Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2021 – 12:03 PM EST

PDB ID	:	1XPQ
Title	:	Crystal structure of fms1, a polyamine oxidase from yeast
Authors	:	Huang, Q.; Liu, Q.; Hao, Q.
Deposited on	:	2004-10-09
Resolution	:	2.51 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

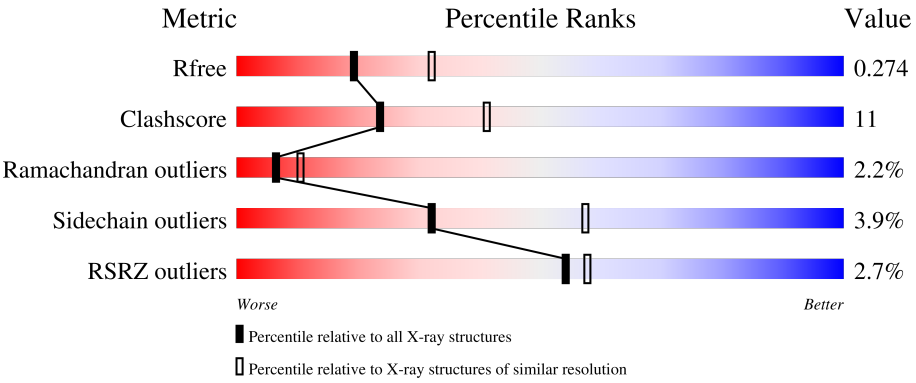
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	513	3% 71% 25%
1	B	513	2% 74% 21%
1	C	513	2% 73% 22%
1	D	513	4% 66% 27%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SPM	A	601	-	X	-	-
2	SPM	B	601	-	X	-	-
2	SPM	C	601	-	X	-	-
2	SPM	D	601	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16450 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.

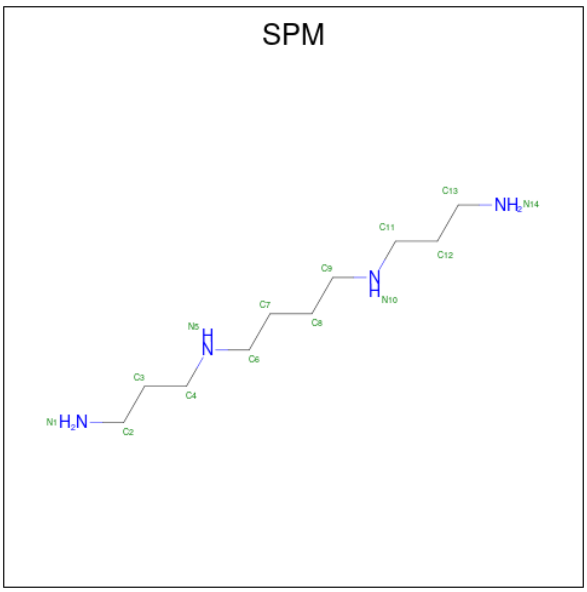
- Molecule 1 is a protein called Polyamine oxidase FMS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	502	Total	C	N	O	S	74	0	0
			4024	2541	703	758	22			
1	B	496	Total	C	N	O	S	124	0	0
			3973	2511	691	749	22			
1	C	499	Total	C	N	O	S	118	0	0
			3994	2524	694	754	22			
1	D	494	Total	C	N	O	S	141	0	0
			3956	2499	688	747	22			

There are 20 discrepancies between the modelled and reference sequences:

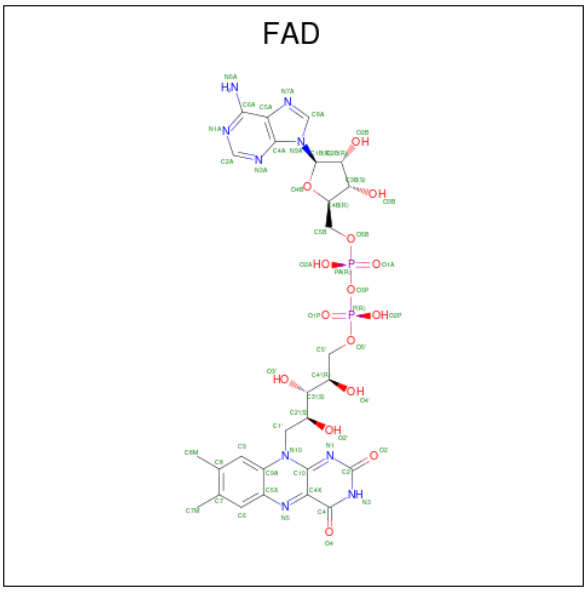
Chain	Residue	Modelled	Actual	Comment	Reference
A	509	LEU	-	expression tag	UNP P50264
A	510	GLU	-	expression tag	UNP P50264
A	511	HIS	-	expression tag	UNP P50264
A	512	HIS	-	expression tag	UNP P50264
A	513	HIS	-	expression tag	UNP P50264
B	509	LEU	-	expression tag	UNP P50264
B	510	GLU	-	expression tag	UNP P50264
B	511	HIS	-	expression tag	UNP P50264
B	512	HIS	-	expression tag	UNP P50264
B	513	HIS	-	expression tag	UNP P50264
C	509	LEU	-	expression tag	UNP P50264
C	510	GLU	-	expression tag	UNP P50264
C	511	HIS	-	expression tag	UNP P50264
C	512	HIS	-	expression tag	UNP P50264
C	513	HIS	-	expression tag	UNP P50264
D	509	LEU	-	expression tag	UNP P50264
D	510	GLU	-	expression tag	UNP P50264
D	511	HIS	-	expression tag	UNP P50264
D	512	HIS	-	expression tag	UNP P50264
D	513	HIS	-	expression tag	UNP P50264

- Molecule 2 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N 14 10 4	0	0
2	B	1	Total C N 14 10 4	0	0
2	C	1	Total C N 14 10 4	0	0
2	D	1	Total C N 14 10 4	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
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is water.

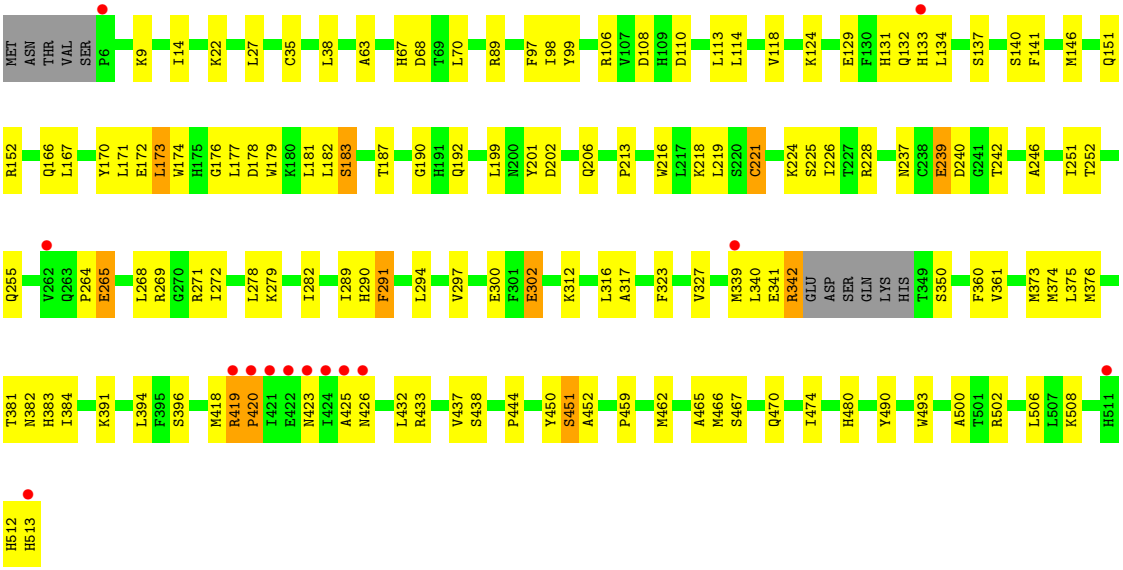
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	60	Total	O	0	0
			60	60		
4	B	46	Total	O	0	0
			46	46		
4	C	73	Total	O	0	0
			73	73		
4	D	56	Total	O	0	0
			56	56		

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.

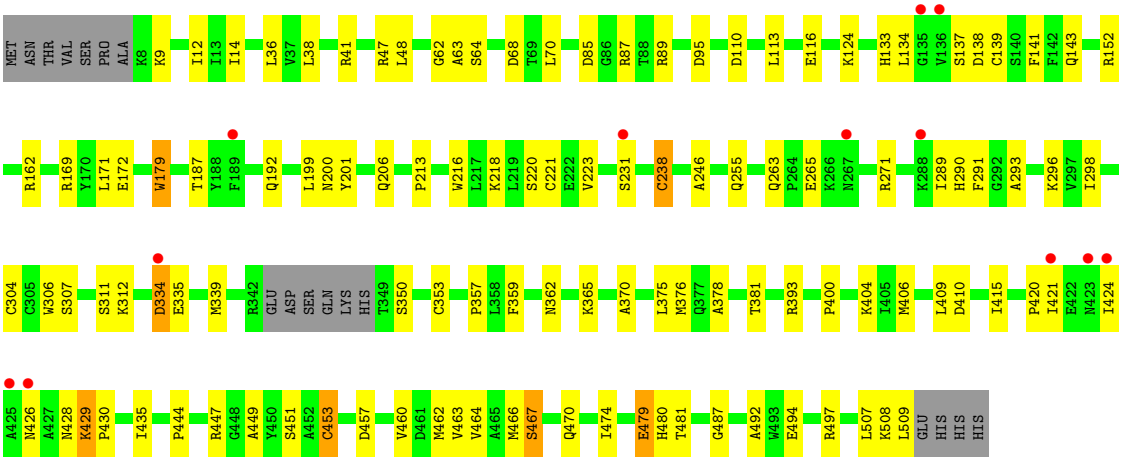
• Molecule 1: Polyamine oxidase FMS1

Chain A:



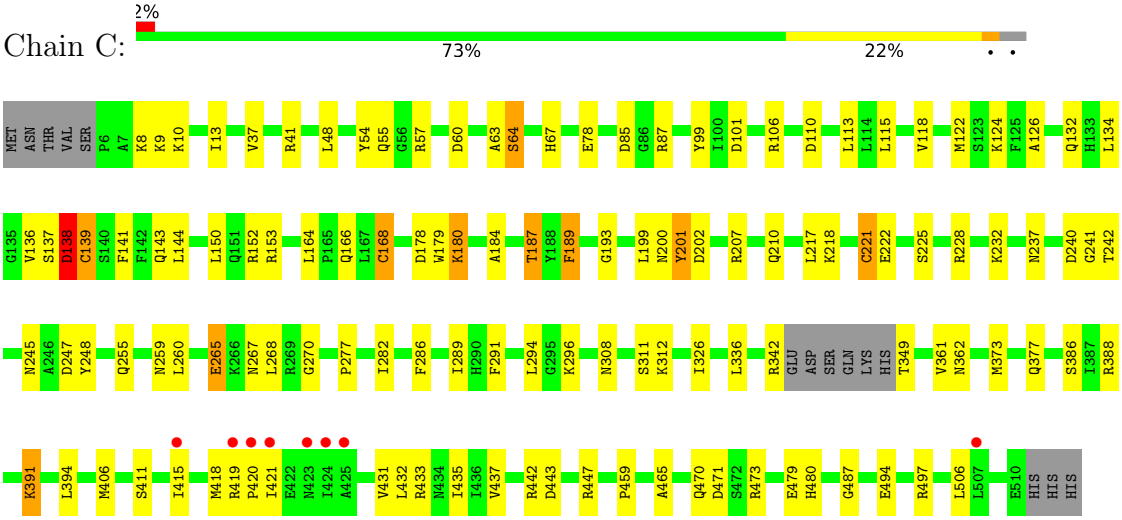
• Molecule 1: Polyamine oxidase FMS1

Chain B:



