Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2020 – 04:43 pm BST

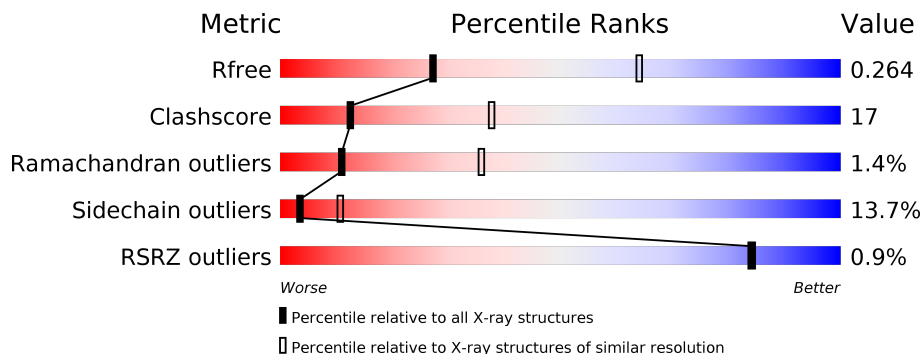|		
PDB ID	:	1T9G
Title	:	Structure of the human MCAD:ETF complex
Authors	:	Toogood, H.S.; van Thiel, A.; Basran, J.; Sutcliffe, M.J.; Scrutton, N.S.; Leys, D.
Deposited on	:	2004-05-17
Resolution	:	2.90 Å(reported)

---

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.90 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	Percentile Ranks	Value
Rfree		0.264
Clashscore		17
Ramachandran outliers		1.4%
Sidechain outliers		13.7%
RSRZ outliers		0.9%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	396	66% 26% 6% ••
1	B	396	% 62% 30% 6% ••
1	C	396	65% 27% 6% ••
1	D	396	61% 30% 6% ••
2	R	333	% 35% 18% • 45%
3	S	255	3% 54% 29% 5% • 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14998 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 Acyl-CoA dehydrogenase, medium-chain specific, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			2929	1859	495	557	18			
1	B	387	Total	C	N	O	S	0	0	0
			2930	1857	496	559	18			
1	C	388	Total	C	N	O	S	0	0	0
			2951	1870	507	556	18			
1	D	387	Total	C	N	O	S	0	0	0
			2957	1872	507	560	18			

- Molecule 2 is a protein called Electron transfer flavoprotein alpha-subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	184	Total	C	N	O	S	0	0	0
			1323	835	221	261	6			

- Molecule 3 is a protein called Electron transfer flavoprotein beta-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	228	Total	C	N	O	S	0	0	0
			1673	1062	282	321	8			

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

FAD

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

• Molecule 5 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).

AMP
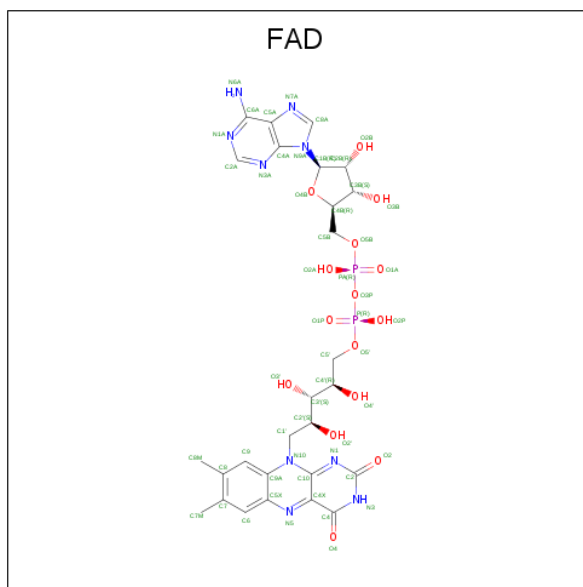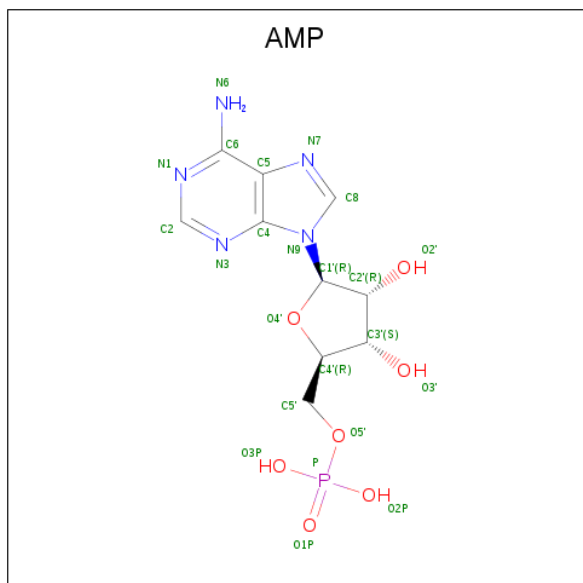
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	S	1	23	10	5	7	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Acyl-CoA dehydrogenase, medium-chain specific, mitochondrial
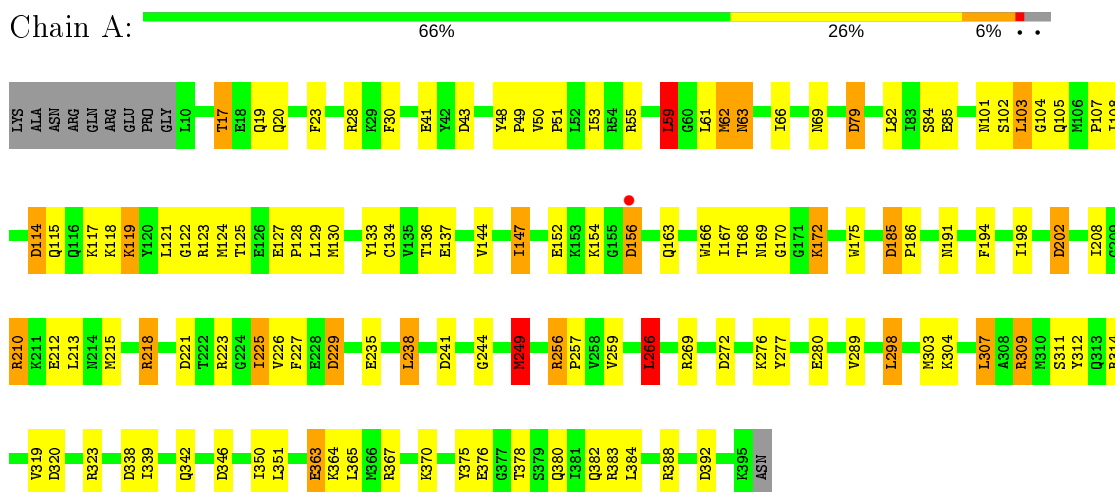
• Molecule 1: Acyl-CoA dehydrogenase, medium-chain specific, mitochondrial

• Molecule 1: Acyl-CoA dehydrogenase, medium-chain specific, mitochondrial

Chain C: 65% 27% 6%

• Molecule 1: Acyl-CoA dehydrogenase, medium-chain specific, mitochondrial

Chain D: 61% 30% 6%

• Molecule 2: Electron transfer flavoprotein alpha-subunit, mitochondrial

Chain R: % 35% 18% 45%
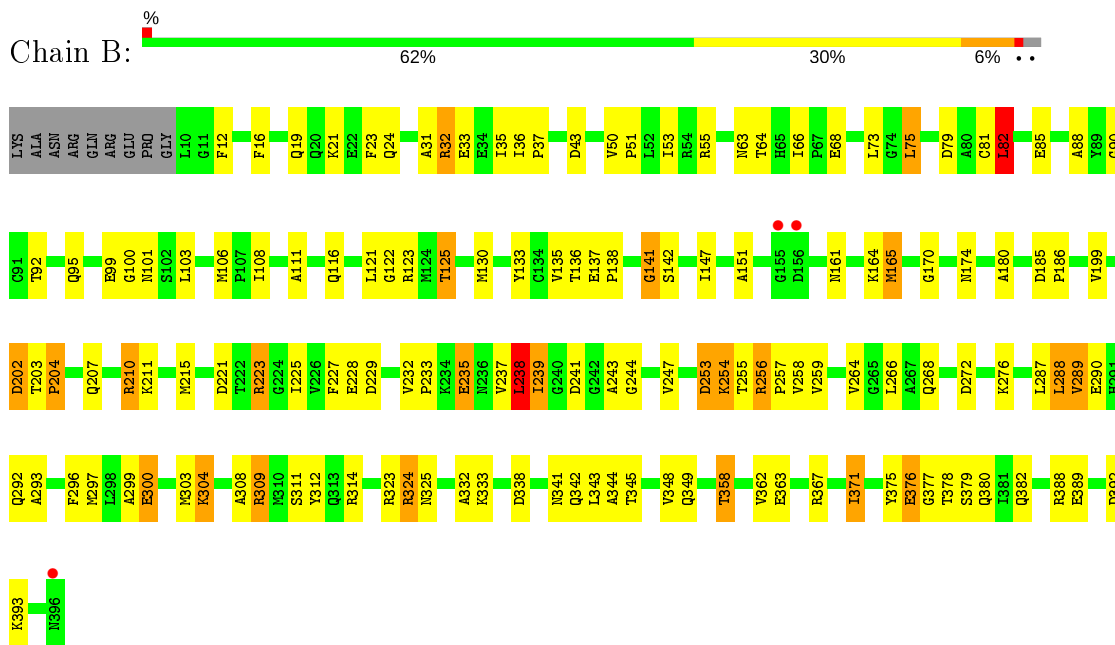
VAL ALA ASP LEU PHE LYS VAL VAL PRO GLU MET THR GLU ILE LEU LYS LYS LYS

• Molecule 3: Electron transfer flavoprotein beta-subunit

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	94.33Å 101.32Å 244.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.90) 98.3 (20.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$<I/\sigma(I)>$ [1]	2.47 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.191 , 0.263 0.191 , 0.264	Depositor DCC
R_{free} test set	2614 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å²)	52.6	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.32 , 35.9	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	0.93	EDS
Total number of atoms	14998	wwPDB-VP
Average B, all atoms (Å²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, 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	0.96	0/2984	1.06	17/4036 (0.4%)
1	B	0.94	0/2985	1.03	9/4039 (0.2%)
1	C	0.93	0/3006	1.07	9/4062 (0.2%)
1	D	0.97	1/3012 (0.0%)	1.06	13/4067 (0.3%)
2	R	0.75	1/1342 (0.1%)	0.94	2/1832 (0.1%)
3	S	0.79	0/1694	1.02	8/2306 (0.3%)
All	All	0.92	2/15023 (0.0%)	1.04	58/20342 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
3	S	0	3
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	305	VAL	CB-CG2	-6.23	1.39	1.52
2	R	158	LYS	CG-CD	5.37	1.70	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	C	338	ASP	CB-CG-OD1	8.26	125.73	118.30
1	D	392	ASP	CB-CG-OD2	8.21	125.69	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	ASP	CB-CG-OD2	8.14	125.63	118.30
1	D	202	ASP	CB-CG-OD2	7.65	125.19	118.30
1	B	202	ASP	CB-CG-OD2	7.57	125.11	118.30
1	C	221	ASP	CB-CG-OD2	7.41	124.97	118.30
1	C	266	LEU	CA-CB-CG	7.18	131.81	115.30
1	C	320	ASP	CB-CG-OD2	7.16	124.75	118.30
1	A	269	ARG	NE-CZ-NH2	-7.15	116.72	120.30
3	S	167	ASP	CB-CG-OD2	7.10	124.69	118.30
1	A	79	ASP	CB-CG-OD2	7.05	124.64	118.30
1	A	338	ASP	CB-CG-OD2	7.00	124.60	118.30
1	D	266	LEU	CA-CB-CG	6.80	130.95	115.30
1	D	28	ARG	NE-CZ-NH1	-6.69	116.95	120.30
2	R	66	ASP	CB-CG-OD2	6.66	124.29	118.30
3	S	15	ASP	CB-CG-OD2	6.40	124.06	118.30
1	D	229	ASP	CB-CG-OD2	6.36	124.02	118.30
1	D	79	ASP	CB-CG-OD2	6.35	124.01	118.30
1	B	79	ASP	CB-CG-OD1	6.31	123.98	118.30
1	D	28	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	D	178	LEU	CA-CB-CG	6.13	129.41	115.30
3	S	143	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	202	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	43	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	249	MET	CG-SD-CE	6.10	109.96	100.20
1	C	272	ASP	CB-CG-OD2	6.08	123.77	118.30
2	R	174	ASP	CB-CG-OD2	5.98	123.68	118.30
1	B	309	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	C	43	ASP	CB-CG-OD2	5.87	123.58	118.30
3	S	178	PRO	N-CD-CG	-5.86	94.42	103.20
1	B	338	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	253	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	309	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	114	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	238	LEU	CA-CB-CG	-5.75	102.07	115.30
1	C	229	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	156	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	241	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	388	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	C	221	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	A	229	ASP	CB-CG-OD2	5.50	123.25	118.30
3	S	177	LEU	N-CA-C	5.40	125.58	111.00
3	S	213	ASP	CB-CG-OD2	5.35	123.12	118.30
1	B	43	ASP	CB-CG-OD2	5.33	123.10	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	59	LEU	CA-CB-CG	5.31	127.51	115.30
1	D	221	ASP	CB-CG-OD2	5.28	123.05	118.30
1	C	368	ASP	CB-CG-OD1	5.28	123.05	118.30
1	D	179	LEU	CA-CB-CG	5.23	127.33	115.30
1	B	82	LEU	CB-CG-CD2	-5.21	102.14	111.00
1	B	309	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	D	241	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	266	LEU	CA-CB-CG	5.14	127.13	115.30
3	S	25	ASP	CB-CG-OD2	5.13	122.91	118.30
3	S	32	ASP	CB-CG-OD2	5.12	122.90	118.30
1	A	28	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	D	54	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	D	185	ASP	CB-CG-OD2	5.04	122.83	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	324	ARG	Peptide
3	S	176	LYS	Peptide
3	S	177	LEU	Peptide
3	S	230	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2929	0	2844	96	0
1	B	2930	0	2826	104	0
1	C	2951	0	2888	96	0
1	D	2957	0	2895	101	0
2	R	1323	0	1320	50	0
3	S	1673	0	1694	88	0
4	A	53	0	31	9	0
4	B	53	0	31	5	0
4	C	53	0	31	2	0
4	D	53	0	31	8	0

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	S	23	0	12	4	0
All	All	14998	0	14603	496	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 17.

