Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:53 AM GMT

PDB ID	:	2OK7
Title	:	Ferredoxin-NADP+ reductase from Plasmodium falciparum with 2'P-AMP
Authors	:	Milani, M.; Mastrangelo, E.; Bolognesi, M.
Deposited on	:	2007-01-16
Resolution	:	2.70 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:

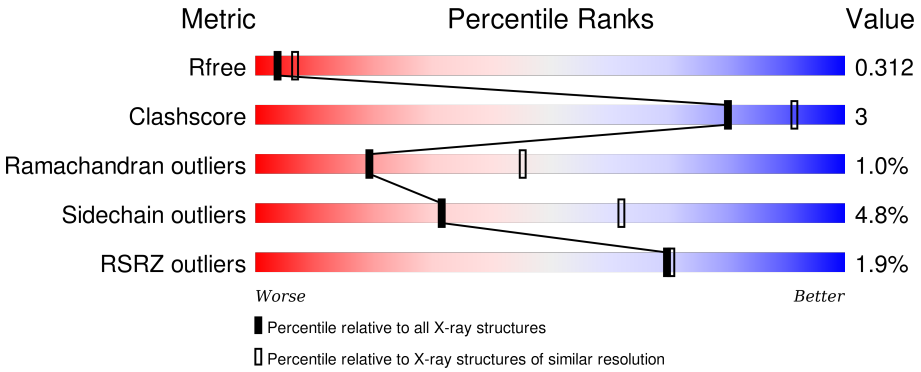
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	316	74% 9% 17%
1	B	316	72% 10% 17%
1	C	316	75% 8% 16%
1	D	316	73% 8% 17%
1	E	316	72% 7% 20%

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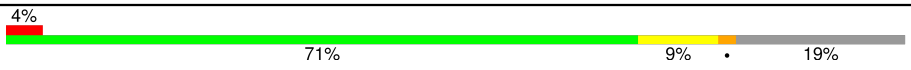
Mol	Chain	Length	Quality of chain
1	F	316	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13658 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.

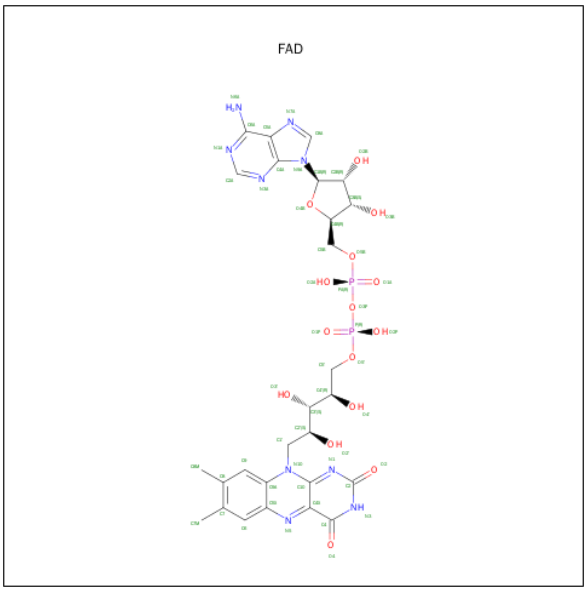
- Molecule 1 is a protein called Putative ferredoxin–NADP reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			2184	1421	357	397	9			
1	B	261	Total	C	N	O	S	0	0	0
			2171	1414	356	392	9			
1	C	266	Total	C	N	O	S	0	0	0
			2198	1429	362	398	9			
1	D	262	Total	C	N	O	S	0	0	0
			2170	1411	354	396	9			
1	E	254	Total	C	N	O	S	0	0	0
			2110	1375	343	383	9			
1	F	257	Total	C	N	O	S	0	0	0
			2116	1382	345	380	9			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

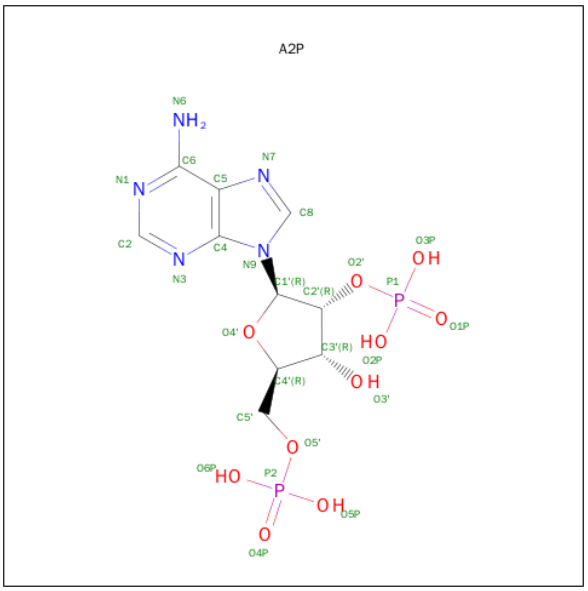
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- 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		
3	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is ADENOSINE-2'-5'-DIPHOSPHATE (three-letter code: A2P) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

