Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:50 AM GMT

PDB ID	:	2UZZ
Title	:	X-ray structure of N-methyl-L-tryptophan oxidase (MTOX)
Authors	:	Ilari, A.; Fiorillo, A.; Franceschini, S.; Bonamore, A.; Colotti, G.; Boffi, A.
Deposited on	:	2007-05-03
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

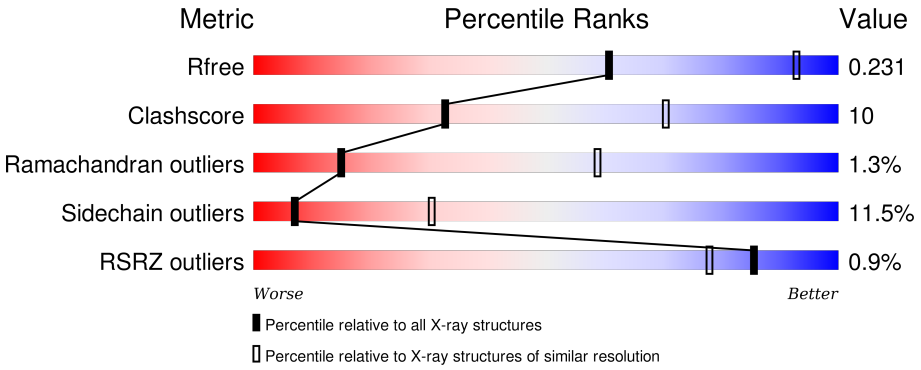
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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. 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	372	70% 25%
1	B	372	72% 23% 5%
1	C	372	69% 26% 5%
1	D	372	75% 21%

2 Entry composition

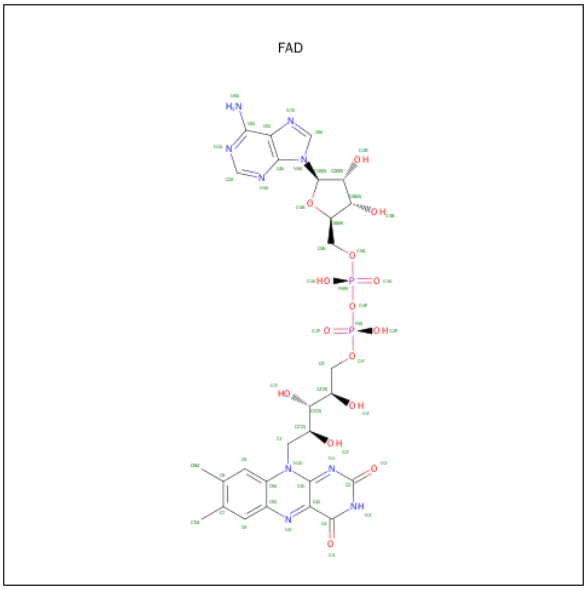
There are 3 unique types of molecules in this entry. The entry contains 11719 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 N-METHYL-L-TRYPTOPHAN OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2881	1833	495	543	10			
1	B	372	Total	C	N	O	S	0	0	0
			2889	1838	496	544	11			
1	C	369	Total	C	N	O	S	0	0	0
			2861	1819	492	540	10			
1	D	370	Total	C	N	O	S	0	0	0
			2872	1828	493	541	10			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

Continued on next page...

Continued from previous page...

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

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

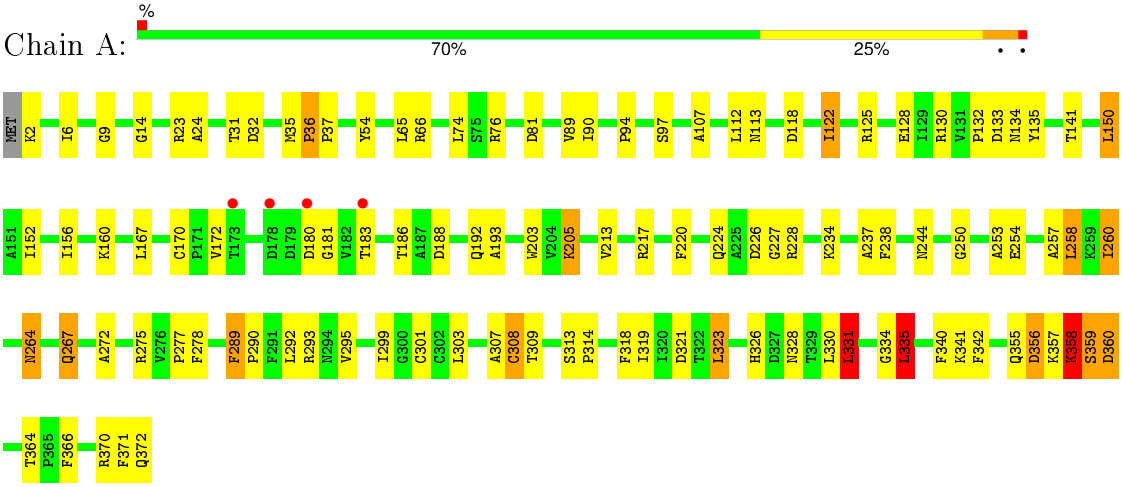
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		

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 errors 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.

