



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 04:13 PM EDT

PDB ID : 1Y9D
Title : Pyruvate Oxidase variant V265A from *Lactobacillus plantarum*
Authors : Wille, G.; Ritter, M.; Weiss, M.S.; Konig, S.; Mantele, W.; Hubner, G.
Deposited on : 2004-12-15
Resolution : 2.20 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 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 : 2.23.2
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) : 2.23.2

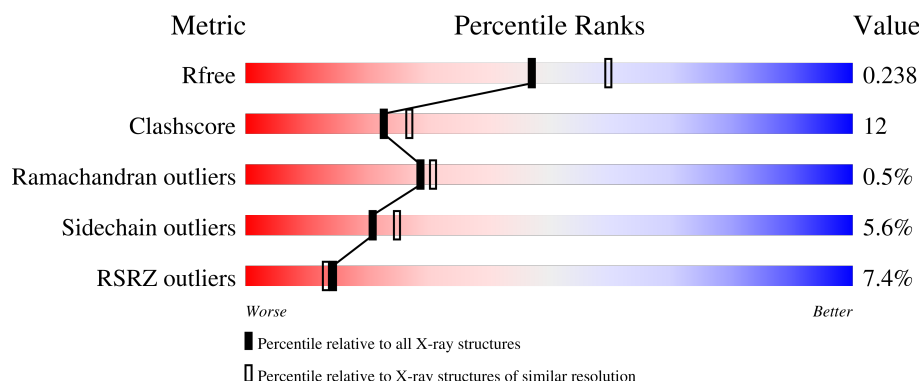
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	603	<div> <div>9%</div> <div> <div></div> <div>73%</div> <div>16%</div> <div>• 7%</div> </div> </div>
1	B	603	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>18%</div> <div>• 5%</div> </div> </div>
1	C	603	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>• 8%</div> </div> </div>
1	D	603	<div> <div>7%</div> <div> <div></div> <div>72%</div> <div>18%</div> <div>• 7%</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19404 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pyruvate oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	0
			4298	2722	746	818	12			
1	B	572	Total	C	N	O	S	0	0	0
			4423	2804	767	839	13			
1	C	556	Total	C	N	O	S	0	0	0
			4282	2711	744	815	12			
1	D	560	Total	C	N	O	S	0	0	0
			4315	2732	748	823	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	ALA	VAL	engineered mutation	UNP P37063
B	265	ALA	VAL	engineered mutation	UNP P37063
C	265	ALA	VAL	engineered mutation	UNP P37063
D	265	ALA	VAL	engineered mutation	UNP P37063

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

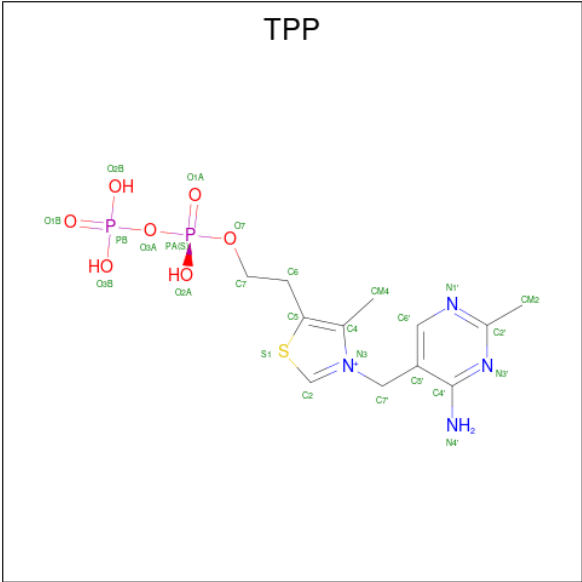
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



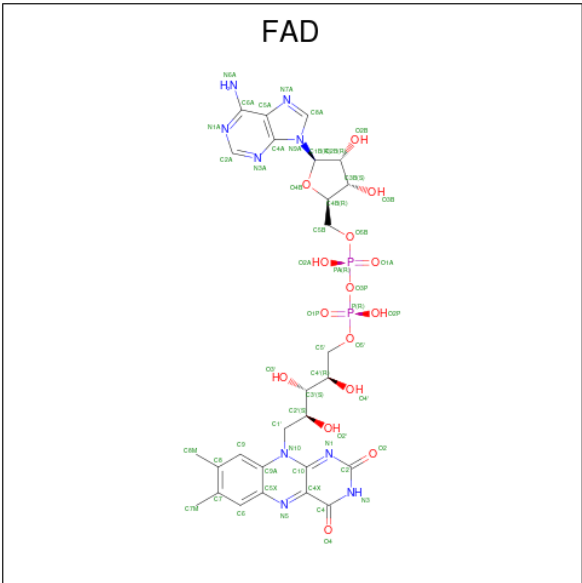
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



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

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

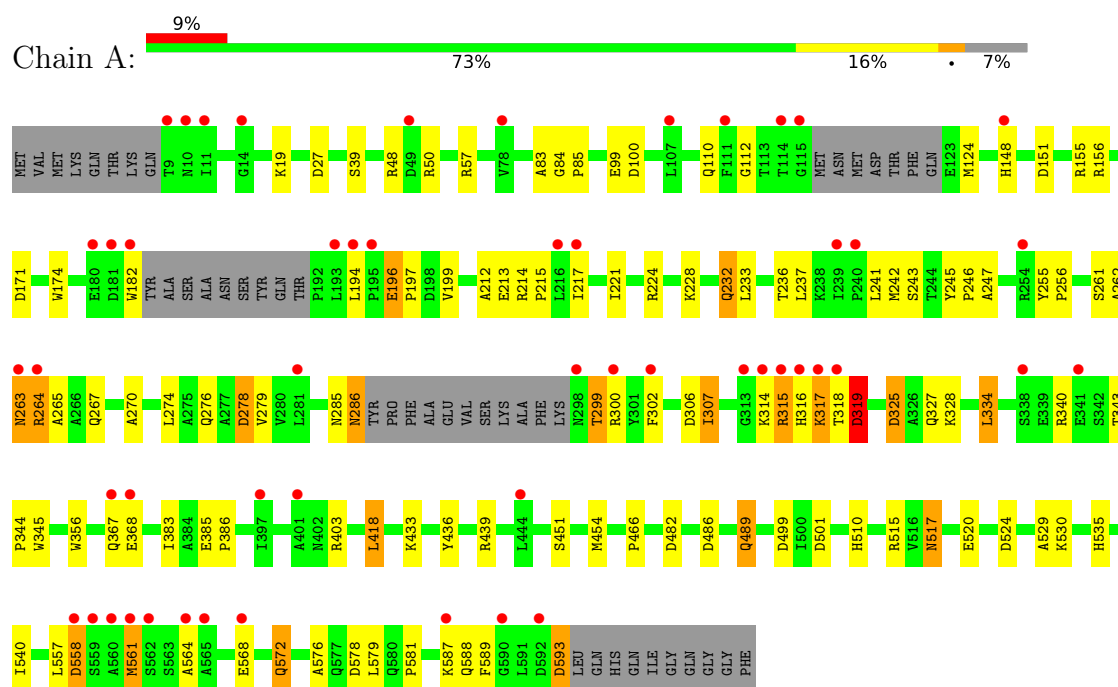
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	402	Total	O	0	0
			402	402		
7	B	532	Total	O	0	0
			532	532		
7	C	426	Total	O	0	0
			426	426		
7	D	488	Total	O	0	0
			488	488		

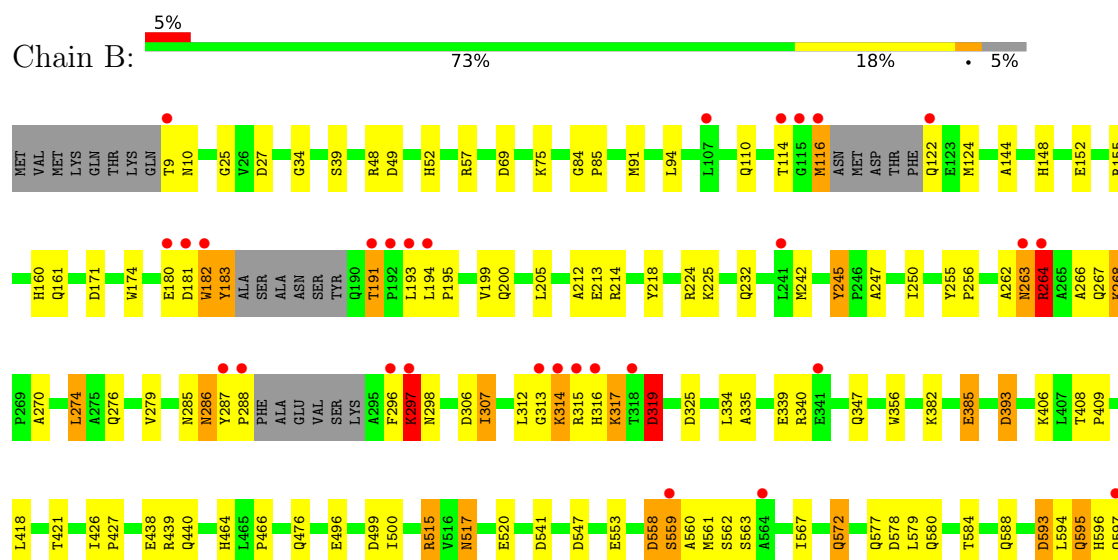
3 Residue-property plots [i](#)

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

• Molecule 1: Pyruvate oxidase



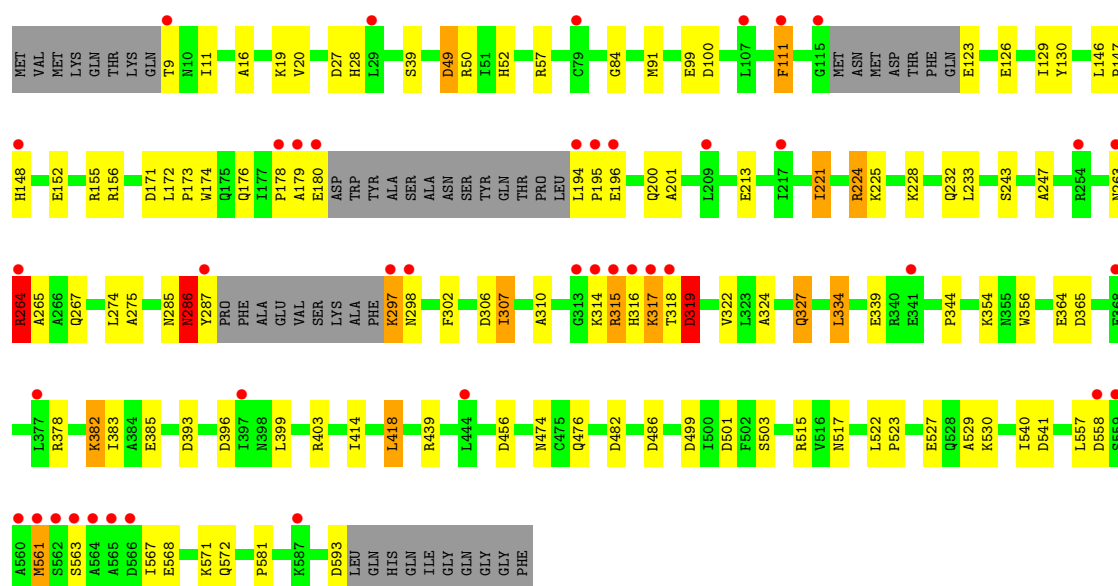
• Molecule 1: Pyruvate oxidase



ILE
GLY
GLN
GLY
GLY
PHE

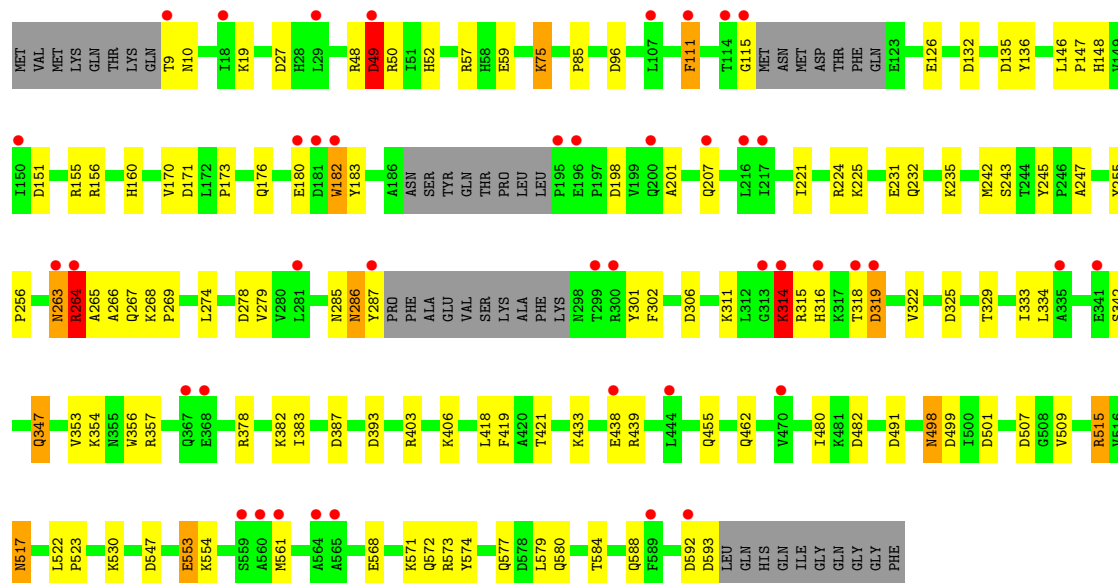
• Molecule 1: Pyruvate oxidase

Chain C: 7% 73% 17% 8%



• Molecule 1: Pyruvate oxidase

Chain D: 7% 72% 18% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.66Å 155.78Å 100.75Å 90.00° 92.92° 90.00°	Depositor
Resolution (Å)	27.30 – 2.20 27.32 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (27.30-2.20) 99.7 (27.32-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.178 , 0.238 0.179 , 0.238	Depositor DCC
R_{free} test set	7369 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19404	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, TPP, FAD, MG, SO4

