Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2022 – 04:20 pm BST

PDB ID	:	7P0X
Title	:	Crystal structure of Thioredoxin reductase from Brugia Malayi
Authors	:	Fata, F.; Ardini, M.; Silvestri, I.; Gabriele, F.; Cheng, Q.; Arner, E.S.J.; Williams, D.L.
Deposited on	:	2021-06-30
Resolution	:	2.55 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:

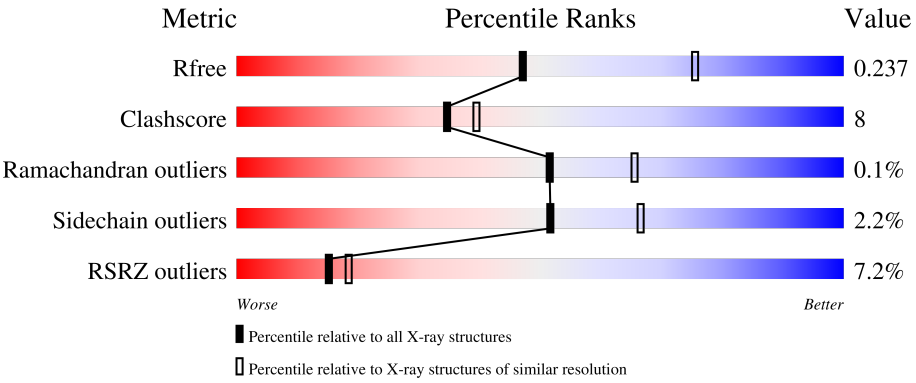
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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

Mol	Chain	Length	Quality of chain
1	A	598	3% 85% 11% ·
1	B	598	% 85% 12% ·
2	C	598	16% 73% 18% · 8%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13517 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.

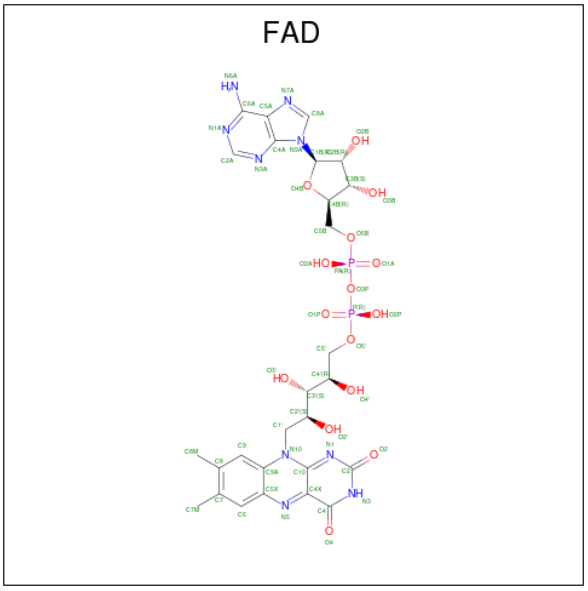
- Molecule 1 is a protein called Glutaredoxin domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S				
1	A	576	4486	2862	752	843	29		0	1	0
			Total	C	N	O	S	Se			
1	B	581	4511	2875	757	848	30	1	0	1	0

- Molecule 2 is a protein called Glutaredoxin domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	550	4270	2732	718	792	28	0	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

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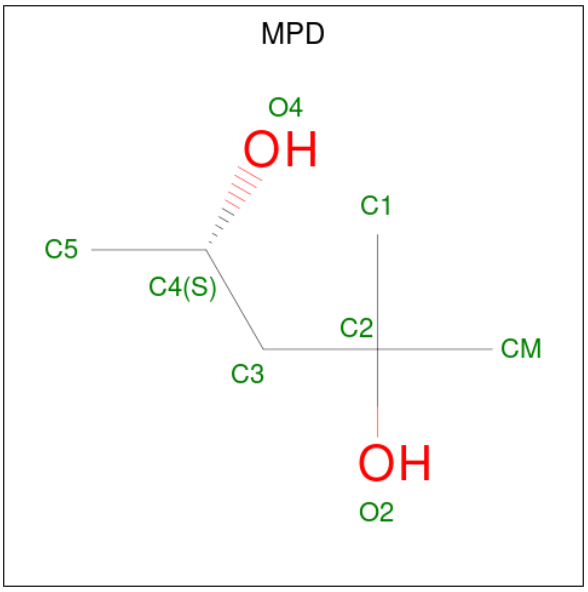
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O P 53 27 9 15 2	0	0
3	C	1	Total C N O P 53 27 9 15 2	0	0

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Na 2 2	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	3	Total Cl 3 3	0	0

- Molecule 7 is water.

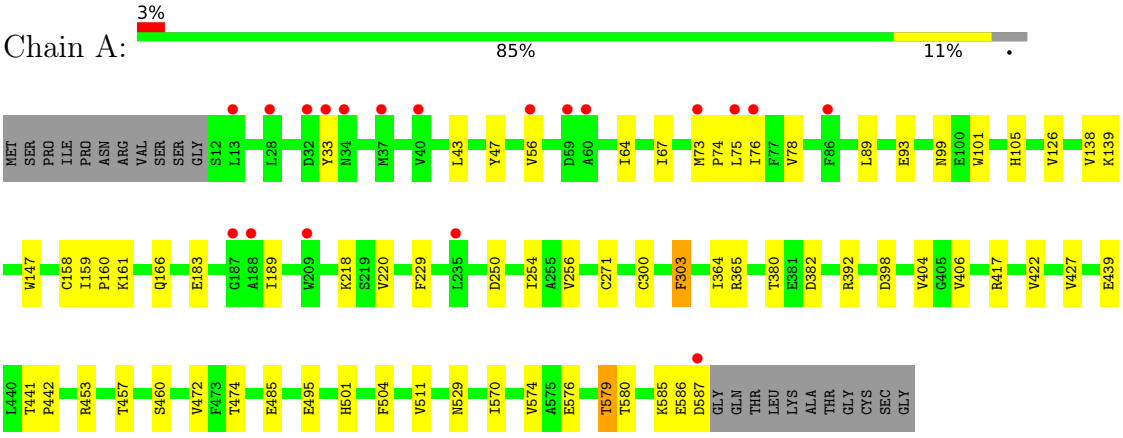
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	34	Total O 34 34	0	0
7	B	26	Total O 26 26	0	0
7	C	2	Total O 2 2	0	0

3 Residue-property plots (i)

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

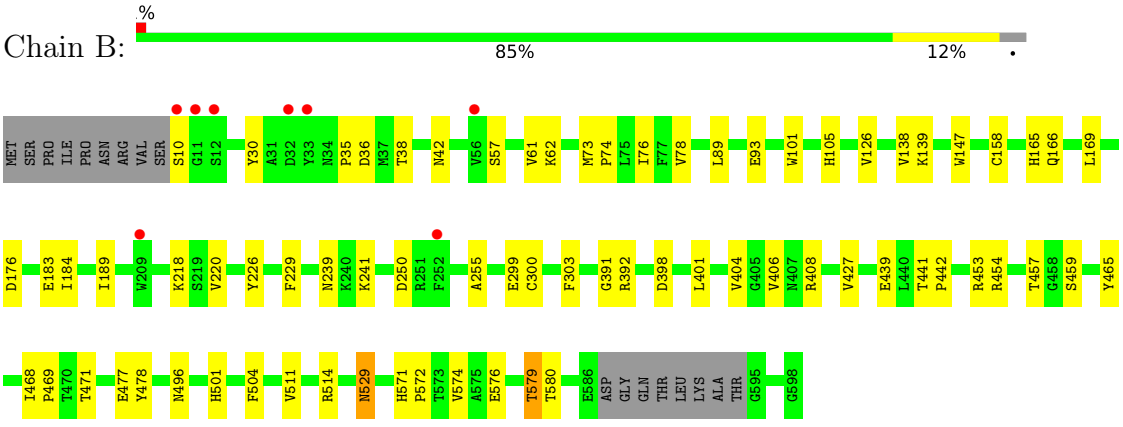
• Molecule 1: Glutaredoxin domain-containing protein