All (496) 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)
4:A:399:FAD:N10	4:A:399:FAD:C1'	1.78	1.47
1:A:124:MET:CE	1:A:175:TRP:HE1	1.63	1.11
1:A:363:GLU:HG3	1:B:215:MET:HB2	1.24	1.09
3:S:194:THR:HG22	3:S:196:PRO:HD2	1.06	1.02
3:S:7:LEU:HD11	3:S:64:VAL:CG1	1.90	1.01
1:B:378:THR:HG21	4:B:399:FAD:O2B	1.60	1.00
3:S:64:VAL:HG21	3:S:108:LEU:HD21	1.39	1.00
3:S:7:LEU:HD11	3:S:64:VAL:HG13	1.41	0.99
3:S:4:LEU:HD11	3:S:155:LEU:HD21	1.46	0.95
3:S:194:THR:CG2	3:S:196:PRO:HD2	1.97	0.94
1:D:54:ARG:HH11	1:D:54:ARG:HG2	1.31	0.94
2:R:110:ALA:HB3	2:R:120:LEU:HD11	1.51	0.93
1:A:124:MET:HE3	1:A:175:TRP:HE1	1.32	0.93
3:S:194:THR:HG22	3:S:196:PRO:CD	1.97	0.93
3:S:64:VAL:HG21	3:S:108:LEU:CD2	2.00	0.92
1:B:378:THR:HG22	1:B:380:GLN:H	1.35	0.91
1:D:304:LYS:HE2	1:D:342:GLN:NE2	1.86	0.90
1:A:108:ILE:HD11	1:A:198:ILE:HG12	1.52	0.90
1:A:124:MET:HE1	1:A:175:TRP:HE1	1.35	0.89
3:S:158:ASP:O	3:S:177:LEU:HB2	1.72	0.89
1:C:213:LEU:O	1:D:358:THR:HB	1.73	0.89
1:B:256:ARG:CG	1:B:256:ARG:HH11	1.86	0.89
3:S:106:ARG:HH11	3:S:106:ARG:HG2	1.37	0.89
1:C:256:ARG:HH11	1:C:256:ARG:HG3	1.38	0.88
2:R:199:TRP:HZ2	2:R:202:GLN:HG3	1.40	0.86
1:D:73:LEU:HG	3:S:199:MET:CE	2.06	0.85
1:D:304:LYS:HE2	1:D:342:GLN:HE21	1.42	0.85
1:B:24:GLN:HB2	1:B:82:LEU:HD11	1.59	0.84
1:A:17:THR:HG22	1:A:20:GLN:H	1.43	0.83
2:R:147:THR:HB	2:R:151:GLY:HA2	1.60	0.83
3:S:14:ILE:HD12	3:S:14:ILE:H	1.43	0.82
1:A:79:ASP:HA	1:A:82:LEU:HD12	1.61	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:LYS:HG2	3:S:192:TYR:HE1	1.45	0.81
3:S:106:ARG:NH1	3:S:106:ARG:HG2	1.95	0.81
1:B:256:ARG:HG2	1:B:256:ARG:HH11	1.45	0.80
1:B:16:PHE:HE2	1:B:82:LEU:HD13	1.46	0.80
1:A:249:MET:HA	1:A:249:MET:HE2	1.62	0.79
1:C:161:ASN:ND2	1:C:229:ASP:H	1.80	0.79
1:A:123:ARG:CG	1:A:124:MET:HE2	2.13	0.78
1:C:281:ARG:NH1	4:D:399:FAD:O2A	2.15	0.78
1:D:19:GLN:NE2	3:S:199:MET:HG2	1.99	0.78
1:B:311:SER:OG	1:B:332:ALA:HA	1.84	0.77
1:A:124:MET:HE1	1:A:175:TRP:NE1	1.98	0.77
3:S:64:VAL:CG2	3:S:108:LEU:HD21	2.15	0.77
3:S:132:ASN:ND2	3:S:136:GLN:HE22	1.84	0.76
2:R:36:ILE:HA	2:R:39:ASN:ND2	2.01	0.76
2:R:122:ARG:HH11	3:S:146:GLN:NE2	1.82	0.76
1:B:32:ARG:HH11	1:B:32:ARG:CG	1.99	0.76
1:A:364:LYS:HA	1:A:367:ARG:NH1	2.02	0.75
1:D:29:LYS:HG2	3:S:192:TYR:CE1	2.21	0.75
3:S:28:GLY:HA2	3:S:227:VAL:HG21	1.68	0.74
3:S:6:VAL:HG13	3:S:119:LEU:HB3	1.67	0.73
1:D:54:ARG:HH11	1:D:54:ARG:CG	2.01	0.73
1:D:123:ARG:HH11	1:D:174:ASN:HD21	1.37	0.73
1:D:73:LEU:HG	3:S:199:MET:HE1	1.69	0.73
1:D:259:VAL:HG21	1:D:376:GLU:OE1	1.89	0.72
1:A:124:MET:CE	1:A:175:TRP:NE1	2.46	0.72
2:R:135:ILE:HD11	2:R:168:VAL:HG22	1.71	0.72
3:S:69:ALA:HA	3:S:88:HIS:HE1	1.54	0.72
3:S:7:LEU:CD1	3:S:64:VAL:HG13	2.18	0.72
1:B:108:ILE:HG21	1:B:121:LEU:HD13	1.72	0.72
1:A:304:LYS:HE2	1:A:342:GLN:HE22	1.55	0.71
1:B:233:PRO:HB2	1:B:235:GLU:HG2	1.72	0.71
1:C:215:MET:HB2	1:D:363:GLU:HG3	1.72	0.71
1:D:91:CYS:HB3	1:D:94:VAL:HG13	1.73	0.71
1:B:244:GLY:O	1:B:247:VAL:HG22	1.91	0.70
1:A:123:ARG:HG3	1:A:129:LEU:HD12	1.70	0.70
1:C:358:THR:HB	1:D:213:LEU:O	1.91	0.70
1:B:324:ARG:NH2	1:B:389:GLU:OE2	2.24	0.70
1:A:123:ARG:HG2	1:A:124:MET:HE2	1.73	0.69
1:D:106:MET:CE	1:D:110:ILE:HG23	2.22	0.69
1:B:259:VAL:HG21	1:B:376:GLU:HG3	1.72	0.69
1:B:378:THR:HG22	1:B:380:GLN:N	2.07	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ILE:N	1:C:108:ILE:CD1	2.56	0.68
1:C:119:LYS:HG2	1:C:123:ARG:HH21	1.56	0.68
1:A:213:LEU:O	1:B:358:THR:HB	1.93	0.68
2:R:83:VAL:HG21	2:R:193:PRO:HB3	1.75	0.68
1:B:266:LEU:C	1:B:266:LEU:HD23	2.13	0.68
1:B:32:ARG:HH11	1:B:32:ARG:HG3	1.56	0.67
4:A:399:FAD:C1'	4:A:399:FAD:C10	2.72	0.67
2:R:199:TRP:CZ2	2:R:202:GLN:HG3	2.28	0.67
3:S:39:ASN:ND2	3:S:127:ILE:H	1.93	0.67
1:D:54:ARG:HG2	1:D:54:ARG:NH1	2.07	0.67
1:D:165:MET:HE3	1:D:166:TRP:H	1.60	0.66
1:D:304:LYS:O	1:D:339:ILE:HD13	1.94	0.66
1:B:363:GLU:OE2	1:B:367:ARG:NE	2.27	0.66
1:C:122:GLY:O	1:C:125:THR:HB	1.96	0.65
1:D:66:ILE:HG22	1:D:72:GLY:HA3	1.77	0.65
1:A:363:GLU:CG	1:B:215:MET:HB2	2.14	0.65
1:B:268:GLN:HE21	1:B:309:ARG:HH22	1.43	0.65
1:D:301:MET:HG2	1:D:343:LEU:HG	1.78	0.65
3:S:14:ILE:H	3:S:14:ILE:CD1	2.08	0.64
1:D:325:ASN:H	1:D:325:ASN:HD22	1.46	0.64
1:A:249:MET:CE	1:A:249:MET:HA	2.26	0.64
1:B:239:ILE:HD11	1:B:243:ALA:HB1	1.79	0.64
1:D:165:MET:HE2	1:D:212:GLU:HG3	1.80	0.64
1:D:85:GLU:OE1	1:D:309:ARG:HD3	1.98	0.64
1:B:123:ARG:HH11	1:B:174:ASN:HD21	1.46	0.63
1:A:137:GLU:HG2	1:A:163:GLN:O	1.98	0.63
2:R:110:ALA:CB	2:R:120:LEU:HD11	2.26	0.63
3:S:4:LEU:HA	3:S:118:ASP:OD2	1.98	0.63
3:S:39:ASN:HD21	3:S:127:ILE:H	1.46	0.63
1:C:161:ASN:HD21	1:C:229:ASP:H	1.47	0.63
1:A:266:LEU:HD12	1:A:266:LEU:C	2.19	0.63
1:B:199:VAL:HG22	1:B:232:VAL:HG11	1.80	0.63
2:R:122:ARG:HH11	3:S:146:GLN:HE21	1.46	0.63
2:R:73:ILE:O	2:R:183:ALA:HB2	1.98	0.63
1:D:73:LEU:HG	3:S:199:MET:HE3	1.80	0.62
1:A:256:ARG:N	1:A:257:PRO:CD	2.62	0.62
1:D:108:ILE:HD11	1:D:198:ILE:HG12	1.81	0.62
2:R:132:ILE:HD11	2:R:159:CYS:HB2	1.82	0.62
1:A:85:GLU:OE2	1:A:309:ARG:HD3	2.00	0.62
2:R:54:LEU:HD21	2:R:95:LEU:CD1	2.30	0.62
1:A:144:VAL:O	1:A:147:ILE:HG23	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:THR:OG1	4:D:399:FAD:H1'1	2.00	0.61
1:A:147:ILE:O	1:A:147:ILE:HG13	1.99	0.61
1:C:281:ARG:HH21	1:D:139:GLY:HA2	1.64	0.61
3:S:124:LYS:HE3	3:S:125:GLN:HE21	1.64	0.61
1:C:256:ARG:CG	1:C:256:ARG:HH11	2.12	0.61
1:A:63:ASN:HD21	1:A:101:ASN:HD22	1.49	0.61
1:C:94:VAL:O	1:C:98:ILE:HG12	2.00	0.61
1:D:119:LYS:HD3	1:D:120:TYR:CE1	2.35	0.61
1:B:63:ASN:HB3	1:B:66:ILE:HD12	1.82	0.61
1:C:62:MET:HG3	1:C:98:ILE:HG23	1.82	0.61
1:B:66:ILE:HG23	1:B:121:LEU:HD23	1.82	0.60
2:R:36:ILE:HA	2:R:39:ASN:HD22	1.64	0.60
1:B:136:THR:HG23	1:B:141:GLY:HA2	1.82	0.60
1:A:298:LEU:HD23	1:D:391:ILE:HD11	1.84	0.60
1:C:123:ARG:HG3	1:C:129:LEU:HD23	1.84	0.60
3:S:4:LEU:CD1	3:S:155:LEU:HD21	2.28	0.60
1:B:50:VAL:N	1:B:51:PRO:HD2	2.17	0.60
1:B:123:ARG:NH1	1:B:174:ASN:HD21	1.99	0.60
1:B:378:THR:CG2	1:B:380:GLN:HE21	2.15	0.60
1:B:161:ASN:ND2	1:B:229:ASP:H	1.99	0.60
1:D:378:THR:O	1:D:382:GLN:HG2	2.02	0.60
2:R:109:CYS:HB3	2:R:166:PHE:CZ	2.37	0.59
3:S:122:LEU:HD23	5:S:600:AMP:H1'	1.84	0.59
1:B:256:ARG:CG	1:B:256:ARG:NH1	2.55	0.59
1:D:381:ILE:C	1:D:381:ILE:HD12	2.23	0.59
2:R:111:GLY:O	2:R:113:SER:N	2.30	0.59
1:D:106:MET:HE2	1:D:110:ILE:HG23	1.83	0.59
1:A:134:CYS:HA	1:A:167:ILE:HD12	1.85	0.59
1:D:81:CYS:HB3	1:D:312:TYR:CE1	2.38	0.59
3:S:142:LEU:HD13	3:S:144:TRP:CZ2	2.37	0.59
1:B:161:ASN:HA	1:B:227:PHE:O	2.02	0.58
1:A:346:ASP:O	1:A:350:ILE:HG12	2.04	0.58
3:S:7:LEU:HD11	3:S:64:VAL:HG11	1.80	0.58
1:C:215:MET:HB2	1:D:363:GLU:CG	2.33	0.58
1:C:382:GLN:NE2	1:C:382:GLN:HA	2.18	0.58
3:S:142:LEU:HD13	3:S:144:TRP:CE2	2.38	0.58
1:B:371:ILE:HD12	1:B:371:ILE:N	2.18	0.58
3:S:14:ILE:N	3:S:14:ILE:HD12	2.17	0.58
3:S:76:ARG:HG3	3:S:76:ARG:HH11	1.69	0.58
3:S:128:ASP:OD1	3:S:129:ASP:N	2.34	0.57
1:C:106:MET:N	1:C:107:PRO:CD	2.67	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:ASP:O	1:D:118:LYS:HG2	2.05	0.57
2:R:124:ALA:HB1	2:R:131:PRO:HD3	1.87	0.57
1:C:166:TRP:O	4:C:399:FAD:C4X	2.53	0.57
1:C:17:THR:HG22	1:C:19:GLN:HB3	1.86	0.57
1:A:170:GLY:O	1:A:221:ASP:OD2	2.22	0.57
1:A:30:PHE:HE1	1:A:55:ARG:HG2	1.69	0.56
1:B:378:THR:HG21	1:B:380:GLN:HE21	1.70	0.56
2:R:201:ASP:OD1	2:R:202:GLN:N	2.38	0.56
1:B:256:ARG:HG3	1:B:256:ARG:HH11	1.69	0.56
1:B:108:ILE:CG2	1:B:121:LEU:HD13	2.34	0.56
1:C:379:SER:HB3	1:C:383:ARG:NH1	2.21	0.56
