W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:23 pm GMT

PDB ID	:	1D4A
Title	:	CRYSTAL STRUCTURE OF HUMAN NAD[P]H-QUINONE OXIDORE-DUCTASE AT 1.7 A RESOLUTION
Authors	:	Faig, M.; Bianchet, M.A.; Chen, S.; Winski, S.; Ross, D.; Amzel, L.M.
Deposited on	:	1999-10-01
Resolution	:	1.70 Å(reported)

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

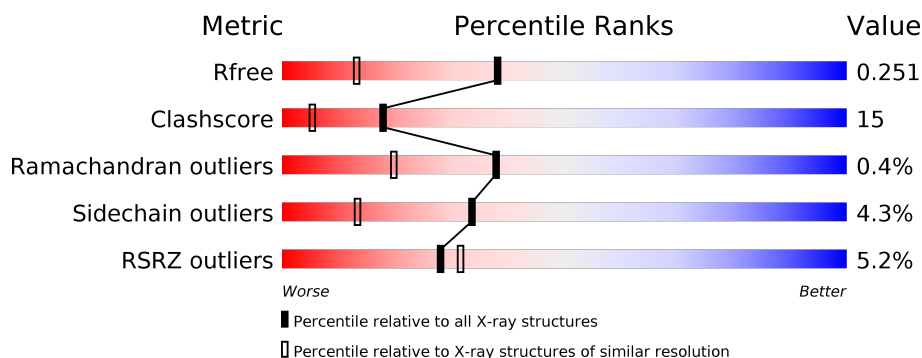|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1   Overall quality at a glance   ⓘ

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

The reported resolution of this entry is 1.70 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	Percentile Ranks	Value
Rfree		0.251
Clashscore		15
Ramachandran outliers		0.4%
Sidechain outliers		4.3%
RSRZ outliers		5.2%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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	273	5% 75% 22% •
1	B	273	4% 71% 25% •
1	C	273	7% 74% 22% •
1	D	273	5% 69% 29% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FAD	B	602	-	-	-	X

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 9496 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 QUINONE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2173	1412	365	389	7			
1	B	273	Total	C	N	O	S	0	0	0
			2173	1412	365	389	7			
1	C	273	Total	C	N	O	S	0	0	0
			2173	1412	365	389	7			
1	D	273	Total	C	N	O	S	0	0	0
			2173	1412	365	389	7			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).
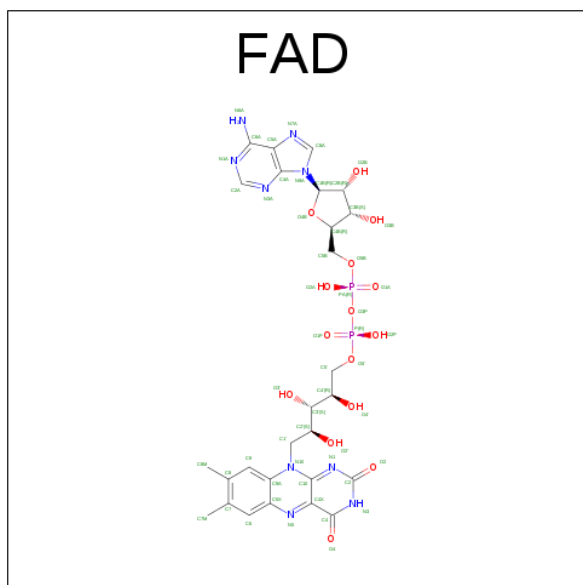
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	145	Total 145	O 145	0	0
3	B	170	Total 170	O 170	0	0
3	C	133	Total 133	O 133	0	0
3	D	144	Total 144	O 144	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: QUINONE REDUCTASE

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- Molecule 1: QUINONE REDUCTASE

V255 G256 T265 D266 N267 A271 R272 K273

• Molecule 1: QUINONE REDUCTASE

Chain D:

5%

69%

29%

V1 G2 R3 R4 L9 R14 F17 N18 Y19 A20 M21 K22 E23 A24 A25 A26 A27 A28 L29 K30 K31 K32 E35 I49 I50 S51 R52 K53 D54 K58 L59 K60 D61 N64 F65 Q66 Y67 P68 A69 E70 S71 V72 L73 K76 Q88 K89 K90 L91 E92 K113

E117 R118 V119 F120 I121 G122 E123 T127 Y128 A129 A130 M131 Y132 D133 K134 R138 V143 S151 G152 S153 M154 Q158 G159 I160 W169 P170 H177 G180 F181 Q182 V183 L184 T189 H194 A197 D198 A199 R200 I201 Q202 I203 L204 E205 K208 L211

I214 W215 P219 D229 L230 N231 F232 Q233 A234 G235 F236 L237 M238 K239 K240 E241 V242 Q243 S254 V255 G256 N267 R272 K273

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	55.68Å 57.03Å 97.40Å 77.04° 76.72° 86.89°	Depositor
Resolution (Å)	43.63 – 1.70 43.63 – 1.70	Depositor EDS
% Data completeness (in resolution range)	78.6 (43.63-1.70) 76.7 (43.63-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 1.70Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.209 , 0.253 0.207 , 0.251	Depositor DCC
R_{free} test set	9755 reflections (9.91%)	DCC
Wilson B-factor (Å^2)	20.2	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9496	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.42	0/2231	0.64	1/3012 (0.0%)
1	B	0.42	0/2231	0.65	0/3012
1	C	0.40	0/2231	0.60	1/3012 (0.0%)
1	D	0.41	0/2231	0.61	1/3012 (0.0%)
All	All	0.41	0/8924	0.62	3/12048 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	182	GLN	N-CA-C	-5.53	96.06	111.00
1	D	182	GLN	N-CA-C	-5.41	96.40	111.00
1	C	182	GLN	N-CA-C	-5.23	96.87	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2173	0	2172	64	0
1	B	2173	0	2172	72	0
1	C	2173	0	2172	64	0
1	D	2173	0	2172	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	53	0	31	4	0
2	B	53	0	31	2	0
2	C	53	0	31	1	0
2	D	53	0	31	1	0
3	A	145	0	0	3	0
3	B	170	0	0	5	0
3	C	133	0	0	6	0
3	D	144	0	0	9	0
All	All	9496	0	8812	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 15.

