42
2:C:477:VAL:O	2:C:481:GLN:HG3	2.19	0.42
2:C:530:ARG:H	2:C:530:ARG:HG2	1.66	0.42
2:A:141:VAL:O	2:A:171:PRO:HD2	2.19	0.42
2:A:368:LEU:HD12	2:A:368:LEU:O	2.20	0.42
2:B:498:ILE:HD12	2:D:507:PHE:HA	2.01	0.42
1:G:28:LEU:HD22	1:G:72:LEU:HD11	2.02	0.42
2:D:32:THR:O	2:D:80:CYS:HA	2.20	0.42
2:D:514:LEU:O	2:D:516:ASN:HB2	2.20	0.42
2:A:278:LEU:HD11	2:A:304:ILE:HG13	2.02	0.42
2:B:524:LEU:HD23	2:B:524:LEU:HA	1.90	0.42
2:A:81:MET:HA	2:A:108:ILE:O	2.19	0.42
2:A:266:VAL:HG13	2:A:269:THR:HG23	2.02	0.42
2:B:209:ASN:ND2	2:B:339:GLU:H	2.17	0.42
2:C:353:LEU:HD23	2:C:353:LEU:HA	1.91	0.42
2:D:77:PRO:HD3	2:D:159:GLN:HG3	2.01	0.42
2:D:454:MET:HE3	2:D:507:PHE:CD2	2.54	0.42
2:B:201:ILE:CD1	2:B:201:ILE:H	2.33	0.42
2:B:242:MET:CE	2:B:249:MET:N	2.82	0.42
2:D:43:TYR:HE2	2:D:54:HIS:ND1	2.16	0.42
1:E:15:VAL:HB	1:E:21:VAL:HG21	2.01	0.42
2:A:136:LYS:HD3	2:A:157:ILE:HG22	2.02	0.42
2:A:269:THR:HA	2:A:272:ILE:HB	2.02	0.42
1:F:68:GLN:O	1:F:71:LYS:HB3	2.20	0.42
2:B:59:HIS:CD2	2:D:449:MET:HE3	2.54	0.42
2:B:222:VAL:HA	2:B:327:VAL:HG21	2.02	0.42
2:B:444:ASP:OD1	2:B:445:GLY:N	2.53	0.42
2:C:263:MET:HA	2:C:550:VAL:HB	2.02	0.42
2:C:371:TYR:OH	2:C:400:GLN:NE2	2.51	0.42
2:C:216:LEU:HD12	2:C:280:ILE:O	2.20	0.42
2:A:147:LEU:HD12	2:A:147:LEU:HA	1.80	0.42
2:A:465:LYS:NZ	2:A:532:GLY:O	2.48	0.42
2:B:201:ILE:HG23	2:B:334:LEU:CD1	2.50	0.42
2:B:208:ILE:HG12	2:B:280:ILE:HD13	2.01	0.42
2:B:86:PRO:HB3	2:D:418:THR:HG23	2.01	0.41
2:A:485:TYR:HB3	2:C:44:ASP:OD2	2.20	0.41
2:B:387:ILE:HG13	2:B:402:TYR:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:419:MET:SD	4:D:602:TPP:H72	2.60	0.41
2:A:31:VAL:O	2:A:54:HIS:HA	2.21	0.41
2:A:200:SER:HB2	2:A:323:ILE:HD11	2.03	0.41
2:A:419:MET:HB2	2:A:449:MET:SD	2.60	0.41
2:A:521:GLN:O	2:A:524:LEU:N	2.53	0.41
2:B:39:ILE:HG13	2:B:39:ILE:O	2.21	0.41
2:B:327:VAL:HG13	3:B:601:FAD:H2A	2.02	0.41
1:H:44:ILE:CD1	1:H:51:HIS:CD2	3.01	0.41
1:H:88:PHE:O	1:H:91:ILE:HG12	2.19	0.41
2:D:353:LEU:HD23	2:D:353:LEU:HA	1.92	0.41
2:B:239:PRO:CB	2:B:258:LEU:HD11	2.51	0.41
2:B:373:LEU:HD22	2:B:538:VAL:HG21	2.01	0.41
2:C:242:MET:HE1	2:C:249:MET:N	2.35	0.41
2:D:391:VAL:HG21	2:D:417:GLY:C	2.40	0.41
2:A:235:LYS:HE3	2:A:338:VAL:O	2.20	0.41
2:A:427:ILE:HG23	2:A:462:LEU:CD1	2.51	0.41
1:F:65:MET:O	1:F:69:ILE:HG13	2.20	0.41
2:B:153:ASP:O	2:B:157:ILE:HG13	2.20	0.41
2:B:239:PRO:HG3	2:B:346:TRP:HE1	1.85	0.41
2:C:419:MET:HG3	4:C:602:TPP:C4'	2.50	0.41
2:C:458:SER:O	2:C:461:GLN:HG2	2.21	0.41
1:F:10:ILE:HB	1:F:81:ASN:HB3	2.03	0.41
1:G:94:PHE:CD1	1:H:87:MET:HE1	2.55	0.41
2:D:444:ASP:OD2	2:D:472:GLU:HA	2.20	0.41
2:B:276:ALA:O	2:B:301:ALA:HB2	2.21	0.41
2:D:81:MET:HA	2:D:108:ILE:O	2.21	0.41
2:D:510:GLU:OE1	2:D:530:ARG:NH2	2.54	0.41
3:D:601:FAD:H9	3:D:601:FAD:H1'1	1.85	0.41
2:A:109:THR:HG22	2:A:169:ASP:OD2	2.21	0.41
2:A:128:TYR:CE1	2:A:132:ILE:HD11	2.55	0.41
2:B:419:MET:HB3	2:B:419:MET:HE2	1.96	0.41
2:B:427:ILE:HG23	2:B:462:LEU:CD1	2.50	0.41
2:D:213:ARG:HG2	2:D:346:TRP:CZ3	2.56	0.41
2:A:137:HIS:O	2:A:166:VAL:HG13	2.21	0.41
2:B:26:GLN:HA	2:B:187:MET:HG3	2.02	0.41
2:B:48:GLN:HE21	2:B:48:GLN:HB2	1.66	0.41
2:B:335:ILE:N	2:B:336:PRO:HD2	2.36	0.41
2:C:32:THR:O	2:C:80:CYS:HA	2.21	0.41
2:C:238:LEU:O	2:C:240:THR:HG23	2.20	0.41
2:C:550:VAL:HG22	2:C:559:MET:HG3	2.02	0.41
2:D:31:VAL:O	2:D:54:HIS:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:111:GLN:O	2:D:171:PRO:HA	2.21	0.41
2:A:238:LEU:O	2:A:240:THR:HG23	2.21	0.41
2:A:290:ALA:HB2	3:A:601:FAD:O2	2.20	0.41
1:H:15:VAL:HB	1:H:21:VAL:HG11	2.03	0.41
1:E:10:ILE:HA	1:E:54:LEU:O	2.22	0.40
1:F:14:THR:HB	1:F:77:LYS:HB2	2.02	0.40
1:H:21:VAL:HG23	1:H:21:VAL:H	1.57	0.40
2:D:54:HIS:CD2	2:D:54:HIS:C	2.94	0.40
2:D:145:GLU:CD	2:D:145:GLU:H	2.24	0.40
2:D:242:MET:HB3	2:D:246:ALA:HB3	2.03	0.40
2:A:437:LYS:HZ1	2:A:465:LYS:HE2	1.80	0.40
2:B:251:PRO:HA	2:B:405:ASN:HA	2.02	0.40
2:B:449:MET:HE3	2:D:59:HIS:CD2	2.56	0.40
2:D:82:ALA:O	2:D:109:THR:HA	2.21	0.40
2:D:251:PRO:HG2	2:D:254:HIS:HB2	2.02	0.40
2:B:380:CYS:O	2:B:525:GLN:NE2	2.52	0.40
1:G:15:VAL:HG12	1:G:75:VAL:HG12	2.04	0.40
1:H:87:MET:HE3	1:H:90:LYS:HD2	2.03	0.40
2:D:514:LEU:HD11	2:D:539:ARG:N	2.32	0.40
2:A:65:PHE:HA	2:A:68:GLN:HB2	2.03	0.40
2:A:555:ALA:HB3	2:A:558:GLU:HG2	2.03	0.40
1:F:62:LEU:O	1:F:66:ILE:HG13	2.21	0.40
2:C:36:GLY:H	2:C:39:ILE:HG22	1.86	0.40
2:C:537:HIS:CD2	2:C:537:HIS:C	2.94	0.40
2:D:319:PRO:HG2	2:D:322:ALA:HB2	2.04	0.40
2:A:402:TYR:CD1	2:A:403:PRO:HD2	2.55	0.40
2:A:459:GLU:CD	2:C:495:PRO:HD2	2.42	0.40
2:B:216:LEU:HD12	2:B:280:ILE:O	2.21	0.40
2:C:30:ILE:HB	2:C:70:MET:HE1	2.03	0.40
1:H:19:PRO:HA	1:H:20:GLY:HA2	1.60	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	E	87/127 (68%)	83 (95%)	4 (5%)	0	100	100
1	F	87/127 (68%)	82 (94%)	5 (6%)	0	100	100
1	G	86/127 (68%)	78 (91%)	7 (8%)	1 (1%)	13	28
1	H	86/127 (68%)	78 (91%)	8 (9%)	0	100	100
2	A	521/562 (93%)	505 (97%)	16 (3%)	0	100	100
2	B	533/562 (95%)	515 (97%)	18 (3%)	0	100	100
2	C	525/562 (93%)	507 (97%)	18 (3%)	0	100	100
2	D	519/562 (92%)	505 (97%)	14 (3%)	0	100	100
All	All	2444/2756 (89%)	2353 (96%)	90 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	19	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	76/104 (73%)	76 (100%)	0	100	100
1	F	81/104 (78%)	80 (99%)	1 (1%)	71	85
1	G	78/104 (75%)	78 (100%)	0	100	100
1	H	81/104 (78%)	79 (98%)	2 (2%)	47	71
2	A	410/446 (92%)	405 (99%)	5 (1%)	71	85
2	B	397/446 (89%)	392 (99%)	5 (1%)	69	84
2	C	397/446 (89%)	390 (98%)	7 (2%)	59	78
2	D	393/446 (88%)	387 (98%)	6 (2%)	65	82
All	All	1913/2200 (87%)	1887 (99%)	26 (1%)	67	83

