Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 07:50 PM EDT

PDB ID	:	1T9D
Title	:	Crystal Structure Of Yeast Acetohydroxyacid Synthase In Complex With A Sulfonylurea Herbicide, Metsulfuron methyl
Authors	:	McCourt, J.A.; Pang, S.S.; Guddat, L.W.; Duggleby, R.G.
Deposited on	:	2004-05-16
Resolution	:	2.30 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:

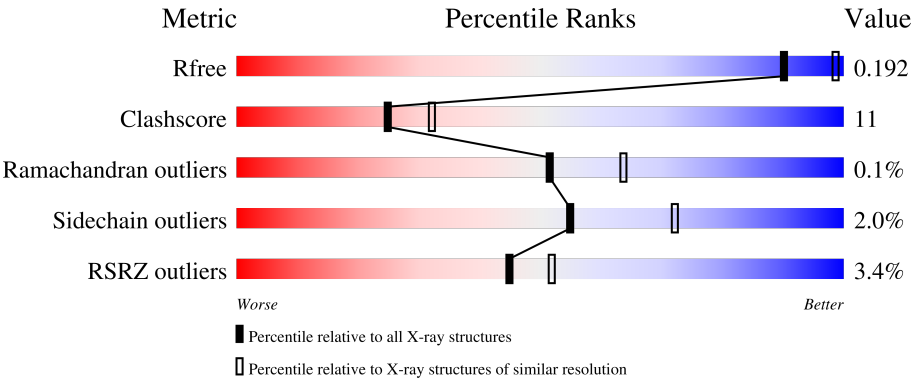
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	677	74% 13% • 12%
1	B	677	% 67% 18% 14%
1	C	677	11% 63% 20% • 15%
1	D	677	74% 14% • 12%

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
4	1MM	A	695	-	X	-	-
4	1MM	B	1695	-	X	-	-
4	1MM	C	2695	-	X	-	-
4	1MM	C	3695	-	X	-	-
6	PYD	A	703	-	X	-	-
6	PYD	B	1703	-	X	-	-
6	PYD	C	2703	-	X	-	-
6	PYD	D	3703	-	X	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 20377 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, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	6	0
			4548	2879	783	865	21			
1	B	582	Total	C	N	O	S	0	3	0
			4392	2788	758	827	19			
1	C	575	Total	C	N	O	S	0	2	0
			4323	2742	746	816	19			
1	D	596	Total	C	N	O	S	0	5	0
			4528	2867	781	860	20			

There are 188 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	cloning artifact	UNP P07342
A	12	HIS	-	cloning artifact	UNP P07342
A	13	HIS	-	cloning artifact	UNP P07342
A	14	HIS	-	cloning artifact	UNP P07342
A	15	HIS	-	cloning artifact	UNP P07342
A	16	HIS	-	cloning artifact	UNP P07342
A	17	HIS	-	cloning artifact	UNP P07342
A	18	SER	-	cloning artifact	UNP P07342
A	19	SER	-	cloning artifact	UNP P07342
A	20	GLY	-	cloning artifact	UNP P07342
A	21	LEU	-	cloning artifact	UNP P07342
A	22	VAL	-	cloning artifact	UNP P07342
A	23	PRO	-	cloning artifact	UNP P07342
A	24	ARG	-	cloning artifact	UNP P07342
A	25	GLY	-	cloning artifact	UNP P07342
A	26	SER	-	cloning artifact	UNP P07342
A	27	GLY	-	cloning artifact	UNP P07342
A	28	MET	-	cloning artifact	UNP P07342
A	29	LYS	-	cloning artifact	UNP P07342
A	30	GLU	-	cloning artifact	UNP P07342
A	31	THR	-	cloning artifact	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ALA	-	cloning artifact	UNP P07342
A	33	ALA	-	cloning artifact	UNP P07342
A	34	ALA	-	cloning artifact	UNP P07342
A	35	LYS	-	cloning artifact	UNP P07342
A	36	PHE	-	cloning artifact	UNP P07342
A	37	GLU	-	cloning artifact	UNP P07342
A	38	ARG	-	cloning artifact	UNP P07342
A	39	GLN	-	cloning artifact	UNP P07342
A	40	HIS	-	cloning artifact	UNP P07342
A	41	MET	-	cloning artifact	UNP P07342
A	42	ASP	-	cloning artifact	UNP P07342
A	43	SER	-	cloning artifact	UNP P07342
A	44	PRO	-	cloning artifact	UNP P07342
A	45	ASP	-	cloning artifact	UNP P07342
A	46	LEU	-	cloning artifact	UNP P07342
A	47	GLY	-	cloning artifact	UNP P07342
A	48	THR	-	cloning artifact	UNP P07342
A	49	ASP	-	cloning artifact	UNP P07342
A	50	ASP	-	cloning artifact	UNP P07342
A	51	ASP	-	cloning artifact	UNP P07342
A	52	ASP	-	cloning artifact	UNP P07342
A	53	LYS	-	cloning artifact	UNP P07342
A	54	ALA	-	cloning artifact	UNP P07342
A	55	MET	-	cloning artifact	UNP P07342
A	56	GLY	-	cloning artifact	UNP P07342
A	57	SER	-	cloning artifact	UNP P07342
B	11	MET	-	cloning artifact	UNP P07342
B	12	HIS	-	cloning artifact	UNP P07342
B	13	HIS	-	cloning artifact	UNP P07342
B	14	HIS	-	cloning artifact	UNP P07342
B	15	HIS	-	cloning artifact	UNP P07342
B	16	HIS	-	cloning artifact	UNP P07342
B	17	HIS	-	cloning artifact	UNP P07342
B	18	SER	-	cloning artifact	UNP P07342
B	19	SER	-	cloning artifact	UNP P07342
B	20	GLY	-	cloning artifact	UNP P07342
B	21	LEU	-	cloning artifact	UNP P07342
B	22	VAL	-	cloning artifact	UNP P07342
B	23	PRO	-	cloning artifact	UNP P07342
B	24	ARG	-	cloning artifact	UNP P07342
B	25	GLY	-	cloning artifact	UNP P07342
B	26	SER	-	cloning artifact	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
B	27	GLY	-	cloning artifact	UNP P07342
B	28	MET	-	cloning artifact	UNP P07342
B	29	LYS	-	cloning artifact	UNP P07342
B	30	GLU	-	cloning artifact	UNP P07342
B	31	THR	-	cloning artifact	UNP P07342
B	32	ALA	-	cloning artifact	UNP P07342
B	33	ALA	-	cloning artifact	UNP P07342
B	34	ALA	-	cloning artifact	UNP P07342
B	35	LYS	-	cloning artifact	UNP P07342
B	36	PHE	-	cloning artifact	UNP P07342
B	37	GLU	-	cloning artifact	UNP P07342
B	38	ARG	-	cloning artifact	UNP P07342
B	39	GLN	-	cloning artifact	UNP P07342
B	40	HIS	-	cloning artifact	UNP P07342
B	41	MET	-	cloning artifact	UNP P07342
B	42	ASP	-	cloning artifact	UNP P07342
B	43	SER	-	cloning artifact	UNP P07342
B	44	PRO	-	cloning artifact	UNP P07342
B	45	ASP	-	cloning artifact	UNP P07342
B	46	LEU	-	cloning artifact	UNP P07342
B	47	GLY	-	cloning artifact	UNP P07342
B	48	THR	-	cloning artifact	UNP P07342
B	49	ASP	-	cloning artifact	UNP P07342
B	50	ASP	-	cloning artifact	UNP P07342
B	51	ASP	-	cloning artifact	UNP P07342
B	52	ASP	-	cloning artifact	UNP P07342
B	53	LYS	-	cloning artifact	UNP P07342
B	54	ALA	-	cloning artifact	UNP P07342
B	55	MET	-	cloning artifact	UNP P07342
B	56	GLY	-	cloning artifact	UNP P07342
B	57	SER	-	cloning artifact	UNP P07342
C	11	MET	-	cloning artifact	UNP P07342
C	12	HIS	-	cloning artifact	UNP P07342
C	13	HIS	-	cloning artifact	UNP P07342
C	14	HIS	-	cloning artifact	UNP P07342
C	15	HIS	-	cloning artifact	UNP P07342
C	16	HIS	-	cloning artifact	UNP P07342
C	17	HIS	-	cloning artifact	UNP P07342
C	18	SER	-	cloning artifact	UNP P07342
C	19	SER	-	cloning artifact	UNP P07342
C	20	GLY	-	cloning artifact	UNP P07342
C	21	LEU	-	cloning artifact	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
C	22	VAL	-	cloning artifact	UNP P07342
C	23	PRO	-	cloning artifact	UNP P07342
C	24	ARG	-	cloning artifact	UNP P07342
C	25	GLY	-	cloning artifact	UNP P07342
C	26	SER	-	cloning artifact	UNP P07342
C	27	GLY	-	cloning artifact	UNP P07342
C	28	MET	-	cloning artifact	UNP P07342
C	29	LYS	-	cloning artifact	UNP P07342
C	30	GLU	-	cloning artifact	UNP P07342
C	31	THR	-	cloning artifact	UNP P07342
C	32	ALA	-	cloning artifact	UNP P07342
C	33	ALA	-	cloning artifact	UNP P07342
C	34	ALA	-	cloning artifact	UNP P07342
C	35	LYS	-	cloning artifact	UNP P07342
C	36	PHE	-	cloning artifact	UNP P07342
C	37	GLU	-	cloning artifact	UNP P07342
C	38	ARG	-	cloning artifact	UNP P07342
C	39	GLN	-	cloning artifact	UNP P07342
C	40	HIS	-	cloning artifact	UNP P07342
C	41	MET	-	cloning artifact	UNP P07342
C	42	ASP	-	cloning artifact	UNP P07342
C	43	SER	-	cloning artifact	UNP P07342
C	44	PRO	-	cloning artifact	UNP P07342
C	45	ASP	-	cloning artifact	UNP P07342
C	46	LEU	-	cloning artifact	UNP P07342
C	47	GLY	-	cloning artifact	UNP P07342
C	48	THR	-	cloning artifact	UNP P07342
C	49	ASP	-	cloning artifact	UNP P07342
C	50	ASP	-	cloning artifact	UNP P07342
C	51	ASP	-	cloning artifact	UNP P07342
C	52	ASP	-	cloning artifact	UNP P07342
C	53	LYS	-	cloning artifact	UNP P07342
C	54	ALA	-	cloning artifact	UNP P07342
C	55	MET	-	cloning artifact	UNP P07342
C	56	GLY	-	cloning artifact	UNP P07342
C	57	SER	-	cloning artifact	UNP P07342
D	11	MET	-	cloning artifact	UNP P07342
D	12	HIS	-	cloning artifact	UNP P07342
D	13	HIS	-	cloning artifact	UNP P07342
D	14	HIS	-	cloning artifact	UNP P07342
D	15	HIS	-	cloning artifact	UNP P07342
D	16	HIS	-	cloning artifact	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
D	17	HIS	-	cloning artifact	UNP P07342
D	18	SER	-	cloning artifact	UNP P07342
D	19	SER	-	cloning artifact	UNP P07342
D	20	GLY	-	cloning artifact	UNP P07342
D	21	LEU	-	cloning artifact	UNP P07342
D	22	VAL	-	cloning artifact	UNP P07342
D	23	PRO	-	cloning artifact	UNP P07342
D	24	ARG	-	cloning artifact	UNP P07342
D	25	GLY	-	cloning artifact	UNP P07342
D	26	SER	-	cloning artifact	UNP P07342
D	27	GLY	-	cloning artifact	UNP P07342
D	28	MET	-	cloning artifact	UNP P07342
D	29	LYS	-	cloning artifact	UNP P07342
D	30	GLU	-	cloning artifact	UNP P07342
D	31	THR	-	cloning artifact	UNP P07342
D	32	ALA	-	cloning artifact	UNP P07342
D	33	ALA	-	cloning artifact	UNP P07342
D	34	ALA	-	cloning artifact	UNP P07342
D	35	LYS	-	cloning artifact	UNP P07342
D	36	PHE	-	cloning artifact	UNP P07342
D	37	GLU	-	cloning artifact	UNP P07342
D	38	ARG	-	cloning artifact	UNP P07342
D	39	GLN	-	cloning artifact	UNP P07342
D	40	HIS	-	cloning artifact	UNP P07342
D	41	MET	-	cloning artifact	UNP P07342
D	42	ASP	-	cloning artifact	UNP P07342
D	43	SER	-	cloning artifact	UNP P07342
D	44	PRO	-	cloning artifact	UNP P07342
D	45	ASP	-	cloning artifact	UNP P07342
D	46	LEU	-	cloning artifact	UNP P07342
D	47	GLY	-	cloning artifact	UNP P07342
D	48	THR	-	cloning artifact	UNP P07342
D	49	ASP	-	cloning artifact	UNP P07342
D	50	ASP	-	cloning artifact	UNP P07342
D	51	ASP	-	cloning artifact	UNP P07342
D	52	ASP	-	cloning artifact	UNP P07342
D	53	LYS	-	cloning artifact	UNP P07342
D	54	ALA	-	cloning artifact	UNP P07342
D	55	MET	-	cloning artifact	UNP P07342
D	56	GLY	-	cloning artifact	UNP P07342
D	57	SER	-	cloning artifact	UNP P07342

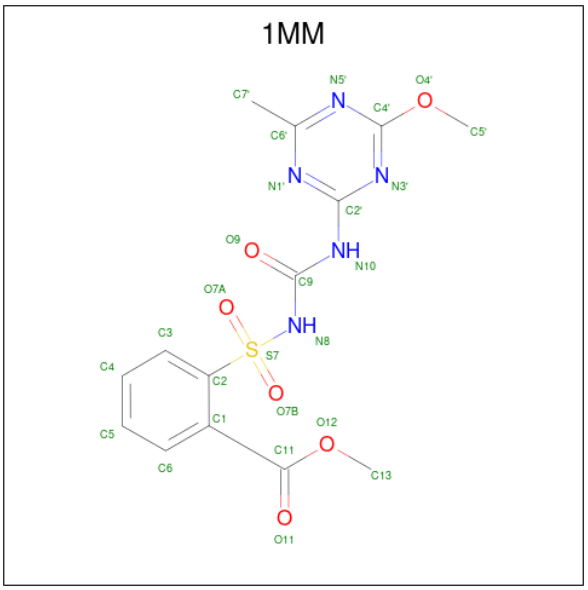
- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is METHYL 2-[({[(4-METHOXY-6-METHYL-1,3,5-TRIAZIN-2-YL)AMINO]CARBONYL}AMINO)SULFONYL]BENZOATE (three-letter code: 1MM) (formula: $C_{14}H_{15}N_5O_6S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 26 14 5 6 1	0	0

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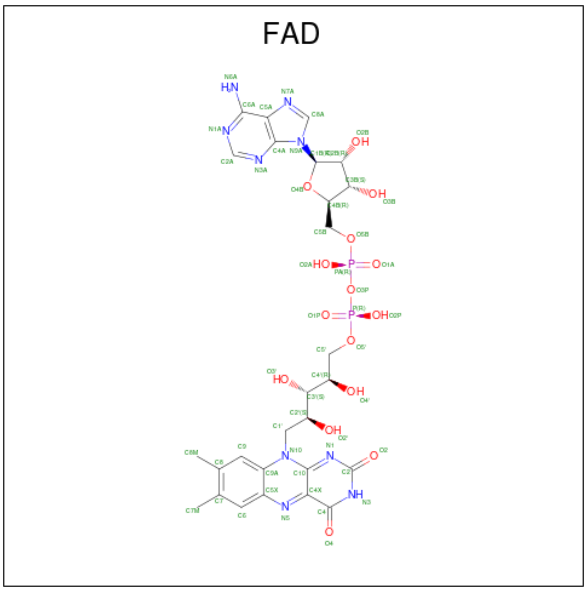
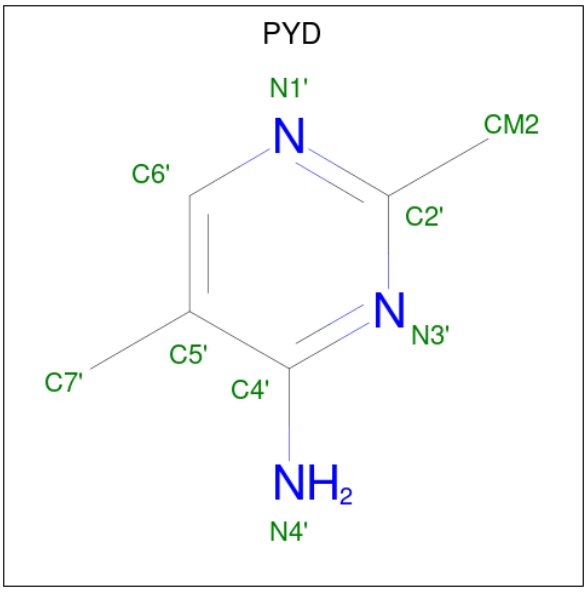
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			26	14	5	6	1		
4	C	1	Total	C	N	O	S	0	0
			26	14	5	6	1		
4	C	1	Total	C	N	O	S	0	0
			26	14	5	6	1		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



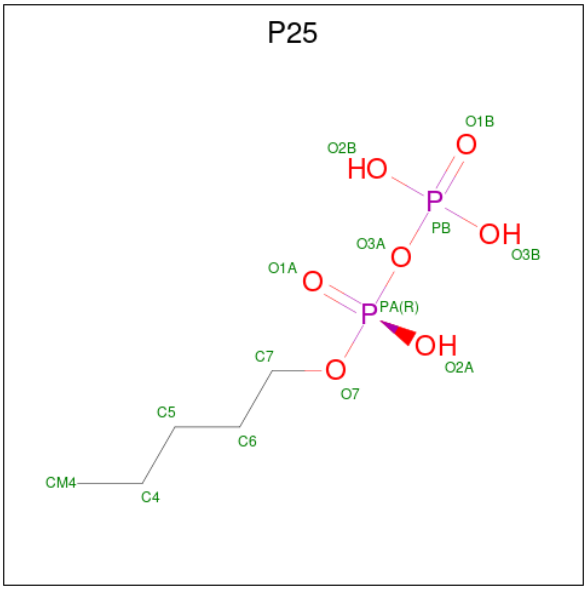
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is 2,5-DIMETHYL-PYRIMIDIN-4-YLAMINE (three-letter code: PYD) (formula: $C_6H_9N_3$).