Chain A:



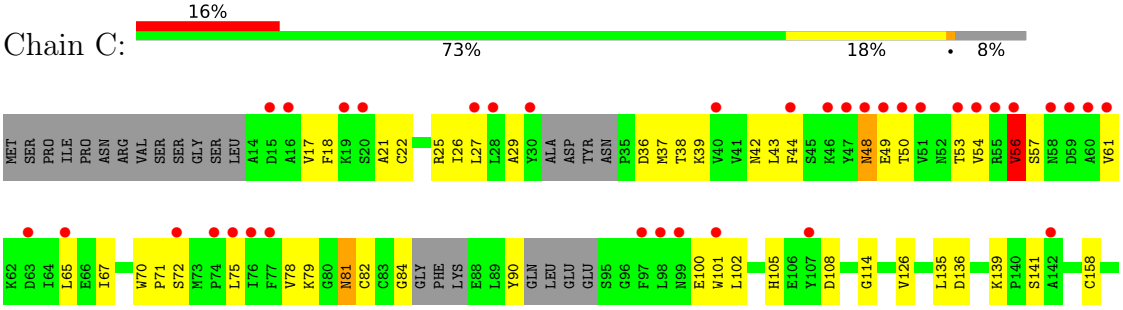
• Molecule 1: Glutaredoxin domain-containing protein

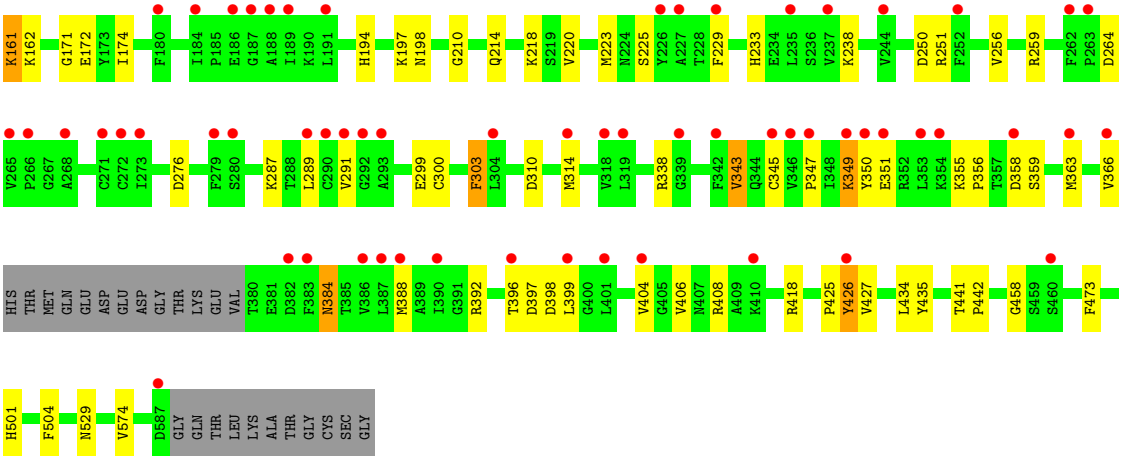
Chain B:



• Molecule 2: Glutaredoxin domain-containing protein

Chain C:




K161 K162 G171 E172 Y173 I174 F180 I184 P185 E186 G187 A188 I189 K190 L191 H194 K197 N198 G210 Q214 K218 S219 V220 M223 N224 S225 Y226 A227 T228 F229 H233 E234 L235 S236 V237 K238 V244 D250 R251 F252 V256 R259 F262 P263 D264
V265 P266 G267 A268 C271 C272 I273 D276 F279 S280 K287 T288 L289 C290 V291 G292 A293 E299 C300 F303 L304 D310 M314 V318 L319 R338 G339 F342 V343 Q344 C345 V346 P347 I348 K349 Y350 E351 R352 L353 K354 K355 P356 T357 D358 S359 M363 V366
HIS THR MET GLN GLU ASP GLU ASP GLY THR LYS GLU VAL T380 E381 D382 F383 N384 T385 V386 L387 M388 A389 I390 G391 R392 T396 D397 D398 L399 G400 L401 V404 G405 V406 N407 R408 A409 K410 R418 P425 Y426 V427 L434 Y435 T441 P442 G458 S459 S460 F473
H501 F504 N529 V574 D587 GLY GLN THR LEU LYS ALA THR GLY CYS SEC GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	146.92Å 258.99Å 129.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.90 – 2.55 48.85 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.90-2.55) 99.9 (48.85-2.55)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.197 , 0.237 0.200 , 0.237	Depositor DCC
R_{free} test set	3847 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	73.3	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.018 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.015 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13517	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEC, CSO, NA, CL, FAD, MPD

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	0.78	0/4570	0.87	0/6177
1	B	0.76	0/4584	0.84	0/6190
2	C	0.74	0/4352	0.88	5/5878 (0.1%)
All	All	0.76	0/13506	0.86	5/18245 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	349	LYS	N-CA-C	11.27	141.42	111.00
2	C	349	LYS	CB-CA-C	-8.82	92.76	110.40
2	C	81	ASN	N-CA-C	6.94	129.74	111.00
2	C	426	TYR	CB-CA-C	5.89	122.19	110.40
2	C	359	SER	CB-CA-C	-5.28	100.08	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4486	0	4510	50	0
1	B	4511	0	4530	62	0
2	C	4270	0	4320	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	53	0	31	1	0
3	B	53	0	31	3	0
3	C	53	0	31	9	0
4	A	16	0	28	4	0
4	B	8	0	14	5	0
5	A	2	0	0	0	0
6	B	3	0	0	2	0
7	A	34	0	0	0	0
7	B	26	0	0	1	0
7	C	2	0	0	0	0
All	All	13517	0	13495	224	0

