



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:38 AM UTC

PDB ID : 1Y9D / pdb_00001y9d
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 types of validation reports are described at

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

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

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

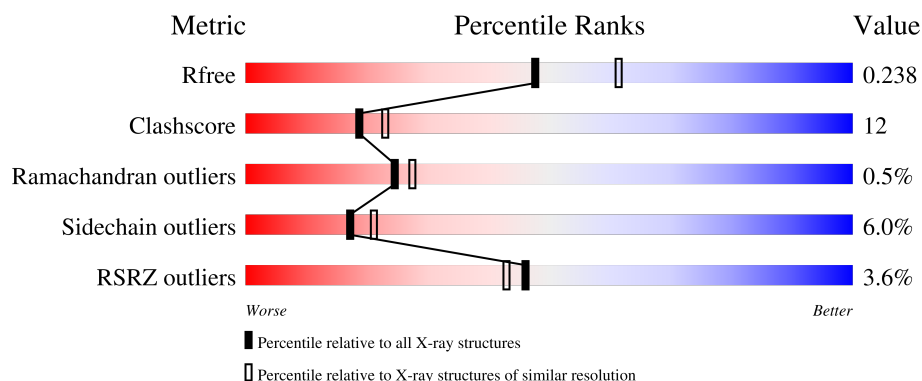
1 Overall quality at a glance

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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	3% 73% 16% • 7%
1	B	603	4% 72% 18% • 5%
1	C	603	2% 73% 15% • 8%
1	D	603	4% 74% 16% • 7%

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

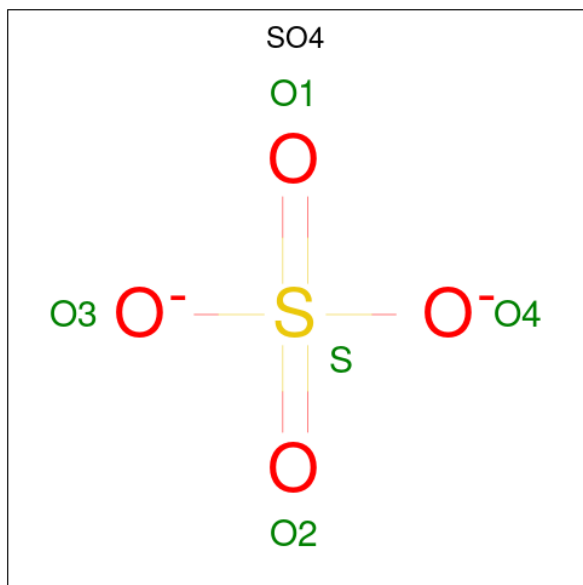
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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 (CCD ID: NA) (formula: Na).

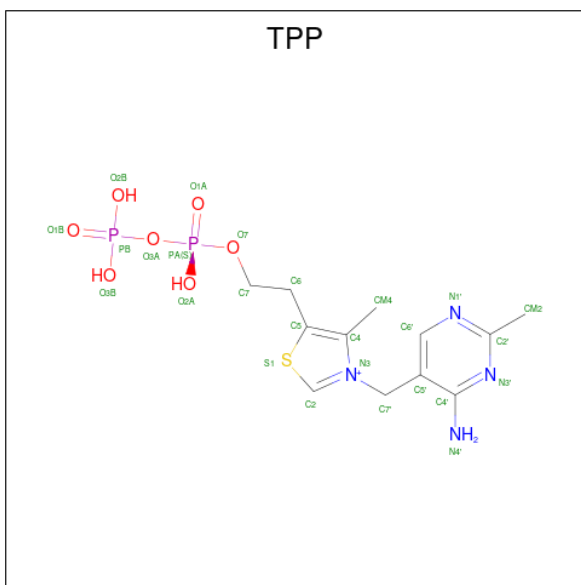
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



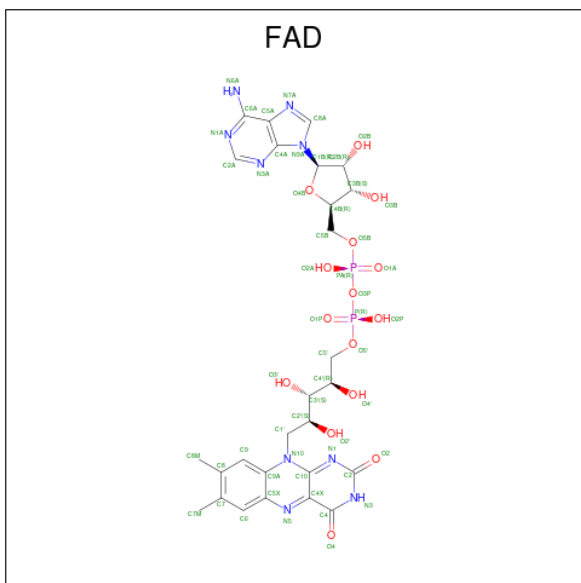
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is THIAMINE DIPHOSPHATE (CCD ID: 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 (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



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		

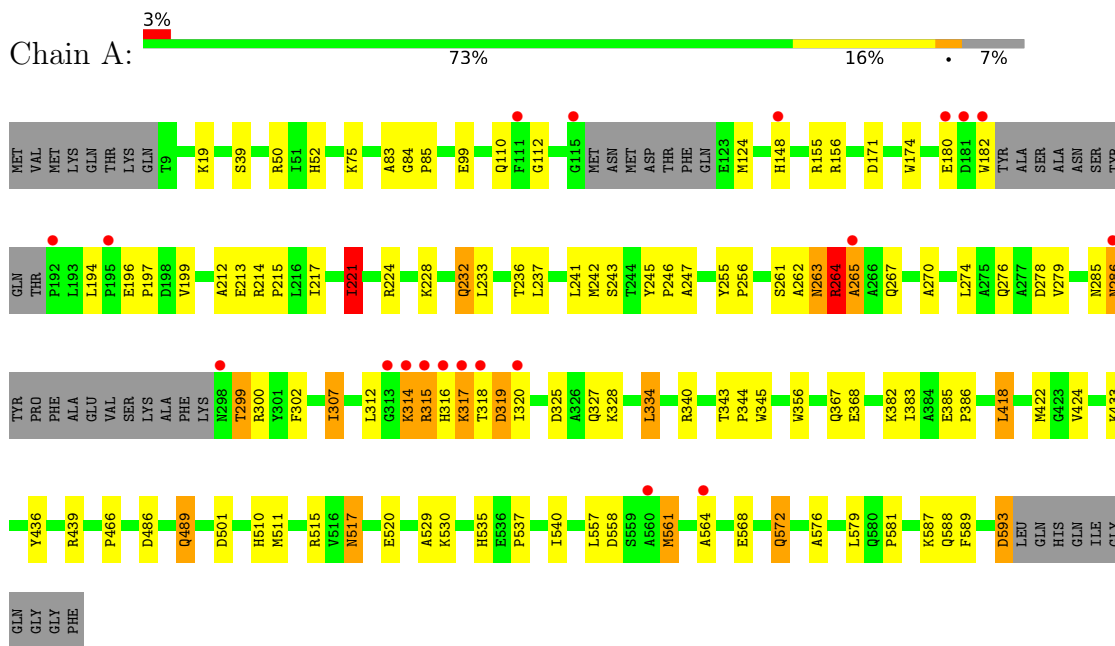
- Molecule 7 is water.

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		

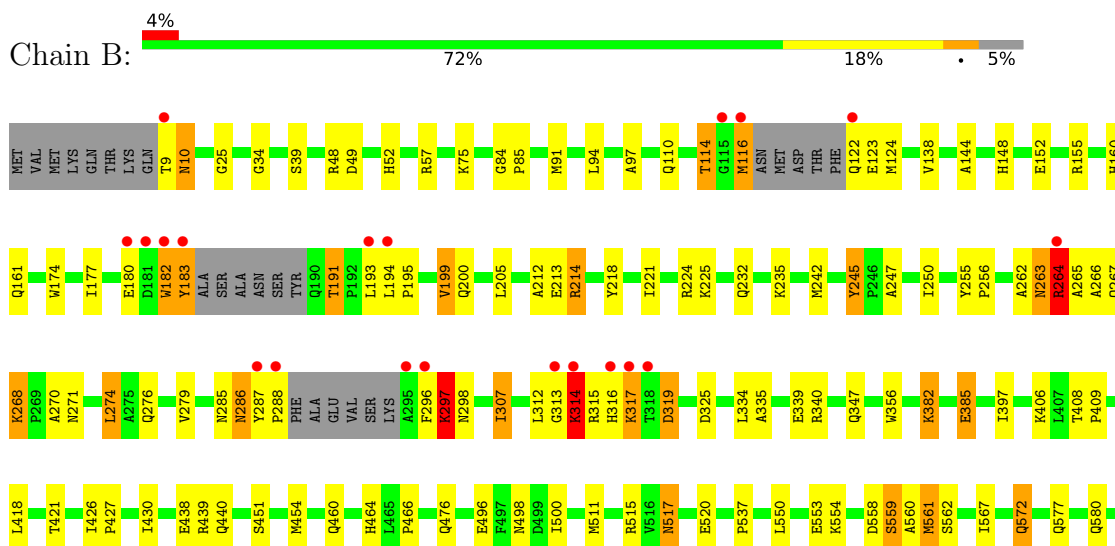
3 Residue-property plots [i](#)