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:B:135:GLY:O	1:B:138:ARG:HG3	1.56	1.05
1:A:127:THR:HG22	1:A:129:ALA:H	1.35	0.92
1:D:60:LYS:HG3	1:D:70:GLU:OE1	1.70	0.90
1:B:108:VAL:HG13	1:B:112:LEU:HB3	1.59	0.84
1:A:189:THR:HG22	3:A:674:HOH:O	1.79	0.82
1:B:143:VAL:HG22	1:B:184:LEU:HB2	1.62	0.81
1:B:50:ILE:HD12	1:B:117:GLU:HB3	1.63	0.80
1:C:59:LEU:HB2	1:C:62:PRO:HG3	1.63	0.80
1:D:17:PHE:HB2	2:D:604:FAD:H52A	1.64	0.78
1:B:236:PHE:HB3	1:D:160:ILE:HG13	1.68	0.76
1:D:127:THR:CG2	1:D:130:ALA:HB3	2.15	0.75
1:A:58:LYS:N	1:A:58:LYS:HD2	2.01	0.75
1:D:240:LYS:HD2	1:D:240:LYS:H	1.53	0.74
1:B:221:TYR:HB3	1:B:273:LYS:HA	1.70	0.74
1:A:108:VAL:HG13	1:A:112:LEU:HB3	1.70	0.74
1:A:202:GLN:HE21	1:A:202:GLN:HA	1.53	0.73
1:C:209:LYS:HD3	1:C:210:ARG:N	2.03	0.73
1:D:189:THR:HG22	3:D:629:HOH:O	1.88	0.72
1:B:271:ALA:O	1:B:272:ARG:HB2	1.89	0.72
1:A:17:PHE:HB2	2:A:601:FAD:H52A	1.70	0.71
1:D:255:VAL:HG23	1:D:267:ASN:HD22	1.55	0.71
1:C:273:LYS:HD2	1:C:273:LYS:H	1.54	0.70
1:D:25:ALA:O	1:D:29:LEU:HD13	1.91	0.70
1:B:88:GLN:O	1:B:92:GLU:HG3	1.91	0.70
1:C:122:GLY:O	1:C:123:GLU:HB2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:ILE:HG22	1:C:118:ARG:HG2	1.73	0.70
1:A:68:PRO:O	1:A:72:VAL:HG23	1.92	0.69
1:A:1:VAL:HA	1:A:215:TRP:CD1	2.28	0.69
1:B:3:ARG:HA	1:B:3:ARG:HE	1.56	0.69
1:D:151:SER:H	1:D:154:MET:HE3	1.57	0.69
1:B:50:ILE:HG12	1:B:67:TYR:CZ	2.28	0.69
1:A:108:VAL:CG1	1:A:112:LEU:HB3	2.23	0.69
1:C:17:PHE:HB2	2:C:603:FAD:H52A	1.75	0.68
1:C:143:VAL:HG22	1:C:184:LEU:HB2	1.74	0.68
1:D:50:ILE:HG22	1:D:118:ARG:HG2	1.76	0.68
1:D:88:GLN:O	1:D:92:GLU:HG3	1.94	0.68
1:A:231:ASN:HD22	1:A:233:GLN:HG3	1.58	0.68
1:D:4:ARG:HG2	3:D:670:HOH:O	1.94	0.68
1:B:40:ASP:O	1:B:44:MET:HG2	1.94	0.67
1:B:17:PHE:HB2	2:B:602:FAD:H52A	1.75	0.67
1:C:233:GLN:HA	1:C:233:GLN:HE21	1.58	0.66
1:C:76:LYS:HE2	1:C:123:GLU:OE2	1.95	0.66
1:A:231:ASN:ND2	1:A:233:GLN:HG3	2.11	0.66
1:C:14:ARG:NH1	1:C:14:ARG:HB2	2.12	0.65
1:D:60:LYS:HG2	1:D:73:LEU:CD2	2.27	0.65
1:B:202:GLN:HE21	1:B:202:GLN:HA	1.62	0.65
1:B:221:TYR:CB	1:B:273:LYS:HA	2.27	0.64
1:D:60:LYS:CD	1:D:73:LEU:HD22	2.27	0.63
1:A:271:ALA:O	1:A:272:ARG:HB3	1.99	0.63
1:B:192:ILE:HD11	1:B:200:ARG:HD3	1.80	0.63
1:B:50:ILE:HG13	1:B:118:ARG:HG2	1.80	0.63
1:B:64:ASN:HB2	3:B:715:HOH:O	1.99	0.63
1:A:200:ARG:NH1	2:A:601:FAD:H1B	2.14	0.62
1:C:243:GLN:O	1:C:247:LYS:HG3	2.00	0.62
1:A:246:GLU:OE1	1:A:249:LYS:HD2	1.98	0.62
1:D:231:ASN:OD1	1:D:233:GLN:HB3	1.99	0.62
1:A:148:THR:HG23	2:A:601:FAD:O2	2.00	0.61
1:A:50:ILE:HD12	1:A:117:GLU:HB3	1.82	0.61
1:C:169:TRP:HB3	1:C:170:PRO:HD3	1.81	0.61
1:B:236:PHE:HD2	1:D:160:ILE:HD11	1.65	0.61
1:D:189:THR:HG23	3:D:644:HOH:O	2.01	0.61
1:A:143:VAL:HG22	1:A:184:LEU:HB2	1.83	0.61
1:B:127:THR:HG22	1:B:129:ALA:H	1.66	0.61
1:B:255:VAL:HG23	1:B:267:ASN:HD22	1.64	0.61
1:A:264:PRO:HG3	1:A:273:LYS:HE3	1.83	0.61
1:A:160:ILE:CG1	1:C:236:PHE:HB3	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ALA:HA	1:B:200:ARG:NH1	2.17	0.59
