Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:01 PM GMT

PDB ID	:	1W87
Title	:	FERREDOXIN-NADP REDUCTASE (MUTATION: Y 303 W) COMPLEXED WITH NADP BY COCRYSTALLIZATION
Authors	:	Hermoso, J.A.; Perez-Dorado, I.; Maya, C.
Deposited on	:	2004-09-16
Resolution	:	3.00 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:

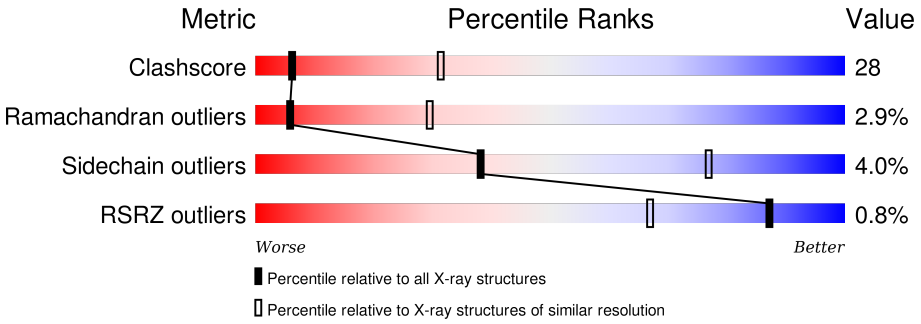
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	304	52% 41% 5% ·
1	B	304	2% 52% 41% · ·

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4882 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.

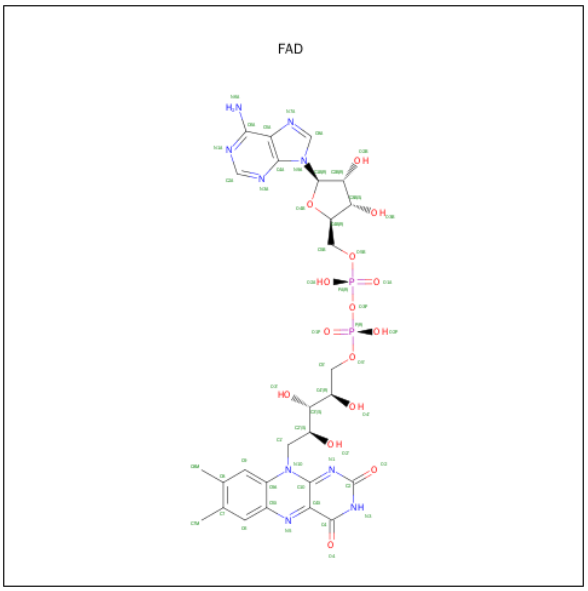
- Molecule 1 is a protein called FERREDOXIN-NADP REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2340	1490	400	441	9			
1	B	295	Total	C	N	O	S	0	0	0
			2340	1490	400	441	9			

There are 4 discrepancies between the modelled and reference sequences:

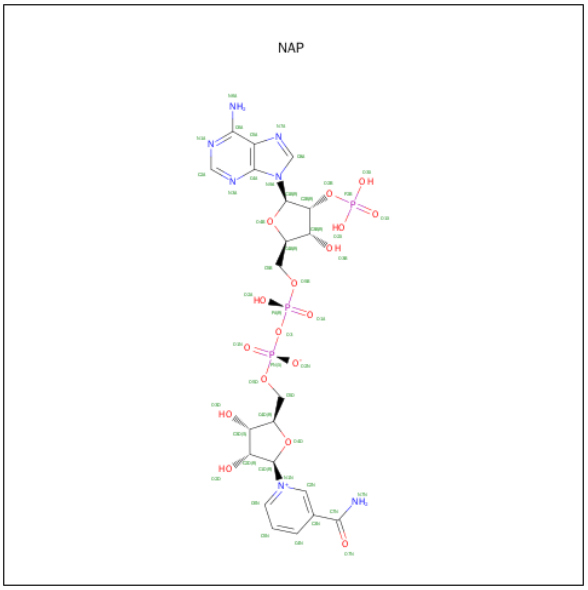
Chain	Residue	Modelled	Actual	Comment	Reference
A	246	GLN	GLU	CONFLICT	UNP P21890
A	303	TRP	TYR	ENGINEERED MUTATION	UNP P21890
B	246	GLN	GLU	CONFLICT	UNP P21890
B	303	TRP	TYR	ENGINEERED MUTATION	UNP P21890

- 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		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



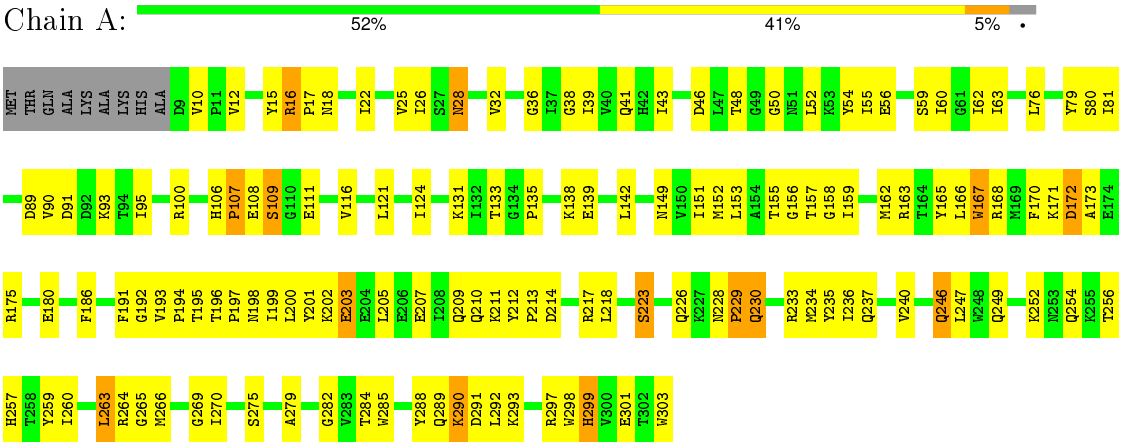
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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.