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

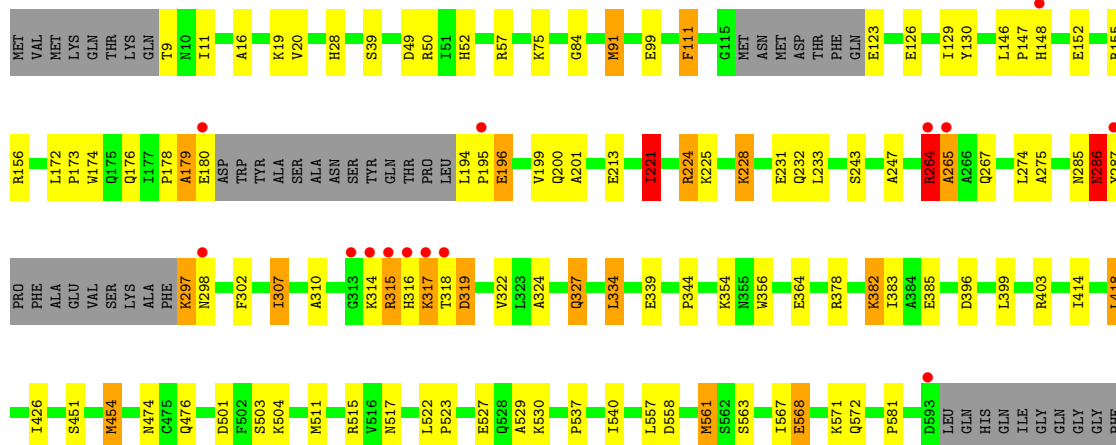
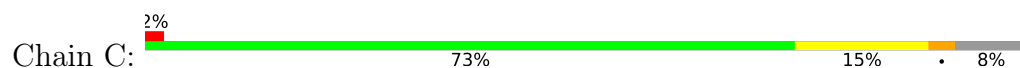


• Molecule 1: Pyruvate oxidase

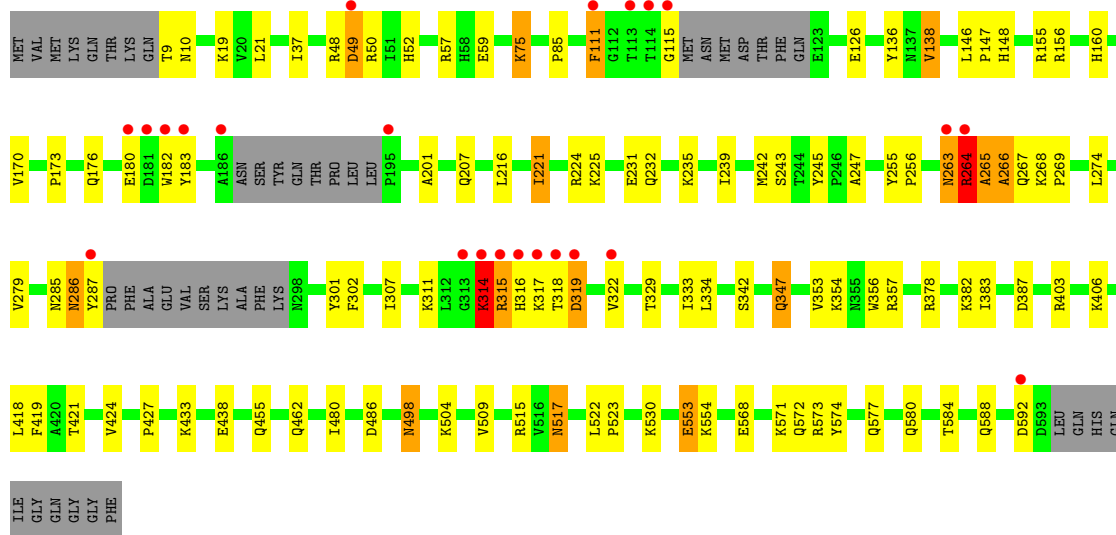
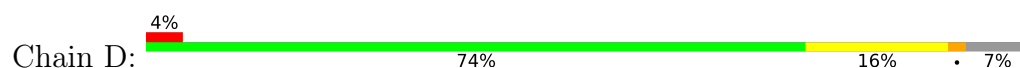




● Molecule 1: Pyruvate oxidase



● Molecule 1: Pyruvate oxidase



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 27.30 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (27.30-2.20) 99.7 (27.30-2.20)	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 (5.00%)	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)	0.38 , 58.4	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, FAD, TPP, 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	0.95	2/4383 (0.0%)	1.09	7/5964 (0.1%)
1	B	1.15	9/4513 (0.2%)	1.12	9/6141 (0.1%)
1	C	1.03	2/4365 (0.0%)	1.08	7/5937 (0.1%)
1	D	1.04	4/4401 (0.1%)	1.07	8/5988 (0.1%)
All	All	1.05	17/17662 (0.1%)	1.09	31/24030 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	2
1	D	0	1
All	All	0	6

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	426	ILE	CA-CB	7.86	1.58	1.54
1	C	221	ILE	CA-CB	7.04	1.63	1.54
1	A	221	ILE	CA-CB	6.97	1.63	1.54
1	B	397	ILE	CA-CB	6.32	1.62	1.54
1	B	268	LYS	CE-NZ	6.09	1.67	1.49
1	B	177	ILE	CA-CB	5.59	1.62	1.54
1	D	239	ILE	CA-C	5.47	1.56	1.52
1	D	37	ILE	CA-CB	5.38	1.61	1.54
1	B	97	ALA	CA-CB	5.35	1.61	1.53
1	A	424	VAL	CA-CB	5.34	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	593	ASP	CA-C	5.34	1.59	1.52
1	D	504	LYS	C-O	5.29	1.30	1.24
1	B	214	ARG	CA-C	5.21	1.58	1.53
1	B	430	ILE	N-CA	5.15	1.52	1.46
1	B	314	LYS	N-CA	5.10	1.52	1.46
1	D	387	ASP	CA-C	5.09	1.59	1.52
1	B	199	VAL	CA-CB	5.03	1.60	1.54

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	265	ALA	N-CA-C	-9.55	102.24	112.93
1	D	265	ALA	N-CA-C	-8.84	102.58	112.57
1	C	179	ALA	N-CA-C	-7.74	102.84	111.82
1	C	265	ALA	N-CA-C	-7.73	100.24	111.30
1	A	264	ARG	N-CA-C	7.63	120.14	110.61
1	A	265	ALA	N-CA-C	-7.18	101.75	111.87
1	D	264	ARG	N-CA-C	7.01	125.74	110.80
1	B	319	ASP	N-CA-C	6.95	118.74	111.03
1	A	486	ASP	N-CA-C	6.86	118.76	111.28
1	D	314	LYS	N-CA-C	6.79	125.25	110.80
1	B	594	LEU	N-CA-C	-6.75	102.97	113.02
1	B	235	LYS	N-CA-C	6.45	119.30	111.82
1	B	382	LYS	N-CA-C	6.28	118.12	111.28
1	D	315	ARG	N-CA-C	6.11	118.02	111.36
1	B	460	GLN	N-CA-C	-5.87	104.88	111.28
1	B	138	VAL	N-CA-C	5.79	118.30	108.86
1	A	314	LYS	N-CA-C	5.73	118.30	111.71
1	B	10	ASN	N-CA-C	5.62	122.78	110.80
1	D	266	ALA	N-CA-C	5.45	117.92	110.24
1	D	138	VAL	N-CA-C	5.37	116.46	108.46
1	C	231	GLU	CA-C-N	5.35	127.77	120.54
1	C	231	GLU	C-N-CA	5.35	127.77	120.54
1	A	320	ILE	N-CA-C	5.31	115.50	107.80
1	A	52	HIS	N-CA-C	5.30	117.27	108.20
1	D	21	LEU	N-CA-C	5.28	117.44	111.11
1	C	454	MET	N-CA-C	5.20	117.62	111.33
1	A	312	LEU	N-CA-C	5.15	117.95	108.58
1	C	91	MET	N-CA-C	5.14	117.28	111.11
1	B	561	MET	N-CA-C	5.09	119.11	113.01
1	C	264	ARG	N-CA-C	5.06	121.58	110.80
1	D	486	ASP	N-CA-C	5.02	117.65	111.82