1:A:50:ILE:CD1	1:A:117:GLU:HB3	2.32	0.59
1:B:25:ALA:O	1:B:29:LEU:HD13	2.02	0.59
1:D:169:TRP:CZ2	1:D:256:GLY:HA3	2.38	0.59
1:C:84:ILE:O	1:C:88:GLN:HG3	2.02	0.59
1:C:238:MET:HE3	1:C:243:GLN:HG2	1.83	0.59
1:D:89:LYS:HD2	3:D:717:HOH:O	2.03	0.59
1:B:108:VAL:HG22	1:B:112:LEU:HD13	1.84	0.59
1:B:148:THR:HG22	2:B:602:FAD:O2	2.02	0.59
1:D:20:ALA:HA	1:D:23:GLU:OE2	2.03	0.59
1:C:189:THR:HG22	3:C:721:HOH:O	2.02	0.58
1:A:160:ILE:HG13	1:C:236:PHE:HB3	1.84	0.58
1:B:48:PRO:HG3	1:D:49:ILE:HD11	1.86	0.58
1:B:89:LYS:HG3	3:B:703:HOH:O	2.04	0.58
1:B:236:PHE:HD2	1:D:160:ILE:CD1	2.18	0.57
1:A:238:MET:HE3	1:A:243:GLN:HA	1.87	0.57
1:B:236:PHE:HB3	1:D:160:ILE:CG1	2.33	0.57
1:D:127:THR:HG23	1:D:130:ALA:HB3	1.84	0.57
1:A:148:THR:HG22	1:A:150:GLY:N	2.18	0.57
1:C:7:ILE:N	1:C:7:ILE:HD12	2.20	0.57
1:D:169:TRP:HB3	1:D:170:PRO:HD3	1.87	0.57
1:B:108:VAL:CG1	1:B:112:LEU:HB3	2.33	0.57
1:B:272:ARG:O	1:B:273:LYS:HB2	2.05	0.56
1:C:27:ALA:O	1:C:31:LYS:HD3	2.05	0.56
1:A:238:MET:CE	1:A:243:GLN:HG2	2.35	0.56
1:B:202:GLN:NE2	1:B:202:GLN:HA	2.21	0.56
1:D:29:LEU:CD1	1:D:211:LEU:HD13	2.36	0.55
1:A:138:ARG:HA	1:A:180:GLY:O	2.06	0.55
1:C:255:VAL:HG23	1:C:267:ASN:HD22	1.72	0.55
1:C:204:LEU:O	1:C:208:LYS:HG3	2.07	0.55
1:D:58:LYS:NZ	1:D:58:LYS:HB2	2.22	0.54
1:A:238:MET:HE3	1:A:243:GLN:HG2	1.89	0.54
1:D:122:GLY:O	1:D:123:GLU:HB2	2.07	0.54
1:B:169:TRP:CZ2	1:B:256:GLY:HA3	2.43	0.54
1:B:169:TRP:HB3	1:B:170:PRO:HD3	1.88	0.54
1:B:143:VAL:CG2	1:B:184:LEU:HD12	2.38	0.54
1:C:14:ARG:CB	1:C:14:ARG:HH11	2.20	0.54
1:C:158:GLN:NE2	1:C:158:GLN:H	2.06	0.54
1:A:231:ASN:HD21	1:A:233:GLN:HE21	1.57	0.53
1:B:246:GLU:O	1:B:261:LYS:NZ	2.41	0.53
1:B:148:THR:HG21	1:B:155:TYR:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:THR:HG23	1:D:130:ALA:H	1.74	0.53
1:A:127:THR:HG22	1:A:129:ALA:N	2.16	0.53
1:D:201:ILE:O	1:D:205:GLU:HG2	2.08	0.53
1:A:14:ARG:H	1:A:14:ARG:CD	2.21	0.53
1:B:108:VAL:CG2	1:B:112:LEU:HD13	2.39	0.53
1:B:230:LEU:HD22	1:D:160:ILE:HD13	1.91	0.53
1:C:195:THR:HG22	1:C:199:ALA:HB3	1.91	0.53
1:D:273:LYS:HB3	3:D:648:HOH:O	2.09	0.52
1:D:127:THR:HG21	1:D:130:ALA:HB3	1.90	0.52
1:C:76:LYS:HE3	1:C:123:GLU:HG3	1.90	0.52
1:A:122:GLY:O	1:A:123:GLU:HB3	2.09	0.52
1:A:147:THR:HG22	1:A:189:THR:OG1	2.10	0.52
1:A:273:LYS:HG2	1:A:273:LYS:OXT	2.09	0.52
1:C:169:TRP:CZ2	1:C:256:GLY:HA3	2.44	0.52
1:D:255:VAL:H	1:D:267:ASN:ND2	2.08	0.52
1:C:231:ASN:OD1	1:C:233:GLN:HB3	2.10	0.52
1:B:189:THR:HG23	3:B:608:HOH:O	2.09	0.52
1:D:27:ALA:O	1:D:31:LYS:HG3	2.10	0.51
1:C:197:ALA:HA	1:C:200:ARG:NH1	2.25	0.51
1:B:195:THR:HG22	1:B:199:ALA:HB3	1.93	0.51
1:A:198:ASP:O	1:A:202:GLN:HG2	2.11	0.51
1:B:231:ASN:ND2	1:B:233:GLN:HB3	2.26	0.51
1:D:197:ALA:HA	1:D:200:ARG:NH1	2.25	0.51
1:A:200:ARG:HH11	2:A:601:FAD:H1B	1.76	0.51
1:C:272:ARG:H	1:C:273:LYS:HZ3	1.58	0.51
1:C:189:THR:HG23	3:C:642:HOH:O	2.11	0.51
1:D:60:LYS:HG2	1:D:73:LEU:HD23	1.93	0.51
1:B:4:ARG:HB3	3:B:700:HOH:O	2.10	0.51
1:D:138:ARG:HA	1:D:180:GLY:O	2.11	0.51