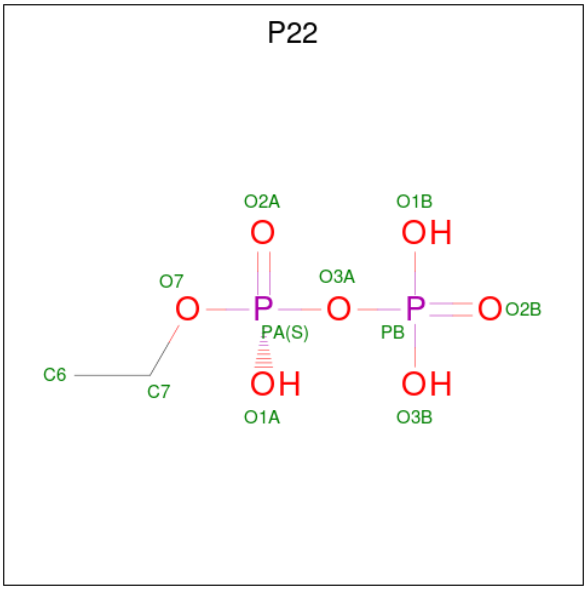
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N 9 6 3	0	0
6	B	1	Total C N 9 6 3	0	0
6	C	1	Total C N 9 6 3	0	0
6	D	1	Total C N 9 6 3	0	0

- Molecule 7 is PENTYL TRIHYDROGEN DIPHOSPHATE (three-letter code: P25) (formula: $C_5H_{14}O_7P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O P 14 5 7 2	0	0
7	B	1	Total C O P 14 5 7 2	0	0

- Molecule 8 is ETHYL DIHYDROGEN DIPHOSPHATE (three-letter code: P22) (formula: $C_2H_8O_7P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C O P 11 2 7 2	0	0
8	D	1	Total C O P 11 2 7 2	0	0

- Molecule 9 is water.

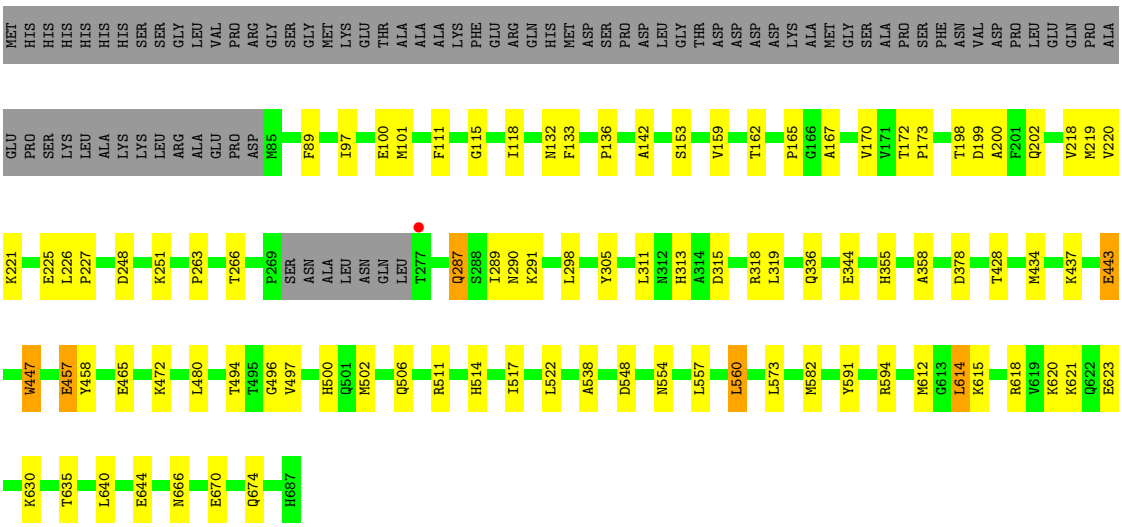
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	671	Total O 671 671	1	0
9	B	468	Total O 468 468	0	0
9	C	400	Total O 400 400	0	0
9	D	637	Total O 637 637	0	0

3 Residue-property plots (i)

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

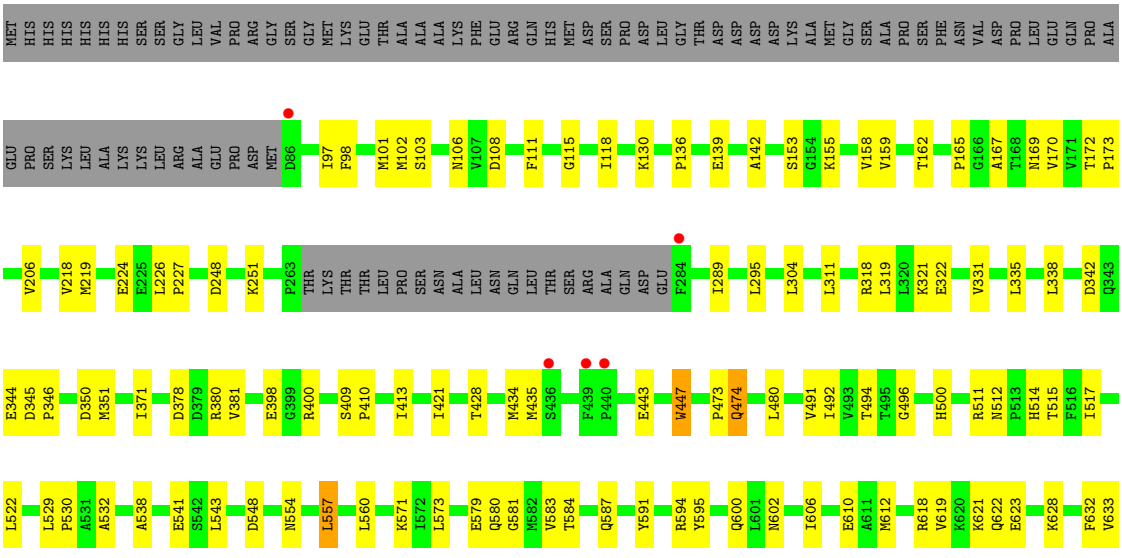
• Molecule 1: Acetolactate synthase, mitochondrial

Chain A:



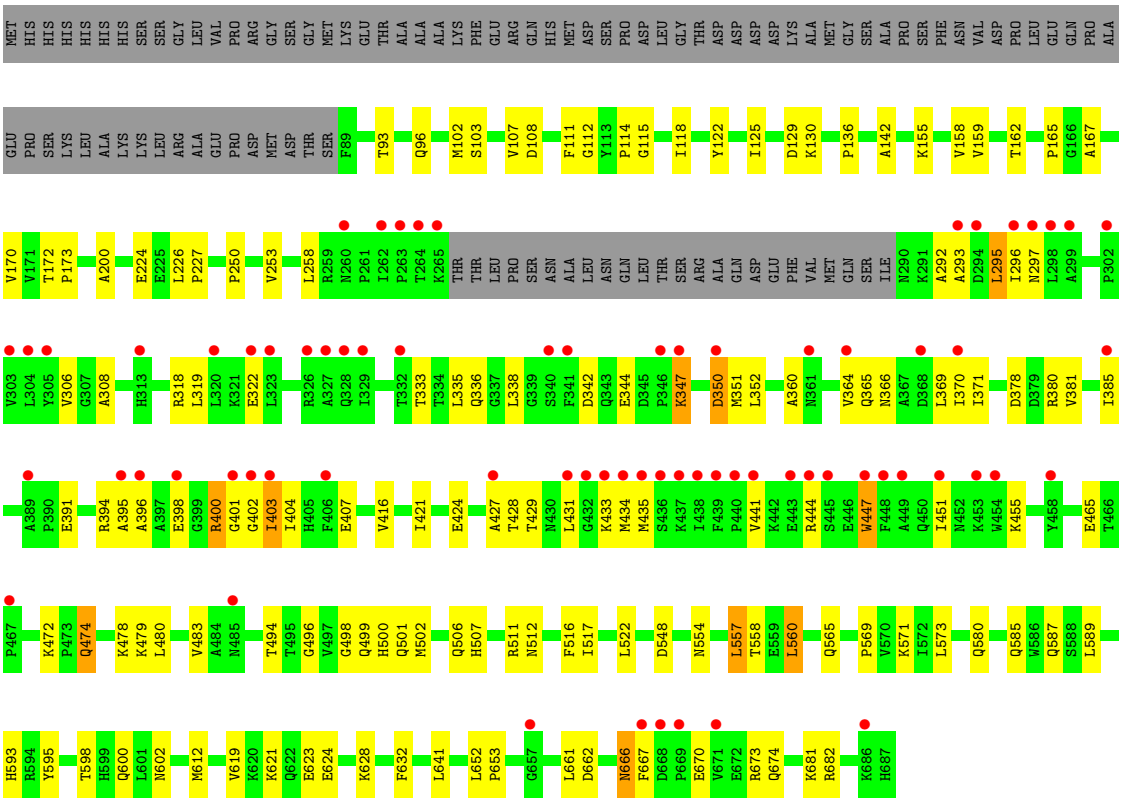
• Molecule 1: Acetolactate synthase, mitochondrial

Chain B:



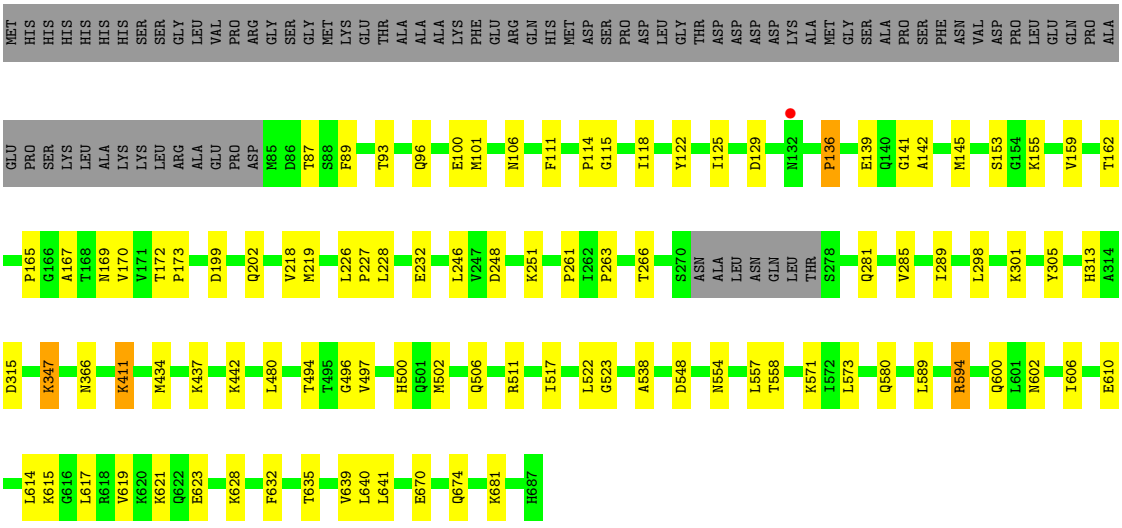
• Molecule 1: Acetolactate synthase, mitochondrial

Chain C:



• Molecule 1: Acetolactate synthase, mitochondrial

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	218.35Å 218.35Å 361.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 94.27 – 2.30	Depositor EDS
% Data completeness (in resolution range)	80.1 (50.00-2.30) 79.9 (94.27-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.73 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.164 , 0.195 0.162 , 0.192	Depositor DCC
R_{free} test set	15994 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å^2)	28.5	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 62.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20377	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: PYD, P25, MG, P22, 1MM, FAD, K

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	0.32	0/4666	0.59	0/6332
1	B	0.29	0/4497	0.55	0/6111
1	C	0.27	0/4423	0.53	0/6014
1	D	0.31	0/4642	0.58	0/6301
All	All	0.30	0/18228	0.56	0/24758

There are no bond length outliers.

There are no bond angle outliers.

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	4548	0	4521	77	0
1	B	4392	0	4352	106	0
1	C	4323	0	4263	135	0
1	D	4528	0	4494	83	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	26	0	15	2	0
4	B	26	0	15	5	0
4	C	52	0	30	4	0
5	A	53	0	31	1	0
5	B	53	0	31	1	0
5	C	53	0	31	1	0
5	D	53	0	31	1	0
6	A	9	0	9	0	0
6	B	9	0	9	0	0
6	C	9	0	9	0	0
6	D	9	0	9	0	0
7	A	14	0	11	2	0
7	B	14	0	11	1	0
8	C	11	0	5	0	0
8	D	11	0	5	1	0
9	A	671	0	0	9	0
9	B	468	0	0	12	0
9	C	400	0	0	18	0
9	D	637	0	0	12	0
All	All	20377	0	17882	389	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 11.