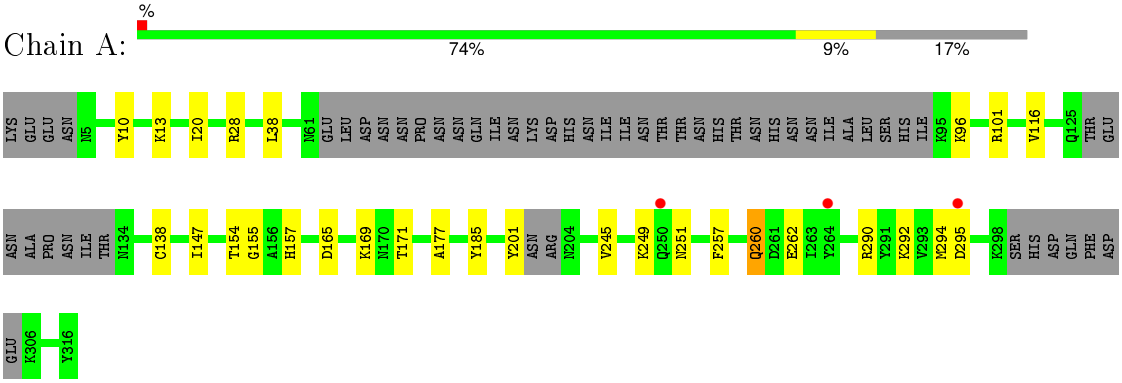
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	49	Total	O	0	0
			49	49		
5	B	47	Total	O	0	0
			47	47		
5	C	46	Total	O	0	0
			46	46		
5	D	38	Total	O	0	0
			38	38		
5	E	24	Total	O	0	0
			24	24		
5	F	24	Total	O	0	0
			24	24		

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.

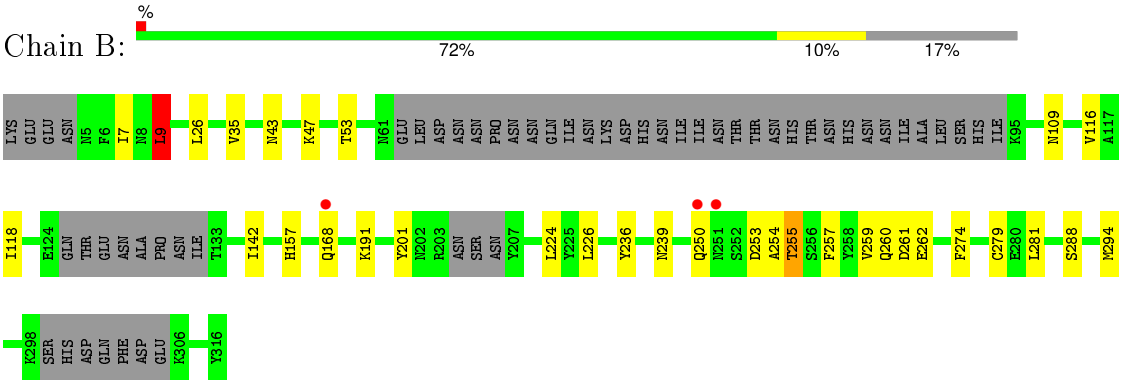
- Molecule 1: Putative ferredoxin–NADP reductase

Chain A:



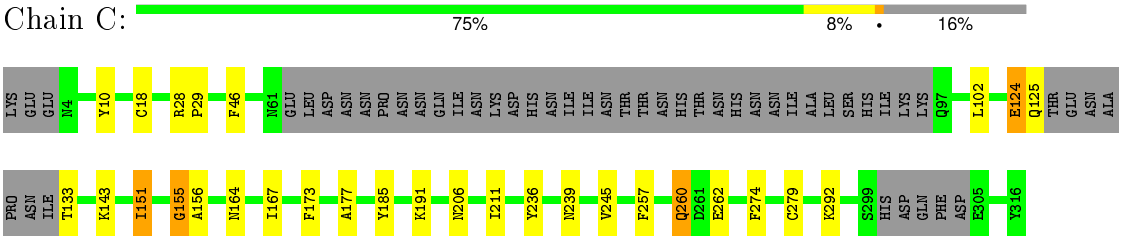
- Molecule 1: Putative ferredoxin–NADP reductase

Chain B:



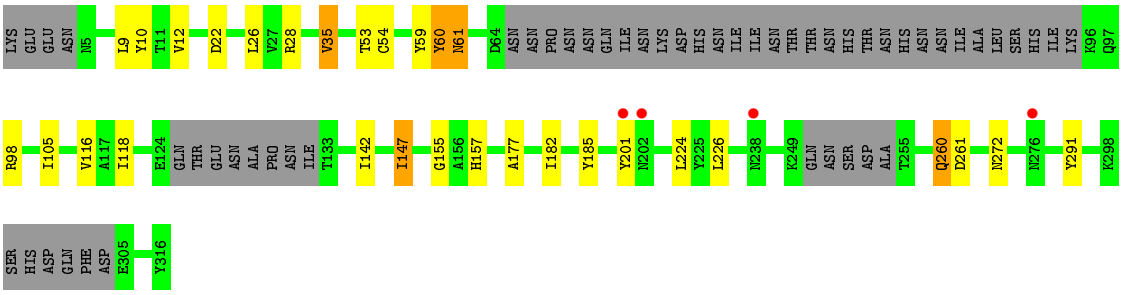
- Molecule 1: Putative ferredoxin–NADP reductase

Chain C:

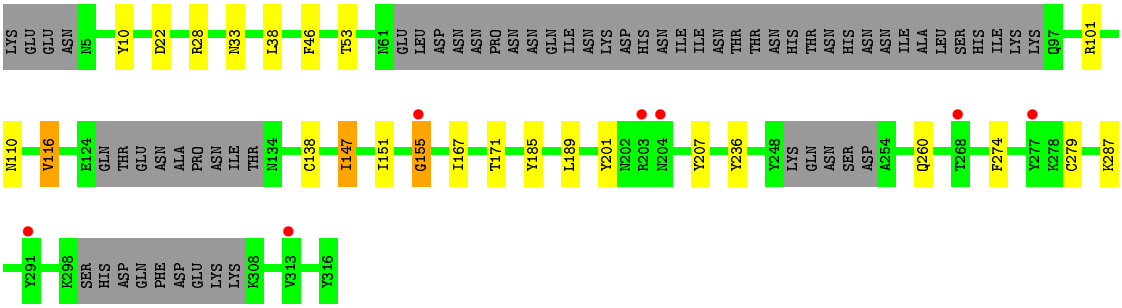


- Molecule 1: Putative ferredoxin–NADP reductase

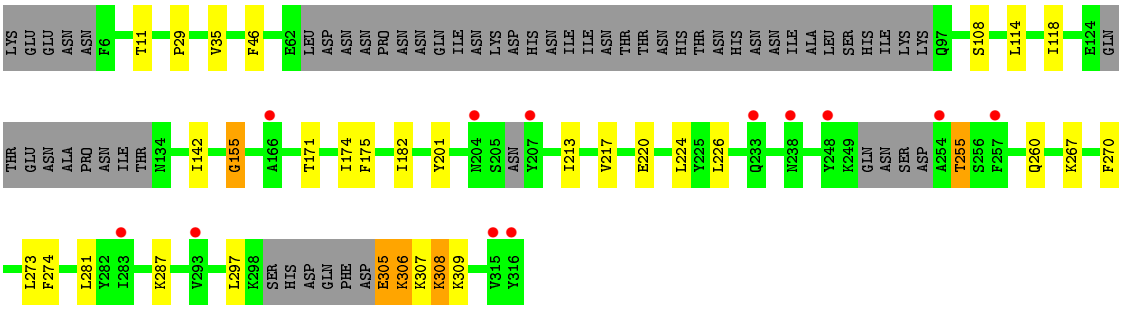
Chain D:



• Molecule 1: Putative ferredoxin–NADP reductase



• Molecule 1: Putative ferredoxin–NADP reductase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	123.13Å 123.13Å 133.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.70 61.56 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-2.70) 98.5 (61.56-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.260 , 0.321 0.256 , 0.312	Depositor DCC
R_{free} test set	3082 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , -8.6	EDS
Estimated twinning fraction	0.000 for -h,-k,l 0.467 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 61385 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13658	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.29 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.1126e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: A2P, 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	0.47	0/2237	0.62	0/3018
1	B	0.53	2/2224 (0.1%)	0.66	1/3002 (0.0%)
1	C	0.48	0/2252	0.64	0/3042
1	D	0.54	2/2223 (0.1%)	0.73	8/3003 (0.3%)
1	E	0.48	0/2163	0.60	0/2925
1	F	0.48	0/2168	0.64	1/2927 (0.0%)
All	All	0.50	4/13267 (0.0%)	0.65	10/17917 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	9	LEU	CG-CD1	-7.58	1.23	1.51
1	D	9	LEU	CG-CD2	-7.57	1.23	1.51
1	D	9	LEU	CG-CD1	-5.03	1.33	1.51
1	B	9	LEU	CG-CD2	-5.02	1.33	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	305	GLU	C-N-CA	-6.78	104.76	121.70
1	D	60	TYR	CB-CG-CD2	6.42	124.85	121.00
1	B	9	LEU	CB-CG-CD1	6.34	121.78	111.00
1	D	9	LEU	CB-CG-CD2	6.21	121.55	111.00
1	D	60	TYR	N-CA-C	5.78	126.60	111.00
1	D	60	TYR	CA-C-N	5.64	129.61	117.20
1	D	60	TYR	CB-CG-CD1	-5.61	117.64	121.00
1	D	60	TYR	C-N-CA	-5.46	108.04	121.70
1	D	61	ASN	N-CA-C	5.42	125.63	111.00
1	D	61	ASN	CA-C-N	5.24	128.73	117.20

There are no chirality outliers.

There are no planarity outliers.

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	2184	0	2139	15	0
1	B	2171	0	2125	13	0
1	C	2198	0	2136	19	0
1	D	2170	0	2101	20	0
1	E	2110	0	2045	11	0
1	F	2116	0	2051	10	0
2	A	1	0	0	0	0
3	A	53	0	31	1	0
3	B	53	0	31	1	0
3	C	53	0	31	3	0
3	D	53	0	31	0	0
3	E	53	0	31	0	0
3	F	53	0	31	0	0
4	A	27	0	11	3	0
4	B	27	0	11	2	0
4	C	27	0	11	3	0
4	D	27	0	11	2	0
4	E	27	0	11	1	0
4	F	27	0	11	0	0
5	A	49	0	0	0	0
5	B	47	0	0	0	0
5	C	46	0	0	0	0
5	D	38	0	0	1	0
5	E	24	0	0	0	0
5	F	24	0	0	0	0
All	All	13658	0	12849	90	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 3.