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	0.74	0/4383	0.89	14/5964 (0.2%)
1	B	0.92	2/4513 (0.0%)	0.94	16/6141 (0.3%)
1	C	0.82	0/4365	0.90	14/5937 (0.2%)
1	D	0.82	1/4401 (0.0%)	0.91	24/5988 (0.4%)
All	All	0.83	3/17662 (0.0%)	0.91	68/24030 (0.3%)

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	A	0	1
1	B	0	2
1	C	0	2
1	D	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	268	LYS	CE-NZ	7.43	1.67	1.49
1	B	268	LYS	CD-CE	5.81	1.65	1.51
1	D	182	TRP	CB-CG	5.10	1.59	1.50

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	ASP	CB-CG-OD2	8.35	125.81	118.30
1	D	27	ASP	CB-CG-OD2	8.10	125.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	439	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A	524	ASP	CB-CG-OD2	7.47	125.03	118.30
1	D	491	ASP	CB-CG-OD2	6.92	124.52	118.30
1	A	578	ASP	CB-CG-OD2	6.88	124.50	118.30
1	D	515	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	B	593	ASP	CB-CG-OD2	6.55	124.20	118.30
1	A	325	ASP	CB-CG-OD2	6.38	124.04	118.30
1	B	541	ASP	CB-CG-OD2	6.34	124.00	118.30
1	B	499	ASP	CB-CG-OD2	6.12	123.81	118.30
1	D	593	ASP	CB-CG-OD2	6.09	123.78	118.30
1	B	547	ASP	CB-CG-OD2	6.08	123.77	118.30
1	C	365	ASP	CB-CG-OD2	6.07	123.77	118.30
1	A	482	ASP	CB-CG-OD2	6.02	123.72	118.30
1	C	171	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	306	ASP	CB-CG-OD2	6.01	123.71	118.30
1	C	49	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	27	ASP	CB-CG-OD2	5.97	123.67	118.30
1	B	515	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	C	499	ASP	CB-CG-OD2	5.95	123.65	118.30
1	B	69	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	274	LEU	CB-CG-CD1	-5.91	100.95	111.00
1	C	319	ASP	CB-CG-OD2	5.89	123.60	118.30
1	D	135	ASP	CB-CG-OD2	5.82	123.54	118.30
1	D	325	ASP	CB-CG-OD2	5.79	123.52	118.30
1	B	558	ASP	CB-CG-OD2	5.77	123.49	118.30
1	D	579	LEU	CA-CB-CG	5.77	128.56	115.30
1	D	439	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	C	306	ASP	CB-CG-OD2	5.76	123.48	118.30
1	B	319	ASP	CB-CG-OD2	5.72	123.45	118.30
1	C	456	ASP	CB-CG-OD2	5.70	123.42	118.30
1	D	547	ASP	CB-CG-OD2	5.67	123.41	118.30
1	A	100	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	499	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	578	ASP	CB-CG-OD2	5.63	123.37	118.30
1	D	151	ASP	CB-CG-OD2	5.60	123.34	118.30
1	C	482	ASP	CB-CG-OD2	5.58	123.32	118.30
1	C	541	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	558	ASP	CB-CG-OD2	5.57	123.31	118.30
1	D	96	ASP	CB-CG-OD2	5.57	123.31	118.30
1	D	499	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	319	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	486	ASP	CB-CG-OD2	5.48	123.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	264	ARG	N-CA-C	5.46	125.74	111.00
1	D	49	ASP	CB-CG-OD2	5.43	123.18	118.30
1	C	593	ASP	CB-CG-OD2	5.41	123.17	118.30
1	D	278	ASP	CB-CG-OD2	5.41	123.17	118.30
1	C	27	ASP	CB-CG-OD2	5.41	123.17	118.30
1	C	100	ASP	CB-CG-OD2	5.40	123.16	118.30
1	D	198	ASP	CB-CG-OD2	5.38	123.14	118.30
1	D	171	ASP	CB-CG-OD2	5.35	123.12	118.30
1	B	181	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	306	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	151	ASP	CB-CG-OD2	5.30	123.07	118.30
1	C	486	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	314	LYS	N-CA-C	5.28	125.25	111.00
1	D	501	ASP	CB-CG-OD1	5.28	123.05	118.30
1	B	579	LEU	CA-CB-CG	5.24	127.35	115.30
1	D	482	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	171	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	278	ASP	CB-CG-OD2	5.15	122.94	118.30
1	D	132	ASP	CB-CG-OD2	5.13	122.92	118.30
1	D	515	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	D	387	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	393	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	403	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	D	507	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	264	ARG	Peptide
1	B	264	ARG	Peptide
1	B	312	LEU	Peptide
1	C	264	ARG	Peptide
1	C	265	ALA	Peptide
1	D	264	ARG	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	A	4298	0	4260	97	0
1	B	4423	0	4377	116	0
1	C	4282	0	4249	94	0
1	D	4315	0	4264	99	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
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	26	0	16	0	0
5	B	26	0	16	1	0
5	C	26	0	16	0	0
5	D	26	0	16	1	0
6	A	27	0	12	2	0
6	B	27	0	12	1	0
6	C	27	0	12	1	0
6	D	27	0	12	1	0
7	A	402	0	0	37	0
7	B	532	0	0	46	0
7	C	426	0	0	25	0
7	D	488	0	0	40	0
All	All	19404	0	17262	401	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 12.