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	74	ASP
2	A	107	CYS
2	A	179	PHE
2	A	217	TYR
2	A	539	ARG
1	F	64	GLN
2	B	51	GLN
2	B	179	PHE
2	B	217	TYR
2	B	539	ARG
2	B	544	GLU
2	C	107	CYS
2	C	179	PHE
2	C	217	TYR
2	C	305	HIS
2	C	390	ASP
2	C	406	ARG
2	C	461	GLN
1	H	61	ARG
1	H	65	MET
2	D	107	CYS
2	D	179	PHE
2	D	217	TYR
2	D	267	ARG
2	D	419	MET
2	D	514	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	68	GLN
2	A	54	HIS
2	A	254	HIS
2	A	318	GLN
2	A	409	GLN
2	A	452	GLN
2	A	481	GLN
2	A	502	GLN
1	F	57	ASN
2	B	61	GLN
2	B	111	GLN

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Mol	Chain	Res	Type
2	B	123	GLN
2	B	137	HIS
2	B	450	ASN
2	B	479	GLN
1	G	64	GLN
1	G	68	GLN
2	C	48	GLN
2	C	54	HIS
2	C	61	GLN
2	C	393	GLN
2	C	400	GLN
2	C	405	ASN
2	C	479	GLN
2	C	537	HIS
1	H	51	HIS
2	D	48	GLN
2	D	54	HIS
2	D	393	GLN
2	D	479	GLN
2	D	480	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	TPP	A	602	5	22,27,27	1.53	4 (18%)	29,40,40	1.84	9 (31%)
3	FAD	A	601	-	53,58,58	0.73	1 (1%)	68,89,89	0.61	1 (1%)
3	FAD	C	601	-	53,58,58	0.50	0	68,89,89	0.55	1 (1%)
3	FAD	D	601	-	53,58,58	0.46	0	68,89,89	0.62	3 (4%)
3	FAD	B	601	-	53,58,58	0.57	1 (1%)	68,89,89	0.51	1 (1%)
4	TPP	D	602	5	22,27,27	1.65	4 (18%)	29,40,40	1.92	8 (27%)
4	TPP	C	602	5	22,27,27	1.56	5 (22%)	29,40,40	1.87	6 (20%)
4	TPP	B	602	5	22,27,27	1.64	6 (27%)	29,40,40	1.84	9 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TPP	A	602	5	-	5/16/17/17	0/2/2/2
3	FAD	A	601	-	-	10/30/50/50	0/6/6/6
3	FAD	C	601	-	-	6/30/50/50	0/6/6/6
3	FAD	D	601	-	-	10/30/50/50	0/6/6/6
3	FAD	B	601	-	-	9/30/50/50	0/6/6/6
4	TPP	D	602	5	-	5/16/17/17	0/2/2/2
4	TPP	C	602	5	-	7/16/17/17	0/2/2/2
4	TPP	B	602	5	-	2/16/17/17	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	602	TPP	C4-N3	-4.82	1.35	1.39
4	A	602	TPP	C4-N3	-4.44	1.35	1.39
3	A	601	FAD	P-O2P	-4.11	1.36	1.55
4	C	602	TPP	C4-N3	-3.74	1.36	1.39
4	D	602	TPP	C2'-N1'	3.15	1.39	1.34
4	B	602	TPP	C7'-N3	-3.06	1.43	1.48
4	B	602	TPP	C4-N3	-3.06	1.37	1.39
4	C	602	TPP	C2'-N1'	3.02	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	TPP	C4'-N3'	2.87	1.39	1.35
4	B	602	TPP	C2'-N3'	2.73	1.38	1.34
4	A	602	TPP	C2'-N1'	2.73	1.38	1.34
4	B	602	TPP	C6-C5	-2.72	1.49	1.50
4	C	602	TPP	C2'-N3'	2.48	1.38	1.34
4	B	602	TPP	C2'-N1'	2.47	1.38	1.34
4	A	602	TPP	C7'-N3	-2.37	1.44	1.48
4	D	602	TPP	C6'-N1'	2.34	1.39	1.34
4	D	602	TPP	C2'-N3'	2.22	1.38	1.34
4	C	602	TPP	C6'-N1'	2.21	1.39	1.34
3	B	601	FAD	P-O2P	-2.16	1.45	1.55
4	A	602	TPP	C2'-N3'	2.08	1.37	1.34
4	C	602	TPP	C4'-N3'	2.07	1.38	1.35

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	602	TPP	CM2-C2'-N1'	5.21	122.87	117.14
4	D	602	TPP	C6-C5-C4	4.25	130.84	127.43
4	C	602	TPP	CM2-C2'-N1'	4.23	121.79	117.14
4	A	602	TPP	CM4-C4-N3	4.16	127.84	122.53
4	B	602	TPP	CM4-C4-N3	4.08	127.73	122.53
4	A	602	TPP	CM2-C2'-N1'	3.81	121.33	117.14
4	C	602	TPP	C6-C5-C4	3.72	130.41	127.43
4	C	602	TPP	C5'-C7'-N3	-3.67	107.17	113.28
4	B	602	TPP	C6-C5-C4	3.66	130.37	127.43
4	D	602	TPP	PA-O3A-PB	-3.50	120.81	132.83
4	C	602	TPP	CM4-C4-N3	3.47	126.96	122.53
4	B	602	TPP	C5'-C7'-N3	-3.42	107.59	113.28
4	D	602	TPP	N1'-C2'-N3'	-3.26	119.92	125.54
4	A	602	TPP	C5'-C7'-N3	-3.16	108.02	113.28
4	B	602	TPP	PA-O3A-PB	-3.16	122.00	132.83
4	C	602	TPP	PA-O3A-PB	-2.98	122.59	132.83
4	A	602	TPP	C6'-C5'-C4'	2.97	119.76	115.72
4	B	602	TPP	N1'-C2'-N3'	-2.93	120.50	125.54
4	C	602	TPP	N1'-C2'-N3'	-2.84	120.65	125.54
4	A	602	TPP	N1'-C2'-N3'	-2.77	120.78	125.54
4	D	602	TPP	C6'-C5'-C4'	2.75	119.46	115.72
4	A	602	TPP	PA-O3A-PB	-2.68	123.62	132.83
4	D	602	TPP	C5'-C6'-N1'	-2.52	119.63	123.82
4	B	602	TPP	C6'-N1'-C2'	2.51	120.23	115.96
4	D	602	TPP	C6'-N1'-C2'	2.41	120.07	115.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	602	TPP	CM4-C4-C5	-2.41	122.34	127.60
4	A	602	TPP	O2B-PB-O3A	2.38	112.61	104.64
3	A	601	FAD	C5A-C6A-N6A	2.32	123.88	120.35
3	D	601	FAD	C5A-C6A-N6A	2.31	123.86	120.35
3	B	601	FAD	C5A-C6A-N6A	2.29	123.83	120.35
4	B	602	TPP	CM2-C2'-N3'	2.23	120.63	117.15
3	C	601	FAD	C5A-C6A-N6A	2.22	123.72	120.35
4	D	602	TPP	O3B-PB-O3A	2.14	111.81	104.64
4	A	602	TPP	C5'-C6'-N1'	-2.13	120.26	123.82
3	D	601	FAD	O2P-P-O1P	2.07	122.46	112.24
4	B	602	TPP	O3B-PB-O3A	2.05	111.52	104.64
4	B	602	TPP	C6'-C5'-C4'	2.02	118.47	115.72
3	D	601	FAD	P-O3P-PA	-2.01	125.93	132.83

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	FAD	C5B-O5B-PA-O1A
3	A	601	FAD	C5B-O5B-PA-O2A
3	A	601	FAD	C3B-C4B-C5B-O5B
3	A	601	FAD	C5'-O5'-P-O1P
3	B	601	FAD	C5B-O5B-PA-O3P
3	B	601	FAD	C3B-C4B-C5B-O5B
3	B	601	FAD	C5'-O5'-P-O1P
3	B	601	FAD	C5'-O5'-P-O3P
3	C	601	FAD	P-O3P-PA-O5B
3	C	601	FAD	C5'-O5'-P-O1P
3	C	601	FAD	C5'-O5'-P-O3P
3	D	601	FAD	C5B-O5B-PA-O1A
3	D	601	FAD	C5B-O5B-PA-O2A
3	D	601	FAD	C3B-C4B-C5B-O5B
4	A	602	TPP	C4-C5-C6-C7
4	A	602	TPP	C5-C6-C7-O7
4	A	602	TPP	C7-O7-PA-O1A
4	A	602	TPP	C7-O7-PA-O3A
4	C	602	TPP	C5-C6-C7-O7
4	C	602	TPP	C7-O7-PA-O3A
4	C	602	TPP	PA-O3A-PB-O3B
4	D	602	TPP	C5-C6-C7-O7
4	D	602	TPP	C7-O7-PA-O3A
3	C	601	FAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	C	601	FAD	C3B-C4B-C5B-O5B
3	B	601	FAD	O4B-C4B-C5B-O5B
3	D	601	FAD	O4B-C4B-C5B-O5B
3	A	601	FAD	O4B-C4B-C5B-O5B
3	D	601	FAD	C3'-C4'-C5'-O5'
3	D	601	FAD	PA-O3P-P-O1P
3	A	601	FAD	C5'-O5'-P-O3P
3	D	601	FAD	C5B-O5B-PA-O3P
3	A	601	FAD	PA-O3P-P-O2P
3	B	601	FAD	PA-O3P-P-O2P
3	D	601	FAD	PA-O3P-P-O2P
3	B	601	FAD	C5B-O5B-PA-O1A
3	B	601	FAD	C5'-O5'-P-O2P
3	C	601	FAD	C5'-O5'-P-O2P
4	D	602	TPP	C7-O7-PA-O2A
4	D	602	TPP	C4-C5-C6-C7
3	D	601	FAD	O4'-C4'-C5'-O5'
3	A	601	FAD	C2'-C3'-C4'-O4'
4	B	602	TPP	PA-O3A-PB-O1B
4	C	602	TPP	PA-O3A-PB-O2B
3	A	601	FAD	C5B-O5B-PA-O3P
3	A	601	FAD	PA-O3P-P-O1P
3	B	601	FAD	PA-O3P-P-O1P
3	D	601	FAD	C5'-O5'-P-O1P
4	A	602	TPP	C7-O7-PA-O2A
4	B	602	TPP	C7-O7-PA-O1A
4	C	602	TPP	C7-O7-PA-O1A
4	C	602	TPP	C7-O7-PA-O2A
4	D	602	TPP	C7-O7-PA-O1A
4	C	602	TPP	PA-O3A-PB-O1B