3:S:144:TRP:HB3	3:S:145:PRO:CD	2.36	0.56
1:D:142:SER:OG	4:D:399:FAD:O1A	2.23	0.56
2:R:140:SER:HB2	2:R:141:PRO:HD2	1.88	0.56
1:A:208:ILE:HG23	1:A:223:ARG:HD2	1.88	0.55
1:A:50:VAL:N	1:A:51:PRO:HD2	2.22	0.55
1:B:116:GLN:NE2	1:B:237:VAL:O	2.38	0.55
1:C:370:LYS:HZ2	1:D:345:THR:HG22	1.71	0.55
1:B:210:ARG:HH11	1:B:210:ARG:CG	2.18	0.55
1:D:22:GLU:HB2	3:S:198:ILE:HG21	1.88	0.55
1:C:108:ILE:N	1:C:108:ILE:HD13	2.22	0.55
1:B:101:ASN:OD1	1:B:130:MET:HA	2.07	0.55
1:B:151:ALA:HB2	1:B:180:ALA:HB3	1.89	0.55
1:A:122:GLY:O	1:A:125:THR:HB	2.06	0.55
1:C:18:GLU:OE1	1:C:18:GLU:HA	2.07	0.55
3:S:122:LEU:O	3:S:182:THR:HA	2.07	0.55
1:B:378:THR:HG21	4:B:399:FAD:HO2A	1.68	0.55
1:B:122:GLY:O	1:B:125:THR:HB	2.06	0.55
1:A:319:VAL:HG13	1:A:320:ASP:N	2.20	0.54
1:C:99:GLU:O	1:C:100:GLY:C	2.45	0.54
1:C:159:ILE:HA	1:C:230:VAL:O	2.06	0.54
1:C:31:ALA:O	1:C:36:ILE:HG13	2.07	0.54
1:C:18:GLU:OE1	1:C:21:LYS:HD2	2.08	0.54
1:C:297:MET:O	1:C:301:MET:HG3	2.07	0.54
2:R:55:VAL:O	2:R:55:VAL:HG13	2.07	0.54
1:B:287:LEU:HB2	1:B:290:GLU:OE1	2.08	0.54
1:B:85:GLU:OE1	1:B:264:VAL:HG12	2.07	0.54
1:C:117:LYS:O	1:C:121:LEU:HB2	2.07	0.54
1:B:106:MET:HE2	1:B:254:LYS:HG3	1.88	0.54
1:B:81:CYS:HB3	1:B:312:TYR:CE1	2.42	0.54
1:A:62:MET:CG	1:A:63:ASN:H	2.21	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:ILE:HD12	1:B:371:ILE:H	1.73	0.53
1:D:28:ARG:O	1:D:32:ARG:HG2	2.08	0.53
1:D:387:ALA:O	1:D:391:ILE:HG12	2.08	0.53
1:C:168:THR:O	1:C:169:ASN:HB2	2.08	0.53
1:B:296:PHE:O	1:B:300:GLU:HG2	2.08	0.53
1:A:363:GLU:HG2	1:B:215:MET:SD	2.48	0.53
1:A:115:GLN:O	1:A:119:LYS:HB2	2.09	0.53
3:S:133:GLN:O	3:S:137:MET:HG3	2.08	0.53
1:C:165:MET:HE3	1:C:166:TRP:H	1.74	0.53
3:S:70:GLN:N	3:S:70:GLN:NE2	2.57	0.53
2:R:36:ILE:HG12	2:R:111:GLY:HA3	1.92	0.52
1:C:119:LYS:HG2	1:C:123:ARG:NH2	2.24	0.52
2:R:121:PRO:O	3:S:137:MET:HG2	2.10	0.52
1:B:138:PRO:HD3	1:B:165:MET:HB2	1.90	0.52
1:B:348:VAL:HA	1:B:362:VAL:HG21	1.91	0.52
1:D:106:MET:HE3	1:D:110:ILE:HG23	1.91	0.52
1:D:259:VAL:CG2	1:D:376:GLU:OE1	2.57	0.52
1:C:296:PHE:O	1:C:300:GLU:HG3	2.10	0.52
1:D:117:LYS:O	1:D:121:LEU:HB2	2.10	0.52
3:S:60:GLU:OE2	3:S:85:ARG:HD3	2.10	0.52
1:D:299:ALA:O	1:D:303:MET:HG2	2.10	0.51
1:C:210:ARG:O	1:C:223:ARG:HG2	2.10	0.51
1:D:325:ASN:N	1:D:325:ASN:HD22	2.06	0.51
1:B:378:THR:CG2	1:B:380:GLN:NE2	2.74	0.51
2:R:94:PRO:HA	2:R:97:LEU:HD12	1.93	0.51
2:R:29:ALA:O	2:R:32:SER:HB3	2.10	0.51
1:B:308:ALA:O	1:B:311:SER:HB3	2.11	0.51
1:A:123:ARG:HG2	1:A:124:MET:CE	2.40	0.51
3:S:44:ILE:HG23	3:S:188:ASN:ND2	2.26	0.51
1:D:88:ALA:HB3	1:D:265:GLY:HA3	1.93	0.50
3:S:54:GLU:C	3:S:56:LYS:H	2.15	0.50
1:D:137:GLU:O	1:D:139:GLY:N	2.44	0.50
1:C:312:TYR:C	1:C:312:TYR:CD1	2.85	0.50
1:B:202:ASP:O	1:B:203:THR:C	2.50	0.50
1:C:62:MET:HG3	1:C:98:ILE:CG2	2.42	0.50
1:A:303:MET:HG3	1:D:331:ILE:HG23	1.94	0.50
1:D:339:ILE:HG13	1:D:340:ALA:N	2.27	0.50
1:C:370:LYS:NZ	1:D:345:THR:HG22	2.27	0.50
2:R:122:ARG:NH1	3:S:146:GLN:HE21	2.08	0.50
1:C:77:THR:HG22	1:C:316:ALA:CB	2.42	0.50
1:B:299:ALA:HB2	1:C:387:ALA:HB2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:109:CYS:HA	2:R:166:PHE:O	2.11	0.50
3:S:126:ALA:N	5:S:600:AMP:O3P	2.37	0.50
3:S:144:TRP:HB3	3:S:145:PRO:HD2	1.93	0.50
1:B:123:ARG:HH11	1:B:174:ASN:ND2	2.09	0.49
3:S:24:PRO:C	3:S:26:ARG:H	2.15	0.49
3:S:9:ALA:HB1	5:S:600:AMP:N3	2.27	0.49
1:C:81:CYS:HB3	1:C:312:TYR:CE1	2.47	0.49
1:C:106:MET:N	1:C:107:PRO:HD3	2.28	0.49
1:D:50:VAL:HB	1:D:51:PRO:HD3	1.94	0.49
2:R:97:LEU:HD21	2:R:126:LYS:HB3	1.93	0.49
3:S:106:ARG:CG	3:S:106:ARG:HH11	2.17	0.49
1:A:62:MET:CG	1:A:63:ASN:N	2.75	0.49
1:B:161:ASN:HD21	1:B:229:ASP:H	1.60	0.49
4:B:399:FAD:H9	4:B:399:FAD:H2'	1.95	0.49
1:D:134:CYS:HA	1:D:167:ILE:HD12	1.94	0.49
1:A:166:TRP:O	4:A:399:FAD:C4X	2.61	0.49
1:C:184:PRO:O	1:C:186:PRO:HD3	2.13	0.49
1:C:132:ALA:HB3	1:C:176:TYR:HD2	1.78	0.49
1:C:68:GLU:HA	1:C:72:GLY:O	2.13	0.49
2:R:93:THR:N	2:R:94:PRO:HD2	2.28	0.49
1:D:101:ASN:HD21	1:D:130:MET:HA	1.77	0.49
1:D:112:GLY:O	1:D:117:LYS:HD3	2.13	0.49
1:A:218:ARG:HH11	1:A:218:ARG:HG2	1.78	0.48
1:D:81:CYS:HB3	1:D:312:TYR:HE1	1.77	0.48
2:R:110:ALA:HB3	2:R:120:LEU:CD1	2.33	0.48
3:S:123:GLY:O	5:S:600:AMP:H4'	2.13	0.48
1:C:17:THR:CG2	1:C:19:GLN:HB3	2.43	0.48
1:D:153:LYS:O	1:D:154:LYS:HD3	2.13	0.48
1:A:249:MET:CA	1:A:249:MET:CE	2.91	0.48
1:A:314:ARG:HA	1:D:14:PHE:CE1	2.48	0.48
2:R:136:ILE:HB	2:R:172:SER:OG	2.13	0.48
1:B:256:ARG:HG3	1:B:256:ARG:NH1	2.26	0.48
2:R:113:SER:HB2	3:S:167:ASP:OD2	2.14	0.48
1:A:259:VAL:HG21	1:A:376:GLU:OE1	2.14	0.48
1:A:303:MET:O	1:A:307:LEU:HD22	2.13	0.48
1:C:134:CYS:HA	1:C:167:ILE:HD12	1.96	0.48
1:D:164:LYS:HE2	1:D:178:LEU:CD2	2.43	0.48
1:B:255:THR:O	1:B:258:VAL:HG22	2.13	0.47
1:D:18:GLU:OE2	3:S:76:ARG:HG3	2.14	0.47
1:C:113:ASN:OD1	1:C:113:ASN:C	2.52	0.47
3:S:177:LEU:O	3:S:177:LEU:CD2	2.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:PHE:O	1:D:249:MET:HG2	2.15	0.47
1:D:165:MET:CE	1:D:212:GLU:HG3	2.43	0.47
1:C:344:ALA:HB1	1:C:366:MET:HA	1.97	0.47
1:D:149:THR:O	1:D:180:ALA:HB1	2.15	0.47
1:A:194:PHE:O	1:A:244:GLY:N	2.45	0.47
1:C:157:GLU:OE1	1:C:231:LYS:HD2	2.15	0.47
1:A:17:THR:HB	1:A:20:GLN:OE1	2.15	0.47
1:A:277:TYR:CD2	1:A:351:LEU:HG	2.49	0.47
1:C:330:SER:HB3	1:C:386:VAL:HG23	1.97	0.47
3:S:24:PRO:O	3:S:26:ARG:N	2.48	0.47
1:A:123:ARG:HG3	1:A:129:LEU:CD1	2.43	0.47
1:A:225:ILE:HD11	1:A:227:PHE:CZ	2.50	0.47
4:A:399:FAD:H2'	4:A:399:FAD:H9	1.96	0.47
1:B:378:THR:O	1:B:382:GLN:HG2	2.14	0.47
1:A:136:THR:OG1	4:A:399:FAD:H1'1	2.14	0.47
1:B:136:THR:HG23	1:B:141:GLY:CA	2.44	0.47
1:B:16:PHE:HB2	1:B:21:LYS:HG3	1.97	0.47
2:R:139:LYS:O	2:R:140:SER:HB3	2.14	0.47
1:A:30:PHE:CE1	1:A:55:ARG:HG2	2.48	0.46
1:D:91:CYS:HB3	1:D:94:VAL:CG1	2.44	0.46
2:R:95:LEU:HD13	2:R:95:LEU:C	2.36	0.46
3:S:71:CYS:O	3:S:75:ILE:HD12	2.15	0.46
1:C:256:ARG:NH1	1:C:256:ARG:CG	2.77	0.46
1:A:48:TYR:CE2	1:A:172:LYS:HG2	2.51	0.46
2:R:142:ASP:HB2	2:R:159:CYS:O	2.15	0.46
1:A:304:LYS:CE	1:A:342:GLN:HE22	2.26	0.46
1:B:73:LEU:HB3	1:B:75:LEU:HD13	1.97	0.46
1:C:312:TYR:CD1	1:C:313:GLN:N	2.84	0.46
1:A:63:ASN:HB3	1:A:66:ILE:CD1	2.45	0.46
1:B:256:ARG:N	1:B:257:PRO:CD	2.79	0.46
3:S:100:GLY:O	3:S:104:VAL:HG23	2.16	0.46
1:B:31:ALA:HA	1:B:35:ILE:HD12	1.97	0.46
1:C:221:ASP:OD2	1:C:223:ARG:HD2	2.16	0.46
1:A:370:LYS:HZ2	1:B:349:GLN:HE21	1.64	0.46
1:B:289:VAL:HG22	1:C:391:ILE:CD1	2.46	0.46
1:A:154:LYS:O	1:A:154:LYS:HG2	2.15	0.45
1:B:12:PHE:HA	1:C:13:SER:O	2.16	0.45
1:D:210:ARG:HG3	1:D:210:ARG:H	1.34	0.45
1:A:104:GLY:O	1:A:107:PRO:HD2	2.16	0.45
4:A:399:FAD:H2'	4:A:399:FAD:C9	2.46	0.45
1:C:136:THR:OG1	4:C:399:FAD:H1'1	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ILE:CG2	1:D:223:ARG:HD2	2.46	0.45
3:S:132:ASN:HD21	3:S:136:GLN:HE22	1.60	0.45
3:S:76:ARG:CG	3:S:76:ARG:HH11	2.29	0.45
4:A:399:FAD:C1'	4:A:399:FAD:C9A	2.85	0.45
1:D:19:GLN:NE2	3:S:199:MET:CG	2.76	0.45
2:R:23:LEU:HD12	2:R:24:VAL:N	2.31	0.45
1:A:103:LEU:HD22	1:A:133:TYR:CD1	2.51	0.45
1:B:292:GLN:HB3	1:D:292:GLN:HB2	1.99	0.45
1:C:98:ILE:O	1:C:101:ASN:HB2	2.16	0.45
1:D:263:ALA:HB3	1:D:336:ALA:HB1	1.98	0.45
1:B:151:ALA:HB2	1:B:180:ALA:CB	2.47	0.45
1:B:221:ASP:OD2	1:B:223:ARG:HD3	2.17	0.45
1:B:210:ARG:HH11	1:B:210:ARG:HG3	1.82	0.45
1:B:88:ALA:HB1	1:B:92:THR:HG22	1.99	0.45
1:C:382:GLN:HE21	1:C:382:GLN:HA	1.82	0.45
1:B:289:VAL:HG22	1:C:391:ILE:HD13	1.99	0.45
3:S:165:GLU:HG3	3:S:184:ASP:OD2	2.17	0.45