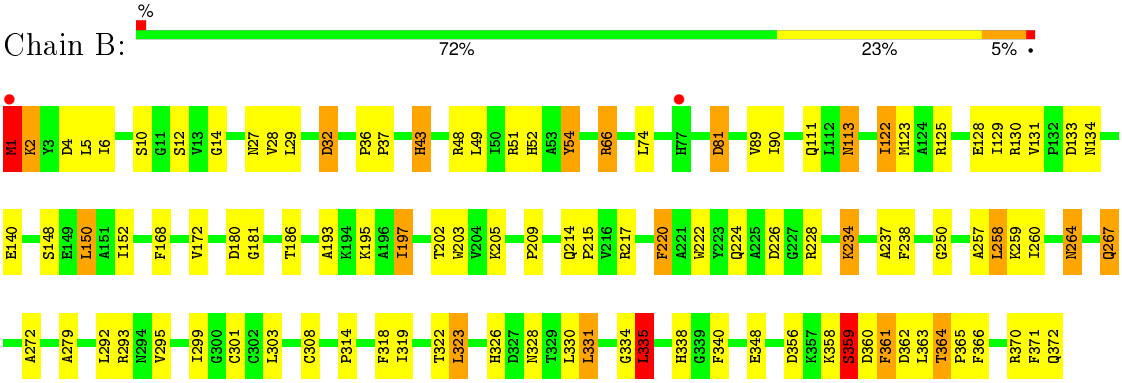
- Molecule 1: N-METHYL-L-TRYPTOPHAN OXIDASE

Chain A:



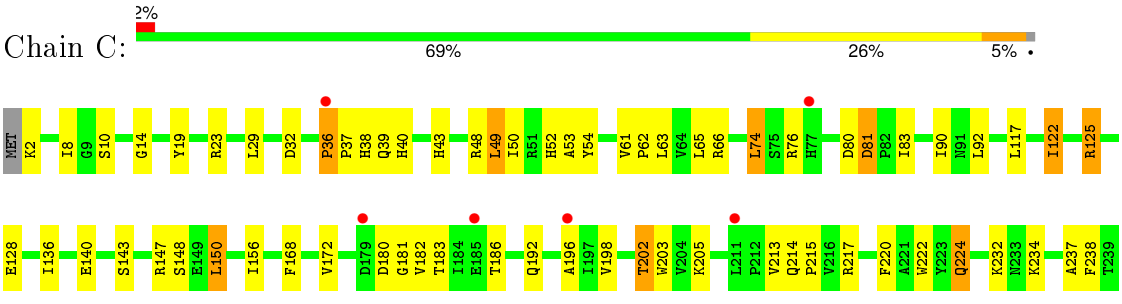
- Molecule 1: N-METHYL-L-TRYPTOPHAN OXIDASE

Chain B:

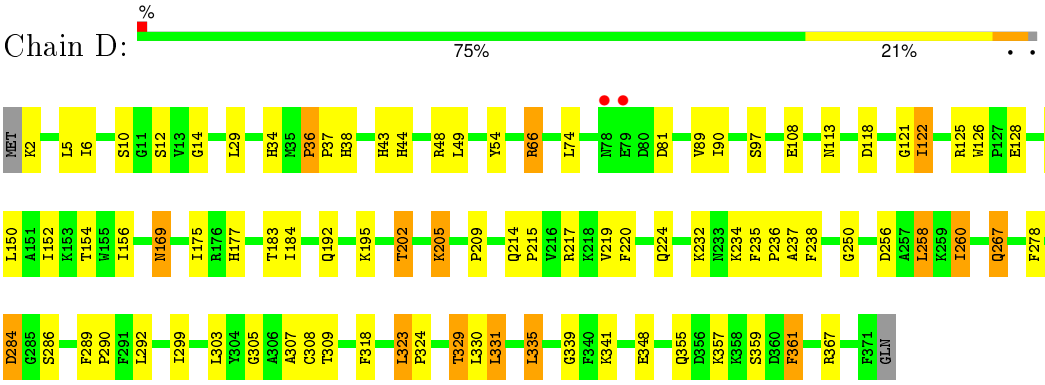


- Molecule 1: N-METHYL-L-TRYPTOPHAN OXIDASE

Chain C:



- Molecule 1: N-METHYL-L-TRYPTOPHAN OXIDASE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	88.19Å 89.81Å 91.92Å 90.00° 104.75° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 40.08 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (40.00-3.20) 99.0 (40.08-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.71 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.236 , 0.313 0.232 , 0.231	Depositor DCC
R_{free} test set	1175 reflections (5.41%)	DCC
Wilson B-factor (Å^2)	49.6	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 34.0	EDS
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 22911 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	11719	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 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	0.44	2/2957 (0.1%)	0.60	5/4020 (0.1%)
1	B	0.38	1/2965 (0.0%)	0.63	4/4030 (0.1%)
1	C	0.33	0/2936	0.55	1/3992 (0.0%)
1	D	0.33	0/2948	0.55	2/4008 (0.0%)
All	All	0.37	3/11806 (0.0%)	0.58	12/16050 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	SER	C-O	10.18	1.42	1.23
1	B	359	SER	C-O	6.40	1.35	1.23
1	A	358	LYS	C-N	-5.79	1.20	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1	MET	O-C-N	-14.45	99.58	122.70
1	B	1	MET	CA-C-N	9.91	139.01	117.20
1	B	331	LEU	CA-CB-CG	6.32	129.83	115.30
1	D	330	LEU	CA-CB-CG	6.06	129.24	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	331	LEU	CA-CB-CG	5.91	128.89	115.30
1	A	359	SER	CA-C-O	-5.75	108.03	120.10
1	A	358	LYS	C-N-CA	5.68	135.91	121.70
1	C	331	LEU	CA-CB-CG	5.62	128.22	115.30
1	A	360	ASP	N-CA-C	5.51	125.88	111.00
1	A	330	LEU	CA-CB-CG	5.44	127.82	115.30
1	A	331	LEU	CA-CB-CG	5.29	127.46	115.30
1	B	330	LEU	CA-CB-CG	5.21	127.30	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	358	LYS	Mainchain
1	A	359	SER	Peptide
1	B	1	MET	Mainchain
1	B	358	LYS	Mainchain,Peptide
1	B	359	SER	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	2881	0	2764	53	1
1	B	2889	0	2777	61	1
1	C	2861	0	2747	63	0
1	D	2872	0	2756	65	0
2	A	53	0	29	6	0
2	B	53	0	29	7	0
2	C	53	0	29	6	0
2	D	53	0	29	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	11719	0	11160	238	1

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 10.