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

All (224) 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:300:CYS:HA	1:B:303:PHE:CE2	1.67	1.29
1:B:38:THR:HG22	1:B:42:ASN:OD1	1.54	1.08
1:A:105:HIS:HD2	1:A:250:ASP:OD1	1.39	1.05
2:C:50:THR:O	2:C:50:THR:HG22	1.64	0.95
2:C:81:ASN:HD21	2:C:426:TYR:CA	1.82	0.90
2:C:81:ASN:HD21	2:C:426:TYR:N	1.70	0.90
1:A:105:HIS:CD2	1:A:250:ASP:OD1	2.29	0.84
2:C:75:LEU:HD13	2:C:82:CYS:SG	2.18	0.82
2:C:81:ASN:ND2	2:C:426:TYR:HA	1.95	0.81
2:C:233:HIS:NE2	2:C:426:TYR:CE1	2.50	0.80
2:C:65:LEU:HD13	2:C:72:SER:HA	1.65	0.78
2:C:48:ASN:OD1	2:C:49:GLU:N	2.17	0.78
2:C:81:ASN:ND2	2:C:426:TYR:CA	2.48	0.76
2:C:161:LYS:HE2	2:C:299:GLU:OE2	1.84	0.76
2:C:36:ASP:C	2:C:38:THR:H	1.87	0.76
2:C:81:ASN:HD21	2:C:426:TYR:HA	1.52	0.74
1:B:300:CYS:CA	1:B:303:PHE:CE2	2.61	0.74
1:A:579:THR:HG22	1:A:580:THR:HG23	1.68	0.73
1:A:365:ARG:HD3	1:A:382:ASP:OD1	1.89	0.73
2:C:75:LEU:CD1	2:C:82:CYS:SG	2.77	0.71
2:C:256:VAL:O	3:C:601:FAD:H8A	1.91	0.71
2:C:36:ASP:C	2:C:38:THR:N	2.44	0.71
1:A:576:GLU:O	1:A:579:THR:HB	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:GLU:HA	1:A:586:GLU:OE2	1.92	0.69
1:A:139:LYS:NZ	1:A:398:ASP:OD2	2.26	0.68
1:B:139:LYS:NZ	1:B:398:ASP:OD2	2.27	0.68
2:C:434:LEU:HD23	2:C:435:TYR:N	2.09	0.67
1:A:56:VAL:HG21	1:A:73:MET:CE	2.25	0.67
1:B:165:HIS:HE1	1:B:477:GLU:OE2	1.76	0.67
1:B:579:THR:HG22	1:B:580:THR:HG23	1.76	0.67
2:C:139:LYS:NZ	2:C:398:ASP:OD2	2.29	0.65
1:B:576:GLU:O	1:B:579:THR:HB	1.96	0.64
1:B:76:ILE:HD13	1:B:89:LEU:HD22	1.79	0.64
1:A:166:GLN:NE2	6:B:603:CL:CL	2.67	0.64
1:B:35:PRO:O	1:B:36:ASP:HB2	1.98	0.63
2:C:65:LEU:CD1	2:C:72:SER:HA	2.28	0.63
2:C:349:LYS:HE2	2:C:351:GLU:OE2	1.99	0.63
1:A:392:ARG:H	4:A:603:MPD:H4	1.64	0.62
2:C:50:THR:O	2:C:50:THR:CG2	2.37	0.62
2:C:256:VAL:HB	3:C:601:FAD:N7A	2.15	0.62
2:C:81:ASN:HD21	2:C:426:TYR:H	1.46	0.61
2:C:397:ASP:HA	2:C:408:ARG:HH22	1.66	0.61
2:C:21:ALA:HB2	2:C:27:LEU:HD23	1.81	0.61
2:C:355:LYS:N	2:C:356:PRO:CD	2.63	0.60
1:B:453:ARG:O	1:B:457:THR:HB	2.01	0.60
2:C:36:ASP:O	2:C:38:THR:N	2.34	0.60
1:A:453:ARG:O	1:A:457:THR:HB	2.02	0.60
2:C:349:LYS:CE	2:C:351:GLU:OE2	2.50	0.60
2:C:194:HIS:HD2	2:C:197:LYS:HE2	1.65	0.60
2:C:161:LYS:NZ	3:C:601:FAD:O4	2.33	0.59
2:C:287:LYS:HG2	2:C:310:ASP:HB3	1.84	0.59
1:A:73:MET:O	1:A:74:PRO:C	2.35	0.59
1:B:166:GLN:NE2	6:B:604:CL:CL	2.72	0.59
1:B:165:HIS:CE1	1:B:169:LEU:HD11	2.38	0.59
1:B:300:CYS:HA	1:B:303:PHE:HE2	1.56	0.59
2:C:102:LEU:O	2:C:102:LEU:HD23	2.03	0.59
2:C:229:PHE:CD2	2:C:404:VAL:HG21	2.38	0.58
2:C:396:THR:HG23	2:C:399:LEU:HD12	1.86	0.58
1:A:365:ARG:HD2	1:A:380:THR:HB	1.86	0.58
2:C:171:GLY:O	2:C:174:ILE:HG12	2.04	0.58
1:A:76:ILE:HD13	1:A:89:LEU:HD22	1.84	0.57
2:C:135:LEU:HD11	2:C:223:MET:HE3	1.86	0.57
2:C:194:HIS:HA	2:C:197:LYS:HG2	1.87	0.57
1:A:229:PHE:CD1	1:A:404:VAL:HG21	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:GLU:O	1:B:303:PHE:CD2	2.57	0.57
1:A:43:LEU:HD11	1:A:93:GLU:HG3	1.87	0.56
2:C:108:ASP:O	2:C:251:ARG:HG3	2.06	0.56
2:C:355:LYS:N	2:C:356:PRO:HD2	2.20	0.56
2:C:81:ASN:ND2	2:C:426:TYR:HB3	2.20	0.56
2:C:48:ASN:OD1	2:C:49:GLU:O	2.23	0.56
2:C:314:MET:HG2	2:C:345:CYS:HB3	1.87	0.56
1:A:73:MET:O	1:A:75:LEU:N	2.39	0.56
2:C:197:LYS:HG3	2:C:198:ASN:N	2.21	0.56
1:B:38:THR:O	1:B:42:ASN:N	2.23	0.56
1:B:454:ARG:HG3	1:B:459:SER:O	2.05	0.55
1:B:300:CYS:HA	1:B:303:PHE:CZ	2.36	0.55
1:B:299:GLU:O	1:B:303:PHE:HD2	1.91	0.54
2:C:425:PRO:O	2:C:426:TYR:CD2	2.61	0.54
2:C:172:GLU:HG3	2:C:338:ARG:HH12	1.72	0.54
1:B:229:PHE:CD1	1:B:404[A]:VAL:HG21	2.43	0.54
1:A:56:VAL:HG21	1:A:73:MET:HE1	1.90	0.54
2:C:81:ASN:OD1	2:C:81:ASN:C	2.44	0.54
2:C:291:VAL:HG12	2:C:388:MET:HA	1.90	0.54
1:B:391:GLY:HA3	4:B:602:MPD:HM2	1.90	0.53
2:C:57:SER:O	2:C:61:VAL:HG23	2.08	0.53
2:C:67:ILE:O	2:C:418:ARG:NH2	2.42	0.53
1:B:496:ASN:HB3	1:B:529:ASN:ND2	2.23	0.53
4:A:603:MPD:H52	4:A:603:MPD:O2	2.09	0.53
2:C:347:PRO:HB3	2:C:350:TYR:CZ	2.44	0.53
1:A:189:ILE:HG23	1:B:183:GLU:O	2.09	0.52
1:B:126:VAL:HG11	1:B:218:LYS:HB3	1.90	0.52
2:C:259:ARG:NH2	2:C:276:ASP:OD2	2.42	0.52
2:C:349:LYS:O	2:C:349:LYS:HG2	2.09	0.52
1:B:38:THR:CG2	1:B:42:ASN:OD1	2.42	0.52
1:B:105:HIS:HD2	1:B:250:ASP:OD1	1.92	0.52
1:A:439:GLU:OE2	4:A:603:MPD:H12	2.10	0.52
2:C:126:VAL:HG11	2:C:218:LYS:HB3	1.92	0.51
1:B:105:HIS:CD2	1:B:250:ASP:OD1	2.63	0.51
2:C:44:PHE:HB3	2:C:48:ASN:HD22	1.76	0.51
2:C:70:TRP:CE2	2:C:84:GLY:O	2.64	0.51
1:B:176:ASP:OD2	1:B:514:ARG:NH1	2.44	0.50
2:C:105:HIS:CD2	2:C:250:ASP:OD1	2.63	0.50
2:C:287:LYS:HB2	2:C:384:ASN:OD1	2.10	0.50
2:C:48:ASN:CG	2:C:49:GLU:N	2.63	0.50
2:C:172:GLU:HG3	2:C:338:ARG:NH1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:CYS:HA	1:B:303:PHE:CD2	2.39	0.50
2:C:71:PRO:O	2:C:72:SER:C	2.50	0.50
1:A:404:VAL:HG12	1:A:404:VAL:O	2.11	0.50
1:B:38:THR:HG22	1:B:42:ASN:CG	2.28	0.50
2:C:233:HIS:CE1	2:C:426:TYR:CE1	3.00	0.49
2:C:349:LYS:O	2:C:349:LYS:CG	2.50	0.49
2:C:404:VAL:HG12	2:C:404:VAL:O	2.12	0.49
2:C:225:SER:OG	2:C:238:LYS:N	2.46	0.49
1:A:56:VAL:HG21	1:A:73:MET:HE3	1.95	0.49
2:C:17:VAL:HG22	2:C:54:VAL:HG11	1.94	0.49
2:C:29:ALA:HA	2:C:54:VAL:O	2.12	0.49
2:C:105:HIS:HD2	2:C:250:ASP:OD1	1.95	0.49
2:C:404:VAL:HG11	2:C:427:VAL:HG21	1.95	0.48