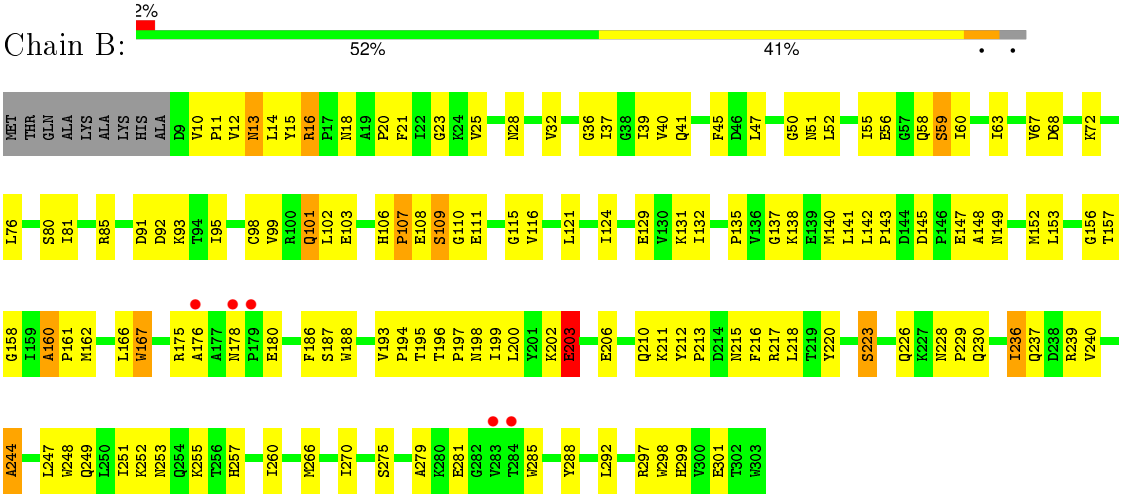
- Molecule 1: FERREDOXIN-NADP REDUCTASE

Chain A:



- Molecule 1: FERREDOXIN-NADP REDUCTASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	221.27Å 221.27Å 37.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.99 – 3.00 34.99 – 2.98	Depositor EDS
% Data completeness (in resolution range)	88.5 (34.99-3.00) 87.6 (34.99-2.98)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 3.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.225 , 0.272 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	1.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.0	EDS
Estimated twinning fraction	0.019 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 16865 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	4882	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: NAP, 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	0.39	0/2397	0.65	0/3248
1	B	0.37	0/2397	0.65	0/3248
All	All	0.38	0/4794	0.65	0/6496

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2340	0	2315	130	0
1	B	2340	0	2315	130	0
2	A	53	0	31	1	0
2	B	53	0	31	6	0
3	A	48	0	25	6	0
3	B	48	0	25	4	0
All	All	4882	0	4742	269	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 28.