All (238) 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:308:CYS:SG	2:A:1373:FAD:HM71	1.49	1.47
1:A:308:CYS:SG	2:A:1373:FAD:C7M	2.29	1.17
1:D:220:PHE:CD2	2:D:1372:FAD:HM72	1.83	1.12
1:D:220:PHE:HD2	2:D:1372:FAD:HM72	1.11	1.10
1:C:125:ARG:HH11	1:C:125:ARG:HG2	1.17	1.06
1:D:38:HIS:H	1:D:43:HIS:HE1	1.11	0.97
1:A:125:ARG:HH11	1:A:125:ARG:HG2	1.38	0.87
1:D:125:ARG:HG2	1:D:125:ARG:HH11	1.43	0.82
1:C:125:ARG:CG	1:C:125:ARG:HH11	1.93	0.81
1:A:357:LYS:HG2	1:A:358:LYS:H	1.51	0.75
1:C:258:LEU:HD12	1:C:260:ILE:HD11	1.69	0.74
1:C:38:HIS:H	1:C:43:HIS:HE1	1.36	0.73
1:B:1:MET:O	1:B:2:LYS:HB2	1.88	0.73
1:C:258:LEU:HD12	1:C:260:ILE:CD1	2.19	0.72
1:D:38:HIS:H	1:D:43:HIS:CE1	2.03	0.72
1:A:258:LEU:HD12	1:A:260:ILE:CD1	2.19	0.72
1:B:220:PHE:CD2	2:B:1373:FAD:HM72	2.25	0.71
1:B:81:ASP:HB3	1:B:150:LEU:HD11	1.72	0.71
1:D:202:THR:HG21	1:D:309:THR:HB	1.73	0.70
1:C:220:PHE:HD2	2:C:1371:FAD:HM72	1.56	0.70
1:C:220:PHE:CD2	2:C:1371:FAD:HM72	2.25	0.70
1:B:181:GLY:HA2	1:B:328:ASN:HD21	1.56	0.70
1:C:292:LEU:HD22	1:C:299:ILE:HG21	1.75	0.69
1:A:36:PRO:HB2	1:A:37:PRO:HD3	1.74	0.69
1:B:258:LEU:HD12	1:B:260:ILE:CD1	2.24	0.68
1:B:258:LEU:HD12	1:B:260:ILE:HD11	1.76	0.68
1:C:10:SER:HA	1:C:14:GLY:HA3	1.77	0.67
1:A:125:ARG:HG2	1:A:125:ARG:NH1	2.10	0.67
1:C:36:PRO:HB2	1:C:37:PRO:HD3	1.76	0.67
1:A:258:LEU:HD12	1:A:260:ILE:HD13	1.76	0.66
1:C:125:ARG:NH1	1:C:125:ARG:HG2	1.97	0.66
1:B:1:MET:O	1:B:2:LYS:CB	2.42	0.66
1:C:2:LYS:HA	1:C:192:GLN:O	1.97	0.65
1:B:122:ILE:HD11	1:B:131:VAL:HG21	1.80	0.63
1:B:172:VAL:HA	1:B:186:THR:HG22	1.81	0.63
1:C:364:THR:O	1:C:367:ARG:HG3	1.98	0.63
1:C:323:LEU:HG	1:C:324:PRO:HD2	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:CYS:HB3	2:B:1373:FAD:HM71	1.81	0.62
1:A:224:GLN:HE21	1:A:301:CYS:H	1.44	0.62
1:D:260:ILE:HG13	1:D:292:LEU:HD11	1.82	0.62
1:D:323:LEU:HD23	1:D:324:PRO:HD2	1.80	0.61
1:A:220:PHE:CD2	2:A:1373:FAD:HM72	2.35	0.60
1:C:318:PHE:CD2	1:C:335:LEU:HA	2.37	0.60
1:C:81:ASP:HB3	1:C:150:LEU:HD11	1.83	0.59
1:D:335:LEU:HD13	2:D:1372:FAD:H5'2	1.85	0.59
1:B:340:PHE:HB2	2:B:1373:FAD:H2'	1.85	0.59
1:C:303:LEU:HD22	1:D:286:SER:HB3	1.82	0.59
1:A:226:ASP:OD1	1:A:228:ARG:HG2	2.03	0.59
1:A:118:ASP:O	1:A:122:ILE:HG12	2.03	0.59
1:A:371:PHE:O	1:A:372:GLN:HB2	2.03	0.59
1:C:304:TYR:CZ	1:D:282:VAL:HG12	2.39	0.58
1:A:181:GLY:C	1:A:328:ASN:HD21	2.07	0.58
1:A:357:LYS:HG2	1:A:358:LYS:N	2.17	0.58
1:D:217:ARG:HB3	1:D:267:GLN:HG2	1.84	0.57
1:D:10:SER:HA	1:D:14:GLY:HA3	1.87	0.57
1:A:170:CYS:SG	1:A:188:ASP:HB2	2.44	0.57
1:A:81:ASP:HB3	1:A:150:LEU:HD11	1.87	0.57
1:D:220:PHE:HD2	2:D:1372:FAD:C7M	2.00	0.57
1:C:335:LEU:HD13	2:C:1371:FAD:H5'2	1.87	0.57
1:C:224:GLN:HE21	1:C:301:CYS:H	1.53	0.57
1:C:202:THR:HG22	1:C:311:ASP:HB2	1.87	0.56
1:B:319:ILE:H	1:B:334:GLY:HA3	1.70	0.56
1:B:123:MET:HG2	1:B:129:ILE:O	2.05	0.56
1:D:220:PHE:CE2	2:D:1372:FAD:HM72	2.38	0.56
1:B:319:ILE:N	1:B:334:GLY:HA3	2.20	0.56
1:A:264:ASN:ND2	1:A:264:ASN:H	2.04	0.56
1:B:217:ARG:HB3	1:B:267:GLN:HG2	1.87	0.56
1:C:147:ARG:NH2	1:C:254:GLU:OE1	2.39	0.56
1:C:238:PHE:CZ	1:C:250:GLY:HA3	2.41	0.55
1:C:264:ASN:H	1:C:264:ASN:HD22	1.54	0.55
1:C:308:CYS:HB3	2:C:1371:FAD:HM71	1.87	0.55
1:A:253:ALA:HA	1:A:257:ALA:O	2.07	0.55
1:A:172:VAL:HA	1:A:186:THR:HG22	1.88	0.55
1:D:36:PRO:HB2	1:D:37:PRO:HD3	1.88	0.55
1:B:36:PRO:HB2	1:B:37:PRO:HD3	1.88	0.55
1:D:175:ILE:HG12	1:D:184:ILE:HG22	1.89	0.54
1:B:10:SER:HA	1:B:14:GLY:HA3	1.89	0.54