All (389) 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:D:594[A]:ARG:HG3	1:D:594[A]:ARG:HH11	1.16	1.04
1:C:114:PRO:HG2	1:D:580:GLN:HE22	1.25	1.00
1:A:313:HIS:HD2	1:A:315:ASP:H	1.19	0.91
1:C:619:VAL:HG22	1:C:628:LYS:HG3	1.54	0.89
1:B:580:GLN:HG3	7:B:698:P25:H72	1.54	0.87
1:D:313:HIS:HD2	1:D:315:ASP:H	1.21	0.86
1:B:335:LEU:HD12	1:B:351:MET:HE1	1.58	0.84
1:B:619:VAL:HG22	1:B:628:LYS:HG3	1.60	0.82
1:B:103:SER:HB2	1:B:130:LYS:HD3	1.59	0.82
1:D:155:LYS:HE2	9:D:5257:HOH:O	1.78	0.82
1:C:114:PRO:HG2	1:D:580:GLN:NE2	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:580:GLN:HE22	1:D:114:PRO:HG2	1.46	0.79
1:C:370:ILE:HB	1:C:403:ILE:CG2	2.13	0.79
1:B:579:GLU:OE1	1:B:584[A]:THR:HG21	1.83	0.79
1:C:441:VAL:HG11	1:C:444:ARG:HD3	1.66	0.76
1:A:318:ARG:HD3	9:A:6062:HOH:O	1.86	0.76
1:C:398:GLU:HB2	1:C:400:ARG:HG2	1.68	0.75
1:D:594[A]:ARG:HG3	1:D:594[A]:ARG:NH1	1.93	0.75
1:C:385:ILE:HD13	1:C:416:VAL:HG12	1.68	0.75
1:D:411:LYS:NZ	1:D:411:LYS:HB3	2.02	0.75
1:B:289:ILE:HG23	1:B:434:MET:HB3	1.67	0.75
1:B:581:GLY:O	1:B:584[A]:THR:HG22	1.85	0.75
1:C:335:LEU:HA	1:C:351:MET:HE2	1.68	0.74
1:C:474:GLN:H	1:C:474:GLN:HE21	1.36	0.73
1:C:344:GLU:HG3	1:C:511:ARG:CZ	2.19	0.73
1:B:591:TYR:O	1:B:594:ARG:HG3	1.90	0.72
1:A:263:PRO:HB2	1:A:266:THR:HG23	1.72	0.71
1:B:619:VAL:HG23	1:B:641:LEU:HD11	1.71	0.70
1:C:587:GLN:NE2	1:C:595:TYR:HA	2.06	0.70
1:C:394:ARG:HD2	1:C:400:ARG:HH12	1.57	0.69
1:C:366:ASN:HA	1:C:391:GLU:HG3	1.75	0.68
1:A:378:ASP:HB2	9:A:4126:HOH:O	1.93	0.68
1:A:221:LYS:HE2	9:A:5512:HOH:O	1.93	0.67
1:A:594[A]:ARG:HG3	1:A:594[A]:ARG:HH11	1.58	0.67
1:D:619:VAL:HG22	1:D:628:LYS:HG3	1.77	0.67
1:B:474:GLN:H	1:B:474:GLN:HE21	1.43	0.67
1:C:560:LEU:HD23	1:C:612:MET:HG3	1.77	0.66
1:C:102:MET:HE2	1:C:158:VAL:HG11	1.77	0.66
1:A:355:HIS:HB2	1:A:502:MET:HE2	1.76	0.66
1:B:600:GLN:CD	1:B:600:GLN:H	1.98	0.66
1:C:352:LEU:HD23	1:C:352:LEU:H	1.60	0.66
1:C:370:ILE:HB	1:C:403:ILE:HG22	1.77	0.66
1:A:621:LYS:HB3	1:A:623:GLU:OE2	1.95	0.66
1:B:491:VAL:HA	9:B:5714:HOH:O	1.96	0.66
1:C:474:GLN:H	1:C:474:GLN:NE2	1.93	0.66
1:B:338:LEU:HD11	1:B:351:MET:HE3	1.76	0.65
1:C:335:LEU:HD12	1:C:351:MET:HE1	1.79	0.65
1:C:371:ILE:N	1:C:371:ILE:HD12	2.12	0.64
1:A:511:ARG:NH2	1:D:511:ARG:HH21	1.95	0.64
1:B:560:LEU:HD23	1:B:612:MET:HG3	1.80	0.64
1:C:102:MET:CE	1:C:158:VAL:HG11	2.28	0.64
1:A:251:LYS:HE2	9:B:5931:HOH:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:PRO:HG3	1:C:142:ALA:HB2	1.81	0.63
1:C:580:GLN:HE22	1:D:114:PRO:CG	2.12	0.63
1:B:338:LEU:HD11	1:B:351:MET:CE	2.28	0.63
1:C:451:ILE:HG22	1:C:455:LYS:HE2	1.80	0.63
1:C:554:ASN:HA	1:C:557[A]:LEU:HD12	1.79	0.63
1:D:411:LYS:HB3	1:D:411:LYS:HZ3	1.62	0.63
1:A:251:LYS:NZ	4:B:1695:1MM:HN8	1.97	0.63
1:B:102:MET:HE2	1:B:158:VAL:HG11	1.80	0.62
1:B:496:GLY:H	1:B:500:HIS:HE1	1.48	0.62
1:C:292:ALA:HB2	1:C:421:ILE:HG21	1.80	0.62
1:A:496:GLY:H	1:A:500:HIS:HE1	1.48	0.62
1:A:511:ARG:NH2	1:D:511:ARG:NH2	2.47	0.62
1:B:304:LEU:HD23	1:B:371:ILE:HB	1.82	0.62
1:B:666:ASN:ND2	1:B:667:PHE:H	1.98	0.62
1:C:499:GLN:HE21	1:C:585:GLN:HE21	1.47	0.62
1:B:474:GLN:H	1:B:474:GLN:NE2	1.97	0.61
1:D:172:THR:HB	1:D:173:PRO:HD3	1.82	0.61
1:C:396:ALA:HB2	1:C:402:GLY:HA2	1.82	0.61
1:C:600:GLN:H	1:C:600:GLN:CD	2.04	0.61
1:D:594[A]:ARG:HD3	9:D:4998:HOH:O	1.99	0.61
1:A:313:HIS:CD2	1:A:315:ASP:H	2.11	0.61
1:B:102:MET:CE	1:B:158:VAL:HG11	2.29	0.61
1:C:522:LEU:HG	1:D:165:PRO:HD3	1.83	0.61
1:B:492:ILE:N	9:B:5714:HOH:O	2.29	0.61
1:C:370:ILE:HB	1:C:403:ILE:HG23	1.82	0.61
1:C:499:GLN:HE21	1:C:585:GLN:NE2	1.99	0.61
1:A:594[A]:ARG:HG3	1:A:594[A]:ARG:NH1	2.16	0.61
1:B:136:PRO:HG3	1:B:142:ALA:HB2	1.82	0.61
1:B:335:LEU:HA	1:B:351:MET:HE2	1.82	0.61
1:A:172:THR:HB	1:A:173:PRO:HD3	1.83	0.60
1:B:600:GLN:H	1:B:600:GLN:NE2	1.99	0.60
1:C:347:LYS:HB2	1:C:347:LYS:NZ	2.15	0.60
1:C:347:LYS:NZ	9:C:5476:HOH:O	2.33	0.60
1:C:293:ALA:HB2	1:C:434:MET:HG3	1.83	0.60
1:A:136:PRO:HG3	1:A:142:ALA:HB2	1.84	0.59
1:C:666:ASN:ND2	1:C:667:PHE:H	2.00	0.59
1:C:385:ILE:HB	9:C:5765:HOH:O	2.01	0.59
1:C:360:ALA:O	1:C:364:VAL:HG23	2.02	0.58
1:D:621:LYS:HD2	9:D:5367:HOH:O	2.04	0.58
1:A:219:MET:HG3	1:A:248:ASP:HB3	1.84	0.58
1:A:226:LEU:HB3	1:A:227:PRO:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:619:VAL:HG23	1:C:641:LEU:HD11	1.85	0.58
1:C:512:ASN:HB2	9:C:5769:HOH:O	2.02	0.58
1:C:496:GLY:H	1:C:500:HIS:HE1	1.49	0.58
1:A:457:GLU:HG2	1:A:458:TYR:CE1	2.38	0.58
1:B:554:ASN:HA	1:B:557:LEU:HD13	1.86	0.57
1:A:355:HIS:HB2	1:A:502:MET:CE	2.34	0.57
1:C:435:MET:HG2	9:C:5209:HOH:O	2.04	0.57
1:D:289:ILE:HG23	1:D:434:MET:HB2	1.84	0.57
1:C:480:LEU:HD22	1:C:573:LEU:HD22	1.86	0.57
1:B:172:THR:HB	1:B:173:PRO:HD3	1.87	0.57
1:C:226:LEU:HB3	1:C:227:PRO:HD3	1.85	0.57
1:A:443:GLU:HG2	9:A:5554:HOH:O	2.05	0.56
1:C:580:GLN:NE2	9:C:4765:HOH:O	2.37	0.56
1:B:623:GLU:CD	1:B:623:GLU:H	2.09	0.56
1:C:557[A]:LEU:HD11	1:D:558:THR:OG1	2.06	0.56
1:A:251:LYS:HZ2	4:B:1695:1MM:HN8	1.53	0.56
1:B:670:GLU:O	1:B:674:GLN:HG3	2.06	0.56
1:D:670:GLU:O	1:D:674:GLN:HG3	2.06	0.56
1:D:496:GLY:H	1:D:500:HIS:HE1	1.53	0.56
1:A:522:LEU:HG	1:B:165:PRO:HD3	1.87	0.56
1:A:132[B]:ASN:HD22	1:A:133:PHE:N	2.04	0.56
1:C:522:LEU:O	1:D:202:GLN:HG2	2.06	0.56
1:C:347:LYS:HE2	9:C:5476:HOH:O	2.06	0.55
1:C:335:LEU:HA	1:C:351:MET:CE	2.35	0.55
4:C:3695:1MM:O7B	1:D:251:LYS:HD3	2.06	0.55
1:C:224:GLU:HG3	1:C:258:LEU:CD1	2.37	0.55
1:C:512:ASN:N	1:C:512:ASN:HD22	2.03	0.55
1:C:682:ARG:NH2	9:C:5797:HOH:O	2.38	0.55
1:D:594[B]:ARG:HD3	9:D:4998:HOH:O	2.06	0.55
1:C:429:THR:HG22	1:C:433:LYS:HE3	1.87	0.55
1:D:313:HIS:CD2	1:D:315:ASP:H	2.11	0.55
1:D:615:LYS:HE2	1:D:635:THR:HG21	1.88	0.55
1:C:557[B]:LEU:HD23	1:C:558:THR:N	2.22	0.55
9:A:4096:HOH:O	1:B:600:GLN:HB3	2.06	0.55
1:B:410:PRO:HA	1:B:413:ILE:HD12	1.89	0.55
1:C:394:ARG:CD	1:C:400:ARG:HH12	2.20	0.55
1:D:89:PHE:CE1	1:D:100[A]:GLU:HG2	2.42	0.54
4:C:2695:1MM:H5'2	5:D:3701:FAD:HM72	1.89	0.54
1:A:251:LYS:HD3	4:B:1695:1MM:O7B	2.07	0.54
1:C:565:GLN:HE22	1:D:600:GLN:HA	1.71	0.54
1:A:511:ARG:HH21	1:D:511:ARG:NH2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:571:LYS:HB3	1:D:632:PHE:CZ	2.43	0.54
1:B:638:PRO:HD3	9:B:4328:HOH:O	2.07	0.54
1:C:554:ASN:HD21	1:C:602:ASN:ND2	2.05	0.53
1:B:335:LEU:HA	1:B:351:MET:CE	2.38	0.53
1:C:494:THR:HA	1:C:517:ILE:O	2.08	0.53
1:B:640:LEU:C	1:B:640:LEU:HD23	2.29	0.53
1:A:89:PHE:CE2	1:A:100[A]:GLU:HG2	2.44	0.53
1:B:681:LYS:HB2	1:B:681:LYS:NZ	2.24	0.53
1:D:226:LEU:HB3	1:D:227:PRO:HD3	1.89	0.53
1:C:624:GLU:HA	9:C:6033:HOH:O	2.07	0.53
1:C:108:ASP:HB3	9:C:5011:HOH:O	2.09	0.53
1:D:96:GLN:O	1:D:100[B]:GLU:HG2	2.09	0.52
1:B:554:ASN:HD21	1:B:602:ASN:ND2	2.07	0.52
1:C:103:SER:HB2	1:C:130:LYS:HD3	1.91	0.52
1:B:167:ALA:O	1:B:170:VAL:HG22	2.10	0.52
1:C:167:ALA:O	1:C:170:VAL:HG22	2.09	0.52
1:C:172:THR:HB	1:C:173:PRO:HD3	1.91	0.52
1:D:494:THR:HA	1:D:517:ILE:O	2.09	0.52
1:A:344:GLU:HG3	9:A:6037:HOH:O	2.10	0.52
1:B:606:ILE:HD13	1:B:618:ARG:NH2	2.25	0.52
1:C:600:GLN:H	1:C:600:GLN:NE2	2.07	0.52
1:D:115:GLY:HA3	1:D:162:THR:HB	1.91	0.52
1:A:640:LEU:C	1:A:640:LEU:HD23	2.30	0.51
1:B:304:LEU:HB2	1:B:331:VAL:HG22	1.92	0.51
1:C:118:ILE:HG13	1:C:118:ILE:O	2.10	0.51
1:C:600:GLN:HB3	9:D:5772:HOH:O	2.10	0.51
1:B:335:LEU:CD1	1:B:351:MET:HE1	2.36	0.51
1:D:619:VAL:HG23	1:D:641:LEU:HD11	1.92	0.51
1:D:199:ASP:HA	9:D:6150:HOH:O	2.11	0.51
4:A:695:1MM:H5'2	5:A:701:FAD:HM72	1.92	0.51
1:C:335:LEU:CD1	1:C:351:MET:HE1	2.40	0.51
1:A:497:VAL:O	7:A:1698:P25:H62	2.10	0.51
1:B:295:LEU:HD12	1:B:421:ILE:HD12	1.93	0.51
1:C:306:VAL:HB	1:C:333:THR:HG22	1.92	0.51
1:C:347:LYS:CE	9:C:5476:HOH:O	2.59	0.50
1:A:591:TYR:O	1:A:594[A]:ARG:HG3	2.11	0.50
1:D:480:LEU:HD22	1:D:573:LEU:HD22	1.92	0.50
4:A:695:1MM:O7B	1:B:251:LYS:HD3	2.12	0.50
1:C:338:LEU:HD11	1:C:351:MET:CE	2.42	0.50
1:B:584[B]:THR:HG21	1:B:648:LYS:HD3	1.94	0.50
1:D:136:PRO:HG3	1:D:142:ALA:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:PRO:HB2	1:D:266:THR:HG23	1.94	0.50
1:A:582:MET:HG2	7:A:1698:P25:HM43	1.94	0.50
1:B:170:VAL:C	1:B:173:PRO:HD2	2.32	0.50
1:B:496:GLY:N	1:B:500:HIS:HE1	2.07	0.50
1:C:381:VAL:O	1:C:661:LEU:HD21	2.12	0.50
1:D:93:THR:H	1:D:96:GLN:HE21	1.59	0.50
1:B:606:ILE:O	1:B:610:GLU:HG3	2.12	0.49
4:B:1695:1MM:H5'2	5:B:1701:FAD:HM72	1.94	0.49
1:A:480:LEU:HD22	1:A:573:LEU:HD22	1.94	0.49
1:D:141:GLY:O	1:D:145:MET:HG3	2.12	0.49
1:B:584[A]:THR:HG23	9:B:4460:HOH:O	2.11	0.49
1:A:319:LEU:HD12	1:A:428:THR:HG23	1.95	0.49
1:B:322:GLU:OE2	1:B:435:MET:HG2	2.12	0.49
9:A:4937:HOH:O	1:D:347:LYS:HD3	2.12	0.49
1:C:111:PHE:O	1:C:159:VAL:HA	2.12	0.49
1:D:101:MET:HA	1:D:101:MET:CE	2.42	0.49
1:B:344:GLU:HG3	1:B:511:ARG:CZ	2.43	0.49
1:C:338:LEU:HD11	1:C:351:MET:HE3	1.94	0.49
1:D:442:LYS:HE2	9:D:4193:HOH:O	2.13	0.49
1:B:342:ASP:OD2	1:B:344:GLU:HB2	2.13	0.49
1:B:512:ASN:HB2	1:B:515:THR:HG21	1.95	0.49
1:A:591:TYR:O	1:A:594[B]:ARG:HG3	2.13	0.49
1:B:118:ILE:HG13	1:B:118:ILE:O	2.13	0.49
1:B:622:GLN:HG3	9:B:5959:HOH:O	2.13	0.48
1:C:496:GLY:N	1:C:500:HIS:HE1	2.11	0.48
1:B:218:VAL:HG22	1:B:219:MET:N	2.29	0.48
1:B:494:THR:HA	1:B:517:ILE:O	2.12	0.48
1:C:122:TYR:HA	1:C:125:ILE:HG12	1.95	0.48
1:D:87:THR:HG22	1:D:261:PRO:HG3	1.96	0.48
1:B:111:PHE:O	1:B:159:VAL:HA	2.13	0.48
1:B:226:LEU:HB3	1:B:227:PRO:HD3	1.96	0.48
1:B:289:ILE:CG2	1:B:434:MET:HB3	2.39	0.48
1:C:580:GLN:HE21	1:C:598:THR:HA	1.79	0.48
5:C:2701:FAD:HM72	4:C:3695:1MM:H5'2	1.95	0.48
1:D:170:VAL:C	1:D:173:PRO:HD2	2.34	0.48
1:A:319:LEU:HD12	1:A:428:THR:CG2	2.43	0.48
1:C:170:VAL:C	1:C:173:PRO:HD2	2.34	0.48
1:D:502:MET:O	1:D:506:GLN:HG3	2.13	0.48
1:C:593:HIS:ND1	1:C:682:ARG:NH1	2.62	0.48
1:B:587:GLN:NE2	1:B:595:TYR:HA	2.29	0.47
1:C:465:GLU:HG3	1:C:472:LYS:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:554:ASN:HD21	1:D:602:ASN:ND2	2.11	0.47
1:D:580:GLN:NE2	9:D:4830:HOH:O	2.44	0.47
1:C:250:PRO:HB2	1:C:253:VAL:HG23	1.97	0.47
1:A:170:VAL:C	1:A:173:PRO:HD2	2.34	0.47
1:B:571:LYS:HB3	1:B:632:PHE:CZ	2.49	0.47
1:B:606:ILE:HD13	1:B:618:ARG:CZ	2.45	0.47
1:C:396:ALA:HB2	1:C:402:GLY:CA	2.44	0.47
1:B:98:PHE:O	1:B:102:MET:HG2	2.13	0.47
1:A:494:THR:HA	1:A:517:ILE:O	2.14	0.47
1:B:581:GLY:HA2	1:B:584[A]:THR:HG22	1.96	0.47
1:D:167:ALA:O	1:D:170:VAL:HG22	2.14	0.47
1:A:594[A]:ARG:HD3	9:A:4406:HOH:O	2.14	0.47
1:C:378:ASP:OD2	1:C:380:ARG:HB2	2.15	0.47
1:B:557:LEU:C	1:B:557:LEU:HD23	2.35	0.46
1:D:218:VAL:HG22	1:D:219:MET:N	2.30	0.46
1:C:557[B]:LEU:CD2	1:D:558:THR:HB	2.45	0.46
1:C:673:ARG:C	1:C:673:ARG:HD2	2.36	0.46
1:B:219:MET:HA	1:B:248:ASP:HB3	1.98	0.46
1:C:297:ASN:HA	9:C:5207:HOH:O	2.16	0.46
1:C:395:ALA:HB1	1:C:401:GLY:HA3	1.98	0.46
1:C:571:LYS:HB3	1:C:632:PHE:CZ	2.50	0.46
1:C:112:GLY:O	1:C:136:PRO:HD2	2.16	0.46
1:B:543:LEU:HG	1:B:543:LEU:O	2.16	0.46
1:A:200:ALA:HB1	4:B:1695:1MM:H5	1.97	0.46
1:C:103:SER:HA	9:C:5182:HOH:O	2.16	0.46
1:C:308:ALA:HB2	1:C:336:GLN:HB3	1.98	0.46
1:C:512:ASN:N	1:C:512:ASN:ND2	2.64	0.46
1:A:289:ILE:HG23	1:A:434:MET:HB2	1.98	0.46
1:B:344:GLU:HG3	1:B:511:ARG:NE	2.31	0.46
1:C:295:LEU:HD13	1:C:295:LEU:O	2.16	0.46
1:C:338:LEU:HD12	1:C:516:PHE:CE2	2.51	0.46
1:B:447:TRP:HA	1:B:447:TRP:CE3	2.51	0.45
1:C:569:PRO:HD2	9:C:5452:HOH:O	2.16	0.45
1:B:378:ASP:OD2	1:B:380:ARG:HB2	2.17	0.45
1:B:409:SER:HB3	9:B:4265:HOH:O	2.16	0.45
1:D:122:TYR:HA	1:D:125:ILE:HG12	1.96	0.45
1:A:618:ARG:HD3	1:A:620:LYS:HE2	1.99	0.45
1:C:395:ALA:HA	1:C:400:ARG:HG3	1.98	0.45
1:C:600:GLN:NE2	9:C:5050:HOH:O	2.49	0.45
1:D:129:ASP:HA	9:D:4852:HOH:O	2.16	0.45
1:D:571:LYS:HD2	1:D:639:VAL:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:606:ILE:HD11	1:D:617:LEU:O	2.16	0.45
1:A:447:TRP:HA	1:A:447:TRP:CE3	2.52	0.45
1:A:290:ASN:OD1	1:A:437:LYS:HD3	2.17	0.45
1:D:219:MET:HG3	1:D:248:ASP:HB3	1.99	0.45
1:D:153:SER:HB3	1:D:538:ALA:HB1	1.99	0.45
1:A:115:GLY:HA3	1:A:162:THR:HB	1.99	0.45
1:C:108:ASP:OD2	1:C:155:LYS:HE2	2.17	0.45
1:C:369:LEU:HD11	1:C:404:ILE:HG13	1.98	0.45
1:C:447:TRP:CE3	1:C:447:TRP:HA	2.51	0.45
1:C:502:MET:O	1:C:506:GLN:HG3	2.17	0.45
1:D:228:LEU:HB2	1:D:266:THR:HB	1.99	0.45
1:A:132[B]:ASN:HD22	1:A:133:PHE:H	1.64	0.45
1:D:118:ILE:O	1:D:118:ILE:HG13	2.17	0.45
1:B:543:LEU:HD21	1:B:633[A]:VAL:HG23	1.98	0.44
1:C:621:LYS:HB3	1:C:623:GLU:OE1	2.17	0.44
1:B:319:LEU:HD12	1:B:428:THR:HG23	1.99	0.44
1:C:365:GLN:HG3	1:C:662:ASP:HB3	1.99	0.44
1:D:606:ILE:O	1:D:610[B]:GLU:HG3	2.17	0.44
1:A:670:GLU:O	1:A:674:GLN:HG3	2.18	0.44
1:D:89:PHE:HE1	1:D:100[A]:GLU:HG2	1.82	0.44
1:D:640:LEU:HD23	1:D:640:LEU:C	2.38	0.44
1:A:620:LYS:HE2	1:A:644:GLU:OE2	2.18	0.44
1:B:447:TRP:HA	1:B:447:TRP:HE3	1.82	0.44
1:D:496:GLY:N	1:D:500:HIS:HE1	2.14	0.44
1:A:167:ALA:O	1:A:170:VAL:HG22	2.18	0.44
1:B:139:GLU:HB2	1:B:169:ASN:HB3	1.99	0.44
1:B:473:PRO:HD3	1:B:645:VAL:HB	1.98	0.44
1:D:111:PHE:O	1:D:159:VAL:HA	2.18	0.44
1:B:206:VAL:HG21	9:B:4244:HOH:O	2.17	0.44
1:B:443:GLU:HA	9:B:4454:HOH:O	2.16	0.44
1:C:447:TRP:HA	1:C:447:TRP:HE3	1.83	0.44
1:C:478:LYS:HE3	1:C:507:HIS:ND1	2.32	0.44
1:C:653:PRO:HB2	9:C:5079:HOH:O	2.18	0.44
1:D:313:HIS:HD2	1:D:315:ASP:N	2.03	0.44
1:D:623:GLU:HG3	9:D:5898:HOH:O	2.17	0.44
1:A:165:PRO:HD3	1:B:522:LEU:HG	1.99	0.44
1:D:594[A]:ARG:NH1	1:D:594[A]:ARG:CG	2.70	0.44
1:B:480:LEU:HD22	1:B:573:LEU:HD22	2.00	0.44
1:C:427:ALA:O	1:C:431:LEU:HB2	2.18	0.43
1:C:554:ASN:HA	1:C:557[B]:LEU:HD13	1.99	0.43
1:D:228:LEU:O	1:D:232:GLU:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:MET:HE2	1:A:221:LYS:HD3	2.01	0.43
1:A:298:LEU:C	1:A:298:LEU:HD12	2.39	0.43
1:A:465:GLU:HG3	1:A:472:LYS:HG2	2.00	0.43
1:A:554:ASN:HA	1:A:557:LEU:HD23	2.00	0.43
1:C:342:ASP:OD1	1:C:344:GLU:HB2	2.18	0.43
1:A:97:ILE:O	1:A:101:MET:HG2	2.18	0.43
1:A:202:GLN:HG2	1:B:522:LEU:O	2.18	0.43
1:A:218:VAL:HG22	1:A:219:MET:N	2.34	0.43
1:B:318:ARG:HD3	9:B:4309:HOH:O	2.18	0.43
1:C:347:LYS:HB2	1:C:347:LYS:HZ2	1.80	0.43
1:C:479:LYS:O	1:C:483:VAL:HG23	2.19	0.43
9:A:4194:HOH:O	1:D:442:LYS:HE3	2.17	0.43
1:C:494:THR:HG22	1:C:517:ILE:HB	2.00	0.43
1:D:621:LYS:HD3	9:D:6160:HOH:O	2.18	0.43
1:A:132[B]:ASN:ND2	1:A:133:PHE:N	2.67	0.43
1:B:115:GLY:HA3	1:B:162:THR:HB	2.01	0.43
1:B:621:LYS:HB3	1:B:623:GLU:OE1	2.18	0.43
1:C:200:ALA:HB1	4:C:2695:1MM:H5	2.00	0.43
1:D:93:THR:H	1:D:96:GLN:NE2	2.16	0.43
1:A:358:ALA:HB3	1:A:458:TYR:HB3	2.01	0.43
1:A:447:TRP:HA	1:A:447:TRP:HE3	1.83	0.43
1:B:311:LEU:O	1:B:514:HIS:HE1	2.01	0.43
1:C:165:PRO:HD3	1:D:522:LEU:HG	2.01	0.43
1:C:292:ALA:O	1:C:296:ILE:HG13	2.18	0.43
1:B:579:GLU:OE1	1:B:584[B]:THR:HG21	2.18	0.43
1:B:591:TYR:O	1:B:594:ARG:CG	2.65	0.43
1:C:474:GLN:HE21	1:C:474:GLN:N	2.11	0.43
1:D:139:GLU:HB2	1:D:169:ASN:HB3	2.00	0.43
1:D:497:VAL:O	8:D:2702:P22:H62	2.18	0.43
1:A:287[A]:GLN:NE2	1:A:291:LYS:NZ	2.66	0.43
1:D:554:ASN:HA	1:D:557:LEU:HD23	2.00	0.43
1:B:681:LYS:HG2	9:B:4342:HOH:O	2.19	0.43
1:C:670:GLU:O	1:C:674:GLN:HG3	2.18	0.43
1:D:437:LYS:HG2	9:D:5562:HOH:O	2.19	0.43
1:C:652:LEU:HD13	1:C:667:PHE:HA	2.01	0.42
1:A:198:THR:O	1:A:199:ASP:HB2	2.20	0.42
1:B:295:LEU:HD12	1:B:421:ILE:CD1	2.49	0.42
1:B:512:ASN:N	1:B:512:ASN:ND2	2.65	0.42
1:C:407:GLU:O	1:C:424:GLU:HA	2.19	0.42
1:B:381:VAL:O	1:B:661:LEU:HD21	2.20	0.42
1:C:102:MET:HE1	1:C:158:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LEU:O	1:A:514:HIS:HE1	2.02	0.42
1:A:336:GLN:HA	1:A:336:GLN:OE1	2.20	0.42
1:A:494:THR:HG22	1:A:517:ILE:HB	2.01	0.42
1:B:153:SER:HB3	1:B:538:ALA:HB1	2.02	0.42
1:D:301:LYS:HE2	1:D:366:ASN:O	2.19	0.42
1:B:398:GLU:HB2	1:B:400:ARG:HG2	2.01	0.42
1:C:398:GLU:HB2	1:C:400:ARG:CG	2.41	0.42
1:A:560:LEU:HG	1:A:614:LEU:HD21	2.02	0.42
1:B:679:ARG:HG2	1:B:687:HIS:OXT	2.20	0.42
1:C:352:LEU:HD13	1:C:364:VAL:HG21	2.02	0.42
1:C:623:GLU:CD	1:C:623:GLU:H	2.23	0.42
1:D:115:GLY:HA3	1:D:162:THR:CB	2.50	0.42
1:C:129:ASP:HB3	9:C:5994:HOH:O	2.20	0.41
1:A:496:GLY:N	1:A:500:HIS:HE1	2.13	0.41
1:C:318:ARG:HG2	1:C:322:GLU:OE2	2.20	0.41
1:C:498:GLY:O	1:C:501:GLN:HB3	2.21	0.41
1:D:246:LEU:C	1:D:246:LEU:HD23	2.40	0.41
1:A:615:LYS:HD3	1:A:635:THR:HG21	2.02	0.41
1:B:108:ASP:OD2	1:B:155:LYS:HE2	2.20	0.41
1:B:600:GLN:CD	1:B:600:GLN:N	2.71	0.41
1:C:589:LEU:HG	9:C:6026:HOH:O	2.19	0.41
1:C:93:THR:OG1	1:C:96:GLN:HG3	2.20	0.41
1:C:619:VAL:CG2	1:C:641:LEU:HD11	2.48	0.41
1:A:594[A]:ARG:HH11	1:A:594[A]:ARG:CG	2.29	0.41
1:C:102:MET:HE1	1:C:107:VAL:HG11	2.02	0.41
1:C:319:LEU:HD12	1:C:428:THR:CG2	2.51	0.41
1:A:118:ILE:HG13	1:A:118:ILE:O	2.21	0.41
1:A:153:SER:HB3	1:A:538:ALA:HB1	2.02	0.41
1:B:580:GLN:HG2	1:B:583:VAL:CG2	2.51	0.41
1:C:350:ASP:HB2	9:C:5038:HOH:O	2.19	0.41
1:A:111:PHE:O	1:A:159:VAL:HA	2.21	0.41
1:B:170:VAL:O	1:B:173:PRO:HD2	2.20	0.41
1:B:345:ASP:HA	1:B:346:PRO:HD3	1.92	0.41
1:C:102:MET:CE	1:C:107:VAL:HG11	2.50	0.41
1:C:681:LYS:HB2	1:C:681:LYS:NZ	2.36	0.41
1:A:115:GLY:HA3	1:A:162:THR:CB	2.51	0.41
1:C:115:GLY:HA3	1:C:162:THR:HB	2.03	0.41
1:A:220:VAL:HG13	1:A:225:GLU:HG3	2.03	0.41
1:B:606:ILE:HD11	1:B:618:ARG:HB2	2.03	0.41
1:A:560:LEU:HD23	1:A:612:MET:HG3	2.03	0.40
1:B:97:ILE:O	1:B:101:MET:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:THR:HG21	1:B:532:ALA:HA	2.02	0.40
1:D:281:GLN:O	1:D:285:VAL:HG23	2.21	0.40
1:A:502:MET:O	1:A:506:GLN:HG3	2.21	0.40
1:B:319:LEU:HD12	1:B:428:THR:CG2	2.51	0.40
1:D:497:VAL:HG21	1:D:523:GLY:C	2.41	0.40
1:D:571:LYS:HD2	1:D:639:VAL:HG12	2.02	0.40
1:B:321:LYS:NZ	9:B:4719:HOH:O	2.54	0.40
1:B:529:LEU:HB3	1:B:530:PRO:CD	2.52	0.40
1:B:606:ILE:HD12	1:B:606:ILE:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	598/677 (88%)	587 (98%)	11 (2%)	0	100	100
1	B	581/677 (86%)	568 (98%)	12 (2%)	1 (0%)	47	58
1	C	573/677 (85%)	551 (96%)	21 (4%)	1 (0%)	47	58
1	D	597/677 (88%)	586 (98%)	11 (2%)	0	100	100
All	All	2349/2708 (87%)	2292 (98%)	55 (2%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	350	ASP
1	C	350	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	488/556 (88%)	477 (98%)	11 (2%)	50	67
1	B	464/556 (84%)	457 (98%)	7 (2%)	65	79
1	C	453/556 (82%)	442 (98%)	11 (2%)	49	66
1	D	483/556 (87%)	471 (98%)	12 (2%)	47	65
All	All	1888/2224 (85%)	1847 (98%)	41 (2%)	55	69