All (269) 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:289:GLN:HA	1:A:292:LEU:HD23	1.56	0.88
1:B:39:ILE:HD12	1:B:101:GLN:HE21	1.39	0.87
1:A:263:LEU:HD12	1:A:263:LEU:H	1.39	0.87
3:A:305:NAP:C2N	3:A:305:NAP:H51N	2.04	0.87
1:A:217:ARG:HH22	1:A:246:GLN:HE22	1.21	0.87
1:A:109:SER:OG	1:A:111:GLU:HG2	1.74	0.86
1:B:28:ASN:HD21	1:B:41:GLN:HB3	1.39	0.86
1:B:14:LEU:HD12	1:B:52:LEU:HD12	1.56	0.84
1:A:25:VAL:HG21	1:A:124:ILE:HG12	1.59	0.81
3:A:305:NAP:C5D	3:A:305:NAP:H2N	2.11	0.81
3:A:305:NAP:H2N	3:A:305:NAP:H51N	1.61	0.81
1:B:68:ASP:OD2	1:B:72:LYS:HB2	1.81	0.80
1:A:217:ARG:NH2	1:A:246:GLN:HE22	1.78	0.80
1:B:249:GLN:HE22	1:B:252:LYS:NZ	1.80	0.80
1:B:12:VAL:HG12	1:B:13:ASN:ND2	1.97	0.79
1:A:228:ASN:ND2	1:A:230:GLN:H	1.79	0.79
1:B:152:MET:HE2	1:B:162:MET:HB3	1.64	0.79
1:B:115:GLY:HA3	2:B:304:FAD:O2P	1.83	0.78
1:B:257:HIS:HD2	1:B:299:HIS:HE1	1.32	0.76
1:A:59:SER:HA	1:A:81:ILE:HG13	1.68	0.75
1:B:249:GLN:HE22	1:B:252:LYS:HZ1	1.36	0.73
3:B:305:NAP:H51N	3:B:305:NAP:H2N	1.70	0.73
1:B:59:SER:HA	1:B:81:ILE:HG13	1.71	0.72
1:B:149:ASN:ND2	1:B:186:PHE:H	1.88	0.72
1:B:211:LYS:HG2	1:B:212:TYR:CE2	2.25	0.72
1:B:153:LEU:HD13	1:B:270:ILE:HD13	1.73	0.71
1:A:194:PRO:HA	1:A:223:SER:OG	1.91	0.70
1:B:60:ILE:HD12	1:B:132:ILE:HG23	1.73	0.69
1:B:20:PRO:HG3	1:B:131:LYS:HD3	1.73	0.69
1:B:10:VAL:HG13	1:B:11:PRO:HD2	1.74	0.68
1:B:193:VAL:HB	1:B:194:PRO:HD2	1.76	0.68
1:A:16:ARG:HH11	1:A:16:ARG:HG3	1.57	0.68
1:B:194:PRO:HA	1:B:223:SER:HB3	1.76	0.68
1:A:153:LEU:HD13	1:A:270:ILE:HD13	1.75	0.67
1:B:109:SER:OG	1:B:111:GLU:HG2	1.94	0.67
1:A:192:GLY:N	1:A:236:ILE:HD11	2.10	0.67
1:B:80:SER:HB3	1:B:161:PRO:HD3	1.77	0.66
1:B:12:VAL:HG21	1:B:138:LYS:HE3	1.78	0.65
1:A:207:GLU:O	1:A:210:GLN:HB2	1.96	0.65
1:B:52:LEU:HD11	1:B:135:PRO:HD3	1.78	0.65
1:B:28:ASN:ND2	1:B:41:GLN:HB3	2.09	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:GLN:O	1:A:213:PRO:HD3	1.98	0.64
1:B:228:ASN:HB2	1:B:229:PRO:HD2	1.78	0.64
1:B:63:ILE:HG12	1:B:76:LEU:HB3	1.79	0.64
1:A:26:ILE:HD11	1:A:46:ASP:HB2	1.80	0.64
1:B:226:GLN:NE2	1:B:239:ARG:HH21	1.94	0.64
1:A:162:MET:O	1:A:166:LEU:HG	1.98	0.63
1:B:229:PRO:HB2	1:B:230:GLN:OE1	1.98	0.63
1:B:248:TRP:CZ2	1:B:252:LYS:HD3	2.35	0.62
1:A:195:THR:OG1	1:A:197:PRO:HD2	1.98	0.62
1:B:175:ARG:HH11	1:B:175:ARG:HG2	1.64	0.62
3:A:305:NAP:C5D	3:A:305:NAP:C2N	2.74	0.62
1:B:32:VAL:HG23	1:B:40:VAL:HB	1.80	0.62
1:B:236:ILE:HG21	1:B:266:MET:HE3	1.82	0.62
1:A:275:SER:HA	1:A:285:TRP:HB2	1.83	0.61
1:A:63:ILE:HG12	1:A:76:LEU:HB3	1.83	0.61
1:A:211:LYS:HB3	1:A:212:TYR:CD2	2.36	0.60
1:A:56:GLU:H	1:A:56:GLU:CD	2.04	0.60
1:A:288:TYR:O	1:A:291:ASP:HB2	2.02	0.60
1:A:254:GLN:HA	1:A:297:ARG:NH2	2.17	0.60
1:A:228:ASN:HD21	1:A:230:GLN:HB2	1.65	0.60
1:A:59:SER:HB3	1:A:80:SER:HA	1.85	0.59
1:A:151:ILE:HD13	1:A:247:LEU:HD22	1.85	0.58
1:B:58:GLN:HG2	1:B:137:GLY:O	2.03	0.58
3:B:305:NAP:C5D	3:B:305:NAP:H2N	2.33	0.58
1:A:153:LEU:CD1	1:A:270:ILE:HD13	2.33	0.58
1:A:168:ARG:HH11	1:A:168:ARG:HG3	1.69	0.58
1:A:228:ASN:HD22	1:A:230:GLN:H	1.50	0.58
1:A:28:ASN:HD21	1:A:41:GLN:HB3	1.68	0.58
1:A:60:ILE:HG23	1:A:81:ILE:HD11	1.84	0.58
1:B:67:VAL:HA	1:B:72:LYS:O	2.04	0.57
1:B:106:HIS:CD2	1:B:108:GLU:H	2.22	0.57
1:A:10:VAL:HG22	1:A:55:ILE:HD11	1.86	0.57
1:B:102:LEU:HD12	1:B:103:GLU:H	1.69	0.57
1:A:60:ILE:HD13	1:A:95:ILE:HD13	1.86	0.57
1:B:160:ALA:HB3	1:B:161:PRO:CD	2.35	0.57
1:B:292:LEU:HD12	1:B:297:ARG:HB2	1.87	0.57
1:B:115:GLY:CA	2:B:304:FAD:O2P	2.52	0.57
1:A:211:LYS:HB3	1:A:212:TYR:CE2	2.40	0.56
1:B:107:PRO:CG	2:B:304:FAD:H2A	2.36	0.56
1:B:260:ILE:HD11	1:B:298:TRP:CZ2	2.40	0.56
1:B:266:MET:O	1:B:270:ILE:HG13	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:SER:N	1:B:215:ASN:O	2.38	0.56
1:A:263:LEU:HD12	1:A:263:LEU:N	2.15	0.56
1:A:193:VAL:HB	1:A:194:PRO:HD2	1.87	0.56
1:A:108:GLU:O	1:A:109:SER:HB3	2.06	0.56
1:B:15:TYR:CE1	1:B:21:PHE:HB2	2.42	0.55
1:A:108:GLU:OE1	1:A:108:GLU:HA	2.07	0.55
1:B:106:HIS:HB3	1:B:109:SER:OG	2.07	0.55
1:B:152:MET:HE3	1:B:166:LEU:HG	1.87	0.55