All (90) 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:D:60:TYR:CD2	1:D:60:TYR:O	1.89	1.24
1:D:61:ASN:O	1:D:61:ASN:CG	1.78	1.21
1:D:60:TYR:CG	1:D:60:TYR:O	1.98	1.08
1:D:61:ASN:O	1:D:61:ASN:OD1	1.71	1.08
1:F:306:LYS:CB	1:F:308:LYS:HE3	1.95	0.96
1:E:260:GLN:HE22	4:E:416:A2P:H2	1.43	0.84
1:C:260:GLN:HE22	4:C:416:A2P:H2	1.46	0.80
1:F:305:GLU:O	1:F:306:LYS:CB	2.21	0.80
1:C:10:TYR:HB2	1:C:155:GLY:H	1.48	0.76
1:B:260:GLN:HE22	4:B:416:A2P:H2	1.56	0.70
1:D:260:GLN:HE22	4:D:416:A2P:H2	1.55	0.69
1:D:182:ILE:HD11	1:D:224:LEU:HB2	1.79	0.64
1:C:257:PHE:HE2	1:C:262:GLU:HG2	1.62	0.64
1:E:10:TYR:HB2	1:E:155:GLY:H	1.64	0.62
1:A:257:PHE:HE2	1:A:262:GLU:HG2	1.63	0.62
1:B:118:ILE:HG21	1:B:142:ILE:HD13	1.82	0.61
1:A:260:GLN:HE22	4:A:416:A2P:H2	1.66	0.60
1:E:101:ARG:HG3	1:E:138:CYS:HB2	1.84	0.59
1:B:53:THR:HG23	1:B:157:HIS:HB2	1.84	0.58
1:F:46:PHE:CZ	1:F:155:GLY:O	2.58	0.57
1:F:118:ILE:HG21	1:F:142:ILE:HD13	1.86	0.56
1:D:260:GLN:NE2	4:D:416:A2P:H2	2.19	0.56
1:A:154:THR:O	1:A:157:HIS:NE2	2.38	0.56
1:B:260:GLN:NE2	4:B:416:A2P:H2	2.21	0.56
1:D:260:GLN:NE2	1:D:260:GLN:H	2.05	0.55
1:C:260:GLN:HB3	1:C:292:LYS:HD2	1.90	0.53
1:B:43:ASN:HD22	1:C:206:ASN:HD21	1.56	0.52
1:C:18:CYS:HB2	1:C:151:ILE:HD12	1.92	0.50
1:C:10:TYR:H	1:C:155:GLY:HA2	1.76	0.50
1:D:53:THR:HG23	1:D:157:HIS:HB2	1.93	0.50
1:C:10:TYR:HB2	1:C:155:GLY:N	2.24	0.49
1:F:182:ILE:HD11	1:F:224:LEU:HB2	1.93	0.49
1:B:236:TYR:HB3	1:B:239:ASN:HB2	1.95	0.49
1:F:307:LYS:C	1:F:309:LYS:H	2.16	0.49
1:A:260:GLN:HE22	4:A:416:A2P:C2	2.25	0.48
1:A:101:ARG:HG3	1:A:138:CYS:HB2	1.96	0.48
1:C:274:PHE:HA	1:C:279:CYS:HB2	1.95	0.48
3:B:415:FAD:H1'1	3:B:415:FAD:H9	1.73	0.48
1:A:260:GLN:NE2	4:A:416:A2P:H2	2.29	0.47
1:D:22:ASP:HA	1:D:147:ILE:HD11	1.97	0.47
1:B:168:GLN:HE21	1:E:236:TYR:HA	1.80	0.47
1:C:177:ALA:HB2	1:C:185:TYR:HE2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:306:LYS:CB	1:F:308:LYS:HG3	2.45	0.47
1:E:10:TYR:H	1:E:155:GLY:HA2	1.79	0.47
1:D:118:ILE:HD13	1:D:142:ILE:HG13	1.96	0.47
1:F:270:PHE:HA	1:F:273:LEU:HD12	1.96	0.47
1:B:118:ILE:HD13	1:B:142:ILE:HD13	1.98	0.46
1:E:46:PHE:CZ	1:E:155:GLY:O	2.69	0.46
1:C:177:ALA:HB2	1:C:185:TYR:CE2	2.50	0.45
1:D:26:LEU:HB2	1:D:35:VAL:HG22	1.98	0.45
1:A:257:PHE:CE2	1:A:262:GLU:HG2	2.47	0.44
1:A:165:ASP:HB3	1:A:169:LYS:HG3	2.00	0.44
1:E:38:LEU:HB2	1:E:116:VAL:HG12	1.99	0.44
1:B:9:LEU:HD22	1:B:47:LYS:HB2	1.99	0.44
1:B:259:VAL:HG12	1:B:260:GLN:HE21	1.83	0.44
1:A:177:ALA:HB2	1:A:185:TYR:CE2	2.52	0.44
1:B:257:PHE:HE2	1:B:262:GLU:HG2	1.81	0.44
1:D:10:TYR:H	1:D:155:GLY:HA3	1.82	0.44
1:E:274:PHE:HA	1:E:279:CYS:HB2	2.00	0.44
1:E:167:ILE:HG23	1:E:207:TYR:HB2	2.00	0.44
1:A:10:TYR:HB2	1:A:155:GLY:H	1.84	0.43
1:C:260:GLN:NE2	4:C:416:A2P:H2	2.25	0.43
1:A:245:VAL:HG22	1:A:262:GLU:HG3	2.01	0.43
1:E:185:TYR:O	1:E:189:LEU:HG	2.19	0.43
1:C:46:PHE:CZ	1:C:155:GLY:O	2.72	0.42
1:A:260:GLN:HB3	1:A:292:LYS:HD2	2.01	0.42
1:D:28:ARG:NH1	5:D:441:HOH:O	2.52	0.42
1:C:260:GLN:HE22	4:C:416:A2P:C2	2.22	0.42
1:C:102:LEU:HD12	3:C:415:FAD:HM82	2.01	0.42
1:D:177:ALA:HB2	1:D:185:TYR:HE1	1.85	0.42
1:C:167:ILE:HD11	1:C:191:LYS:HE3	2.01	0.42
1:A:177:ALA:HB2	1:A:185:TYR:HE2	1.85	0.42
1:D:177:ALA:HB2	1:D:185:TYR:CE1	2.54	0.42
1:C:245:VAL:HG22	1:C:262:GLU:HG3	2.01	0.42
1:C:173:PHE:HB2	1:C:211:ILE:HG12	2.01	0.42
1:B:274:PHE:HA	1:B:279:CYS:HB2	2.02	0.42
1:D:260:GLN:H	1:D:260:GLN:HE21	1.64	0.42
1:D:54:CYS:HB3	1:D:105:ILE:HD11	2.02	0.42
1:F:175:PHE:HB2	1:F:213:ILE:HG12	2.01	0.42
1:C:236:TYR:HB3	1:C:239:ASN:HB2	2.01	0.42
1:A:20:ILE:HD12	1:A:38:LEU:HD22	2.02	0.41
1:B:26:LEU:HD13	1:B:224:LEU:HB3	2.02	0.41
1:A:290:ARG:O	1:A:294:MET:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:TYR:HB2	1:D:155:GLY:H	1.85	0.41
3:C:415:FAD:O2A	3:C:415:FAD:H8A	2.20	0.41
1:D:10:TYR:HB2	1:D:155:GLY:N	2.36	0.41
3:A:415:FAD:H1'1	3:A:415:FAD:H9	1.81	0.41
1:F:274:PHE:HE1	1:F:281:LEU:HB2	1.87	0.40
1:E:22:ASP:HA	1:E:147:ILE:HD11	2.01	0.40
3:C:415:FAD:H1'1	3:C:415:FAD:H9	1.81	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	252/316 (80%)	242 (96%)	9 (4%)	1 (0%)	39 69
1	B	251/316 (79%)	238 (95%)	11 (4%)	2 (1%)	24 51
1	C	258/316 (82%)	244 (95%)	10 (4%)	4 (2%)	12 30
1	D	252/316 (80%)	242 (96%)	8 (3%)	2 (1%)	24 51
1	E	244/316 (77%)	232 (95%)	11 (4%)	1 (0%)	39 69
1	F	245/316 (78%)	225 (92%)	15 (6%)	5 (2%)	9 24
All	All	1502/1896 (79%)	1423 (95%)	64 (4%)	15 (1%)	19 45