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	287[A]	GLN
1	A	287[B]	GLN
1	A	305	TYR
1	A	443	GLU
1	A	447	TRP
1	A	457	GLU
1	A	548	ASP
1	A	560	LEU
1	A	614	LEU
1	A	630	LYS
1	A	666	ASN
1	B	106	ASN
1	B	224	GLU
1	B	447	TRP
1	B	474	GLN
1	B	541	GLU
1	B	548	ASP
1	B	557	LEU
1	C	295	LEU
1	C	347	LYS
1	C	400	ARG
1	C	403	ILE
1	C	447	TRP
1	C	474	GLN

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Mol	Chain	Res	Type
1	C	548	ASP
1	C	557[A]	LEU
1	C	557[B]	LEU
1	C	560	LEU
1	C	666	ASN
1	D	106	ASN
1	D	136	PRO
1	D	298	LEU
1	D	305	TYR
1	D	347	LYS
1	D	411	LYS
1	D	548	ASP
1	D	589	LEU
1	D	594[A]	ARG
1	D	594[B]	ARG
1	D	614	LEU
1	D	681	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	312	ASN
1	A	313	HIS
1	A	500	HIS
1	A	565	GLN
1	A	666	ASN
1	B	99	ASN
1	B	106	ASN
1	B	126	HIS
1	B	132	ASN
1	B	169	ASN
1	B	312	ASN
1	B	474	GLN
1	B	500	HIS
1	B	512	ASN
1	B	514	HIS
1	B	587	GLN
1	B	600	GLN
1	B	602	ASN
1	B	666	ASN
1	C	99	ASN

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Mol	Chain	Res	Type
1	C	132	ASN
1	C	169	ASN
1	C	312	ASN
1	C	412	ASN
1	C	452	ASN
1	C	474	GLN
1	C	500	HIS
1	C	512	ASN
1	C	514	HIS
1	C	565	GLN
1	C	580	GLN
1	C	585	GLN
1	C	587	GLN
1	C	600	GLN
1	C	602	ASN
1	C	666	ASN
1	D	96	GLN
1	D	106	ASN
1	D	127	ASN
1	D	169	ASN
1	D	312	ASN
1	D	313	HIS
1	D	450	GLN
1	D	500	HIS
1	D	580	GLN
1	D	602	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
6	PYD	A	703	-	9,9,9	8.04	6 (66%)	11,12,12	3.88	6 (54%)
6	PYD	C	2703	-	9,9,9	8.26	6 (66%)	11,12,12	3.91	7 (63%)
7	P25	B	698	3	11,13,13	1.93	4 (36%)	15,18,18	3.32	5 (33%)
4	1MM	B	1695	-	27,27,27	3.88	19 (70%)	36,38,38	4.22	16 (44%)
4	1MM	C	2695	-	27,27,27	3.73	19 (70%)	36,38,38	4.15	18 (50%)
5	FAD	B	1701	-	53,58,58	2.75	23 (43%)	68,89,89	1.55	8 (11%)
8	P22	D	2702	3	8,10,10	2.01	4 (50%)	12,15,15	1.87	1 (8%)
6	PYD	D	3703	-	9,9,9	8.13	6 (66%)	11,12,12	3.83	7 (63%)
5	FAD	A	701	-	53,58,58	2.56	21 (39%)	68,89,89	1.50	9 (13%)
6	PYD	B	1703	-	9,9,9	8.06	6 (66%)	11,12,12	3.92	6 (54%)
5	FAD	D	3701	-	53,58,58	2.64	23 (43%)	68,89,89	1.52	8 (11%)
4	1MM	C	3695	-	27,27,27	3.87	19 (70%)	36,38,38	4.25	16 (44%)
4	1MM	A	695	-	27,27,27	3.67	19 (70%)	36,38,38	4.17	16 (44%)
7	P25	A	1698	3	11,13,13	1.96	4 (36%)	15,18,18	3.35	5 (33%)
8	P22	C	3702	3	8,10,10	1.93	3 (37%)	12,15,15	1.98	1 (8%)
5	FAD	C	2701	-	53,58,58	2.83	24 (45%)	68,89,89	1.56	9 (13%)

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
6	PYD	A	703	-	-	-	0/1/1/1
7	P25	B	698	3	-	0/13/13/13	-
6	PYD	C	2703	-	-	-	0/1/1/1
4	1MM	B	1695	-	-	12/23/23/23	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1MM	C	2695	-	-	12/23/23/23	0/2/2/2
5	FAD	B	1701	-	-	1/30/50/50	0/6/6/6
8	P22	D	2702	3	-	2/10/10/10	-
6	PYD	D	3703	-	-	-	0/1/1/1
5	FAD	A	701	-	-	1/30/50/50	0/6/6/6
6	PYD	B	1703	-	-	-	0/1/1/1
5	FAD	D	3701	-	-	1/30/50/50	0/6/6/6
4	1MM	C	3695	-	-	9/23/23/23	0/2/2/2
4	1MM	A	695	-	-	11/23/23/23	0/2/2/2
7	P25	A	1698	3	-	2/13/13/13	-
8	P22	C	3702	3	-	1/10/10/10	-
5	FAD	C	2701	-	-	1/30/50/50	0/6/6/6