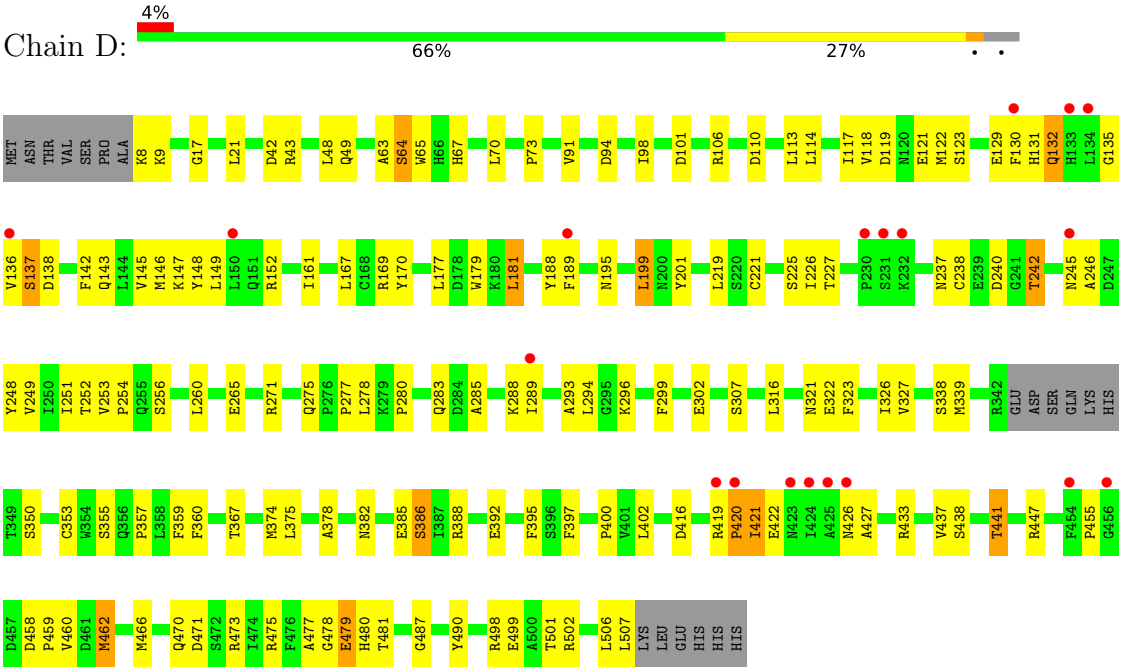
• Molecule 1: Polyamine oxidase FMS1

Chain C:



• Molecule 1: Polyamine oxidase FMS1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.05Å 98.13Å 123.83Å 90.00° 103.28° 90.00°	Depositor
Resolution (Å)	42.93 – 2.51 49.84 – 2.51	Depositor EDS
% Data completeness (in resolution range)	80.4 (42.93-2.51) 73.5 (49.84-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.200 , 0.276 0.198 , 0.274	Depositor DCC
R_{free} test set	2000 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å^2)	41.3	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16450	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: SPM, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.46	0/4109	0.67	1/5557 (0.0%)
1	B	0.47	0/4054	0.65	0/5483
1	C	0.48	1/4076 (0.0%)	0.67	0/5513
1	D	0.44	0/4037	0.65	1/5461 (0.0%)
All	All	0.46	1/16276 (0.0%)	0.66	2/22014 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	168	CYS	CB-SG	-7.10	1.70	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	199	LEU	CA-CB-CG	-7.00	99.21	115.30
1	A	173	LEU	CB-CG-CD1	-5.44	101.75	111.00