1:B:108:GLU:O	1:B:109:SER:HB3	2.06	0.55
1:B:257:HIS:CD2	1:B:299:HIS:HE1	2.18	0.54
1:B:228:ASN:HB2	1:B:229:PRO:CD	2.37	0.54
1:A:10:VAL:HG13	1:A:55:ILE:HD11	1.89	0.54
1:B:36:GLY:CA	1:B:197:PRO:HB2	2.37	0.54
1:B:275:SER:HA	1:B:285:TRP:HB2	1.88	0.54
1:A:28:ASN:ND2	1:A:41:GLN:HB3	2.22	0.54
1:A:175:ARG:HH11	1:A:175:ARG:HG2	1.71	0.54
1:B:247:LEU:O	1:B:251:ILE:HG13	2.08	0.54
1:B:156:GLY:C	1:B:158:GLY:H	2.11	0.54
1:B:288:TYR:O	1:B:292:LEU:HD23	2.09	0.53
1:A:152:MET:HE1	1:A:162:MET:HB3	1.91	0.53
1:A:254:GLN:HA	1:A:297:ARG:HH22	1.72	0.53
1:A:12:VAL:HG21	1:A:138:LYS:HE2	1.90	0.53
1:A:167:TRP:CD1	1:A:171:LYS:HG3	2.43	0.53
1:A:236:ILE:HG21	1:A:266:MET:CE	2.39	0.53
1:B:47:LEU:HD11	1:B:95:ILE:HB	1.90	0.52
1:B:102:LEU:HD12	1:B:103:GLU:N	2.24	0.52
1:A:263:LEU:HD23	1:B:110:GLY:C	2.30	0.52
1:A:170:PHE:HB3	1:A:212:TYR:CD2	2.44	0.52
1:A:89:ASP:HB2	1:A:91:ASP:OD1	2.09	0.52
1:B:156:GLY:O	1:B:158:GLY:N	2.42	0.52
1:A:159:ILE:HB	1:A:191:PHE:CE1	2.45	0.52
1:A:36:GLY:CA	1:A:197:PRO:HB2	2.39	0.52
1:A:223:SER:O	1:A:233:ARG:HG2	2.09	0.52
1:A:229:PRO:HB2	1:A:230:GLN:OE1	2.10	0.51
1:B:15:TYR:OH	1:B:50:GLY:HA3	2.11	0.51
1:A:106:HIS:HB2	1:A:111:GLU:HG3	1.93	0.51
1:A:109:SER:HG	1:A:111:GLU:HG2	1.72	0.51
1:A:153:LEU:O	1:A:260:ILE:HA	2.10	0.51
1:A:16:ARG:HG3	1:A:16:ARG:NH1	2.25	0.51
1:A:249:GLN:HA	1:A:252:LYS:HZ3	1.76	0.51
1:B:236:ILE:HG21	1:B:266:MET:HB2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:304:FAD:O2'	2:B:304:FAD:H9	2.11	0.51
1:A:54:TYR:CE2	1:A:81:ILE:HG21	2.45	0.50
1:B:80:SER:CB	1:B:161:PRO:HD3	2.41	0.50
1:B:25:VAL:HG21	1:B:124:ILE:HG12	1.94	0.50
1:A:196:THR:N	1:A:197:PRO:CD	2.74	0.50
1:A:52:LEU:HD11	1:A:135:PRO:HD3	1.92	0.50
1:A:106:HIS:O	1:A:108:GLU:N	2.44	0.50
1:B:175:ARG:HG2	1:B:175:ARG:NH1	2.26	0.50
1:B:37:ILE:HD12	1:B:194:PRO:HB2	1.94	0.49
1:B:188:TRP:CD2	1:B:217:ARG:HD3	2.47	0.49
2:B:304:FAD:H8A	2:B:304:FAD:H3B	1.93	0.49
1:A:230:GLN:OE1	1:A:230:GLN:N	2.46	0.49
1:B:188:TRP:CE2	1:B:217:ARG:HD3	2.47	0.49
1:B:203:GLU:OE1	1:B:203:GLU:N	2.46	0.49
1:B:142:LEU:HD12	1:B:143:PRO:HD2	1.95	0.49
1:B:153:LEU:HD12	1:B:260:ILE:HG12	1.95	0.49
1:B:156:GLY:C	1:B:158:GLY:N	2.67	0.48
1:B:196:THR:HA	1:B:199:ILE:HG13	1.93	0.48
1:A:279:ALA:O	1:A:282:GLY:N	2.42	0.48
1:A:155:THR:OG1	1:A:263:LEU:HD12	2.13	0.48
1:A:25:VAL:HG21	1:A:124:ILE:CG1	2.37	0.48
1:B:223:SER:OG	3:B:305:NAP:O2X	2.20	0.48
1:A:235:TYR:HB3	1:A:237:GLN:OE1	2.14	0.48
1:A:156:GLY:O	1:A:158:GLY:N	2.46	0.48
1:A:59:SER:HB2	1:A:79:TYR:O	2.14	0.48
1:B:236:ILE:HG21	1:B:266:MET:CE	2.43	0.48
1:B:195:THR:OG1	1:B:197:PRO:HD2	2.13	0.48
1:B:257:HIS:CD2	1:B:297:ARG:HA	2.49	0.48
1:B:107:PRO:HG3	2:B:304:FAD:H2A	1.96	0.48
1:A:299:HIS:N	1:A:299:HIS:ND1	2.62	0.48
1:A:257:HIS:CD2	1:A:299:HIS:CE1	3.02	0.47
1:A:52:LEU:CD1	1:A:135:PRO:HD3	2.44	0.47
1:A:226:GLN:HE21	1:A:234:MET:HG2	1.79	0.47
1:B:98:CYS:SG	1:B:200:LEU:HD13	2.54	0.47
1:B:188:TRP:HD1	1:B:217:ARG:O	1.97	0.47
1:A:48:THR:HG22	1:A:93:LYS:HG2	1.96	0.47
1:B:152:MET:HE2	1:B:162:MET:CB	2.41	0.47
1:B:152:MET:CE	1:B:166:LEU:HG	2.45	0.47
1:B:63:ILE:HG12	1:B:76:LEU:CB	2.44	0.47
1:B:15:TYR:CZ	1:B:21:PHE:HB2	2.49	0.47
1:B:91:ASP:O	1:B:93:LYS:HG3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ARG:HB3	1:A:18:ASN:OD1	2.14	0.47
1:A:210:GLN:O	1:A:211:LYS:C	2.52	0.47
1:B:202:LYS:O	1:B:203:GLU:C	2.53	0.47
1:A:257:HIS:HD2	1:A:299:HIS:CE1	2.32	0.47
1:A:257:HIS:HB3	1:A:259:TYR:CE1	2.49	0.47
1:A:149:ASN:HB2	1:A:256:THR:HA	1.96	0.47
1:A:152:MET:HE3	1:A:165:TYR:HB2	1.97	0.47
1:A:168:ARG:HG3	1:A:168:ARG:NH1	2.29	0.47
1:A:89:ASP:C	1:A:90:VAL:HG23	2.36	0.47
1:B:147:GLU:HB3	1:B:255:LYS:HE2	1.97	0.47
1:A:263:LEU:H	1:A:263:LEU:CD1	2.18	0.46
1:A:257:HIS:CD2	1:A:299:HIS:HE1	2.33	0.46
1:B:28:ASN:HD21	1:B:41:GLN:CB	2.18	0.46
1:A:121:LEU:O	1:A:124:ILE:HG22	2.15	0.46
1:B:249:GLN:HE22	1:B:252:LYS:HZ3	1.59	0.46
1:B:288:TYR:CE2	1:B:292:LEU:HD21	2.50	0.46
1:B:218:LEU:HD11	1:B:220:TYR:CE1	2.51	0.46
3:A:305:NAP:O2N	3:A:305:NAP:N7N	2.48	0.46