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

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	100	0
1	B	4423	0	4377	119	0
1	C	4282	0	4249	99	0
1	D	4315	0	4264	103	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	1	0
5	B	26	0	16	1	0
5	C	26	0	16	0	0
5	D	26	0	16	0	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	38	0
7	B	532	0	0	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	426	0	0	26	0
7	D	488	0	0	41	0
All	All	19404	0	17262	415	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 (415) 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
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:A:242:MET:HE1	1:A:274:LEU:HB2	1.52	0.90
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:A:84:GLY:HA2	1:A:124:MET:HE1	1.57	0.85
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:286:ASN:O	1:D:286:ASN:CG	2.29	0.75
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
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:C:286:ASN:O	1:C:286:ASN:CG	2.32	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:B:84:GLY:HA2	1:B:124:MET:HE1	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:91:MET:HA	1:B:91:MET:HE2	1.75	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:B:593:ASP:CG	1:B:594:LEU:H	2.02	0.68
1:D:517:ASN:HD22	1:D:517:ASN:H	1.40	0.68
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
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: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:205:LEU:C	1:B:205:LEU:HD23	2.22	0.64
1:B:262:ALA:O	1:B:263:ASN:HB2	1.96	0.64
1:B:317:LYS:HE2	7:B:3338:HOH:O	1.97	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:511:MET:HE2	1:B:537:PRO:HB2	1.82	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: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
1:B:270:ALA:O	1:B:274:LEU:HD12	2.00	0.60
1:B:286:ASN:O	1:B:286:ASN:CG	2.44	0.60
1:B:287:TYR:CD1	1:B:288:PRO:HD2	2.36	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:C:501:ASP:OD1	1:C:503:SER:OG	2.16	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:511:MET:HE2	1:A:537:PRO:HB2	1.85	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:D:317:LYS:NZ	7:D:3322:HOH:O	2.31	0.58
1:C:111:PHE:HD2	1:C:111:PHE:H	1.48	0.57
1:C:511:MET:HE2	1:C:537:PRO:HB2	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:242:MET:HE1	1:D:274:LEU:HD13	1.86	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: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
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: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:91:MET:HE1	1:C:130:TYR:CD1	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:264:ARG:C	1:B:266:ALA:H	2.17	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: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:O	1:D:286:ASN:ND2	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
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:C:196:GLU:CD	1:C:196:GLU:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:122:GLN:HG3	1:B:124:MET:HE2	1.93	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:A:182:TRP:CD1	7:A:3142:HOH:O	2.65	0.49
1:B:421:THR:HB	1:D:85:PRO:HB3	1.95	0.49
1:B:91:MET:HE1	1:B:94:LEU:HD12	1.94	0.48
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
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:C:317:LYS:HD2	1:C:317:LYS:C	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:39:SER:HB3	1:A:174:TRP:CD2	2.50	0.46
1:B:212:ALA:HB2	1:B:279:VAL:HG21	1.97	0.46
1:D:216:LEU:HD13	1:D:242:MET:HE2	1.96	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:C:176:GLN:CD	7:C:3222:HOH:O	2.58	0.46
1:B:319:ASP:OD1	1:B:319:ASP:N	2.48	0.46
1:B:558:ASP:C	1:B:560:ALA:N	2.74	0.46
1:C:84:GLY:H	1:C:126:GLU:CD	2.24	0.46
1:A:242:MET:CE	1:A:270:ALA:O	2.64	0.46
1:C:504:LYS:NZ	7:C:2954:HOH:O	2.35	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
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:A:422:MET:HE3	5:A:2602:TPP:H72	1.98	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: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:D:264:ARG:HA	1:D:266:ALA:N	2.27	0.45
1:B:245:TYR:C	1:B:245:TYR:CD2	2.94	0.45
1:D:268:LYS:HB3	1:D:269:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:286:ASN:ND2	1:A:286:ASN:C	2.75	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
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:D:245:TYR:C	1:D:245:TYR:CD2	2.96	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:D:424:VAL:C	1:D:427:PRO:HD2	2.43	0.43
1:C:156:ARG:HD3	7:C:3211:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:399:LEU:C	1:C:399:LEU:HD23	2.45	0.42
1:C:451:SER:HA	1:C:454:MET:HE3	2.01	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:A:180:GLU:H	1:A:180:GLU:CD	2.28	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:A:267:GLN:HE21	1:A:356:TRP:NE1	2.02	0.42
1:B:438:GLU:HB3	7:B:3417:HOH:O	2.19	0.42
1:B:550:LEU:C	1:B:550:LEU:HD23	2.45	0.42
1:C:91:MET:HE1	1:C:130:TYR:CE1	2.54	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:B:451:SER:HA	1:B:454:MET:HE3	2.01	0.41
1:C:195:PRO:HD2	1:C:307:ILE:CD1	2.50	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/603 (91%)	529 (96%)	19 (4%)	2 (0%)	30	34
1	B	564/603 (94%)	537 (95%)	20 (4%)	7 (1%)	10	8
1	C	548/603 (91%)	517 (94%)	30 (6%)	1 (0%)	43	51
1	D	552/603 (92%)	530 (96%)	21 (4%)	1 (0%)	43	51
All	All	2214/2412 (92%)	2113 (95%)	90 (4%)	11 (0%)	24	27

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%)	20	25
1	B	459/484 (95%)	427 (93%)	32 (7%)	14	16
1	C	444/484 (92%)	417 (94%)	27 (6%)	17	20
1	D	446/484 (92%)	422 (95%)	24 (5%)	20	25
All	All	1795/1936 (93%)	1688 (94%)	107 (6%)	17	21

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LYS
1	A	156	ARG
1	A	194	LEU
1	A	199	VAL
1	A	221	ILE
1	A	228	LYS
1	A	232	GLN
1	A	286	ASN
1	A	299	THR
1	A	300	ARG
1	A	307	ILE

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Mol	Chain	Res	Type
1	A	315	ARG
1	A	317	LYS
1	A	319	ASP
1	A	327	GLN
1	A	334	LEU
1	A	382	LYS
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	114	THR
1	B	116	MET
1	B	123	GLU
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	221	ILE
1	B	232	GLN
1	B	245	TYR
1	B	264	ARG
1	B	271	ASN
1	B	274	LEU
1	B	286	ASN
1	B	297	LYS
1	B	307	ILE
1	B	314	LYS
1	B	334	LEU
1	B	339	GLU
1	B	385	GLU
1	B	418	LEU
1	B	498	ASN
1	B	515	ARG
1	B	517	ASN
1	B	554	LYS
1	B	562	SER

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Mol	Chain	Res	Type
1	B	572	GLN
1	B	595	GLN
1	B	597	GLN
1	C	75	LYS
1	C	111	PHE
1	C	123	GLU
1	C	196	GLU
1	C	199	VAL
1	C	221	ILE
1	C	224	ARG
1	C	228	LYS
1	C	232	GLN
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	414	ILE
1	C	418	LEU
1	C	515	ARG
1	C	517	ASN
1	C	561	MET
1	C	563	SER
1	C	568	GLU
1	C	572	GLN
1	D	49	ASP
1	D	75	LYS
1	D	111	PHE
1	D	138	VAL
1	D	207	GLN
1	D	221	ILE
1	D	263	ASN
1	D	286	ASN
1	D	307	ILE
1	D	311	LYS
1	D	314	LYS
1	D	319	ASP

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Mol	Chain	Res	Type
1	D	334	LEU
1	D	347	GLN
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	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 (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	HIS
1	A	176	GLN
1	A	267	GLN
1	A	276	GLN
1	A	304	GLN
1	A	417	ASN
1	A	435	ASN
1	A	476	GLN
1	A	489	GLN
1	A	517	ASN
1	A	572	GLN
1	A	588	GLN
1	B	10	ASN
1	B	122	GLN
1	B	127	ASN
1	B	167	GLN
1	B	190	GLN
1	B	267	GLN
1	B	276	GLN
1	B	298	ASN
1	B	316	HIS
1	B	336	GLN
1	B	476	GLN
1	B	517	ASN
1	B	534	GLN
1	B	596	HIS

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Mol	Chain	Res	Type
1	B	597	GLN
1	C	101	HIS
1	C	125	ASN
1	C	200	GLN
1	C	207	GLN
1	C	263	ASN
1	C	267	GLN
1	C	276	GLN
1	C	316	HIS
1	C	435	ASN
1	C	443	ASN
1	C	460	GLN
1	C	469	ASN
1	C	476	GLN
1	C	580	GLN
1	D	10	ASN
1	D	101	HIS
1	D	110	GLN
1	D	142	ASN
1	D	160	HIS
1	D	175	GLN
1	D	176	GLN
1	D	263	ASN
1	D	267	GLN
1	D	327	GLN
1	D	336	GLN
1	D	347	GLN
1	D	417	ASN
1	D	443	ASN
1	D	460	GLN
1	D	469	ASN
1	D	476	GLN
1	D	498	ASN
1	D	517	ASN
1	D	534	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0.46	0	6,6,6	0.32	0
4	SO4	D	2704	-	4,4,4	0.29	0	6,6,6	0.77	0
5	TPP	A	2602	2	26,27,27	1.90	7 (26%)	38,40,40	1.85	10 (26%)
6	FAD	D	2903	-	28,29,58	1.28	5 (17%)	43,45,89	1.93	10 (23%)
6	FAD	A	2603	-	28,29,58	1.26	5 (17%)	43,45,89	1.87	10 (23%)
5	TPP	C	2802	2	26,27,27	1.77	8 (30%)	38,40,40	1.78	9 (23%)
4	SO4	B	2904	-	4,4,4	0.18	0	6,6,6	0.40	0
4	SO4	A	2804	-	4,4,4	0.39	0	6,6,6	0.22	0
5	TPP	B	2702	2	26,27,27	1.62	6 (23%)	38,40,40	2.10	13 (34%)
6	FAD	C	2803	-	28,29,58	1.32	4 (14%)	43,45,89	1.93	9 (20%)
6	FAD	B	2703	-	28,29,58	1.17	2 (7%)	43,45,89	1.91	11 (25%)
5	TPP	D	2902	2	26,27,27	1.61	5 (19%)	38,40,40	1.97	13 (34%)

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	A	2602	2	-	3/17/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FAD	D	2903	-	-	3/16/32/50	0/3/3/6
6	FAD	A	2603	-	-	3/16/32/50	0/3/3/6
5	TPP	C	2802	2	-	4/17/17/17	0/2/2/2
5	TPP	B	2702	2	-	2/17/17/17	0/2/2/2
6	FAD	C	2803	-	-	1/16/32/50	0/3/3/6
6	FAD	B	2703	-	-	3/16/32/50	0/3/3/6
5	TPP	D	2902	2	-	3/17/17/17	0/2/2/2

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2602	TPP	C2-N3	4.05	1.42	1.32
5	C	2802	TPP	C5-S1	-3.83	1.62	1.72
5	D	2902	TPP	C2-N3	3.81	1.41	1.32
5	B	2702	TPP	C6'-N1'	3.45	1.41	1.34
5	B	2702	TPP	C2-N3	3.41	1.40	1.32
5	D	2902	TPP	C4'-N3'	3.34	1.39	1.35
5	A	2602	TPP	C2'-N3'	3.31	1.39	1.34
5	A	2602	TPP	C2'-N1'	3.29	1.39	1.34
6	C	2803	FAD	PA-O3P	3.28	1.63	1.59
5	A	2602	TPP	PA-O3A	3.24	1.63	1.59
5	B	2702	TPP	C5-S1	-3.19	1.64	1.72
5	C	2802	TPP	C2-N3	3.13	1.40	1.32
5	C	2802	TPP	C4'-N3'	3.12	1.39	1.35
5	D	2902	TPP	C5-S1	-3.04	1.64	1.72
5	C	2802	TPP	C6'-N1'	3.02	1.40	1.34
6	C	2803	FAD	C8A-N7A	3.00	1.37	1.31
5	A	2602	TPP	C5-C4	2.94	1.41	1.35
5	B	2702	TPP	C2'-N1'	2.87	1.38	1.34
6	A	2603	FAD	C2A-N1A	2.86	1.39	1.33
6	D	2903	FAD	C8A-N7A	2.83	1.37	1.31
5	A	2602	TPP	C5-S1	-2.81	1.65	1.72
5	C	2802	TPP	C5-C4	2.80	1.41	1.35
6	D	2903	FAD	P-O5'	2.73	1.64	1.54
6	C	2803	FAD	P-O5'	2.69	1.64	1.54
5	D	2902	TPP	C6'-N1'	2.65	1.39	1.34
6	B	2703	FAD	C8A-N7A	2.60	1.36	1.31
6	D	2903	FAD	C2A-N3A	2.55	1.38	1.33
6	A	2603	FAD	C8A-N7A	2.55	1.36	1.31
6	A	2603	FAD	PA-O3P	2.48	1.62	1.59
5	B	2702	TPP	C2'-N3'	2.37	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2802	TPP	C2'-N3'	2.34	1.38	1.34
5	A	2602	TPP	C6'-C5'	2.32	1.42	1.37
5	C	2802	TPP	C7'-C5'	2.32	1.55	1.51
5	D	2902	TPP	C5-C4	2.27	1.40	1.35
6	D	2903	FAD	PA-O3P	2.25	1.61	1.59
5	B	2702	TPP	C4'-N3'	2.17	1.37	1.35
6	A	2603	FAD	P-O5'	2.12	1.62	1.54
6	D	2903	FAD	C2A-N1A	2.10	1.37	1.33
6	C	2803	FAD	O4B-C4B	-2.06	1.40	1.45
6	A	2603	FAD	C2A-N3A	2.04	1.37	1.33
5	C	2802	TPP	C2'-N1'	2.04	1.37	1.34
6	B	2703	FAD	C5A-N7A	-2.03	1.35	1.39