1:B:230:LEU:CD2	1:D:160:ILE:HD13	2.41	0.50
1:C:271:ALA:O	1:C:272:ARG:HB2	2.10	0.50
1:D:204:LEU:O	1:D:208:LYS:HG3	2.11	0.50
1:B:237:LEU:HD21	1:D:153:SER:HB2	1.92	0.50
1:B:201:ILE:O	1:B:205:GLU:HG2	2.12	0.50
1:C:25:ALA:O	1:C:29:LEU:HD13	2.12	0.50
1:B:236:PHE:HB3	1:D:160:ILE:CD1	2.42	0.49
1:B:47:ASN:ND2	1:B:49:ILE:H	2.09	0.49
1:C:60:LYS:NZ	1:C:60:LYS:HB3	2.27	0.49
1:D:19:TYR:O	1:D:23:GLU:HG2	2.12	0.49
1:C:197:ALA:O	1:C:201:ILE:HG13	2.11	0.49
1:C:89:LYS:HG3	3:C:623:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:VAL:CG2	1:C:184:LEU:HD12	2.43	0.49
1:D:60:LYS:HB2	1:D:60:LYS:NZ	2.28	0.49
1:C:138:ARG:HA	1:C:180:GLY:O	2.11	0.49
1:C:14:ARG:HH11	1:C:14:ARG:HB2	1.77	0.49
1:A:253:LEU:O	1:A:273:LYS:HE3	2.13	0.49
1:B:112:LEU:HD22	1:B:116:PHE:CE2	2.48	0.49
1:B:77:GLU:HB2	1:B:79:HIS:CE1	2.48	0.48
1:C:273:LYS:HD2	1:C:273:LYS:N	2.27	0.48
1:D:113:LYS:O	1:D:117:GLU:HG3	2.13	0.48
1:A:169:TRP:CZ2	1:A:256:GLY:HA3	2.48	0.48
1:A:270:LYS:O	1:A:272:ARG:NH1	2.46	0.48
1:A:264:PRO:HG3	1:A:273:LYS:CE	2.42	0.48
1:B:46:PHE:O	1:B:48:PRO:HD3	2.14	0.48
1:C:151:SER:H	1:C:154:MET:HE2	1.79	0.48
1:C:233:GLN:HA	1:C:233:GLN:NE2	2.26	0.48
1:B:271:ALA:O	1:B:272:ARG:CB	2.61	0.48
1:C:55:ILE:HD12	1:C:55:ILE:N	2.29	0.48
1:D:197:ALA:HA	1:D:200:ARG:CZ	2.44	0.48
1:A:202:GLN:NE2	1:A:202:GLN:HA	2.23	0.47
1:D:23:GLU:HG3	3:D:687:HOH:O	2.14	0.47
1:D:60:LYS:HG2	1:D:73:LEU:HD22	1.96	0.47
1:D:4:ARG:HG3	1:D:35:GLU:HB2	1.96	0.47
1:D:68:PRO:O	1:D:72:VAL:HG23	2.14	0.47
1:D:272:ARG:O	1:D:273:LYS:HE3	2.14	0.47
1:A:50:ILE:HG13	1:A:118:ARG:HG2	1.95	0.47
1:C:14:ARG:HG2	1:C:19:TYR:CZ	2.50	0.47
1:D:60:LYS:HD3	1:D:73:LEU:HD22	1.97	0.47
1:D:240:LYS:CD	1:D:240:LYS:H	2.23	0.47
1:B:202:GLN:NE2	1:B:202:GLN:CA	2.78	0.47
1:C:131:MET:HE3	3:C:689:HOH:O	2.15	0.46
1:C:200:ARG:HA	1:C:203:ILE:HD12	1.98	0.46
1:A:67:TYR:HB3	1:A:68:PRO:HD3	1.97	0.46
1:C:272:ARG:H	1:C:273:LYS:NZ	2.13	0.46
1:A:243:GLN:O	1:A:247:LYS:HG3	2.15	0.46
1:D:238:MET:HE3	1:D:243:GLN:HG2	1.98	0.46
1:D:32:LYS:HA	1:D:32:LYS:HD2	1.75	0.46
1:B:236:PHE:CD2	1:D:160:ILE:HD11	2.48	0.45
1:C:155:TYR:HB3	1:C:164:MET:HB2	1.98	0.45
1:C:7:ILE:HD13	1:C:36:VAL:HG13	1.99	0.45
1:D:229:ASP:O	1:D:236:PHE:HA	2.16	0.45
1:A:163:ASP:OD2	1:A:165:ASN:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:ASP:O	1:B:202:GLN:HG2	2.16	0.45
1:A:258:HIS:HB3	1:A:263:ILE:HG12	1.98	0.45
1:A:148:THR:CG2	1:A:149:GLY:N	2.79	0.45
3:B:734:HOH:O	1:D:52:ARG:HD3	2.16	0.45
1:D:29:LEU:HD11	1:D:211:LEU:HD13	1.97	0.45
1:D:54:ASP:OD2	1:D:118:ARG:HD2	2.17	0.45
1:D:132:TYR:O	1:D:180:GLY:HA2	2.16	0.45
1:A:272:ARG:N	1:A:272:ARG:HD3	2.32	0.45
1:C:185:GLU:HG3	3:C:662:HOH:O	2.15	0.45
1:B:236:PHE:CD2	1:D:160:ILE:CD1	3.00	0.45
1:D:233:GLN:HA	1:D:233:GLN:HE21	1.82	0.45
1:A:14:ARG:N	1:A:14:ARG:HD2	2.32	0.45
1:B:154:MET:CE	1:B:160:ILE:HD11	2.47	0.45
1:A:202:GLN:CA	1:A:202:GLN:NE2	2.80	0.44
1:B:158:GLN:HE21	1:D:238:MET:CE	2.31	0.44
1:D:132:TYR:HA	1:D:177:HIS:O	2.18	0.44
1:D:1:VAL:HA	1:D:215:TRP:NE1	2.32	0.44