2:C:81:ASN:ND2	2:C:426:TYR:CB	2.77	0.48
2:C:233:HIS:NE2	2:C:426:TYR:CD1	2.81	0.48
2:C:78:VAL:HB	2:C:101:TRP:CH2	2.48	0.48
2:C:289:LEU:HD22	2:C:366:VAL:HG21	1.94	0.48
1:B:165:HIS:CE1	1:B:477:GLU:OE2	2.63	0.48
1:A:56:VAL:CG2	1:A:73:MET:CE	2.92	0.48
1:B:78:VAL:HB	1:B:101:TRP:CH2	2.49	0.48
2:C:17:VAL:HG21	2:C:56:VAL:HG13	1.95	0.48
2:C:75:LEU:HD11	2:C:82:CYS:SG	2.53	0.47
2:C:314:MET:HG2	2:C:343:VAL:HG22	1.96	0.47
2:C:21:ALA:CB	2:C:27:LEU:HD23	2.44	0.47
1:A:138:VAL:HG11	1:A:147:TRP:CE2	2.49	0.47
2:C:434:LEU:HD23	2:C:434:LEU:C	2.33	0.47
2:C:135:LEU:HD13	2:C:223:MET:HB2	1.96	0.47
1:B:10:SER:O	1:B:57:SER:HA	2.14	0.47
1:B:404[A]:VAL:HG12	1:B:404[A]:VAL:O	2.13	0.47
1:B:579:THR:CG2	7:B:726:HOH:O	2.63	0.47
1:B:439:GLU:OE2	4:B:602:MPD:O4	2.32	0.47
1:B:404[A]:VAL:HG11	1:B:427:VAL:HG21	1.96	0.46
2:C:79:LYS:O	2:C:251:ARG:NH1	2.48	0.46
2:C:291:VAL:CG1	2:C:388:MET:HA	2.46	0.46
1:B:126:VAL:HG21	1:B:220:VAL:HG22	1.96	0.46
1:A:78:VAL:HB	1:A:101:TRP:CH2	2.50	0.46
1:A:441:THR:HB	1:A:442:PRO:HD3	1.97	0.46
1:A:417:ARG:NH1	1:A:422:VAL:O	2.46	0.46
2:C:399:LEU:HD21	3:C:601:FAD:H61A	1.81	0.46
1:A:406:VAL:HG21	1:A:427:VAL:HG11	1.97	0.46
2:C:256:VAL:HB	3:C:601:FAD:C8A	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:VAL:HG11	1:A:218:LYS:HB3	1.98	0.46
2:C:363:MET:HG2	2:C:384:ASN:HA	1.97	0.46
2:C:256:VAL:HG12	3:C:601:FAD:N7A	2.31	0.45
1:A:495:GLU:CD	1:A:495:GLU:H	2.20	0.45
1:A:56:VAL:HG11	1:A:64:ILE:HD12	1.99	0.45
1:B:504:PHE:CE1	1:B:574:VAL:HG13	2.51	0.45
1:A:47:TYR:HE1	1:A:99:ASN:HD22	1.64	0.45
1:B:401:LEU:HD12	1:B:408:ARG:HD3	1.98	0.44
2:C:194:HIS:CD2	2:C:197:LYS:HE2	2.50	0.44
2:C:406:VAL:HG21	2:C:427:VAL:HG11	1.99	0.44
1:A:183:GLU:O	1:B:189:ILE:HG23	2.18	0.44
2:C:26:ILE:HD12	2:C:78:VAL:HG22	1.99	0.44
1:B:126:VAL:HG21	1:B:220:VAL:CG2	2.48	0.44
2:C:171:GLY:O	2:C:174:ILE:CG1	2.65	0.44
2:C:504:PHE:CE1	2:C:574:VAL:HG13	2.53	0.44
1:A:404:VAL:O	1:A:404:VAL:CG1	2.66	0.44
3:B:601:FAD:H9	3:B:601:FAD:H1'1	1.84	0.44
2:C:418:ARG:HH21	2:C:418:ARG:HG3	1.83	0.44
1:B:61:VAL:HG13	1:B:62:LYS:N	2.32	0.44
1:B:239:ASN:HD21	1:B:241:LYS:HG2	1.82	0.43
1:B:406:VAL:HG21	1:B:427:VAL:HG11	2.01	0.43
1:B:138:VAL:HG11	1:B:147:TRP:CE2	2.53	0.43
2:C:256:VAL:CB	3:C:601:FAD:N7A	2.81	0.43
2:C:396:THR:HG22	2:C:396:THR:O	2.18	0.43
1:B:226:TYR:CZ	3:B:601:FAD:N6A	2.86	0.43
2:C:392:ARG:CZ	3:C:601:FAD:HM81	2.48	0.43
1:A:485:GLU:OE2	1:A:585:LYS:HE2	2.19	0.43
1:B:496:ASN:HB3	1:B:529:ASN:HD22	1.83	0.43
1:B:255:ALA:O	3:B:601:FAD:H52A	2.18	0.43
1:B:439:GLU:OE2	4:B:602:MPD:C4	2.66	0.43
2:C:18:PHE:HB3	2:C:458:GLY:O	2.18	0.43
2:C:300:CYS:HA	2:C:303:PHE:CE2	2.53	0.43
1:A:73:MET:O	1:A:73:MET:SD	2.77	0.43
1:A:33:TYR:HD1	1:A:33:TYR:O	2.02	0.43
3:A:601:FAD:H9	3:A:601:FAD:H1'1	1.88	0.43
1:B:571:HIS:HA	1:B:572:PRO:HA	1.81	0.42
2:C:425:PRO:O	2:C:426:TYR:CG	2.72	0.42
1:A:67:ILE:HD13	1:A:460:SER:HB3	2.01	0.42
1:A:504:PHE:CE1	1:A:574:VAL:HG13	2.54	0.42
1:B:441:THR:HB	1:B:442:PRO:HD3	2.00	0.42
2:C:135:LEU:CD1	2:C:223:MET:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:126:VAL:HG21	2:C:220:VAL:CG2	2.50	0.42
1:A:126:VAL:HG21	1:A:220:VAL:HG22	2.02	0.42
2:C:25:ARG:O	2:C:26:ILE:HD13	2.20	0.42
2:C:256:VAL:CG1	3:C:601:FAD:N7A	2.83	0.42
1:A:404:VAL:HG11	1:A:427:VAL:HG21	2.01	0.42
2:C:291:VAL:CG1	2:C:388:MET:SD	3.08	0.42
1:B:73:MET:HB3	1:B:74:PRO:HA	2.01	0.42
1:B:30:TYR:CD1	1:B:30:TYR:C	2.93	0.42
1:B:465:TYR:HA	1:B:468:ILE:HD11	2.02	0.42
2:C:26:ILE:HD13	2:C:78:VAL:HA	2.01	0.42
1:B:93:GLU:C	1:B:93:GLU:OE1	2.58	0.42
1:B:239:ASN:HD21	1:B:241:LYS:CD	2.33	0.41
4:A:603:MPD:H53	4:A:603:MPD:HM1	2.02	0.41
2:C:126:VAL:HG21	2:C:220:VAL:HG22	2.02	0.41
1:A:472:VAL:HG12	1:A:474:THR:HG23	2.02	0.41
2:C:162:LYS:HE3	2:C:473:PHE:CE2	2.55	0.41
1:B:404[A]:VAL:O	1:B:404[A]:VAL:CG1	2.68	0.41
2:C:349:LYS:HE3	2:C:351:GLU:OE2	2.20	0.41
1:A:93:GLU:C	1:A:93:GLU:OE1	2.60	0.41
1:A:159:ILE:HB	1:A:160:PRO:CD	2.51	0.41
1:A:570:ILE:HD11	1:B:469:PRO:HB2	2.03	0.41
1:A:254:ILE:HG22	1:A:256:VAL:HG13	2.03	0.41
1:A:300:CYS:HA	1:A:303:PHE:CE2	2.56	0.41
1:B:392:ARG:N	4:B:602:MPD:H11	2.36	0.41
1:B:392:ARG:O	4:B:602:MPD:H31	2.20	0.41
2:C:39:LYS:HA	2:C:42:ASN:HB2	2.02	0.41
2:C:229:PHE:CD2	2:C:404:VAL:CG2	3.03	0.41
2:C:314:MET:SD	2:C:345:CYS:HB3	2.61	0.41
1:A:271:CYS:HB3	1:A:364:ILE:HG12	2.03	0.40
1:B:471:THR:HA	1:B:478:TYR:O	2.22	0.40
1:A:159:ILE:HB	1:A:160:PRO:HD3	2.03	0.40
2:C:210:GLY:O	2:C:214:GLN:HB2	2.20	0.40
1:A:254:ILE:CG2	1:A:256:VAL:HG13	2.51	0.40
2:C:114:GLY:HA3	2:C:136:ASP:HB2	2.02	0.40
1:B:239:ASN:ND2	1:B:241:LYS:HG2	2.36	0.40
2:C:404:VAL:O	2:C:404:VAL:CG1	2.70	0.40
2:C:441:THR:HB	2:C:442:PRO:HD3	2.03	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	574/598 (96%)	553 (96%)	21 (4%)	0	100	100
1	B	576/598 (96%)	553 (96%)	23 (4%)	0	100	100
2	C	540/598 (90%)	504 (93%)	34 (6%)	2 (0%)	34	46
All	All	1690/1794 (94%)	1610 (95%)	78 (5%)	2 (0%)	51	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	37	MET
2	C	56	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	488/503 (97%)	479 (98%)	9 (2%)	59	74
1	B	489/503 (97%)	483 (99%)	6 (1%)	71	81
2	C	465/504 (92%)	448 (96%)	17 (4%)	34	46
All	All	1442/1510 (96%)	1410 (98%)	32 (2%)	52	66