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	4024	0	3935	92	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3973	0	3900	70	0
1	C	3994	0	3919	80	2
1	D	3956	0	3876	106	0
2	A	14	0	26	6	0
2	B	14	0	26	2	0
2	C	14	0	26	2	0
2	D	14	0	26	7	0
3	A	53	0	31	3	0
3	B	53	0	31	9	0
3	C	53	0	31	2	0
3	D	53	0	31	5	0
4	A	60	0	0	11	0
4	B	46	0	0	5	0
4	C	73	0	0	5	0
4	D	56	0	0	1	0
All	All	16450	0	15858	347	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (347) 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:A:451:SER:OG	4:A:701:HOH:O	1.91	0.89
1:C:228:ARG:HH21	1:C:473:ARG:HG3	1.39	0.88
1:B:238:CYS:SG	4:B:742:HOH:O	2.35	0.84
1:A:452:ALA:O	4:A:702:HOH:O	1.95	0.84
1:A:173:LEU:HD12	1:A:375:LEU:HB3	1.60	0.83
1:B:206:GLN:NE2	4:B:701:HOH:O	2.10	0.82
1:D:260:LEU:HB3	1:D:271:ARG:HG3	1.60	0.81
1:D:67:HIS:HE2	2:D:601:SPM:H121	1.46	0.81
1:D:130:PHE:O	1:D:132:GLN:N	2.15	0.80
1:A:171:LEU:HD23	1:A:187:THR:HG22	1.64	0.79
1:D:149:LEU:HD22	1:D:161:ILE:HD13	1.62	0.79
1:B:64:SER:HB2	1:B:296:LYS:HZ3	1.48	0.78
1:B:12:ILE:HD12	1:B:246:ALA:HB2	1.64	0.78
1:B:311:SER:HB3	1:B:365:LYS:HE3	1.66	0.78
1:D:419:ARG:O	1:D:421:ILE:N	2.18	0.76
1:D:278:LEU:HA	1:D:470:GLN:HE22	1.50	0.76
1:A:291:PHE:HA	1:A:451:SER:HA	1.67	0.75
1:A:173:LEU:CD1	1:A:375:LEU:HB3	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:ILE:HD11	1:B:429:LYS:HD3	1.70	0.74
1:C:13:ILE:HB	1:C:37:VAL:HG12	1.71	0.73
1:D:8:LYS:N	1:D:245:ASN:OD1	2.23	0.72
1:D:353:CYS:SG	1:D:400:PRO:HG2	2.30	0.71
1:D:466:MET:HE1	1:D:480:HIS:CD2	2.25	0.71
1:C:349:THR:N	4:C:702:HOH:O	2.23	0.70
1:B:463:VAL:O	1:B:467:SER:OG	2.10	0.70
1:B:293:ALA:HB3	1:B:378:ALA:HB2	1.74	0.70
1:C:37:VAL:HG23	1:C:217:LEU:HA	1.73	0.70
1:D:478:GLY:O	1:D:481:THR:HG22	1.92	0.69
1:C:180:LYS:NZ	4:C:703:HOH:O	2.24	0.69
1:A:383:HIS:NE2	4:A:709:HOH:O	2.26	0.69
1:A:182:LEU:HD21	1:A:187:THR:HG23	1.74	0.68
1:A:110:ASP:HB3	1:A:113:LEU:HB2	1.75	0.67
1:B:169:ARG:HB3	1:B:357:PRO:HG3	1.77	0.67
1:B:470:GLN:HB3	1:B:474:ILE:HB	1.77	0.67
1:D:63:ALA:HA	3:D:602:FAD:N5	2.10	0.67
1:A:297:VAL:HG22	1:A:437:VAL:HG13	1.78	0.66
1:B:63:ALA:HA	3:B:602:FAD:N5	2.12	0.65
1:A:98:ILE:HG12	1:A:106:ARG:NH2	2.11	0.65
1:B:213:PRO:HG2	1:B:216:TRP:CE2	2.32	0.65
1:D:385:GLU:OE1	1:D:441:THR:OG1	2.14	0.65
1:D:289:ILE:HG13	1:D:459:PRO:HA	1.79	0.65
1:B:110:ASP:HB3	1:B:113:LEU:HB2	1.77	0.65
1:D:477:ALA:HA	1:D:481:THR:HG21	1.78	0.65
1:B:453:CYS:HB2	1:B:457:ASP:HB2	1.80	0.64
1:D:240:ASP:OD1	1:D:242:THR:HG23	1.97	0.64
1:A:14:ILE:HD13	1:A:251:ILE:HG13	1.79	0.64
1:D:119:ASP:O	1:D:122:MET:HB3	1.97	0.64
1:D:359:PHE:HB3	1:D:375:LEU:HB2	1.79	0.64
1:C:419:ARG:O	1:C:421:ILE:N	2.31	0.64
1:B:38:LEU:HG	4:B:742:HOH:O	1.98	0.64
1:A:129:GLU:OE2	4:A:703:HOH:O	2.15	0.63
1:D:225:SER:OG	1:D:237:ASN:ND2	2.31	0.62
1:C:63:ALA:HA	3:C:602:FAD:N5	2.15	0.62
1:C:178:ASP:OD1	1:C:180:LYS:HE2	2.00	0.62
1:B:85:ASP:OD2	1:B:89:ARG:NH2	2.31	0.62
1:C:67:HIS:NE2	2:C:601:SPM:H121	2.15	0.62
1:C:479:GLU:OE1	1:C:487:GLY:HA2	2.00	0.62
1:D:289:ILE:HG12	1:D:462:MET:HB2	1.82	0.61
1:A:63:ALA:HA	3:A:602:FAD:N5	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ILE:HG12	1:C:465:ALA:HB1	1.83	0.61
1:D:67:HIS:HE1	2:D:601:SPM:H82	1.65	0.61
1:D:110:ASP:HB3	1:D:113:LEU:HB2	1.83	0.60
1:B:95:ASP:OD2	1:B:365:LYS:HE2	2.01	0.60
1:B:221:CYS:SG	4:B:742:HOH:O	2.57	0.59
1:A:376:MET:HE1	1:A:384:ILE:HG21	1.84	0.59
1:B:171:LEU:HD13	1:B:187:THR:HG22	1.83	0.59
1:C:391:LYS:HB2	1:C:419:ARG:HH22	1.68	0.59
1:A:9:LYS:O	1:A:246:ALA:HA	2.02	0.59
1:A:323:PHE:O	1:A:327:VAL:HG23	2.03	0.58
1:A:268:LEU:HD12	1:A:271:ARG:HD2	1.84	0.58
1:C:55:GLN:HE22	1:C:57:ARG:NH2	2.02	0.58
1:C:218:LYS:NZ	1:C:221:CYS:HB2	2.18	0.58
1:D:181:LEU:O	1:D:455:PRO:HD3	2.04	0.57
1:C:406:MET:HB3	1:C:411:SER:HB3	1.86	0.57
1:A:302:GLU:HG2	1:A:433:ARG:HE	1.69	0.57
1:B:62:GLY:O	1:B:296:LYS:NZ	2.27	0.57
1:D:9:LYS:O	1:D:246:ALA:HA	2.05	0.57
1:A:99:TYR:H	1:A:108:ASP:HB3	1.70	0.56
1:A:290:HIS:N	4:A:702:HOH:O	2.19	0.56
1:D:94:ASP:OD1	2:D:601:SPM:H21	2.05	0.56
1:D:248:TYR:HE2	1:D:507:LEU:HD21	1.70	0.56
1:B:426:ASN:O	1:B:428:ASN:N	2.35	0.56
1:D:359:PHE:HD2	1:D:375:LEU:HG	1.71	0.56
1:B:116:GLU:OE1	1:B:116:GLU:N	2.30	0.56
1:A:462:MET:HE2	1:A:466:MET:HG2	1.88	0.56
1:C:247:ASP:O	1:C:473:ARG:HD2	2.06	0.56
1:C:54:TYR:CE2	1:C:433:ARG:HG3	2.41	0.56
1:D:251:ILE:HG22	1:D:253:VAL:HG22	1.88	0.55
1:B:63:ALA:HA	3:B:602:FAD:C5X	2.36	0.55
1:A:282:ILE:HG12	1:A:465:ALA:HB1	1.88	0.55
1:C:240:ASP:OD1	1:C:242:THR:HG23	2.07	0.55
1:D:302:GLU:OE1	1:D:433:ARG:HD3	2.07	0.55
1:D:385:GLU:OE2	1:D:438:SER:OG	2.24	0.55
1:B:311:SER:HA	1:B:362:ASN:HB3	1.89	0.54
1:C:126:ALA:HB2	1:C:144:LEU:HD21	1.89	0.54
1:C:143:GLN:NE2	4:C:706:HOH:O	2.30	0.54
1:C:391:LYS:HA	1:C:394:LEU:HD12	1.90	0.54
1:B:494:GLU:HG3	1:B:497:ARG:NH2	2.23	0.54
1:B:48:LEU:CD2	1:B:63:ALA:HB3	2.37	0.54
1:B:353:CYS:SG	1:B:400:PRO:HB2	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:MET:SD	1:C:435:ILE:HD12	2.47	0.54
1:D:114:LEU:HB3	1:D:117:ILE:HD12	1.90	0.54
1:D:322:GLU:O	1:D:326:ILE:HG13	2.08	0.53
1:A:68:ASP:HB3	1:A:192:GLN:HB2	1.90	0.53
1:A:131:HIS:O	4:A:704:HOH:O	2.19	0.53
1:D:67:HIS:HA	1:D:195:ASN:HD22	1.73	0.53
1:D:458:ASP:OD1	1:D:460:VAL:HG12	2.08	0.53
1:D:280:PRO:HA	1:D:283:GLN:HB3	1.89	0.53
1:A:167:LEU:HA	1:A:316:LEU:HD21	1.90	0.53
1:A:202:ASP:OD1	1:A:202:ASP:N	2.33	0.53
1:A:360:PHE:CD1	1:A:374:MET:HB2	2.43	0.53
1:B:64:SER:HB2	1:B:296:LYS:NZ	2.23	0.52
1:B:479:GLU:OE1	1:B:487:GLY:HA2	2.09	0.52
1:B:312:LYS:NZ	2:B:601:SPM:H22	2.25	0.52
1:C:78:GLU:OE2	1:C:207:ARG:NH2	2.43	0.52
1:C:248:TYR:HD1	1:C:473:ARG:HA	1.75	0.52
1:A:423:ASN:HB3	1:A:426:ASN:ND2	2.25	0.52
1:B:289:ILE:HD12	1:B:290:HIS:H	1.75	0.52
1:C:388:ARG:HB2	1:C:437:VAL:HB	1.92	0.52
1:A:224:LYS:HE2	1:A:239:GLU:HB2	1.92	0.52
1:C:255:GLN:HB2	1:C:480:HIS:CG	2.44	0.51
1:C:432:LEU:HD21	1:C:435:ILE:HD11	1.92	0.51
1:B:311:SER:O	1:B:312:LYS:HD3	2.11	0.51
1:D:475:ARG:HD3	1:D:502:ARG:HH21	1.75	0.51
1:A:226:ILE:HD12	1:A:272:ILE:HG21	1.91	0.51
1:B:255:GLN:HB2	1:B:480:HIS:CG	2.46	0.51
1:C:110:ASP:HB3	1:C:113:LEU:HB2	1.91	0.51
1:A:97:PHE:HZ	2:A:601:SPM:H21	1.76	0.51
1:C:118:VAL:HG23	1:C:164:LEU:HD13	1.92	0.51
1:C:225:SER:HB2	1:C:237:ASN:HB2	1.92	0.51
1:C:289:ILE:CG1	1:C:459:PRO:HA	2.40	0.51
1:D:67:HIS:NE2	2:D:601:SPM:H121	2.20	0.51
1:D:43:ARG:CZ	1:D:49:GLN:HE21	2.23	0.50
1:D:478:GLY:HA2	3:D:602:FAD:O2P	2.11	0.50
1:A:174:TRP:HZ2	2:A:601:SPM:H22	1.76	0.50
1:A:218:LYS:NZ	1:A:221:CYS:HB2	2.26	0.50
1:A:67:HIS:NE2	2:A:601:SPM:H131	2.26	0.50
1:D:395:PHE:CE2	1:D:416:ASP:HB2	2.47	0.50
1:A:339:MET:O	1:A:341:GLU:N	2.44	0.50
1:A:152:ARG:CZ	1:B:70:LEU:HD23	2.41	0.50
1:A:312:LYS:HE3	2:A:601:SPM:H41	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:GLY:HA2	1:D:121:GLU:HG3	1.94	0.50
1:C:265:GLU:O	1:C:267:ASN:N	2.45	0.50
1:A:265:GLU:HG3	1:A:268:LEU:HD21	1.93	0.50
1:A:391:LYS:HA	1:A:394:LEU:HD12	1.94	0.50
1:C:248:TYR:CD1	1:C:473:ARG:HA	2.47	0.50
1:D:256:SER:O	1:D:260:LEU:HD13	2.12	0.50
1:D:466:MET:HE3	1:D:481:THR:HB	1.93	0.50
1:D:481:THR:HG23	1:D:498:ARG:HH22	1.77	0.50
1:B:289:ILE:HG21	1:B:462:MET:HB2	1.94	0.50
1:B:41:ARG:NH1	3:B:602:FAD:O2B	2.44	0.49
1:A:132:GLN:HB2	4:A:704:HOH:O	2.12	0.49
1:A:278:LEU:HA	1:A:470:GLN:NE2	2.27	0.49
1:A:131:HIS:CD2	1:A:132:GLN:H	2.30	0.49
1:B:139:CYS:HB2	1:B:143:GLN:HB3	1.94	0.49
1:C:259:ASN:ND2	4:C:715:HOH:O	2.45	0.49
1:D:293:ALA:HB3	1:D:378:ALA:HB2	1.94	0.49
1:D:502:ARG:NH1	1:D:506:LEU:HD11	2.27	0.49
1:A:89:ARG:N	4:A:711:HOH:O	2.29	0.49
1:D:122:MET:HE3	1:D:145:VAL:HG22	1.94	0.49
1:D:63:ALA:HA	3:D:602:FAD:C5X	2.43	0.49
1:A:70:LEU:HD23	1:B:152:ARG:CZ	2.42	0.49
1:B:68:ASP:HB3	1:B:192:GLN:HB2	1.94	0.49
1:C:308:ASN:O	4:C:701:HOH:O	2.20	0.49
1:A:174:TRP:CZ2	2:A:601:SPM:H22	2.48	0.48
1:B:141:PHE:CD1	1:B:187:THR:HG21	2.47	0.48
1:A:213:PRO:HB2	1:A:216:TRP:CD1	2.49	0.48
1:A:252:THR:O	3:A:602:FAD:H52A	2.13	0.48
1:D:98:ILE:HG12	1:D:106:ARG:NH2	2.28	0.48