1:B:249:GLN:NE2	1:B:252:LYS:NZ	2.59	0.46
1:B:149:ASN:HD22	1:B:186:PHE:H	1.61	0.46
1:B:12:VAL:CG2	1:B:138:LYS:HE3	2.45	0.45
1:B:203:GLU:H	1:B:203:GLU:CD	2.19	0.45
1:B:230:GLN:N	1:B:230:GLN:CD	2.70	0.45
1:B:142:LEU:CD1	1:B:143:PRO:HD2	2.46	0.45
1:B:142:LEU:HG	1:B:143:PRO:HD2	1.97	0.45
1:A:213:PRO:HG2	1:A:214:ASP:H	1.81	0.45
1:B:10:VAL:CG1	1:B:11:PRO:HD2	2.43	0.45
1:B:167:TRP:N	1:B:167:TRP:HE3	2.15	0.45
1:A:291:ASP:O	1:A:292:LEU:C	2.56	0.45
1:B:47:LEU:HD22	1:B:52:LEU:HD23	1.98	0.45
1:B:50:GLY:O	1:B:51:ASN:C	2.55	0.45
1:A:156:GLY:C	1:A:158:GLY:H	2.21	0.45
1:A:168:ARG:O	1:A:168:ARG:HG2	2.18	0.44
1:B:202:LYS:NZ	1:B:206:GLU:OE1	2.47	0.44
1:B:108:GLU:O	1:B:109:SER:CB	2.65	0.44
1:A:12:VAL:CG2	1:A:138:LYS:HE2	2.47	0.44
1:B:279:ALA:C	1:B:281:GLU:H	2.20	0.44
1:B:211:LYS:HG2	1:B:212:TYR:CD2	2.53	0.44
1:B:10:VAL:CG1	1:B:55:ILE:HD11	2.48	0.44
1:A:163:ARG:HG3	1:A:167:TRP:CZ3	2.53	0.44
1:A:195:THR:CB	1:A:197:PRO:HD2	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ARG:HH11	1:B:16:ARG:HG3	1.83	0.44
1:A:38:GLY:HA3	1:A:100:ARG:NH1	2.33	0.43
1:A:293:LYS:HE3	1:A:298:TRP:CD1	2.53	0.43
1:B:252:LYS:HA	1:B:288:TYR:OH	2.18	0.43
1:A:196:THR:HB	1:A:197:PRO:HD3	2.00	0.43
1:A:257:HIS:HB3	1:A:259:TYR:HE1	1.83	0.43
1:B:37:ILE:N	1:B:198:ASN:OD1	2.44	0.43
1:A:180:GLU:OE1	1:A:180:GLU:N	2.48	0.43
1:A:109:SER:C	1:A:111:GLU:H	2.20	0.43
1:B:56:GLU:OE2	1:B:85:ARG:HG2	2.18	0.43
1:B:45:PHE:N	1:B:45:PHE:CD1	2.86	0.43
1:A:22:ILE:CD1	1:A:131:LYS:HG2	2.48	0.43
1:A:62:ILE:HG21	1:A:121:LEU:HD21	2.01	0.43
3:B:305:NAP:N7N	3:B:305:NAP:O2N	2.51	0.43
1:B:148:ALA:HA	1:B:255:LYS:HB3	2.01	0.43
1:A:289:GLN:O	1:A:290:LYS:C	2.57	0.43
1:A:175:ARG:HG2	1:A:175:ARG:NH1	2.33	0.43
1:B:108:GLU:OE1	1:B:108:GLU:HA	2.19	0.42
1:A:76:LEU:HD12	1:A:76:LEU:C	2.39	0.42
1:A:156:GLY:C	1:A:158:GLY:N	2.73	0.42
1:B:180:GLU:N	1:B:180:GLU:OE1	2.52	0.42
1:A:209:GLN:OE1	1:A:218:LEU:N	2.49	0.42
1:A:194:PRO:HG2	1:A:195:THR:H	1.85	0.42
1:B:99:VAL:HG21	1:B:121:LEU:HD13	2.01	0.42
1:B:16:ARG:HB3	1:B:18:ASN:OD1	2.19	0.42
1:A:237:GLN:CB	1:A:269:GLY:HA3	2.50	0.42
1:B:140:MET:SD	1:B:299:HIS:HB3	2.60	0.42
1:B:10:VAL:O	1:B:12:VAL:HG23	2.20	0.42
1:A:289:GLN:C	1:A:291:ASP:N	2.71	0.42
1:B:230:GLN:H	1:B:230:GLN:CD	2.23	0.42
1:B:40:VAL:HG11	1:B:200:LEU:CD2	2.49	0.42
1:A:266:MET:HE2	1:A:270:ILE:HD11	2.02	0.41
1:A:17:PRO:HA	1:A:133:THR:HG21	2.01	0.41
1:A:15:TYR:OH	1:A:50:GLY:O	2.29	0.41
1:A:264:ARG:NH1	1:A:264:ARG:HB2	2.35	0.41
1:A:205:LEU:HA	1:A:205:LEU:HD23	1.87	0.41
1:A:199:ILE:HB	1:A:202:LYS:HB2	2.02	0.41
1:B:236:ILE:HG13	1:B:266:MET:HE3	2.02	0.41
1:B:187:SER:O	1:B:216:PHE:HA	2.20	0.41
1:A:172:ASP:O	1:A:173:ALA:C	2.58	0.41
1:B:236:ILE:CG2	1:B:237:GLN:N	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLU:O	1:A:299:HIS:HB3	2.21	0.41
1:B:142:LEU:CG	1:B:143:PRO:HD2	2.50	0.41
1:B:210:GLN:O	1:B:213:PRO:HD3	2.19	0.41
1:B:240:VAL:O	1:B:244:ALA:N	2.53	0.41
1:B:39:ILE:HB	1:B:101:GLN:HB2	2.02	0.41
1:B:10:VAL:HG21	1:B:141:LEU:HD13	2.03	0.41
1:A:264:ARG:HH11	1:A:264:ARG:CB	2.33	0.41
1:A:32:VAL:HG13	1:A:198:ASN:ND2	2.36	0.41
1:B:23:GLY:O	1:B:129:GLU:HA	2.20	0.41
1:A:200:LEU:O	1:A:201:TYR:HB2	2.20	0.41
1:A:109:SER:HG	1:A:111:GLU:CG	2.34	0.41
1:A:43:ILE:CD1	1:A:121:LEU:HB3	2.51	0.41
1:A:39:ILE:HG23	1:A:41:GLN:OE1	2.21	0.41
1:B:160:ALA:HB3	1:B:161:PRO:HD3	2.02	0.40
1:A:149:ASN:ND2	1:A:186:PHE:H	2.19	0.40
1:A:108:GLU:O	1:A:109:SER:CB	2.68	0.40
1:A:203:GLU:OE1	1:A:203:GLU:N	2.54	0.40
1:A:263:LEU:C	1:A:265:GLY:N	2.73	0.40
1:A:303:TRP:O	3:A:305:NAP:H5N	2.21	0.40
1:A:153:LEU:HD22	1:A:240:VAL:CG2	2.52	0.40
1:A:142:LEU:HD13	1:A:165:TYR:CD1	2.56	0.40
1:B:176:ALA:C	1:B:178:ASN:H	2.25	0.40
1:A:107:PRO:CG	2:A:304:FAD:H2A	2.51	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	293/304 (96%)	253 (86%)	34 (12%)	6 (2%)	9 41
1	B	293/304 (96%)	247 (84%)	35 (12%)	11 (4%)	4 22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	586/608 (96%)	500 (85%)	69 (12%)	17 (3%)	6 29