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	CYS

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Mol	Chain	Res	Type
1	A	161	LYS
1	A	303	PHE
1	A	501	HIS
1	A	511	VAL
1	A	529[A]	ASN
1	A	529[B]	ASN
1	A	579	THR
1	A	587	ASP
1	B	158	CYS
1	B	184	ILE
1	B	501	HIS
1	B	511	VAL
1	B	529	ASN
1	B	579	THR
2	C	22	CYS
2	C	43	LEU
2	C	48	ASN
2	C	53	THR
2	C	56	VAL
2	C	90	TYR
2	C	100	GLU
2	C	141	SER
2	C	158	CYS
2	C	161	LYS
2	C	264	ASP
2	C	303	PHE
2	C	343	VAL
2	C	358	ASP
2	C	384	ASN
2	C	501	HIS
2	C	529	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	105	HIS
1	B	165	HIS
1	B	166	GLN
1	B	529	ASN
2	C	81	ASN
2	C	99	ASN

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Mol	Chain	Res	Type
2	C	420	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CSO	A	345	1	3,6,7	0.62	0	0,6,8	-	-
1	CSO	B	345	1	3,6,7	0.67	0	0,6,8	-	-

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
1	CSO	A	345	1	-	1/1/5/7	-
1	CSO	B	345	1	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	CSO	N-CA-CB-SG
1	B	345	CSO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	MPD	B	602	-	7,7,7	0.25	0	9,10,10	0.51	0
3	FAD	B	601	-	51,58,58	1.23	5 (9%)	60,89,89	1.80	7 (11%)
3	FAD	A	601	5	51,58,58	1.30	6 (11%)	60,89,89	1.88	10 (16%)
4	MPD	A	602	-	7,7,7	0.11	0	9,10,10	0.45	0
4	MPD	A	603	-	7,7,7	0.21	0	9,10,10	0.72	0
3	FAD	C	601	-	51,58,58	1.16	3 (5%)	60,89,89	1.78	6 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	B	602	-	-	0/5/5/5	-
3	FAD	B	601	-	-	3/30/50/50	0/6/6/6
3	FAD	A	601	5	-	3/30/50/50	0/6/6/6
4	MPD	A	602	-	-	0/5/5/5	-
4	MPD	A	603	-	-	3/5/5/5	-
3	FAD	C	601	-	-	3/30/50/50	0/6/6/6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	FAD	C4X-C10	5.13	1.44	1.38
3	B	601	FAD	C4X-C10	4.90	1.43	1.38
3	A	601	FAD	C4X-C10	4.90	1.43	1.38
3	A	601	FAD	C2-N1	-2.70	1.32	1.38
3	A	601	FAD	C2-N3	-2.57	1.33	1.38
3	C	601	FAD	C4-N3	2.43	1.37	1.33
3	B	601	FAD	C2-N1	-2.31	1.33	1.38
3	C	601	FAD	C2-N1	-2.28	1.33	1.38
3	A	601	FAD	C4X-N5	-2.24	1.30	1.33
3	B	601	FAD	C2-N3	-2.23	1.33	1.38
3	B	601	FAD	C4X-N5	-2.18	1.30	1.33
3	A	601	FAD	C4X-C4	-2.14	1.37	1.41
3	B	601	FAD	C4-N3	2.12	1.36	1.33
3	A	601	FAD	C8A-N7A	-2.02	1.31	1.34

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	FAD	C2-N3-C4	8.40	122.23	115.14
3	C	601	FAD	C2-N3-C4	8.01	121.91	115.14
3	B	601	FAD	C2-N3-C4	7.97	121.88	115.14
3	A	601	FAD	C10-C4X-N5	5.82	125.28	121.26
3	B	601	FAD	C10-C4X-N5	5.62	125.14	121.26
3	A	601	FAD	C10-C4X-C4	-5.44	116.35	119.95
3	C	601	FAD	C10-C4X-N5	5.32	124.94	121.26
3	C	601	FAD	C10-C4X-C4	-5.23	116.49	119.95
3	B	601	FAD	C10-C4X-C4	-5.15	116.54	119.95
3	C	601	FAD	C4X-C4-N3	-4.14	117.77	123.43
3	A	601	FAD	C4X-C4-N3	-4.05	117.89	123.43
3	B	601	FAD	C4X-C4-N3	-3.99	117.98	123.43
3	B	601	FAD	C4X-C10-N10	-3.94	116.25	120.30
3	A	601	FAD	C4X-C10-N10	-3.77	116.43	120.30
3	C	601	FAD	C4X-C10-N10	-3.70	116.50	120.30
3	A	601	FAD	O4B-C1B-C2B	-3.25	102.17	106.93
3	B	601	FAD	O4B-C1B-C2B	-3.13	102.36	106.93
3	C	601	FAD	C5A-C6A-N6A	2.34	123.91	120.35
3	B	601	FAD	C5A-C6A-N6A	2.25	123.77	120.35
3	A	601	FAD	C5A-C6A-N6A	2.18	123.67	120.35
3	A	601	FAD	C3B-C2B-C1B	-2.17	97.71	100.98
3	A	601	FAD	O3B-C3B-C2B	-2.05	105.18	111.82
3	A	601	FAD	C1'-N10-C9A	2.01	119.88	118.29