1:D:135:GLY:O	1:D:137:SER:N	2.46	0.48
1:D:143:GLN:O	1:D:147:LYS:HG3	2.13	0.48
1:D:447:ARG:NH1	1:D:447:ARG:HG2	2.29	0.48
1:B:47:ARG:NE	3:B:602:FAD:O2A	2.33	0.48
1:A:342:ARG:O	4:A:705:HOH:O	2.20	0.48
1:D:477:ALA:CA	1:D:481:THR:HG21	2.44	0.47
1:C:48:LEU:CD2	1:C:63:ALA:HB3	2.44	0.47
1:A:141:PHE:CD1	1:A:187:THR:HG21	2.49	0.47
1:C:199:LEU:HD23	1:C:199:LEU:HA	1.75	0.47
1:B:263:GLN:O	1:B:271:ARG:NH1	2.48	0.47
1:C:361:VAL:HB	1:C:373:MET:HB3	1.96	0.47
1:D:65:TRP:CD2	2:D:601:SPM:H62	2.49	0.47
1:D:130:PHE:C	1:D:132:GLN:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:PHE:CE2	1:D:374:MET:HG3	2.50	0.47
1:A:269:ARG:CZ	1:A:444:PRO:HG3	2.44	0.47
1:B:9:LYS:HG3	1:B:36:LEU:HG	1.96	0.47
1:D:67:HIS:CE1	2:D:601:SPM:H82	2.46	0.47
1:D:73:PRO:HD2	1:D:490:TYR:CD1	2.49	0.47
1:D:148:TYR:CE1	1:D:152:ARG:HG3	2.50	0.47
1:D:260:LEU:HB3	1:D:271:ARG:CG	2.37	0.47
1:D:288:LYS:O	1:D:289:ILE:HD12	2.14	0.47
1:B:453:CYS:CB	1:B:457:ASP:HB2	2.45	0.47
1:C:277:PRO:O	1:C:470:GLN:NE2	2.42	0.47
1:B:406:MET:HG3	1:B:430:PRO:HG3	1.97	0.46
1:C:222:GLU:OE2	1:C:270:GLY:N	2.33	0.46
1:A:124:LYS:HD2	1:A:124:LYS:HA	1.74	0.46
1:C:55:GLN:HE22	1:C:57:ARG:HH21	1.63	0.46
1:A:151:GLN:OE1	4:A:706:HOH:O	2.20	0.46
1:A:289:ILE:HD13	1:A:459:PRO:HB3	1.97	0.46
1:B:444:PRO:O	1:B:447:ARG:NE	2.49	0.46
1:A:279:LYS:HB2	1:A:470:GLN:OE1	2.15	0.46
1:B:304:CYS:HA	1:B:306:TRP:CZ3	2.51	0.46
1:D:299:PHE:CD1	1:D:402:LEU:HD11	2.50	0.46
1:A:166:GLN:OE1	1:A:317:ALA:HB3	2.16	0.46
1:A:173:LEU:HD13	1:A:173:LEU:HA	1.63	0.46
1:A:255:GLN:HB2	1:A:480:HIS:CG	2.51	0.46
2:B:601:SPM:HN0	3:B:602:FAD:C4X	2.28	0.46
1:C:122:MET:HE3	1:C:168:CYS:SG	2.56	0.46
1:D:289:ILE:CG1	1:D:459:PRO:HA	2.45	0.46
1:C:99:TYR:O	1:C:106:ARG:HA	2.16	0.46
1:C:240:ASP:OD1	1:C:241:GLY:N	2.48	0.46
1:C:255:GLN:HG2	1:C:286:PHE:HE2	1.81	0.46
1:A:361:VAL:HB	1:A:373:MET:HB3	1.97	0.45
1:B:298:ILE:O	1:B:435:ILE:HA	2.16	0.45
1:C:202:ASP:OD1	1:C:202:ASP:N	2.49	0.45
1:A:490:TYR:HA	1:A:493:TRP:HB3	1.99	0.45
1:C:124:LYS:HA	1:C:124:LYS:HD3	1.75	0.45
1:C:166:GLN:OE1	1:C:166:GLN:HA	2.15	0.45
1:D:302:GLU:OE1	1:D:433:ARG:NH1	2.47	0.45
1:D:110:ASP:OD1	1:D:113:LEU:N	2.46	0.45
1:A:294:LEU:HD12	1:A:376:MET:O	2.16	0.45
1:D:447:ARG:HG2	1:D:447:ARG:HH11	1.81	0.45
1:A:502:ARG:O	1:A:506:LEU:HD23	2.16	0.45
1:D:48:LEU:CD2	1:D:63:ALA:HB3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:GLU:OE2	1:B:179:TRP:N	2.42	0.45
1:B:466:MET:HB3	1:B:481:THR:HB	1.99	0.45
1:C:255:GLN:HB2	1:C:480:HIS:CD2	2.51	0.45
1:C:326:ILE:HG22	1:C:336:LEU:HD12	1.98	0.45
1:D:142:PHE:O	1:D:146:MET:HG2	2.16	0.45
1:C:415:ILE:HB	1:C:431:VAL:HG22	1.99	0.45
1:D:323:PHE:O	1:D:327:VAL:HG23	2.16	0.45
1:D:420:PRO:O	1:D:422:GLU:N	2.50	0.45
1:A:202:ASP:O	1:A:206:GLN:HG2	2.17	0.45
1:B:404:LYS:HD2	1:B:404:LYS:HA	1.74	0.45
1:A:178:ASP:HB3	1:A:181:LEU:HD12	1.99	0.45
1:A:225:SER:OG	1:A:237:ASN:HB2	2.16	0.45
1:A:418:MET:O	1:A:420:PRO:HD3	2.17	0.45
1:B:460:VAL:O	1:B:464:VAL:HG23	2.16	0.45
1:C:471:ASP:OD1	1:C:473:ARG:N	2.41	0.45
1:A:110:ASP:O	1:A:114:LEU:HD23	2.17	0.45
1:A:508:LYS:O	1:A:513:HIS:CE1	2.70	0.45
1:C:10:LYS:O	1:C:247:ASP:HB2	2.16	0.45
1:C:113:LEU:HB3	1:C:115:LEU:HG	1.98	0.45
1:B:507:LEU:O	1:B:509:LEU:N	2.50	0.44
1:D:123:SER:HG	1:D:188:TYR:HE1	1.62	0.44
1:C:41:ARG:NH2	1:C:443:ASP:OD2	2.43	0.44
1:A:27:LEU:HG	1:A:500:ALA:HB1	2.00	0.44
1:A:172:GLU:HG2	1:A:177:LEU:O	2.18	0.44
1:D:17:GLY:O	1:D:21:LEU:HG	2.16	0.44
1:D:64:SER:HB2	1:D:296:LYS:NZ	2.32	0.44
1:D:294:LEU:HD11	1:D:375:LEU:HD13	1.99	0.44
1:A:22:LYS:NZ	4:A:717:HOH:O	2.50	0.44
1:D:382:ASN:O	1:D:386:SER:HB3	2.17	0.44
1:A:240:ASP:OD1	1:A:242:THR:OG1	2.26	0.44
1:D:219:LEU:HD23	1:D:219:LEU:HA	1.78	0.44
1:C:260:LEU:HD11	1:C:447:ARG:NE	2.33	0.44
1:C:494:GLU:HG2	1:C:497:ARG:NH2	2.32	0.44
1:A:278:LEU:HA	1:A:470:GLN:HE22	1.83	0.44
1:C:189:PHE:N	1:C:189:PHE:CD1	2.86	0.44
1:A:167:LEU:O	1:A:170:TYR:HD1	2.01	0.43
1:D:392:GLU:OE2	1:D:419:ARG:HD3	2.18	0.43
1:D:248:TYR:HD1	1:D:473:ARG:HA	1.83	0.43
1:D:479:GLU:OE1	1:D:487:GLY:HA2	2.18	0.43
1:A:376:MET:SD	1:A:381:THR:HA	2.58	0.43
1:B:89:ARG:HG3	1:B:89:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:LEU:HD23	1:B:199:LEU:HA	1.92	0.43
1:C:85:ASP:OD1	1:C:87:ARG:HB2	2.18	0.43
1:D:199:LEU:HD21	1:D:367:THR:HG22	2.01	0.43
1:D:278:LEU:HA	1:D:470:GLN:NE2	2.25	0.43
1:C:152:ARG:CZ	1:D:70:LEU:HD23	2.49	0.43
1:D:326:ILE:HG23	1:D:339:MET:HG2	1.99	0.43
1:D:475:ARG:HB3	1:D:499:GLU:OE1	2.19	0.43
1:A:63:ALA:HA	3:A:602:FAD:C5X	2.49	0.43
1:D:91:VAL:HG22	1:D:199:LEU:HD11	2.01	0.43
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.78	0.43
1:B:221:CYS:HB3	4:B:742:HOH:O	2.18	0.43
1:C:126:ALA:CB	1:C:144:LEU:HD21	2.49	0.43
1:C:386:SER:HA	1:C:442:ARG:HE	1.83	0.43
1:C:391:LYS:HB2	1:C:419:ARG:NH2	2.33	0.43
1:D:65:TRP:CE3	2:D:601:SPM:H62	2.52	0.43
1:D:227:THR:HG23	1:D:275:GLN:HB2	1.99	0.43
1:A:38:LEU:HD22	1:A:221:CYS:SG	2.58	0.43
1:C:144:LEU:HD22	1:C:184:ALA:HB1	2.01	0.43
1:D:260:LEU:CB	1:D:271:ARG:HG3	2.41	0.43
1:C:64:SER:HB2	1:C:296:LYS:HZ1	1.82	0.43
1:A:35:CYS:HB2	1:A:216:TRP:CZ3	2.53	0.43
1:D:122:MET:CE	1:D:145:VAL:HA	2.49	0.43
1:C:218:LYS:HZ3	1:C:221:CYS:HB2	1.81	0.43
1:D:471:ASP:OD1	1:D:473:ARG:N	2.33	0.43
1:A:300:GLU:O	1:A:432:LEU:HD12	2.18	0.42
1:C:8:LYS:O	1:C:9:LYS:HD2	2.19	0.42
1:C:248:TYR:CE1	1:C:473:ARG:HD3	2.54	0.42
1:C:311:SER:HA	1:C:362:ASN:HB3	2.01	0.42
1:A:177:LEU:HD22	1:A:452:ALA:HB3	2.01	0.42
1:A:224:LYS:CE	1:A:239:GLU:HB2	2.49	0.42
1:A:290:HIS:O	1:A:451:SER:HB2	2.19	0.42
1:D:122:MET:HE1	1:D:145:VAL:HA	2.00	0.42
1:D:226:ILE:HD13	1:D:249:VAL:HG11	2.02	0.42
1:C:141:PHE:CE2	1:C:187:THR:HG21	2.55	0.42
1:D:101:ASP:HB2	1:D:316:LEU:HD12	2.01	0.42
1:D:195:ASN:ND2	4:D:710:HOH:O	2.52	0.42
1:B:36:LEU:HB3	1:B:38:LEU:CD1	2.50	0.42
1:B:63:ALA:HA	3:B:602:FAD:C4X	2.49	0.42
1:D:177:LEU:HD12	1:D:177:LEU:HA	1.84	0.42
1:D:252:THR:HG22	1:D:477:ALA:HB3	2.01	0.42
1:A:228:ARG:HB2	1:A:474:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:TYR:O	1:A:451:SER:CB	2.67	0.42
1:B:359:PHE:HD2	1:B:375:LEU:HD22	1.85	0.42
1:D:167:LEU:O	1:D:170:TYR:HD2	2.02	0.42
1:C:189:PHE:N	1:C:189:PHE:HD1	2.17	0.42
1:C:232:LYS:O	1:C:473:ARG:NE	2.53	0.42
1:D:114:LEU:HD22	1:D:117:ILE:HD12	2.02	0.41
1:B:14:ILE:CD1	1:B:223:VAL:HG21	2.50	0.41
1:D:169:ARG:HB3	1:D:357:PRO:HG3	2.02	0.41
1:D:254:PRO:HD3	3:D:602:FAD:H51A	2.02	0.41
1:C:150:LEU:O	1:C:153:ARG:HG2	2.20	0.41
1:C:289:ILE:HG13	1:C:459:PRO:HA	2.00	0.41
2:C:601:SPM:H122	3:C:602:FAD:C4X	2.51	0.41
2:A:601:SPM:H72	2:A:601:SPM:H42	1.70	0.41
1:B:479:GLU:HG2	3:B:602:FAD:H5'1	2.02	0.41
1:C:138:ASP:O	1:C:139:CYS:HB3	2.20	0.41
1:D:253:VAL:HG12	3:D:602:FAD:C8A	2.51	0.41
1:B:14:ILE:HD12	1:B:223:VAL:HG21	2.03	0.41
1:B:376:MET:HG3	1:B:381:THR:OG1	2.20	0.41
1:B:89:ARG:HG3	1:B:89:ARG:HH11	1.84	0.41
1:B:334:ASP:N	1:B:334:ASP:OD1	2.53	0.41
1:B:449:ALA:HB1	3:B:602:FAD:HM83	2.03	0.41
1:D:285:ALA:O	1:D:289:ILE:HD13	2.20	0.41
1:A:183:SER:O	1:A:187:THR:OG1	2.36	0.41
1:A:255:GLN:HB2	1:A:480:HIS:CD2	2.55	0.41
1:B:409:LEU:O	1:B:410:ASP:HB2	2.21	0.41
1:B:492:ALA:HB2	3:B:602:FAD:H5'2	2.03	0.41
1:C:311:SER:O	1:C:312:LYS:HD3	2.20	0.41
1:D:48:LEU:HD22	1:D:63:ALA:HB3	2.03	0.41
1:A:192:GLN:HA	1:A:192:GLN:HE21	1.86	0.40
1:A:289:ILE:HG13	1:A:290:HIS:N	2.36	0.40
1:A:342:ARG:HD3	1:A:342:ARG:N	2.36	0.40
1:C:60:ASP:OD2	1:C:201:TYR:HB2	2.22	0.40
1:D:388:ARG:HB2	1:D:437:VAL:HB	2.03	0.40
1:B:255:GLN:NE2	1:B:289:ILE:HG13	2.36	0.40
1:C:8:LYS:HA	1:C:245:ASN:O	2.21	0.40
1:D:385:GLU:O	1:D:388:ARG:HD2	2.22	0.40
1:D:42:ASP:O	1:D:219:LEU:HD13	2.21	0.40
1:A:172:GLU:O	1:A:176:GLY:N	2.55	0.40
1:A:423:ASN:OD1	1:A:425:ALA:N	2.55	0.40
1:B:335:GLU:HG3	1:B:339:MET:SD	2.61	0.40
1:C:289:ILE:HD11	1:C:459:PRO:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:353:CYS:HB3	1:D:397:PHE:O	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ARG:NH2	1:C:210:GLN:OE1[2_646]	2.10	0.10
1:A:219:LEU:O	1:C:442:ARG:NH1[2_646]	2.19	0.01