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	SER
1	B	109	SER
1	B	223	SER
1	A	223	SER
1	B	116	VAL
1	A	157	THR
1	B	157	THR
1	B	244	ALA
1	A	172	ASP
1	B	203	GLU
1	B	253	ASN
1	A	116	VAL
1	A	107	PRO
1	B	13	ASN
1	B	145	ASP
1	B	160	ALA
1	B	107	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	250/256 (98%)	238 (95%)	12 (5%)	31 71
1	B	250/256 (98%)	242 (97%)	8 (3%)	46 82
All	All	500/512 (98%)	480 (96%)	20 (4%)	38 77

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	28	ASN
1	A	167	TRP
1	A	203	GLU
1	A	229	PRO
1	A	230	GLN
1	A	246	GLN
1	A	263	LEU
1	A	284	THR
1	A	290	LYS
1	A	299	HIS
1	A	301	GLU
1	B	16	ARG
1	B	59	SER
1	B	92	ASP
1	B	101	GLN
1	B	167	TRP
1	B	203	GLU
1	B	236	ILE
1	B	301	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	51	ASN
1	A	70	ASN
1	A	101	GLN
1	A	106	HIS
1	A	149	ASN
1	A	182	GLN
1	A	226	GLN
1	A	228	ASN
1	A	246	GLN
1	A	249	GLN
1	A	257	HIS
1	A	289	GLN
1	A	299	HIS
1	B	13	ASN
1	B	28	ASN
1	B	101	GLN
1	B	106	HIS
1	B	149	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	182	GLN
1	B	226	GLN
1	B	243	HIS
1	B	249	GLN
1	B	257	HIS
1	B	289	GLN
1	B	299	HIS