1:A:301:CYS:HG	1:B:301:CYS:HG	1.50	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLN:HB3	1:A:303:LEU:HD21	1.90	0.53
1:A:264:ASN:HD22	1:A:264:ASN:H	1.57	0.53
1:D:34:HIS:HA	1:D:169:ASN:ND2	2.24	0.53
1:A:94:PRO:HG2	1:A:97:SER:HB3	1.91	0.52
1:C:278:PHE:CG	1:C:305:GLY:HA3	2.45	0.52
1:D:278:PHE:O	1:D:284:ASP:OD2	2.28	0.52
1:B:5:LEU:HD11	1:B:197:ILE:HD12	1.92	0.52
1:D:260:ILE:HD12	1:D:292:LEU:HD21	1.92	0.52
1:D:224:GLN:HB3	1:D:303:LEU:HD21	1.92	0.52
1:D:292:LEU:HD22	1:D:299:ILE:HG21	1.91	0.51
1:C:222:TRP:HB3	1:C:257:ALA:HB1	1.92	0.51
1:B:238:PHE:CZ	1:B:250:GLY:HA3	2.45	0.51
1:A:340:PHE:HB2	2:A:1373:FAD:H2'	1.93	0.51
1:C:224:GLN:HB3	1:C:303:LEU:HD21	1.90	0.51
1:D:6:ILE:HG21	1:D:184:ILE:HG12	1.92	0.51
1:A:275:ARG:HD2	1:A:307:ALA:O	2.11	0.51
1:B:52:HIS:HB2	1:B:140:GLU:OE1	2.10	0.51
1:D:318:PHE:CD2	1:D:335:LEU:HA	2.46	0.50
1:A:238:PHE:CZ	1:A:250:GLY:HA3	2.46	0.50
1:C:258:LEU:HD12	1:C:260:ILE:HD13	1.94	0.50
1:C:36:PRO:O	1:C:43:HIS:CE1	2.65	0.50
1:B:318:PHE:CD2	1:B:335:LEU:HA	2.46	0.50
1:D:38:HIS:O	1:D:44:HIS:HB3	2.10	0.50
1:B:130:ARG:O	1:B:295:VAL:HA	2.12	0.50
1:D:66:ARG:HG3	1:D:361:PHE:HZ	1.75	0.50
1:C:62:PRO:HG2	1:C:63:LEU:HD12	1.93	0.50
1:C:289:PHE:N	1:C:290:PRO:HD2	2.28	0.49
1:A:89:VAL:HA	1:A:237:ALA:O	2.12	0.49
1:B:292:LEU:HD22	1:B:299:ILE:HG12	1.94	0.49
1:D:238:PHE:CZ	1:D:250:GLY:HA3	2.48	0.49
1:B:224:GLN:HE21	1:B:301:CYS:H	1.61	0.49
1:A:107:ALA:HA	1:A:112:LEU:HD12	1.94	0.49
1:C:364:THR:N	1:C:365:PRO:HD2	2.28	0.49
1:B:32:ASP:O	1:B:168:PHE:O	2.31	0.49
1:C:172:VAL:HA	1:C:186:THR:HG22	1.94	0.49
1:A:292:LEU:HD22	1:A:299:ILE:HG21	1.95	0.48
1:D:49:LEU:O	1:D:341:LYS:HE3	2.13	0.48
1:D:202:THR:HG21	1:D:309:THR:CB	2.43	0.48
1:A:289:PHE:N	1:A:290:PRO:HD2	2.27	0.48
1:B:205:LYS:O	1:B:209:PRO:HA	2.13	0.48
1:D:38:HIS:N	1:D:43:HIS:HE1	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:TYR:OH	1:B:338:HIS:HB2	2.14	0.48
1:B:6:ILE:HG13	1:B:193:ALA:HB2	1.95	0.48
1:C:340:PHE:HB2	2:C:1371:FAD:H2'	1.95	0.48
1:A:357:LYS:CG	1:A:358:LYS:H	2.22	0.48
1:B:125:ARG:HH12	1:B:234:LYS:HB3	1.78	0.48
1:C:203:TRP:CZ2	1:C:272:ALA:HA	2.49	0.48
1:D:5:LEU:HA	1:D:195:LYS:O	2.13	0.48
1:B:258:LEU:HD12	1:B:260:ILE:HD13	1.95	0.48
1:C:196:ALA:HB3	1:C:329:THR:HG22	1.95	0.47
1:B:220:PHE:CE2	2:B:1373:FAD:HM72	2.50	0.47
1:D:125:ARG:NH1	1:D:125:ARG:HG2	2.20	0.47
1:D:278:PHE:CD2	1:D:305:GLY:HA3	2.50	0.47
1:D:278:PHE:CG	1:D:305:GLY:HA3	2.50	0.47
1:A:205:LYS:HE2	1:A:213:VAL:O	2.14	0.47
1:D:118:ASP:HB3	1:D:121:GLY:H	1.80	0.47
1:A:323:LEU:HD22	1:A:326:HIS:HD2	1.78	0.47
1:C:276:VAL:HG12	1:C:277:PRO:HD2	1.96	0.47
1:B:314:PRO:HG2	1:B:371:PHE:CE1	2.50	0.47
1:A:220:PHE:CE2	2:A:1373:FAD:HM72	2.50	0.46
1:C:38:HIS:HD1	1:C:40:HIS:H	1.61	0.46
1:A:203:TRP:CZ2	1:A:272:ALA:HA	2.50	0.46
1:D:202:THR:HG22	1:D:215:PRO:HB3	1.97	0.46
1:C:74:LEU:HD13	1:C:83:ILE:HD13	1.98	0.46
1:D:308:CYS:HB3	2:D:1372:FAD:HM71	1.97	0.46
1:A:130:ARG:O	1:A:295:VAL:HA	2.15	0.46
1:D:205:LYS:O	1:D:209:PRO:HA	2.15	0.46
1:D:308:CYS:SG	1:D:309:THR:N	2.88	0.46
1:B:359:SER:HB2	1:B:361:PHE:O	2.16	0.46
1:B:1:MET:SD	1:B:180:ASP:HB3	2.56	0.46
1:D:152:ILE:HG22	1:D:156:ILE:HD13	1.97	0.46
1:D:48:ARG:HD2	2:D:1372:FAD:C10	2.45	0.46
1:C:48:ARG:HD2	2:C:1371:FAD:C10	2.46	0.46
1:A:24:ALA:HB1	1:A:355:GLN:HE22	1.80	0.46
1:A:308:CYS:SG	1:A:309:THR:N	2.88	0.46
1:D:36:PRO:O	1:D:43:HIS:CE1	2.68	0.46
1:B:222:TRP:CE2	1:B:259:LYS:HG3	2.51	0.46
1:D:122:ILE:HG22	1:D:126:TRP:HZ3	1.81	0.45
1:A:217:ARG:HD3	1:A:267:GLN:OE1	2.16	0.45
1:B:66:ARG:NH1	1:B:348:GLU:OE1	2.49	0.45