All (401) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:LYS:NZ	1:B:268:LYS:CE	1.67	1.53
1:B:286:ASN:HB2	7:B:3415:HOH:O	1.16	1.32
1:D:318:THR:HG22	7:D:3379:HOH:O	1.39	1.23
1:A:155:ARG:HD3	7:A:3196:HOH:O	1.53	1.08
7:A:3092:HOH:O	1:B:155:ARG:HD3	1.55	1.07
1:C:286:ASN:HB2	7:C:2934:HOH:O	1.54	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:THR:HA	7:D:3235:HOH:O	1.57	1.04
1:C:155:ARG:HD2	7:D:3010:HOH:O	1.59	1.03
1:D:342:SER:HB3	1:D:347:GLN:HE22	1.25	1.01
1:C:19:LYS:NZ	1:C:50:ARG:HH21	1.61	0.98
1:A:368:GLU:HB3	7:A:3182:HOH:O	1.64	0.98
1:C:267:GLN:HE21	1:C:356:TRP:HE1	1.12	0.98
1:B:561:MET:HA	7:B:2979:HOH:O	1.62	0.97
1:B:285:ASN:O	1:B:286:ASN:ND2	1.98	0.97
1:D:319:ASP:HB3	7:D:3267:HOH:O	1.64	0.96
1:A:489:GLN:HG2	7:A:3173:HOH:O	1.65	0.96
1:B:319:ASP:HB3	7:B:2987:HOH:O	1.64	0.95
1:D:286:ASN:HB2	7:D:3370:HOH:O	1.67	0.92
1:B:267:GLN:HE21	1:B:356:TRP:HE1	1.14	0.92
1:D:267:GLN:HE21	1:D:356:TRP:HE1	1.13	0.92
1:B:110:GLN:HG2	7:B:3341:HOH:O	1.69	0.91
1:B:148:HIS:HB2	7:B:2968:HOH:O	1.70	0.90
1:C:19:LYS:HZ2	1:C:50:ARG:HH21	1.13	0.90
1:A:182:TRP:CZ3	7:A:3157:HOH:O	2.24	0.88
1:A:267:GLN:HE21	1:A:356:TRP:HE1	1.20	0.87
1:B:116:MET:CG	7:B:3346:HOH:O	2.23	0.85
1:D:49:ASP:HB3	7:D:3046:HOH:O	1.77	0.85
1:B:264:ARG:O	1:B:264:ARG:HG3	1.77	0.83
1:B:152:GLU:OE1	1:B:155:ARG:NH1	2.11	0.83
1:B:593:ASP:OD2	1:B:594:LEU:N	2.13	0.82
1:A:299:THR:HG21	7:A:3118:HOH:O	1.78	0.81
1:A:558:ASP:HB3	1:A:561:MET:HB2	1.60	0.81
1:C:287:TYR:HB3	1:C:315:ARG:HD2	1.61	0.81
1:C:152:GLU:OE1	1:C:155:ARG:NH2	2.14	0.80
1:B:116:MET:HG3	7:B:3346:HOH:O	1.81	0.80
1:A:568:GLU:HB3	7:A:2964:HOH:O	1.80	0.80
1:C:286:ASN:O	1:C:286:ASN:ND2	2.15	0.79
1:B:382:LYS:HD3	7:B:3323:HOH:O	1.85	0.77
1:B:182:TRP:CE3	1:B:183:TYR:HA	2.19	0.77
1:C:148:HIS:HB2	7:C:2979:HOH:O	1.83	0.77
1:A:262:ALA:O	1:A:263:ASN:HB2	1.83	0.77
1:C:267:GLN:NE2	1:C:356:TRP:HE1	1.83	0.77
1:C:567:ILE:O	1:C:571:LYS:HG3	1.85	0.76
1:B:182:TRP:HB3	7:B:3416:HOH:O	1.84	0.76
1:D:267:GLN:NE2	1:D:356:TRP:HE1	1.84	0.75
1:B:114:THR:HG23	7:B:3333:HOH:O	1.88	0.74
1:D:49:ASP:OD2	1:D:50:ARG:NH2	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:523:PRO:O	1:C:527:GLU:HG2	1.88	0.73
1:C:224:ARG:HD3	7:C:3105:HOH:O	1.88	0.73
1:D:285:ASN:O	1:D:286:ASN:ND2	2.18	0.73
1:B:267:GLN:NE2	1:B:356:TRP:HE1	1.84	0.73
1:A:267:GLN:NE2	1:A:356:TRP:HE1	1.86	0.72
1:B:182:TRP:HE3	1:B:183:TYR:HA	1.52	0.72
1:D:148:HIS:CD2	7:D:3337:HOH:O	2.41	0.72
1:B:347:GLN:HG2	7:B:3029:HOH:O	1.88	0.72
1:B:553:GLU:HB3	7:B:3339:HOH:O	1.90	0.72
1:A:564:ALA:O	1:A:568:GLU:HG2	1.89	0.72
1:C:57:ARG:HD2	7:C:2988:HOH:O	1.90	0.72
1:D:264:ARG:HA	1:D:266:ALA:H	1.55	0.71
1:A:299:THR:CG2	7:A:3118:HOH:O	2.33	0.71
1:D:406:LYS:HE3	7:D:2929:HOH:O	1.89	0.71
1:A:196:GLU:HB2	1:A:197:PRO:HD3	1.72	0.71
1:A:110:GLN:HG3	7:A:3138:HOH:O	1.89	0.71
1:D:286:ASN:O	1:D:286:ASN:CG	2.29	0.71
1:A:433:LYS:HE2	1:A:466:PRO:HD2	1.73	0.70
1:B:116:MET:HG2	7:B:3346:HOH:O	1.87	0.70
1:C:314:LYS:O	1:C:314:LYS:HG2	1.91	0.70
1:C:319:ASP:OD2	1:C:319:ASP:N	2.25	0.70
1:C:9:THR:HA	7:C:3213:HOH:O	1.90	0.70
1:B:183:TYR:CE2	7:B:2973:HOH:O	2.45	0.70
1:A:50:ARG:HD2	7:A:2860:HOH:O	1.92	0.69
1:B:286:ASN:ND2	1:B:286:ASN:O	2.24	0.69
1:D:243:SER:HB2	1:D:247:ALA:HB3	1.73	0.69
1:D:342:SER:CB	1:D:347:GLN:HE22	2.05	0.69
1:D:342:SER:HB3	1:D:347:GLN:NE2	2.06	0.68
1:A:535:HIS:ND1	7:A:2990:HOH:O	2.26	0.68
1:B:270:ALA:O	1:B:274:LEU:CD1	2.42	0.68
1:C:286:ASN:O	1:C:286:ASN:CG	2.32	0.68
1:D:517:ASN:HD22	1:D:517:ASN:H	1.40	0.68
1:B:91:MET:HA	1:B:91:MET:HE2	1.76	0.67
1:D:433:LYS:HE2	7:D:2930:HOH:O	1.93	0.67
1:A:221:ILE:O	1:A:224:ARG:HG3	1.95	0.67
1:C:344:PRO:HD2	7:C:2860:HOH:O	1.93	0.67
1:D:182:TRP:CD1	7:D:3372:HOH:O	2.47	0.67
1:A:315:ARG:HD2	7:A:2910:HOH:O	1.95	0.67
1:B:213:GLU:HG2	1:B:214:ARG:HG3	1.75	0.67
1:C:385:GLU:OE2	7:C:3200:HOH:O	2.13	0.66
7:B:3291:HOH:O	1:D:498:ASN:HB3	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:GLY:HA2	7:B:3247:HOH:O	1.96	0.66
1:A:285:ASN:O	6:A:2603:FAD:H4B	1.94	0.66
1:B:287:TYR:O	1:B:315:ARG:NH2	2.29	0.66
1:B:262:ALA:O	1:B:263:ASN:HB2	1.96	0.65
1:C:568:GLU:HG3	7:C:3047:HOH:O	1.96	0.65
1:C:287:TYR:CB	1:C:315:ARG:HD2	2.27	0.65
1:B:317:LYS:HE2	7:B:3338:HOH:O	1.97	0.64
1:A:242:MET:HE3	1:A:274:LEU:HB2	1.80	0.64
1:D:318:THR:CG2	7:D:3379:HOH:O	2.14	0.64
1:A:367:GLN:O	1:A:368:GLU:HG3	1.97	0.64
1:A:224:ARG:HD3	7:A:3009:HOH:O	1.98	0.64
1:D:438:GLU:HB3	7:D:3166:HOH:O	1.96	0.64
1:D:160:HIS:HD2	7:D:3105:HOH:O	1.79	0.63
1:A:317:LYS:HD2	7:A:2854:HOH:O	1.98	0.63
1:B:593:ASP:CG	1:B:594:LEU:H	2.02	0.63
1:D:263:ASN:O	1:D:266:ALA:HB2	1.98	0.63
1:A:274:LEU:HB3	7:A:3199:HOH:O	1.99	0.62
1:B:335:ALA:HB3	7:B:3431:HOH:O	1.99	0.62
1:B:84:GLY:HA2	1:B:124:MET:HE1	1.81	0.62
1:B:572:GLN:HG2	7:B:3410:HOH:O	1.99	0.62
1:C:19:LYS:NZ	1:C:50:ARG:NH2	2.42	0.62
1:B:594:LEU:HD12	1:B:594:LEU:O	2.00	0.62
1:C:287:TYR:HB3	1:C:315:ARG:CD	2.29	0.62
1:A:383:ILE:HB	1:A:530:LYS:HD2	1.82	0.62
1:C:561:MET:HG3	7:C:3085:HOH:O	1.97	0.62
1:C:111:PHE:HD2	1:C:111:PHE:N	1.97	0.62
1:A:285:ASN:O	6:A:2603:FAD:O1A	2.17	0.62
1:B:25:GLY:O	1:B:75:LYS:HE3	1.98	0.62
7:B:3291:HOH:O	1:D:498:ASN:CB	2.47	0.62
1:A:83:ALA:O	1:A:85:PRO:HD2	2.00	0.61
1:A:214:ARG:N	1:A:278:ASP:OD1	2.26	0.61
1:D:264:ARG:NH2	7:D:3364:HOH:O	2.33	0.61
1:D:553:GLU:HG3	7:D:3388:HOH:O	1.98	0.61
1:A:593:ASP:HB3	7:A:3184:HOH:O	2.01	0.61
1:C:111:PHE:N	1:C:111:PHE:CD2	2.68	0.61
1:D:286:ASN:HA	7:D:2960:HOH:O	2.01	0.61
1:C:364:GLU:HB3	1:C:378:ARG:HB2	1.81	0.61
1:C:501:ASP:OD1	1:C:503:SER:OG	2.16	0.61
1:A:212:ALA:HB2	1:A:279:VAL:HG21	1.83	0.60
1:C:302:PHE:CE2	1:C:316:HIS:HB3	2.36	0.60
1:C:302:PHE:HB2	1:C:318:THR:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ALA:O	1:B:274:LEU:HD12	2.00	0.60
1:B:287:TYR:CD1	1:B:288:PRO:HD2	2.36	0.60
1:B:205:LEU:C	1:B:205:LEU:HD23	2.22	0.60
1:D:182:TRP:HD1	7:D:3372:HOH:O	1.84	0.60
1:C:530:LYS:HE2	7:C:3198:HOH:O	2.02	0.59
1:D:225:LYS:HD2	7:D:3231:HOH:O	2.01	0.59
1:C:39:SER:HB3	1:C:174:TRP:CD2	2.38	0.59
1:D:148:HIS:HB2	7:D:3135:HOH:O	2.02	0.59
1:A:243:SER:HB2	1:A:247:ALA:HB3	1.84	0.59
1:C:287:TYR:CA	1:C:315:ARG:HD2	2.33	0.59
1:B:144:ALA:O	7:B:3416:HOH:O	2.17	0.58
1:A:433:LYS:NZ	7:A:2927:HOH:O	2.36	0.58
1:D:148:HIS:HD2	7:D:3337:HOH:O	1.82	0.58
1:A:262:ALA:O	1:A:263:ASN:CB	2.52	0.58
1:B:264:ARG:O	1:B:264:ARG:CG	2.49	0.58
1:C:11:ILE:HB	1:C:179:ALA:HB2	1.85	0.58
1:C:111:PHE:HD2	1:C:111:PHE:H	1.48	0.57
1:D:245:TYR:HD1	1:D:265:ALA:HB3	1.68	0.57
1:A:232:GLN:HG3	7:A:3194:HOH:O	2.04	0.57
1:A:314:LYS:HB3	7:A:2896:HOH:O	2.05	0.57
1:D:403:ARG:HG3	7:D:3002:HOH:O	2.04	0.57
1:C:557:LEU:HB3	1:C:581:PRO:HD3	1.87	0.57
1:A:182:TRP:HB3	7:A:3142:HOH:O	2.05	0.57
1:B:160:HIS:HD2	7:B:3355:HOH:O	1.87	0.56
1:B:315:ARG:NH2	7:B:3428:HOH:O	2.37	0.56
1:A:343:THR:HB	1:A:344:PRO:HD2	1.87	0.56
7:B:3027:HOH:O	1:D:57:ARG:HD2	2.05	0.56
1:D:75:LYS:HG2	7:D:3359:HOH:O	2.04	0.56
1:D:287:TYR:HB3	1:D:315:ARG:HG3	1.87	0.56
1:A:196:GLU:HA	7:A:3197:HOH:O	2.05	0.56
1:D:52:HIS:CD2	7:D:3182:HOH:O	2.58	0.56
1:C:200:GLN:HG3	7:C:2998:HOH:O	2.05	0.56
1:A:245:TYR:HD1	1:A:265:ALA:HB3	1.70	0.56
1:C:275:ALA:O	1:C:298:ASN:ND2	2.38	0.56
1:B:286:ASN:O	1:B:286:ASN:CG	2.44	0.55
1:C:9:THR:O	1:C:180:GLU:HG3	2.05	0.55
1:C:49:ASP:HB2	7:C:2986:HOH:O	2.07	0.55
1:D:314:LYS:HB3	7:D:3032:HOH:O	2.05	0.55
1:C:19:LYS:HZ1	1:C:50:ARG:HH21	1.50	0.55
1:A:319:ASP:N	7:A:2869:HOH:O	2.39	0.55
1:C:522:LEU:HB2	1:C:523:PRO:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:TRP:HZ3	7:A:3157:HOH:O	1.77	0.55
1:C:316:HIS:CD2	7:C:2850:HOH:O	2.60	0.55
1:D:126:GLU:CG	7:D:3005:HOH:O	2.54	0.55
1:A:245:TYR:HD1	1:A:265:ALA:CB	2.20	0.55
1:C:146:LEU:HB3	1:C:147:PRO:HD3	1.88	0.55
1:D:242:MET:HE1	1:D:274:LEU:HD13	1.89	0.55
1:B:577:GLN:OE1	7:B:3432:HOH:O	2.18	0.54
1:A:367:GLN:HG3	7:A:2921:HOH:O	2.06	0.54
1:A:517:ASN:H	1:A:517:ASN:HD22	1.55	0.54
1:B:161:GLN:HG3	7:B:3225:HOH:O	2.08	0.54
1:B:426:ILE:HB	1:B:427:PRO:HD3	1.88	0.54
1:A:196:GLU:HB2	1:A:197:PRO:CD	2.36	0.54
1:C:243:SER:HB2	1:C:247:ALA:HB3	1.88	0.54
1:C:285:ASN:O	1:C:286:ASN:ND2	2.38	0.54
1:B:57:ARG:HD2	7:D:3114:HOH:O	2.08	0.54
1:B:214:ARG:NH1	1:B:276:GLN:HE21	2.05	0.54
1:D:10:ASN:HB3	1:D:176:GLN:NE2	2.23	0.54
1:D:182:TRP:CE3	1:D:183:TYR:HA	2.43	0.54
1:D:573:ARG:HD3	1:D:574:TYR:CZ	2.44	0.53
1:A:436:TYR:HB3	1:A:439:ARG:HG3	1.91	0.53
1:C:529:ALA:HB2	1:C:540:ILE:HD11	1.90	0.53
1:A:148:HIS:HB2	7:A:2906:HOH:O	2.07	0.53
1:A:276:GLN:HE22	1:A:593:ASP:HA	1.73	0.53
1:A:557:LEU:HB3	1:A:581:PRO:HD3	1.91	0.53
1:D:517:ASN:HD22	1:D:517:ASN:N	2.02	0.53
1:B:225:LYS:HG3	7:B:3089:HOH:O	2.08	0.53
1:B:595:GLN:HG3	1:B:596:HIS:CD2	2.44	0.52
1:C:9:THR:HG21	7:C:2984:HOH:O	2.08	0.52
1:B:595:GLN:HG2	7:B:3409:HOH:O	2.08	0.52
1:A:302:PHE:HB2	1:A:318:THR:HA	1.91	0.52
1:C:172:LEU:HB2	1:C:173:PRO:HD3	1.92	0.52
1:B:224:ARG:NH1	7:B:3023:HOH:O	2.33	0.52
1:B:285:ASN:O	6:B:2703:FAD:O1A	2.28	0.52
1:B:558:ASP:O	1:B:561:MET:N	2.43	0.52
1:D:126:GLU:HG2	7:D:3005:HOH:O	2.09	0.52
1:A:242:MET:CE	1:A:274:LEU:HB2	2.40	0.51
1:C:233:LEU:HD13	1:C:334:LEU:HD13	1.92	0.51
1:A:317:LYS:HE2	7:A:3035:HOH:O	2.09	0.51
1:D:286:ASN:ND2	1:D:286:ASN:O	2.44	0.51
1:A:243:SER:O	1:A:261:SER:HA	2.11	0.51
1:C:178:PRO:HG3	7:C:3021:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:TYR:O	7:B:3428:HOH:O	2.19	0.51
1:D:52:HIS:CE1	7:D:3389:HOH:O	2.63	0.51
1:A:233:LEU:HD13	1:A:334:LEU:HD13	1.92	0.50
1:B:182:TRP:O	1:B:183:TYR:HB2	2.11	0.50
1:D:111:PHE:HD1	1:D:115:GLY:O	1.94	0.50
1:C:126:GLU:HG2	1:C:129:ILE:HD12	1.93	0.50
1:C:310:ALA:O	1:D:155:ARG:NH1	2.35	0.50
1:B:408:THR:HB	1:B:409:PRO:HD2	1.93	0.50
1:C:558:ASP:HB3	1:C:561:MET:HG2	1.93	0.50
1:B:194:LEU:HD13	1:B:307:ILE:HD11	1.92	0.50
1:C:195:PRO:HB2	1:C:324:ALA:HA	1.94	0.50
1:C:221:ILE:HG13	6:C:2803:FAD:O2P	2.10	0.50
1:C:287:TYR:N	1:C:315:ARG:HD2	2.26	0.50
1:B:262:ALA:O	1:B:263:ASN:CB	2.60	0.50
1:B:464:HIS:O	1:B:466:PRO:HD3	2.10	0.50
1:D:329:THR:O	1:D:333:ILE:HG13	2.11	0.50
1:A:212:ALA:HB2	1:A:279:VAL:CG2	2.42	0.50
1:B:558:ASP:HB3	1:B:561:MET:CB	2.42	0.49
1:C:50:ARG:HG2	1:C:50:ARG:HH11	1.76	0.49
1:D:170:VAL:O	1:D:173:PRO:HD2	2.13	0.49
1:D:231:GLU:O	1:D:235:LYS:HG2	2.12	0.49
1:B:517:ASN:HD22	1:B:517:ASN:H	1.60	0.49
1:D:279:VAL:HG22	1:D:301:TYR:HB2	1.93	0.49
1:D:232:GLN:HG2	7:D:3244:HOH:O	2.12	0.49
1:B:439:ARG:NH2	7:B:3392:HOH:O	2.36	0.49
1:B:594:LEU:HD13	7:B:3407:HOH:O	2.11	0.49
1:A:286:ASN:HA	7:A:2910:HOH:O	2.13	0.49
1:C:339:GLU:HG2	7:C:3205:HOH:O	2.12	0.49
1:D:201:ALA:HB1	1:D:322:VAL:HG22	1.94	0.49
1:B:421:THR:HB	1:D:85:PRO:HB3	1.95	0.49
1:B:340:ARG:HD3	7:B:3184:HOH:O	2.13	0.48
1:D:160:HIS:CD2	7:D:3105:HOH:O	2.61	0.48
1:A:245:TYR:HB3	1:A:246:PRO:HD3	1.96	0.48
1:A:588:GLN:HG2	1:A:588:GLN:O	2.13	0.48
1:C:264:ARG:NH2	7:C:3132:HOH:O	2.45	0.48
1:C:396:ASP:OD2	7:C:3173:HOH:O	2.19	0.48
1:C:314:LYS:O	1:C:314:LYS:CG	2.60	0.48
1:D:571:LYS:HD3	1:D:577:GLN:HA	1.95	0.48
1:A:112:GLY:HA2	1:A:171:ASP:OD1	2.14	0.48
1:B:91:MET:CE	1:B:94:LEU:HD12	2.42	0.48
1:A:517:ASN:HD22	1:A:517:ASN:N	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:GLN:HG2	1:B:496:GLU:HG2	1.96	0.48
1:D:319:ASP:CB	7:D:3267:HOH:O	2.40	0.48
1:D:319:ASP:OD1	1:D:319:ASP:N	2.47	0.48
1:D:263:ASN:O	1:D:264:ARG:HB2	2.14	0.48
1:C:297:LYS:HE3	1:C:297:LYS:N	2.29	0.47
1:D:10:ASN:HB3	1:D:176:GLN:HE21	1.80	0.47
1:B:52:HIS:CE1	7:B:3326:HOH:O	2.68	0.47
1:B:122:GLN:NE2	1:D:419:PHE:O	2.47	0.47
1:C:50:ARG:HG2	1:C:50:ARG:NH1	2.30	0.47
1:B:559:SER:HA	1:B:567:ILE:CD1	2.44	0.47
1:C:194:LEU:HD11	7:C:3155:HOH:O	2.15	0.47
1:C:317:LYS:HD2	1:C:318:THR:N	2.29	0.47
1:B:39:SER:HB3	1:B:174:TRP:CD2	2.50	0.47
1:B:406:LYS:HE3	7:B:3032:HOH:O	2.14	0.47
1:D:48:ARG:HD2	7:D:3118:HOH:O	2.13	0.47
1:D:146:LEU:HB3	1:D:147:PRO:HD3	1.97	0.47
1:D:221:ILE:O	1:D:224:ARG:HG3	2.14	0.47
1:A:217:ILE:HB	1:A:241:LEU:HD23	1.97	0.47
1:B:225:LYS:CG	7:B:3089:HOH:O	2.63	0.47
1:B:264:ARG:C	1:B:266:ALA:H	2.17	0.47
1:C:354:LYS:HE3	7:C:3084:HOH:O	2.13	0.47
1:A:19:LYS:HA	1:A:19:LYS:HD2	1.66	0.46
1:B:270:ALA:O	1:B:274:LEU:HD13	2.13	0.46
1:B:319:ASP:N	1:B:319:ASP:OD1	2.48	0.46
1:A:39:SER:HB3	1:A:174:TRP:CD2	2.50	0.46
1:A:84:GLY:HA2	1:A:124:MET:CE	2.45	0.46
1:B:212:ALA:HB2	1:B:279:VAL:HG21	1.97	0.46
1:D:498:ASN:ND2	7:D:3216:HOH:O	2.49	0.46
1:A:328:LYS:HD2	7:A:3204:HOH:O	2.16	0.46
1:B:212:ALA:HB2	1:B:279:VAL:CG2	2.45	0.46
1:D:57:ARG:NH2	1:D:462:GLN:OE1	2.47	0.46
1:D:302:PHE:CE1	1:D:316:HIS:CE1	3.03	0.46
1:B:182:TRP:HE3	1:B:183:TYR:CA	2.26	0.46
1:C:383:ILE:HB	1:C:530:LYS:HD2	1.97	0.46
1:D:315:ARG:HG2	7:D:3032:HOH:O	2.16	0.46
1:B:264:ARG:HG2	7:B:3201:HOH:O	2.14	0.46
1:A:245:TYR:CD1	1:A:265:ALA:CB	2.98	0.46
1:A:242:MET:CE	1:A:270:ALA:O	2.64	0.46
1:C:196:GLU:CD	1:C:196:GLU:H	2.20	0.46
1:D:285:ASN:O	6:D:2903:FAD:O1A	2.34	0.46
1:A:99:GLU:O	1:A:418:LEU:HD23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:GLU:HG2	7:A:2891:HOH:O	2.15	0.45
1:A:299:THR:HG22	7:A:3118:HOH:O	2.11	0.45
1:D:530:LYS:HD3	7:D:3380:HOH:O	2.16	0.45
1:D:115:GLY:HA3	7:D:3024:HOH:O	2.16	0.45
1:D:522:LEU:HB2	1:D:523:PRO:HD3	1.99	0.45
1:A:84:GLY:HA2	1:A:124:MET:HE1	1.99	0.45
1:C:19:LYS:HZ1	1:C:50:ARG:NH2	2.10	0.45
1:A:255:TYR:HA	1:A:256:PRO:HD3	1.84	0.45
1:A:302:PHE:O	1:A:318:THR:HG23	2.16	0.45
1:C:91:MET:HE2	1:C:130:TYR:CE1	2.52	0.45
1:D:264:ARG:HA	1:D:266:ALA:N	2.27	0.45
1:D:268:LYS:HB3	1:D:269:PRO:HD3	1.99	0.45
1:A:529:ALA:CB	1:A:540:ILE:HD11	2.47	0.45
1:B:584:THR:O	1:B:588:GLN:HG3	2.16	0.45
5:B:2702:TPP:N1'	1:D:59:GLU:OE2	2.49	0.45
1:C:316:HIS:HD2	7:C:2850:HOH:O	2.00	0.45
1:A:501:ASP:HA	1:A:515:ARG:NH1	2.32	0.44
1:B:500:ILE:HG12	1:D:509:VAL:HG12	1.98	0.44
1:A:264:ARG:HB2	7:A:3117:HOH:O	2.16	0.44
1:A:529:ALA:HB2	1:A:540:ILE:HD11	1.99	0.44
1:B:296:PHE:O	1:B:298:ASN:N	2.45	0.44
1:B:307:ILE:HD12	1:B:325:ASP:HA	1.99	0.44
1:C:213:GLU:HG2	7:C:3217:HOH:O	2.17	0.44
1:B:195:PRO:HG2	7:B:3331:HOH:O	2.18	0.44
1:B:316:HIS:O	1:B:317:LYS:O	2.35	0.44
1:B:558:ASP:O	1:B:560:ALA:N	2.51	0.44
1:C:399:LEU:HD21	1:C:403:ARG:CZ	2.48	0.44
1:C:228:LYS:HE3	7:C:3123:HOH:O	2.17	0.44
1:A:317:LYS:CE	7:A:3035:HOH:O	2.65	0.44
1:B:558:ASP:HB3	1:B:561:MET:HB3	1.99	0.44
1:C:201:ALA:HB1	1:C:322:VAL:HG22	1.98	0.44
1:D:19:LYS:NZ	1:D:50:ARG:HH11	2.16	0.43
1:B:114:THR:CG2	7:B:3333:HOH:O	2.55	0.43
1:B:247:ALA:HB1	1:B:250:ILE:HD12	2.00	0.43
1:C:99:GLU:HB3	1:C:418:LEU:HB3	2.00	0.43
1:D:286:ASN:OD1	1:D:314:LYS:HD3	2.17	0.43
1:A:214:ARG:HH12	1:A:276:GLN:NE2	2.15	0.43
1:A:263:ASN:HB3	1:A:264:ARG:H	1.73	0.43
1:A:315:ARG:HD3	7:A:2900:HOH:O	2.17	0.43
1:C:39:SER:HB3	1:C:174:TRP:CE3	2.53	0.43
1:D:180:GLU:HA	7:D:3371:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:MET:CE	1:C:130:TYR:CE1	3.01	0.43
1:A:572:GLN:HE21	1:A:572:GLN:HB3	1.61	0.43
1:B:268:LYS:HE3	1:B:580:GLN:O	2.18	0.43
1:A:307:ILE:HD12	1:A:325:ASP:HA	2.01	0.43
1:D:255:TYR:HA	1:D:256:PRO:HD3	1.80	0.43
1:A:317:LYS:NZ	7:A:3035:HOH:O	2.51	0.43
1:B:9:THR:HG23	7:B:3369:HOH:O	2.19	0.43
1:D:353:VAL:O	1:D:357:ARG:HG3	2.18	0.43
1:B:91:MET:HE1	1:B:94:LEU:HD12	2.00	0.43
1:C:156:ARG:HD3	7:C:3211:HOH:O	2.18	0.42
1:C:378:ARG:O	1:C:382:LYS:HG2	2.18	0.42
1:D:584:THR:O	1:D:588:GLN:HG3	2.19	0.42
1:A:368:GLU:HG2	1:A:520:GLU:HB3	2.01	0.42
1:A:385:GLU:HB3	1:A:386:PRO:HD2	1.99	0.42
1:C:28:HIS:HA	1:C:52:HIS:O	2.19	0.42
1:D:378:ARG:HD3	1:D:382:LYS:HE2	2.01	0.42
1:A:236:THR:HG22	1:A:237:LEU:HD23	2.01	0.42
1:A:328:LYS:HG2	7:A:2876:HOH:O	2.20	0.42
1:D:383:ILE:HB	1:D:530:LYS:HD2	2.01	0.42
1:B:85:PRO:HB3	1:D:421:THR:HB	2.01	0.42
1:B:317:LYS:HG2	7:B:3303:HOH:O	2.20	0.42
1:B:408:THR:HB	1:B:409:PRO:CD	2.49	0.42
1:C:317:LYS:HD2	1:C:317:LYS:C	2.39	0.42
1:A:315:ARG:HB2	1:A:316:HIS:H	1.71	0.42
1:D:136:TYR:CD1	1:D:156:ARG:HG3	2.55	0.42
1:B:218:TYR:HE2	1:B:287:TYR:CD1	2.37	0.42
1:B:315:ARG:HG2	7:B:3428:HOH:O	2.19	0.42
1:B:438:GLU:HB3	7:B:3417:HOH:O	2.19	0.42
1:A:307:ILE:CD1	1:A:325:ASP:HA	2.50	0.41
1:C:39:SER:HB3	1:C:174:TRP:CE2	2.54	0.41
1:B:307:ILE:CD1	1:B:325:ASP:HA	2.50	0.41
1:A:340:ARG:HG2	7:A:3104:HOH:O	2.19	0.41
1:C:195:PRO:HD2	1:C:307:ILE:CD1	2.50	0.41
1:A:451:SER:HA	1:A:454:MET:HE2	2.01	0.41
1:C:176:GLN:CD	7:C:3222:HOH:O	2.58	0.41
1:C:194:LEU:HB2	1:C:307:ILE:HD11	2.02	0.41
1:D:49:ASP:OD1	1:D:49:ASP:N	2.47	0.41
1:B:48:ARG:HD2	7:B:3306:HOH:O	2.20	0.41
1:B:245:TYR:C	1:B:245:TYR:CD2	2.94	0.41
1:C:16:ALA:O	1:C:20:VAL:HG23	2.20	0.41
1:C:286:ASN:OD1	1:C:314:LYS:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:LYS:HB3	1:D:354:LYS:HE2	1.89	0.41
1:A:215:PRO:HD2	1:A:345:TRP:CD1	2.56	0.41
1:B:558:ASP:C	1:B:560:ALA:N	2.74	0.41
1:C:84:GLY:H	1:C:126:GLU:CD	2.24	0.41
1:D:285:ASN:O	1:D:286:ASN:CB	2.68	0.41
1:B:559:SER:HA	1:B:567:ILE:HD13	2.03	0.41
1:A:589:PHE:HE1	7:A:3079:HOH:O	2.03	0.41
1:B:34:GLY:HA2	1:D:480:ILE:HD12	2.03	0.41
1:B:385:GLU:HG3	1:B:440:GLN:HB2	2.02	0.41
1:B:520:GLU:OE2	7:B:3297:HOH:O	2.22	0.41
1:D:57:ARG:HB2	1:D:455:GLN:HG2	2.03	0.41
5:D:2902:TPP:H61	5:D:2902:TPP:HM41	1.96	0.41
1:B:191:THR:HG23	7:B:3138:HOH:O	2.20	0.41
1:D:148:HIS:HD2	7:D:3305:HOH:O	2.04	0.41
1:C:285:ASN:O	1:C:286:ASN:CB	2.69	0.40
1:B:84:GLY:HA2	1:B:124:MET:CE	2.51	0.40
1:B:242:MET:SD	1:B:274:LEU:HD11	2.62	0.40
1:D:316:HIS:CE1	7:D:3284:HOH:O	2.74	0.40
1:A:368:GLU:HA	1:A:520:GLU:OE1	2.21	0.40
1:D:263:ASN:HD22	1:D:263:ASN:HA	1.59	0.40
1:B:296:PHE:O	1:B:297:LYS:HG2	2.21	0.40
1:C:225:LYS:O	1:C:327:GLN:HG3	2.22	0.40
1:C:474:ASN:O	1:C:476:GLN:HG3	2.22	0.40
1:D:156:ARG:HD2	7:D:3083:HOH:O	2.22	0.40
1:A:576:ALA:HB1	1:A:579:LEU:HD12	2.04	0.40
1:B:255:TYR:HA	1:B:256:PRO:HD3	1.91	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	550/603 (91%)	529 (96%)	19 (4%)	2 (0%)	34	37
1	B	564/603 (94%)	537 (95%)	20 (4%)	7 (1%)	13	10
1	C	548/603 (91%)	517 (94%)	30 (6%)	1 (0%)	47	55
1	D	552/603 (92%)	530 (96%)	21 (4%)	1 (0%)	47	55
All	All	2214/2412 (92%)	2113 (95%)	90 (4%)	11 (0%)	29	31