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	498/513 (97%)	452 (91%)	35 (7%)	11 (2%)	6 10
1	B	492/513 (96%)	445 (90%)	34 (7%)	13 (3%)	5 8
1	C	495/513 (96%)	459 (93%)	27 (6%)	9 (2%)	8 14
1	D	490/513 (96%)	445 (91%)	34 (7%)	11 (2%)	6 10
All	All	1975/2052 (96%)	1801 (91%)	130 (7%)	44 (2%)	6 10

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	LEU
1	B	137	SER
1	B	138	ASP
1	B	265	GLU
1	B	424	ILE
1	C	137	SER
1	C	420	PRO
1	D	131	HIS

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Mol	Chain	Res	Type
1	D	132	GLN
1	D	137	SER
1	D	265	GLU
1	D	350	SER
1	D	420	PRO
1	A	133	HIS
1	A	264	PRO
1	B	133	HIS
1	D	136	VAL
1	A	438	SER
1	A	512	HIS
1	B	420	PRO
1	C	136	VAL
1	C	138	ASP
1	C	265	GLU
1	D	421	ILE
1	D	427	ALA
1	A	350	SER
1	A	420	PRO
1	B	134	LEU
1	B	200	ASN
1	B	231	SER
1	B	370	ALA
1	B	508	LYS
1	C	139	CYS
1	C	187	THR
1	D	138	ASP
1	A	137	SER
1	A	265	GLU
1	A	451	SER
1	B	350	SER
1	B	421	ILE
1	C	134	LEU
1	C	200	ASN
1	A	190	GLY
1	D	277	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	442/454 (97%)	426 (96%)	16 (4%)	35	61
1	B	438/454 (96%)	421 (96%)	17 (4%)	32	57
1	C	440/454 (97%)	424 (96%)	16 (4%)	35	61
1	D	436/454 (96%)	416 (95%)	20 (5%)	27	50
All	All	1756/1816 (97%)	1687 (96%)	69 (4%)	32	57

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	VAL
1	A	134	LEU
1	A	140	SER
1	A	146	MET
1	A	179	TRP
1	A	183	SER
1	A	201	TYR
1	A	221	CYS
1	A	239	GLU
1	A	291	PHE
1	A	302	GLU
1	A	342	ARG
1	A	382	ASN
1	A	396	SER
1	A	419	ARG
1	A	467	SER
1	B	87	ARG
1	B	124	LYS
1	B	162	ARG
1	B	179	TRP
1	B	201	TYR
1	B	218	LYS
1	B	220	SER
1	B	238	CYS
1	B	291	PHE
1	B	307	SER
1	B	334	ASP
1	B	393	ARG
1	B	429	LYS
1	B	451	SER

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Mol	Chain	Res	Type
1	B	453	CYS
1	B	467	SER
1	B	479	GLU
1	C	64	SER
1	C	101	ASP
1	C	132	GLN
1	C	138	ASP
1	C	179	TRP
1	C	180	LYS
1	C	189	PHE
1	C	201	TYR
1	C	221	CYS
1	C	268	LEU
1	C	291	PHE
1	C	294	LEU
1	C	342	ARG
1	C	377	GLN
1	C	391	LYS
1	C	506	LEU
1	D	64	SER
1	D	118	VAL
1	D	129	GLU
1	D	179	TRP
1	D	181	LEU
1	D	189	PHE
1	D	201	TYR
1	D	221	CYS
1	D	238	CYS
1	D	242	THR
1	D	307	SER
1	D	321	ASN
1	D	338	SER
1	D	355	SER
1	D	386	SER
1	D	426	ASN
1	D	441	THR
1	D	462	MET
1	D	479	GLU
1	D	501	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	HIS
1	A	192	GLN
1	A	513	HIS
1	B	255	GLN
1	C	55	GLN
1	D	49	GLN
1	D	195	ASN
1	D	290	HIS
1	D	382	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands 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	$\#\|Z\| > 2$
3	FAD	A	602	-	51,58,58	1.19	3 (5%)	60,89,89	2.27	9 (15%)
2	SPM	C	601	-	13,13,13	2.99	11 (84%)	12,12,12	2.31	6 (50%)
2	SPM	B	601	-	13,13,13	2.92	11 (84%)	12,12,12	2.43	6 (50%)
3	FAD	D	602	-	51,58,58	1.22	5 (9%)	60,89,89	2.28	7 (11%)
2	SPM	A	601	-	13,13,13	3.02	11 (84%)	12,12,12	2.25	6 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SPM	D	601	-	13,13,13	2.98	11 (84%)	12,12,12	2.26	6 (50%)
3	FAD	C	602	-	51,58,58	1.24	4 (7%)	60,89,89	2.19	7 (11%)
3	FAD	B	602	-	51,58,58	1.26	3 (5%)	60,89,89	2.42	11 (18%)

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
3	FAD	A	602	-	-	7/30/50/50	0/6/6/6
2	SPM	C	601	-	-	8/11/11/11	-
2	SPM	B	601	-	-	4/11/11/11	-
3	FAD	D	602	-	-	12/30/50/50	0/6/6/6
2	SPM	A	601	-	-	7/11/11/11	-
2	SPM	D	601	-	-	9/11/11/11	-
3	FAD	C	602	-	-	7/30/50/50	0/6/6/6
3	FAD	B	602	-	-	9/30/50/50	0/6/6/6

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	FAD	C4X-C10	5.81	1.44	1.38
3	A	602	FAD	C4X-C10	5.58	1.44	1.38
3	D	602	FAD	C4X-C10	5.30	1.44	1.38
3	C	602	FAD	C4X-C10	5.17	1.44	1.38
2	A	601	SPM	C4-N5	-4.25	1.32	1.46
2	B	601	SPM	C4-N5	-4.22	1.32	1.46
2	A	601	SPM	C9-N10	-4.15	1.33	1.46
2	D	601	SPM	C6-N5	-4.10	1.33	1.46
2	C	601	SPM	C11-N10	-4.09	1.33	1.46
2	D	601	SPM	C11-N10	-4.08	1.33	1.46
2	C	601	SPM	C4-N5	-4.07	1.33	1.46
2	A	601	SPM	C6-N5	-4.07	1.33	1.46
2	D	601	SPM	C4-N5	-4.06	1.33	1.46
2	C	601	SPM	C9-N10	-3.99	1.33	1.46
2	C	601	SPM	C6-N5	-3.96	1.33	1.46
2	B	601	SPM	C6-N5	-3.88	1.34	1.46
2	D	601	SPM	C9-N10	-3.83	1.34	1.46
2	B	601	SPM	C9-N10	-3.72	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	SPM	C11-N10	-3.68	1.34	1.46
2	A	601	SPM	C11-N10	-3.66	1.34	1.46
3	C	602	FAD	C4X-N5	-3.50	1.28	1.33
3	B	602	FAD	C4X-N5	-3.46	1.28	1.33
3	D	602	FAD	C4-N3	3.34	1.38	1.33
3	B	602	FAD	C4-N3	3.11	1.38	1.33
2	B	601	SPM	C3-C4	-3.05	1.39	1.51
2	A	601	SPM	C7-C6	-3.02	1.39	1.51
2	A	601	SPM	C8-C9	-2.96	1.39	1.51
2	C	601	SPM	C12-C11	-2.93	1.39	1.51
2	D	601	SPM	C12-C11	-2.92	1.39	1.51
2	C	601	SPM	C7-C6	-2.85	1.39	1.51
2	C	601	SPM	C3-C4	-2.85	1.39	1.51
2	A	601	SPM	C3-C4	-2.84	1.39	1.51
2	C	601	SPM	C8-C9	-2.82	1.40	1.51
2	D	601	SPM	C8-C9	-2.81	1.40	1.51
2	B	601	SPM	C7-C6	-2.80	1.40	1.51
2	D	601	SPM	C7-C6	-2.77	1.40	1.51
2	D	601	SPM	C3-C4	-2.73	1.40	1.51
2	A	601	SPM	C12-C11	-2.65	1.40	1.51
3	C	602	FAD	C4-N3	2.60	1.37	1.33
2	B	601	SPM	C8-C9	-2.57	1.41	1.51
3	A	602	FAD	C4-N3	2.57	1.37	1.33
2	B	601	SPM	C3-C2	-2.52	1.39	1.51
2	B	601	SPM	C12-C11	-2.50	1.41	1.51
2	C	601	SPM	C12-C13	-2.39	1.40	1.51
2	D	601	SPM	C12-C13	-2.34	1.40	1.51
2	D	601	SPM	C3-C2	-2.31	1.40	1.51
3	D	602	FAD	C4-C4X	2.31	1.45	1.41
2	A	601	SPM	C12-C13	-2.31	1.40	1.51
2	B	601	SPM	C12-C13	-2.30	1.40	1.51
2	A	601	SPM	C3-C2	-2.30	1.40	1.51
3	D	602	FAD	C5X-N5	2.28	1.39	1.35
3	A	602	FAD	C9A-N10	2.24	1.41	1.38
3	C	602	FAD	P-O2P	-2.22	1.44	1.55
2	C	601	SPM	C3-C2	-2.19	1.40	1.51
2	A	601	SPM	C8-C7	-2.16	1.39	1.51
2	C	601	SPM	C8-C7	-2.10	1.39	1.51
2	D	601	SPM	C8-C7	-2.06	1.40	1.51
3	D	602	FAD	C9A-N10	2.03	1.41	1.38
2	B	601	SPM	C8-C7	-2.03	1.40	1.51