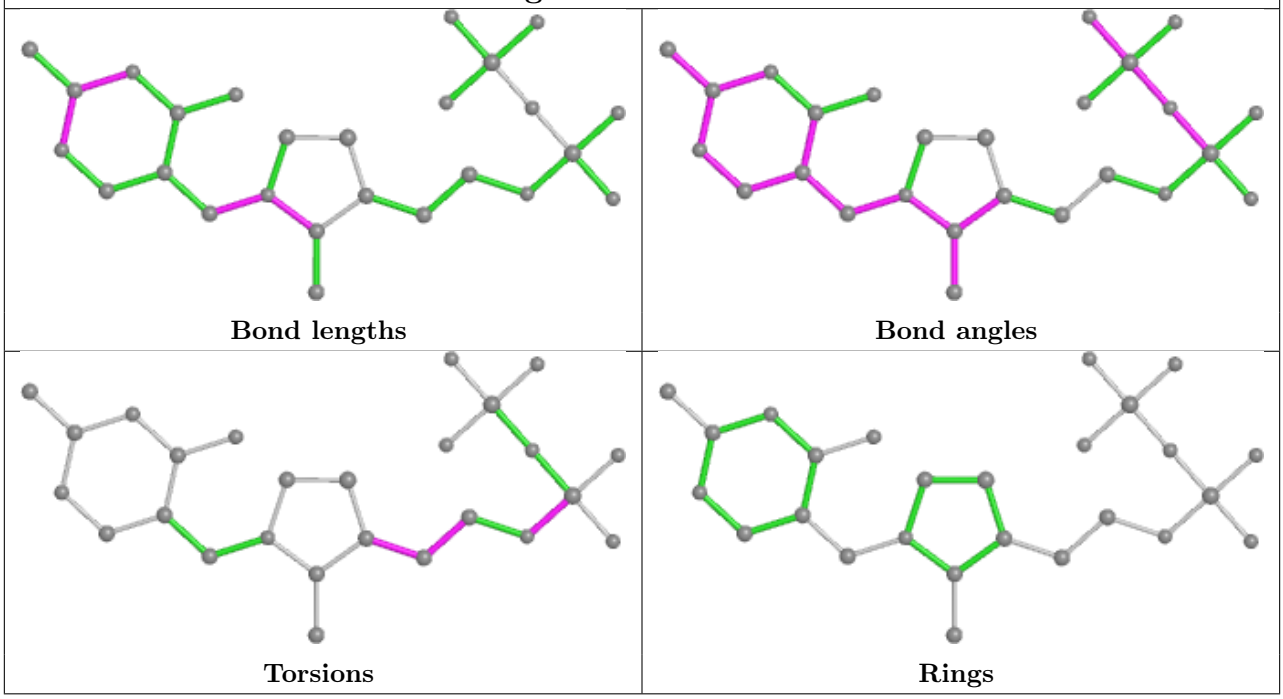
There are no ring outliers.

7 monomers are involved in 19 short contacts:

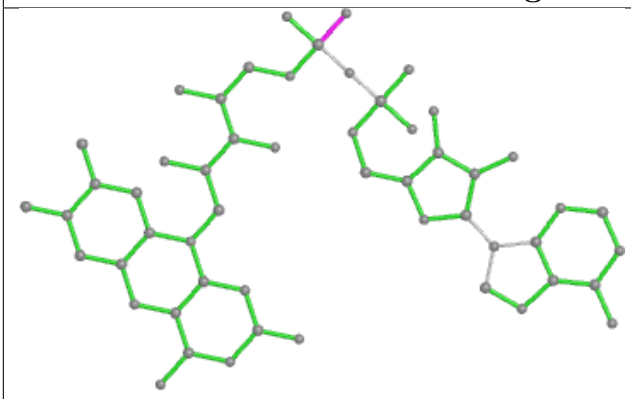
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	TPP	7	0
3	A	601	FAD	2	0
3	D	601	FAD	3	0
3	B	601	FAD	1	0
4	D	602	TPP	1	0
4	C	602	TPP	4	0
4	B	602	TPP	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