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	ASN
1	B	10	ASN
1	B	263	ASN
1	B	314	LYS
1	B	317	LYS
1	D	314	LYS
1	B	182	TRP
1	A	510	HIS
1	B	297	LYS
1	B	559	SER
1	C	286	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	446/484 (92%)	422 (95%)	24 (5%)	22	26
1	B	459/484 (95%)	431 (94%)	28 (6%)	18	21
1	C	444/484 (92%)	419 (94%)	25 (6%)	21	25
1	D	446/484 (92%)	423 (95%)	23 (5%)	23	28
All	All	1795/1936 (93%)	1695 (94%)	100 (6%)	21	25

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	57	ARG
1	A	156	ARG
1	A	194	LEU
1	A	196	GLU
1	A	199	VAL
1	A	228	LYS
1	A	232	GLN
1	A	286	ASN
1	A	299	THR
1	A	300	ARG
1	A	307	ILE
1	A	315	ARG
1	A	317	LYS
1	A	319	ASP
1	A	327	GLN
1	A	334	LEU
1	A	418	LEU
1	A	489	GLN
1	A	517	ASN
1	A	561	MET
1	A	572	GLN
1	A	587	LYS
1	A	593	ASP
1	B	49	ASP
1	B	116	MET
1	B	180	GLU
1	B	183	TYR
1	B	191	THR
1	B	193	LEU
1	B	199	VAL
1	B	200	GLN
1	B	232	GLN
1	B	245	TYR
1	B	264	ARG
1	B	286	ASN
1	B	297	LYS
1	B	307	ILE
1	B	314	LYS
1	B	319	ASP
1	B	334	LEU
1	B	339	GLU
1	B	385	GLU