1:B:288:LEU:HD12	1:B:288:LEU:HA	1.69	0.45
1:D:371:ILE:HD11	4:D:399:FAD:HM83	1.98	0.45
1:D:43:ASP:HB2	1:D:364:LYS:HD2	1.99	0.45
1:A:117:LYS:O	1:A:121:LEU:HB2	2.17	0.45
1:A:304:LYS:HE2	1:A:342:GLN:NE2	2.29	0.45
1:C:266:LEU:HD11	1:C:369:ALA:HB2	1.99	0.45
1:C:77:THR:HG22	1:C:316:ALA:HB1	1.98	0.45
1:D:338:ASP:OD2	1:D:383:ARG:NH2	2.45	0.45
2:R:124:ALA:CB	2:R:131:PRO:HD3	2.46	0.45
2:R:124:ALA:O	2:R:125:ALA:C	2.54	0.44
3:S:38:MET:HE1	3:S:78:ALA:HB2	1.99	0.44
3:S:69:ALA:HA	3:S:88:HIS:CE1	2.42	0.44
1:B:293:ALA:O	1:B:297:MET:HG3	2.17	0.44
1:D:54:ARG:CG	1:D:54:ARG:NH1	2.71	0.44
1:A:166:TRP:O	4:A:399:FAD:N5	2.50	0.44
3:S:12:ARG:HB2	3:S:74:THR:OG1	2.17	0.44
1:A:311:SER:HB3	1:D:307:LEU:CD2	2.48	0.44
1:D:259:VAL:HG21	1:D:376:GLU:CD	2.37	0.44
1:D:269:ARG:NH1	1:D:273:GLU:OE2	2.49	0.44
1:A:185:ASP:HA	1:A:186:PRO:HD3	1.83	0.44
1:A:108:ILE:HD13	1:A:198:ILE:CD1	2.47	0.44
1:A:62:MET:HG3	1:A:63:ASN:H	1.82	0.44
1:C:161:ASN:HD21	1:C:229:ASP:N	2.11	0.44
1:C:311:SER:OG	1:C:332:ALA:HA	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:ILE:HD12	1:D:175:TRP:CZ3	2.53	0.44
1:D:55:ARG:NH1	3:S:192:TYR:HE2	2.16	0.44
3:S:4:LEU:HD23	3:S:4:LEU:N	2.32	0.44
1:A:136:THR:HG22	1:A:137:GLU:N	2.33	0.44
1:A:108:ILE:CD1	1:A:198:ILE:HG12	2.36	0.44
1:D:297:MET:HB3	1:D:301:MET:CE	2.48	0.44
1:D:85:GLU:OE2	1:D:309:ARG:NH1	2.50	0.44
1:D:66:ILE:HA	1:D:67:PRO:HD3	1.85	0.44
3:S:153:VAL:CG1	3:S:154:THR:N	2.80	0.44
1:D:371:ILE:HD11	4:D:399:FAD:C8	2.47	0.44
1:C:166:TRP:CZ3	1:C:212:GLU:HG2	2.52	0.44
1:C:256:ARG:HB2	1:C:257:PRO:HD3	2.00	0.44
1:A:384:LEU:CD2	1:D:296:PHE:HE1	2.29	0.44
1:B:53:ILE:HG21	1:B:130:MET:SD	2.57	0.43
1:C:239:ILE:HG22	1:C:239:ILE:O	2.18	0.43
1:D:324:ARG:NH2	1:D:389:GLU:OE1	2.50	0.43
2:R:194:VAL:HG12	2:R:196:ILE:HG23	2.00	0.43
2:R:86:GLY:HA3	2:R:199:TRP:CD1	2.53	0.43
1:C:174:ASN:OD1	1:C:175:TRP:HD1	2.01	0.43
2:R:203:LYS:HE3	2:R:203:LYS:HB2	1.80	0.43
1:B:344:ALA:O	1:B:348:VAL:HG23	2.18	0.43
1:A:123:ARG:HG3	1:A:124:MET:HE2	1.95	0.43
1:A:19:GLN:NE2	1:A:23:PHE:CZ	2.84	0.43
1:C:75:LEU:HA	1:C:75:LEU:HD12	1.53	0.43
1:C:99:GLU:C	1:C:101:ASN:N	2.68	0.43
1:D:371:ILE:CD1	4:D:399:FAD:HM83	2.48	0.43
1:C:375:TYR:N	1:C:375:TYR:CD1	2.86	0.43
3:S:149:PHE:N	3:S:149:PHE:CD1	2.84	0.43
3:S:38:MET:CE	3:S:78:ALA:HB2	2.48	0.43
1:B:254:LYS:HB3	1:B:254:LYS:HE2	1.67	0.43
4:B:399:FAD:HM71	4:B:399:FAD:HM83	1.77	0.43
1:C:375:TYR:H	1:C:375:TYR:HD1	1.64	0.43
2:R:121:PRO:HB2	3:S:136:GLN:HB2	2.01	0.43
1:C:256:ARG:N	1:C:257:PRO:CD	2.81	0.43
3:S:136:GLN:OE1	3:S:136:GLN:N	2.47	0.43
3:S:65:SER:HB3	3:S:75:ILE:HD11	2.01	0.43
1:B:164:LYS:HA	1:B:164:LYS:HD2	1.81	0.43
1:A:49:PRO:O	1:A:53:ILE:HG13	2.18	0.43
1:B:99:GLU:O	1:B:100:GLY:C	2.56	0.43
3:S:148:THR:OG1	3:S:164:ARG:NH2	2.52	0.43
1:A:215:MET:HB2	1:B:363:GLU:HG2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:THR:O	1:A:382:GLN:HG2	2.19	0.42
2:R:61:ASP:OD1	2:R:61:ASP:N	2.52	0.42
3:S:48:GLU:OE1	3:S:48:GLU:HA	2.18	0.42
1:C:375:TYR:C	1:C:375:TYR:CD1	2.89	0.42
1:A:63:ASN:ND2	1:A:101:ASN:HD22	2.15	0.42
1:A:208:ILE:CG2	1:A:223:ARG:HD2	2.49	0.42
1:A:50:VAL:N	1:A:51:PRO:CD	2.83	0.42
1:B:33:GLU:O	1:B:37:PRO:HG3	2.19	0.42
1:C:208:ILE:HG22	1:C:209:GLY:O	2.20	0.42
1:B:16:PHE:CD1	1:B:16:PHE:N	2.87	0.42
1:B:253:ASP:OD2	1:B:325:ASN:HB2	2.19	0.42
1:B:300:GLU:O	1:B:304:LYS:HG2	2.19	0.42
1:D:89:TYR:C	1:D:89:TYR:CD1	2.93	0.42
1:A:127:GLU:O	1:A:129:LEU:N	2.48	0.42
1:A:63:ASN:ND2	1:A:105:GLN:OE1	2.53	0.42
1:C:371:ILE:HD12	1:C:371:ILE:HA	1.77	0.42
1:A:210:ARG:NH1	1:A:212:GLU:OE1	2.53	0.42
1:B:238:LEU:HA	1:B:238:LEU:HD13	1.94	0.42
1:B:333:LYS:NZ	1:B:377:GLY:O	2.53	0.42
1:C:202:ASP:OD2	1:C:202:ASP:C	2.58	0.42
1:C:238:LEU:HD13	1:C:238:LEU:HA	1.85	0.42
1:C:48:TYR:CD1	1:C:49:PRO:HD2	2.55	0.42
1:D:48:TYR:CE2	1:D:172:LYS:HG2	2.54	0.42
1:C:358:THR:CB	1:D:213:LEU:O	2.66	0.42
1:D:19:GLN:HE22	3:S:199:MET:HG2	1.81	0.42
1:B:111:ALA:HB1	1:B:239:ILE:HG23	2.00	0.42
1:C:134:CYS:HB2	1:C:177:PHE:O	2.19	0.42
3:S:64:VAL:HA	3:S:87:ILE:O	2.20	0.42
1:A:256:ARG:N	1:A:257:PRO:HD3	2.35	0.41
1:A:277:TYR:CE2	1:A:351:LEU:HA	2.55	0.41
1:C:349:GLN:HE21	1:D:370:LYS:NZ	2.18	0.41
2:R:36:ILE:CA	2:R:39:ASN:HD22	2.33	0.41
1:D:364:LYS:HG2	1:D:368:ASP:OD1	2.20	0.41
2:R:109:CYS:HB3	2:R:166:PHE:CE1	2.54	0.41
3:S:72:GLN:HG3	3:S:206:ILE:HD12	2.02	0.41
1:A:266:LEU:HD13	1:A:365:LEU:HD22	2.03	0.41
1:A:62:MET:HG2	1:A:63:ASN:N	2.35	0.41
1:D:304:LYS:HB3	1:D:339:ILE:HG21	2.02	0.41
3:S:149:PHE:HA	3:S:184:ASP:HB2	2.02	0.41
2:R:91:GLU:OE1	2:R:91:GLU:HA	2.20	0.41
1:A:168:THR:O	1:A:169:ASN:HB2	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ASN:N	1:A:221:ASP:O	2.51	0.41
1:B:272:ASP:OD1	1:C:394:TYR:OH	2.19	0.41
1:B:341:ASN:HD22	1:B:341:ASN:H	1.67	0.41
4:B:399:FAD:H2'	4:B:399:FAD:C9	2.50	0.41
1:B:289:VAL:CG2	1:C:391:ILE:HD13	2.50	0.41
2:R:54:LEU:HD21	2:R:95:LEU:HD11	2.03	0.41
3:S:124:LYS:HE3	3:S:125:GLN:NE2	2.33	0.41
2:R:81:HIS:CE1	2:R:83:VAL:HB	2.55	0.41
1:B:19:GLN:OE1	1:B:23:PHE:CZ	2.74	0.41
1:D:371:ILE:HD12	1:D:371:ILE:HA	1.92	0.41
1:D:66:ILE:CG2	1:D:72:GLY:HA3	2.48	0.41
1:A:319:VAL:CG1	1:A:320:ASP:N	2.82	0.41
1:C:300:GLU:O	1:C:303:MET:HB2	2.20	0.41
2:R:23:LEU:HA	2:R:52:SER:O	2.21	0.41
1:A:266:LEU:C	1:A:266:LEU:CD1	2.87	0.41
1:A:53:ILE:HG23	1:A:62:MET:HE1	2.01	0.41
1:B:185:ASP:HA	1:B:186:PRO:HD2	1.77	0.41
1:B:203:THR:HA	1:B:204:PRO:HD2	1.93	0.41
1:C:149:THR:HG23	1:C:162:GLY:HA3	2.02	0.41
1:C:277:TYR:CG	1:C:351:LEU:HG	2.56	0.41
1:C:281:ARG:HG3	1:C:282:LYS:N	2.35	0.41
1:C:98:ILE:HG12	1:C:98:ILE:H	1.49	0.41
1:A:304:LYS:CE	1:A:342:GLN:NE2	2.84	0.41
1:A:55:ARG:O	1:A:59:LEU:HB2	2.21	0.41
1:A:63:ASN:HB3	1:A:66:ILE:HD12	2.03	0.41
1:B:133:TYR:CZ	1:B:135:VAL:HG21	2.56	0.41
1:B:203:THR:HG22	1:B:204:PRO:O	2.20	0.41
1:C:108:ILE:N	1:C:108:ILE:HD12	2.34	0.41
1:C:119:LYS:HD3	1:C:120:TYR:CZ	2.55	0.41
1:C:375:TYR:HD1	1:C:375:TYR:N	2.19	0.41
3:S:112:ALA:HB3	3:S:142:LEU:HD21	2.03	0.41
3:S:25:ASP:OD1	3:S:27:THR:OG1	2.33	0.41
1:A:383:ARG:HH11	1:D:300:GLU:HG2	1.86	0.41
1:A:380:GLN:NE2	4:A:399:FAD:O2B	2.44	0.41
1:B:303:MET:HG2	1:C:331:ILE:HG23	2.02	0.41
1:B:304:LYS:HE3	1:B:342:GLN:OE1	2.21	0.41
1:C:239:ILE:CG2	1:C:239:ILE:O	2.69	0.41
1:D:131:CYS:HA	1:D:173:ALA:HB1	2.03	0.41
1:A:20:GLN:HG2	1:A:82:LEU:HD11	2.03	0.40
1:D:123:ARG:HD2	1:D:174:ASN:ND2	2.36	0.40
1:D:166:TRP:O	4:D:399:FAD:C4X	2.69	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:THR:HG21	1:D:266:LEU:HD23	2.03	0.40
1:C:350:ILE:O	4:D:399:FAD:H4B	2.21	0.40
3:S:195:LEU:N	3:S:196:PRO:CD	2.84	0.40
1:B:272:ASP:O	1:B:276:LYS:HG3	2.21	0.40
1:B:36:ILE:HG13	1:B:90:GLY:HA2	2.03	0.40
1:D:73:LEU:HD12	1:D:73:LEU:HA	1.81	0.40
2:R:130:ALA:HB2	3:S:102:LEU:HD22	2.03	0.40
2:R:55:VAL:O	2:R:55:VAL:CG1	2.70	0.40
1:B:137:GLU:OE2	1:B:147:ILE:HB	2.21	0.40
1:B:170:GLY:O	1:B:225:ILE:HD11	2.22	0.40
1:C:59:LEU:HA	1:C:59:LEU:HD23	1.78	0.40
1:D:144:VAL:O	1:D:147:ILE:HB	2.21	0.40
3:S:39:ASN:HD22	3:S:127:ILE:HG12	1.85	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	384/396 (97%)	352 (92%)	27 (7%)	5 (1%)	12	37
1	B	385/396 (97%)	351 (91%)	30 (8%)	4 (1%)	15	45
1	C	386/396 (98%)	362 (94%)	20 (5%)	4 (1%)	15	45
1	D	385/396 (97%)	361 (94%)	19 (5%)	5 (1%)	12	37
2	R	182/333 (55%)	165 (91%)	11 (6%)	6 (3%)	4	15
3	S	226/255 (89%)	197 (87%)	25 (11%)	4 (2%)	8	29
All	All	1948/2172 (90%)	1788 (92%)	132 (7%)	28 (1%)	11	36