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	FAD	PA-O3P-P-O5'
3	C	601	FAD	PA-O3P-P-O5'
4	A	603	MPD	C2-C3-C4-O4
4	A	603	MPD	C2-C3-C4-C5
3	A	601	FAD	O4B-C4B-C5B-O5B
3	C	601	FAD	O4B-C4B-C5B-O5B
3	C	601	FAD	C3B-C4B-C5B-O5B
3	A	601	FAD	C3B-C4B-C5B-O5B
3	B	601	FAD	PA-O3P-P-O5'
4	A	603	MPD	O2-C2-C3-C4
3	B	601	FAD	O4B-C4B-C5B-O5B
3	B	601	FAD	C3B-C4B-C5B-O5B

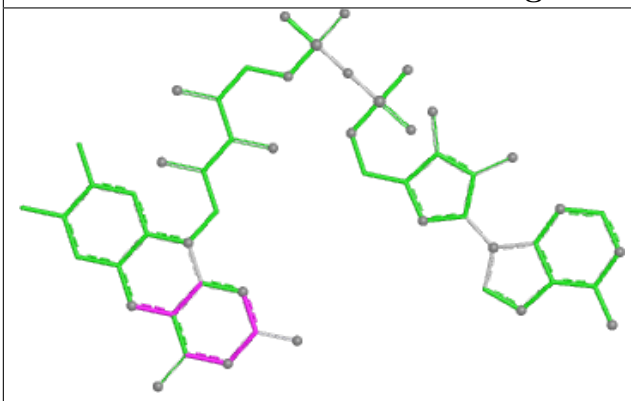
There are no ring outliers.

5 monomers are involved in 22 short contacts:

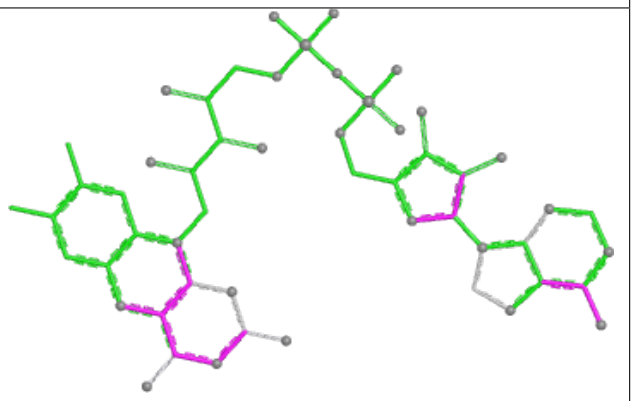
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	MPD	5	0
3	B	601	FAD	3	0
3	A	601	FAD	1	0
4	A	603	MPD	4	0
3	C	601	FAD	9	0