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Mol	Chain	Res	Type
1	B	393	ASP
1	B	418	LEU
1	B	515	ARG
1	B	517	ASN
1	B	562	SER
1	B	563	SER
1	B	572	GLN
1	B	595	GLN
1	B	597	GLN
1	C	111	PHE
1	C	123	GLU
1	C	221	ILE
1	C	224	ARG
1	C	232	GLN
1	C	263	ASN
1	C	264	ARG
1	C	274	LEU
1	C	286	ASN
1	C	297	LYS
1	C	307	ILE
1	C	315	ARG
1	C	317	LYS
1	C	319	ASP
1	C	327	GLN
1	C	334	LEU
1	C	382	LYS
1	C	393	ASP
1	C	414	ILE
1	C	418	LEU
1	C	515	ARG
1	C	517	ASN
1	C	561	MET
1	C	563	SER
1	C	572	GLN
1	D	49	ASP
1	D	75	LYS
1	D	111	PHE
1	D	207	GLN
1	D	263	ASN
1	D	286	ASN
1	D	306	ASP
1	D	311	LYS

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Mol	Chain	Res	Type
1	D	319	ASP
1	D	334	LEU
1	D	347	GLN
1	D	393	ASP
1	D	418	LEU
1	D	498	ASN
1	D	515	ARG
1	D	517	ASN
1	D	553	GLU
1	D	554	LYS
1	D	561	MET
1	D	568	GLU
1	D	572	GLN
1	D	580	GLN
1	D	592	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	176	GLN
1	A	267	GLN
1	A	276	GLN
1	A	476	GLN
1	A	489	GLN
1	A	517	ASN
1	A	572	GLN
1	B	10	ASN
1	B	101	HIS
1	B	122	GLN
1	B	267	GLN
1	B	276	GLN
1	B	304	GLN
1	B	316	HIS
1	B	476	GLN
1	B	517	ASN
1	B	572	GLN
1	B	597	GLN
1	C	101	HIS
1	C	207	GLN
1	C	263	ASN
1	C	267	GLN

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Mol	Chain	Res	Type
1	C	276	GLN
1	C	476	GLN
1	C	517	ASN
1	D	10	ASN
1	D	176	GLN
1	D	232	GLN
1	D	263	ASN
1	D	267	GLN
1	D	276	GLN
1	D	347	GLN
1	D	476	GLN
1	D	517	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 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	SO4	C	2604	-	4,4,4	0.37	0	6,6,6	0.32	0
5	TPP	B	2702	2	22,27,27	1.63	6 (27%)	29,40,40	2.17	9 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FAD	B	2703	-	24,29,58	1.23	2 (8%)	29,45,89	1.46	3 (10%)
6	FAD	D	2903	-	24,29,58	1.32	3 (12%)	29,45,89	1.61	3 (10%)
5	TPP	A	2602	2	22,27,27	2.38	5 (22%)	29,40,40	1.70	7 (24%)
4	SO4	A	2804	-	4,4,4	0.35	0	6,6,6	0.22	0
6	FAD	A	2603	-	24,29,58	1.23	3 (12%)	29,45,89	1.66	6 (20%)
5	TPP	D	2902	2	22,27,27	1.42	4 (18%)	29,40,40	1.91	10 (34%)
5	TPP	C	2802	2	22,27,27	1.58	4 (18%)	29,40,40	1.89	10 (34%)
4	SO4	B	2904	-	4,4,4	0.24	0	6,6,6	0.42	0
4	SO4	D	2704	-	4,4,4	0.24	0	6,6,6	0.90	0
6	FAD	C	2803	-	24,29,58	1.21	3 (12%)	29,45,89	1.56	4 (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
5	TPP	B	2702	2	-	3/16/17/17	0/2/2/2
6	FAD	B	2703	-	-	2/12/32/50	0/3/3/6
6	FAD	D	2903	-	-	2/12/32/50	0/3/3/6
5	TPP	A	2602	2	-	2/16/17/17	0/2/2/2
6	FAD	A	2603	-	-	2/12/32/50	0/3/3/6
5	TPP	D	2902	2	-	2/16/17/17	0/2/2/2
5	TPP	C	2802	2	-	3/16/17/17	0/2/2/2
6	FAD	C	2803	-	-	2/12/32/50	0/3/3/6

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2602	TPP	C6-C5	8.50	1.54	1.50
5	B	2702	TPP	C6-C5	4.20	1.52	1.50
6	D	2903	FAD	C2A-N3A	3.95	1.38	1.32
6	A	2603	FAD	C2A-N3A	3.39	1.37	1.32
5	B	2702	TPP	C6'-N1'	3.33	1.41	1.34
6	B	2703	FAD	C2A-N3A	3.25	1.37	1.32
5	A	2602	TPP	C2'-N3'	3.21	1.39	1.34
5	C	2802	TPP	C6-C5	3.13	1.52	1.50
5	D	2902	TPP	C4'-N3'	3.11	1.39	1.35
5	A	2602	TPP	C2'-N1'	3.11	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	2803	FAD	C2A-N3A	3.04	1.37	1.32
5	A	2602	TPP	C2-N3	2.96	1.42	1.36
5	C	2802	TPP	C6'-N1'	2.91	1.40	1.34
5	C	2802	TPP	C4'-N3'	2.90	1.39	1.35
6	A	2603	FAD	C2A-N1A	2.74	1.39	1.33
5	B	2702	TPP	C2'-N1'	2.71	1.38	1.34
5	D	2902	TPP	C2-N3	2.68	1.41	1.36
6	D	2903	FAD	P-O5'	2.62	1.64	1.54
6	C	2803	FAD	P-O5'	2.59	1.64	1.54
5	D	2902	TPP	C6'-N1'	2.55	1.39	1.34
6	B	2703	FAD	C2B-C1B	-2.33	1.50	1.53
5	D	2902	TPP	C6-C5	2.32	1.51	1.50
5	B	2702	TPP	C2'-N3'	2.30	1.38	1.34
5	C	2802	TPP	C2'-N3'	2.27	1.38	1.34
5	B	2702	TPP	C2-N3	2.21	1.40	1.36
5	A	2602	TPP	C6'-C5'	2.20	1.42	1.37
6	C	2803	FAD	O4B-C4B	-2.05	1.40	1.45
6	A	2603	FAD	P-O5'	2.03	1.62	1.54
6	D	2903	FAD	C2A-N1A	2.02	1.37	1.33
5	B	2702	TPP	C4'-N3'	2.01	1.37	1.35

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	2903	FAD	N3A-C2A-N1A	-6.22	118.96	128.68
6	C	2803	FAD	N3A-C2A-N1A	-5.52	120.05	128.68
6	A	2603	FAD	N3A-C2A-N1A	-5.36	120.30	128.68
6	B	2703	FAD	N3A-C2A-N1A	-4.98	120.90	128.68
5	B	2702	TPP	CM4-C4-N3	4.92	128.81	122.53
5	B	2702	TPP	CM2-C2'-N1'	4.58	122.18	117.14
5	C	2802	TPP	N1'-C2'-N3'	-4.10	118.48	125.54
5	D	2902	TPP	CM2-C2'-N1'	4.10	121.65	117.14
5	B	2702	TPP	N1'-C2'-N3'	-3.96	118.73	125.54
5	D	2902	TPP	CM4-C4-N3	3.80	127.38	122.53
5	D	2902	TPP	N1'-C2'-N3'	-3.74	119.11	125.54
5	A	2602	TPP	C6'-C5'-C4'	3.69	120.74	115.72
5	C	2802	TPP	CM2-C2'-N1'	3.69	121.19	117.14
5	B	2702	TPP	C5'-C7'-N3	-3.29	107.79	113.28
5	B	2702	TPP	CM4-C4-C5	-3.14	120.74	127.60
5	A	2602	TPP	CM2-C2'-N1'	3.11	120.56	117.14
5	C	2802	TPP	CM4-C4-N3	3.09	126.47	122.53
5	C	2802	TPP	C2'-N3'-C4'	2.98	122.73	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2603	FAD	C5A-C6A-N6A	2.91	124.77	120.35
5	B	2702	TPP	C6'-N1'-C2'	2.89	120.88	115.96
5	D	2902	TPP	C6'-N1'-C2'	2.87	120.85	115.96
5	B	2702	TPP	C5'-C6'-N1'	-2.87	119.03	123.82
5	C	2802	TPP	C6-C5-C4	2.82	129.70	127.43
5	B	2702	TPP	C6'-C5'-C4'	2.82	119.55	115.72
5	A	2602	TPP	O3B-PB-O2B	2.79	118.30	107.64
6	A	2603	FAD	PA-O3P-P	-2.77	123.31	132.83
5	B	2702	TPP	C2'-N3'-C4'	2.75	122.36	118.08
5	D	2902	TPP	C2'-N3'-C4'	2.62	122.17	118.08
5	C	2802	TPP	C5'-C7'-N3	-2.60	108.94	113.28
5	C	2802	TPP	C6'-N1'-C2'	2.60	120.39	115.96
6	C	2803	FAD	C4A-C5A-N7A	-2.59	106.70	109.40
5	A	2602	TPP	CM4-C4-N3	2.59	125.83	122.53
6	C	2803	FAD	C5A-C6A-N6A	2.53	124.20	120.35
6	A	2603	FAD	C4A-C5A-N7A	-2.53	106.76	109.40
6	D	2903	FAD	PA-O3P-P	-2.51	124.22	132.83
5	D	2902	TPP	C5'-C7'-N3	-2.49	109.13	113.28
6	D	2903	FAD	O5'-P-O3P	-2.44	96.45	104.64
5	D	2902	TPP	CM4-C4-C5	-2.41	122.33	127.60
5	A	2602	TPP	C5'-C6'-N1'	-2.37	119.86	123.82
5	A	2602	TPP	N1'-C2'-N3'	-2.28	121.61	125.54
6	B	2703	FAD	O3P-P-O1P	-2.28	98.55	111.19
5	D	2902	TPP	O3B-PB-O3A	2.26	112.20	104.64
5	D	2902	TPP	PA-O3A-PB	-2.23	125.17	132.83
6	C	2803	FAD	PA-O3P-P	-2.23	125.19	132.83
5	A	2602	TPP	C5'-C7'-N3	-2.21	109.59	113.28
5	C	2802	TPP	CM4-C4-C5	-2.14	122.91	127.60
6	B	2703	FAD	C1B-N9A-C4A	-2.12	122.92	126.64
6	A	2603	FAD	C1B-N9A-C4A	-2.10	122.96	126.64
6	A	2603	FAD	C2A-N1A-C6A	2.05	122.27	118.75
5	C	2802	TPP	O2B-PB-O3A	-2.05	97.76	104.64
5	D	2902	TPP	C5'-C6'-N1'	-2.05	120.41	123.82
5	C	2802	TPP	CM2-C2'-N3'	2.04	120.33	117.15

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2602	TPP	PA-O3A-PB-O3B
5	B	2702	TPP	PA-O3A-PB-O2B
5	B	2702	TPP	PA-O3A-PB-O3B

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Mol	Chain	Res	Type	Atoms
5	C	2802	TPP	PA-O3A-PB-O2B
5	C	2802	TPP	PA-O3A-PB-O3B
5	D	2902	TPP	PA-O3A-PB-O2B
5	D	2902	TPP	PA-O3A-PB-O3B
6	D	2903	FAD	PA-O3P-P-O2P
6	B	2703	FAD	O4B-C4B-C5B-O5B
6	A	2603	FAD	C4B-C5B-O5B-PA
5	B	2702	TPP	C4-C5-C6-C7
6	C	2803	FAD	C4B-C5B-O5B-PA
6	B	2703	FAD	C4B-C5B-O5B-PA
6	A	2603	FAD	O4B-C4B-C5B-O5B
5	C	2802	TPP	PA-O3A-PB-O1B
6	D	2903	FAD	O4B-C4B-C5B-O5B
5	A	2602	TPP	PA-O3A-PB-O2B
6	C	2803	FAD	O4B-C4B-C5B-O5B

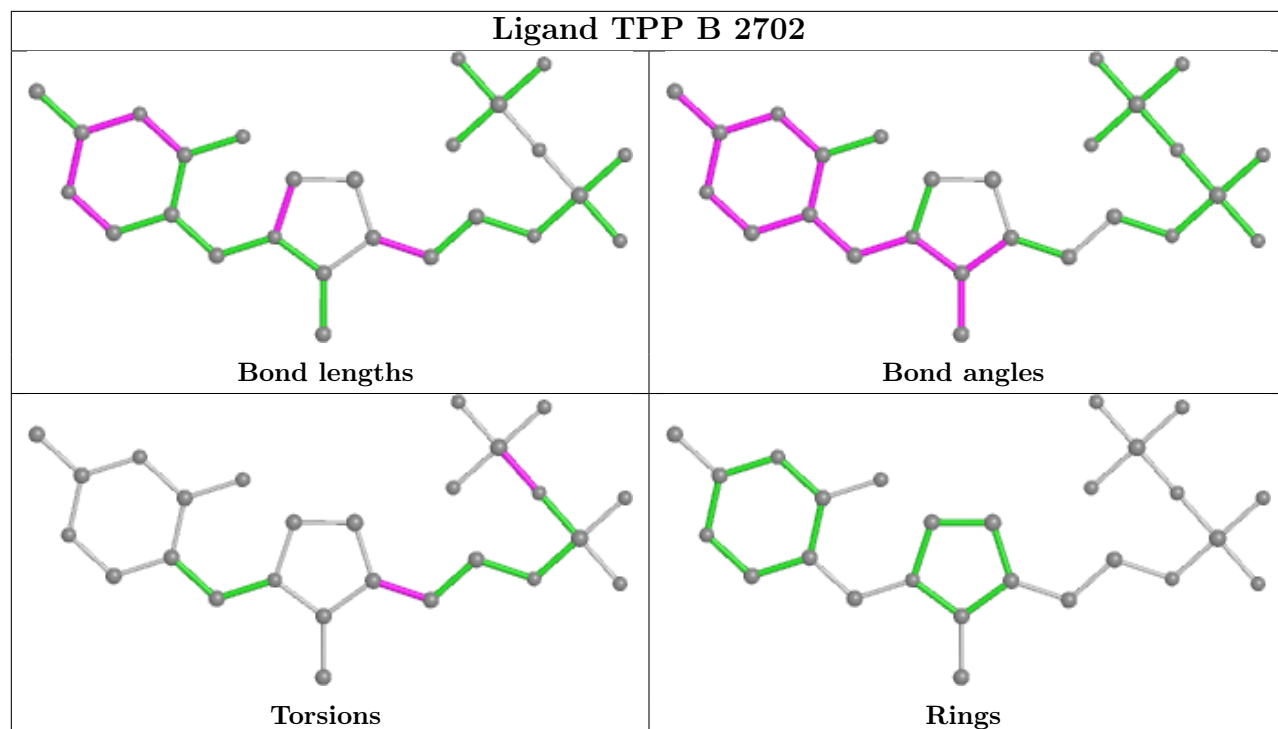
There are no ring outliers.