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	234	LYS
1	D	156	ASP
1	D	234	LYS
2	R	112	ALA
3	S	25	ASP
1	A	63	ASN
1	A	202	ASP
2	R	36	ILE
2	R	150	ALA
3	S	68	PRO
1	A	229	ASP
1	B	141	GLY
1	B	393	LYS
2	R	141	PRO
1	A	69	ASN
2	R	81	HIS
1	B	238	LEU
1	D	155	GLY
1	A	128	PRO
1	C	204	PRO
2	R	149	TYR
1	D	138	PRO
1	D	141	GLY
3	S	157	GLY
1	C	11	GLY
1	B	204	PRO
1	C	109	ILE
3	S	107	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	286/311 (92%)	247 (86%)	39 (14%)	3	11
1	B	284/311 (91%)	248 (87%)	36 (13%)	4	13
1	C	290/311 (93%)	247 (85%)	43 (15%)	3	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	292/311 (94%)	244 (84%)	48 (16%)	2	7
2	R	139/262 (53%)	123 (88%)	16 (12%)	5	17
3	S	174/214 (81%)	155 (89%)	19 (11%)	6	19
All	All	1465/1720 (85%)	1264 (86%)	201 (14%)	3	11

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	41	GLU
1	A	59	LEU
1	A	61	LEU
1	A	62	MET
1	A	84	SER
1	A	102	SER
1	A	103	LEU
1	A	114	ASP
1	A	118	LYS
1	A	119	LYS
1	A	130	MET
1	A	147	ILE
1	A	152	GLU
1	A	156	ASP
1	A	172	LYS
1	A	185	ASP
1	A	191	ASN
1	A	210	ARG
1	A	218	ARG
1	A	225	ILE
1	A	226	VAL
1	A	235	GLU
1	A	238	LEU
1	A	241	ASP
1	A	249	MET
1	A	256	ARG
1	A	266	LEU
1	A	276	LYS
1	A	280	GLU
1	A	289	VAL
1	A	298	LEU
1	A	307	LEU