1:B:203:TRP:CZ2	1:B:272:ALA:HA	2.51	0.45
1:D:125:ARG:CG	1:D:125:ARG:HH11	2.20	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:SER:OG	2:B:1373:FAD:O5'	2.34	0.45
1:B:264:ASN:HD22	1:B:264:ASN:H	1.65	0.45
1:B:364:THR:N	1:B:365:PRO:HD2	2.32	0.45
1:D:177:HIS:HE1	1:D:329:THR:CG2	2.29	0.45
1:D:258:LEU:HD12	1:D:260:ILE:CD1	2.48	0.44
1:C:181:GLY:C	1:C:328:ASN:HD21	2.20	0.44
1:C:52:HIS:HB2	1:C:140:GLU:OE1	2.18	0.44
1:A:132:PRO:O	1:A:135:TYR:HB2	2.18	0.44
1:C:278:PHE:CD2	1:C:305:GLY:HA3	2.53	0.44
1:A:318:PHE:CD2	1:A:335:LEU:HA	2.53	0.44
1:D:89:VAL:HA	1:D:237:ALA:O	2.18	0.44
1:C:198:VAL:HB	1:C:331:LEU:HB2	2.00	0.44
1:C:8:ILE:HD13	1:C:198:VAL:HG22	1.99	0.44
1:B:148:SER:O	1:B:152:ILE:HG12	2.17	0.44
1:D:289:PHE:N	1:D:290:PRO:HD2	2.32	0.44
1:A:152:ILE:HG22	1:A:156:ILE:HD13	2.00	0.44
1:B:222:TRP:HB3	1:B:257:ALA:HB1	1.99	0.43
1:C:182:VAL:HG22	1:C:328:ASN:ND2	2.32	0.43
1:D:183:THR:HG22	1:D:192:GLN:HB3	1.98	0.43
1:C:92:LEU:O	1:C:240:GLY:HA2	2.18	0.43
1:D:214:GLN:HA	1:D:215:PRO:HD2	1.90	0.43
1:B:122:ILE:CD1	1:B:131:VAL:HG21	2.48	0.43
1:B:48:ARG:HD2	2:B:1373:FAD:C10	2.47	0.43
1:D:284:ASP:N	1:D:284:ASP:OD1	2.50	0.43
1:A:278:PHE:HD1	1:B:279:ALA:HB2	1.83	0.43
1:C:50:ILE:O	1:C:143:SER:OG	2.35	0.43
1:D:66:ARG:NH1	1:D:348:GLU:OE1	2.52	0.43
1:C:293:ARG:HD3	1:C:293:ARG:O	2.19	0.43
1:A:319:ILE:N	1:A:334:GLY:HA3	2.34	0.43
1:C:61:VAL:N	1:C:62:PRO:HD2	2.34	0.43
1:D:232:LYS:HD3	1:D:232:LYS:HA	1.89	0.43
1:A:6:ILE:HG13	1:A:193:ALA:HB2	2.01	0.43
1:A:9:GLY:O	1:A:14:GLY:HA3	2.19	0.42
1:D:12:SER:HA	1:D:152:ILE:CD1	2.49	0.42
1:B:214:GLN:HA	1:B:215:PRO:HD2	1.94	0.42
1:A:31:THR:HA	1:A:167:LEU:O	2.20	0.42
1:B:366:PHE:HA	1:B:370:ARG:NH2	2.34	0.42
1:C:301:CYS:SG	1:D:289:PHE:HZ	2.43	0.42
1:B:36:PRO:O	1:B:43:HIS:CE1	2.73	0.42
1:A:313:SER:HB2	1:A:314:PRO:HD2	2.00	0.42
1:C:214:GLN:HA	1:C:215:PRO:HD2	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:LYS:HE3	1:B:356:ASP:OD1	2.19	0.42
1:C:220:PHE:CD1	1:C:306:ALA:HB2	2.54	0.42
1:D:49:LEU:HD11	1:D:237:ALA:HB1	2.01	0.42
1:D:148:SER:O	1:D:152:ILE:HG12	2.20	0.42
1:B:49:LEU:HD11	1:B:237:ALA:HB1	2.01	0.42
1:B:48:ARG:HD2	2:B:1373:FAD:C4X	2.50	0.42
1:C:148:SER:HA	1:C:340:PHE:CZ	2.55	0.42
1:C:19:TYR:CZ	1:C:23:ARG:HD3	2.55	0.42
1:B:113:ASN:HD22	1:B:113:ASN:C	2.23	0.42
1:D:339:GLY:H	2:D:1372:FAD:H1'2	1.84	0.41
1:A:321:ASP:O	1:A:331:LEU:HD13	2.20	0.41
1:C:49:LEU:HD11	1:C:237:ALA:HB1	2.02	0.41
1:B:224:GLN:HB3	1:B:303:LEU:HD21	2.02	0.41
1:B:51:ARG:HG2	1:B:89:VAL:HG11	2.01	0.41
1:B:226:ASP:OD1	1:B:228:ARG:HG2	2.19	0.41
1:A:371:PHE:O	1:A:372:GLN:CB	2.68	0.41
1:D:48:ARG:HD2	2:D:1372:FAD:C4X	2.50	0.41
1:B:361:PHE:CD1	1:B:361:PHE:N	2.88	0.41
1:C:217:ARG:HB3	1:C:267:GLN:HG2	2.02	0.41
1:B:12:SER:HA	1:B:152:ILE:HD12	2.02	0.41
1:D:355:GLN:C	1:D:357:LYS:H	2.24	0.41
1:C:125:ARG:NH1	1:C:125:ARG:CG	2.62	0.41
1:D:122:ILE:HG12	1:D:122:ILE:H	1.72	0.41
1:C:205:LYS:HE2	1:C:213:VAL:O	2.21	0.41
1:D:12:SER:HA	1:D:152:ILE:HD12	2.02	0.41
1:C:319:ILE:H	1:C:334:GLY:HA3	1.85	0.41
1:A:366:PHE:HA	1:A:370:ARG:NH2	2.35	0.41
1:B:4:ASP:N	1:B:27:ASN:O	2.51	0.41
1:C:122:ILE:HG12	1:C:122:ILE:H	1.61	0.41
1:B:5:LEU:HB3	1:B:28:VAL:HG22	2.02	0.41
1:C:32:ASP:O	1:C:168:PHE:O	2.39	0.40
2:A:1373:FAD:H1'1	2:A:1373:FAD:H9	1.81	0.40
1:B:323:LEU:HD22	1:B:326:HIS:HD2	1.86	0.40
1:A:341:LYS:HG3	1:A:342:PHE:CD1	2.55	0.40
1:D:235:PHE:HA	1:D:236:PRO:HD3	1.93	0.40
1:D:125:ARG:NH1	1:D:125:ARG:CG	2.82	0.40
1:D:2:LYS:O	1:D:2:LYS:HG3	2.20	0.40