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	2903	FAD	N3A-C2A-N1A	-6.36	118.96	128.58
6	C	2803	FAD	N3A-C2A-N1A	-5.64	120.05	128.58
6	A	2603	FAD	N3A-C2A-N1A	-5.47	120.30	128.58
6	B	2703	FAD	N3A-C2A-N1A	-5.08	120.90	128.58
6	B	2703	FAD	N9A-C8A-N7A	-4.70	107.27	113.94
5	B	2702	TPP	CM2-C2'-N1'	4.68	122.18	117.20
6	C	2803	FAD	C5A-C4A-N3A	-4.60	120.38	126.72
5	C	2802	TPP	N1'-C2'-N3'	-4.24	118.48	125.53
5	A	2602	TPP	C6'-C5'-C4'	4.22	120.74	115.55
5	D	2902	TPP	C2-N3-C4	-4.22	108.36	114.06
5	B	2702	TPP	C2-N3-C4	-4.18	108.41	114.06
5	D	2902	TPP	CM2-C2'-N1'	4.18	121.65	117.20
6	A	2603	FAD	N9A-C8A-N7A	-4.10	108.12	113.94
6	D	2903	FAD	C5A-C4A-N3A	-4.10	121.08	126.72
5	B	2702	TPP	N1'-C2'-N3'	-4.09	118.73	125.53
6	C	2803	FAD	N9A-C8A-N7A	-4.05	108.19	113.94
6	D	2903	FAD	O2A-PA-O3P	4.05	118.22	107.27
5	D	2902	TPP	N1'-C2'-N3'	-3.86	119.11	125.53
5	A	2602	TPP	C2-N3-C4	-3.86	108.84	114.06
6	B	2703	FAD	C5A-N7A-C8A	3.83	109.47	103.45
6	A	2603	FAD	C5A-N7A-C8A	3.77	109.37	103.45
6	B	2703	FAD	C5A-C4A-N3A	-3.76	121.55	126.72
5	C	2802	TPP	CM2-C2'-N1'	3.75	121.19	117.20
6	B	2703	FAD	O2A-PA-O3P	3.71	117.31	107.27
6	C	2803	FAD	C5A-N7A-C8A	3.69	109.25	103.45
6	D	2903	FAD	C2A-N3A-C4A	3.60	120.63	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2702	TPP	CM4-C4-N3	3.57	128.81	120.57
6	C	2803	FAD	C2A-N3A-C4A	3.57	120.55	111.83
5	C	2802	TPP	C2-N3-C4	-3.54	109.28	114.06
6	C	2803	FAD	O2A-PA-O3P	3.41	116.50	107.27
6	C	2803	FAD	C4A-C5A-N7A	-3.40	106.70	110.58
5	D	2902	TPP	C4-C5-S1	3.40	115.86	110.56
6	A	2603	FAD	C5A-C4A-N3A	-3.37	122.07	126.72
6	A	2603	FAD	C4A-C5A-N7A	-3.34	106.76	110.58
5	B	2702	TPP	C4-C5-S1	3.28	115.68	110.56
5	B	2702	TPP	C6'-C5'-C4'	3.26	119.55	115.55
5	A	2602	TPP	C4-C5-S1	3.26	115.64	110.56
6	A	2603	FAD	O2A-PA-O3P	3.24	116.03	107.27
6	D	2903	FAD	O3P-PA-O1A	-3.21	101.05	110.70
5	A	2602	TPP	CM2-C2'-N1'	3.16	120.56	117.20
6	D	2903	FAD	N9A-C8A-N7A	-3.14	109.48	113.94
5	D	2902	TPP	S1-C2-N3	3.11	116.24	112.30
5	D	2902	TPP	C2-S1-C5	-3.05	89.19	91.22
5	C	2802	TPP	C2'-N3'-C4'	3.01	122.73	118.10
5	D	2902	TPP	CM4-C4-N3	2.95	127.38	120.57
5	B	2702	TPP	C5'-C6'-N1'	-2.95	119.03	123.83
6	B	2703	FAD	C2A-N3A-C4A	2.93	118.99	111.83
5	B	2702	TPP	C6'-N1'-C2'	2.93	120.88	116.07
5	D	2902	TPP	C6'-N1'-C2'	2.91	120.85	116.07
5	B	2702	TPP	S1-C2-N3	2.89	115.96	112.30
5	A	2602	TPP	O3B-PB-O2B	2.80	118.30	107.80
5	B	2702	TPP	C2'-N3'-C4'	2.77	122.36	118.10
5	A	2602	TPP	S1-C2-N3	2.77	115.80	112.30
6	A	2603	FAD	O3P-PA-O1A	-2.74	102.45	110.70
5	B	2702	TPP	CM4-C4-C5	-2.74	120.74	127.75
6	B	2703	FAD	C4A-C5A-N7A	-2.73	107.46	110.58
6	A	2603	FAD	C2A-N3A-C4A	2.72	118.46	111.83
5	A	2602	TPP	C2-S1-C5	-2.66	89.45	91.22
5	D	2902	TPP	C2'-N3'-C4'	2.64	122.17	118.10
5	C	2802	TPP	C6'-N1'-C2'	2.63	120.39	116.07
5	B	2702	TPP	C2-S1-C5	-2.62	89.48	91.22
6	D	2903	FAD	C5A-N7A-C8A	2.56	107.48	103.45
5	C	2802	TPP	CM4-C4-N3	2.56	126.47	120.57
6	C	2803	FAD	C5A-C4A-N9A	2.53	108.56	105.81
6	B	2703	FAD	O3P-PA-O1A	-2.46	103.32	110.70
6	D	2903	FAD	O5'-P-O3P	-2.44	96.45	104.64
5	A	2602	TPP	C5'-C6'-N1'	-2.44	119.86	123.83
5	B	2702	TPP	C5'-C7'-N3	-2.40	107.79	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	2703	FAD	O3P-P-O1P	-2.37	98.55	111.04
5	A	2602	TPP	N1'-C2'-N3'	-2.36	121.61	125.53
6	C	2803	FAD	N3A-C4A-N9A	2.29	131.06	127.17
5	A	2602	TPP	CM4-C4-N3	2.28	125.83	120.57
6	A	2603	FAD	C5A-C4A-N9A	2.27	108.28	105.81
6	D	2903	FAD	N3A-C4A-N9A	2.26	131.01	127.17
6	D	2903	FAD	C4A-C5A-N7A	-2.26	108.00	110.58
5	D	2902	TPP	O3B-PB-O3A	2.26	112.20	104.64
6	B	2703	FAD	C4A-N9A-C8A	2.22	108.07	105.74
6	A	2603	FAD	C2A-N1A-C6A	2.15	122.27	118.73
5	C	2802	TPP	C4-C5-S1	2.15	113.92	110.56
5	C	2802	TPP	CM2-C2'-N3'	2.14	120.33	117.13
5	D	2902	TPP	CM4-C4-C5	-2.12	122.33	127.75
5	D	2902	TPP	C5'-C6'-N1'	-2.10	120.41	123.83
6	B	2703	FAD	N3A-C4A-N9A	2.09	130.73	127.17
5	D	2902	TPP	C6'-C5'-C4'	2.06	118.07	115.55
5	C	2802	TPP	O2B-PB-O3A	-2.05	97.76	104.64

There are no chirality outliers.