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	308	LYS
1	B	254	ALA
1	C	155	GLY
1	D	59	TYR
1	E	155	GLY

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Mol	Chain	Res	Type
1	C	124	GLU
1	C	156	ALA
1	D	98	ARG
1	A	251	ASN
1	C	29	PRO
1	F	29	PRO
1	F	255	THR
1	F	306	LYS
1	B	255	THR
1	F	155	GLY

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	241/295 (82%)	231 (96%)	10 (4%)	37	69
1	B	238/295 (81%)	223 (94%)	15 (6%)	22	48
1	C	239/295 (81%)	231 (97%)	8 (3%)	45	76
1	D	237/295 (80%)	227 (96%)	10 (4%)	36	68
1	E	231/295 (78%)	221 (96%)	10 (4%)	35	66
1	F	228/295 (77%)	213 (93%)	15 (7%)	21	45
All	All	1414/1770 (80%)	1346 (95%)	68 (5%)	31	62

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	28	ARG
1	A	96	LYS
1	A	116	VAL
1	A	147	ILE
1	A	171	THR
1	A	201	TYR
1	A	249	LYS

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Mol	Chain	Res	Type
1	A	260	GLN
1	A	295	ASP
1	B	7	ILE
1	B	9	LEU
1	B	35	VAL
1	B	109	ASN
1	B	116	VAL
1	B	191	LYS
1	B	201	TYR
1	B	226	LEU
1	B	250	GLN
1	B	253	ASP
1	B	255	THR
1	B	261	ASP
1	B	281	LEU
1	B	288	SER
1	B	294	MET
1	C	28	ARG
1	C	124	GLU
1	C	125	GLN
1	C	133	THR
1	C	143	LYS
1	C	151	ILE
1	C	164	ASN
1	C	260	GLN
1	D	12	VAL
1	D	35	VAL
1	D	116	VAL
1	D	147	ILE
1	D	201	TYR
1	D	226	LEU
1	D	260	GLN
1	D	261	ASP
1	D	272	ASN
1	D	291	TYR
1	E	28	ARG
1	E	33	ASN
1	E	53	THR
1	E	110	ASN
1	E	116	VAL
1	E	147	ILE
1	E	151	ILE