All (1) 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:357:LYS:CE	1:B:359:SER:OG[1_545]	1.67	0.53

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	369/372 (99%)	327 (89%)	35 (10%)	7 (2%)	10	50
1	B	370/372 (100%)	327 (88%)	40 (11%)	3 (1%)	24	69
1	C	367/372 (99%)	328 (89%)	34 (9%)	5 (1%)	14	57
1	D	368/372 (99%)	335 (91%)	29 (8%)	4 (1%)	17	62
All	All	1474/1488 (99%)	1317 (89%)	138 (9%)	19 (1%)	15	59

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	ASP
1	B	360	ASP
1	C	247	GLN
1	A	335	LEU
1	B	2	LYS
1	C	224	GLN
1	A	36	PRO
1	D	256	ASP
1	A	356	ASP
1	C	36	PRO
1	C	53	ALA
1	C	307	ALA
1	D	169	ASN
1	A	254	GLU
1	B	335	LEU
1	D	307	ALA
1	A	227	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	277	PRO
1	D	36	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	299/301 (99%)	263 (88%)	36 (12%)	6	28
1	B	300/301 (100%)	268 (89%)	32 (11%)	8	34
1	C	297/301 (99%)	258 (87%)	39 (13%)	5	24
1	D	298/301 (99%)	268 (90%)	30 (10%)	9	36
All	All	1194/1204 (99%)	1057 (88%)	137 (12%)	7	30