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	FAD	C4-N3-C2	13.16	126.25	115.14
3	D	602	FAD	C4-N3-C2	13.04	126.15	115.14
3	A	602	FAD	C4-N3-C2	12.96	126.08	115.14
3	C	602	FAD	C4-N3-C2	12.45	125.65	115.14
3	D	602	FAD	C4X-C4-N3	-7.18	113.60	123.43
3	B	602	FAD	C4X-C4-N3	-6.99	113.87	123.43
3	C	602	FAD	C4X-C4-N3	-6.74	114.21	123.43
3	A	602	FAD	C4X-C4-N3	-6.67	114.31	123.43
3	B	602	FAD	C10-C4X-N5	5.40	124.99	121.26
3	C	602	FAD	C10-C4X-N5	5.03	124.73	121.26
3	A	602	FAD	C10-C4X-N5	5.01	124.72	121.26
3	D	602	FAD	C10-C4X-N5	4.65	124.47	121.26
2	B	601	SPM	C8-C9-N10	4.51	124.31	112.14
3	D	602	FAD	C4-C4X-C10	-3.98	117.32	119.95
2	A	601	SPM	C7-C6-N5	3.95	122.79	112.14
3	A	602	FAD	C4-C4X-C10	-3.81	117.43	119.95
3	B	602	FAD	O5B-PA-O1A	3.80	123.90	109.07
3	B	602	FAD	C4X-C10-N10	-3.78	116.42	120.30
2	C	601	SPM	C12-C11-N10	3.77	122.32	112.14
3	C	602	FAD	C4-C4X-C10	-3.72	117.49	119.95
2	D	601	SPM	C12-C11-N10	3.64	121.96	112.14
2	B	601	SPM	C7-C6-N5	3.58	121.81	112.14
3	A	602	FAD	C4X-C10-N10	-3.55	116.66	120.30
3	D	602	FAD	C1'-N10-C9A	3.50	121.04	118.29
2	D	601	SPM	C7-C6-N5	3.47	121.50	112.14
3	C	602	FAD	C4X-C10-N10	-3.45	116.75	120.30
2	A	601	SPM	C12-C11-N10	3.45	121.45	112.14
2	B	601	SPM	C12-C11-N10	3.45	121.44	112.14
3	B	602	FAD	C4-C4X-C10	-3.43	117.68	119.95
3	C	602	FAD	C1'-N10-C9A	3.34	120.92	118.29
3	D	602	FAD	C4X-C10-N10	-3.32	116.89	120.30
2	D	601	SPM	C3-C4-N5	3.24	120.89	112.14
2	C	601	SPM	C8-C9-N10	3.22	120.83	112.14
2	C	601	SPM	C7-C6-N5	3.22	120.83	112.14
2	A	601	SPM	C8-C9-N10	3.17	120.70	112.14
3	A	602	FAD	C1'-N10-C9A	3.12	120.75	118.29
3	B	602	FAD	C1'-N10-C9A	3.07	120.71	118.29
2	D	601	SPM	C8-C9-N10	3.03	120.32	112.14
2	C	601	SPM	C3-C4-N5	2.89	119.94	112.14
3	B	602	FAD	O2A-PA-O5B	-2.83	94.62	107.75
2	B	601	SPM	C3-C4-N5	2.82	119.75	112.14
2	A	601	SPM	C3-C4-N5	2.44	118.72	112.14
3	A	602	FAD	O5'-P-O1P	-2.39	99.74	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	SPM	C11-C12-C13	2.38	122.99	114.28
3	B	602	FAD	C5A-C6A-N6A	2.36	123.94	120.35
2	C	601	SPM	C4-C3-C2	2.34	122.84	114.28
2	B	601	SPM	C11-C12-C13	2.31	122.73	114.28
2	A	601	SPM	C4-C3-C2	2.28	122.64	114.28
3	A	602	FAD	C5A-C6A-N6A	2.20	123.70	120.35
3	D	602	FAD	C5A-C6A-N6A	2.17	123.65	120.35
3	B	602	FAD	O5B-C5B-C4B	-2.08	101.82	108.99
2	B	601	SPM	C8-C7-C6	2.05	123.27	113.56
2	C	601	SPM	C11-C12-C13	2.05	121.78	114.28
3	A	602	FAD	O2P-P-O5'	2.04	117.20	107.75
3	C	602	FAD	C5A-C6A-N6A	2.03	123.44	120.35
2	D	601	SPM	C4-C3-C2	2.01	121.63	114.28
2	D	601	SPM	C7-C8-C9	2.01	123.06	113.56
3	B	602	FAD	O4B-C1B-C2B	-2.00	104.00	106.93

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	FAD	C5B-O5B-PA-O1A
3	B	602	FAD	O4'-C4'-C5'-O5'
3	B	602	FAD	C5'-O5'-P-O1P
3	B	602	FAD	C5'-O5'-P-O2P
3	D	602	FAD	C3'-C4'-C5'-O5'
3	D	602	FAD	C5'-O5'-P-O1P
3	D	602	FAD	C5'-O5'-P-O2P
3	D	602	FAD	C5'-O5'-P-O3P
2	A	601	SPM	C7-C6-N5-C4
3	D	602	FAD	O3'-C3'-C4'-O4'
3	D	602	FAD	C2'-C3'-C4'-O4'
2	B	601	SPM	C2-C3-C4-N5
2	B	601	SPM	C7-C8-C9-N10
2	D	601	SPM	C7-C8-C9-N10
2	A	601	SPM	C2-C3-C4-N5
2	C	601	SPM	C2-C3-C4-N5
2	C	601	SPM	C8-C9-N10-C11
2	D	601	SPM	C8-C9-N10-C11
2	D	601	SPM	C12-C11-N10-C9
3	B	602	FAD	O4B-C4B-C5B-O5B
3	B	602	FAD	C3B-C4B-C5B-O5B
2	D	601	SPM	N10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
3	D	602	FAD	O3'-C3'-C4'-C5'
3	D	602	FAD	C2'-C3'-C4'-C5'
2	A	601	SPM	C8-C9-N10-C11
2	C	601	SPM	C12-C11-N10-C9
3	A	602	FAD	C2'-C3'-C4'-O4'
3	C	602	FAD	C2'-C3'-C4'-O4'
2	A	601	SPM	C7-C8-C9-N10
3	D	602	FAD	O4'-C4'-C5'-O5'
2	A	601	SPM	C11-C12-C13-N14
2	C	601	SPM	N1-C2-C3-C4
2	D	601	SPM	C11-C12-C13-N14
2	A	601	SPM	N10-C11-C12-C13
3	B	602	FAD	C3'-C4'-C5'-O5'
2	B	601	SPM	C3-C4-N5-C6
2	D	601	SPM	C6-C7-C8-C9
3	A	602	FAD	O3'-C3'-C4'-O4'
2	C	601	SPM	C7-C6-N5-C4
3	A	602	FAD	C2'-C3'-C4'-C5'
3	A	602	FAD	PA-O3P-P-O5'
3	B	602	FAD	PA-O3P-P-O5'
2	C	601	SPM	C3-C4-N5-C6
2	D	601	SPM	N1-C2-C3-C4
3	C	602	FAD	C5'-O5'-P-O3P
3	C	602	FAD	O3'-C3'-C4'-O4'
2	B	601	SPM	C6-C7-C8-C9
3	D	602	FAD	C5B-O5B-PA-O1A
2	C	601	SPM	C6-C7-C8-C9
2	D	601	SPM	C7-C6-N5-C4
3	C	602	FAD	C2'-C3'-C4'-C5'
2	D	601	SPM	C3-C4-N5-C6
3	D	602	FAD	O4B-C4B-C5B-O5B
2	C	601	SPM	C11-C12-C13-N14
3	A	602	FAD	O3'-C3'-C4'-C5'
3	C	602	FAD	O3'-C3'-C4'-C5'
3	B	602	FAD	C5'-O5'-P-O3P
3	D	602	FAD	C5B-O5B-PA-O3P
3	A	602	FAD	P-O3P-PA-O2A
2	A	601	SPM	C3-C4-N5-C6
3	C	602	FAD	C3'-C4'-C5'-O5'
3	A	602	FAD	O4B-C4B-C5B-O5B
3	C	602	FAD	O4B-C4B-C5B-O5B

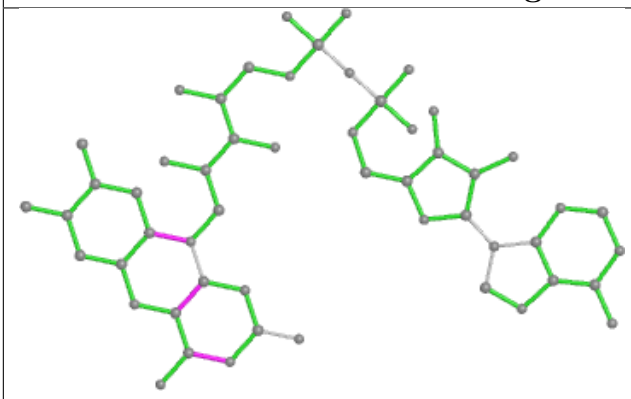
There are no ring outliers.

8 monomers are involved in 34 short contacts:

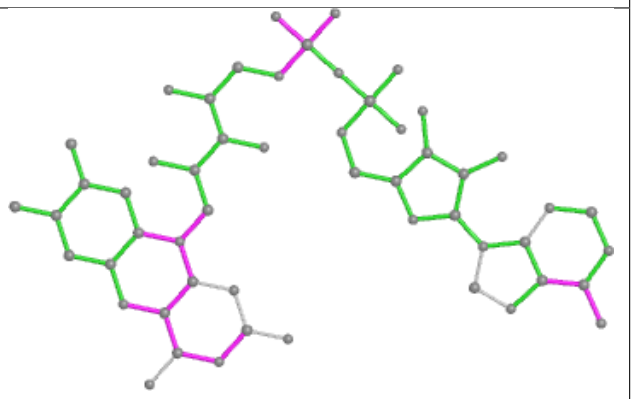
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	FAD	3	0
2	C	601	SPM	2	0
2	B	601	SPM	2	0
3	D	602	FAD	5	0
2	A	601	SPM	6	0
2	D	601	SPM	7	0
3	C	602	FAD	2	0
3	B	602	FAD	9	0

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.