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Mol	Chain	Res	Type
1	E	171	THR
1	E	201	TYR
1	E	287	LYS
1	F	11	THR
1	F	35	VAL
1	F	108	SER
1	F	114	LEU
1	F	171	THR
1	F	174	ILE
1	F	201	TYR
1	F	217	VAL
1	F	220	GLU
1	F	226	LEU
1	F	255	THR
1	F	260	GLN
1	F	267	LYS
1	F	287	LYS
1	F	297	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	33	ASN
1	A	241	ASN
1	A	260	GLN
1	B	30	ASN
1	B	168	GLN
1	B	260	GLN
1	B	272	ASN
1	C	8	ASN
1	C	33	ASN
1	C	144	ASN
1	C	199	ASN
1	C	202	ASN
1	C	206	ASN
1	C	241	ASN
1	C	260	GLN
1	D	30	ASN
1	D	260	GLN
1	D	272	ASN
1	E	144	ASN

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Mol	Chain	Res	Type
1	E	202	ASN
1	E	260	GLN
1	F	260	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FAD	A	415	-	48,58,58	1.30	6 (12%)	54,89,89	2.26	9 (16%)
4	A2P	A	416	2	24,29,29	0.93	1 (4%)	29,45,45	1.80	4 (13%)
3	FAD	B	415	-	48,58,58	1.29	6 (12%)	54,89,89	2.28	8 (14%)
4	A2P	B	416	-	24,29,29	0.88	1 (4%)	29,45,45	1.74	4 (13%)
3	FAD	C	415	-	48,58,58	1.29	6 (12%)	54,89,89	2.25	11 (20%)
4	A2P	C	416	-	24,29,29	0.92	1 (4%)	29,45,45	1.79	5 (17%)
3	FAD	D	415	-	48,58,58	1.24	7 (14%)	54,89,89	2.26	9 (16%)
4	A2P	D	416	-	24,29,29	0.93	1 (4%)	29,45,45	1.79	6 (20%)
3	FAD	E	415	-	48,58,58	1.24	5 (10%)	54,89,89	2.18	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	A2P	E	416	-	24,29,29	1.04	1 (4%)	29,45,45	1.71	3 (10%)
3	FAD	F	415	-	48,58,58	1.27	7 (14%)	54,89,89	2.16	7 (12%)
4	A2P	F	416	-	24,29,29	1.00	1 (4%)	29,45,45	1.93	5 (17%)

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	415	-	-	0/30/50/50	0/6/6/6
4	A2P	A	416	2	-	0/11/31/31	0/3/3/3
3	FAD	B	415	-	-	0/30/50/50	0/6/6/6
4	A2P	B	416	-	-	0/11/31/31	0/3/3/3
3	FAD	C	415	-	-	0/30/50/50	0/6/6/6
4	A2P	C	416	-	-	0/11/31/31	0/3/3/3
3	FAD	D	415	-	-	0/30/50/50	0/6/6/6
4	A2P	D	416	-	-	0/11/31/31	0/3/3/3
3	FAD	E	415	-	-	0/30/50/50	0/6/6/6
4	A2P	E	416	-	-	0/11/31/31	0/3/3/3
3	FAD	F	415	-	-	0/30/50/50	0/6/6/6
4	A2P	F	416	-	-	0/11/31/31	0/3/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	415	FAD	C10-N1	2.11	1.39	1.35
3	F	415	FAD	C5X-N5	2.12	1.38	1.35
3	B	415	FAD	C10-N1	2.15	1.39	1.35
3	D	415	FAD	C10-N1	2.15	1.39	1.35
3	A	415	FAD	C1'-N10	2.17	1.50	1.48
3	A	415	FAD	C10-N1	2.17	1.39	1.35
3	F	415	FAD	C10-N1	2.19	1.39	1.35
3	D	415	FAD	C5X-N5	2.21	1.38	1.35
3	D	415	FAD	C1'-N10	2.25	1.50	1.48
3	C	415	FAD	C5X-N5	2.28	1.38	1.35
3	E	415	FAD	C1'-N10	2.28	1.50	1.48
3	F	415	FAD	C1'-N10	2.40	1.50	1.48
3	B	415	FAD	C2A-N1A	2.46	1.38	1.33
3	D	415	FAD	C2A-N1A	2.48	1.38	1.33
3	B	415	FAD	C4-N3	2.55	1.37	1.33
3	F	415	FAD	C2A-N1A	2.64	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	415	FAD	C2A-N1A	2.65	1.38	1.33
3	E	415	FAD	C2A-N1A	2.66	1.39	1.33
3	D	415	FAD	C4-N3	2.71	1.38	1.33
3	A	415	FAD	C2A-N1A	2.76	1.39	1.33
4	A	416	A2P	C5-C4	2.78	1.46	1.40
4	B	416	A2P	C5-C4	2.86	1.46	1.40
4	C	416	A2P	C5-C4	2.87	1.47	1.40
3	B	415	FAD	C1'-N10	2.88	1.51	1.48
3	E	415	FAD	C4-N3	3.00	1.38	1.33
3	A	415	FAD	C4-N3	3.04	1.38	1.33
4	F	416	A2P	C5-C4	3.07	1.47	1.40
4	D	416	A2P	C5-C4	3.11	1.47	1.40
3	F	415	FAD	C4-N3	3.12	1.38	1.33
3	C	415	FAD	C4-N3	3.27	1.39	1.33
4	E	416	A2P	C5-C4	3.27	1.47	1.40
3	C	415	FAD	C4X-N5	3.31	1.38	1.33
3	E	415	FAD	C4X-N5	3.44	1.38	1.33
3	D	415	FAD	C4X-N5	3.51	1.38	1.33
3	F	415	FAD	C4X-N5	3.51	1.38	1.33
3	A	415	FAD	C4X-N5	3.57	1.38	1.33
3	B	415	FAD	C2A-N3A	3.62	1.38	1.32
3	D	415	FAD	C2A-N3A	3.68	1.38	1.32
3	B	415	FAD	C4X-N5	3.78	1.39	1.33
3	E	415	FAD	C2A-N3A	3.80	1.38	1.32
3	C	415	FAD	C2A-N3A	3.82	1.39	1.32
3	A	415	FAD	C2A-N3A	3.83	1.39	1.32
3	F	415	FAD	C2A-N3A	3.87	1.39	1.32