6 monomers are involved in 7 short contacts:

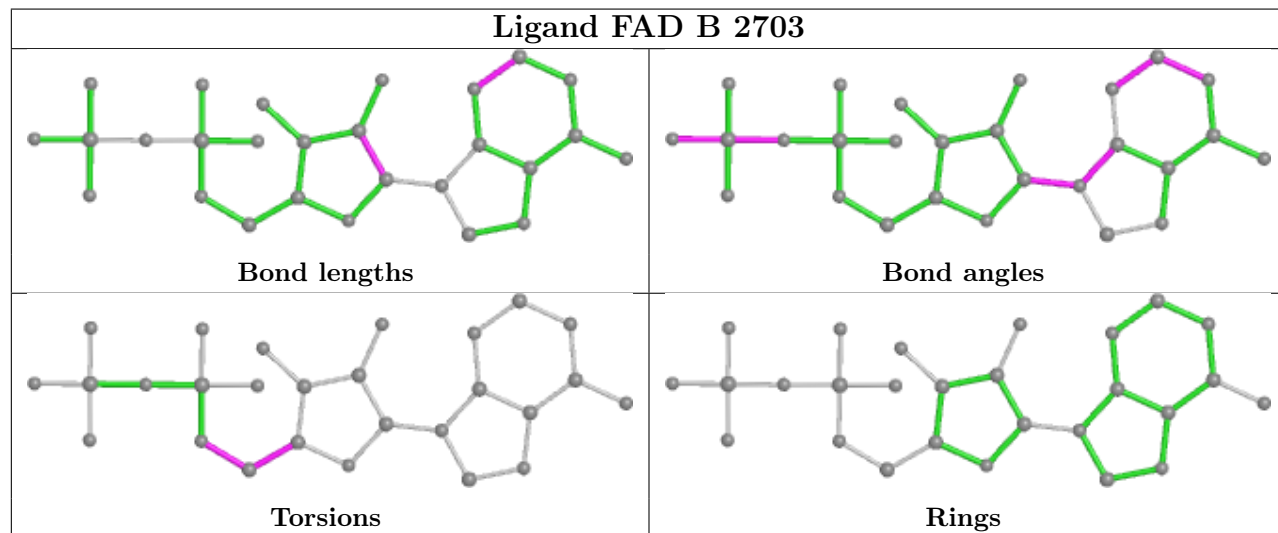
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2702	TPP	1	0
6	B	2703	FAD	1	0
6	D	2903	FAD	1	0
6	A	2603	FAD	2	0
5	D	2902	TPP	1	0
6	C	2803	FAD	1	0