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Mol	Chain	Res	Type
1	A	312	TYR
1	A	323	ARG
1	A	339	ILE
1	A	363	GLU
1	A	375	TYR
1	A	392	ASP
1	B	32	ARG
1	B	55	ARG
1	B	64	THR
1	B	68	GLU
1	B	75	LEU
1	B	82	LEU
1	B	95	GLN
1	B	103	LEU
1	B	125	THR
1	B	142	SER
1	B	165	MET
1	B	207	GLN
1	B	210	ARG
1	B	211	LYS
1	B	223	ARG
1	B	228	GLU
1	B	235	GLU
1	B	238	LEU
1	B	239	ILE
1	B	254	LYS
1	B	256	ARG
1	B	288	LEU
1	B	289	VAL
1	B	300	GLU
1	B	304	LYS
1	B	314	ARG
1	B	323	ARG
1	B	343	LEU
1	B	345	THR
1	B	358	THR
1	B	371	ILE
1	B	375	TYR
1	B	376	GLU
1	B	379	SER
1	B	388	ARG
1	B	392	ASP

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Mol	Chain	Res	Type
1	C	10	LEU
1	C	19	GLN
1	C	34	GLU
1	C	47	GLU
1	C	54	ARG
1	C	75	LEU
1	C	84	SER
1	C	98	ILE
1	C	99	GLU
1	C	103	LEU
1	C	108	ILE
1	C	109	ILE
1	C	119	LYS
1	C	129	LEU
1	C	142	SER
1	C	165	MET
1	C	178	LEU
1	C	179	LEU
1	C	204	PRO
1	C	210	ARG
1	C	213	LEU
1	C	221	ASP
1	C	222	THR
1	C	225	ILE
1	C	226	VAL
1	C	231	LYS
1	C	237	VAL
1	C	238	LEU
1	C	241	ASP
1	C	249	MET
1	C	256	ARG
1	C	259	VAL
1	C	266	LEU
1	C	281	ARG
1	C	282	LYS
1	C	286	LYS
1	C	298	LEU
1	C	307	LEU
1	C	311	SER
1	C	312	TYR
1	C	323	ARG
1	C	358	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	375	TYR
1	D	18	GLU
1	D	19	GLN
1	D	22	GLU
1	D	53	ILE
1	D	54	ARG
1	D	63	ASN
1	D	68	GLU
1	D	73	LEU
1	D	75	LEU
1	D	84	SER
1	D	94	VAL
1	D	98	ILE
1	D	99	GLU
1	D	115	GLN
1	D	117	LYS
1	D	121	LEU
1	D	123	ARG
1	D	129	LEU
1	D	142	SER
1	D	147	ILE
1	D	152	GLU
1	D	156	ASP
1	D	178	LEU
1	D	179	LEU
1	D	181	ARG
1	D	182	SER
1	D	191	ASN
1	D	210	ARG
1	D	213	LEU
1	D	218	ARG
1	D	234	LYS
1	D	238	LEU
1	D	253	ASP
1	D	255	THR
1	D	266	LEU
1	D	269	ARG
1	D	280	GLU
1	D	282	LYS
1	D	286	LYS
1	D	303	MET
1	D	305	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	325	ASN
1	D	345	THR
1	D	358	THR
1	D	375	TYR
1	D	381	ILE
1	D	388	ARG
1	D	395	LYS
2	R	20	GLN
2	R	39	ASN
2	R	45	THR
2	R	58	THR
2	R	83	VAL
2	R	126	LYS
2	R	132	ILE
2	R	133	SER
2	R	146	ARG
2	R	157	VAL
2	R	159	CYS
2	R	163	VAL
2	R	164	LYS
2	R	169	ARG
2	R	174	ASP
2	R	185	SER
3	S	4	LEU
3	S	6	VAL
3	S	31	THR
3	S	72	GLN
3	S	76	ARG
3	S	85	ARG
3	S	118	ASP
3	S	132	ASN
3	S	149	PHE
3	S	152	GLN
3	S	154	THR
3	S	155	LEU
3	S	164	ARG
3	S	170	LEU
3	S	177	LEU
3	S	188	ASN
3	S	189	GLU
3	S	206	ILE
3	S	219	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	105	GLN
1	A	169	ASN
1	A	341	ASN
1	A	342	GLN
1	A	349	GLN
1	A	373	GLN
1	A	380	GLN
1	B	19	GLN
1	B	65	HIS
1	B	95	GLN
1	B	161	ASN
1	B	163	GLN
1	B	174	ASN
1	B	207	GLN
1	B	268	GLN
1	B	325	ASN
1	B	349	GLN
1	B	380	GLN
1	B	382	GLN
1	C	19	GLN
1	C	161	ASN
1	C	313	GLN
1	C	341	ASN
1	C	349	GLN
1	C	373	GLN
1	C	382	GLN
1	D	19	GLN
1	D	115	GLN
1	D	174	ASN
1	D	236	ASN
1	D	325	ASN
1	D	342	GLN
1	D	373	GLN
2	R	39	ASN
2	R	118	ASN
2	R	202	GLN
3	S	39	ASN
3	S	88	HIS
3	S	125	GLN
3	S	132	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	S	146	GLN
3	S	188	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

5 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	$\#|Z| > 2$
4	FAD	B	399	-	51,58,58	1.50	9 (17%)	60,89,89	2.40	18 (30%)
4	FAD	C	399	-	51,58,58	2.02	11 (21%)	60,89,89	2.68	18 (30%)
4	FAD	A	399	-	51,58,58	4.66	13 (25%)	60,89,89	2.83	22 (36%)
4	FAD	D	399	-	51,58,58	1.36	7 (13%)	60,89,89	1.81	13 (21%)
5	AMP	S	600	-	22,25,25	1.29	2 (9%)	25,38,38	1.28	3 (12%)

