Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 11:34 PM GMT

PDB ID	:	5EAI
Title	:	Crystal Structure of NAD(P)H dehydrogenase, quinone 1 complexed with a chemotherapeutic naphthoquinone E6a
Authors	:	Pidugu, L.S.; Mbimba, J.E.; Ahmad, M.; Pozharski, E.; Sausville, E.A.; Emadi, A.; Toth, E.A.
Deposited on	:	2015-10-16
Resolution	:	2.90 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:

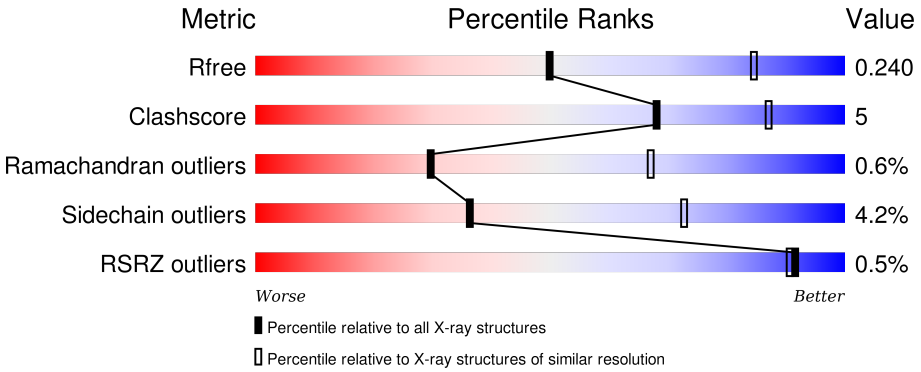
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	277	86% 11% • •
1	B	277	88% 8% • •
1	C	277	86% 11% • •
1	D	277	85% 11% • •
1	E	277	82% 13% • •

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Mol	Chain	Length	Quality of chain
1	F	277	86% 10%
1	G	277	% 81% 14%
1	H	277	87% 10%
1	I	277	81% 16%
1	J	277	84% 13%
1	K	277	% 83% 13%
1	L	277	86% 10%
1	M	277	% 85% 12%
1	N	277	% 83% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31021 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 NAD(P)H dehydrogenase [quinone] 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	46	0	0
			2134	1386	356	385	7			
1	B	270	Total	C	N	O	S	78	0	0
			2122	1379	353	383	7			
1	C	272	Total	C	N	O	S	61	0	0
			2161	1405	362	387	7			
1	D	271	Total	C	N	O	S	45	0	0
			2164	1407	363	387	7			
1	E	271	Total	C	N	O	S	55	0	0
			2155	1402	361	385	7			
1	F	271	Total	C	N	O	S	63	0	0
			2152	1400	359	386	7			
1	G	272	Total	C	N	O	S	78	0	0
			2139	1389	362	381	7			
1	H	271	Total	C	N	O	S	77	0	0
			2158	1403	362	386	7			
1	I	272	Total	C	N	O	S	31	0	0
			2163	1406	363	387	7			
1	J	271	Total	C	N	O	S	62	0	0
			2148	1396	361	384	7			
1	K	271	Total	C	N	O	S	69	0	0
			2154	1401	361	385	7			
1	L	273	Total	C	N	O	S	69	0	0
			2164	1406	364	387	7			
1	M	273	Total	C	N	O	S	80	0	0
			2151	1398	360	386	7			
1	N	271	Total	C	N	O	S	53	0	0
			2134	1391	351	385	7			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P15559