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	23	ARG
1	A	32	ASP
1	A	35	MET
1	A	54	TYR
1	A	65	LEU
1	A	66	ARG
1	A	74	LEU
1	A	76	ARG
1	A	90	ILE
1	A	113	ASN
1	A	122	ILE
1	A	128	GLU
1	A	133	ASP
1	A	134	ASN
1	A	141	THR
1	A	150	LEU
1	A	160	LYS
1	A	180	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	183	THR
1	A	192	GLN
1	A	205	LYS
1	A	234	LYS
1	A	244	ASN
1	A	258	LEU
1	A	260	ILE
1	A	264	ASN
1	A	267	GLN
1	A	289	PHE
1	A	293	ARG
1	A	308	CYS
1	A	323	LEU
1	A	331	LEU
1	A	335	LEU
1	A	356	ASP
1	A	364	THR
1	B	29	LEU
1	B	32	ASP
1	B	43	HIS
1	B	54	TYR
1	B	66	ARG
1	B	74	LEU
1	B	81	ASP
1	B	90	ILE
1	B	111	GLN
1	B	113	ASN
1	B	122	ILE
1	B	128	GLU
1	B	133	ASP
1	B	134	ASN
1	B	150	LEU
1	B	197	ILE
1	B	202	THR
1	B	220	PHE
1	B	234	LYS
1	B	258	LEU
1	B	264	ASN
1	B	267	GLN
1	B	293	ARG
1	B	322	THR
1	B	323	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	331	LEU
1	B	335	LEU
1	B	361	PHE
1	B	362	ASP
1	B	363	LEU
1	B	364	THR
1	B	372	GLN
1	C	29	LEU
1	C	39	GLN
1	C	49	LEU
1	C	54	TYR
1	C	65	LEU
1	C	66	ARG
1	C	74	LEU
1	C	76	ARG
1	C	80	ASP
1	C	81	ASP
1	C	90	ILE
1	C	117	LEU
1	C	122	ILE
1	C	125	ARG
1	C	128	GLU
1	C	136	ILE
1	C	150	LEU
1	C	156	ILE
1	C	180	ASP
1	C	183	THR
1	C	202	THR
1	C	232	LYS
1	C	234	LYS
1	C	258	LEU
1	C	260	ILE
1	C	264	ASN
1	C	267	GLN
1	C	276	VAL
1	C	281	VAL
1	C	293	ARG
1	C	323	LEU
1	C	331	LEU
1	C	335	LEU
1	C	356	ASP
1	C	358	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	359	SER
1	C	361	PHE
1	C	362	ASP
1	C	370	ARG
1	D	29	LEU
1	D	54	TYR
1	D	66	ARG
1	D	74	LEU
1	D	81	ASP
1	D	90	ILE
1	D	97	SER
1	D	108	GLU
1	D	113	ASN
1	D	122	ILE
1	D	128	GLU
1	D	136	ILE
1	D	150	LEU
1	D	154	THR
1	D	202	THR
1	D	205	LYS
1	D	219	VAL
1	D	234	LYS
1	D	258	LEU
1	D	260	ILE
1	D	267	GLN
1	D	281	VAL
1	D	284	ASP
1	D	323	LEU
1	D	329	THR
1	D	331	LEU
1	D	335	LEU
1	D	359	SER
1	D	361	PHE
1	D	367	ARG

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

Mol	Chain	Res	Type
1	A	43	HIS
1	A	113	ASN
1	A	177	HIS
1	A	224	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	244	ASN
1	A	264	ASN
1	A	326	HIS
1	A	328	ASN
1	A	338	HIS
1	A	355	GLN
1	B	91	ASN
1	B	111	GLN
1	B	113	ASN
1	B	177	HIS
1	B	192	GLN
1	B	224	GLN
1	B	264	ASN
1	B	326	HIS
1	B	328	ASN
1	C	43	HIS
1	C	177	HIS
1	C	192	GLN
1	C	224	GLN
1	C	233	ASN
1	C	264	ASN
1	C	328	ASN
1	C	338	HIS
1	D	34	HIS
1	D	43	HIS
1	D	68	GLN
1	D	157	GLN
1	D	177	HIS
1	D	192	GLN
1	D	264	ASN
1	D	294	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	A	1373	1	48,58,58	1.24	6 (12%)	54,89,89	2.14	6 (11%)
2	FAD	B	1373	1,3	48,58,58	1.19	4 (8%)	54,89,89	2.10	6 (11%)
2	FAD	C	1371	1	48,58,58	1.23	6 (12%)	54,89,89	2.11	7 (12%)
2	FAD	D	1372	1,3	48,58,58	1.22	6 (12%)	54,89,89	2.07	6 (11%)

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
2	FAD	A	1373	1	-	0/30/50/50	0/6/6/6
2	FAD	B	1373	1,3	-	0/30/50/50	0/6/6/6
2	FAD	C	1371	1	-	0/30/50/50	0/6/6/6
2	FAD	D	1372	1,3	-	0/30/50/50	0/6/6/6