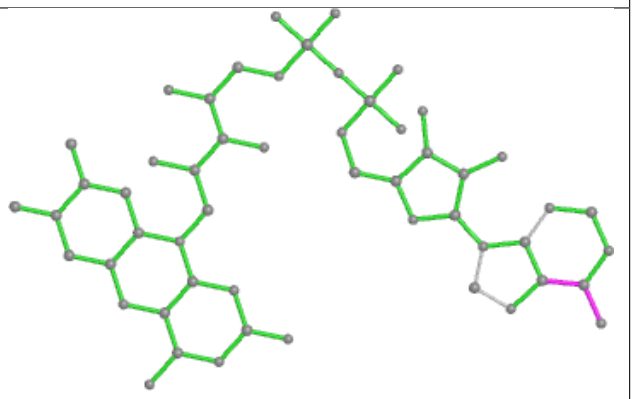
Ligand TPP A 602



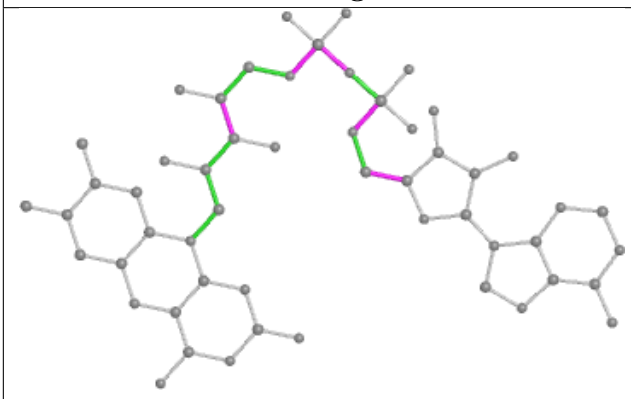
Ligand FAD A 601



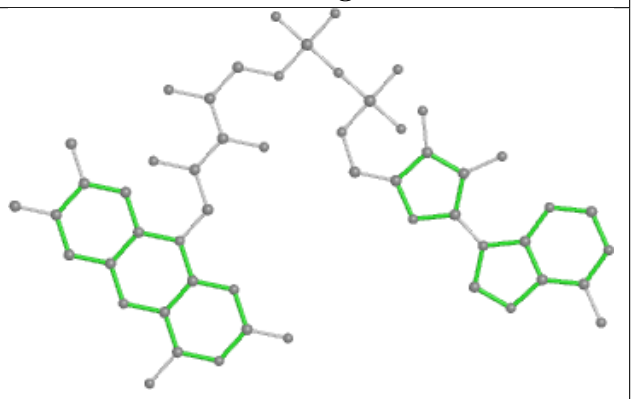
Bond lengths



Bond angles

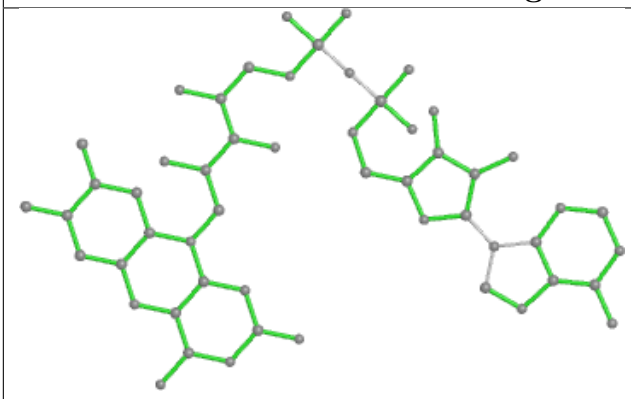


Torsions

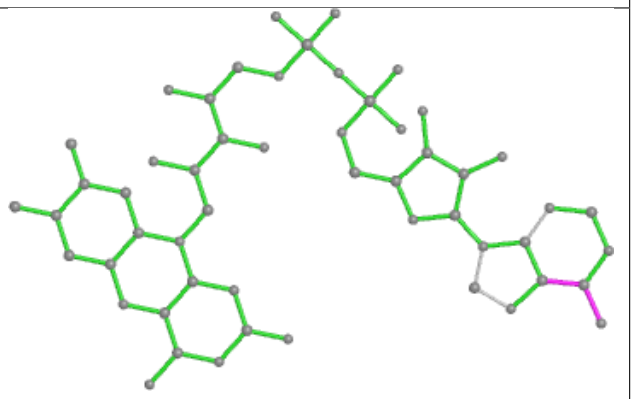


Rings

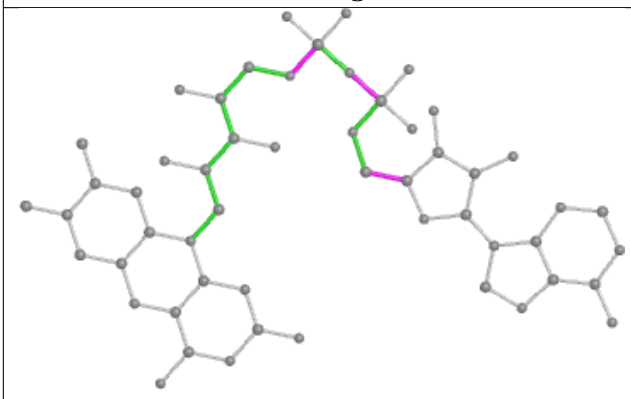
Ligand FAD C 601



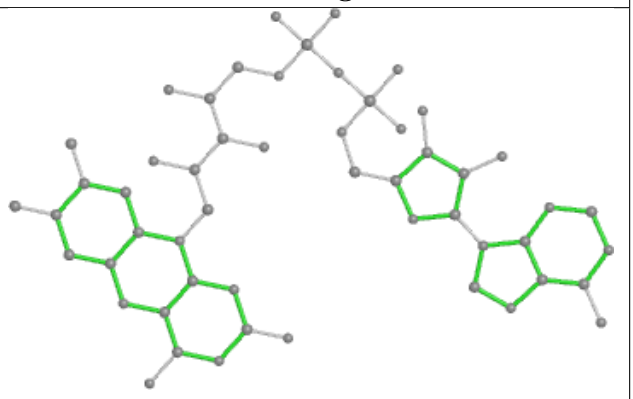
Bond lengths



Bond angles

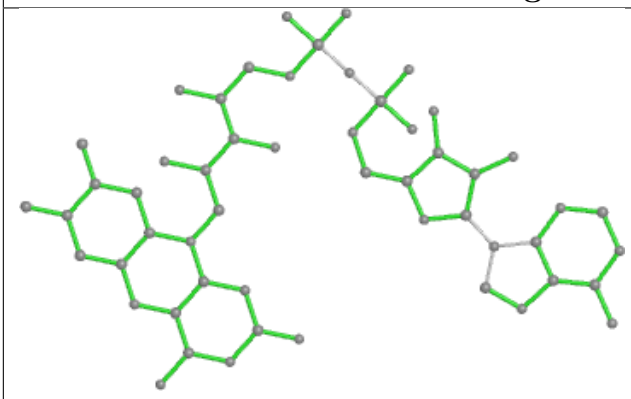


Torsions

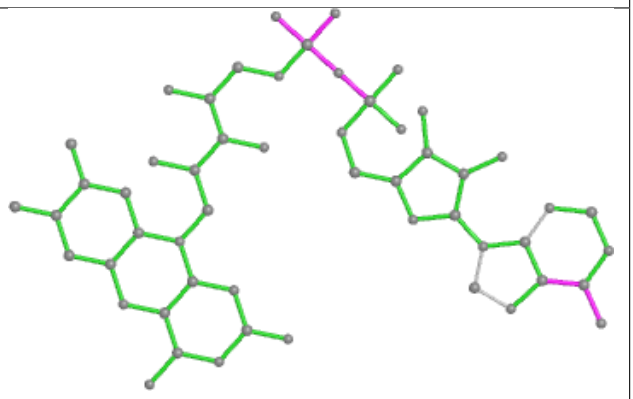


Rings

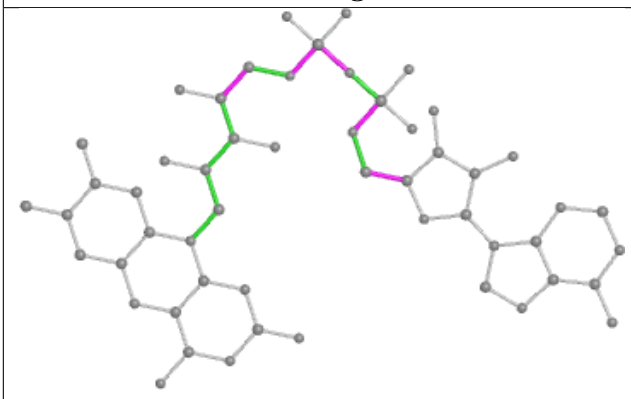
Ligand FAD D 601



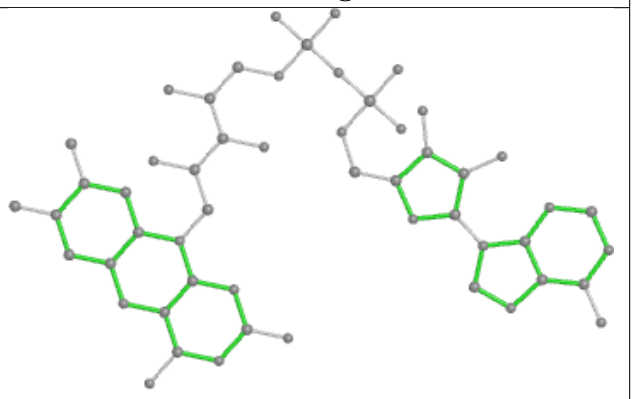
Bond lengths



Bond angles

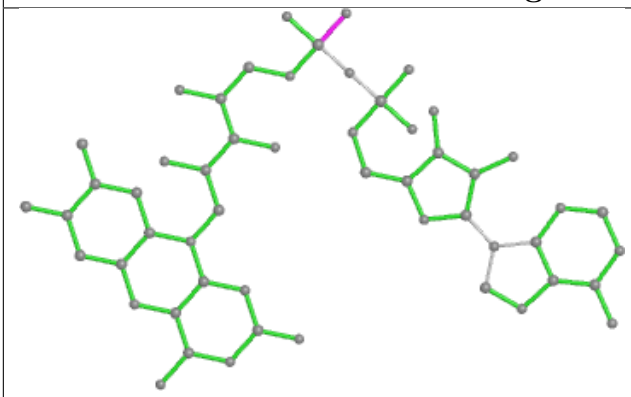


Torsions

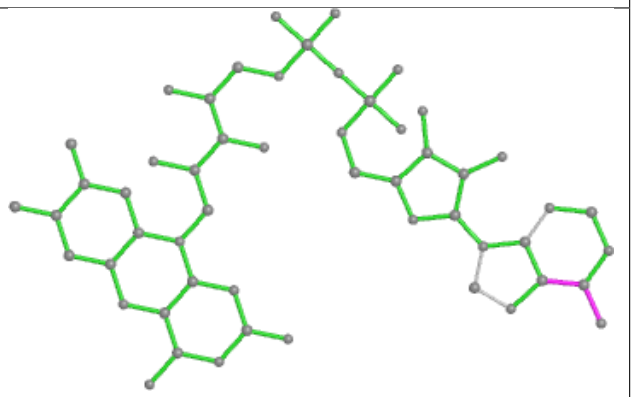


Rings

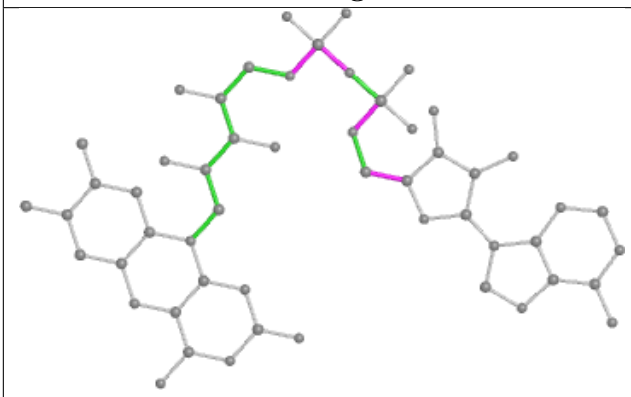
Ligand FAD B 601



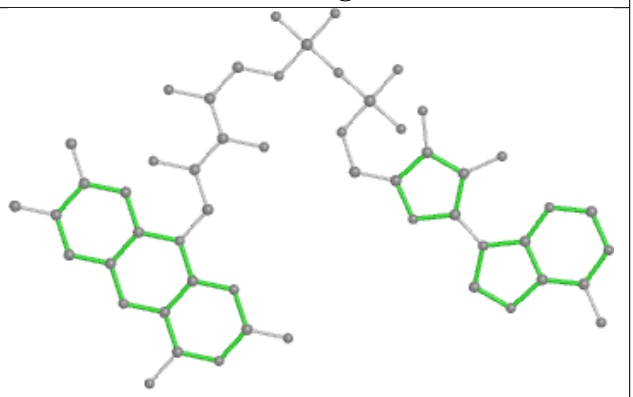
Bond lengths



Bond angles

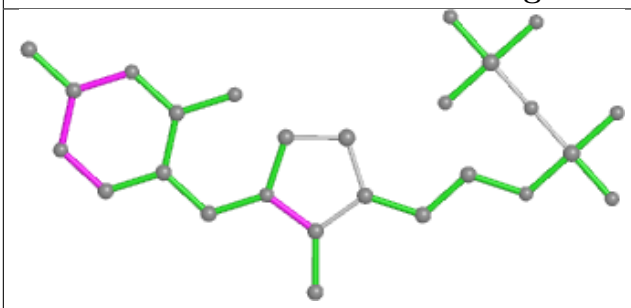


Torsions

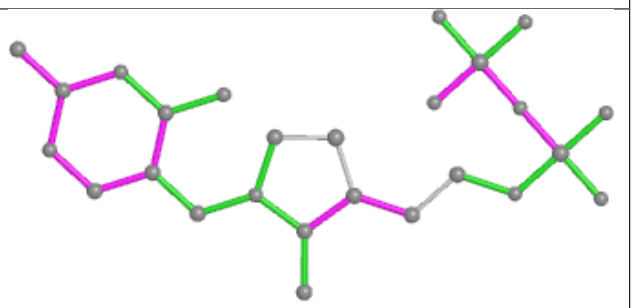


Rings

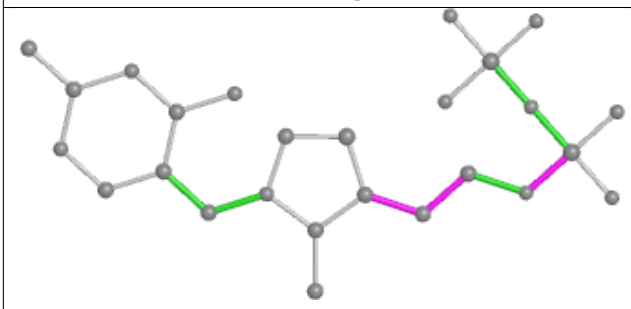
Ligand TPP D 602



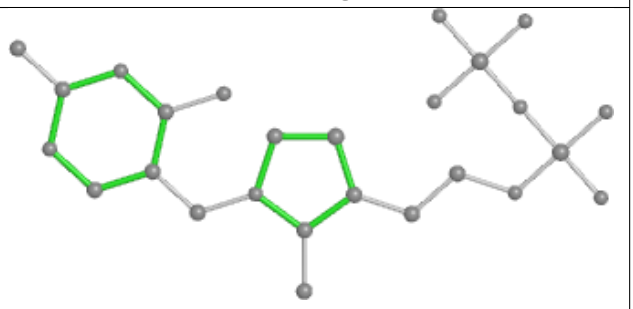
Bond lengths



Bond angles

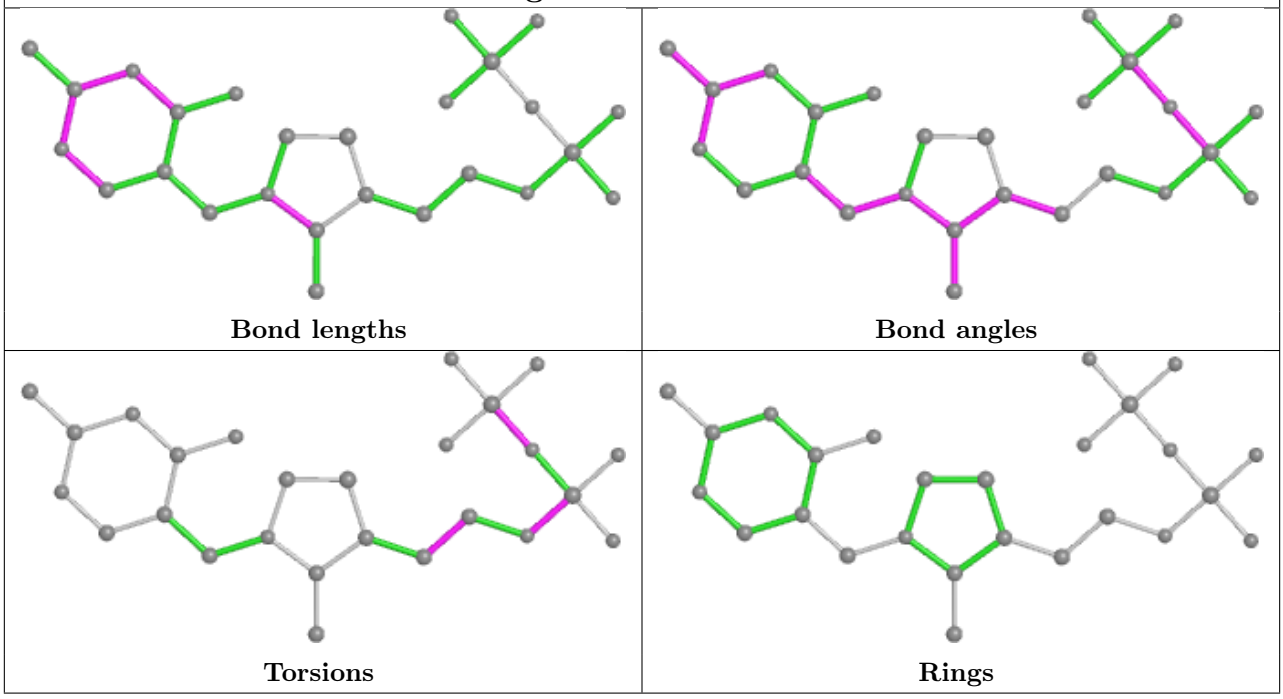


Torsions

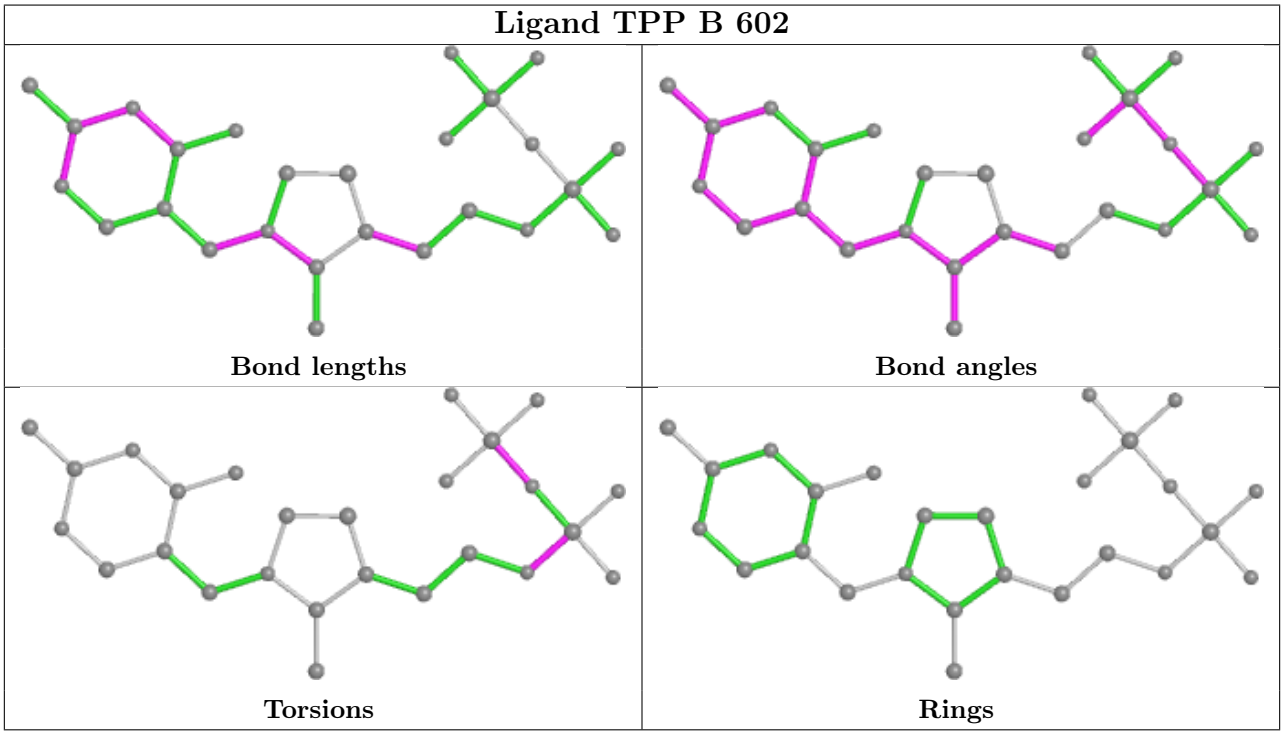


Rings

Ligand TPP C 602



Ligand TPP B 602



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, 95^{th} 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	E	89/127 (70%)	-0.36	1 (1%) 80 78	34, 50, 74, 91	0
1	F	89/127 (70%)	-0.12	3 (3%) 45 37	41, 62, 94, 148	0
1	G	88/127 (69%)	-0.24	2 (2%) 60 55	37, 59, 85, 111	0