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

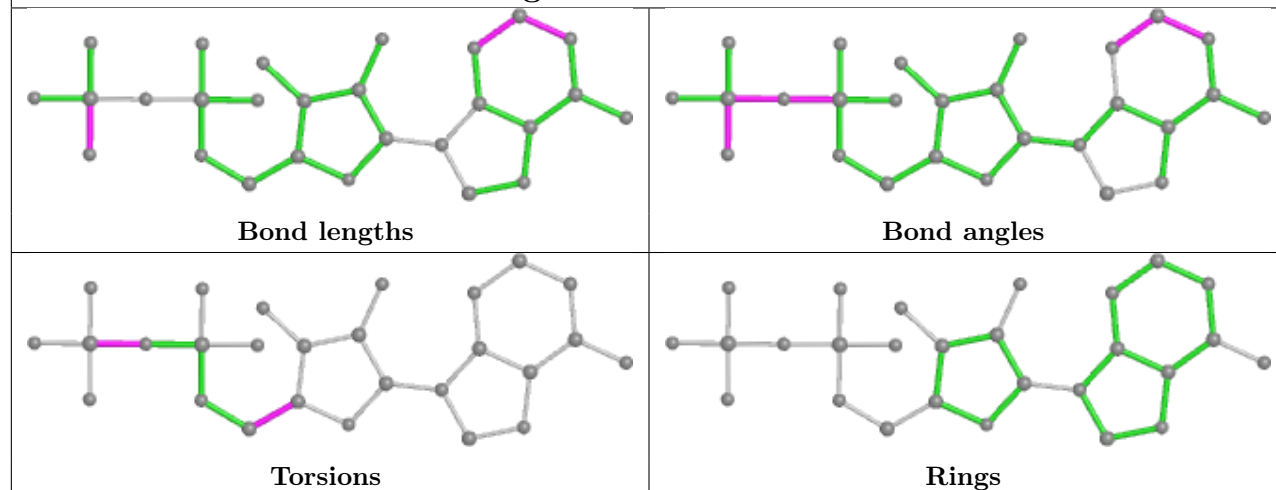
Ligand TPP B 2702



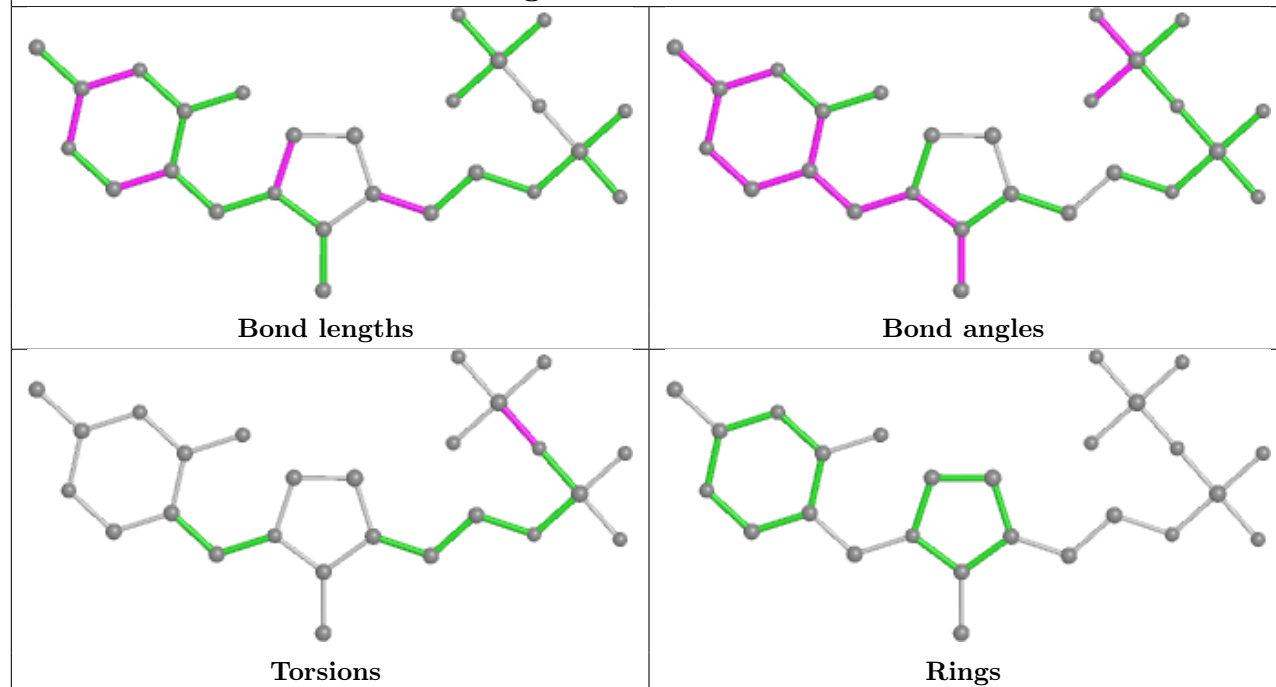
Ligand FAD B 2703



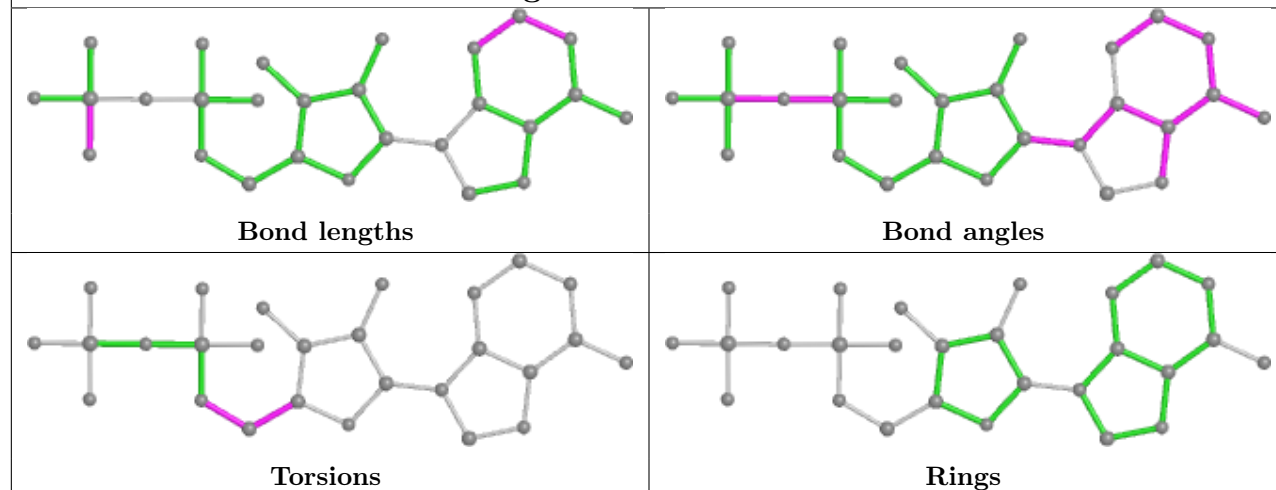
Ligand FAD D 2903



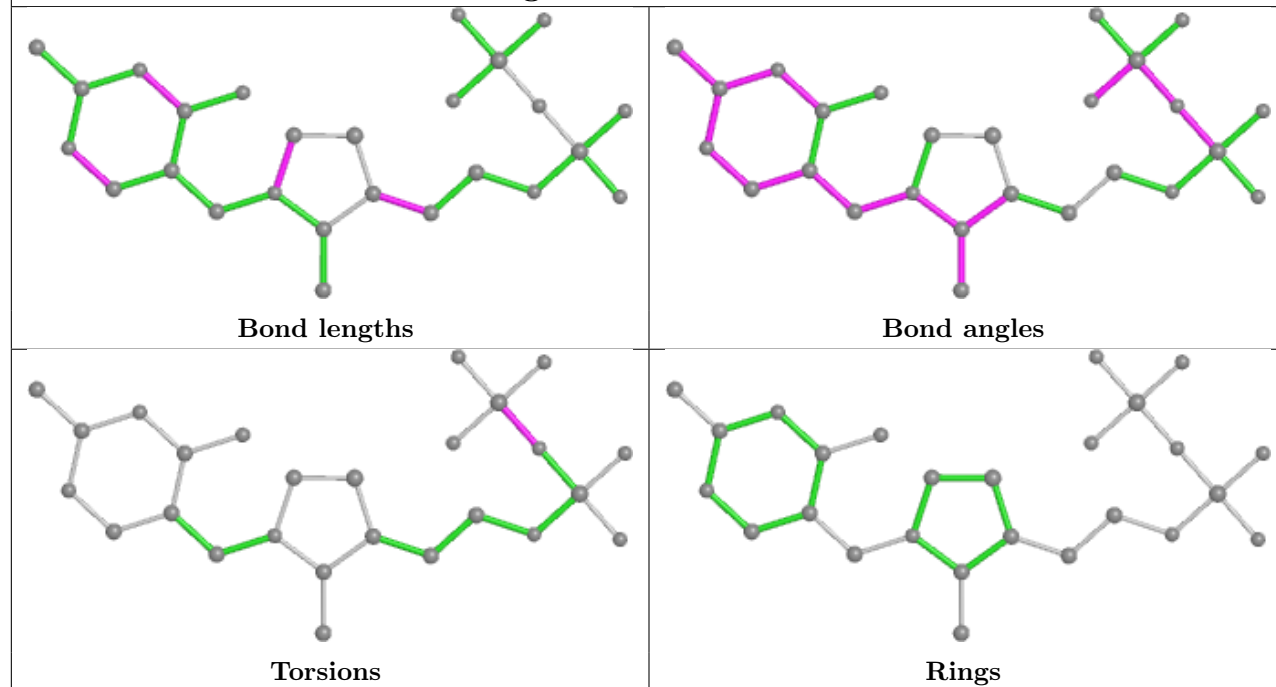
Ligand TPP A 2602

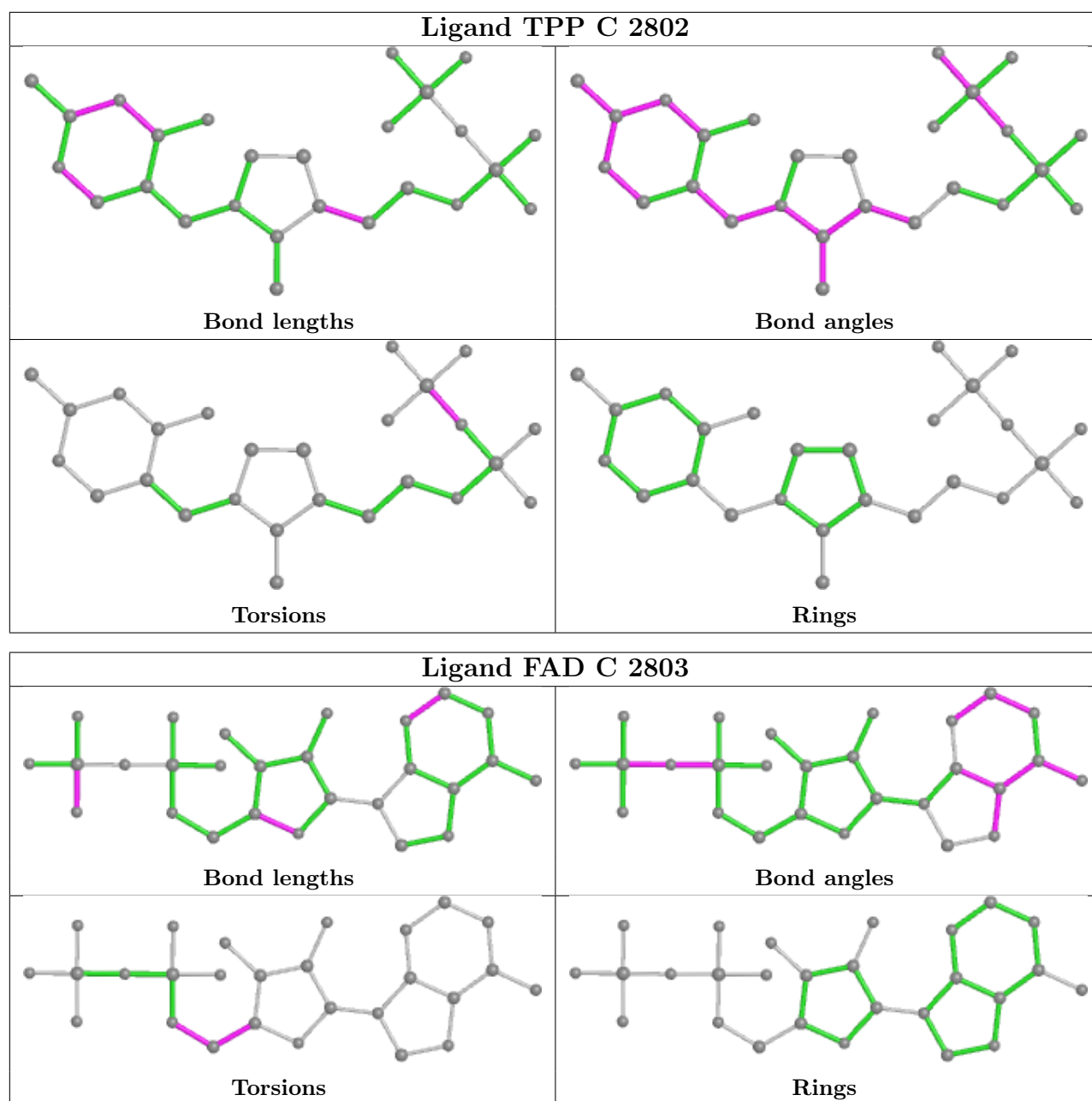


Ligand FAD A 2603



Ligand TPP D 2902





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	558/603 (92%)	0.31	52 (9%) 8 7	28, 46, 80, 96	0
1	B	572/603 (94%)	0.03	29 (5%) 28 26	22, 37, 69, 87	0
1	C	556/603 (92%)	0.22	42 (7%) 13 12	26, 43, 71, 91	0
1	D	560/603 (92%)	0.25	43 (7%) 13 12	25, 42, 78, 93	0
All	All	2246/2412 (93%)	0.20	166 (7%) 14 13	22, 42, 75, 96	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	316	HIS	15.7
1	A	316	HIS	14.4
1	D	318	THR	13.6
1	C	318	THR	12.7
1	A	318	THR	10.4
1	C	287	TYR	10.3
1	B	288	PRO	9.9
1	D	181	ASP	9.4
1	B	318	THR	9.3
1	B	116	MET	8.3
1	B	181	ASP	7.6
1	B	316	HIS	7.4
1	D	180	GLU	7.1
1	C	195	PRO	7.1
1	A	180	GLU	6.9
1	A	181	ASP	6.7
1	B	193	LEU	6.6
1	B	122	GLN	6.6
1	B	180	GLU	6.4
1	C	316	HIS	6.3
1	C	180	GLU	6.3

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Mol	Chain	Res	Type	RSRZ
1	C	194	LEU	6.2
1	B	287	TYR	6.0
1	A	560	ALA	5.8
1	C	560	ALA	5.8
1	D	287	TYR	5.7
1	B	115	GLY	5.7
1	A	590	GLY	5.7
1	D	313	GLY	5.5
1	A	115	GLY	5.4
1	B	9	THR	5.3
1	C	559	SER	5.3
1	C	565	ALA	5.3
1	B	597	GLN	5.2
1	B	313	GLY	5.1
1	C	9	THR	4.9
1	D	111	PHE	4.8
1	B	314	LYS	4.8
1	A	317	LYS	4.7
1	A	313	GLY	4.6
1	D	217	ILE	4.6
1	D	182	TRP	4.5
1	D	114	THR	4.4
1	D	115	GLY	4.2
1	A	182	TRP	4.2
1	C	264	ARG	4.1
1	C	313	GLY	4.0
1	D	592	ASP	4.0
1	C	297	LYS	4.0
1	C	563	SER	3.9
1	C	115	GLY	3.9
1	D	264	ARG	3.8
1	B	191	THR	3.7
1	C	298	ASN	3.7
1	A	314	LYS	3.6
1	D	314	LYS	3.6
1	A	565	ALA	3.5
1	D	195	PRO	3.4
1	B	297	LYS	3.4
1	A	562	SER	3.4
1	C	561	MET	3.2
1	A	300	ARG	3.2
1	A	264	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	315	ARG	3.1
1	A	281	LEU	3.1
1	C	217	ILE	3.1
1	A	111	PHE	3.1
1	D	561	MET	3.1
1	A	559	SER	3.1
1	D	281	LEU	3.1
1	A	195	PRO	3.1
1	D	564	ALA	3.1
1	D	565	ALA	3.1
1	A	194	LEU	3.0
1	D	49	ASP	3.0
1	C	341	GLU	3.0
1	B	264	ARG	3.0
1	C	111	PHE	3.0
1	A	298	ASN	3.0
1	B	182	TRP	3.0
1	C	107	LEU	2.9
1	A	9	THR	2.8
1	A	107	LEU	2.8
1	B	296	PHE	2.8
1	C	196	GLU	2.8
1	C	29	LEU	2.8
1	C	148	HIS	2.8
1	A	368	GLU	2.8
1	B	559	SER	2.7
1	A	568	GLU	2.7
1	A	592	ASP	2.7
1	C	564	ALA	2.7
1	C	317	LYS	2.7
1	B	114	THR	2.7
1	A	114	THR	2.7
1	C	254	ARG	2.6
1	D	335	ALA	2.6
1	A	148	HIS	2.6
1	C	558	ASP	2.6
1	A	216	LEU	2.6
1	C	263	ASN	2.6
1	D	341	GLU	2.6
1	D	368	GLU	2.6
1	A	558	ASP	2.6
1	C	377	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	341	GLU	2.6
1	B	194	LEU	2.6
1	D	200	GLN	2.6
1	C	179	ALA	2.6
1	A	397	ILE	2.5
1	A	561	MET	2.5
1	D	470	VAL	2.5
1	A	444	LEU	2.5
1	C	209	LEU	2.5
1	D	438	GLU	2.4
1	C	314	LYS	2.4
1	C	178	PRO	2.4
1	A	217	ILE	2.4
1	A	239	ILE	2.4
1	D	367	GLN	2.4
1	A	10	ASN	2.4
1	D	263	ASN	2.4
1	A	401	ALA	2.3
1	D	559	SER	2.3
1	A	11	ILE	2.3
1	D	107	LEU	2.3
1	A	49	ASP	2.3
1	A	587	LYS	2.3
1	C	397	ILE	2.3
1	A	341	GLU	2.3
1	C	315	ARG	2.3
1	A	302	PHE	2.3
1	C	587	LYS	2.3
1	D	216	LEU	2.2
1	A	254	ARG	2.2
1	B	107	LEU	2.2
1	D	589	PHE	2.2
1	B	241	LEU	2.2
1	A	367	GLN	2.2
1	B	192	PRO	2.2
1	D	300	ARG	2.2
1	C	562	SER	2.2
1	D	319	ASP	2.2
1	D	9	THR	2.2
1	D	299	THR	2.2
1	A	193	LEU	2.2
1	A	263	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	444	LEU	2.1
1	A	338	SER	2.1
1	D	196	GLU	2.1
1	C	566	ASP	2.1
1	D	207	GLN	2.1
1	B	263	ASN	2.1
1	C	79	CYS	2.1
1	C	444	LEU	2.1
1	D	29	LEU	2.1
1	A	315	ARG	2.1
1	D	18	ILE	2.1
1	A	78	VAL	2.1
1	D	560	ALA	2.0
1	C	368	GLU	2.0
1	A	240	PRO	2.0
1	A	14	GLY	2.0
1	B	564	ALA	2.0
1	D	150	ILE	2.0
1	A	564	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

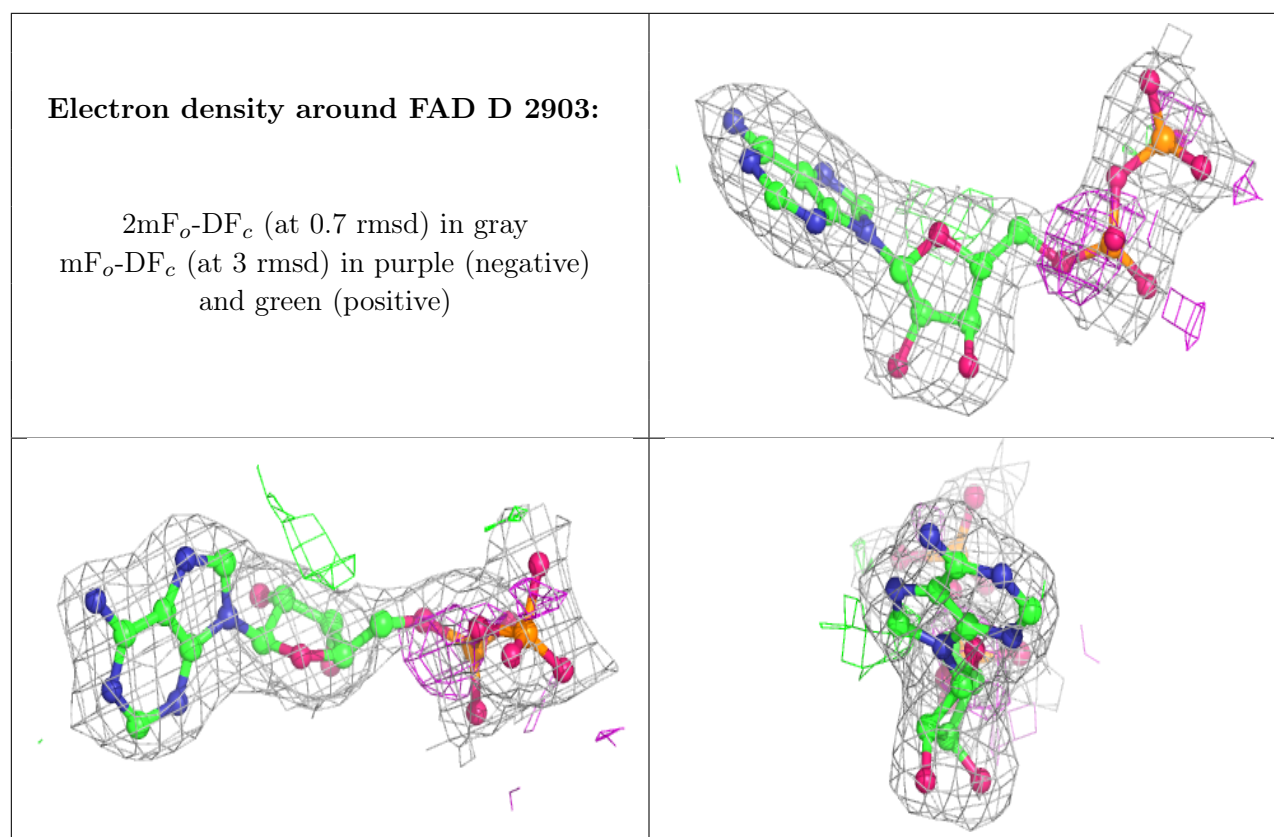
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	C	2801	1/1	0.87	0.18	40,40,40,40	0
6	FAD	D	2903	27/53	0.92	0.13	46,51,68,69	0
6	FAD	C	2803	27/53	0.94	0.13	37,43,61,64	0
2	MG	A	2601	1/1	0.94	0.10	38,38,38,38	0

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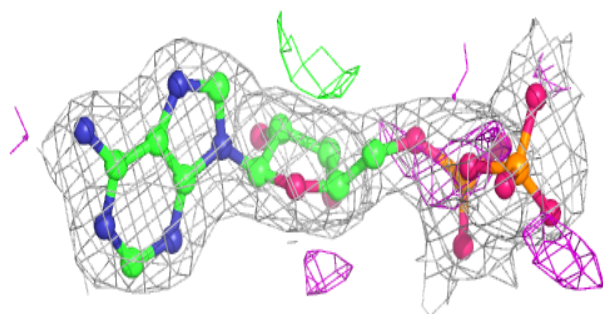
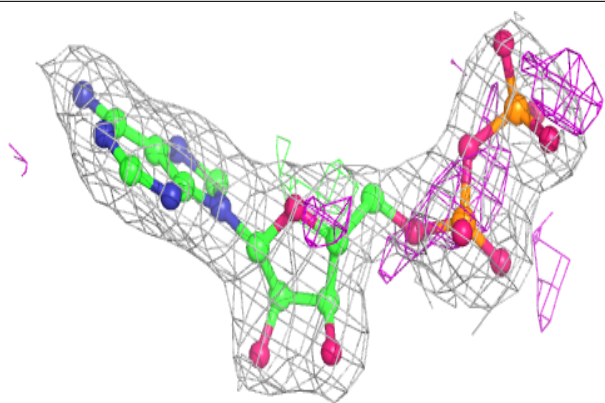
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NA	B	2705	1/1	0.95	0.08	42,42,42,42	0
6	FAD	A	2603	27/53	0.95	0.11	47,52,60,62	0
5	TPP	C	2802	26/26	0.97	0.11	27,36,37,38	0
3	NA	A	2605	1/1	0.97	0.12	48,48,48,48	0
5	TPP	D	2902	26/26	0.98	0.09	21,27,31,33	0
5	TPP	A	2602	26/26	0.98	0.09	26,32,36,37	0
6	FAD	B	2703	27/53	0.98	0.08	31,34,45,48	0
5	TPP	B	2702	26/26	0.98	0.09	21,28,31,32	0
2	MG	B	2701	1/1	0.98	0.07	31,31,31,31	0
2	MG	D	2901	1/1	0.99	0.08	32,32,32,32	0
4	SO4	A	2804	5/5	0.99	0.06	45,46,46,47	0
4	SO4	C	2604	5/5	0.99	0.06	41,42,43,44	0
4	SO4	D	2704	5/5	0.99	0.08	34,36,38,39	0
4	SO4	B	2904	5/5	1.00	0.06	33,34,35,39	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.