All (22) 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
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	A	2603	FAD	C4B-C5B-O5B-PA
6	B	2703	FAD	O4B-C4B-C5B-O5B
6	C	2803	FAD	C4B-C5B-O5B-PA
6	B	2703	FAD	C4B-C5B-O5B-PA
5	C	2802	TPP	PA-O3A-PB-O1B
5	A	2602	TPP	PA-O3A-PB-O2B
5	A	2602	TPP	C5-C6-C7-O7
5	C	2802	TPP	C5-C6-C7-O7
5	D	2902	TPP	C5-C6-C7-O7
6	A	2603	FAD	O4B-C4B-C5B-O5B
6	D	2903	FAD	C2B-C1B-N9A-C8A
6	A	2603	FAD	C2B-C1B-N9A-C8A

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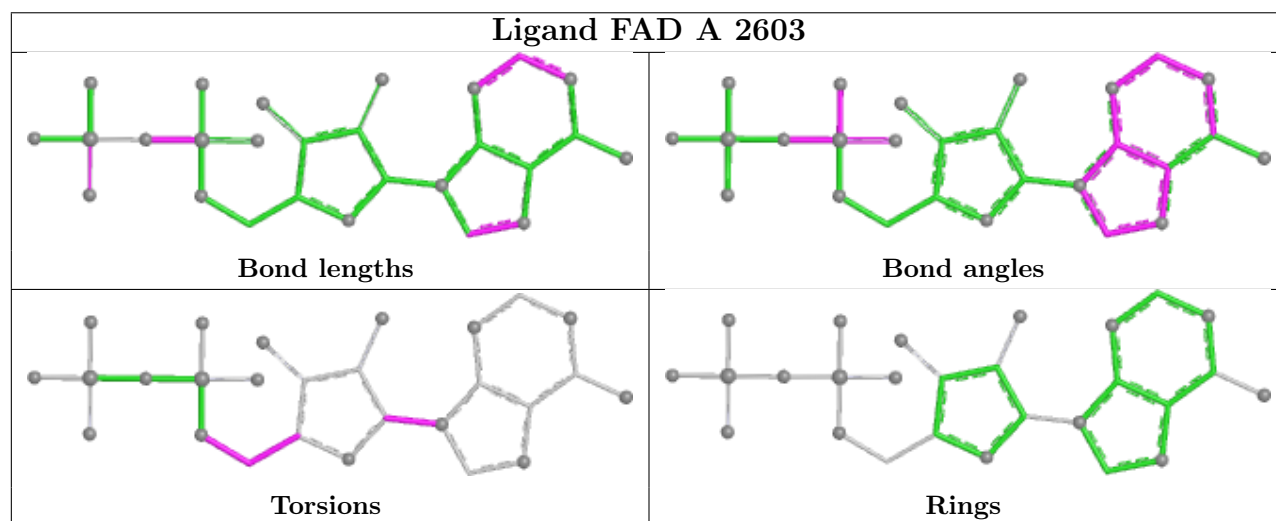
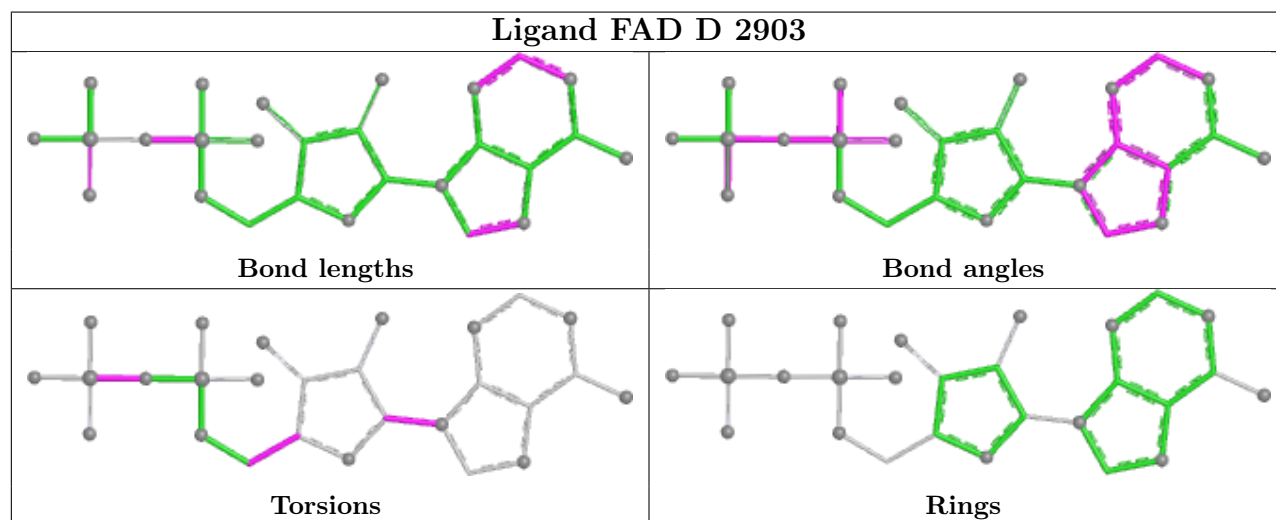
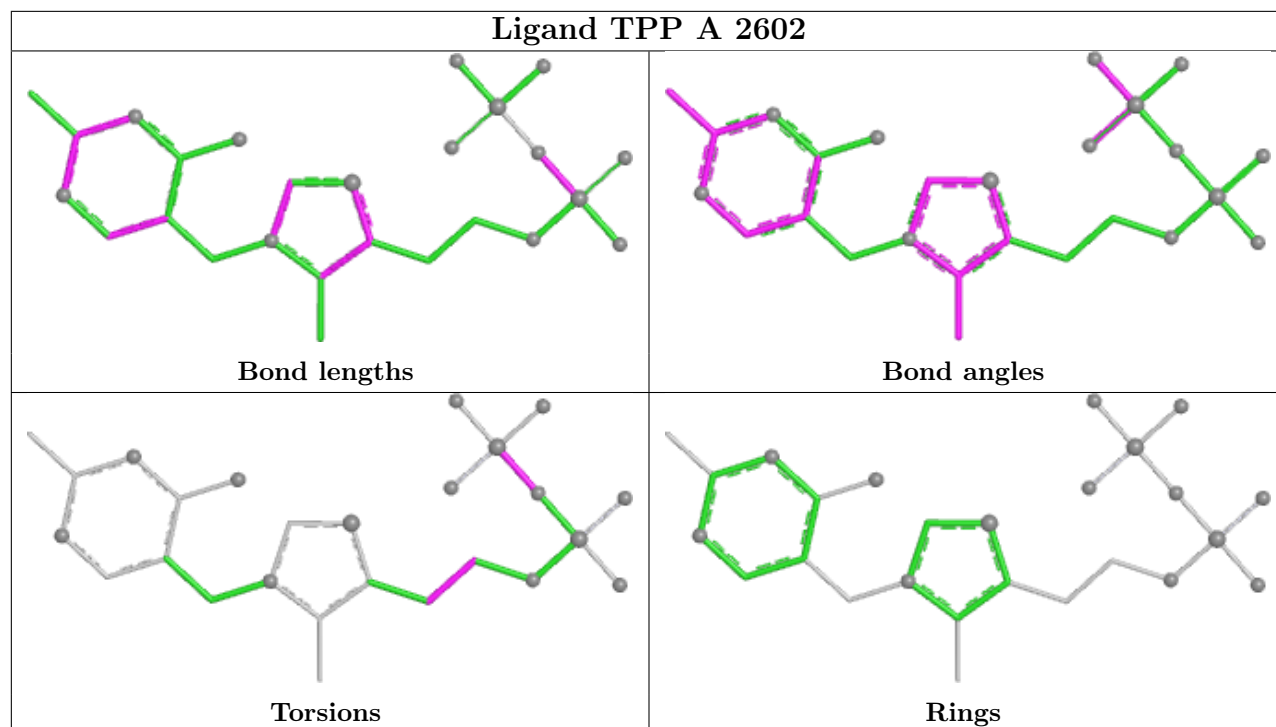
Mol	Chain	Res	Type	Atoms
6	B	2703	FAD	C2B-C1B-N9A-C8A
6	D	2903	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

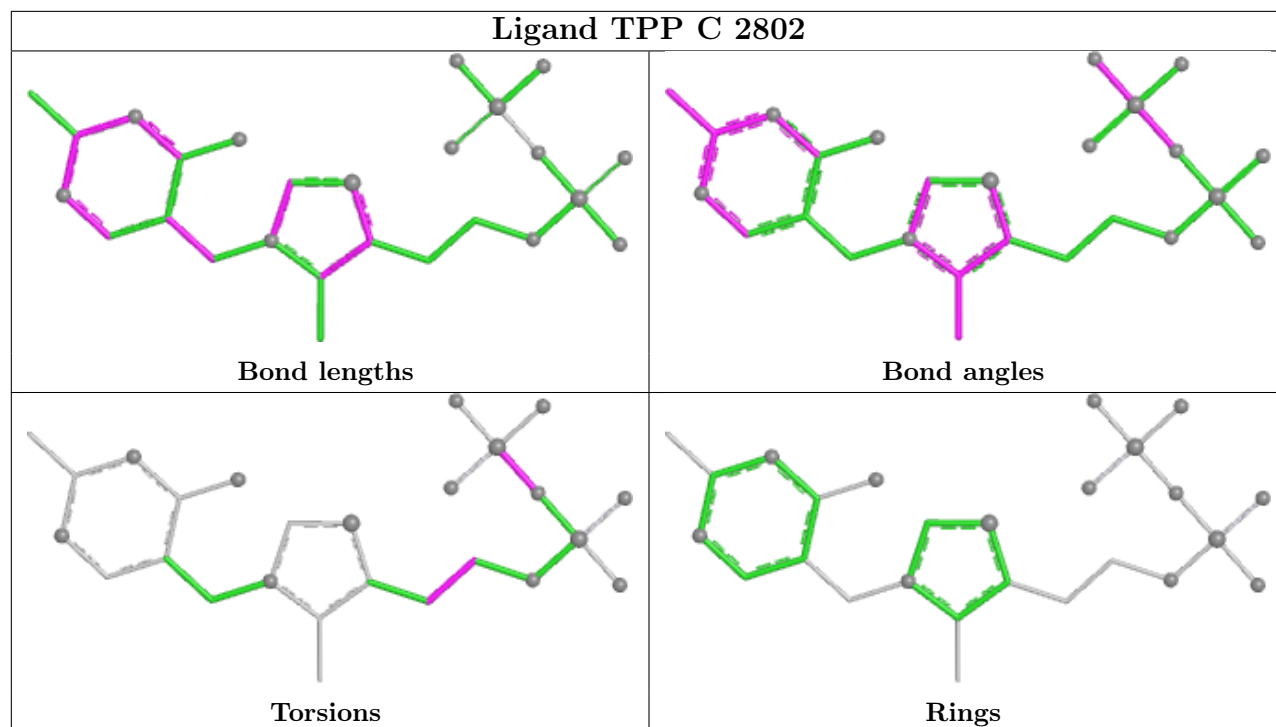
6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2602	TPP	1	0
6	D	2903	FAD	1	0
6	A	2603	FAD	2	0
5	B	2702	TPP	1	0
6	C	2803	FAD	1	0
6	B	2703	FAD	1	0