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	415	FAD	N3A-C2A-N1A	-11.96	119.73	128.89
3	E	415	FAD	N3A-C2A-N1A	-11.90	119.78	128.89
3	C	415	FAD	N3A-C2A-N1A	-11.84	119.83	128.89
3	F	415	FAD	N3A-C2A-N1A	-11.73	119.91	128.89
3	D	415	FAD	N3A-C2A-N1A	-11.67	119.95	128.89
3	A	415	FAD	N3A-C2A-N1A	-11.26	120.27	128.89
4	F	416	A2P	N3-C2-N1	-7.15	123.42	128.89
4	B	416	A2P	N3-C2-N1	-5.88	124.39	128.89
4	E	416	A2P	N3-C2-N1	-5.56	124.63	128.89
4	D	416	A2P	N3-C2-N1	-5.49	124.69	128.89
4	A	416	A2P	N3-C2-N1	-5.29	124.84	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	416	A2P	N3-C2-N1	-5.21	124.91	128.89
3	B	415	FAD	P-O3P-PA	-4.84	119.13	132.73
3	F	415	FAD	P-O3P-PA	-4.30	120.66	132.73
3	E	415	FAD	P-O3P-PA	-3.88	121.83	132.73
3	A	415	FAD	P-O3P-PA	-3.56	122.73	132.73
3	D	415	FAD	P-O3P-PA	-3.39	123.20	132.73
4	A	416	A2P	C4-C5-N7	-3.18	106.56	109.48
4	B	416	A2P	C4-C5-N7	-3.16	106.57	109.48
4	F	416	A2P	C4-C5-N7	-3.08	106.65	109.48
4	E	416	A2P	C4-C5-N7	-2.94	106.78	109.48
3	A	415	FAD	C4X-C4-N3	-2.90	119.62	123.59
3	C	415	FAD	C4X-C4-N3	-2.82	119.73	123.59
3	D	415	FAD	C4X-C4-N3	-2.78	119.79	123.59
3	C	415	FAD	C2B-C1B-N9A	-2.72	110.13	114.29
4	C	416	A2P	C4-C5-N7	-2.72	106.97	109.48
3	A	415	FAD	C4X-C10-N10	-2.63	118.97	120.52
3	B	415	FAD	C4X-C4-N3	-2.62	120.01	123.59
3	E	415	FAD	C4X-C4-N3	-2.62	120.01	123.59
3	F	415	FAD	C4X-C4-N3	-2.57	120.07	123.59
4	D	416	A2P	C4-C5-N7	-2.54	107.14	109.48
4	F	416	A2P	O5P-P2-O5'	-2.39	99.68	106.56
3	C	415	FAD	C4X-C10-N10	-2.34	119.14	120.52
4	D	416	A2P	O5'-P2-O4P	-2.28	101.34	107.14
3	C	415	FAD	P-O3P-PA	-2.23	126.47	132.73
4	B	416	A2P	C1'-N9-C4	-2.16	123.69	126.94
4	D	416	A2P	O2'-P1-O1P	-2.15	101.74	107.11
4	C	416	A2P	C4'-O4'-C1'	-2.10	107.42	109.72
4	F	416	A2P	C4'-O4'-C1'	-2.09	107.42	109.72
4	D	416	A2P	C1'-N9-C4	-2.07	123.82	126.94
4	C	416	A2P	O5'-P2-O4P	-2.03	101.98	107.14
3	D	415	FAD	O3'-C3'-C2'	2.02	113.83	108.75
4	A	416	A2P	O6P-P2-O5P	2.02	115.06	107.38
3	D	415	FAD	O2'-C2'-C3'	2.02	114.10	109.02
3	C	415	FAD	C2B-C3B-C4B	2.10	106.92	102.61
3	A	415	FAD	O3'-C3'-C2'	2.12	114.10	108.75
3	C	415	FAD	O2'-C2'-C3'	2.18	114.50	109.02
3	B	415	FAD	O2'-C2'-C3'	2.19	114.51	109.02
3	C	415	FAD	C5X-C9A-N10	2.23	119.31	117.62
3	F	415	FAD	C4B-O4B-C1B	2.31	112.25	109.72
3	A	415	FAD	C4B-O4B-C1B	2.31	112.26	109.72
3	E	415	FAD	C4B-O4B-C1B	2.32	112.27	109.72
3	B	415	FAD	C4B-O4B-C1B	2.35	112.30	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	416	A2P	O4'-C1'-N9	2.52	113.37	108.10
4	B	416	A2P	O4'-C1'-N9	2.58	113.49	108.10
3	E	415	FAD	C4X-N5-C5X	2.78	119.97	116.76
3	D	415	FAD	C5X-C9A-N10	2.84	119.78	117.62
3	F	415	FAD	C5X-C9A-N10	2.91	119.83	117.62
3	B	415	FAD	C4X-N5-C5X	2.99	120.20	116.76
3	E	415	FAD	C5X-C9A-N10	3.05	119.93	117.62