1:A:172:GLN:NE2	3:A:604:HOH:O	2.50	0.44
1:A:148:THR:HG22	1:A:149:GLY:N	2.32	0.44
1:D:143:VAL:HG22	1:D:184:LEU:HB2	1.99	0.44
1:D:64:ASN:HD21	1:D:66:GLN:NE2	2.15	0.44
1:A:31:LYS:HE3	1:A:31:LYS:HB2	1.79	0.44
1:C:246:GLU:HG3	3:C:670:HOH:O	2.18	0.44
1:B:214:ILE:HG23	1:B:215:TRP:N	2.33	0.43
1:C:272:ARG:HH11	1:C:272:ARG:HG2	1.83	0.43
1:D:52:ARG:HG2	1:D:52:ARG:H	1.57	0.43
1:B:176:LEU:O	1:B:181:PHE:HB2	2.17	0.43
1:C:255:VAL:H	1:C:267:ASN:ND2	2.17	0.43
1:B:141:LYS:HG2	1:B:182:GLN:HB2	2.01	0.43
1:D:239:LYS:HB2	1:D:242:VAL:HG23	2.01	0.43
1:B:238:MET:HE3	1:B:243:GLN:HG2	2.00	0.43
1:D:272:ARG:N	3:D:680:HOH:O	2.50	0.43
1:B:254:SER:HB2	1:B:267:ASN:HD21	1.83	0.43
1:A:41:LEU:HD23	1:A:44:MET:CE	2.49	0.43
1:D:127:THR:HG23	1:D:130:ALA:N	2.32	0.42
1:A:132:TYR:O	1:A:180:GLY:HA2	2.19	0.42
1:A:64:ASN:HB2	3:A:700:HOH:O	2.18	0.42
1:B:132:TYR:O	1:B:180:GLY:HA2	2.19	0.42
1:B:238:MET:CE	1:B:243:GLN:HG2	2.49	0.42
1:C:14:ARG:NH1	1:C:14:ARG:CB	2.78	0.42
1:C:233:GLN:CA	1:C:233:GLN:HE21	2.25	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:VAL:O	1:C:113:LYS:NZ	2.52	0.42
1:B:240:LYS:C	1:B:240:LYS:HD2	2.39	0.42
1:D:91:LEU:HD11	1:D:120:PHE:HE1	1.85	0.42
1:B:67:TYR:HB3	1:B:68:PRO:HD3	2.00	0.42
1:D:130:ALA:HB1	1:D:134:LYS:O	2.20	0.42
1:D:198:ASP:HA	1:D:201:ILE:HD12	2.01	0.42
1:D:211:LEU:HA	1:D:214:ILE:HB	2.00	0.42
1:D:64:ASN:HB2	3:D:744:HOH:O	2.18	0.42
1:B:22:LYS:HD2	1:B:22:LYS:C	2.40	0.42
1:C:132:TYR:O	1:C:180:GLY:HA2	2.19	0.42
1:D:197:ALA:O	1:D:201:ILE:HG13	2.20	0.42
1:C:196:PRO:HB2	1:C:198:ASP:OD1	2.20	0.42
1:B:202:GLN:HE21	1:B:202:GLN:CA	2.26	0.42
1:C:47:ASN:ND2	1:C:49:ILE:H	2.18	0.42
1:B:240:LYS:HE3	1:B:240:LYS:HB3	1.84	0.42
1:A:127:THR:CG2	1:A:129:ALA:HB3	2.50	0.41
1:B:254:SER:HB2	1:B:267:ASN:ND2	2.36	0.41
1:A:161:HIS:HD2	1:C:132:TYR:OH	2.03	0.41
1:B:29:LEU:CD1	1:B:211:LEU:HD13	2.51	0.41
1:D:76:LYS:CE	1:D:123:GLU:HG3	2.51	0.41
1:C:9:LEU:HD22	1:C:22:LYS:HD3	2.01	0.41
1:C:273:LYS:HZ2	1:C:273:LYS:N	2.19	0.41
1:A:58:LYS:CD	1:A:58:LYS:N	2.78	0.41
1:D:219:PRO:HG2	3:D:736:HOH:O	2.21	0.41
1:C:158:GLN:NE2	1:C:158:GLN:N	2.69	0.41
1:C:22:LYS:HE3	1:C:23:GLU:OE1	2.20	0.41
1:D:30:LYS:C	1:D:32:LYS:H	2.22	0.41
1:A:50:ILE:HD11	1:A:117:GLU:O	2.21	0.41
1:D:9:LEU:HD22	1:D:22:LYS:HD3	2.02	0.41
1:D:254:SER:HB2	1:D:267:ASN:HD21	1.86	0.41
1:C:242:VAL:O	1:C:246:GLU:HB2	2.21	0.41
1:A:4:ARG:HE	1:A:35:GLU:CD	2.25	0.40
1:B:27:ALA:O	1:B:31:LYS:HG3	2.20	0.40
1:A:154:MET:HG2	1:A:160:ILE:HD11	2.03	0.40
1:A:91:LEU:HD11	1:A:120:PHE:HE1	1.85	0.40
1:A:202:GLN:CA	1:A:202:GLN:HE21	2.21	0.40
1:D:241:GLU:CD	1:D:241:GLU:H	2.24	0.40
1:D:60:LYS:CG	1:D:73:LEU:HD22	2.49	0.40
1:A:91:LEU:HD11	1:A:120:PHE:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	271/273 (99%)	258 (95%)	11 (4%)	2 (1%)	25	9
1	B	271/273 (99%)	259 (96%)	11 (4%)	1 (0%)	38	20
1	C	271/273 (99%)	259 (96%)	11 (4%)	1 (0%)	38	20
1	D	271/273 (99%)	257 (95%)	14 (5%)	0	100	100
All	All	1084/1092 (99%)	1033 (95%)	47 (4%)	4 (0%)	38	20