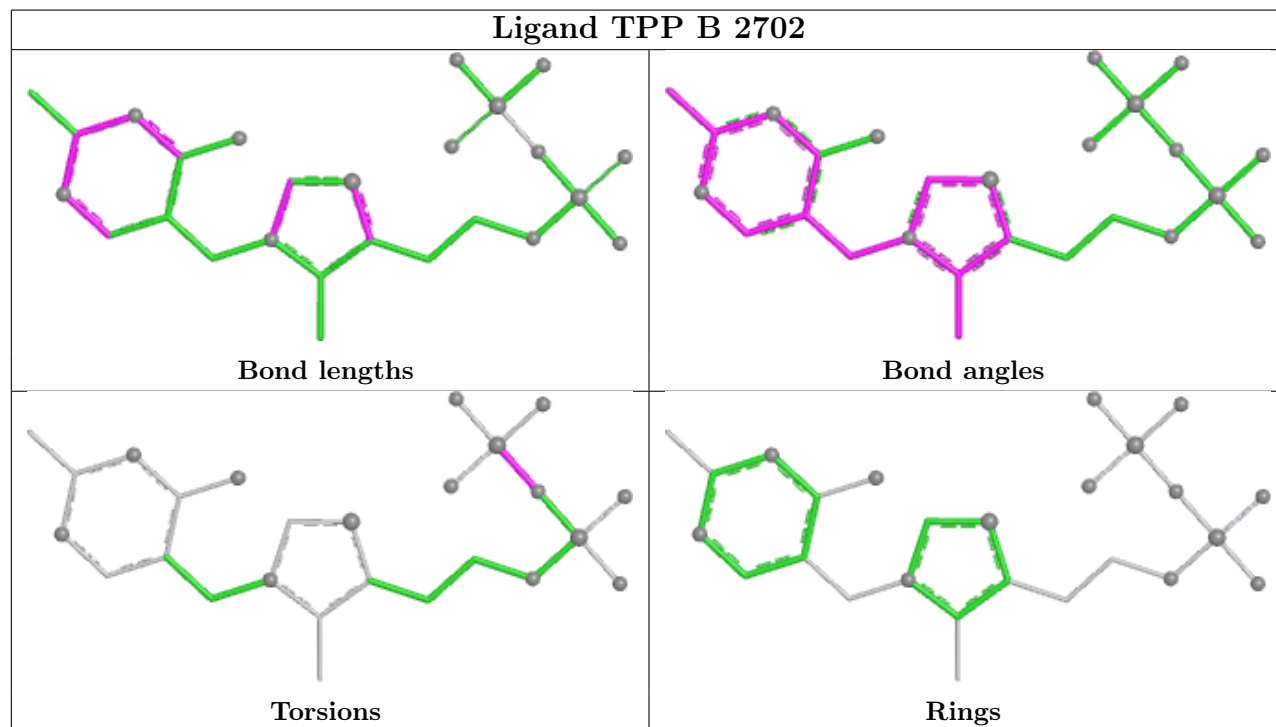
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

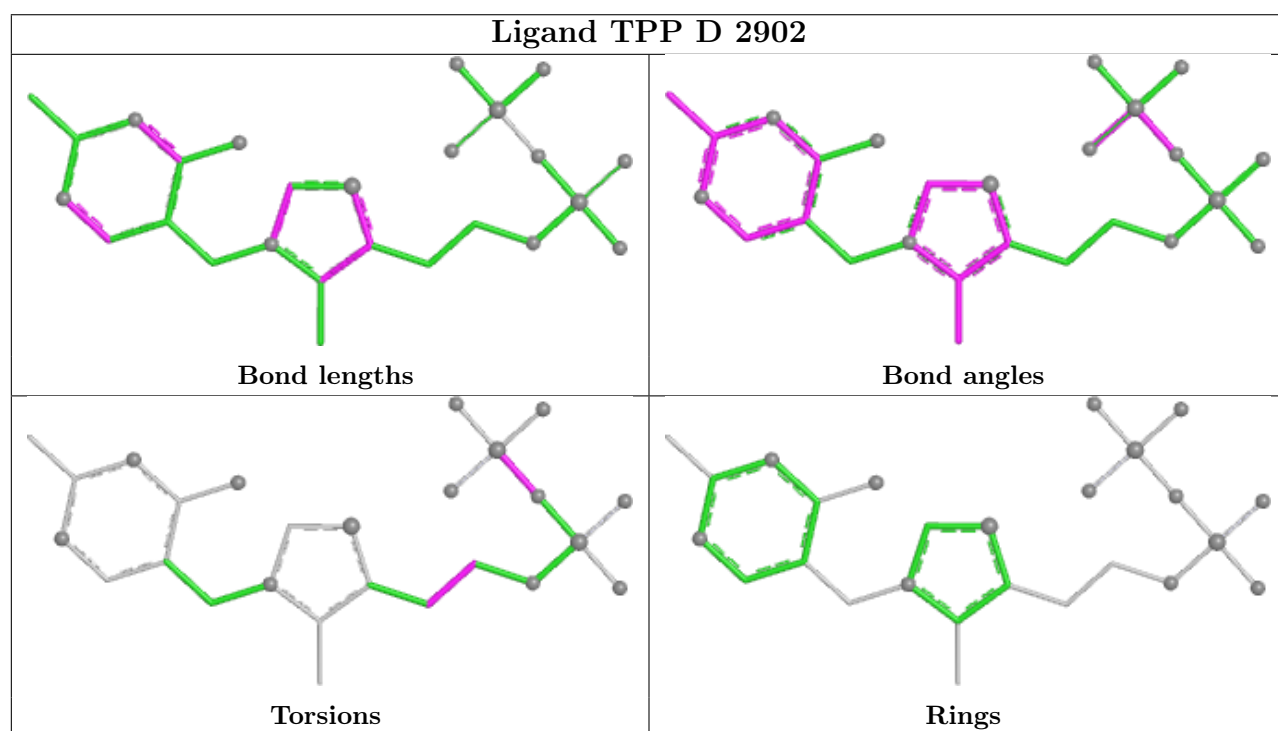
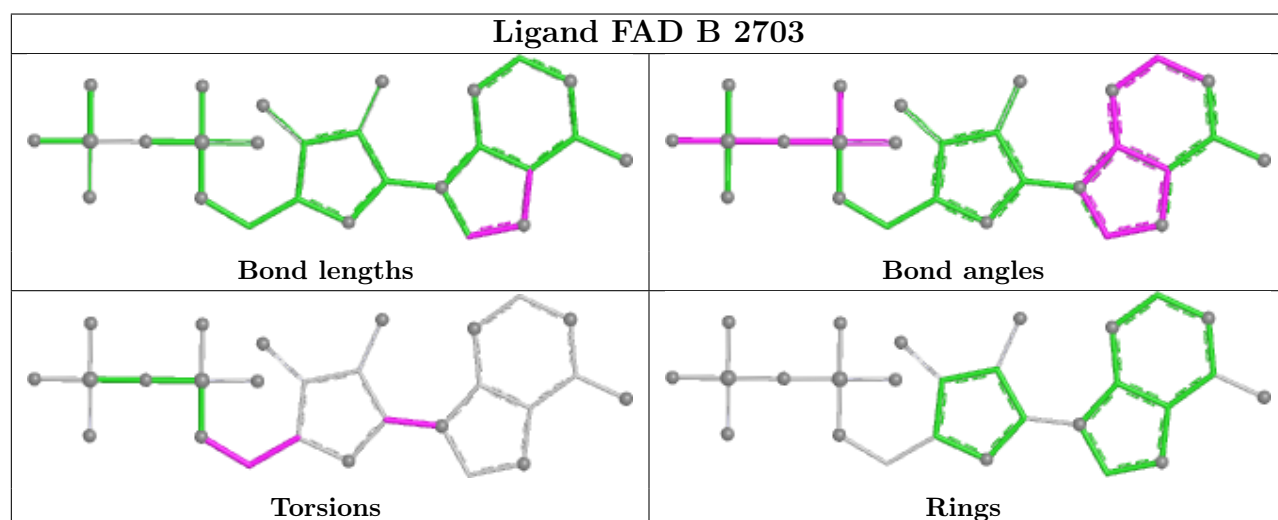
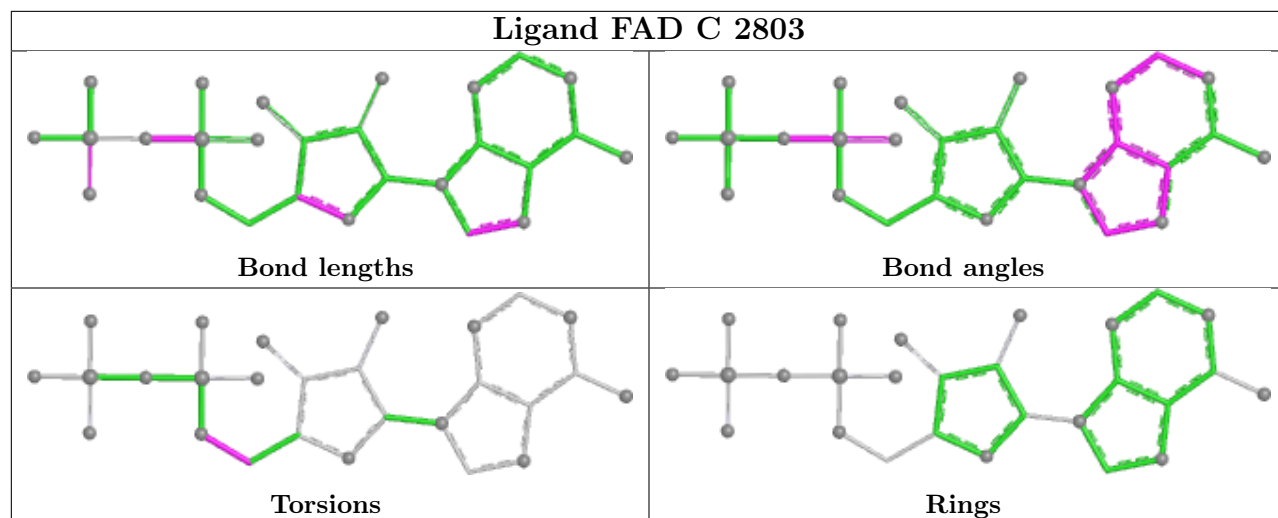