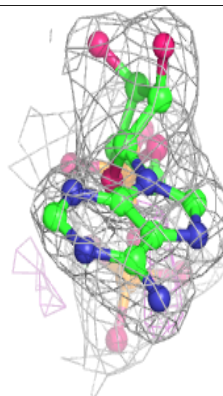
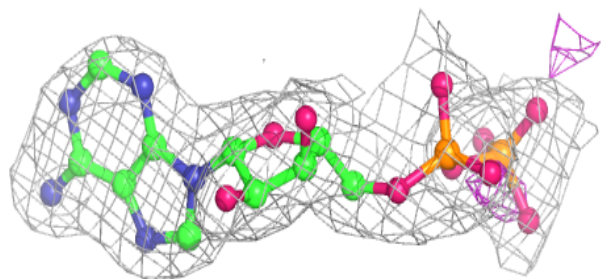
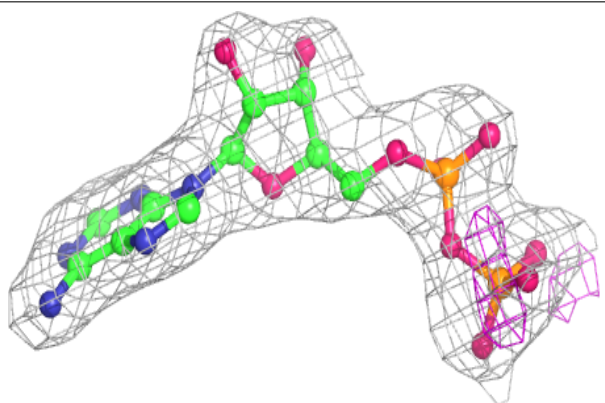


Electron density around FAD C 2803:

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

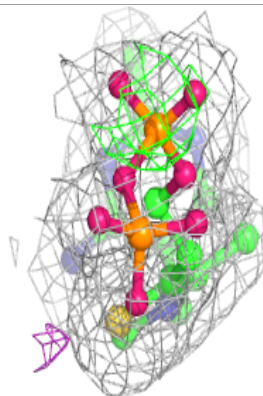
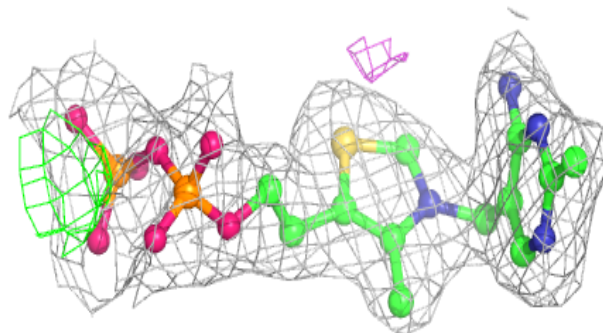
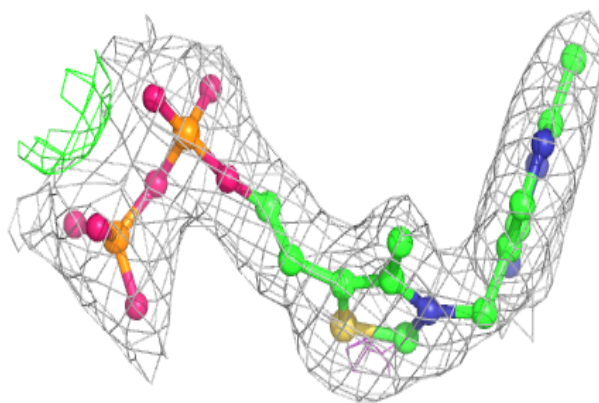
**Electron density around FAD A 2603:**

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

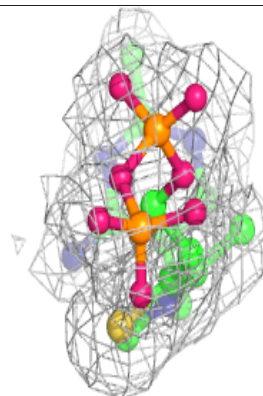
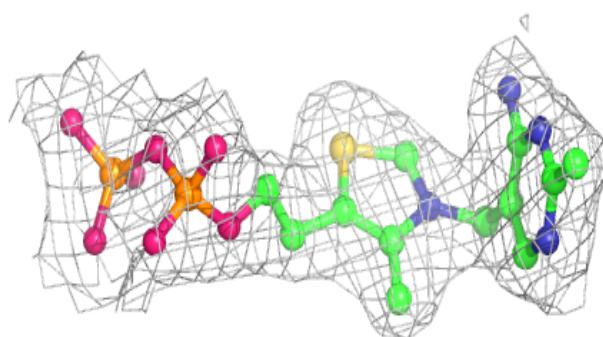
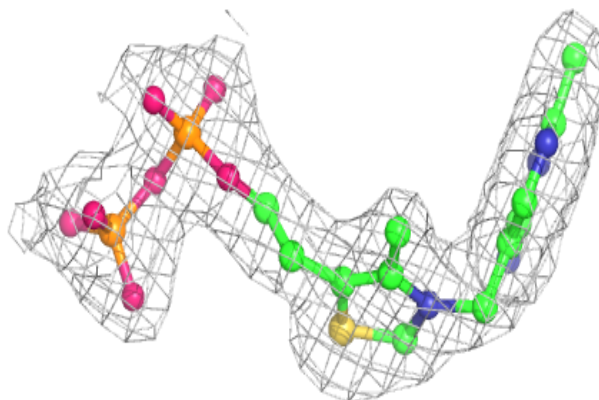


Electron density around TPP C 2802:

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

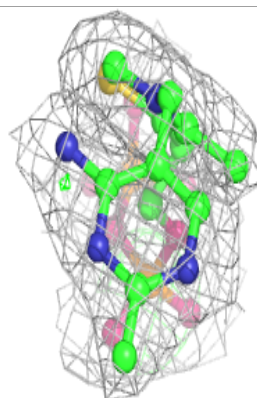
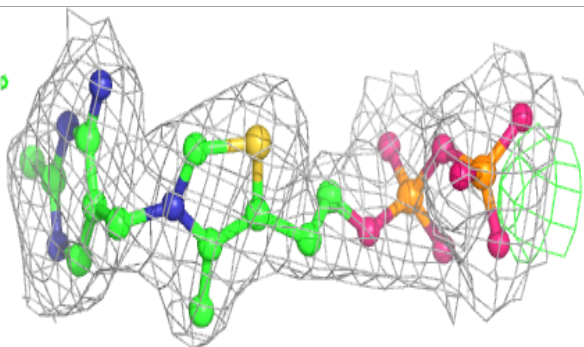
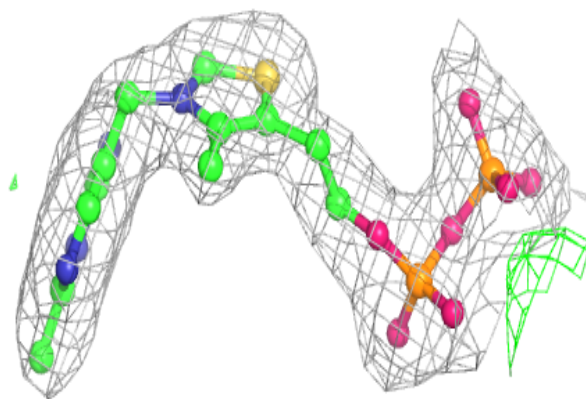
**Electron density around TPP D 2902:**

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

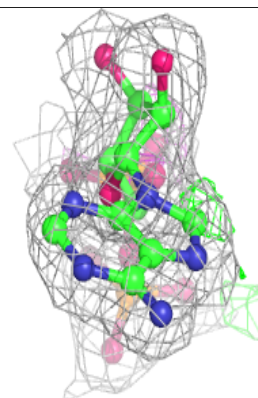
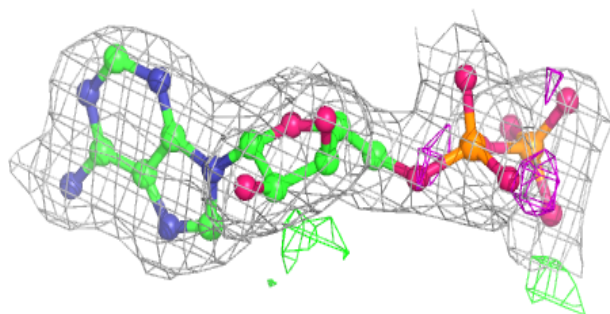
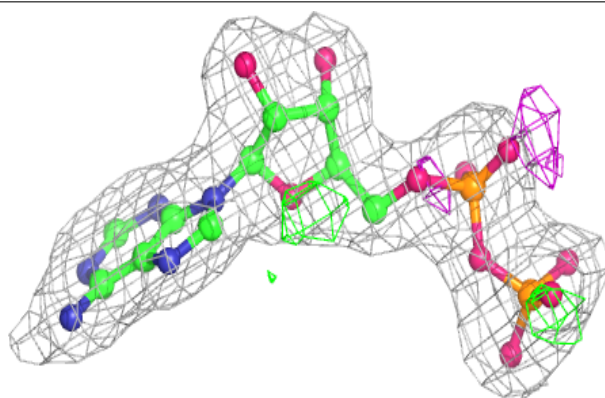


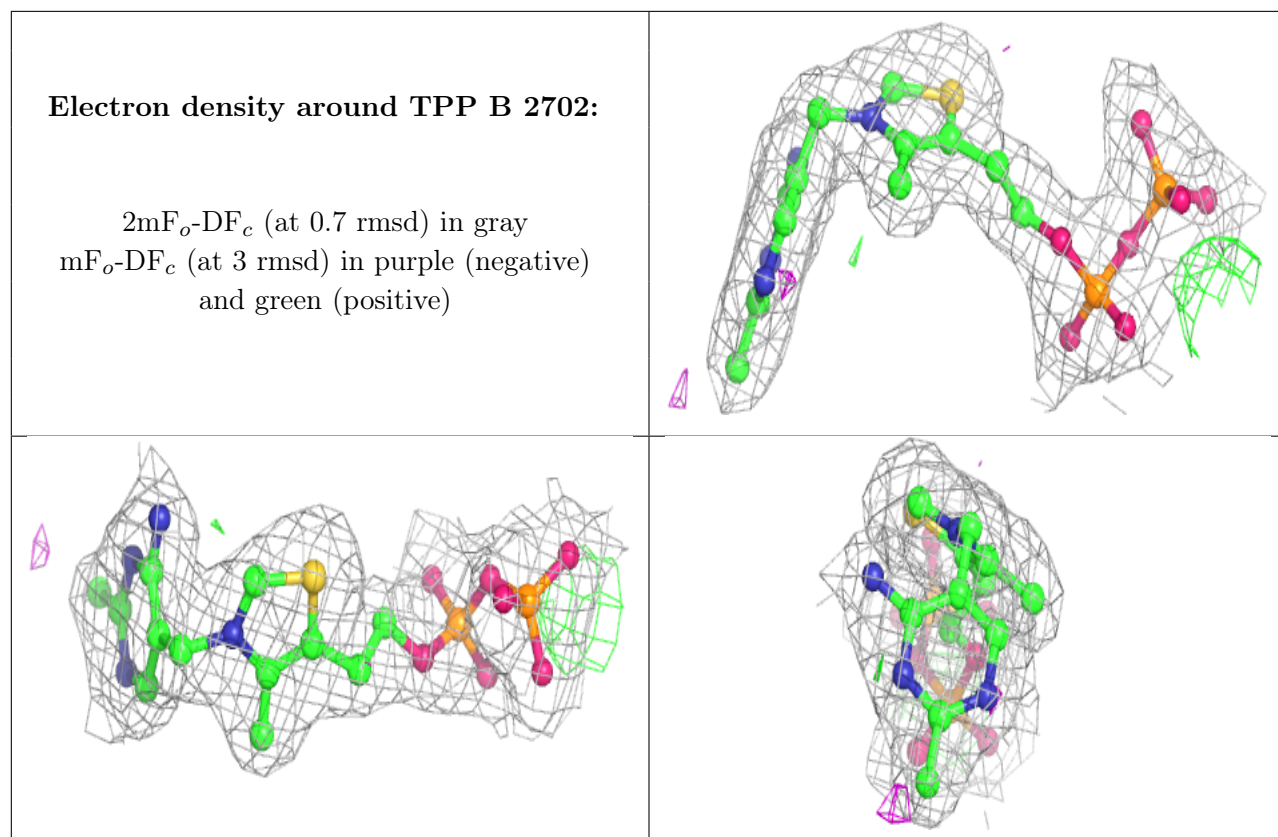
Electron density around TPP A 2602:

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

**Electron density around FAD B 2703:**

$2mF_o-DF_c$ (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.