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1372	FAD	C5X-N5	2.01	1.38	1.35
2	D	1372	FAD	C1'-N10	2.09	1.50	1.48
2	C	1371	FAD	C10-N1	2.10	1.39	1.35
2	A	1373	FAD	C1'-N10	2.16	1.50	1.48
2	A	1373	FAD	C5X-N5	2.25	1.38	1.35
2	C	1371	FAD	C1'-N10	2.32	1.50	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1371	FAD	C2A-N1A	2.56	1.38	1.33
2	A	1373	FAD	C2A-N1A	2.63	1.38	1.33
2	B	1373	FAD	C2A-N1A	2.66	1.39	1.33
2	D	1372	FAD	C2A-N1A	2.70	1.39	1.33
2	D	1372	FAD	C4-N3	2.86	1.38	1.33
2	B	1373	FAD	C4-N3	3.00	1.38	1.33
2	B	1373	FAD	C4X-N5	3.15	1.38	1.33
2	A	1373	FAD	C4-N3	3.15	1.39	1.33
2	C	1371	FAD	C4-N3	3.28	1.39	1.33
2	D	1372	FAD	C4X-N5	3.33	1.38	1.33
2	C	1371	FAD	C4X-N5	3.34	1.38	1.33
2	B	1373	FAD	C2A-N3A	3.53	1.38	1.32
2	A	1373	FAD	C4X-N5	3.56	1.38	1.33
2	C	1371	FAD	C2A-N3A	3.65	1.38	1.32
2	D	1372	FAD	C2A-N3A	3.66	1.38	1.32
2	A	1373	FAD	C2A-N3A	3.81	1.38	1.32

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1373	FAD	N3A-C2A-N1A	-12.13	119.60	128.89
2	A	1373	FAD	N3A-C2A-N1A	-11.67	119.96	128.89
2	C	1371	FAD	N3A-C2A-N1A	-11.66	119.97	128.89
2	D	1372	FAD	N3A-C2A-N1A	-11.58	120.03	128.89
2	C	1371	FAD	P-O3P-PA	-4.16	121.05	132.73
2	B	1373	FAD	P-O3P-PA	-3.99	121.52	132.73
2	D	1372	FAD	P-O3P-PA	-3.98	121.54	132.73
2	A	1373	FAD	P-O3P-PA	-3.37	123.28	132.73
2	A	1373	FAD	C4X-C4-N3	-2.80	119.76	123.59
2	D	1372	FAD	C4X-C4-N3	-2.64	119.98	123.59
2	C	1371	FAD	C4X-C4-N3	-2.63	120.00	123.59
2	B	1373	FAD	C4X-C4-N3	-2.33	120.41	123.59
2	C	1371	FAD	O4B-C1B-N9A	2.41	113.15	108.10
2	C	1371	FAD	C5X-C9A-N10	2.73	119.70	117.62
2	D	1372	FAD	C5X-C9A-N10	2.74	119.70	117.62
2	B	1373	FAD	C5X-C9A-N10	2.80	119.75	117.62
2	C	1371	FAD	C4X-N5-C5X	2.89	120.09	116.76
2	B	1373	FAD	C4X-N5-C5X	2.89	120.09	116.76
2	A	1373	FAD	C4X-N5-C5X	2.90	120.10	116.76
2	D	1372	FAD	C4X-N5-C5X	3.08	120.31	116.76
2	A	1373	FAD	C5X-C9A-N10	3.86	120.55	117.62
2	B	1373	FAD	C4-N3-C2	5.17	119.71	115.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1372	FAD	C4-N3-C2	5.67	120.14	115.25
2	C	1371	FAD	C4-N3-C2	5.73	120.20	115.25
2	A	1373	FAD	C4-N3-C2	5.97	120.41	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1373	FAD	6	0
2	B	1373	FAD	7	0
2	C	1371	FAD	6	0
2	D	1372	FAD	9	0

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	371/372 (99%)	-0.03	4 (1%)	82	72	24, 42, 45, 48	0
1	B	372/372 (100%)	-0.13	2 (0%)	91	87	24, 42, 45, 48	0
1	C	369/372 (99%)	-0.09	6 (1%)	74	62	24, 42, 44, 48	0
1	D	370/372 (99%)	-0.17	2 (0%)	91	87	38, 42, 44, 47	0
All	All	1482/1488 (99%)	-0.10	14 (0%)	85	78	24, 42, 45, 48	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	ASP	3.6
1	B	1	MET	3.0
1	C	36	PRO	2.6
1	A	178	ASP	2.4
1	C	185	GLU	2.4
1	D	78	ASN	2.3
1	C	77	HIS	2.3
1	C	179	ASP	2.2
1	D	79	GLU	2.2
1	A	183	THR	2.2
1	C	211	LEU	2.2
1	A	173	THR	2.1
1	B	77	HIS	2.1
1	C	196	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	NA	A	1374	1/1	0.96	0.22	0.92	3,3,3,3	0
2	FAD	B	1373	53/53	0.92	0.19	-0.34	27,30,39,39	0
2	FAD	C	1371	53/53	0.91	0.19	-0.44	35,37,42,43	0
2	FAD	A	1373	53/53	0.93	0.17	-0.62	29,32,34,34	0
2	FAD	D	1372	53/53	0.93	0.17	-0.82	27,28,39,39	0
3	NA	C	1372	1/1	0.96	0.15	-1.27	9,9,9,9	0
3	NA	B	1374	1/1	0.96	0.12	-2.99	2,2,2,2	0
3	NA	D	1373	1/1	0.97	0.11	-3.34	2,2,2,2	0

6.5 Other polymers (i)

There are no such residues in this entry.