3	A	415	FAD	C5X-C9A-N10	3.16	120.02	117.62
3	F	415	FAD	C4X-N5-C5X	3.18	120.42	116.76
3	D	415	FAD	C4B-O4B-C1B	3.34	113.39	109.72
3	D	415	FAD	C4X-N5-C5X	3.34	120.60	116.76
3	A	415	FAD	C4X-N5-C5X	3.42	120.69	116.76
4	D	416	A2P	O4'-C1'-N9	3.51	115.45	108.10
3	C	415	FAD	C4X-N5-C5X	3.52	120.81	116.76
3	B	415	FAD	C5X-C9A-N10	3.57	120.33	117.62
3	C	415	FAD	C4B-O4B-C1B	3.61	113.69	109.72
4	E	416	A2P	O4'-C1'-N9	3.93	116.33	108.10
4	C	416	A2P	O4'-C1'-N9	4.20	116.89	108.10
4	A	416	A2P	O4'-C1'-N9	4.61	117.75	108.10
3	F	415	FAD	C4-N3-C2	5.78	120.25	115.25
3	E	415	FAD	C4-N3-C2	5.93	120.37	115.25
3	B	415	FAD	C4-N3-C2	5.96	120.40	115.25
3	C	415	FAD	C4-N3-C2	6.20	120.61	115.25
3	D	415	FAD	C4-N3-C2	6.90	121.22	115.25
3	A	415	FAD	C4-N3-C2	6.92	121.23	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	415	FAD	1	0
4	A	416	A2P	3	0
3	B	415	FAD	1	0
4	B	416	A2P	2	0
3	C	415	FAD	3	0
4	C	416	A2P	3	0
4	D	416	A2P	2	0
4	E	416	A2P	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	262/316 (82%)	0.01	3 (1%) 82 83	2, 5, 30, 53	0
1	B	261/316 (82%)	0.04	3 (1%) 82 83	2, 6, 37, 63	0
1	C	266/316 (84%)	-0.01	0 100 100	2, 3, 35, 55	0
1	D	262/316 (82%)	0.10	4 (1%) 76 76	2, 5, 32, 57	0
1	E	254/316 (80%)	0.18	7 (2%) 56 57	3, 17, 50, 73	0
1	F	257/316 (81%)	0.57	12 (4%) 35 34	9, 30, 56, 74	0
All	All	1562/1896 (82%)	0.15	29 (1%) 70 70	2, 10, 46, 74	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	251	ASN	4.7
1	A	295	ASP	3.5
1	F	257	PHE	3.4
1	F	293	VAL	3.4
1	E	291	TYR	3.3
1	B	250	GLN	3.1
1	F	248	TYR	3.0
1	F	238	ASN	2.9
1	E	277	TYR	2.7
1	A	264	TYR	2.7
1	F	204	ASN	2.7
1	E	203	ARG	2.6
1	D	201	TYR	2.6
1	D	202	ASN	2.5
1	E	204	ASN	2.4
1	F	233	GLN	2.4
1	F	316	TYR	2.3
1	F	283	ILE	2.3
1	F	254	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	250	GLN	2.3
1	B	168	GLN	2.3
1	D	238	ASN	2.2
1	E	155	GLY	2.1
1	F	166	ALA	2.1
1	E	313	VAL	2.0
1	F	207	TYR	2.0
1	D	276	ASN	2.0
1	E	268	THR	2.0
1	F	315	VAL	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 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	FAD	B	415	53/53	0.96	0.19	0.23	2,2,10,16	0
3	FAD	F	415	53/53	0.96	0.21	-0.04	2,24,38,44	0
3	FAD	D	415	53/53	0.96	0.18	-0.13	2,2,5,15	0
4	A2P	C	416	27/27	0.98	0.16	-0.17	2,2,6,21	0
3	FAD	E	415	53/53	0.97	0.19	-0.25	2,10,31,40	0
3	FAD	C	415	53/53	0.96	0.18	-0.30	2,2,4,19	0
4	A2P	D	416	27/27	0.97	0.16	-0.76	2,2,3,10	0
4	A2P	F	416	27/27	0.96	0.16	-0.77	2,22,41,48	0
4	A2P	B	416	27/27	0.97	0.15	-1.01	2,2,13,22	0
3	FAD	A	415	53/53	0.97	0.17	-1.03	2,2,7,21	0
4	A2P	A	416	27/27	0.98	0.15	-1.09	2,2,2,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	A2P	E	416	27/27	0.97	0.13	-1.28	2,6,18,22	0
2	NA	A	9001	1/1	0.70	0.19	-	2,2,2,2	0

6.5 Other polymers (i)

There are no such residues in this entry.