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	272	ARG
1	C	272	ARG
1	A	230	LEU
1	B	272	ARG

5.3.2 Protein sidechains ⓘ

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	226/227 (100%)	215 (95%)	11 (5%)	29	10
1	B	226/227 (100%)	216 (96%)	10 (4%)	33	13
1	C	226/227 (100%)	217 (96%)	9 (4%)	36	15
1	D	226/227 (100%)	217 (96%)	9 (4%)	36	15
All	All	904/908 (100%)	865 (96%)	39 (4%)	33	13

W O R L D W I D E
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PROTEIN DATA BANK

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	29	LEU
1	A	112	LEU
1	A	158	GLN
1	A	160	ILE
1	A	198	ASP
1	A	202	GLN
1	A	229	ASP
1	A	233	GLN
1	A	241	GLU
1	A	272	ARG
1	B	3	ARG
1	B	14	ARG
1	B	22	LYS
1	B	47	ASN
1	B	50	ILE
1	B	108	VAL
1	B	112	LEU
1	B	158	GLN
1	B	198	ASP
1	B	240	LYS
1	C	14	ARG
1	C	60	LYS
1	C	158	GLN
1	C	189	THR
1	C	198	ASP
1	C	209	LYS
1	C	233	GLN
1	C	265	THR
1	C	273	LYS
1	D	14	ARG
1	D	52	ARG
1	D	60	LYS
1	D	61	ASP
1	D	127	THR
1	D	158	GLN
1	D	233	GLN
1	D	240	LYS
1	D	273	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	79	HIS
1	A	161	HIS
1	A	172	GLN
1	A	182	GLN
1	A	194	HIS
1	A	202	GLN
1	A	231	ASN
1	A	267	ASN
1	A	268	GLN
1	B	47	ASN
1	B	158	GLN
1	B	172	GLN
1	B	202	GLN
1	B	231	ASN
1	B	267	ASN
1	B	268	GLN
1	C	47	ASN
1	C	64	ASN
1	C	66	GLN
1	C	158	GLN
1	C	172	GLN
1	C	233	GLN
1	C	267	ASN
1	C	268	GLN
1	D	47	ASN
1	D	66	GLN
1	D	158	GLN
1	D	172	GLN
1	D	233	GLN
1	D	243	GLN
1	D	267	ASN
1	D	268	GLN

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	601	-	51,58,58	2.35	17 (33%)	54,89,89	1.78	11 (20%)
2	FAD	B	602	-	51,58,58	2.39	20 (39%)	54,89,89	1.73	7 (12%)
2	FAD	C	603	-	51,58,58	2.40	19 (37%)	54,89,89	1.75	10 (18%)
2	FAD	D	604	-	51,58,58	2.45	21 (41%)	54,89,89	1.74	8 (14%)

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	601	-	-	0/28/50/50	0/6/6/6
2	FAD	B	602	-	-	0/28/50/50	0/6/6/6
2	FAD	C	603	-	-	0/28/50/50	0/6/6/6
2	FAD	D	604	-	-	0/28/50/50	0/6/6/6