1	H	88/127 (69%)	-0.37	0 100 100	36, 55, 83, 100	0
2	A	531/562 (94%)	-0.21	12 (2%) 60 55	34, 57, 84, 137	0
2	B	539/562 (95%)	-0.09	21 (3%) 39 31	31, 65, 110, 135	0
2	C	533/562 (94%)	-0.04	16 (3%) 50 44	31, 66, 100, 115	0
2	D	529/562 (94%)	-0.26	12 (2%) 60 55	27, 63, 99, 132	0
All	All	2486/2756 (90%)	-0.17	67 (2%) 54 49	27, 61, 100, 148	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	193	ALA	4.0
2	D	522	ALA	4.0
2	C	342	PRO	3.9
1	F	60	GLN	3.8
1	G	62	LEU	3.8
2	B	349	LEU	3.7
2	C	271	TYR	3.6
2	B	342	PRO	3.5
2	B	554	ALA	3.5
2	B	352	ASP	3.4
2	B	344	ALA	3.4
2	A	359	CYS	3.2
2	C	524	LEU	3.1
2	B	559	MET	3.1
2	B	435	ASP	3.0
2	A	195	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	557	THR	2.9
2	C	340	ALA	2.9
2	C	523	SER	2.9
2	A	191	ALA	2.9
2	A	512	CYS	2.9
2	C	120	ASP	2.8
2	A	186	ALA	2.8
2	D	353	LEU	2.8
2	B	299	PRO	2.8
2	D	519	ASP	2.8
2	C	350	VAL	2.8
2	C	559	MET	2.7
2	B	351	ALA	2.7
2	D	560	VAL	2.6
2	B	295	GLU	2.6
2	B	558	GLU	2.6
2	A	187	MET	2.6
2	D	553	GLY	2.6
2	B	557	THR	2.5
2	A	422	GLY	2.5
2	D	520	PRO	2.5
2	B	346	TRP	2.5
2	D	552	PRO	2.5
2	D	350	VAL	2.4
2	C	186	ALA	2.4
2	A	358	PRO	2.4
2	C	521	GLN	2.4
2	B	340	ALA	2.4
2	B	275	GLU	2.3
2	B	520	PRO	2.3
2	C	121	ALA	2.3
2	C	349	LEU	2.3
2	D	114	ALA	2.3
2	B	341	GLN	2.2
2	A	192	ALA	2.2
1	F	62	LEU	2.2
2	C	314	GLY	2.2
2	C	558	GLU	2.2
1	E	79	GLN	2.2
2	D	559	MET	2.2
1	G	59	ASP	2.2
2	C	522	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	64	GLN	2.1
2	B	318	GLN	2.1
2	B	551	PRO	2.1
2	A	379	ALA	2.1
2	B	555	ALA	2.1
2	A	51	GLN	2.0
2	C	313	LEU	2.0
2	D	349	LEU	2.0
2	B	348	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