All (206) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	3703	PYD	C4'-N3'	12.92	1.53	1.35
6	C	2703	PYD	C5'-C4'	12.46	1.60	1.41
6	C	2703	PYD	C4'-N3'	12.31	1.52	1.35
6	A	703	PYD	C4'-N3'	12.27	1.52	1.35
6	B	1703	PYD	C4'-N3'	12.26	1.52	1.35
6	D	3703	PYD	C5'-C4'	11.65	1.59	1.41
6	B	1703	PYD	C5'-C4'	11.65	1.59	1.41
6	A	703	PYD	C5'-C4'	11.56	1.59	1.41
6	D	3703	PYD	C6'-C5'	10.25	1.55	1.39
6	A	703	PYD	C2'-N1'	10.13	1.50	1.34
6	B	1703	PYD	C2'-N1'	10.07	1.50	1.34
6	C	2703	PYD	C6'-C5'	10.02	1.54	1.39
6	B	1703	PYD	C6'-N1'	9.97	1.55	1.34
5	C	2701	FAD	C4A-N3A	9.90	1.49	1.35
6	C	2703	PYD	C2'-N1'	9.89	1.50	1.34
6	A	703	PYD	C6'-N1'	9.80	1.55	1.34
6	C	2703	PYD	C6'-N1'	9.77	1.55	1.34
6	D	3703	PYD	C6'-N1'	9.69	1.54	1.34
5	B	1701	FAD	C4A-N3A	9.64	1.49	1.35
6	A	703	PYD	C6'-C5'	9.48	1.54	1.39
6	B	1703	PYD	C6'-C5'	9.43	1.53	1.39
5	D	3701	FAD	C4A-N3A	9.05	1.48	1.35
5	A	701	FAD	C4A-N3A	8.58	1.47	1.35
6	D	3703	PYD	C2'-N1'	8.53	1.48	1.34
4	B	1695	1MM	C3-C2	7.32	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3695	1MM	C3-C2	7.26	1.47	1.39
4	A	695	1MM	C3-C2	7.09	1.47	1.39
4	C	2695	1MM	C4'-N5'	6.93	1.46	1.33
4	A	695	1MM	C4'-N5'	6.92	1.46	1.33
4	B	1695	1MM	C4'-N5'	6.91	1.46	1.33
4	C	3695	1MM	C4'-N5'	6.90	1.46	1.33
4	C	2695	1MM	C3-C2	6.76	1.47	1.39
4	C	3695	1MM	C6'-N1'	6.69	1.45	1.34
5	C	2701	FAD	C2A-N1A	6.64	1.46	1.33
4	B	1695	1MM	C6'-N1'	6.34	1.45	1.34
5	B	1701	FAD	C2A-N1A	6.23	1.45	1.33
4	C	3695	1MM	C6'-N5'	6.16	1.45	1.34
4	A	695	1MM	C6'-N1'	6.14	1.45	1.34
5	D	3701	FAD	C2A-N1A	6.10	1.45	1.33
4	B	1695	1MM	C6'-N5'	6.02	1.44	1.34
4	B	1695	1MM	C1-C2	5.93	1.46	1.40
5	C	2701	FAD	C2A-N3A	5.88	1.41	1.32
5	A	701	FAD	C2A-N1A	5.86	1.44	1.33
4	C	2695	1MM	C6'-N5'	5.84	1.44	1.34
4	A	695	1MM	C6'-N5'	5.78	1.44	1.34
4	C	2695	1MM	C6'-N1'	5.77	1.44	1.34
4	C	3695	1MM	C4'-N3'	5.74	1.44	1.33
4	C	3695	1MM	C1-C2	5.69	1.46	1.40
4	C	2695	1MM	C1-C2	5.59	1.46	1.40
4	B	1695	1MM	C4'-N3'	5.48	1.43	1.33
5	B	1701	FAD	C2A-N3A	5.29	1.40	1.32
4	C	2695	1MM	O12-C11	5.23	1.44	1.33
5	D	3701	FAD	C2A-N3A	5.20	1.40	1.32
4	B	1695	1MM	C2'-N10	-5.16	1.32	1.38
4	C	2695	1MM	C4'-N3'	5.12	1.43	1.33
5	C	2701	FAD	C1'-C2'	-5.07	1.45	1.52
4	A	695	1MM	C2'-N10	-5.03	1.32	1.38
4	C	3695	1MM	O12-C11	5.02	1.44	1.33
5	A	701	FAD	C2A-N3A	4.98	1.40	1.32
4	B	1695	1MM	O12-C11	4.94	1.44	1.33
4	C	2695	1MM	C2'-N10	-4.93	1.32	1.38
4	A	695	1MM	O12-C11	4.88	1.44	1.33
4	A	695	1MM	C1-C2	4.78	1.45	1.40
4	A	695	1MM	C4'-N3'	4.72	1.42	1.33
5	C	2701	FAD	O4'-C4'	4.63	1.53	1.43
5	B	1701	FAD	C1'-C2'	-4.59	1.46	1.52
4	C	3695	1MM	C2'-N10	-4.51	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	701	FAD	O4'-C4'	4.50	1.52	1.43
5	B	1701	FAD	O4'-C4'	4.46	1.52	1.43
5	D	3701	FAD	C1'-C2'	-4.43	1.46	1.52
5	D	3701	FAD	O4'-C4'	4.33	1.52	1.43
5	C	2701	FAD	C9A-C5X	4.22	1.48	1.41
5	A	701	FAD	C1'-C2'	-4.22	1.46	1.52
5	B	1701	FAD	O3'-C3'	4.22	1.52	1.43
5	D	3701	FAD	O3'-C3'	4.20	1.52	1.43
5	B	1701	FAD	C9A-C5X	4.16	1.48	1.41
5	C	2701	FAD	O3'-C3'	4.14	1.52	1.43
4	B	1695	1MM	C4-C3	4.14	1.47	1.38
5	A	701	FAD	O3'-C3'	4.10	1.52	1.43
5	B	1701	FAD	C4X-N5	4.08	1.38	1.30
4	C	3695	1MM	C4-C3	4.05	1.47	1.38
5	A	701	FAD	C9A-C5X	4.01	1.47	1.41
5	D	3701	FAD	C9A-C5X	3.99	1.47	1.41
5	C	2701	FAD	C4X-N5	3.95	1.38	1.30
6	D	3703	PYD	C2'-N3'	3.93	1.41	1.34
4	A	695	1MM	C4-C3	3.92	1.47	1.38
4	C	2695	1MM	C4-C3	3.90	1.47	1.38
7	B	698	P25	PA-O7	-3.89	1.43	1.59
5	C	2701	FAD	C5'-C4'	-3.87	1.46	1.51
4	B	1695	1MM	C2-S7	3.79	1.83	1.77
5	D	3701	FAD	C5'-C4'	-3.78	1.46	1.51
7	A	1698	P25	PA-O7	-3.75	1.44	1.59
4	C	3695	1MM	C6-C1	3.71	1.45	1.39
4	C	2695	1MM	C6-C1	3.69	1.45	1.39
5	A	701	FAD	C4X-N5	3.69	1.37	1.30
5	C	2701	FAD	C6A-C5A	3.67	1.56	1.43
5	B	1701	FAD	C6A-C5A	3.66	1.56	1.43
4	B	1695	1MM	C6-C1	3.64	1.45	1.39
5	D	3701	FAD	C4X-N5	3.58	1.37	1.30
5	A	701	FAD	C6A-C5A	3.54	1.56	1.43
5	B	1701	FAD	C5'-C4'	-3.47	1.46	1.51
5	A	701	FAD	C5'-C4'	-3.46	1.46	1.51
5	C	2701	FAD	C5A-C4A	3.45	1.50	1.40
4	C	3695	1MM	C2-S7	3.43	1.82	1.77
5	D	3701	FAD	C6A-C5A	3.40	1.55	1.43
5	B	1701	FAD	C5A-C4A	3.32	1.49	1.40
4	A	695	1MM	C6-C1	3.30	1.45	1.39
5	B	1701	FAD	C10-N1	3.28	1.39	1.33
4	C	2695	1MM	C2-S7	3.27	1.82	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	695	1MM	C9-N10	-3.27	1.30	1.37
4	C	2695	1MM	C9-N10	-3.25	1.30	1.37
5	C	2701	FAD	C10-N1	3.22	1.39	1.33
5	D	3701	FAD	C10-N1	3.21	1.39	1.33
4	C	3695	1MM	C2'-N1'	3.19	1.44	1.34
6	C	2703	PYD	C2'-N3'	3.18	1.39	1.34
4	A	695	1MM	C2-S7	3.16	1.82	1.77
4	C	2695	1MM	C2'-N1'	3.12	1.44	1.34
5	D	3701	FAD	C5A-C4A	3.12	1.49	1.40
5	A	701	FAD	C5A-C4A	3.11	1.49	1.40
4	B	1695	1MM	C9-N10	-3.10	1.31	1.37
8	D	2702	P22	PA-O7	-3.09	1.46	1.59
4	B	1695	1MM	C2'-N1'	3.09	1.44	1.34
7	A	1698	P25	O7-C7	3.08	1.57	1.44
4	A	695	1MM	C2'-N1'	3.04	1.43	1.34
5	A	701	FAD	C3B-C4B	2.95	1.60	1.53
5	B	1701	FAD	C8A-N7A	-2.90	1.29	1.34
5	C	2701	FAD	C8-C7	2.89	1.48	1.40
5	B	1701	FAD	C3B-C4B	2.86	1.60	1.53
4	C	3695	1MM	C9-N10	-2.86	1.31	1.37
7	B	698	P25	O7-C7	2.84	1.56	1.44
5	D	3701	FAD	C3B-C4B	2.82	1.60	1.53
5	A	701	FAD	C10-N1	2.81	1.39	1.33
5	D	3701	FAD	C8-C7	2.81	1.47	1.40
4	C	3695	1MM	S7-N8	2.79	1.70	1.64
5	C	2701	FAD	C3B-C4B	2.79	1.60	1.53
5	D	3701	FAD	C8A-N7A	-2.78	1.29	1.34
4	C	3695	1MM	C2'-N3'	2.74	1.43	1.34
4	B	1695	1MM	C9-N8	-2.73	1.33	1.39
5	A	701	FAD	C8-C7	2.71	1.47	1.40
4	C	2695	1MM	C2'-N3'	2.70	1.42	1.34
5	D	3701	FAD	C6-C5X	2.68	1.44	1.40
4	B	1695	1MM	C2'-N3'	2.65	1.42	1.34
4	C	3695	1MM	O4'-C4'	2.64	1.39	1.33
5	A	701	FAD	C8A-N7A	-2.64	1.30	1.34
5	A	701	FAD	C9-C9A	2.62	1.43	1.39
5	D	3701	FAD	P-O2P	-2.62	1.43	1.55
4	B	1695	1MM	O4'-C4'	2.61	1.39	1.33
5	B	1701	FAD	C8-C7	2.61	1.47	1.40
5	C	2701	FAD	P-O2P	-2.59	1.43	1.55
5	A	701	FAD	P-O2P	-2.59	1.43	1.55
5	C	2701	FAD	C8A-N7A	-2.57	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1701	FAD	P-O2P	-2.57	1.43	1.55
5	B	1701	FAD	C9-C9A	2.57	1.43	1.39
4	A	695	1MM	C9-N8	-2.56	1.33	1.39
4	A	695	1MM	C2'-N3'	2.56	1.42	1.34
7	A	1698	P25	PB-O2B	-2.53	1.45	1.54
5	B	1701	FAD	C6-C5X	2.53	1.43	1.40
5	C	2701	FAD	C9-C9A	2.52	1.43	1.39
7	B	698	P25	PB-O2B	-2.51	1.45	1.54
7	B	698	P25	PA-O2A	-2.51	1.43	1.55
4	C	2695	1MM	C1-C11	2.50	1.55	1.50
8	C	3702	P22	PA-O2A	-2.50	1.42	1.50
4	C	2695	1MM	O4'-C4'	2.49	1.39	1.33
7	A	1698	P25	PA-O2A	-2.45	1.43	1.55
8	D	2702	P22	PB-O1B	-2.42	1.45	1.54
5	B	1701	FAD	C6-C7	2.41	1.43	1.39
4	A	695	1MM	O4'-C4'	2.40	1.39	1.33
4	C	2695	1MM	C9-N8	-2.40	1.34	1.39
5	C	2701	FAD	C6-C5X	2.39	1.43	1.40
5	D	3701	FAD	PA-O2A	-2.34	1.44	1.55
4	C	2695	1MM	C5-C6	2.32	1.43	1.38
5	C	2701	FAD	C10-N10	2.31	1.42	1.37
4	C	3695	1MM	C5-C6	2.29	1.43	1.38
5	C	2701	FAD	C6A-N1A	2.27	1.47	1.37
5	D	3701	FAD	C6A-N1A	2.26	1.47	1.37
5	C	2701	FAD	C6-C7	2.26	1.42	1.39
6	A	703	PYD	C2'-N3'	2.26	1.38	1.34
5	B	1701	FAD	C10-N10	2.25	1.42	1.37
5	B	1701	FAD	C6A-N1A	2.23	1.47	1.37
5	D	3701	FAD	C6-C7	2.22	1.42	1.39
8	D	2702	P22	PA-O1A	-2.20	1.45	1.55
5	B	1701	FAD	PA-O5B	-2.20	1.50	1.59
4	C	3695	1MM	C1-C11	2.19	1.54	1.50
8	C	3702	P22	PA-O7	-2.19	1.50	1.59
4	B	1695	1MM	C5-C6	2.18	1.43	1.38
4	B	1695	1MM	S7-N8	2.18	1.69	1.64
5	C	2701	FAD	PA-O2A	-2.16	1.45	1.55
5	D	3701	FAD	C10-N10	2.16	1.42	1.37
8	C	3702	P22	PB-O1B	-2.15	1.46	1.54
4	C	2695	1MM	S7-N8	2.14	1.68	1.64
5	D	3701	FAD	C9-C9A	2.13	1.43	1.39
5	A	701	FAD	PA-O2A	-2.13	1.45	1.55
4	A	695	1MM	C1-C11	2.13	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3695	1MM	C9-N8	-2.12	1.34	1.39
4	B	1695	1MM	C1-C11	2.10	1.54	1.50
6	B	1703	PYD	C2'-N3'	2.09	1.37	1.34
4	A	695	1MM	C5-C6	2.09	1.43	1.38
5	B	1701	FAD	PA-O2A	-2.09	1.45	1.55
5	D	3701	FAD	PA-O5B	-2.08	1.50	1.59
5	A	701	FAD	C6A-N1A	2.07	1.46	1.37
5	C	2701	FAD	PA-O5B	-2.07	1.50	1.59
4	A	695	1MM	S7-N8	2.07	1.68	1.64
5	A	701	FAD	C6-C5X	2.06	1.43	1.40
5	A	701	FAD	PA-O5B	-2.06	1.51	1.59
5	C	2701	FAD	C9-C8	2.05	1.42	1.39
8	D	2702	P22	PA-O2A	-2.02	1.43	1.50

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	3695	1MM	C5'-O4'-C4'	14.13	140.19	117.58
4	B	1695	1MM	C5'-O4'-C4'	14.02	140.01	117.58
4	C	2695	1MM	C5'-O4'-C4'	13.94	139.88	117.58
4	A	695	1MM	C5'-O4'-C4'	13.77	139.62	117.58
4	C	2695	1MM	C3-C2-S7	-10.49	103.17	117.42
4	B	1695	1MM	C3-C2-S7	-10.26	103.49	117.42
4	A	695	1MM	C3-C2-S7	-10.23	103.53	117.42
4	C	3695	1MM	C3-C2-S7	-10.14	103.65	117.42
4	C	3695	1MM	C4'-N3'-C2'	9.86	120.76	112.86
4	A	695	1MM	C4'-N3'-C2'	9.52	120.49	112.86
4	B	1695	1MM	C4'-N3'-C2'	9.42	120.41	112.86
4	C	2695	1MM	C4'-N3'-C2'	9.13	120.18	112.86
7	B	698	P25	O7-C7-C6	9.05	139.20	108.99
7	A	1698	P25	O7-C7-C6	8.91	138.71	108.99
6	B	1703	PYD	CM2-C2'-N1'	8.12	126.07	117.14
6	C	2703	PYD	CM2-C2'-N1'	8.09	126.04	117.14
6	A	703	PYD	CM2-C2'-N1'	8.02	125.96	117.14
6	D	3703	PYD	CM2-C2'-N1'	8.02	125.96	117.14
5	C	2701	FAD	C1B-N9A-C4A	6.64	138.31	126.64
5	B	1701	FAD	C1B-N9A-C4A	6.40	137.88	126.64
5	D	3701	FAD	C1B-N9A-C4A	6.13	137.41	126.64
5	A	701	FAD	C1B-N9A-C4A	6.06	137.29	126.64
6	B	1703	PYD	C5'-C6'-N1'	-5.96	119.02	125.11
4	C	3695	1MM	C2-C1-C11	-5.88	116.12	124.25
7	A	1698	P25	C5-C6-C7	5.86	139.48	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	703	PYD	C5'-C6'-N1'	-5.84	119.14	125.11
4	B	1695	1MM	N8-C9-N10	-5.78	107.27	114.93
4	A	695	1MM	C2-C1-C11	-5.70	116.38	124.25
4	C	3695	1MM	N8-C9-N10	-5.63	107.46	114.93
4	A	695	1MM	N8-C9-N10	-5.60	107.50	114.93
7	B	698	P25	C5-C6-C7	5.59	138.27	113.49
4	B	1695	1MM	C2-C1-C11	-5.56	116.56	124.25
4	C	2695	1MM	N8-C9-N10	-5.50	107.63	114.93
6	C	2703	PYD	C5'-C6'-N1'	-5.47	119.52	125.11
8	C	3702	P22	PA-O7-C7	5.26	151.88	121.56
8	D	2702	P22	PA-O7-C7	5.16	151.31	121.56
4	C	2695	1MM	C2-C1-C11	-5.16	117.12	124.25
7	A	1698	P25	PA-O7-C7	5.09	146.65	121.59
6	C	2703	PYD	C6'-N1'-C2'	4.86	124.22	115.96
7	B	698	P25	PA-O7-C7	4.78	145.11	121.59
6	D	3703	PYD	C6'-N1'-C2'	4.76	124.06	115.96
6	B	1703	PYD	C6'-N1'-C2'	4.75	124.04	115.96
4	C	2695	1MM	C2'-N1'-C6'	4.75	122.08	114.61
4	C	3695	1MM	C2'-N1'-C6'	4.74	122.08	114.61
4	B	1695	1MM	C2'-N1'-C6'	4.74	122.06	114.61
6	A	703	PYD	C6'-N1'-C2'	4.73	124.02	115.96
4	A	695	1MM	C2'-N1'-C6'	4.69	122.00	114.61
4	C	3695	1MM	N3'-C2'-N1'	-4.66	118.87	126.23
6	D	3703	PYD	C5'-C6'-N1'	-4.64	120.36	125.11
6	D	3703	PYD	N1'-C2'-N3'	-4.50	117.80	125.54
4	A	695	1MM	N3'-C2'-N1'	-4.43	119.22	126.23
4	B	1695	1MM	N3'-C2'-N1'	-4.43	119.23	126.23
6	C	2703	PYD	N1'-C2'-N3'	-4.40	117.96	125.54
4	B	1695	1MM	O9-C9-N10	4.38	131.04	123.62
4	C	2695	1MM	N3'-C2'-N1'	-4.32	119.39	126.23
4	A	695	1MM	O9-C9-N10	4.28	130.87	123.62
6	A	703	PYD	N1'-C2'-N3'	-4.25	118.22	125.54
6	B	1703	PYD	N1'-C2'-N3'	-4.23	118.25	125.54
4	C	3695	1MM	O9-C9-N10	4.18	130.71	123.62
4	C	3695	1MM	O12-C11-C1	-4.14	105.42	112.30
4	C	2695	1MM	N5'-C6'-N1'	-4.13	118.12	125.72
4	A	695	1MM	N5'-C6'-N1'	-4.12	118.15	125.72
4	C	2695	1MM	O9-C9-N10	4.08	130.52	123.62
4	B	1695	1MM	N5'-C6'-N1'	-4.04	118.28	125.72
4	C	2695	1MM	O12-C11-C1	-4.04	105.59	112.30
4	C	3695	1MM	O12-C11-O11	3.97	131.22	123.45
4	C	3695	1MM	N5'-C6'-N1'	-3.96	118.44	125.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1695	1MM	O12-C11-C1	-3.94	105.74	112.30
4	B	1695	1MM	O12-C11-O11	3.91	131.11	123.45
4	A	695	1MM	O12-C11-O11	3.89	131.06	123.45
4	A	695	1MM	O12-C11-C1	-3.88	105.85	112.30
4	B	1695	1MM	O7B-S7-C2	3.83	113.97	107.66
4	C	2695	1MM	N3'-C4'-N5'	-3.82	120.28	127.63
4	C	3695	1MM	N3'-C4'-N5'	-3.76	120.38	127.63
4	C	3695	1MM	O7B-S7-C2	3.76	113.84	107.66
4	B	1695	1MM	N3'-C4'-N5'	-3.74	120.43	127.63
6	D	3703	PYD	C7'-C5'-C4'	3.67	125.44	121.72
4	A	695	1MM	N3'-C4'-N5'	-3.66	120.59	127.63
4	C	2695	1MM	O12-C11-O11	3.65	130.59	123.45
6	C	2703	PYD	C7'-C5'-C4'	3.49	125.26	121.72
4	C	2695	1MM	O7B-S7-C2	3.47	113.37	107.66
4	A	695	1MM	O7B-S7-C2	3.47	113.37	107.66
4	C	3695	1MM	C6-C1-C11	3.41	125.65	118.66
4	A	695	1MM	C6-C1-C11	3.26	125.36	118.66
5	D	3701	FAD	N3A-C2A-N1A	-3.25	123.60	128.68
6	D	3703	PYD	C2'-N3'-C4'	3.23	123.12	118.08
4	B	1695	1MM	C6-C1-C11	3.20	125.23	118.66
5	A	701	FAD	N3A-C2A-N1A	-3.17	123.73	128.68
6	C	2703	PYD	C2'-N3'-C4'	3.10	122.92	118.08
6	B	1703	PYD	C7'-C5'-C4'	3.09	124.85	121.72
4	C	2695	1MM	C6-C1-C11	3.08	124.98	118.66
5	B	1701	FAD	N3A-C2A-N1A	-3.07	123.89	128.68
6	A	703	PYD	C7'-C5'-C4'	3.03	124.79	121.72
5	C	2701	FAD	N3A-C2A-N1A	-3.01	123.98	128.68
6	B	1703	PYD	C2'-N3'-C4'	2.94	122.66	118.08
6	A	703	PYD	C2'-N3'-C4'	2.90	122.61	118.08
4	C	3695	1MM	C7'-C6'-N1'	2.87	121.63	117.15
4	A	695	1MM	C7'-C6'-N1'	2.86	121.62	117.15
7	A	1698	P25	CM4-C4-C5	2.82	134.84	113.42
5	C	2701	FAD	O2B-C2B-C1B	2.81	121.23	110.85
5	A	701	FAD	O2B-C2B-C3B	2.81	120.90	111.82
5	B	1701	FAD	O2B-C2B-C1B	2.79	121.17	110.85
4	B	1695	1MM	C7'-C6'-N1'	2.78	121.50	117.15
4	C	2695	1MM	C7'-C6'-N1'	2.76	121.46	117.15
5	D	3701	FAD	O2B-C2B-C3B	2.72	120.62	111.82
5	D	3701	FAD	O2B-C2B-C1B	2.72	120.90	110.85
7	A	1698	P25	C4-C5-C6	2.70	140.41	115.30
7	B	698	P25	CM4-C4-C5	2.69	133.88	113.42
5	A	701	FAD	O2B-C2B-C1B	2.69	120.77	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	698	P25	C4-C5-C6	2.66	140.01	115.30
5	C	2701	FAD	O2-C2-N1	-2.66	117.42	121.83
5	B	1701	FAD	O2-C2-N1	-2.65	117.44	121.83
5	B	1701	FAD	O2B-C2B-C3B	2.63	120.33	111.82
4	B	1695	1MM	O7B-S7-N8	-2.61	99.42	106.74
5	A	701	FAD	O2-C2-N1	-2.60	117.52	121.83
5	C	2701	FAD	O2B-C2B-C3B	2.59	120.21	111.82
5	D	3701	FAD	O2-C2-N1	-2.53	117.64	121.83
4	C	3695	1MM	O7B-S7-N8	-2.41	99.96	106.74
4	C	2695	1MM	O7A-S7-C2	2.41	111.63	107.66
6	D	3703	PYD	C6'-C5'-C4'	-2.35	112.17	115.63
5	B	1701	FAD	O4B-C4B-C5B	-2.34	101.69	109.37
5	D	3701	FAD	O3'-C3'-C4'	-2.26	103.35	108.81
4	C	2695	1MM	O7B-S7-N8	-2.24	100.44	106.74
5	A	701	FAD	O4B-C4B-C5B	-2.22	102.06	109.37
5	B	1701	FAD	O3'-C3'-C4'	-2.20	103.48	108.81
5	D	3701	FAD	O4B-C4B-C5B	-2.19	102.15	109.37
5	C	2701	FAD	C3B-C2B-C1B	-2.19	97.69	100.98
5	A	701	FAD	O3'-C3'-C4'	-2.16	103.59	108.81
4	A	695	1MM	O7B-S7-N8	-2.14	100.73	106.74
5	C	2701	FAD	O3'-C3'-C4'	-2.13	103.66	108.81
5	C	2701	FAD	O4-C4-C4X	-2.13	120.94	126.60
5	D	3701	FAD	O4-C4-C4X	-2.12	120.97	126.60
5	C	2701	FAD	O4B-C4B-C5B	-2.10	102.47	109.37
6	C	2703	PYD	C6'-C5'-C4'	-2.09	112.55	115.63
4	C	2695	1MM	C7'-C6'-N5'	2.09	120.42	117.15
5	A	701	FAD	C1'-C2'-C3'	2.08	115.61	109.79
5	B	1701	FAD	O4-C4-C4X	-2.07	121.10	126.60
5	A	701	FAD	O4-C4-C4X	-2.07	121.12	126.60