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	603	FAD	PA-O2A	-3.83	1.35	1.55
2	D	604	FAD	PA-O2A	-3.79	1.36	1.55
2	A	601	FAD	PA-O2A	-3.78	1.36	1.55
2	B	602	FAD	PA-O2A	-3.75	1.36	1.55
2	A	601	FAD	PA-O5B	-3.07	1.46	1.59
2	C	603	FAD	P-O2P	-2.97	1.40	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	FAD	P-O2P	-2.95	1.40	1.55
2	A	601	FAD	P-O2P	-2.93	1.40	1.55
2	D	604	FAD	P-O2P	-2.82	1.41	1.55
2	D	604	FAD	PA-O5B	-2.73	1.47	1.59
2	B	602	FAD	PA-O5B	-2.35	1.49	1.59
2	C	603	FAD	PA-O5B	-2.33	1.49	1.59
2	B	602	FAD	C2-N1	-2.00	1.34	1.38
2	D	604	FAD	C2-N1	-2.00	1.34	1.38
2	C	603	FAD	C5A-C4A	2.00	1.45	1.40
2	D	604	FAD	C6-C5X	2.04	1.44	1.41
2	B	602	FAD	C5A-C4A	2.14	1.45	1.40
2	B	602	FAD	C6-C5X	2.19	1.45	1.41
2	D	604	FAD	C5A-C4A	2.25	1.45	1.40
2	D	604	FAD	O4B-C4B	2.26	1.50	1.45
2	A	601	FAD	O4B-C4B	2.26	1.50	1.45
2	C	603	FAD	C5X-N5	2.36	1.38	1.35
2	A	601	FAD	C4-C4X	2.40	1.45	1.41
2	C	603	FAD	O4B-C4B	2.63	1.51	1.45
2	D	604	FAD	C5X-N5	2.63	1.39	1.35
2	A	601	FAD	C8-C7	2.68	1.47	1.41
2	A	601	FAD	C2A-N1A	2.71	1.39	1.33
2	C	603	FAD	C2A-N1A	2.80	1.39	1.33
2	C	603	FAD	C8-C7	2.84	1.48	1.41
2	A	601	FAD	C4A-N3A	2.84	1.39	1.35
2	A	601	FAD	C2A-N3A	2.86	1.37	1.32
2	A	601	FAD	O5'-C5'	2.87	1.56	1.44
2	D	604	FAD	C8-C7	2.88	1.48	1.41
2	B	602	FAD	C8-C7	2.88	1.48	1.41
2	B	602	FAD	O5'-C5'	2.90	1.56	1.44
2	D	604	FAD	C2A-N1A	2.94	1.39	1.33
2	A	601	FAD	C2-N3	2.94	1.44	1.38
2	C	603	FAD	C2A-N3A	2.99	1.37	1.32
2	C	603	FAD	O5'-C5'	2.99	1.56	1.44
2	B	602	FAD	C5X-N5	3.02	1.39	1.35
2	B	602	FAD	C2A-N3A	3.05	1.37	1.32
2	B	602	FAD	C2-N3	3.08	1.44	1.38
2	D	604	FAD	O5'-C5'	3.10	1.57	1.44
2	B	602	FAD	C4-C4X	3.14	1.47	1.41
2	D	604	FAD	C2A-N3A	3.19	1.37	1.32
2	B	602	FAD	C2A-N1A	3.19	1.39	1.33
2	D	604	FAD	C2-N3	3.24	1.44	1.38
2	B	602	FAD	C4A-N3A	3.27	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	604	FAD	C4A-N3A	3.29	1.40	1.35
2	A	601	FAD	C4X-N5	3.30	1.38	1.33
2	C	603	FAD	C4X-N5	3.34	1.38	1.33
2	D	604	FAD	C4X-N5	3.35	1.38	1.33
2	B	602	FAD	C4X-N5	3.47	1.38	1.33
2	C	603	FAD	C4-C4X	3.51	1.48	1.41
2	C	603	FAD	C10-N1	3.51	1.38	1.33
2	C	603	FAD	C4A-N3A	3.60	1.40	1.35
2	B	602	FAD	C10-N1	3.64	1.38	1.33
2	D	604	FAD	C4-C4X	3.75	1.48	1.41
2	A	601	FAD	C10-N1	3.78	1.38	1.33
2	D	604	FAD	C10-N1	3.78	1.38	1.33
2	C	603	FAD	C2-N3	3.81	1.45	1.38
2	B	602	FAD	C4-N3	4.05	1.40	1.33
2	A	601	FAD	C4-N3	4.29	1.40	1.33
2	C	603	FAD	O4B-C1B	4.51	1.47	1.41
2	D	604	FAD	C4-N3	4.61	1.41	1.33
2	A	601	FAD	O4B-C1B	4.67	1.47	1.41
2	B	602	FAD	O4B-C1B	4.69	1.47	1.41
2	A	601	FAD	C4X-C10	4.71	1.49	1.41
2	C	603	FAD	C4-N3	4.77	1.41	1.33
2	B	602	FAD	C4X-C10	4.90	1.49	1.41
2	D	604	FAD	C4X-C10	5.06	1.49	1.41
2	C	603	FAD	C4X-C10	5.11	1.50	1.41
2	D	604	FAD	O4B-C1B	5.61	1.49	1.41
2	D	604	FAD	C9A-N10	6.93	1.47	1.38
2	C	603	FAD	C9A-N10	7.04	1.48	1.38
2	B	602	FAD	C9A-N10	7.30	1.48	1.38
2	A	601	FAD	C9A-N10	7.95	1.49	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	603	FAD	C4X-C4-N3	-4.71	116.77	123.48
2	D	604	FAD	C4X-C4-N3	-4.66	116.84	123.48
2	B	602	FAD	C4X-C4-N3	-4.46	117.14	123.48
2	A	601	FAD	C4X-C4-N3	-4.27	117.40	123.48
2	B	602	FAD	C4-C4X-C10	-3.50	117.13	119.96
2	D	604	FAD	C4-C4X-C10	-3.31	117.28	119.96