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

4 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	$\#\|Z\| > 2$
2	FAD	A	304	-	48,58,58	1.56	10 (20%)	54,89,89	2.94	13 (24%)
3	NAP	A	305	-	42,52,52	1.81	9 (21%)	54,80,80	2.18	13 (24%)
2	FAD	B	304	-	48,58,58	1.76	13 (27%)	54,89,89	2.83	18 (33%)
3	NAP	B	305	-	42,52,52	1.80	6 (14%)	54,80,80	1.93	13 (24%)

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	304	-	-	0/30/50/50	0/6/6/6
3	NAP	A	305	-	-	0/27/67/67	0/5/5/5
2	FAD	B	304	-	-	0/30/50/50	0/6/6/6
3	NAP	B	305	-	-	0/27/67/67	0/5/5/5

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	304	FAD	C10-N10	-4.62	1.33	1.39
2	B	304	FAD	C9A-N10	-4.34	1.32	1.38
2	B	304	FAD	C6-C5X	-3.87	1.35	1.41
3	B	305	NAP	O4B-C1B	-3.70	1.36	1.41
2	B	304	FAD	C9A-C5X	-3.34	1.35	1.42
2	A	304	FAD	C9A-C5X	-2.96	1.36	1.42
3	A	305	NAP	PN-O2N	-2.86	1.42	1.54
2	A	304	FAD	C6-C5X	-2.86	1.37	1.41
3	A	305	NAP	O4B-C1B	-2.83	1.37	1.41
3	A	305	NAP	C4N-C3N	-2.72	1.34	1.39
2	B	304	FAD	C9-C9A	-2.59	1.35	1.40
3	A	305	NAP	O4B-C4B	-2.40	1.39	1.45
2	B	304	FAD	O5B-C5B	-2.32	1.35	1.44
3	A	305	NAP	PN-O1N	-2.27	1.42	1.51
2	A	304	FAD	C4'-C3'	-2.27	1.48	1.53
2	B	304	FAD	C7M-C7	-2.23	1.46	1.51
3	B	305	NAP	PN-O2N	-2.22	1.45	1.54
3	B	305	NAP	O4B-C4B	-2.14	1.40	1.45
3	A	305	NAP	PA-O1A	-2.12	1.43	1.51
2	A	304	FAD	O2B-C2B	-2.11	1.37	1.43
2	B	304	FAD	C8-C7	-2.06	1.35	1.41
2	B	304	FAD	O4B-C4B	-2.05	1.40	1.45
2	A	304	FAD	O3'-C3'	-2.03	1.38	1.43
2	B	304	FAD	C5'-C4'	2.15	1.55	1.51
2	B	304	FAD	C1'-N10	2.18	1.50	1.48
2	A	304	FAD	C4X-N5	2.21	1.36	1.33
2	B	304	FAD	C4X-N5	2.26	1.36	1.33
2	B	304	FAD	C2A-N1A	2.39	1.38	1.33
2	A	304	FAD	C2A-N3A	2.73	1.37	1.32
3	B	305	NAP	C2A-N3A	2.76	1.37	1.32
3	A	305	NAP	C2A-N1A	2.77	1.39	1.33
3	B	305	NAP	C2A-N1A	2.96	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	304	FAD	C2A-N1A	3.03	1.39	1.33
2	A	304	FAD	C4-N3	3.23	1.39	1.33
2	B	304	FAD	C4-N3	4.07	1.40	1.33
3	A	305	NAP	C2A-N3A	4.23	1.39	1.32
3	A	305	NAP	O7N-C7N	6.27	1.37	1.24
3	B	305	NAP	O7N-C7N	8.01	1.41	1.24