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	695	1MM	N8-C9-N10-C2'
4	B	1695	1MM	N8-C9-N10-C2'
4	C	2695	1MM	N8-C9-N10-C2'
4	C	3695	1MM	N8-C9-N10-C2'
7	A	1698	P25	C6-C7-O7-PA
8	D	2702	P22	C6-C7-O7-PA
4	A	695	1MM	C1-C2-S7-O7A
4	B	1695	1MM	C1-C2-S7-O7A

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Mol	Chain	Res	Type	Atoms
4	C	2695	1MM	C1-C2-S7-O7A
4	C	3695	1MM	C1-C2-S7-O7A
7	A	1698	P25	C4-C5-C6-C7
4	B	1695	1MM	C3-C2-S7-N8
8	C	3702	P22	PA-O3A-PB-O2B
8	D	2702	P22	PA-O3A-PB-O2B
4	A	695	1MM	C3-C2-S7-N8
4	C	2695	1MM	C3-C2-S7-N8
4	C	3695	1MM	C3-C2-S7-N8
4	A	695	1MM	C1-C2-S7-O7B
4	B	1695	1MM	C1-C2-S7-O7B
4	C	2695	1MM	C1-C2-S7-O7B
4	C	3695	1MM	C1-C2-S7-O7B
4	A	695	1MM	C1-C2-S7-N8
4	B	1695	1MM	C1-C2-S7-N8
4	C	2695	1MM	C1-C2-S7-N8
4	C	3695	1MM	C1-C2-S7-N8
4	C	2695	1MM	C6-C1-C11-O12
4	A	695	1MM	C3-C2-S7-O7A
4	A	695	1MM	C3-C2-S7-O7B
4	B	1695	1MM	C3-C2-S7-O7B
4	C	3695	1MM	C3-C2-S7-O7B
4	B	1695	1MM	C6-C1-C11-O12
4	A	695	1MM	O9-C9-N10-C2'
4	B	1695	1MM	O9-C9-N10-C2'
4	C	2695	1MM	O9-C9-N10-C2'
4	C	3695	1MM	O9-C9-N10-C2'
4	C	2695	1MM	C3-C2-S7-O7B
4	A	695	1MM	C6-C1-C11-O12
4	B	1695	1MM	C3-C2-S7-O7A
4	C	2695	1MM	C2-C1-C11-O12
4	C	3695	1MM	C6-C1-C11-O12
5	A	701	FAD	O4B-C4B-C5B-O5B
5	C	2701	FAD	O4B-C4B-C5B-O5B
5	D	3701	FAD	O4B-C4B-C5B-O5B
4	A	695	1MM	C2-C1-C11-O12
4	B	1695	1MM	C2-C1-C11-O12
4	C	2695	1MM	C3-C2-S7-O7A
4	C	3695	1MM	C3-C2-S7-O7A
5	B	1701	FAD	O4B-C4B-C5B-O5B
4	C	2695	1MM	C6-C1-C11-O11
4	A	695	1MM	C2-C1-C11-O11

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Mol	Chain	Res	Type	Atoms
4	C	2695	1MM	C2-C1-C11-O11
4	B	1695	1MM	C6-C1-C11-O11
4	B	1695	1MM	C2-C1-C11-O11

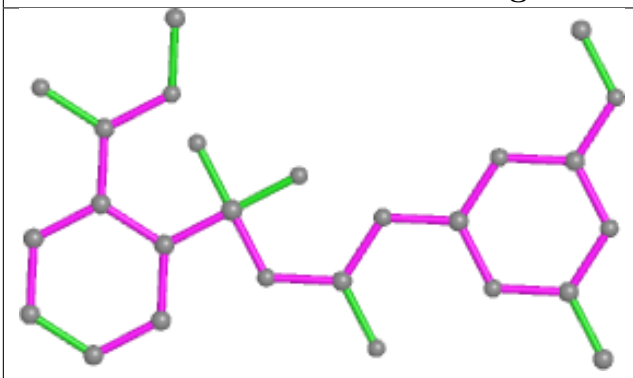
There are no ring outliers.

11 monomers are involved in 15 short contacts:

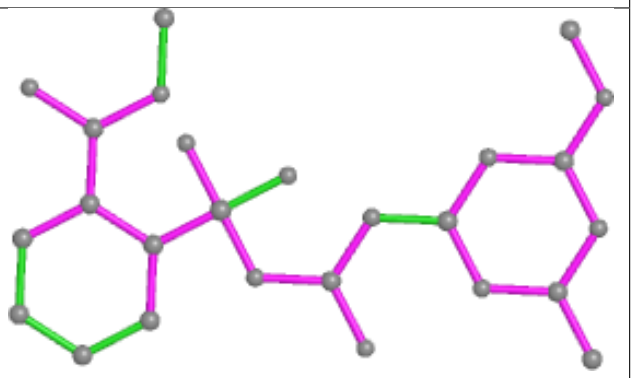
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	698	P25	1	0
4	B	1695	1MM	5	0
4	C	2695	1MM	2	0
5	B	1701	FAD	1	0
8	D	2702	P22	1	0
5	A	701	FAD	1	0
5	D	3701	FAD	1	0
4	C	3695	1MM	2	0
4	A	695	1MM	2	0
7	A	1698	P25	2	0
5	C	2701	FAD	1	0