Ligand TPP C 2802



Ligand TPP B 2702





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%)	0.08	20 (3%) 46 43	28, 46, 80, 96	0
1	B	572/603 (94%)	-0.22	24 (4%) 40 37	22, 37, 69, 87	0
1	C	556/603 (92%)	0.02	14 (2%) 58 55	26, 43, 71, 91	0
1	D	560/603 (92%)	-0.03	23 (4%) 41 38	25, 42, 78, 93	0
All	All	2246/2412 (93%)	-0.04	81 (3%) 46 43	22, 42, 75, 96	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	318	THR	8.7
1	C	318	THR	8.6
1	D	316	HIS	8.6
1	B	318	THR	7.5
1	A	316	HIS	7.0
1	C	287	TYR	6.7
1	D	313	GLY	6.2
1	A	318	THR	6.2
1	B	288	PRO	5.4
1	D	181	ASP	5.2
1	B	287	TYR	5.0
1	C	313	GLY	4.8
1	B	313	GLY	4.7
1	A	313	GLY	4.6
1	C	195	PRO	4.4
1	C	316	HIS	4.2
1	B	122	GLN	4.2
1	B	597	GLN	4.2
1	B	116	MET	4.1
1	D	182	TRP	4.1
1	D	317	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	181	ASP	4.0
1	D	287	TYR	3.7
1	B	193	LEU	3.7
1	D	183	TYR	3.7
1	D	195	PRO	3.7
1	D	264	ARG	3.5
1	A	181	ASP	3.5
1	B	316	HIS	3.5
1	D	180	GLU	3.4
1	A	182	TRP	3.4
1	B	180	GLU	3.3
1	D	49	ASP	3.2
1	B	314	LYS	3.2
1	A	192	PRO	3.2
1	B	594	LEU	3.2
1	D	111	PHE	3.1
1	B	182	TRP	3.1
1	C	317	LYS	3.1
1	A	265	ALA	3.1
1	B	296	PHE	3.1
1	B	183	TYR	3.1
1	B	264	ARG	3.0
1	B	596	HIS	2.9
1	A	317	LYS	2.9
1	D	115	GLY	2.9
1	A	298	ASN	2.9
1	D	319	ASP	2.9
1	B	295	ALA	2.9
1	C	593	ASP	2.8
1	D	314	LYS	2.7
1	B	317	LYS	2.7
1	A	111	PHE	2.7
1	C	148	HIS	2.6
1	A	195	PRO	2.6
1	A	180	GLU	2.6
1	C	264	ARG	2.6
1	A	560	ALA	2.5
1	C	265	ALA	2.5
1	D	186	ALA	2.5
1	A	115	GLY	2.5
1	B	115	GLY	2.5
1	A	286	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	314	LYS	2.4
1	C	180	GLU	2.4
1	A	320	ILE	2.4
1	D	114	THR	2.4
1	D	322	VAL	2.4
1	A	148	HIS	2.4
1	B	593	ASP	2.3
1	D	113	THR	2.3
1	C	314	LYS	2.3
1	A	315	ARG	2.3
1	A	564	ALA	2.3
1	B	194	LEU	2.3
1	C	315	ARG	2.3
1	D	263	ASN	2.2
1	D	315	ARG	2.2
1	B	9	THR	2.2
1	C	298	ASN	2.1
1	D	592	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

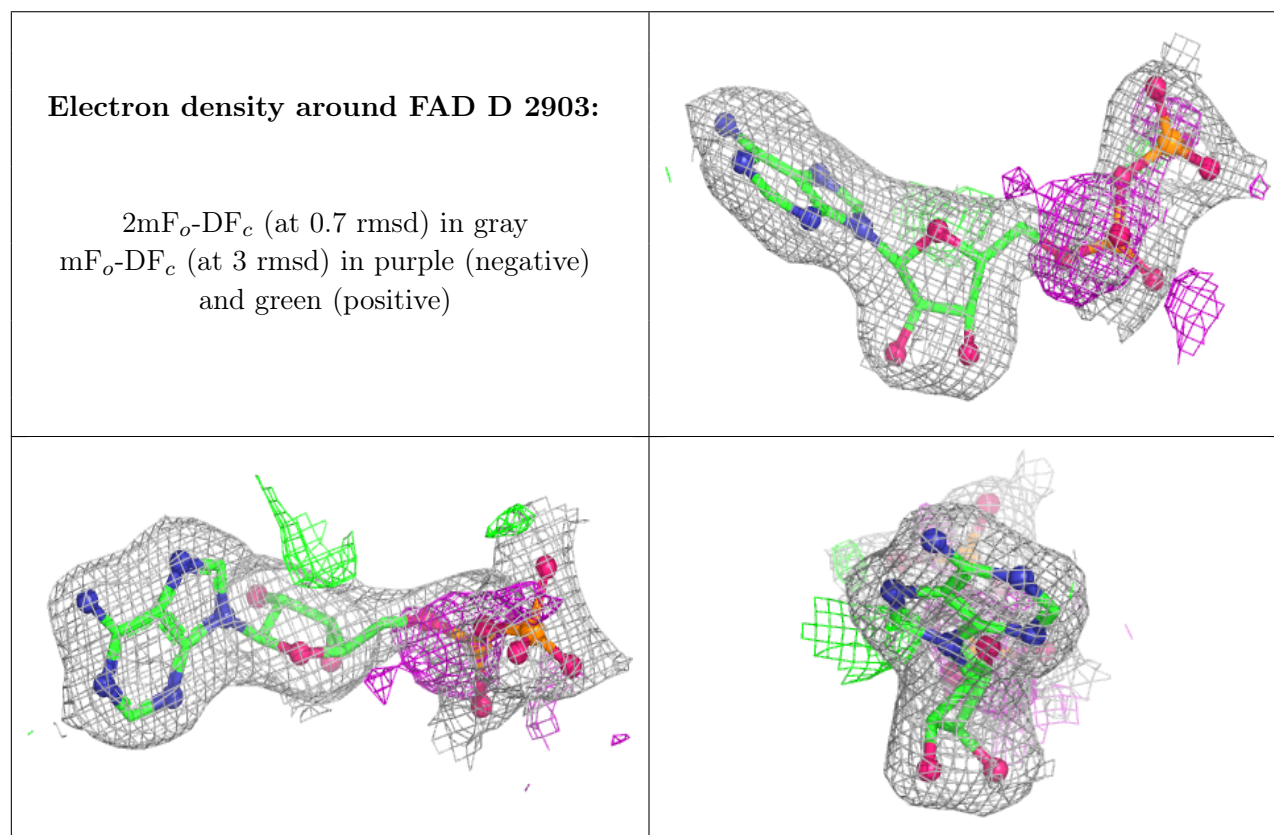
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	2601	1/1	0.76	0.09	38,38,38,38	0
2	MG	C	2801	1/1	0.89	0.08	40,40,40,40	0
6	FAD	D	2903	27/53	0.89	0.10	46,51,68,69	0
2	MG	B	2701	1/1	0.90	0.04	31,31,31,31	0
6	FAD	C	2803	27/53	0.92	0.08	37,43,61,64	0

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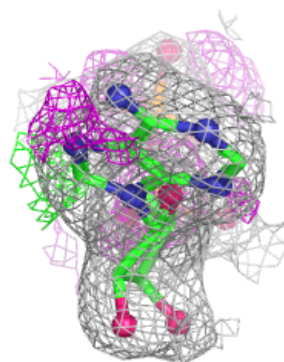
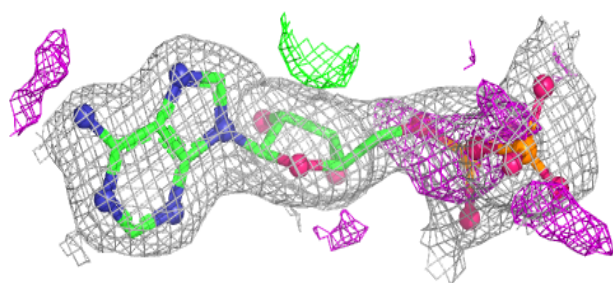
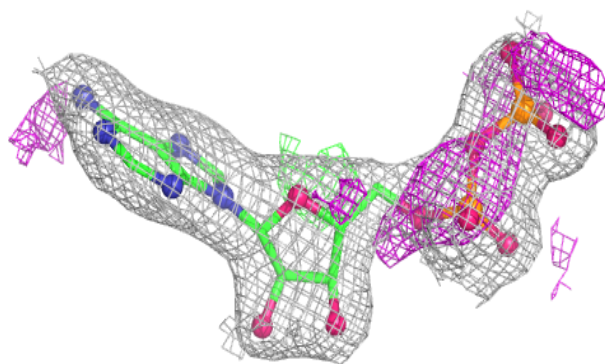
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	FAD	A	2603	27/53	0.93	0.08	47,52,60,62	0
6	FAD	B	2703	27/53	0.95	0.07	31,34,45,48	0
3	NA	B	2705	1/1	0.96	0.06	42,42,42,42	0
3	NA	A	2605	1/1	0.97	0.13	48,48,48,48	0
5	TPP	C	2802	26/26	0.97	0.06	27,36,37,38	0
5	TPP	D	2902	26/26	0.98	0.04	21,27,31,33	0
4	SO4	D	2704	5/5	0.98	0.08	34,36,38,39	0
5	TPP	A	2602	26/26	0.98	0.06	26,32,36,37	0
5	TPP	B	2702	26/26	0.98	0.05	21,28,31,32	0
4	SO4	A	2804	5/5	0.98	0.06	45,46,46,47	0
4	SO4	C	2604	5/5	0.99	0.04	41,42,43,44	0
2	MG	D	2901	1/1	0.99	0.01	32,32,32,32	0
4	SO4	B	2904	5/5	1.00	0.02	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.