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	FAD	B	399	-	-	1/30/50/50	0/6/6/6
4	FAD	C	399	-	-	4/30/50/50	0/6/6/6
4	FAD	A	399	-	-	6/30/50/50	0/6/6/6
4	FAD	D	399	-	-	0/30/50/50	0/6/6/6
5	AMP	S	600	-	-	5/6/26/26	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	399	FAD	C1'-N10	29.32	1.78	1.48
4	A	399	FAD	C8M-C8	-6.76	1.37	1.51
4	C	399	FAD	C1'-N10	6.65	1.55	1.48
4	A	399	FAD	C4X-N5	5.43	1.41	1.33
4	C	399	FAD	C10-N1	5.38	1.40	1.33
4	A	399	FAD	C9A-N10	5.26	1.45	1.38
4	A	399	FAD	C4-C4X	5.22	1.50	1.41
4	C	399	FAD	C4X-N5	4.99	1.40	1.33
4	A	399	FAD	C10-N1	4.47	1.39	1.33
4	B	399	FAD	C2A-N3A	4.42	1.39	1.32
4	C	399	FAD	C2A-N3A	4.33	1.39	1.32
4	A	399	FAD	C2-N1	3.95	1.46	1.38
4	D	399	FAD	C10-N1	3.92	1.38	1.33
4	B	399	FAD	C4X-N5	3.73	1.38	1.33
4	D	399	FAD	C4-N3	3.49	1.39	1.33
5	S	600	AMP	C5-C4	3.38	1.49	1.40
4	A	399	FAD	C2A-N3A	3.32	1.37	1.32
4	A	399	FAD	C4X-C10	3.32	1.42	1.38
4	C	399	FAD	C7M-C7	3.26	1.57	1.51
4	B	399	FAD	C4-N3	3.24	1.38	1.33
4	C	399	FAD	C4-N3	3.24	1.38	1.33
4	B	399	FAD	C2A-N1A	3.23	1.39	1.33
4	C	399	FAD	C8M-C8	3.12	1.57	1.51
4	D	399	FAD	C4X-N5	3.10	1.37	1.33
4	B	399	FAD	C10-N1	2.96	1.37	1.33
4	A	399	FAD	C4-N3	2.85	1.38	1.33
4	B	399	FAD	C1'-N10	2.84	1.51	1.48
4	A	399	FAD	C5X-N5	2.84	1.40	1.35
4	D	399	FAD	C1'-N10	2.81	1.51	1.48
4	B	399	FAD	C2B-C1B	-2.66	1.49	1.53
4	D	399	FAD	C2A-N3A	2.65	1.36	1.32
4	C	399	FAD	O4'-C4'	-2.56	1.37	1.43
4	C	399	FAD	C9A-N10	2.49	1.41	1.38
4	D	399	FAD	C9A-N10	2.49	1.41	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	399	FAD	C6-C5X	-2.45	1.38	1.41
5	S	600	AMP	C2-N3	2.44	1.36	1.32
4	C	399	FAD	O2'-C2'	-2.40	1.38	1.43
4	D	399	FAD	C5X-N5	2.40	1.39	1.35
4	B	399	FAD	O2B-C2B	-2.38	1.37	1.43
4	C	399	FAD	C6-C5X	-2.24	1.38	1.41
4	A	399	FAD	C2A-N1A	2.16	1.37	1.33
4	B	399	FAD	C6-C5X	-2.09	1.38	1.41

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	399	FAD	C1'-N10-C9A	9.95	126.13	118.29
4	A	399	FAD	C4-N3-C2	8.30	122.15	115.14
4	A	399	FAD	C10-C4X-N5	-7.81	115.86	121.26
4	B	399	FAD	C4-N3-C2	7.63	121.59	115.14
4	A	399	FAD	C4-C4X-N5	6.85	126.43	118.60
4	A	399	FAD	C4X-N5-C5X	6.66	123.43	116.77
4	A	399	FAD	C1'-N10-C9A	6.51	123.42	118.29
4	C	399	FAD	O5'-C5'-C4'	-6.11	93.04	109.36
4	C	399	FAD	C4-N3-C2	5.88	120.11	115.14
4	D	399	FAD	C4X-N5-C5X	5.88	122.65	116.77
4	B	399	FAD	N3A-C2A-N1A	-5.86	119.53	128.68
4	A	399	FAD	N3A-C2A-N1A	-5.82	119.58	128.68
4	B	399	FAD	C4X-C4-N3	-5.72	115.61	123.43
4	C	399	FAD	C8M-C8-C9	-5.48	107.24	120.34
4	B	399	FAD	C10-C4X-N5	-5.45	117.49	121.26
4	B	399	FAD	C1'-N10-C9A	5.19	122.38	118.29
4	C	399	FAD	C1'-N10-C10	-5.01	113.92	118.41
4	C	399	FAD	C4X-N5-C5X	5.01	121.77	116.77
4	A	399	FAD	C6-C5X-C9A	4.72	125.24	119.05
4	D	399	FAD	C1'-N10-C9A	4.37	121.73	118.29
4	B	399	FAD	C4X-N5-C5X	4.28	121.05	116.77
4	C	399	FAD	N3A-C2A-N1A	-4.25	122.03	128.68
4	B	399	FAD	C8M-C8-C7	-4.12	112.29	120.74
4	C	399	FAD	C7M-C7-C6	-3.98	110.83	120.34
4	C	399	FAD	C4-C4X-N5	3.94	123.11	118.60
4	B	399	FAD	C7M-C7-C8	-3.93	112.67	120.74
4	C	399	FAD	O2'-C2'-C1'	-3.93	100.14	109.59
4	D	399	FAD	N3A-C2A-N1A	-3.87	122.64	128.68
4	B	399	FAD	C7M-C7-C6	-3.79	111.27	120.34
4	D	399	FAD	C4-N3-C2	3.69	118.26	115.14

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	399	FAD	C5X-C9A-N10	3.69	120.39	117.72
4	B	399	FAD	C8M-C8-C9	-3.63	111.67	120.34
4	A	399	FAD	C4-C4X-C10	-3.63	117.55	119.95
4	A	399	FAD	C6-C5X-N5	-3.59	115.09	119.05
4	A	399	FAD	O2'-C2'-C3'	-3.48	100.64	109.10
4	C	399	FAD	P-O3P-PA	-3.47	120.93	132.83
4	A	399	FAD	P-O3P-PA	-3.36	121.30	132.83
4	C	399	FAD	C10-C4X-N5	-3.30	118.97	121.26
4	A	399	FAD	C9-C9A-C5X	-3.18	114.45	119.88
4	A	399	FAD	C9A-N10-C10	-3.15	117.79	121.91
4	B	399	FAD	C4A-C5A-N7A	-3.09	106.17	109.40
4	D	399	FAD	C10-C4X-N5	-3.09	119.12	121.26
4	C	399	FAD	C4-C4X-C10	-3.08	117.92	119.95
4	B	399	FAD	C4-C4X-C10	3.06	121.97	119.95
4	D	399	FAD	P-O3P-PA	-3.05	122.36	132.83
4	B	399	FAD	P-O3P-PA	-3.00	122.54	132.83
4	A	399	FAD	C5X-C9A-N10	2.96	119.86	117.72
4	A	399	FAD	C4X-C10-N10	2.95	123.33	120.30
4	D	399	FAD	C8M-C8-C7	-2.92	114.74	120.74
4	A	399	FAD	C8M-C8-C9	-2.82	113.61	120.34
4	A	399	FAD	C6-C7-C8	-2.80	115.19	119.91
4	D	399	FAD	C4-C4X-C10	2.76	121.78	119.95
4	D	399	FAD	C4X-C4-N3	-2.70	119.74	123.43
4	D	399	FAD	O3'-C3'-C2'	-2.68	102.34	108.81
5	S	600	AMP	C4-C5-N7	-2.60	106.69	109.40
5	S	600	AMP	N3-C2-N1	-2.58	124.65	128.68
4	D	399	FAD	C7M-C7-C8	-2.46	115.69	120.74
4	C	399	FAD	C6-C5X-C9A	2.46	122.27	119.05
4	C	399	FAD	O4'-C4'-C5'	-2.44	104.42	109.92
4	A	399	FAD	C4X-C4-N3	-2.40	120.14	123.43
4	A	399	FAD	O4'-C4'-C5'	-2.40	104.53	109.92
4	C	399	FAD	C4A-C5A-N7A	-2.37	106.93	109.40
4	B	399	FAD	C4X-C10-N10	2.28	122.65	120.30
4	B	399	FAD	C9A-N10-C10	-2.28	118.92	121.91
4	D	399	FAD	O2'-C2'-C1'	2.27	115.06	109.59
4	A	399	FAD	O3'-C3'-C4'	2.21	114.14	108.81
4	C	399	FAD	C9A-C5X-N5	-2.20	118.91	122.36
4	D	399	FAD	C9A-C5X-N5	-2.14	119.02	122.36
4	B	399	FAD	O4B-C1B-C2B	-2.10	103.86	106.93
4	B	399	FAD	C6-C5X-C9A	2.09	121.79	119.05
4	A	399	FAD	O3B-C3B-C4B	-2.05	105.11	111.05
5	S	600	AMP	C2-N1-C6	2.01	122.19	118.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	399	FAD	C5X-C9A-N10	2.00	119.17	117.72
4	A	399	FAD	C8M-C8-C7	-2.00	116.64	120.74

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	399	FAD	C2'-C1'-N10-C10
4	C	399	FAD	C2'-C1'-N10-C9A
4	C	399	FAD	C2'-C1'-N10-C10
4	A	399	FAD	C2'-C1'-N10-C9A
4	A	399	FAD	C2'-C1'-N10-C10
4	A	399	FAD	N10-C1'-C2'-O2'
4	A	399	FAD	N10-C1'-C2'-C3'
4	A	399	FAD	C1'-C2'-C3'-C4'
5	S	600	AMP	C5'-O5'-P-O2P
5	S	600	AMP	O4'-C4'-C5'-O5'
5	S	600	AMP	C3'-C4'-C5'-O5'
4	A	399	FAD	O2'-C2'-C3'-C4'
5	S	600	AMP	C5'-O5'-P-O1P
5	S	600	AMP	C5'-O5'-P-O3P
4	C	399	FAD	C2'-C3'-C4'-C5'
4	C	399	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

5 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	399	FAD	5	0
4	C	399	FAD	2	0
4	A	399	FAD	9	0
4	D	399	FAD	8	0
5	S	600	AMP	4	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 399