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

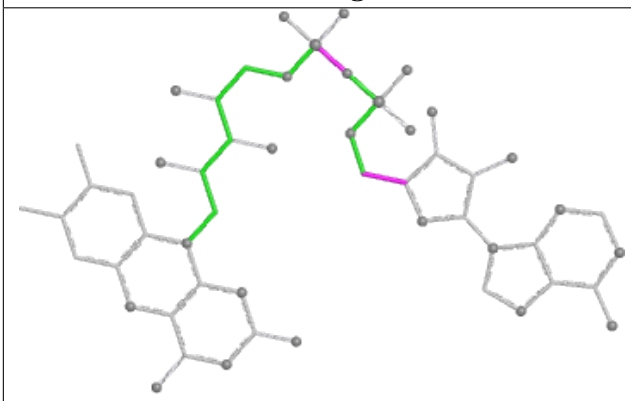
Ligand FAD B 601



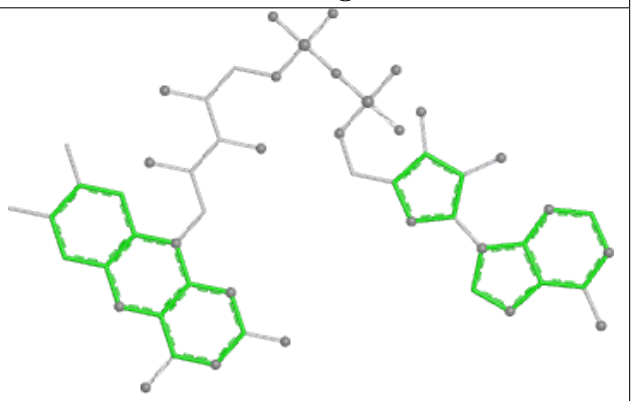
Bond lengths



Bond angles

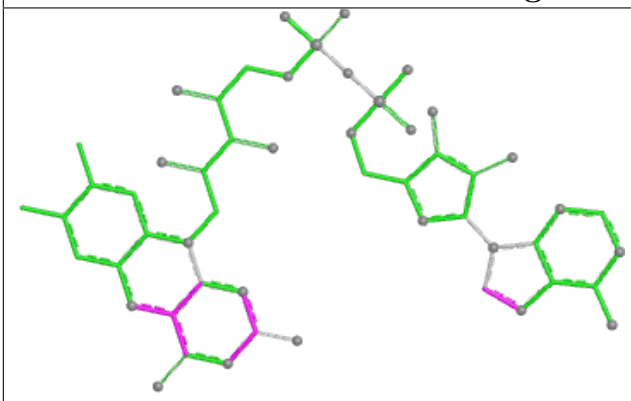


Torsions

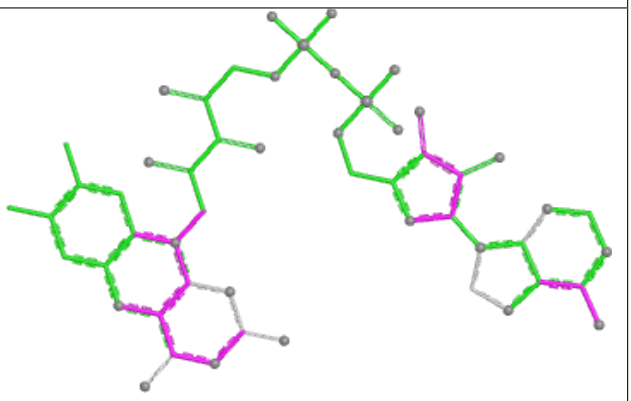


Rings

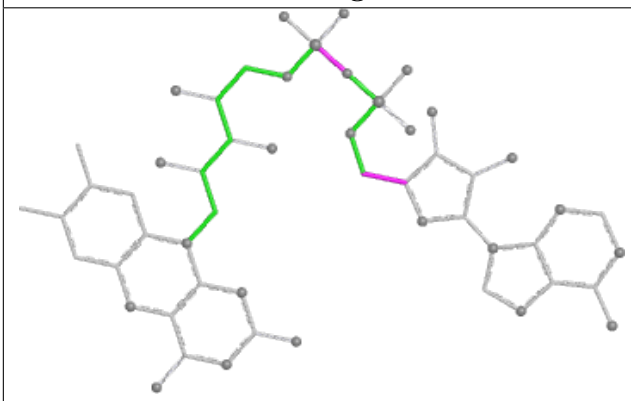
Ligand FAD A 601



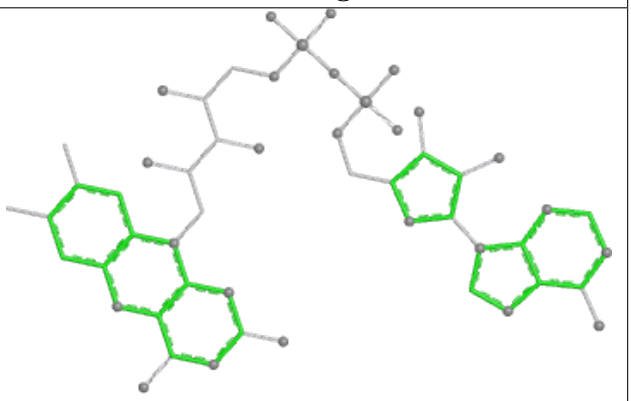
Bond lengths



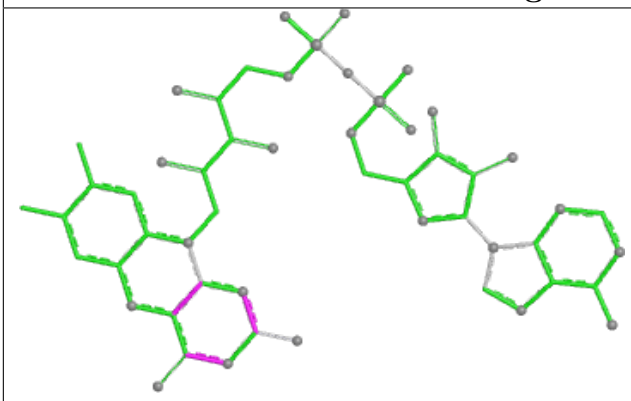
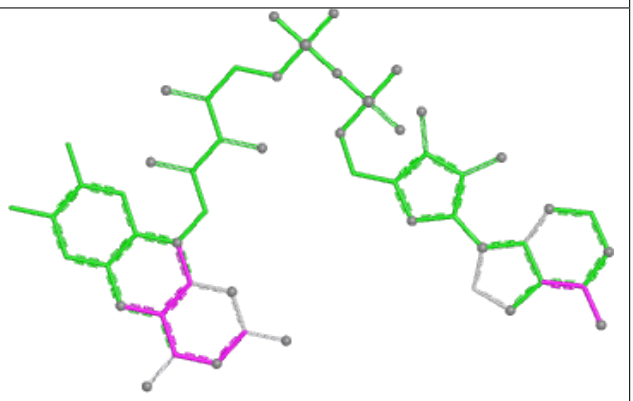
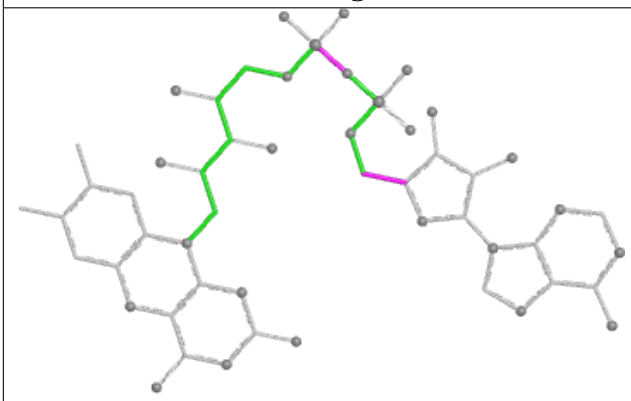
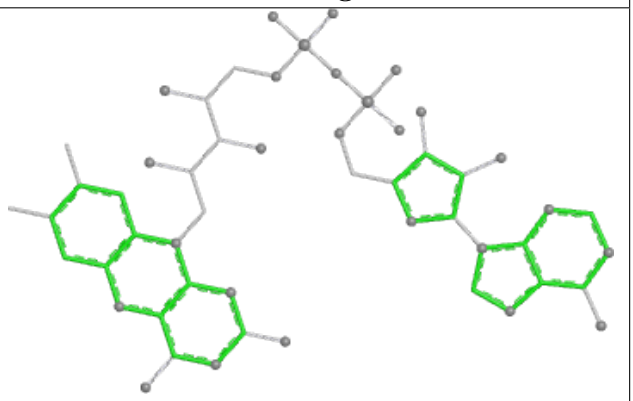
Bond angles



Torsions



Rings

Ligand FAD C 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	575/598 (96%)	0.02	19 (3%) 46 53	50, 78, 136, 206	1 (0%)
1	B	579/598 (96%)	0.02	8 (1%) 75 81	50, 84, 144, 207	0
2	C	550/598 (91%)	0.92	96 (17%) 1 1	59, 128, 205, 268	0
All	All	1704/1794 (94%)	0.31	123 (7%) 15 18	50, 92, 180, 268	1 (0%)

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	44	PHE	10.8
1	A	33	TYR	8.3
2	C	345	CYS	7.4
2	C	229	PHE	7.2
2	C	387	LEU	6.6
1	B	33	TYR	6.3
2	C	77	PHE	6.3
2	C	293	ALA	6.3
2	C	318	VAL	6.2
2	C	347	PRO	6.2
2	C	55	ARG	6.1
2	C	290	CYS	5.9
2	C	252	PHE	5.7
2	C	56	VAL	5.4
2	C	40	VAL	5.4
2	C	27	LEU	5.4
2	C	75	LEU	5.4
2	C	263	PRO	5.3
2	C	383	PHE	5.3
2	C	404	VAL	5.2
2	C	50	THR	5.1
2	C	346	VAL	5.1
2	C	272	CYS	5.1

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Mol	Chain	Res	Type	RSRZ
2	C	350	TYR	5.0
1	B	32	ASP	4.8
2	C	426	TYR	4.5
2	C	61	VAL	4.5
2	C	342	PHE	4.5
2	C	54	VAL	4.3
2	C	58	ASN	4.3
2	C	47	TYR	4.2
2	C	188	ALA	4.0
2	C	74	PRO	4.0
2	C	15	ASP	4.0
2	C	292	GLY	3.9
2	C	291	VAL	3.9
2	C	587	ASP	3.8
2	C	388	MET	3.8
2	C	353	LEU	3.8
2	C	30	TYR	3.8
2	C	262	PHE	3.7
2	C	386	VAL	3.7
1	A	73	MET	3.6
1	A	86	PHE	3.5
2	C	28	LEU	3.5
2	C	266	PRO	3.5
2	C	268	ALA	3.4
1	A	34	ASN	3.4
1	A	13	LEU	3.3
2	C	48	ASN	3.3
2	C	273	ILE	3.2
2	C	51	VAL	3.2
2	C	271	CYS	3.2
2	C	235	LEU	3.2
2	C	399	LEU	3.2
2	C	184	ILE	3.2
2	C	382	ASP	3.1
1	B	56	VAL	3.1
1	B	11	GLY	3.1
2	C	237	VAL	3.1
2	C	279	PHE	3.1
2	C	314	MET	3.1
2	C	97	PHE	3.0
2	C	280	SER	3.0
2	C	363	MET	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	99	ASN	2.9
2	C	59	ASP	2.9
1	B	12	SER	2.9
2	C	20	SER	2.9
2	C	390	ILE	2.9
2	C	186	GLU	2.8
2	C	358	ASP	2.8
2	C	189	ILE	2.8
2	C	72	SER	2.8
1	A	75	LEU	2.8
2	C	65	LEU	2.8
2	C	460	SER	2.8
1	A	235	LEU	2.7
2	C	98	LEU	2.7
2	C	60	ALA	2.7
2	C	226	TYR	2.6
1	A	40	VAL	2.6
2	C	53	THR	2.6
2	C	289	LEU	2.6
2	C	401	LEU	2.6
1	A	60	ALA	2.6
2	C	265	VAL	2.6
1	B	10	SER	2.6
1	B	209	TRP	2.5
1	A	76	ILE	2.5
2	C	49	GLU	2.5
2	C	396	THR	2.5
1	A	28	LEU	2.5
1	A	59	ASP	2.5
2	C	142	ALA	2.5
2	C	107	TYR	2.5
2	C	187	GLY	2.5
2	C	101	TRP	2.5
1	B	252	PHE	2.4
2	C	63	ASP	2.4
2	C	76	ILE	2.4
1	A	209	TRP	2.3
2	C	19	LYS	2.3
2	C	366	VAL	2.3
2	C	339	GLY	2.3
2	C	354	LYS	2.2
1	A	188	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	187	GLY	2.2
2	C	46	LYS	2.1
1	A	32	ASP	2.1
2	C	304	LEU	2.1
1	A	56	VAL	2.1
2	C	410	LYS	2.1
2	C	16	ALA	2.1
2	C	227	ALA	2.1
2	C	244	VAL	2.1
2	C	180	PHE	2.0
2	C	319	LEU	2.0
1	A	37	MET	2.0
1	A	587	ASP	2.0
2	C	351	GLU	2.0
2	C	191	LEU	2.0
2	C	349	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSO	B	345	7/8	0.79	0.12	85,94,123,124	0
1	CSO	A	345	7/8	0.90	0.13	78,85,113,121	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