2	A	601	FAD	C4-C4X-C10	-3.25	117.33	119.96
2	A	601	FAD	C4X-C10-N10	-3.12	118.35	120.52
2	C	603	FAD	C4-C4X-C10	-2.92	117.60	119.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	602	FAD	O5B-PA-O1A	-2.82	97.87	109.25
2	D	604	FAD	O5B-PA-O1A	-2.81	97.91	109.25
2	C	603	FAD	C4X-C10-N10	-2.77	118.60	120.52
2	C	603	FAD	O5B-PA-O1A	-2.77	98.08	109.25
2	A	601	FAD	O5B-PA-O1A	-2.73	98.22	109.25
2	B	602	FAD	C4X-C10-N10	-2.59	118.72	120.52
2	D	604	FAD	C4X-C10-N10	-2.46	118.81	120.52
2	D	604	FAD	N3A-C2A-N1A	-2.42	126.75	128.86
2	C	603	FAD	N3A-C2A-N1A	-2.38	126.78	128.86
2	A	601	FAD	C4B-O4B-C1B	-2.32	107.30	109.77
2	A	601	FAD	N3A-C2A-N1A	-2.20	126.94	128.86
2	D	604	FAD	C5X-C9A-N10	-2.13	116.08	117.66
2	B	602	FAD	N3A-C2A-N1A	-2.11	127.02	128.86
2	B	602	FAD	C5X-C9A-N10	-2.11	116.09	117.66
2	C	603	FAD	C4B-O4B-C1B	-2.07	107.56	109.77
2	A	601	FAD	C5X-C9A-N10	-2.06	116.13	117.66
2	C	603	FAD	C5X-C9A-N10	-2.05	116.13	117.66
2	A	601	FAD	C2A-N1A-C6A	2.01	122.28	118.77
2	A	601	FAD	C5A-C6A-N6A	2.02	124.58	120.47
2	A	601	FAD	C1'-N10-C10	2.06	120.61	118.50
2	C	603	FAD	C2A-N1A-C6A	2.08	122.41	118.77
2	D	604	FAD	C2A-N1A-C6A	2.12	122.48	118.77
2	C	603	FAD	C1'-N10-C10	2.26	120.82	118.50
2	D	604	FAD	C4-N3-C2	7.56	121.77	115.16
2	C	603	FAD	C4-N3-C2	7.58	121.78	115.16
2	B	602	FAD	C4-N3-C2	7.78	121.96	115.16
2	A	601	FAD	C4-N3-C2	7.89	122.06	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	4	0
2	B	602	FAD	2	0
2	C	603	FAD	1	0
2	D	604	FAD	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	273/273 (100%)	0.29	13 (4%)	31	36	9, 20, 41, 50	0
1	B	273/273 (100%)	0.36	12 (4%)	35	40	8, 19, 40, 47	0
1	C	273/273 (100%)	0.39	19 (6%)	17	20	11, 24, 43, 49	0
1	D	273/273 (100%)	0.32	13 (4%)	31	36	9, 22, 40, 49	0
All	All	1092/1092 (100%)	0.34	57 (5%)	28	31	8, 21, 42, 50	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	273	LYS	8.3
1	A	232	PHE	7.1
1	D	232	PHE	7.0
1	C	232	PHE	5.7
1	D	128	TYR	5.6
1	B	273	LYS	5.6
1	A	2	GLY	5.3
1	B	232	PHE	5.1
1	C	272	ARG	5.1
1	A	233	GLN	4.8
1	D	272	ARG	4.8
1	B	233	GLN	4.3
1	C	1	VAL	3.9
1	B	248	ASN	3.9
1	C	128	TYR	3.9
1	C	273	LYS	3.8
1	D	1	VAL	3.8
1	A	128	TYR	3.7
1	C	2	GLY	3.7
1	C	64	ASN	3.6
1	C	57	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	58	LYS	3.4
1	A	272	ARG	3.3
1	A	3	ARG	3.3
1	B	128	TYR	3.0
1	B	1	VAL	3.0
1	A	1	VAL	2.9
1	D	198	ASP	2.8
1	C	233	GLN	2.8
1	A	273	LYS	2.7
1	B	240	LYS	2.7
1	C	240	LYS	2.7
1	D	233	GLN	2.6
1	A	244	ASP	2.6
1	C	198	ASP	2.6
1	A	248	ASN	2.6
1	B	272	ARG	2.5
1	D	240	LYS	2.5
1	D	35	GLU	2.4
1	D	234	ALA	2.4
1	B	3	ARG	2.4
1	B	14	ARG	2.4
1	A	240	LYS	2.3
1	C	31	LYS	2.3
1	C	244	ASP	2.3
1	A	14	ARG	2.3
1	C	202	GLN	2.3
1	D	202	GLN	2.3
1	A	57	GLY	2.3
1	D	2	GLY	2.3
1	C	241	GLU	2.2
1	D	194	HIS	2.2
1	C	194	HIS	2.2
1	B	2	GLY	2.2
1	C	3	ARG	2.1
1	C	63	ALA	2.1
1	B	244	ASP	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 ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FAD	B	602	53/53	0.81	0.17	2.39	24,29,33,34	0
2	FAD	D	604	53/53	0.89	0.12	0.36	15,22,33,35	0
2	FAD	C	603	53/53	0.91	0.10	-0.14	16,22,33,34	0
2	FAD	A	601	53/53	0.91	0.10	-0.18	15,19,27,29	0

6.5 Other polymers ⓘ

There are no such residues in this entry.