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

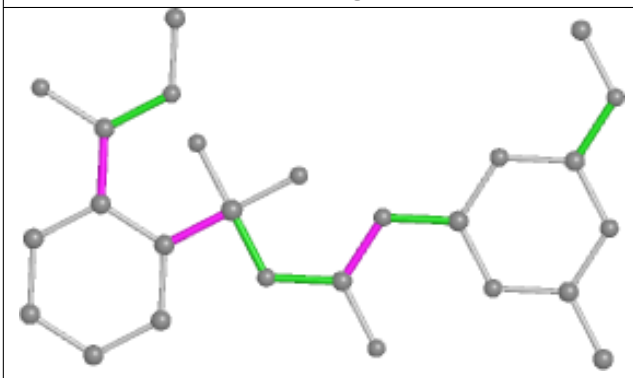
Ligand 1MM B 1695



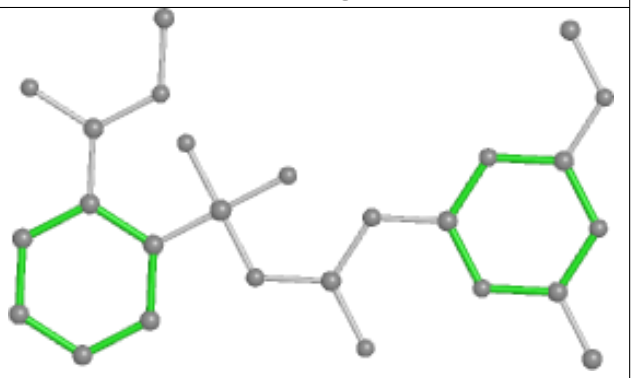
Bond lengths



Bond angles

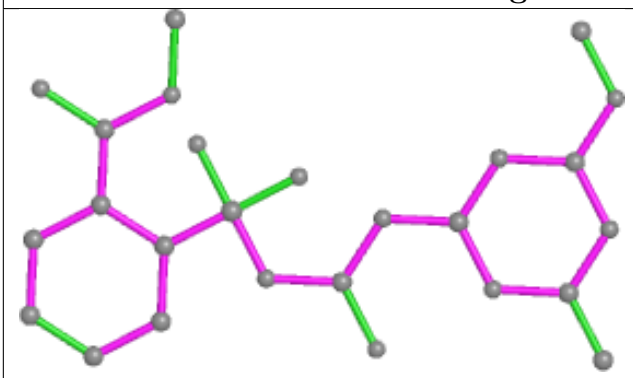


Torsions

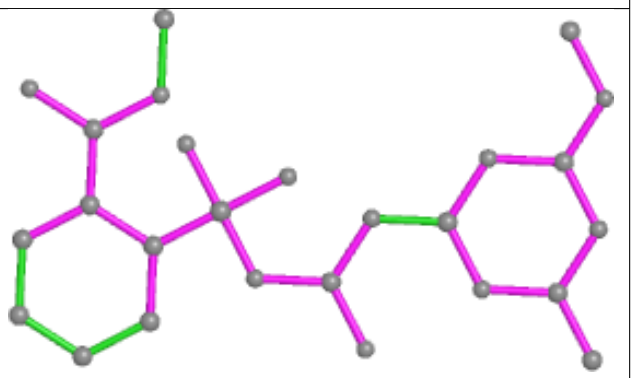


Rings

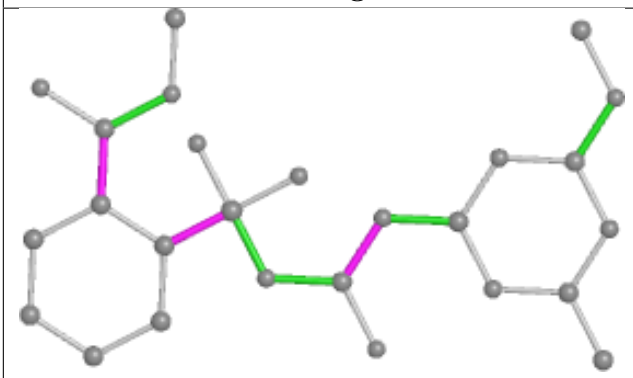
Ligand 1MM C 2695



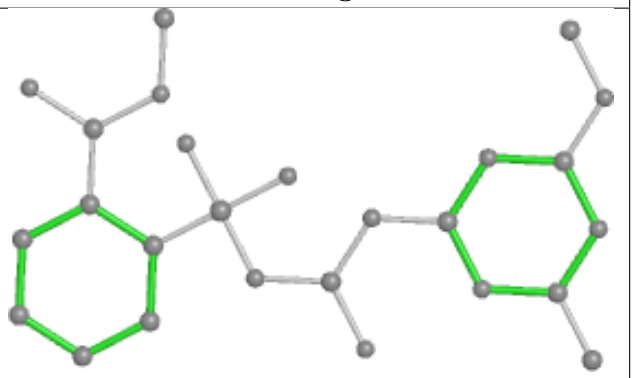
Bond lengths



Bond angles

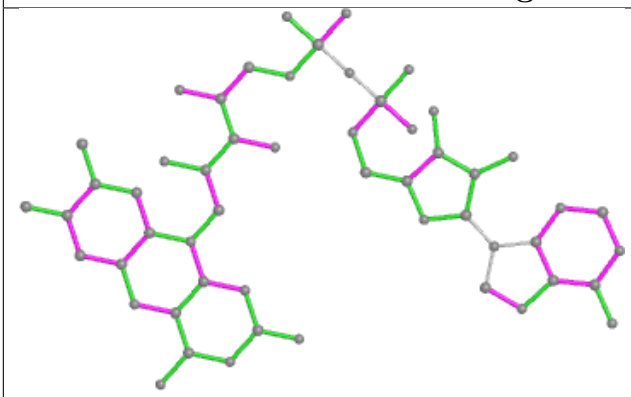


Torsions

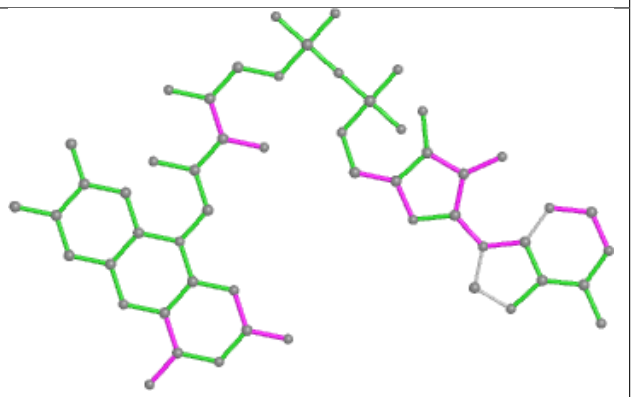


Rings

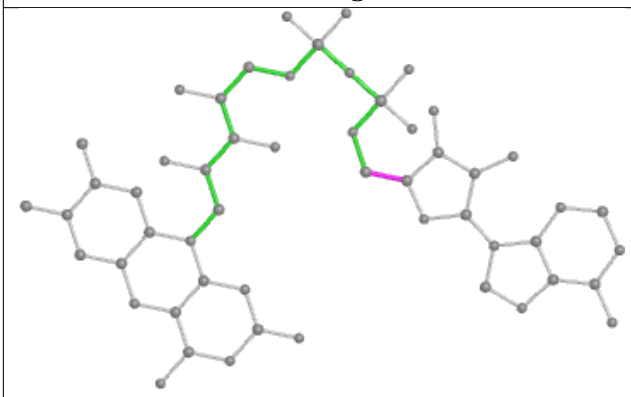
Ligand FAD B 1701



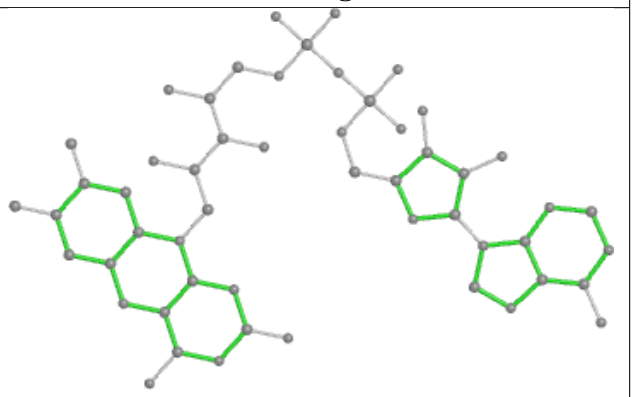
Bond lengths



Bond angles

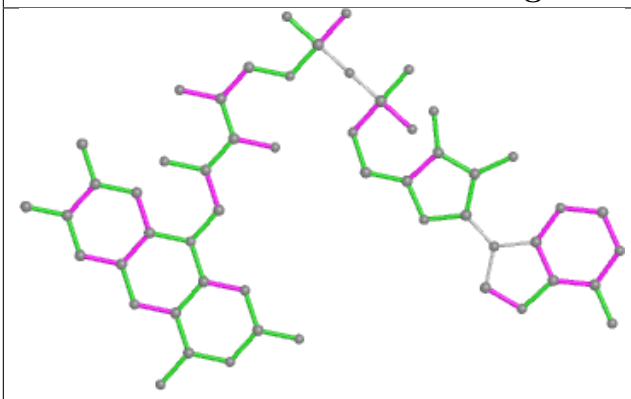


Torsions

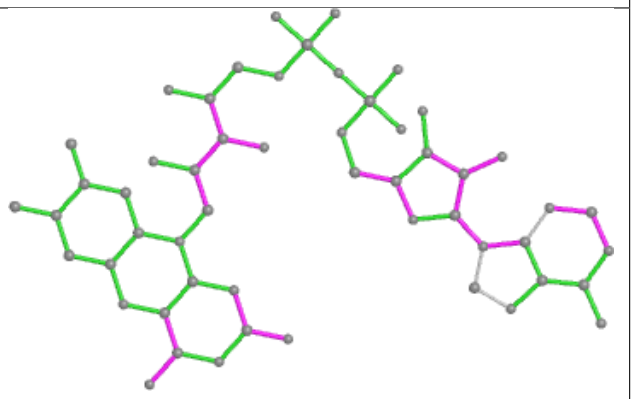


Rings

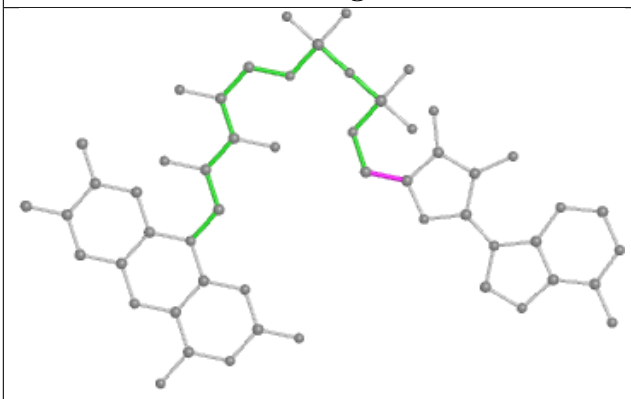
Ligand FAD A 701



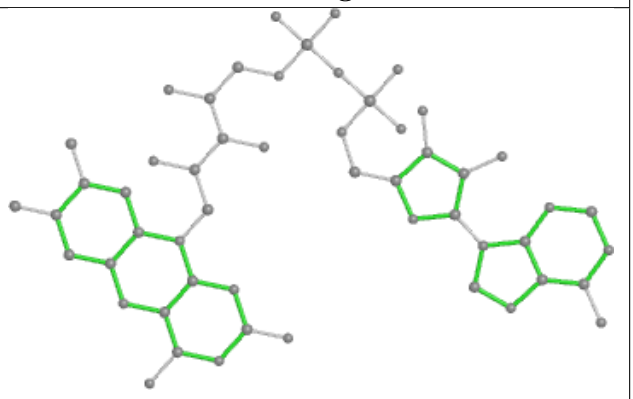
Bond lengths



Bond angles

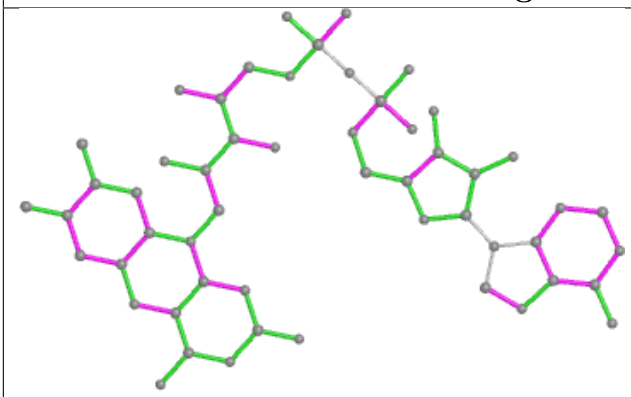


Torsions

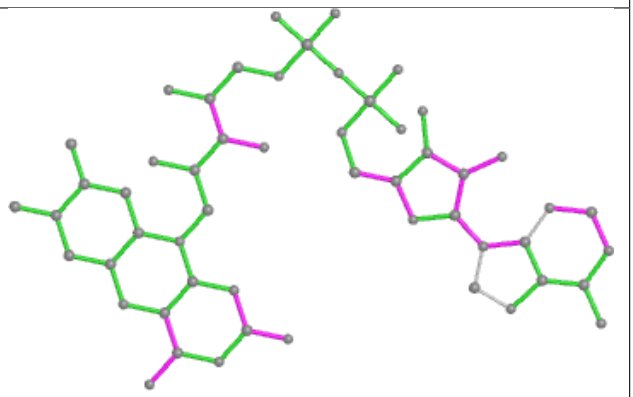


Rings

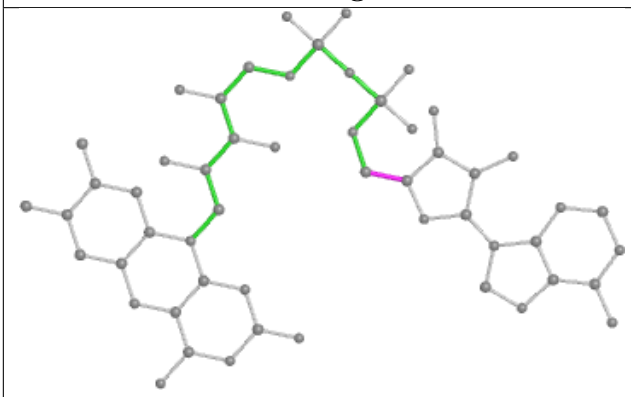
Ligand FAD D 3701



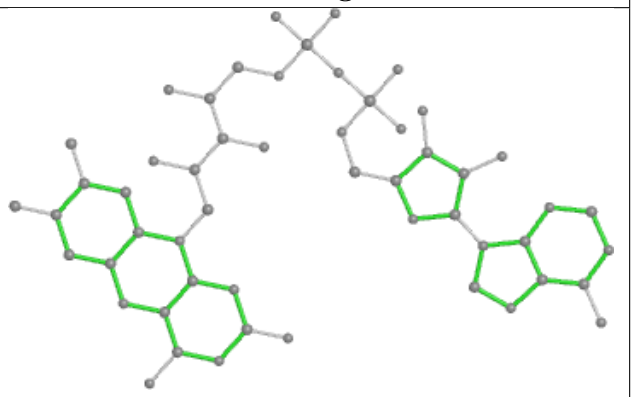
Bond lengths



Bond angles

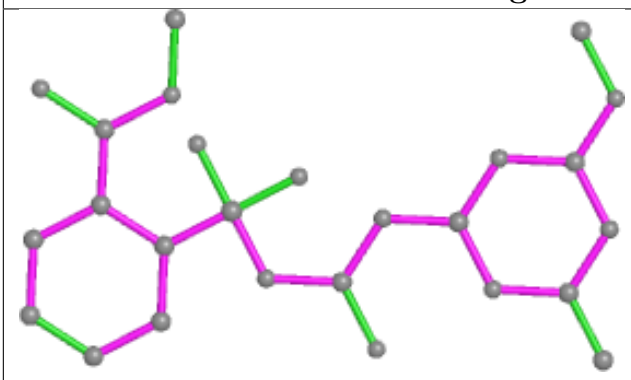


Torsions



Rings

Ligand 1MM C 3695



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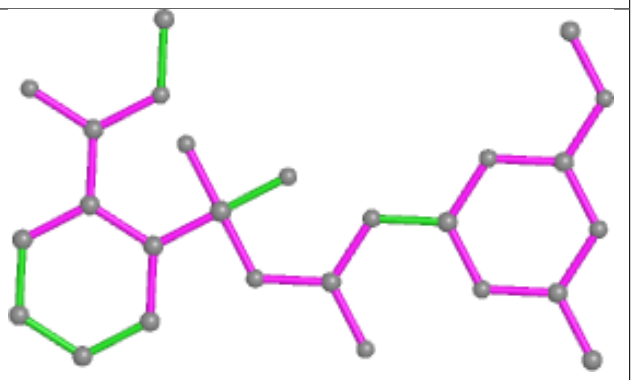
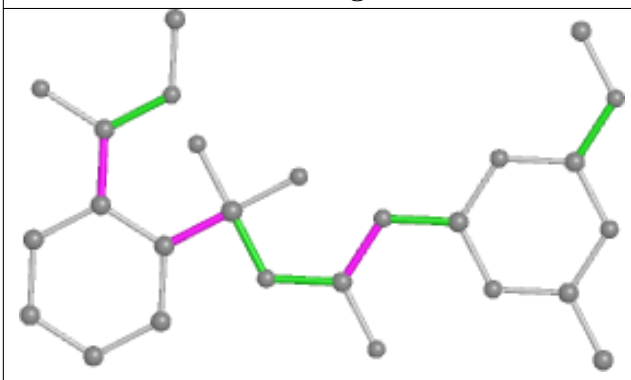
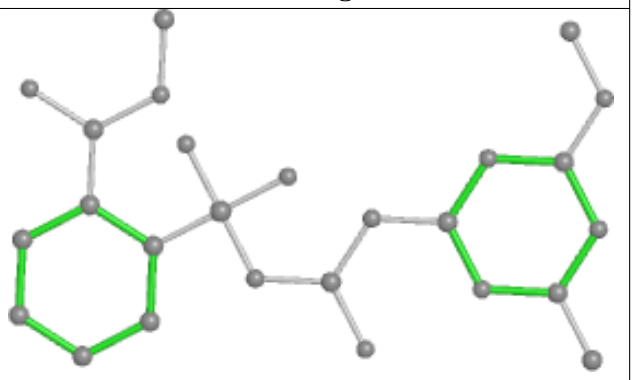


Bond angles

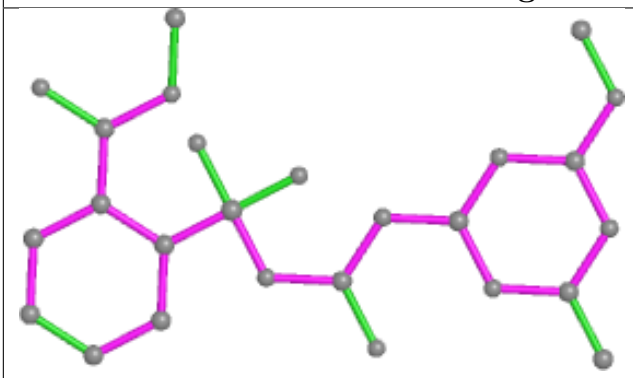


Torsions

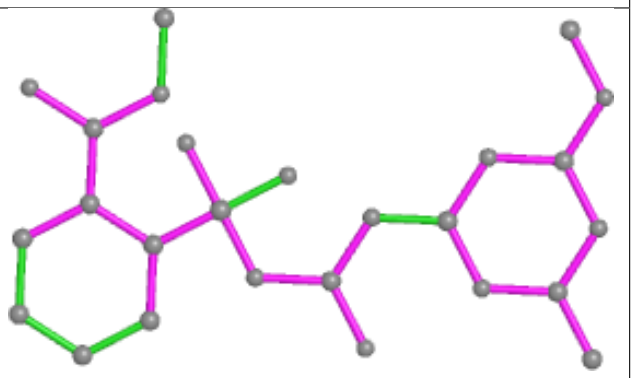


Rings

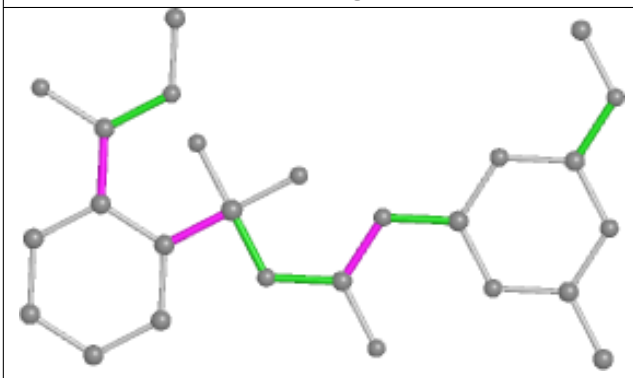
Ligand 1MM A 695



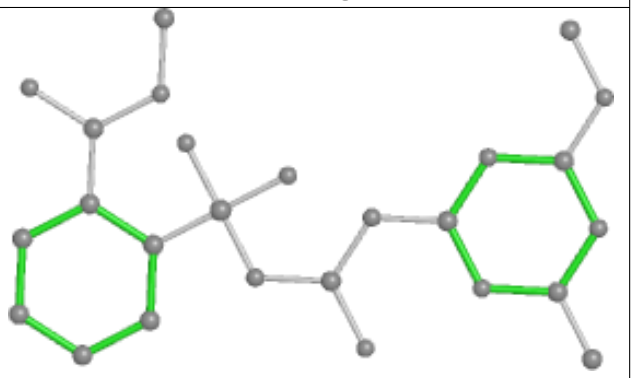
Bond lengths



Bond angles

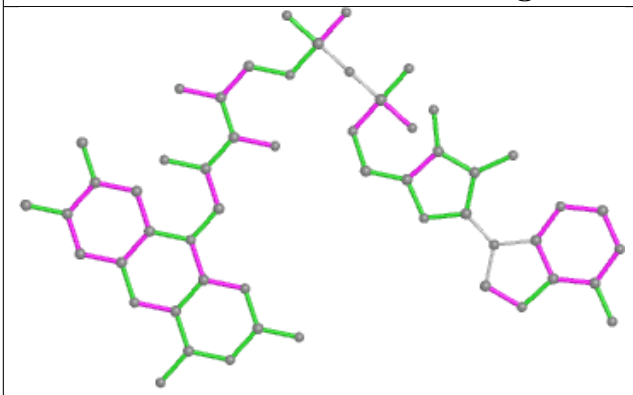


Torsions

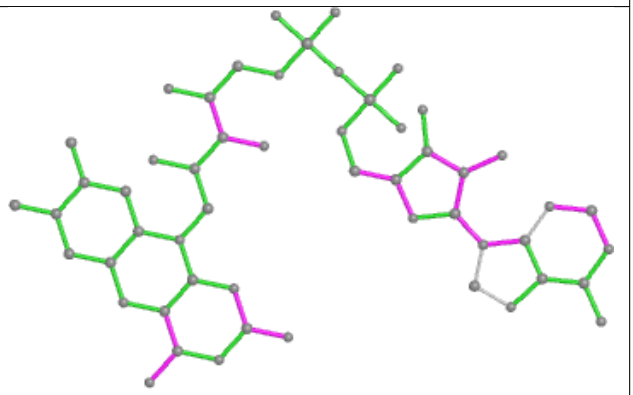


Rings

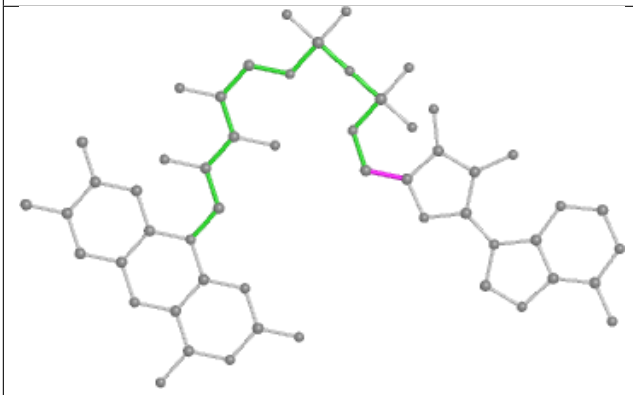
Ligand FAD C 2701



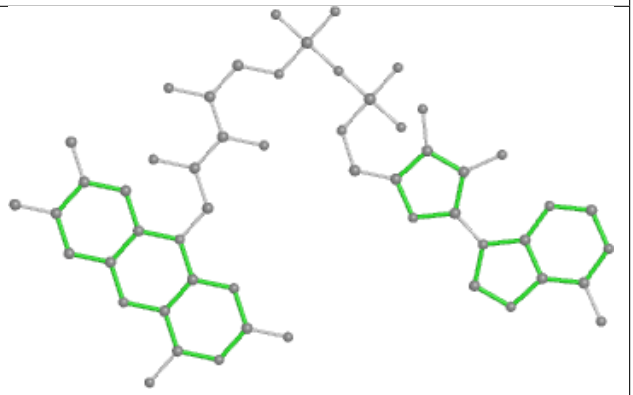
Bond lengths



Bond angles



Torsions



Rings

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	A	596/677 (88%)	-0.25	1 (0%) 95 96	15, 25, 41, 76	0
1	B	582/677 (85%)	-0.14	5 (0%) 84 88	19, 38, 62, 84	0
1	C	575/677 (84%)	0.48	72 (12%) 3 5	23, 49, 99, 114	0
1	D	596/677 (88%)	-0.30	1 (0%) 95 96	18, 28, 43, 74	1 (0%)
All	All	2349/2708 (86%)	-0.06	79 (3%) 45 52	15, 32, 77, 114	1 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	438	ILE	6.9
1	C	264	THR	5.5
1	C	445	SER	5.3
1	C	263	PRO	5.2
1	C	432	GLY	5.0
1	C	293	ALA	4.7
1	C	298	LEU	4.7
1	C	449	ALA	4.7
1	C	431	LEU	4.6
1	C	304	LEU	4.2
1	C	444	ARG	4.1
1	C	447	TRP	4.0
1	C	320	LEU	4.0
1	C	296	ILE	3.9
1	C	265	LYS	3.8
1	C	436	SER	3.8
1	C	439	PHE	3.7
1	C	327	ALA	3.7
1	C	434	MET	3.7
1	C	441	VAL	3.6
1	C	323	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	451	ILE	3.6
1	C	440	PRO	3.6
1	C	458	TYR	3.5
1	C	329	ILE	3.4
1	D	132[A]	ASN	3.4
1	C	299	ALA	3.4
1	C	262	ILE	3.4
1	C	402	GLY	3.2
1	C	313	HIS	3.2
1	C	297	ASN	3.2
1	C	341	PHE	3.1
1	C	364	VAL	3.1
1	C	406	PHE	3.1
1	B	439	PHE	3.0
1	C	294	ASP	3.0
1	C	448	PHE	2.9
1	C	467	PRO	2.9
1	C	443	GLU	2.8
1	C	401	GLY	2.7
1	C	657	GLY	2.7
1	C	454	TRP	2.7
1	C	385	ILE	2.7
1	C	370	ILE	2.6
1	C	389	ALA	2.6
1	C	303	VAL	2.5
1	C	347	LYS	2.5
1	C	368	ASP	2.5
1	C	326	ARG	2.5
1	B	86	ASP	2.5
1	C	305	TYR	2.5
1	C	346	PRO	2.5
1	C	433	LYS	2.4
1	C	667	PHE	2.4
1	C	350	ASP	2.4
1	C	260	ASN	2.4
1	C	435	MET	2.3
1	C	328	GLN	2.3
1	C	485	ASN	2.3
1	C	398	GLU	2.3
1	B	440	PRO	2.3
1	C	427	ALA	2.3
1	C	669	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	302	PRO	2.3
1	C	340	SER	2.3
1	C	671	VAL	2.2
1	C	361	ASN	2.2
1	C	453	LYS	2.2
1	B	284	PHE	2.1
1	C	322	GLU	2.1
1	C	403	ILE	2.1
1	C	395	ALA	2.1
1	C	396	ALA	2.1
1	B	436	SER	2.1
1	C	332	THR	2.0
1	C	686	LYS	2.0
1	A	277	THR	2.0
1	C	437	LYS	2.0
1	C	668	ASP	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
6	PYD	D	3703	9/9	0.81	0.24	43,46,49,51	0
6	PYD	C	2703	9/9	0.84	0.27	39,40,42,44	0
6	PYD	A	703	9/9	0.90	0.22	33,37,39,39	0
6	PYD	B	1703	9/9	0.90	0.26	35,37,38,38	0
3	MG	C	3699	1/1	0.96	0.08	36,36,36,36	0
2	K	C	3696	1/1	0.97	0.06	61,61,61,61	0
3	MG	D	2699	1/1	0.97	0.07	24,24,24,24	0

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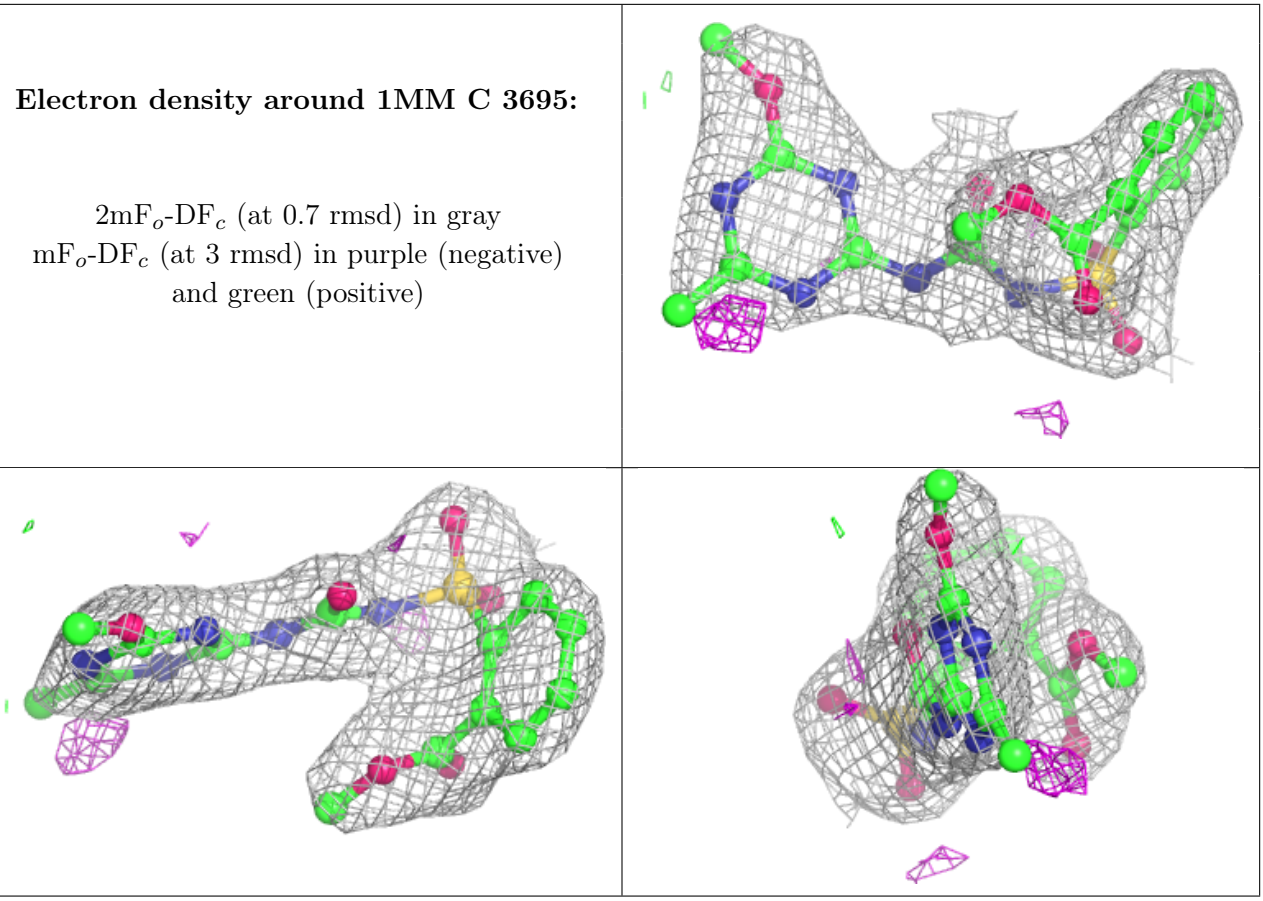
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	1MM	C	3695	26/26	0.97	0.17	48,51,53,56	0
5	FAD	C	2701	53/53	0.97	0.14	48,51,55,57	0
7	P25	B	698	14/14	0.97	0.12	25,29,42,44	0
4	1MM	A	695	26/26	0.98	0.14	21,25,30,30	0
5	FAD	B	1701	53/53	0.98	0.12	30,33,36,37	0
4	1MM	B	1695	26/26	0.98	0.12	30,35,38,39	0
7	P25	A	1698	14/14	0.98	0.14	18,22,33,36	0
4	1MM	C	2695	26/26	0.98	0.12	27,30,31,34	0
8	P22	C	3702	11/11	0.98	0.12	38,40,44,45	0
2	K	D	2696	1/1	0.99	0.12	26,26,26,26	0
5	FAD	A	701	53/53	0.99	0.15	13,18,23,24	0
3	MG	A	1699	1/1	0.99	0.08	19,19,19,19	0
3	MG	B	699	1/1	0.99	0.04	25,25,25,25	0
5	FAD	D	3701	53/53	0.99	0.13	17,21,24,25	0
2	K	B	696	1/1	0.99	0.06	45,45,45,45	0
8	P22	D	2702	11/11	0.99	0.12	21,24,27,30	0
2	K	A	1696	1/1	1.00	0.12	24,24,24,24	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.