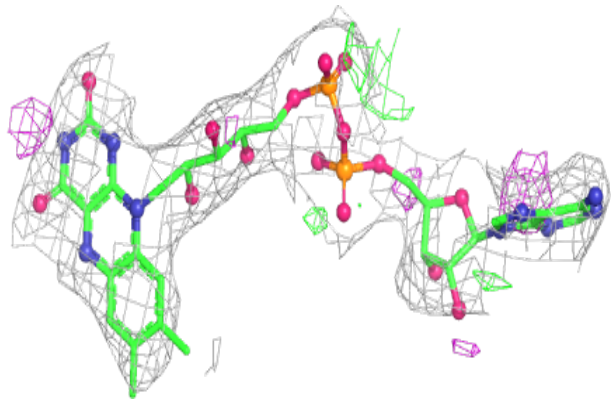
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

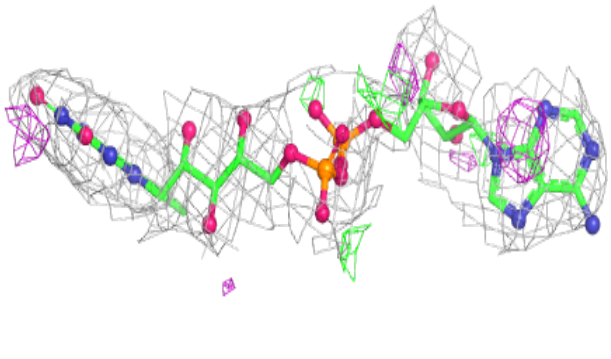
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MPD	B	602	8/8	0.81	0.31	91,104,107,110	0
4	MPD	A	602	8/8	0.85	0.29	90,112,118,119	0
4	MPD	A	603	8/8	0.86	0.24	88,103,105,111	0
5	NA	A	605	1/1	0.88	0.55	66,66,66,66	1
5	NA	A	604	1/1	0.90	0.18	54,54,54,54	1
3	FAD	C	601	53/53	0.93	0.15	86,109,132,137	0
3	FAD	A	601	53/53	0.96	0.18	50,59,69,74	0
3	FAD	B	601	53/53	0.97	0.14	53,66,85,90	0
6	CL	B	603	1/1	0.97	0.65	98,98,98,98	0
6	CL	B	604	1/1	0.97	0.59	98,98,98,98	0
6	CL	B	605	1/1	0.99	0.42	101,101,101,101	0

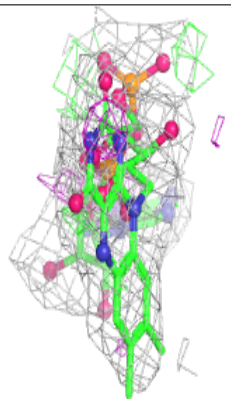
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD C 601:

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

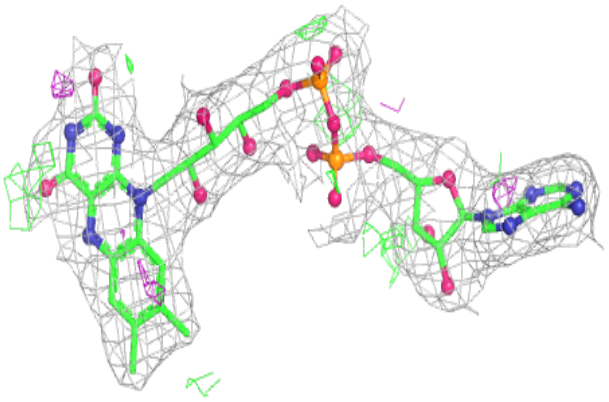


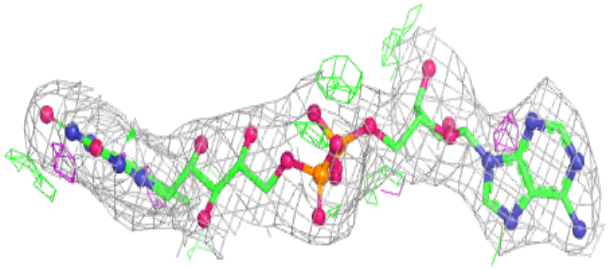


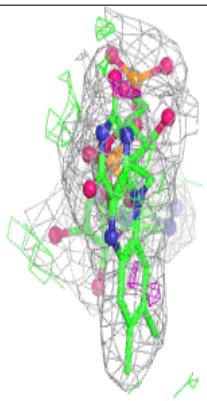


Electron density around FAD A 601:

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

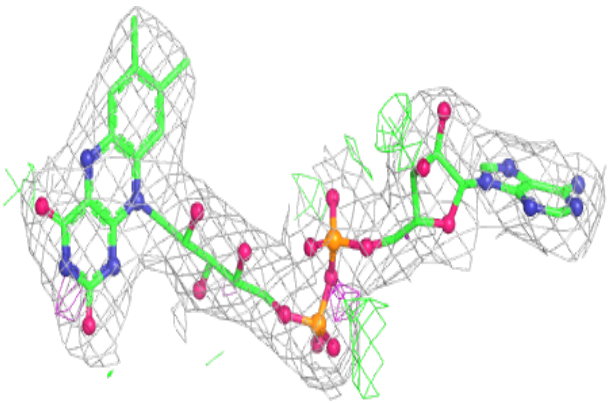


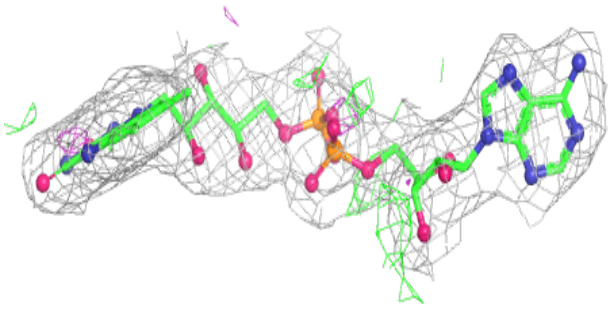


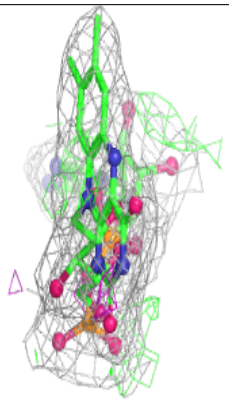


Electron density around FAD B 601:

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







6.5 Other polymers (i)

There are no such residues in this entry.