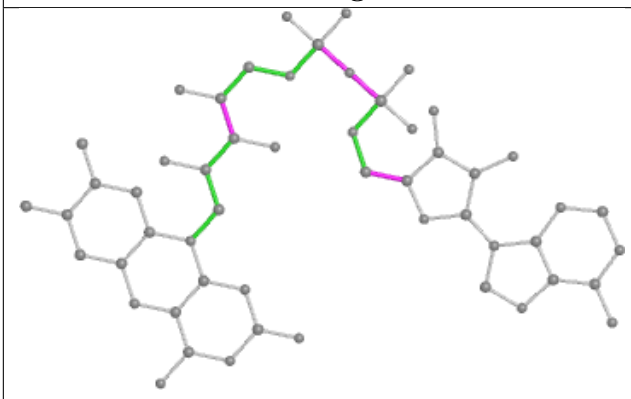
Ligand FAD A 602



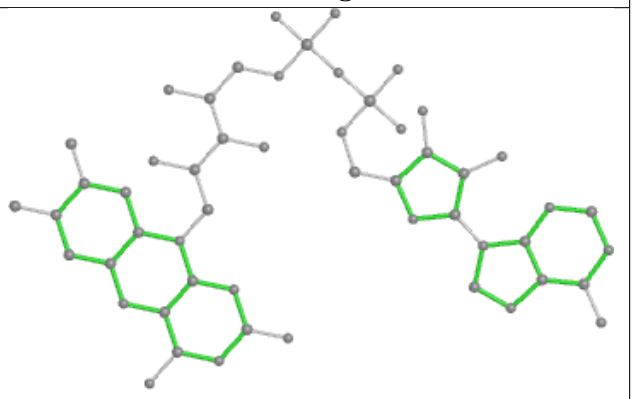
Bond lengths



Bond angles

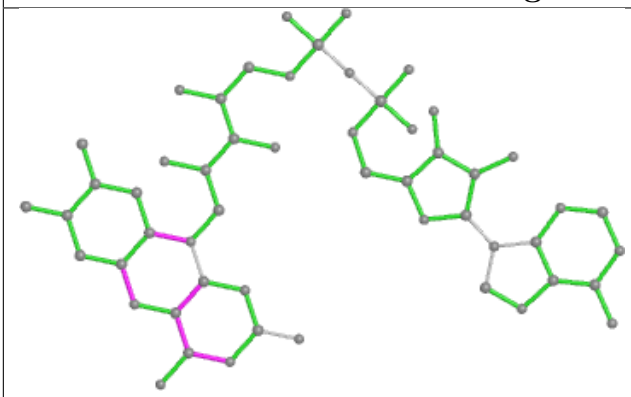


Torsions

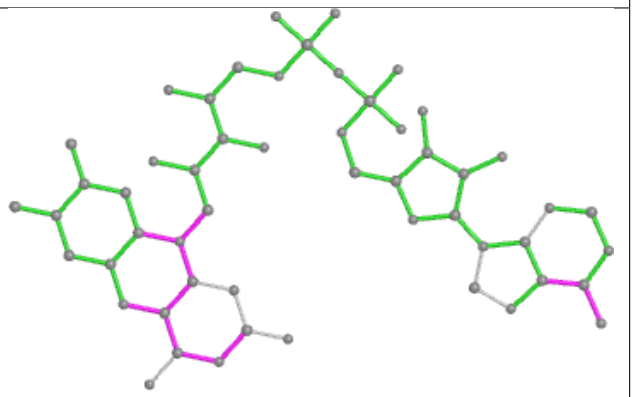


Rings

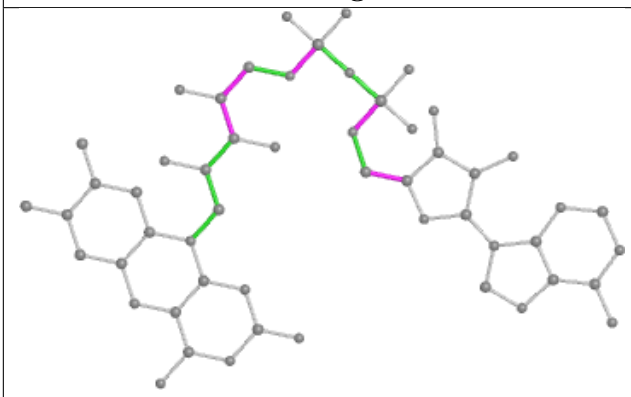
Ligand FAD D 602



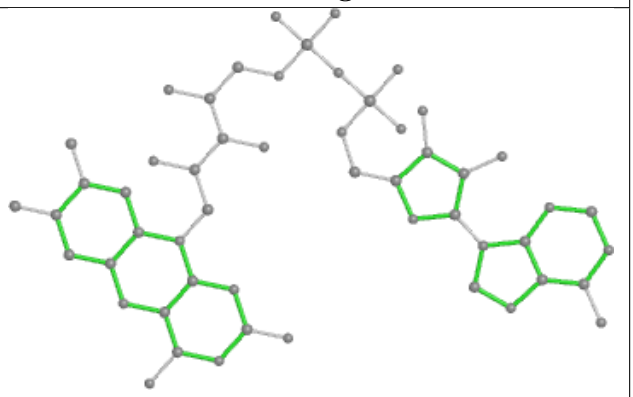
Bond lengths



Bond angles

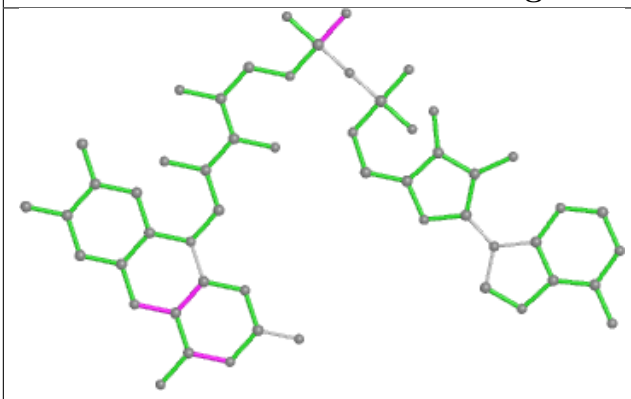


Torsions

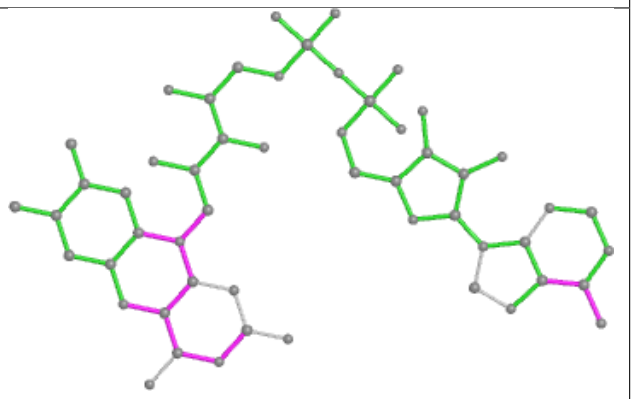


Rings

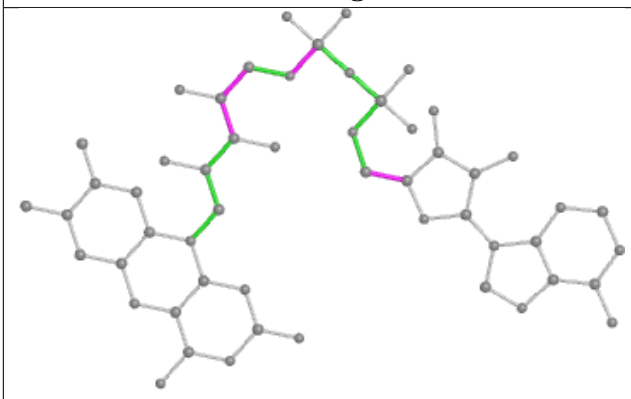
Ligand FAD C 602



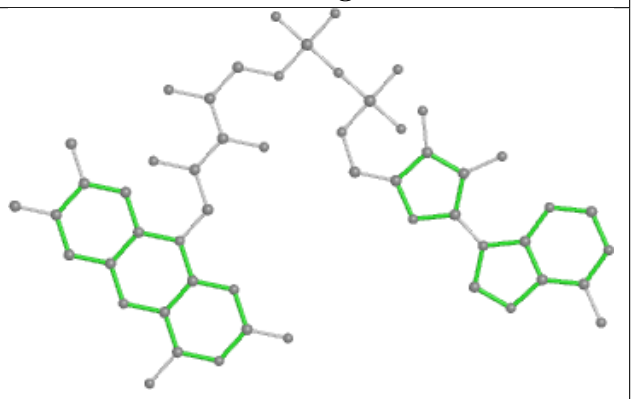
Bond lengths



Bond angles

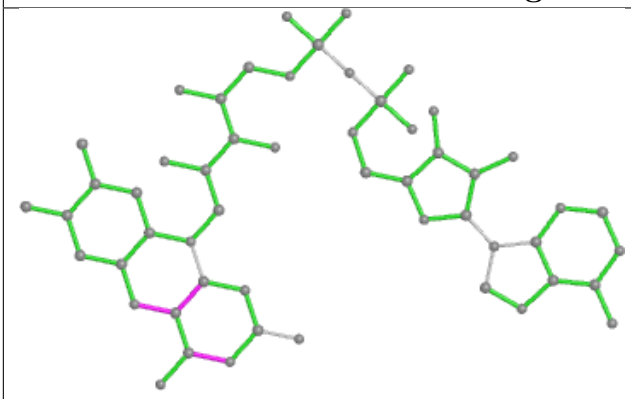


Torsions

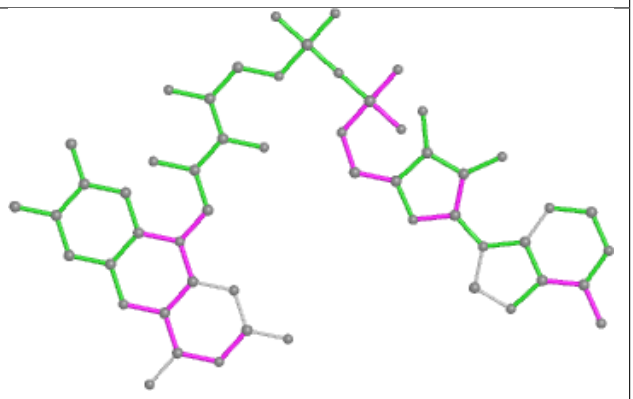


Rings

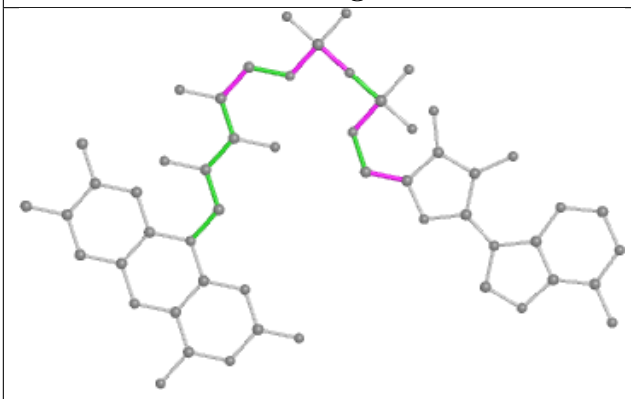
Ligand FAD B 602



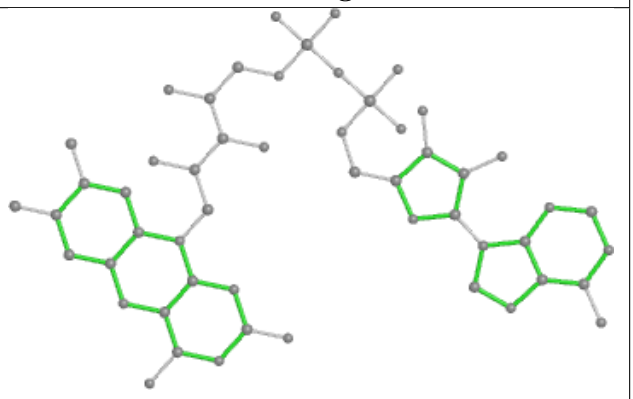
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	502/513 (97%)	-0.26	14 (2%)	53	56	31, 46, 73, 108	20 (3%)
1	B	496/513 (96%)	-0.26	12 (2%)	59	62	35, 46, 74, 99	33 (6%)
1	C	499/513 (97%)	-0.26	8 (1%)	72	74	31, 46, 72, 87	33 (6%)
1	D	494/513 (96%)	-0.15	19 (3%)	40	43	32, 50, 79, 105	33 (6%)
All	All	1991/2052 (97%)	-0.23	53 (2%)	54	58	31, 47, 75, 108	119 (5%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	424	ILE	6.0
1	A	424	ILE	5.8
1	B	135	GLY	4.7
1	A	421	ILE	4.5
1	B	267	ASN	4.4
1	A	423	ASN	4.4
1	D	230	PRO	4.4
1	B	425	ALA	4.2
1	D	231	SER	4.1
1	D	134	LEU	4.0
1	B	424	ILE	4.0
1	D	423	ASN	4.0
1	A	425	ALA	4.0
1	D	425	ALA	4.0
1	D	426	ASN	3.9
1	A	513	HIS	3.8
1	B	421	ILE	3.6
1	C	423	ASN	3.6
1	C	425	ALA	3.4
1	A	426	ASN	3.4
1	D	232	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	136	VAL	3.2
1	A	422	GLU	2.9
1	A	511	HIS	2.9
1	D	289	ILE	2.9
1	D	454	PHE	2.8
1	B	189	PHE	2.8
1	A	419	ARG	2.7
1	D	133	HIS	2.7
1	C	419	ARG	2.7
1	A	262	VAL	2.6
1	B	426	ASN	2.5
1	B	136	VAL	2.5
1	D	189	PHE	2.4
1	A	133	HIS	2.4
1	C	415	ILE	2.4
1	D	419	ARG	2.4
1	C	424	ILE	2.3
1	C	420	PRO	2.3
1	B	231	SER	2.3
1	C	507	LEU	2.2
1	A	420	PRO	2.2
1	D	245	ASN	2.2
1	D	150	LEU	2.1
1	D	130	PHE	2.1
1	A	339	MET	2.1
1	D	420	PRO	2.1
1	A	6	PRO	2.1
1	C	421	ILE	2.1
1	B	334	ASP	2.0
1	D	456	GLY	2.0
1	B	288	LYS	2.0
1	B	423	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