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	304	FAD	N3A-C2A-N1A	-12.28	119.49	128.89
2	A	304	FAD	N3A-C2A-N1A	-10.17	121.11	128.89
3	A	305	NAP	O7N-C7N-N7N	-6.46	113.50	122.59
3	A	305	NAP	N3A-C2A-N1A	-5.84	124.42	128.89
2	A	304	FAD	C4X-C4-N3	-5.81	115.64	123.59
2	B	304	FAD	O3P-P-O5'	-5.46	88.45	102.94
3	B	305	NAP	N3A-C2A-N1A	-5.06	125.02	128.89
3	B	305	NAP	C4D-O4D-C1D	-4.39	104.90	109.72
2	B	304	FAD	P-O3P-PA	-4.30	120.66	132.73
2	B	304	FAD	C1B-N9A-C4A	-4.25	120.53	126.94
2	B	304	FAD	C4X-C4-N3	-3.64	118.61	123.59
3	B	305	NAP	O7N-C7N-N7N	-3.57	117.58	122.59
2	A	304	FAD	P-O3P-PA	-3.55	122.76	132.73
2	B	304	FAD	C2B-C1B-N9A	-3.49	108.95	114.29
2	A	304	FAD	O2'-C2'-C3'	-3.17	101.04	109.02
3	A	305	NAP	O4D-C4D-C5D	-3.00	98.60	109.32
3	A	305	NAP	C4B-O4B-C1B	-2.88	106.55	109.72
2	B	304	FAD	C6-C5X-N5	-2.84	115.31	118.96
3	B	305	NAP	O4B-C1B-C2B	-2.70	101.72	106.60
3	B	305	NAP	O2N-PN-O5D	-2.68	94.93	108.46
2	B	304	FAD	O4B-C4B-C5B	-2.67	99.79	109.32
3	B	305	NAP	C4A-C5A-N7A	-2.58	107.11	109.48
2	A	304	FAD	C4-C4X-C10	-2.54	118.32	119.94
3	B	305	NAP	PN-O3-PA	-2.41	125.95	132.73
3	A	305	NAP	C5N-C4N-C3N	-2.21	117.55	120.33
3	A	305	NAP	C3B-C2B-C1B	-2.20	98.48	102.73
3	A	305	NAP	O2X-P2B-O1X	-2.19	103.53	110.58
3	B	305	NAP	O3-PA-O5B	-2.16	97.21	102.94
2	A	304	FAD	O2B-C2B-C3B	-2.01	105.29	111.83
3	B	305	NAP	O3D-C3D-C4D	2.01	117.08	111.05
2	B	304	FAD	C4-C4X-N5	2.03	121.18	118.72
2	B	304	FAD	O2A-PA-O3P	2.09	114.58	105.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	305	NAP	O3X-P2B-O1X	2.16	117.54	110.58
2	B	304	FAD	O2P-P-O3P	2.20	115.09	105.09
3	B	305	NAP	O5D-PN-O1N	2.23	118.26	109.62
3	A	305	NAP	O3D-C3D-C4D	2.27	117.85	111.05
2	B	304	FAD	C2A-N1A-C6A	2.32	122.91	118.77
2	B	304	FAD	O3'-C3'-C2'	2.48	114.99	108.75
3	A	305	NAP	O2A-PA-O3	2.50	116.43	105.09
3	A	305	NAP	O2B-C2B-C1B	2.52	119.83	110.02
2	A	304	FAD	C7-C6-C5X	2.55	125.09	120.92
2	B	304	FAD	O3B-C3B-C4B	2.83	119.53	111.05
2	A	304	FAD	O2P-P-O3P	2.86	118.05	105.09
3	B	305	NAP	O3X-P2B-O2X	2.92	118.51	107.38
2	A	304	FAD	C4-C4X-N5	3.15	122.55	118.72
2	B	304	FAD	C4X-C10-N10	3.25	122.43	120.52
3	A	305	NAP	C6N-C5N-C4N	3.54	124.79	119.44
2	B	304	FAD	C1'-N10-C9A	3.63	122.94	118.86
3	A	305	NAP	O3X-P2B-O2X	3.67	121.37	107.38
2	B	304	FAD	C5X-C9A-N10	3.70	120.43	117.62
2	A	304	FAD	C5X-C9A-N10	4.57	121.09	117.62
2	A	304	FAD	C1'-N10-C9A	5.56	125.10	118.86
2	A	304	FAD	C4X-C10-N10	6.25	124.20	120.52
3	B	305	NAP	C3N-C7N-N7N	6.49	124.92	117.82
3	A	305	NAP	C3N-C7N-N7N	7.85	126.41	117.82
2	B	304	FAD	C4-N3-C2	8.35	122.47	115.25
2	A	304	FAD	C4-N3-C2	11.17	124.90	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	304	FAD	1	0
3	A	305	NAP	6	0
2	B	304	FAD	6	0
3	B	305	NAP	4	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	295/304 (97%)	-0.39	0 100 100	7, 31, 51, 65	0
1	B	295/304 (97%)	-0.17	5 (1%) 73 45	17, 36, 58, 62	0
All	All	590/608 (97%)	-0.28	5 (0%) 87 67	7, 34, 56, 65	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	283	VAL	4.0
1	B	284	THR	2.4
1	B	176	ALA	2.2
1	B	179	PRO	2.1
1	B	178	ASN	2.1

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

There are no carbohydrates in this entry.

6.4 Ligands

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
2	FAD	B	304	53/53	0.94	0.18	-0.09	23,32,73,81	0
3	NAP	A	305	48/48	0.96	0.18	-0.17	27,40,49,51	0
2	FAD	A	304	53/53	0.95	0.18	-0.29	20,26,65,70	0
3	NAP	B	305	48/48	0.95	0.18	-0.34	23,46,60,62	0

6.5 Other polymers (i)

There are no such residues in this entry.