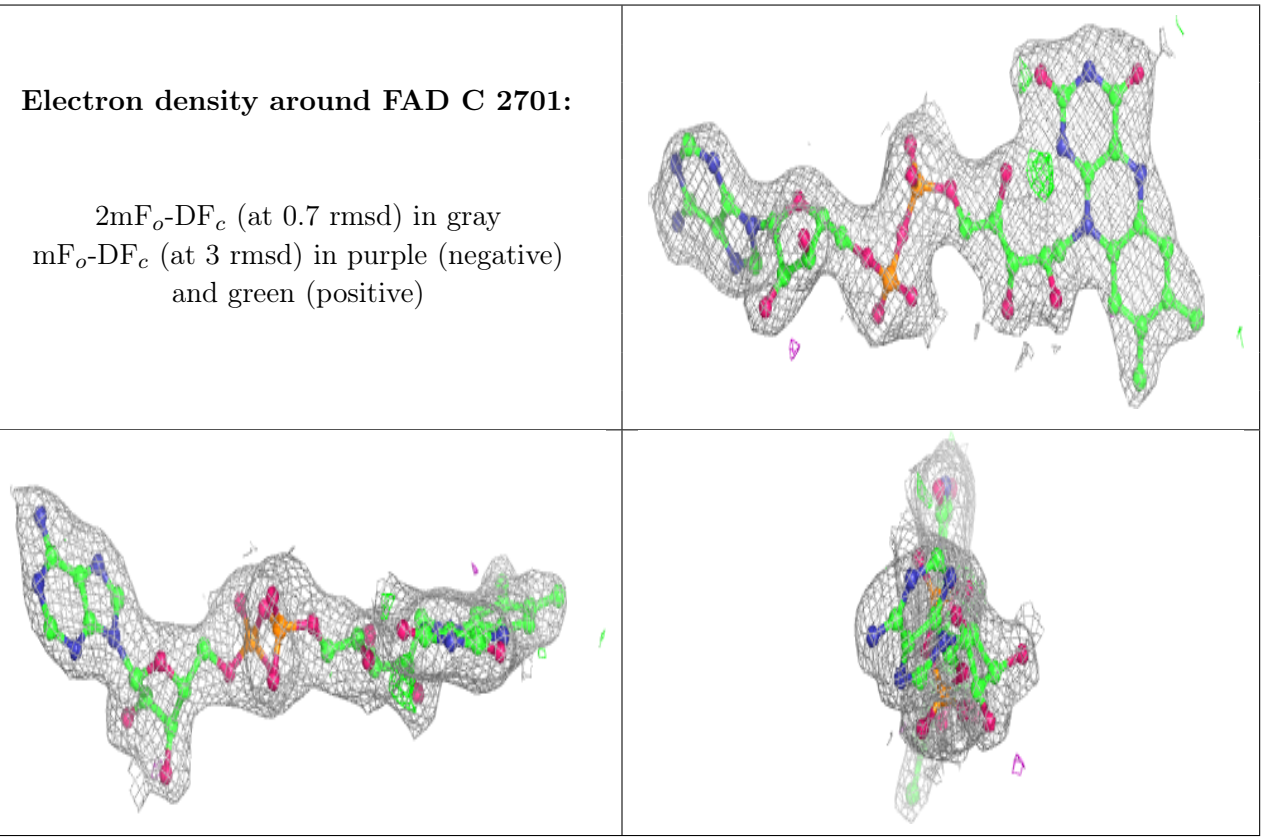
Electron density around 1MM C 3695:

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



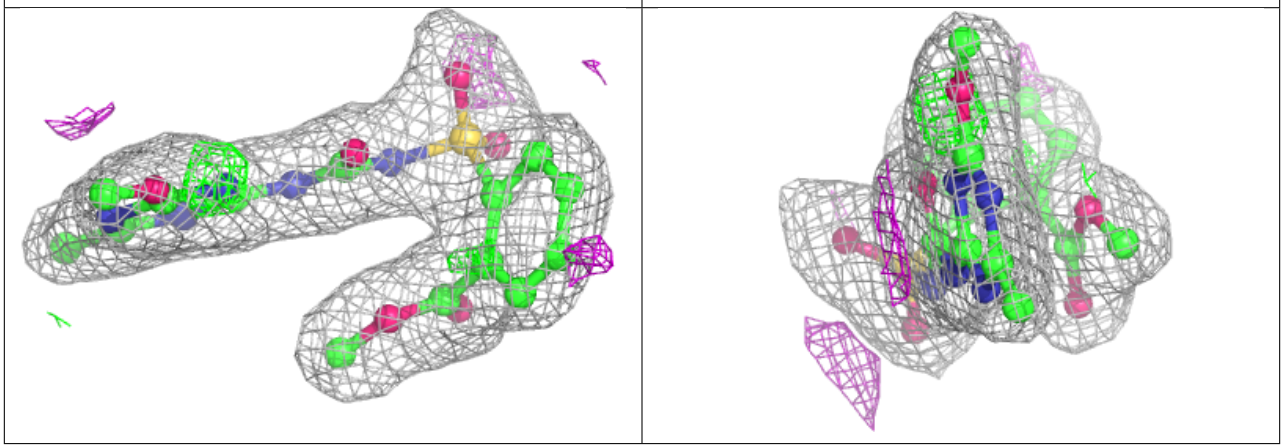
Electron density around FAD C 2701:

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



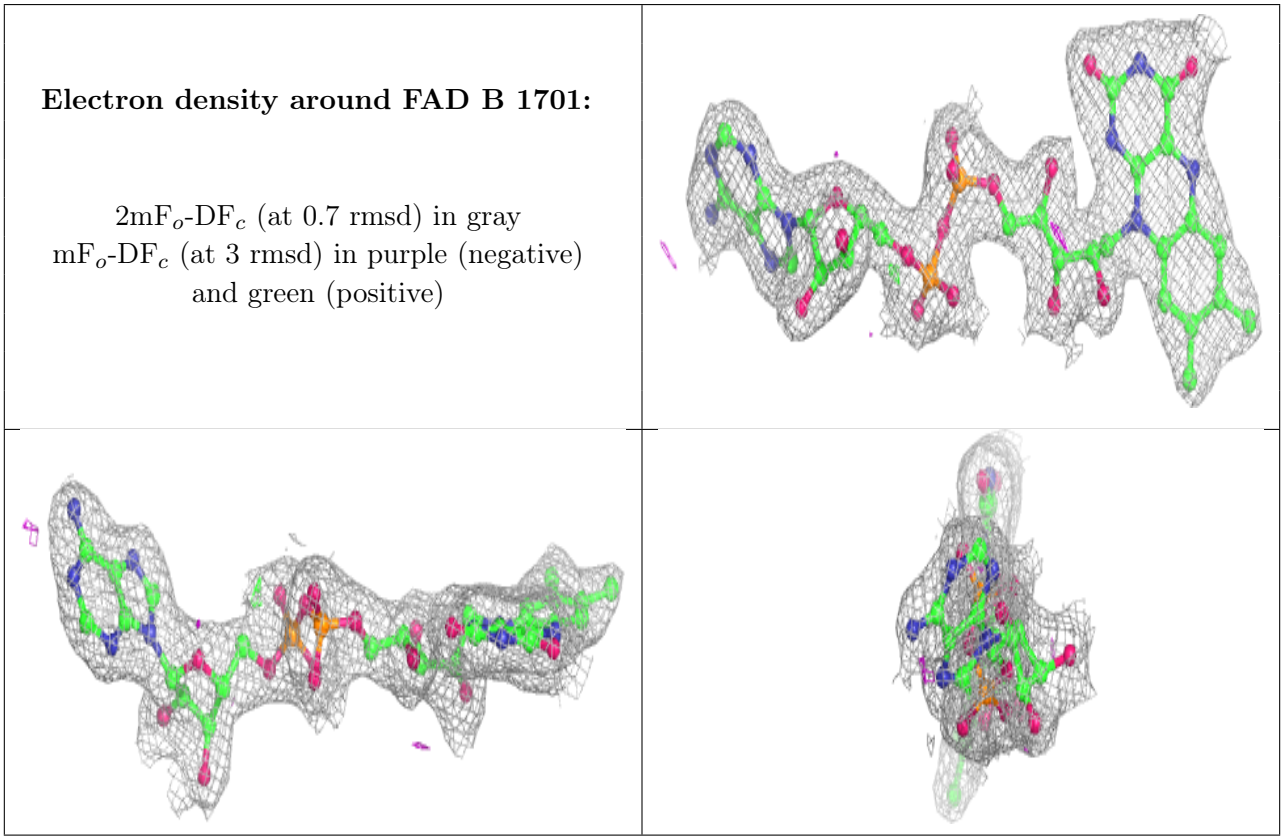
Electron density around 1MM A 695:

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



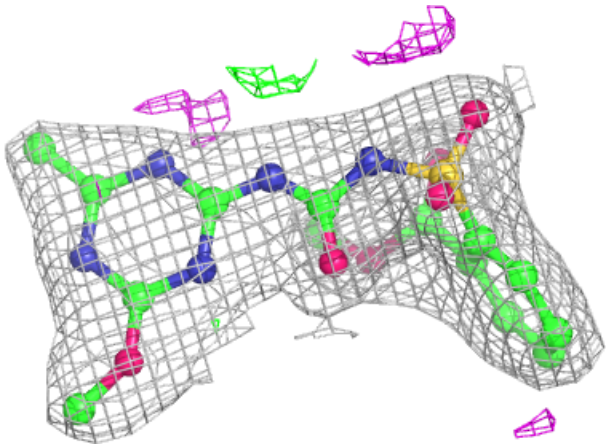
Electron density around FAD B 1701:

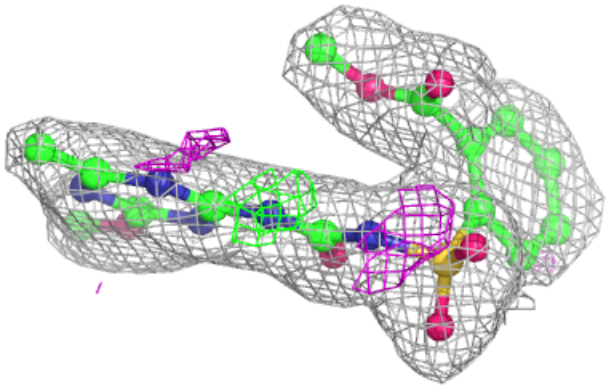
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

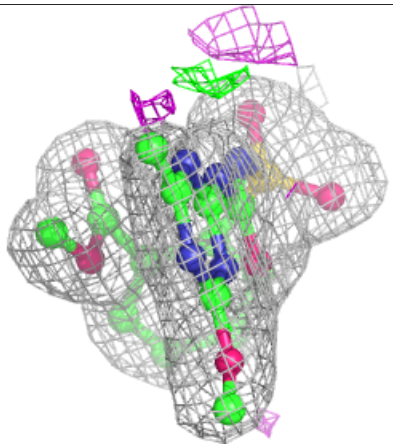


Electron density around 1MM B 1695:

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

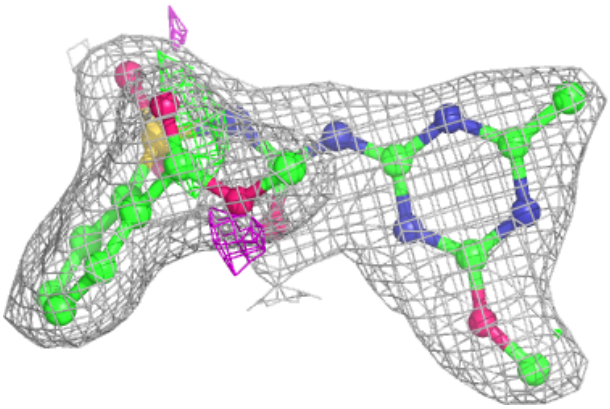


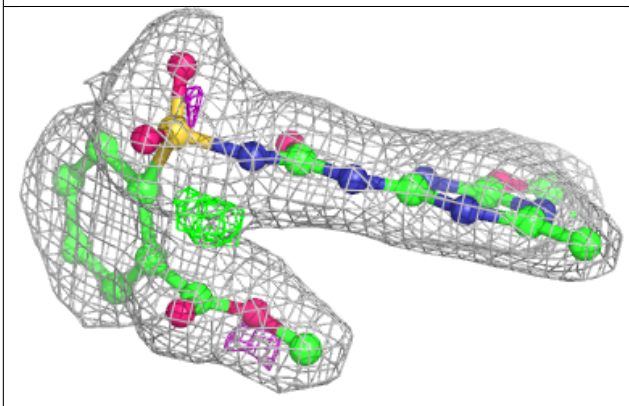


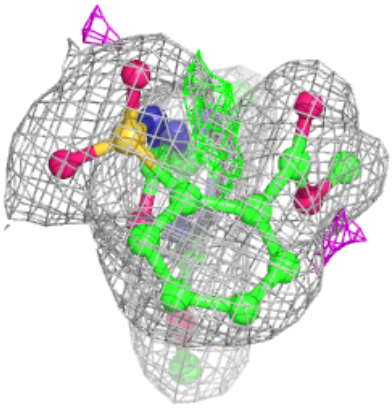


Electron density around 1MM C 2695:

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

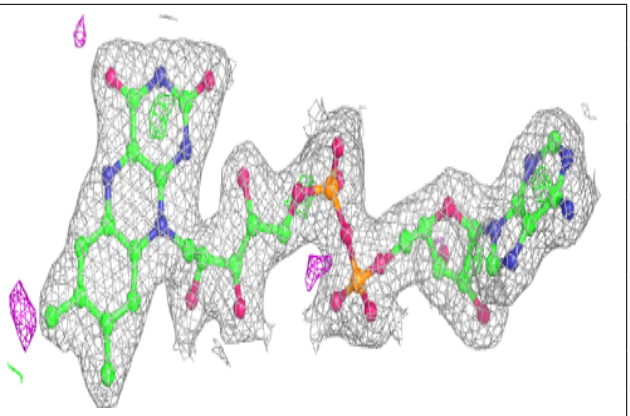


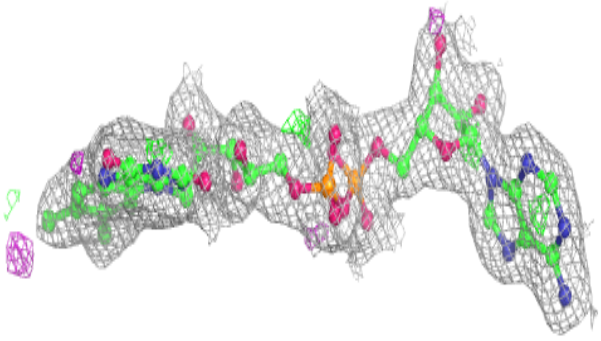


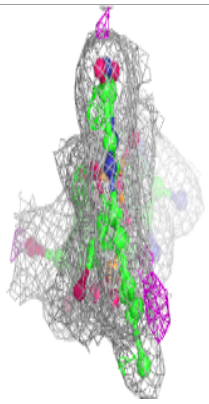


Electron density around FAD A 701:

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

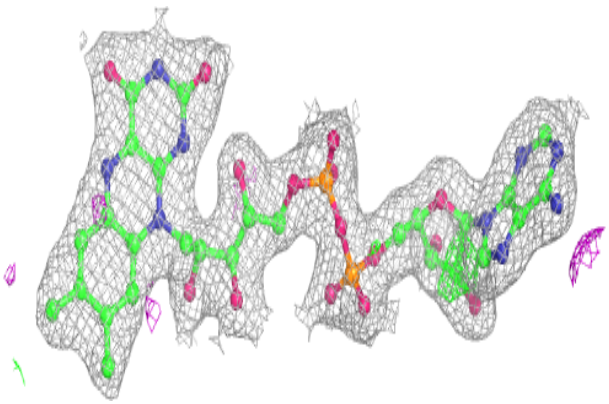


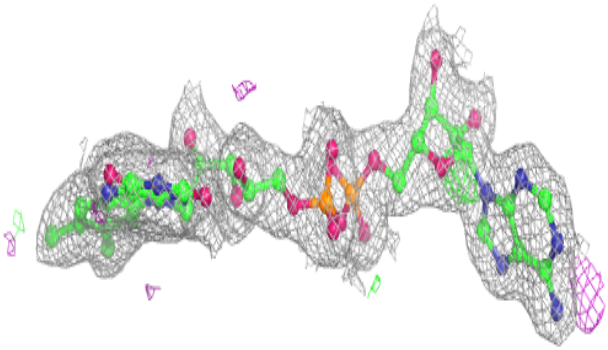


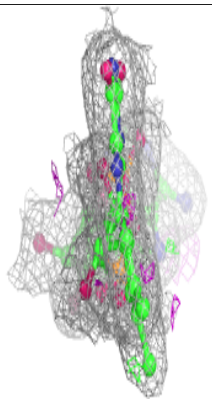


Electron density around FAD D 3701:

$2mF_o$-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.