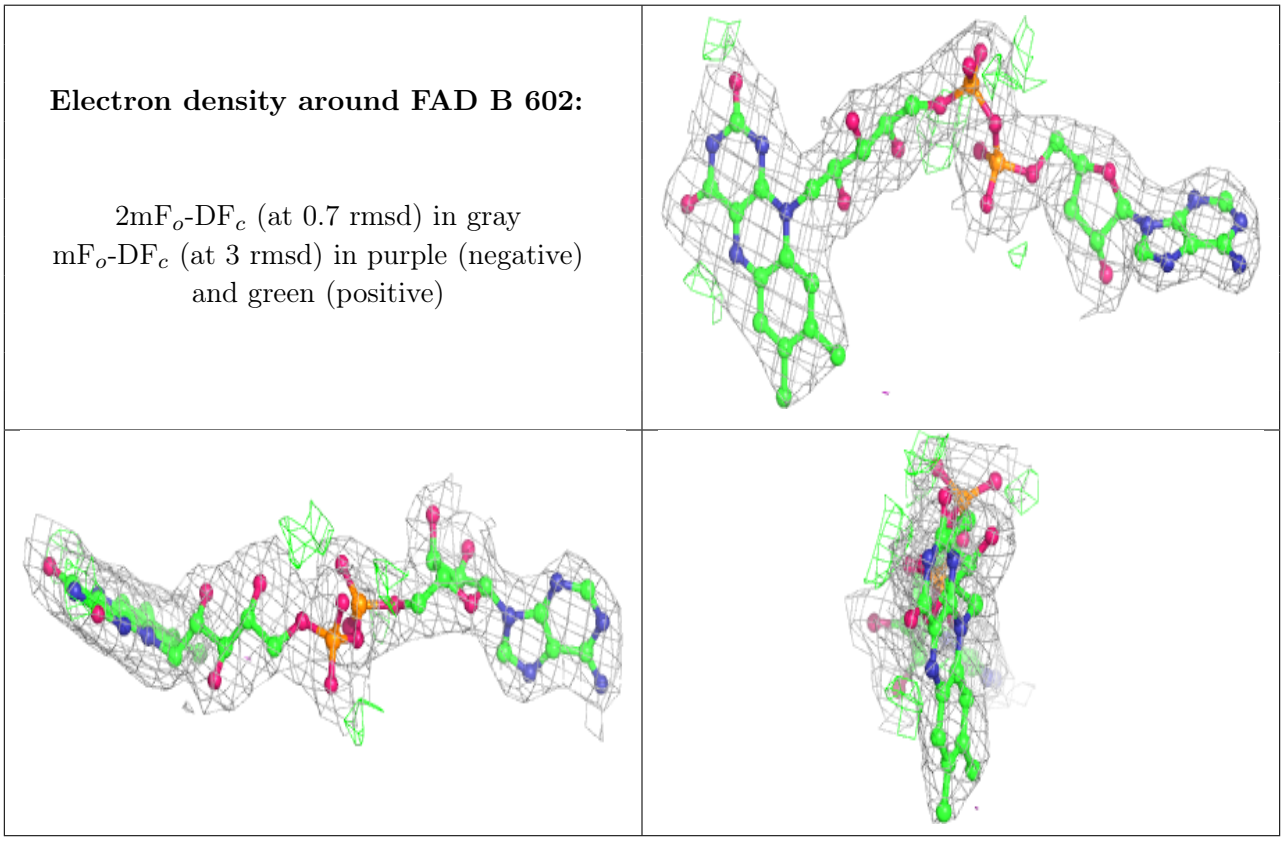
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SPM	D	601	14/14	0.85	0.23	51,57,60,62	0
2	SPM	B	601	14/14	0.89	0.19	44,49,54,62	0
2	SPM	A	601	14/14	0.90	0.22	44,52,61,62	0
2	SPM	C	601	14/14	0.92	0.22	38,54,57,58	0
3	FAD	B	602	53/53	0.96	0.12	33,42,52,54	0
3	FAD	D	602	53/53	0.97	0.13	34,42,54,57	0
3	FAD	C	602	53/53	0.98	0.15	31,38,45,46	0
3	FAD	A	602	53/53	0.98	0.14	32,40,44,46	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.

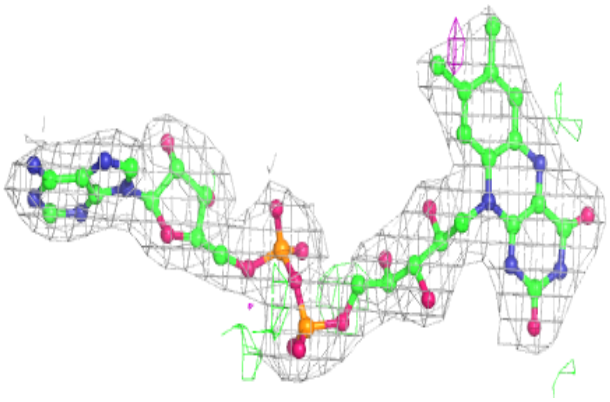
Electron density around FAD B 602:

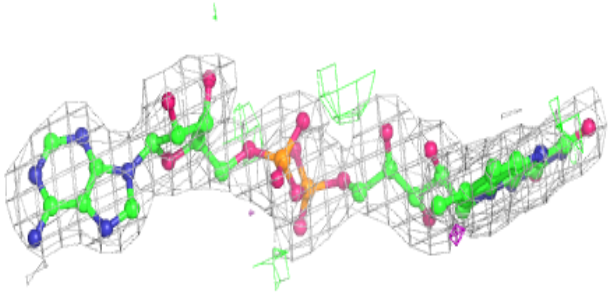
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

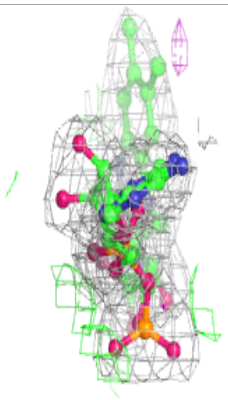


Electron density around FAD D 602:

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

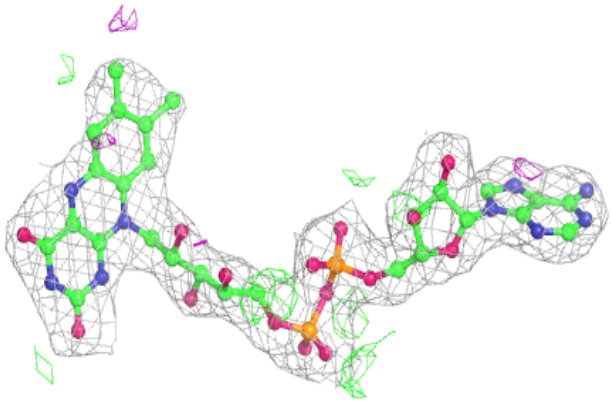


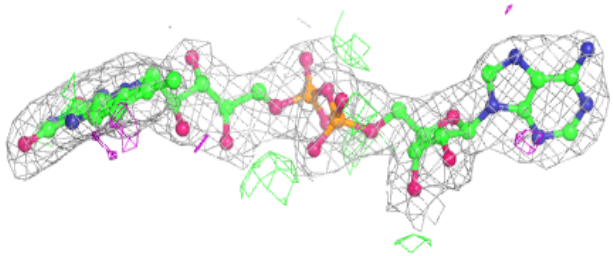


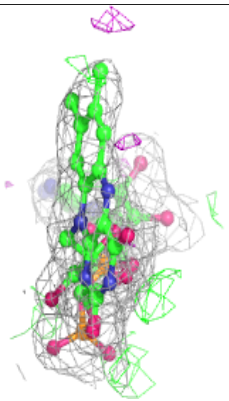


Electron density around FAD C 602:

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

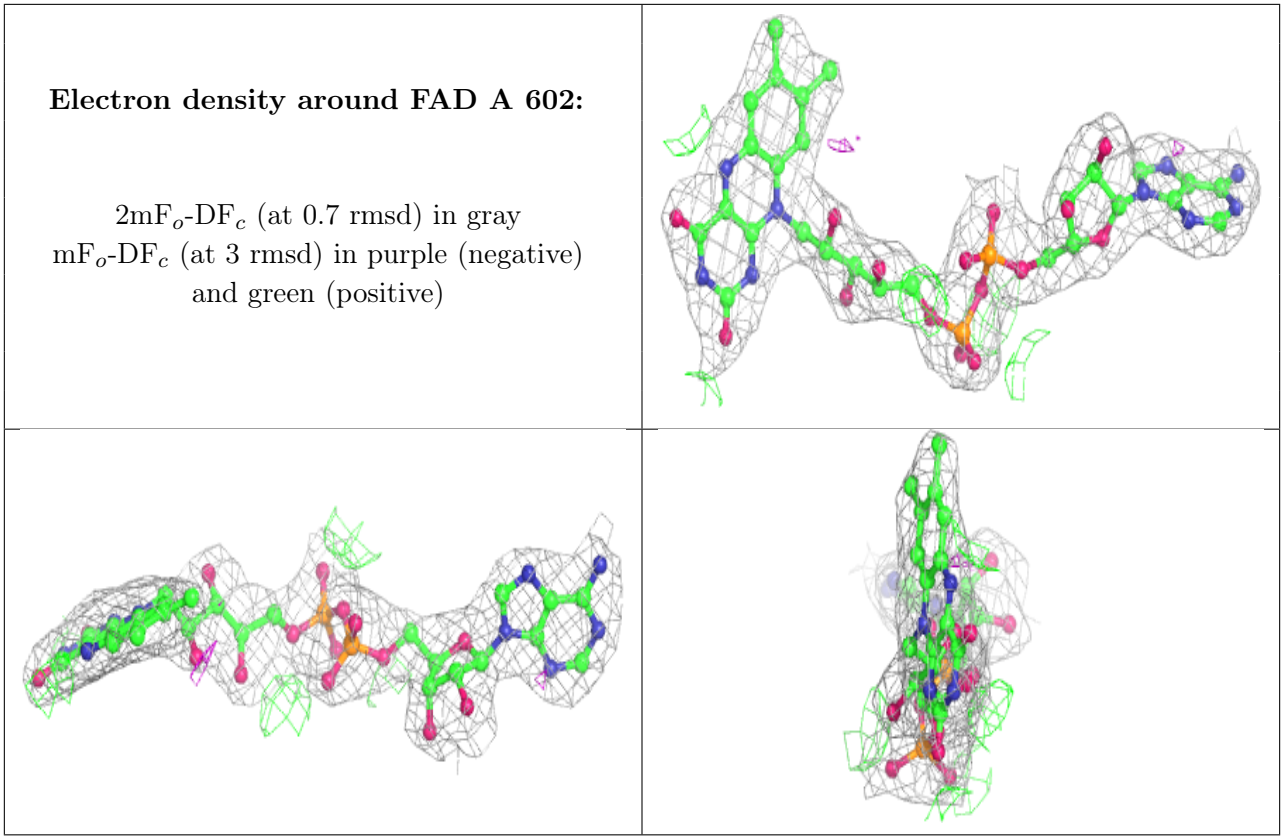






Electron density around FAD A 602:

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



6.5 Other polymers (i)

There are no such residues in this entry.