Bond lengths   Bond angles

Torsions   Rings

Ligand FAD C 399

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 399

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD D 399

Bond lengths

Bond angles

Torsions

Rings

Ligand AMP S 600

Bond lengths

Bond angles

Torsions

Rings
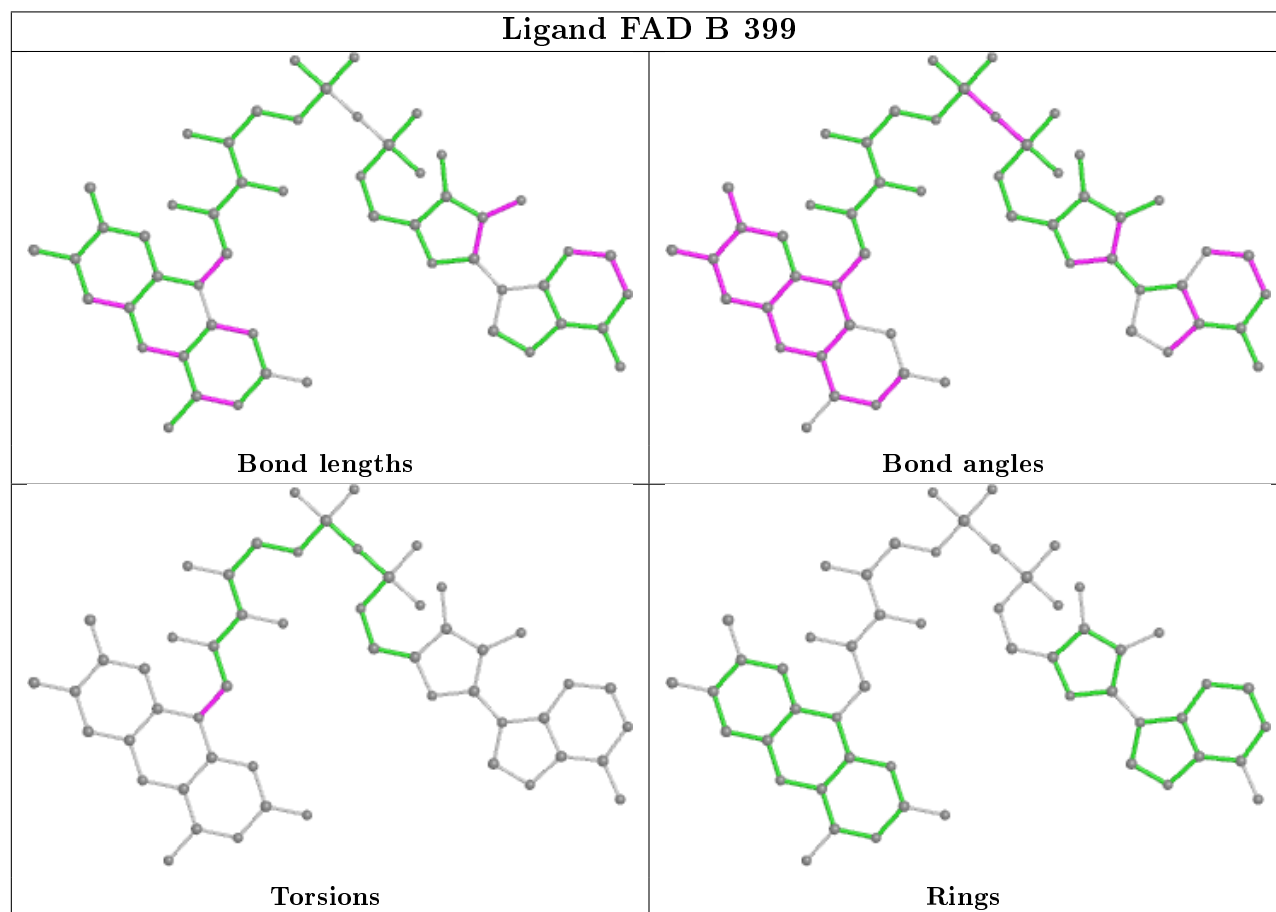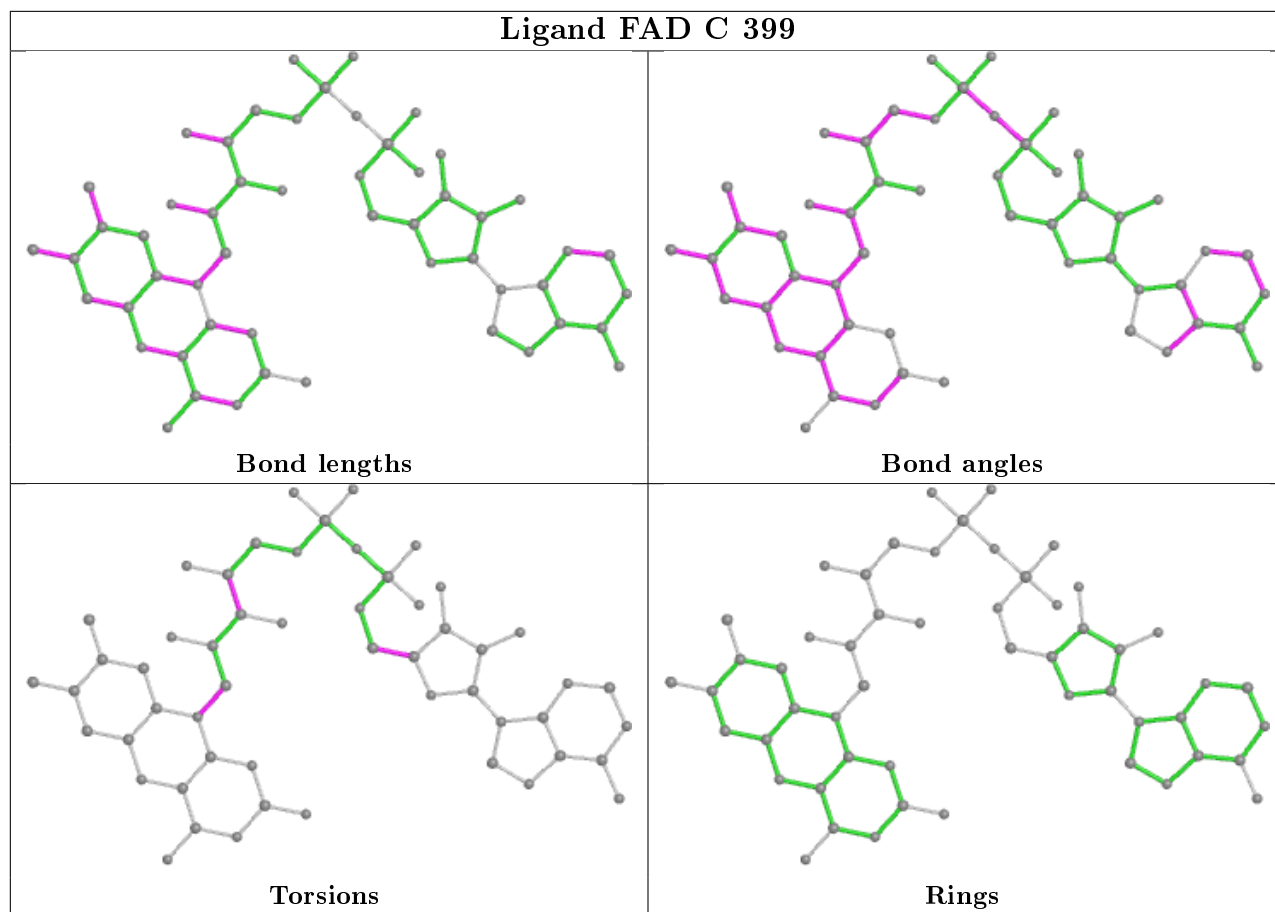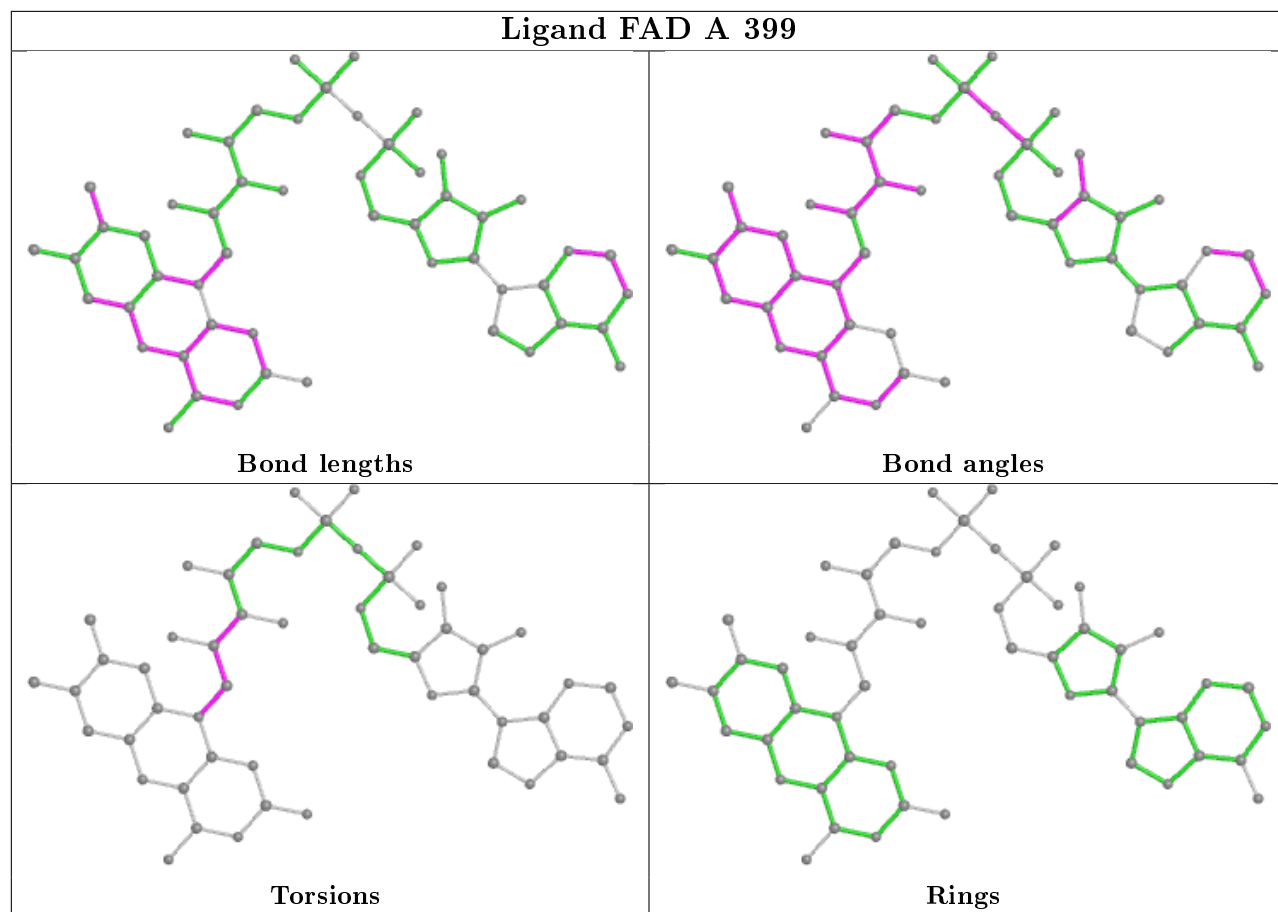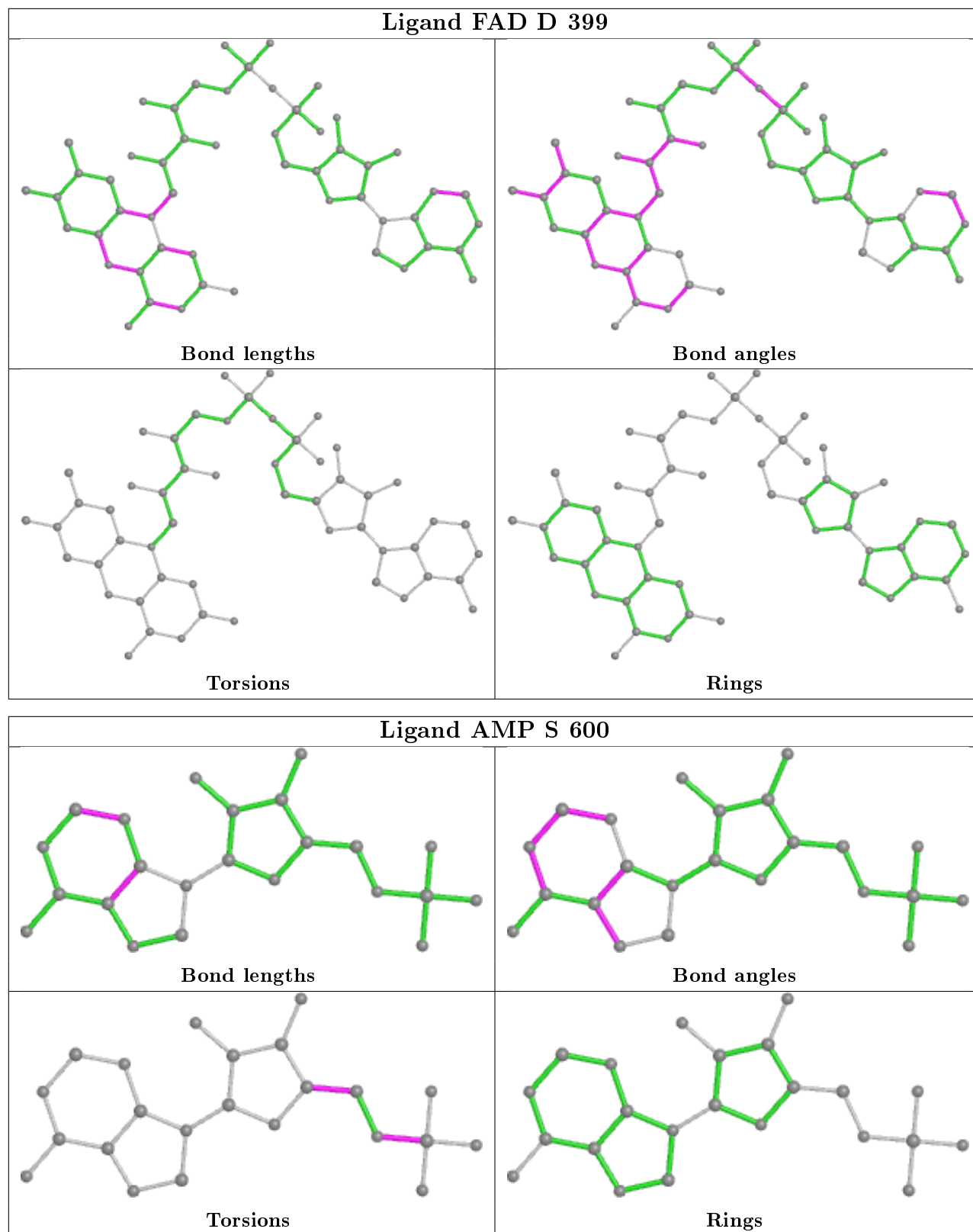
5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	386/396 (97%)	-0.66	1 (0%)	94	94	21, 37, 53, 71	0
1	B	387/396 (97%)	-0.54	3 (0%)	86	86	23, 43, 63, 81	0
1	C	388/396 (97%)	-0.62	1 (0%)	94	94	20, 36, 53, 70	0
1	D	387/396 (97%)	-0.68	1 (0%)	94	94	20, 36, 56, 68	0
2	R	184/333 (55%)	-0.06	4 (2%)	62	59	43, 62, 74, 79	0
3	S	228/255 (89%)	-0.11	7 (3%)	49	44	36, 57, 85, 90	0
All	All	1960/2172 (90%)	-0.51	17 (0%)	84	84	20, 41, 71, 90	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	396	ASN	4.5
2	R	171	THR	3.9
1	C	396	ASN	3.6
3	S	33	GLY	3.3
3	S	32	ASP	3.2
1	D	396	ASN	2.9
1	A	156	ASP	2.9
3	S	219	THR	2.8
3	S	24	PRO	2.7
1	B	155	GLY	2.4
1	B	156	ASP	2.4
3	S	25	ASP	2.3
2	R	182	SER	2.3
3	S	34	VAL	2.2
2	R	181	GLY	2.2
2	R	159	CYS	2.1
3	S	189	GLU	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FAD	A	399	53/53	0.96	0.13	19,28,34,36	0
4	FAD	C	399	53/53	0.97	0.12	24,29,37,39	0
4	FAD	B	399	53/53	0.98	0.10	25,32,37,38	0
4	FAD	D	399	53/53	0.98	0.10	24,31,34,35	0
5	AMP	S	600	23/23	0.98	0.11	37,42,47,51	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 A 399:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
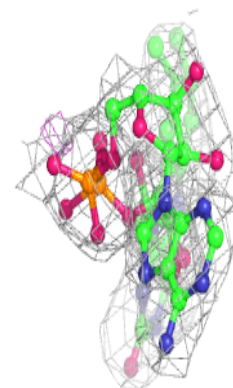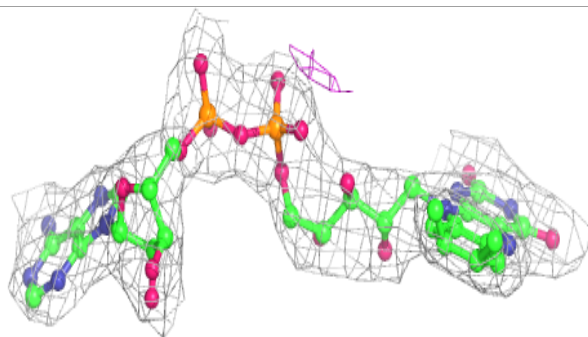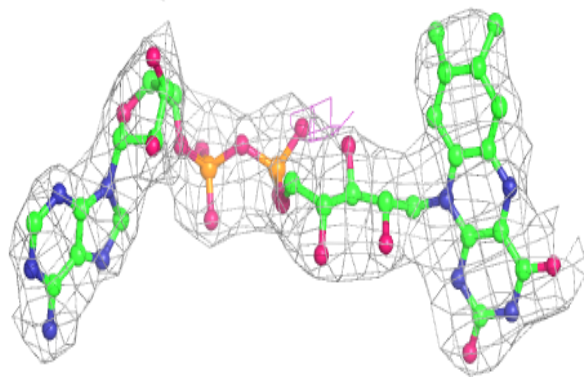and green (positive)
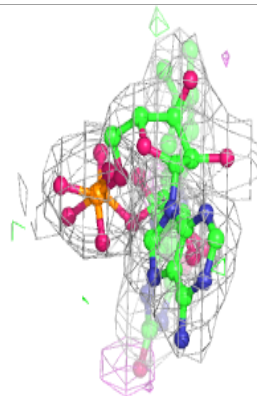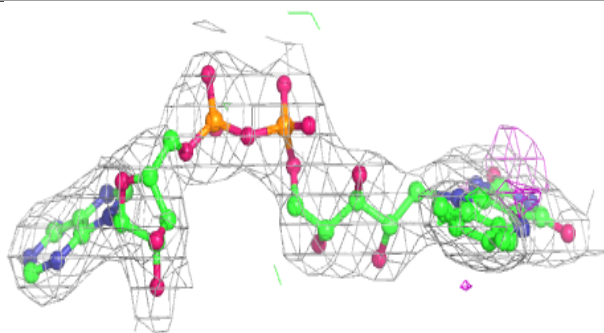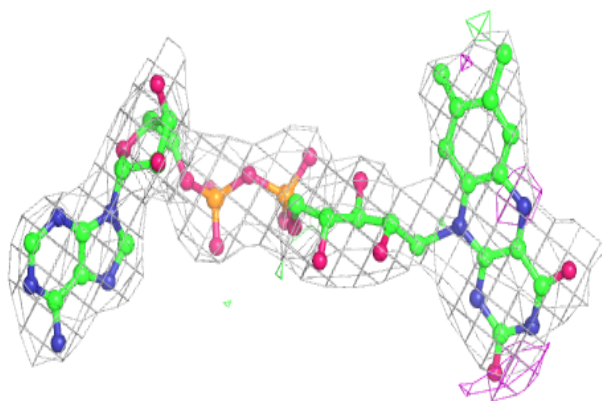
Electron density around FAD C 399:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
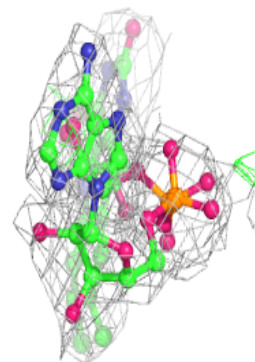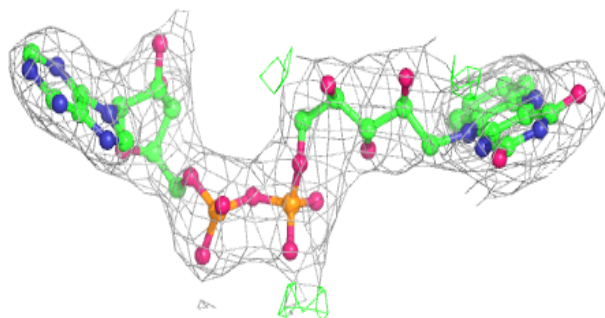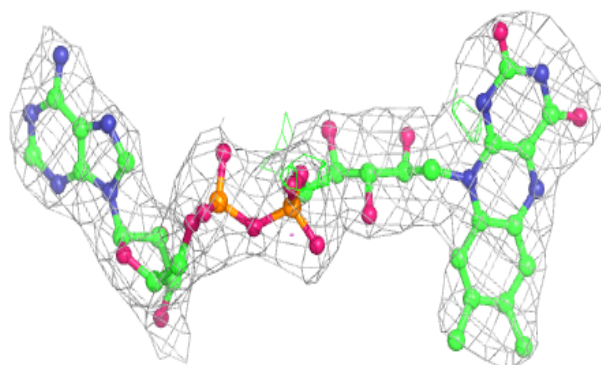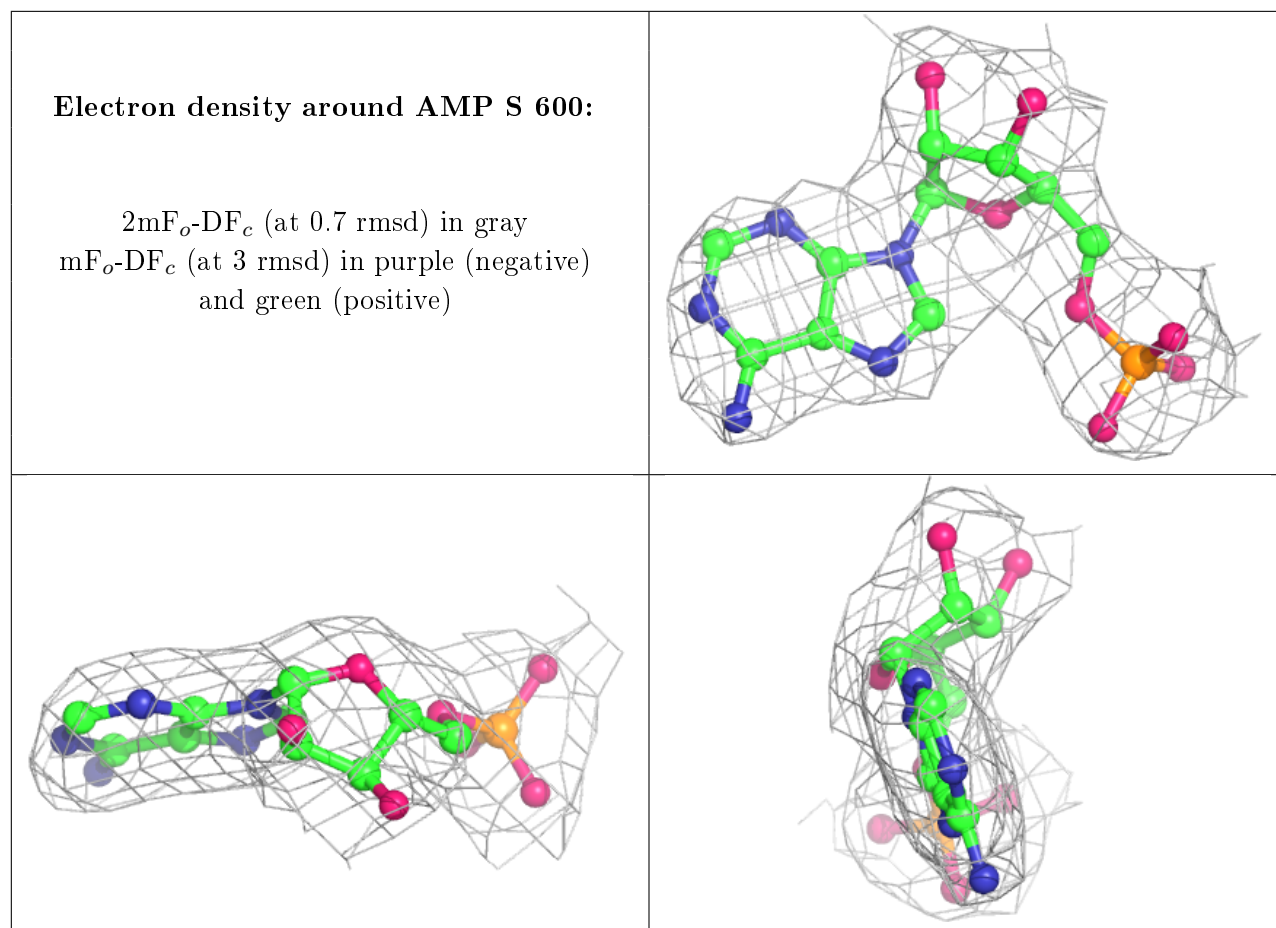and green (positive)
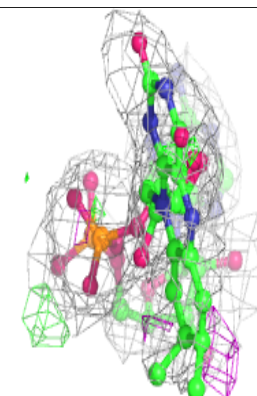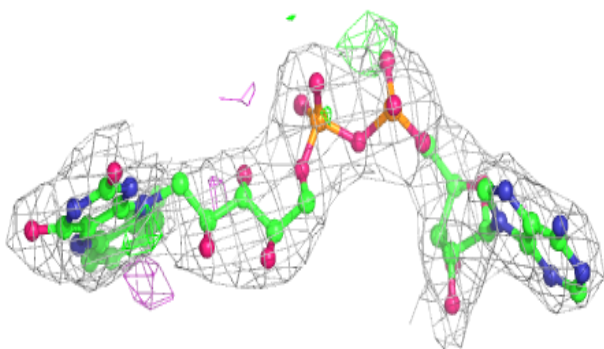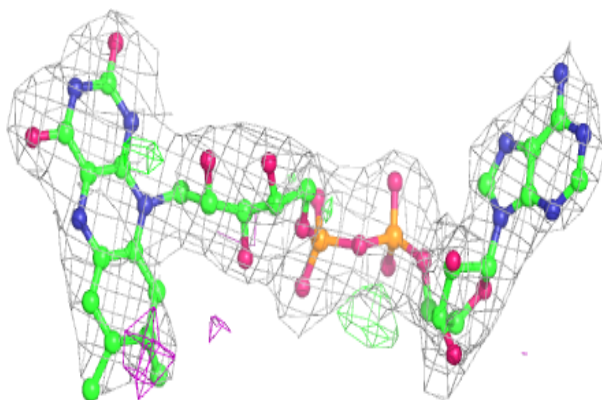
Electron density around FAD B 399:

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

Electron density around FAD D 399:

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

Electron density around AMP S 600:

$2mF_o$-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.