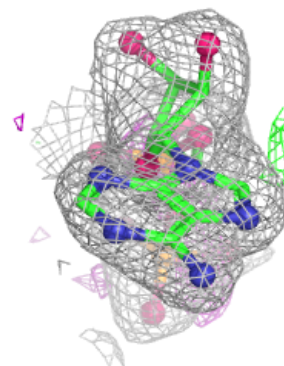
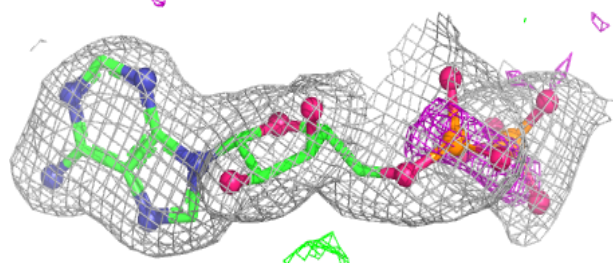
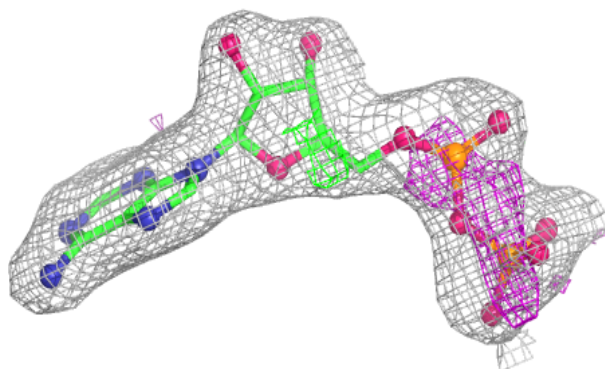


Electron density around FAD C 2803:

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

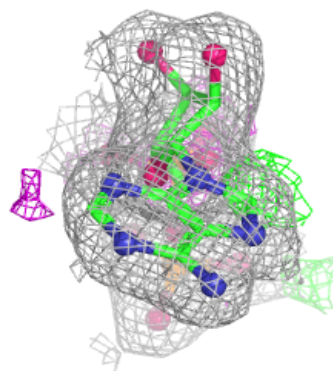
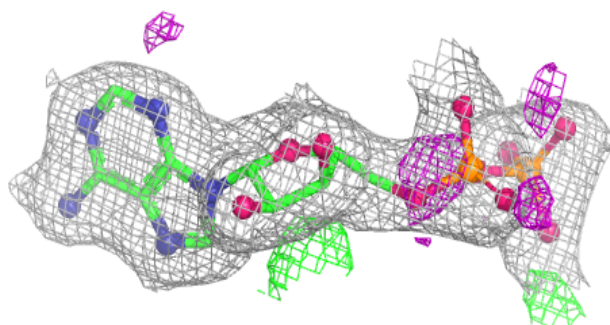
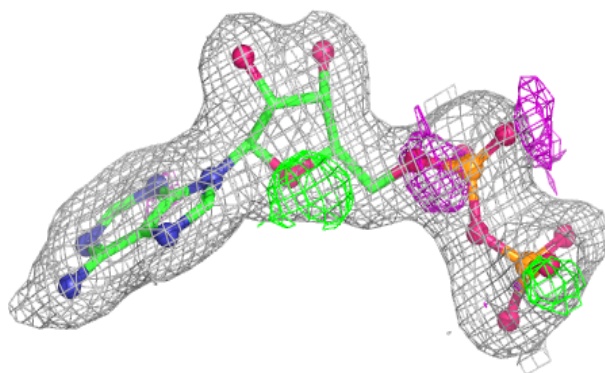
**Electron density around FAD A 2603:**

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

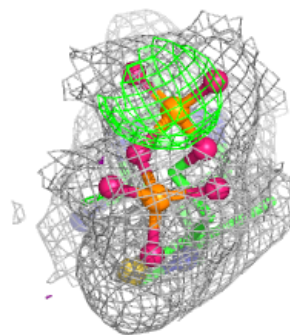
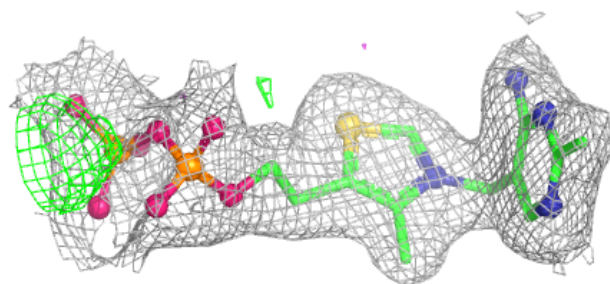
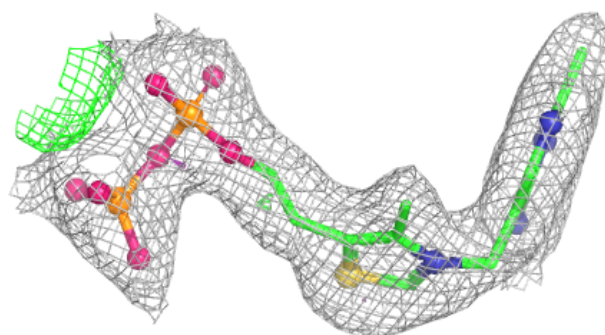


Electron density around FAD B 2703:

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

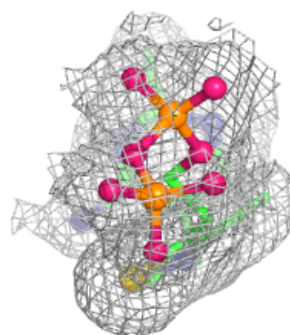
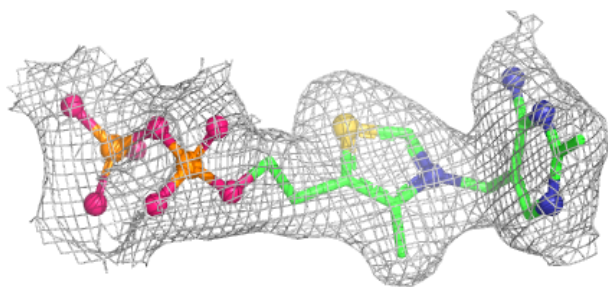
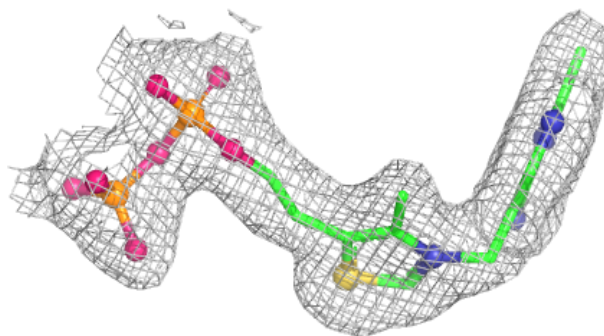
**Electron density around TPP C 2802:**

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

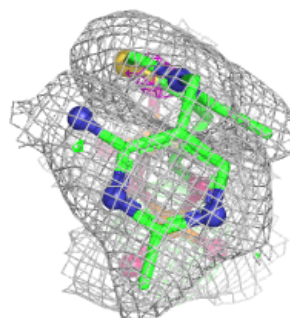
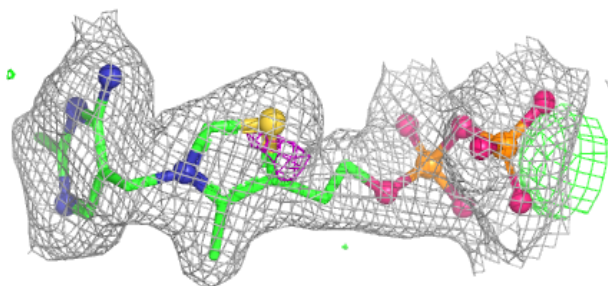
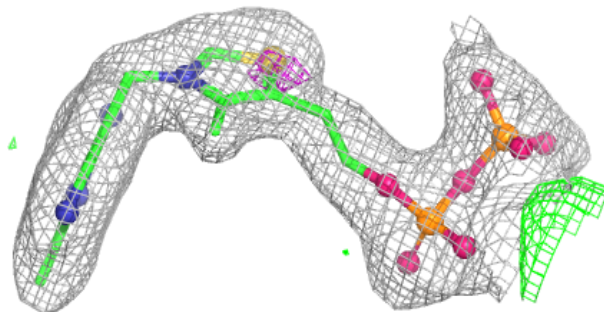


Electron density around TPP D 2902:

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

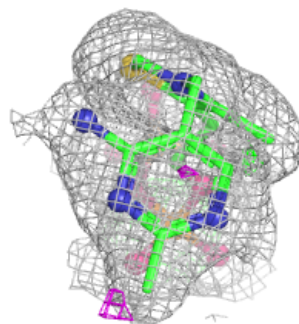
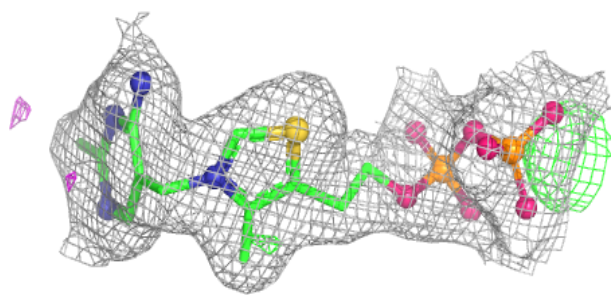
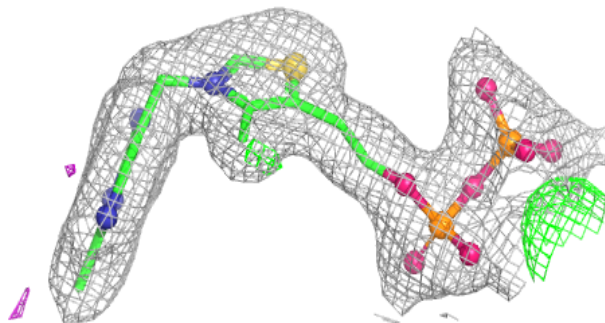
**Electron density around TPP A 2602:**

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



Electron density around TPP B 2702:

$2mF_o - DF_c$ (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.