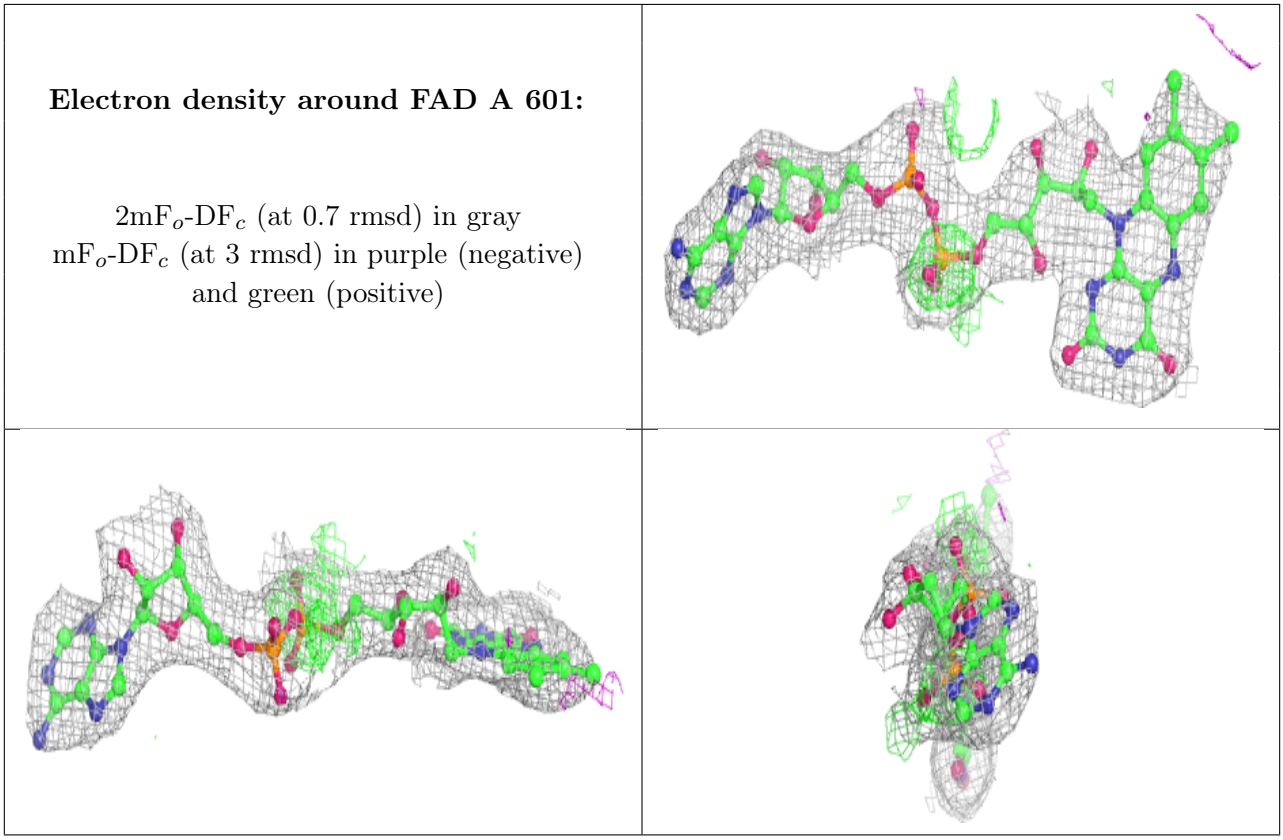
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FAD	A	601	53/53	0.94	0.17	26,41,61,90	0
5	MG	C	603	1/1	0.94	0.19	56,56,56,56	0
3	FAD	C	601	53/53	0.95	0.18	45,67,78,80	0
3	FAD	B	601	53/53	0.95	0.21	49,65,77,80	0
3	FAD	D	601	53/53	0.96	0.15	50,64,73,78	0
4	TPP	C	602	26/26	0.97	0.13	35,52,57,63	0
5	MG	D	603	1/1	0.97	0.09	64,64,64,64	0
4	TPP	D	602	26/26	0.98	0.12	24,47,63,67	0
5	MG	A	603	1/1	0.98	0.16	50,50,50,50	0
4	TPP	B	602	26/26	0.98	0.15	17,43,55,58	0
4	TPP	A	602	26/26	0.98	0.15	23,41,54,60	0
5	MG	B	603	1/1	0.99	0.11	52,52,52,52	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.

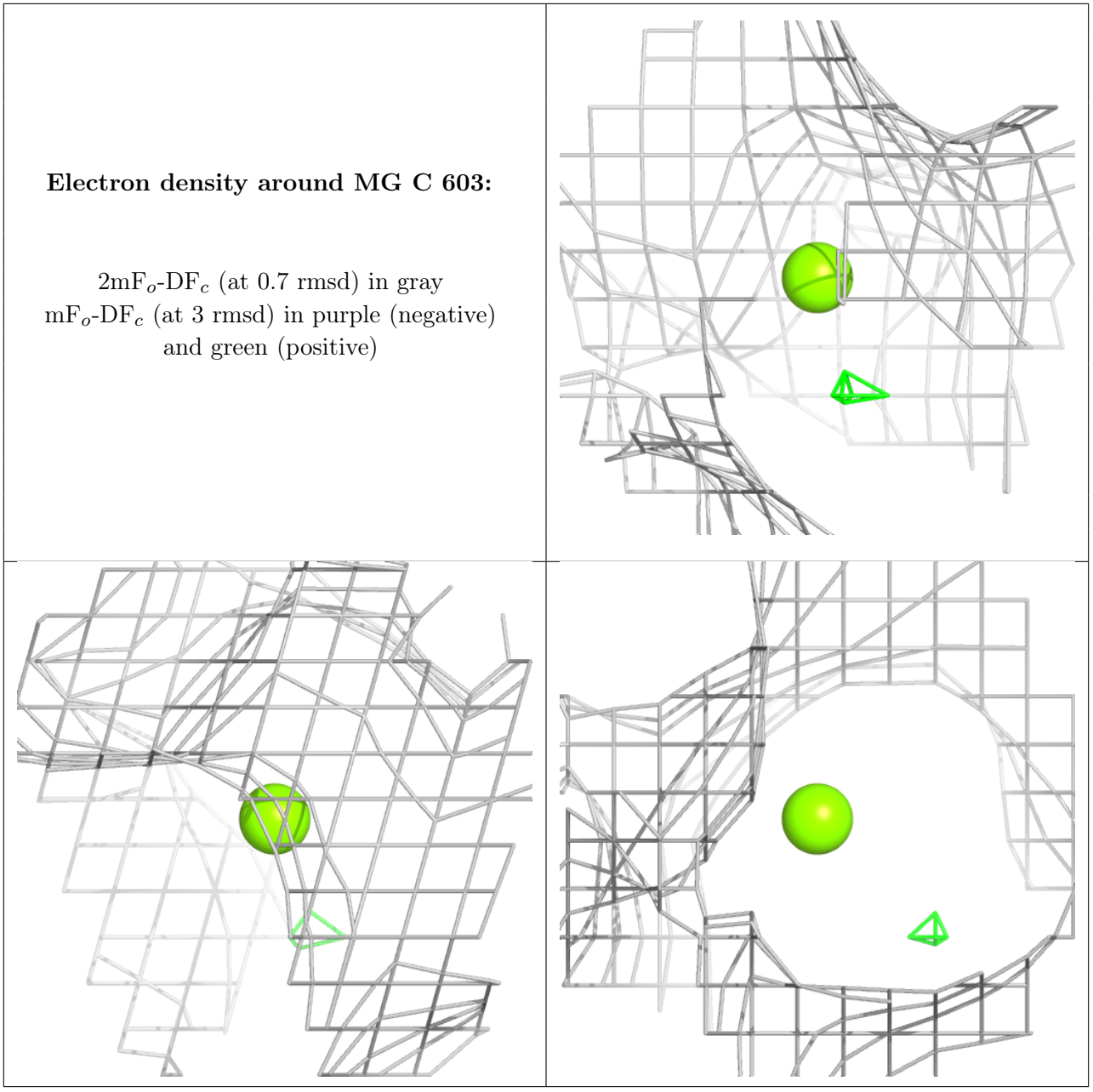
Electron density around FAD A 601:

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



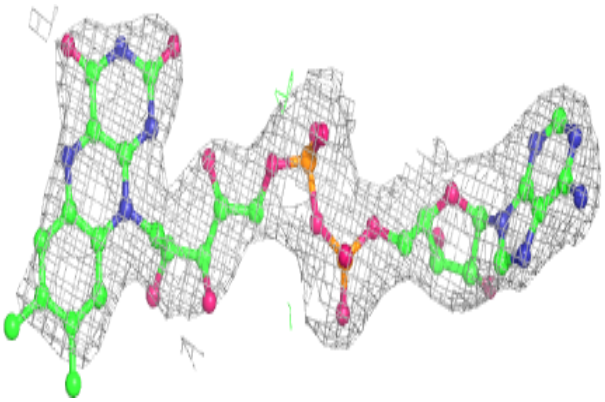
Electron density around MG C 603:

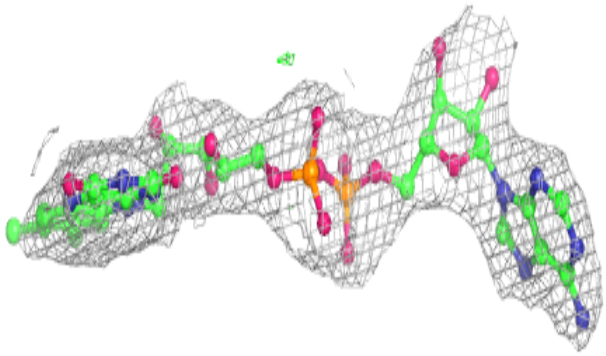
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

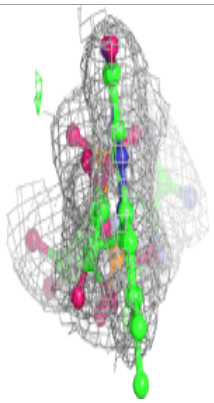


Electron density around FAD C 601:

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

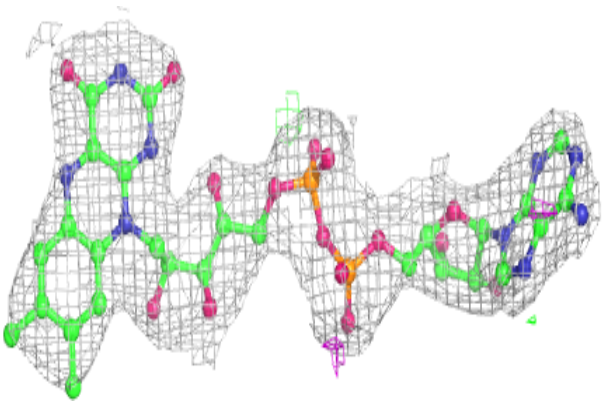


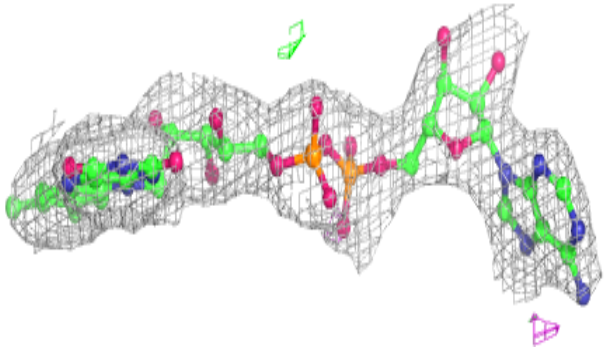


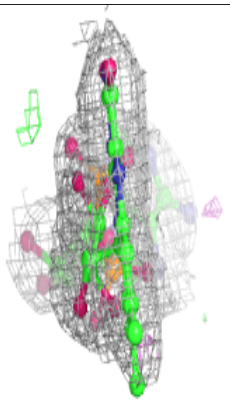


Electron density around FAD B 601:

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

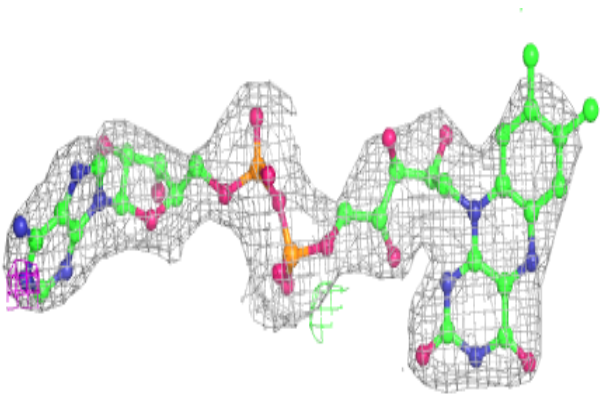


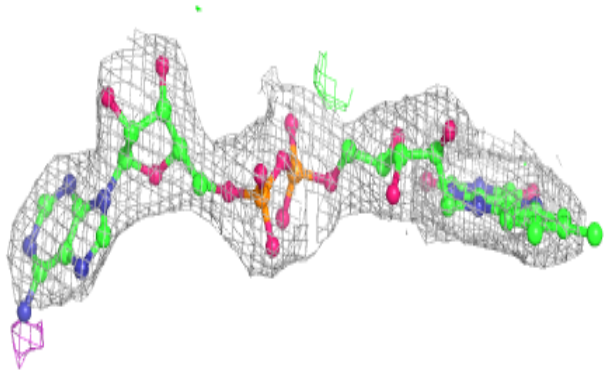


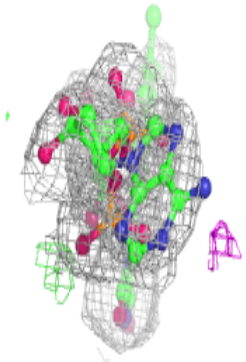


Electron density around FAD D 601:

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

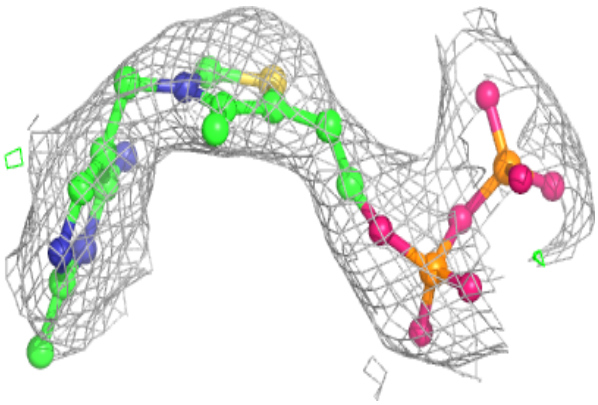


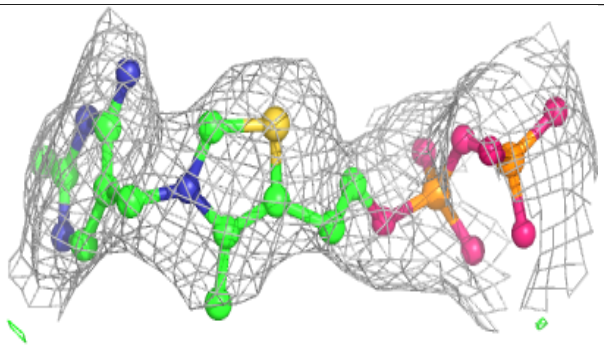


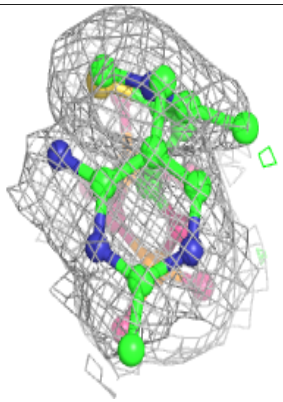


Electron density around TPP C 602:

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

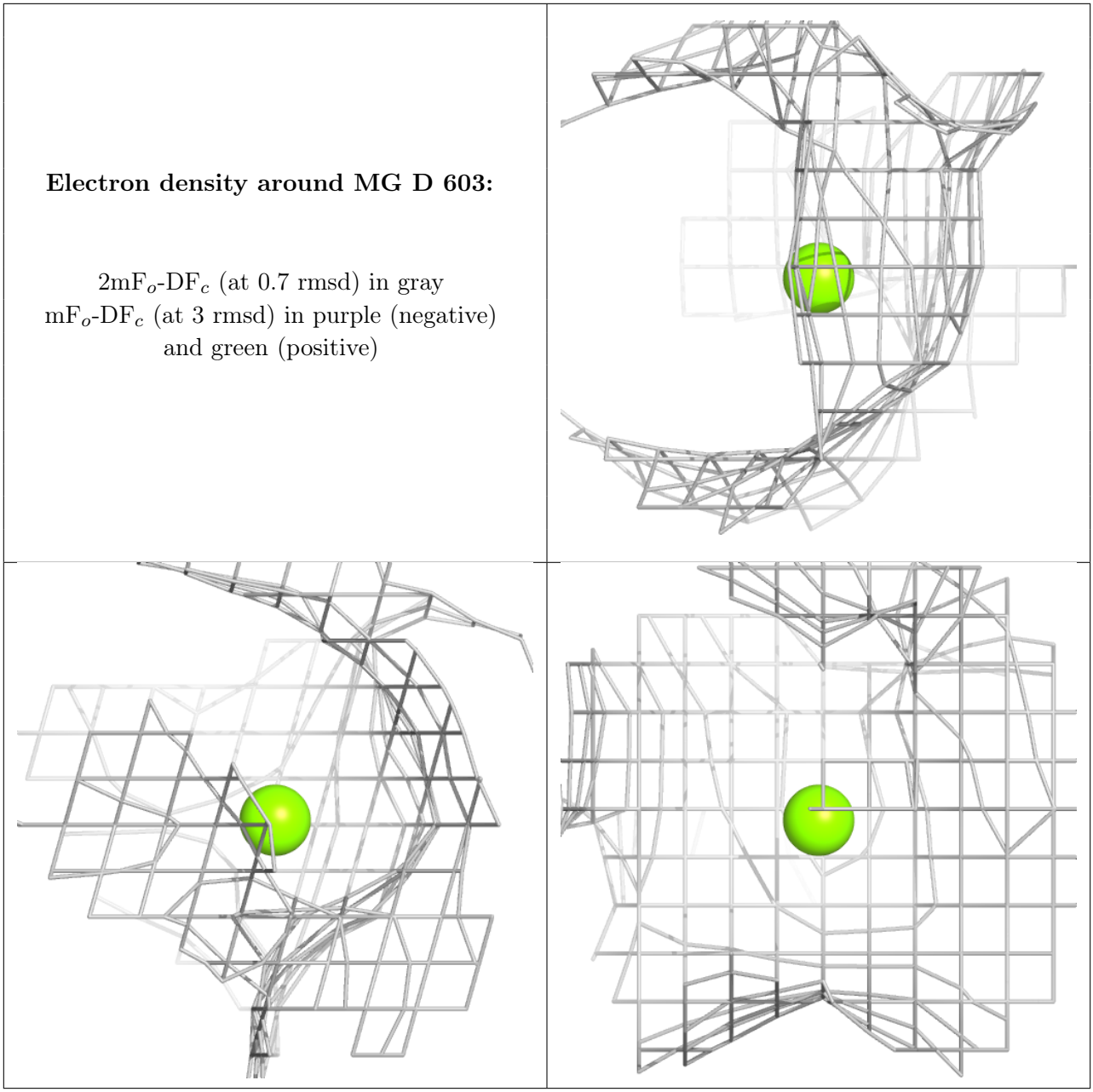






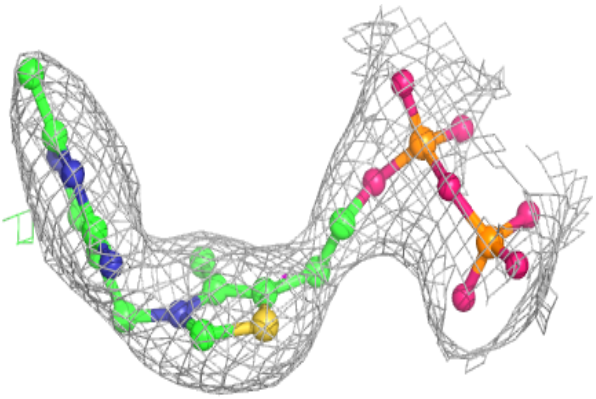
Electron density around MG D 603:

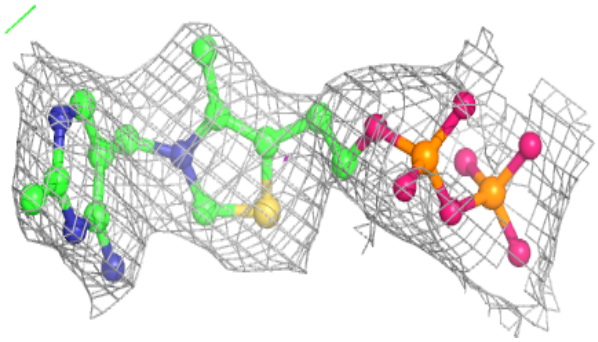
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

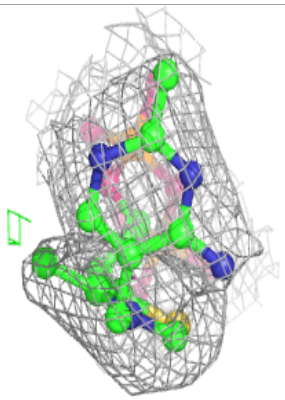


Electron density around TPP D 602:

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

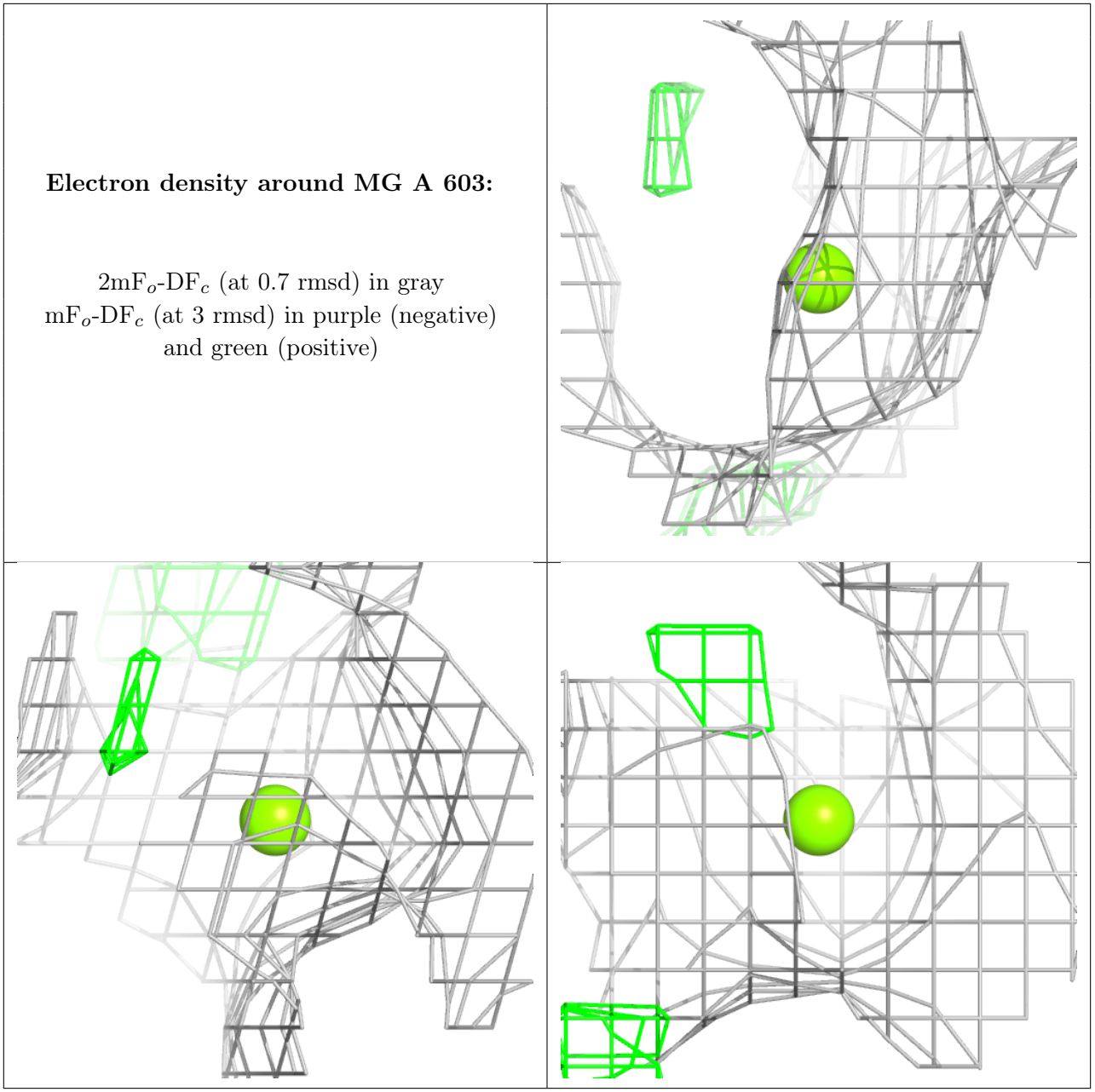






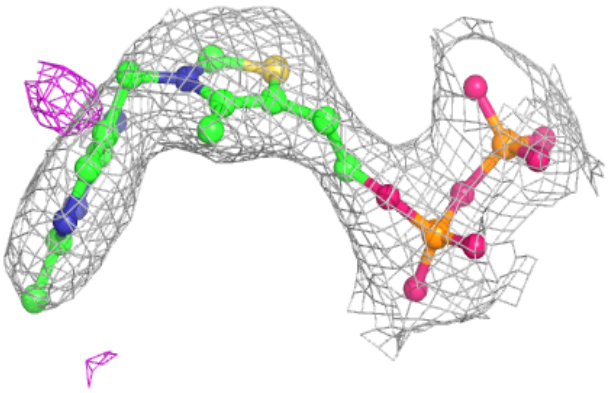
Electron density around MG A 603:

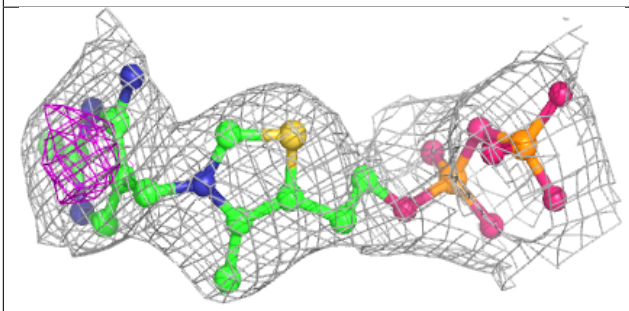
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

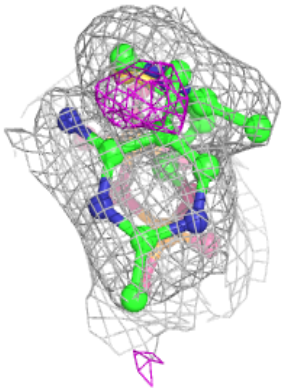


Electron density around TPP B 602:

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

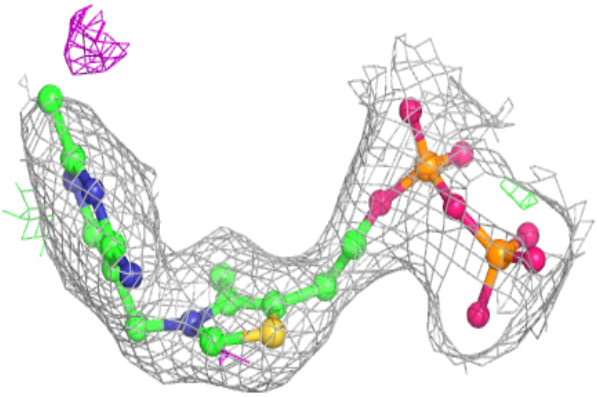


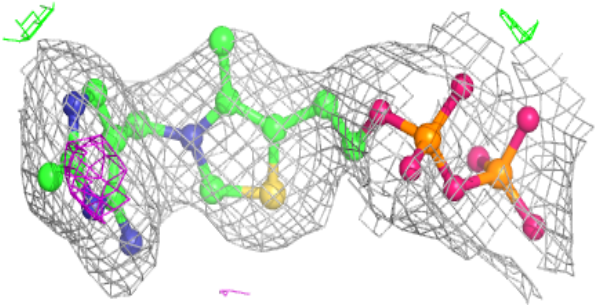


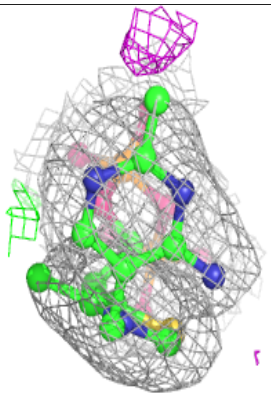


Electron density around TPP A 602:

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

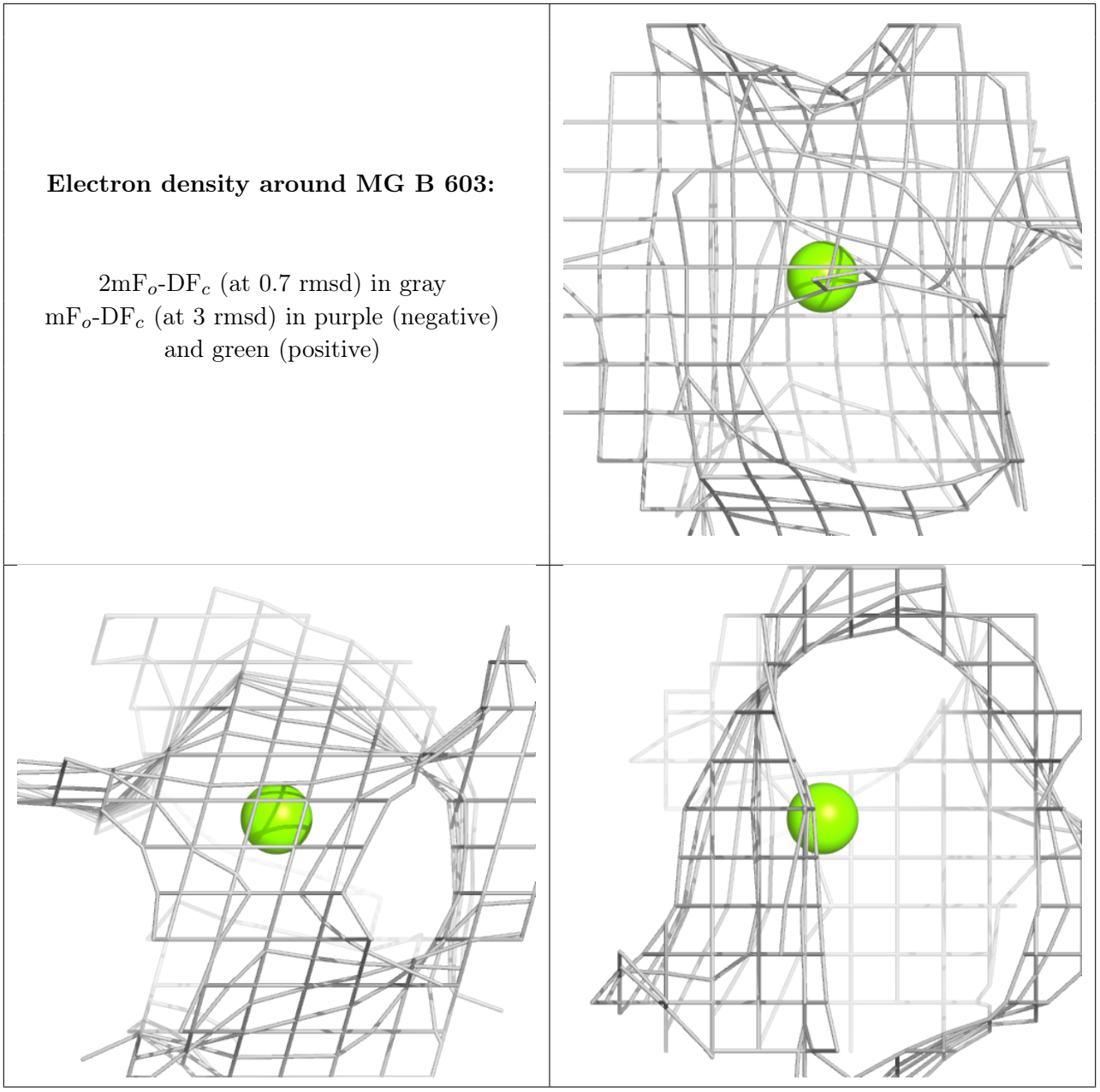






Electron density around MG B 603:

$2mF_o$-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.