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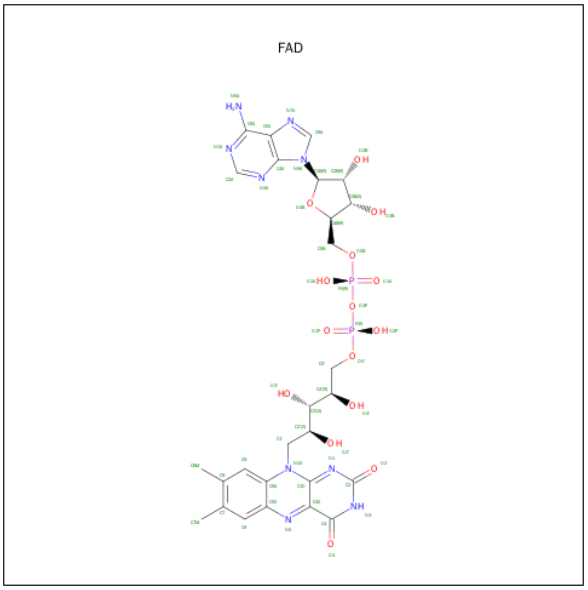
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	PRO	-	expression tag	UNP P15559
A	-1	HIS	-	expression tag	UNP P15559
B	-3	GLY	-	expression tag	UNP P15559
B	-2	PRO	-	expression tag	UNP P15559
B	-1	HIS	-	expression tag	UNP P15559
C	-3	GLY	-	expression tag	UNP P15559
C	-2	PRO	-	expression tag	UNP P15559
C	-1	HIS	-	expression tag	UNP P15559
D	-3	GLY	-	expression tag	UNP P15559
D	-2	PRO	-	expression tag	UNP P15559
D	-1	HIS	-	expression tag	UNP P15559
E	-3	GLY	-	expression tag	UNP P15559
E	-2	PRO	-	expression tag	UNP P15559
E	-1	HIS	-	expression tag	UNP P15559
F	-3	GLY	-	expression tag	UNP P15559
F	-2	PRO	-	expression tag	UNP P15559
F	-1	HIS	-	expression tag	UNP P15559
G	-3	GLY	-	expression tag	UNP P15559
G	-2	PRO	-	expression tag	UNP P15559
G	-1	HIS	-	expression tag	UNP P15559
H	-3	GLY	-	expression tag	UNP P15559
H	-2	PRO	-	expression tag	UNP P15559
H	-1	HIS	-	expression tag	UNP P15559
I	-3	GLY	-	expression tag	UNP P15559
I	-2	PRO	-	expression tag	UNP P15559
I	-1	HIS	-	expression tag	UNP P15559
J	-3	GLY	-	expression tag	UNP P15559
J	-2	PRO	-	expression tag	UNP P15559
J	-1	HIS	-	expression tag	UNP P15559
K	-3	GLY	-	expression tag	UNP P15559
K	-2	PRO	-	expression tag	UNP P15559
K	-1	HIS	-	expression tag	UNP P15559
L	-3	GLY	-	expression tag	UNP P15559
L	-2	PRO	-	expression tag	UNP P15559
L	-1	HIS	-	expression tag	UNP P15559
M	-3	GLY	-	expression tag	UNP P15559
M	-2	PRO	-	expression tag	UNP P15559
M	-1	HIS	-	expression tag	UNP P15559
N	-3	GLY	-	expression tag	UNP P15559
N	-2	PRO	-	expression tag	UNP P15559
N	-1	HIS	-	expression tag	UNP P15559

- 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		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	I	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	J	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	K	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	L	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	M	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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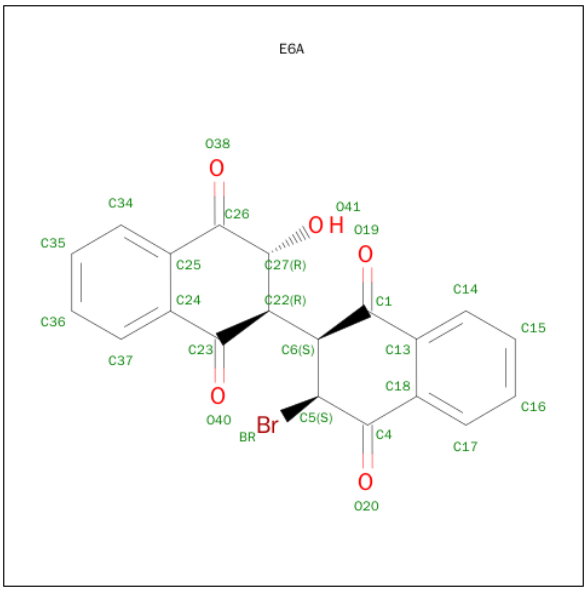
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	N	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is (2 {R},3 {R})-2-[(2 {S},3 {S})-3-bromanyl-1,4-bis(oxidanylidene)-2,3-dihydronaphthalen-2-yl]-3-oxidanyl-2,3-dihydronaphthalene-1,4-dione (three-letter code: E6A) (formula: $C_{20}H_{13}BrO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	Br	C	O	0	0
			26	1	20	5		
3	E	1	Total	Br	C	O	0	0
			26	1	20	5		
3	H	1	Total	Br	C	O	0	0
			26	1	20	5		
3	K	1	Total	Br	C	O	0	0
			26	1	20	5		
3	M	1	Total	Br	C	O	0	0
			26	1	20	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	B	4	Total	O	0	0
			4	4		

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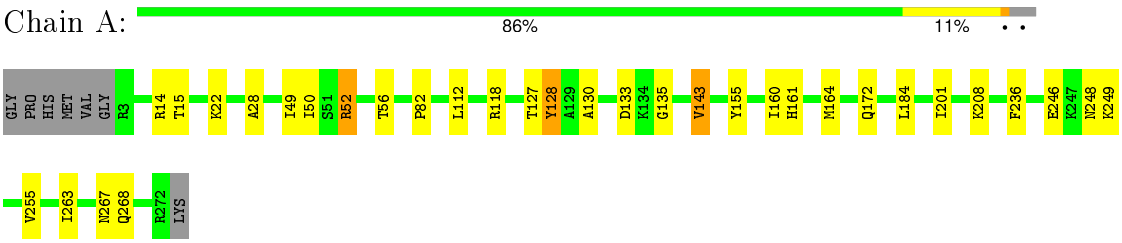
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O 1 1	0	0
4	D	4	Total O 4 4	0	0
4	E	6	Total O 6 6	0	0
4	F	2	Total O 2 2	0	0
4	G	1	Total O 1 1	0	0
4	H	3	Total O 3 3	0	0
4	I	8	Total O 8 8	0	0
4	J	4	Total O 4 4	0	0
4	K	3	Total O 3 3	0	0
4	L	4	Total O 4 4	0	0
4	M	3	Total O 3 3	0	0
4	N	3	Total O 3 3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

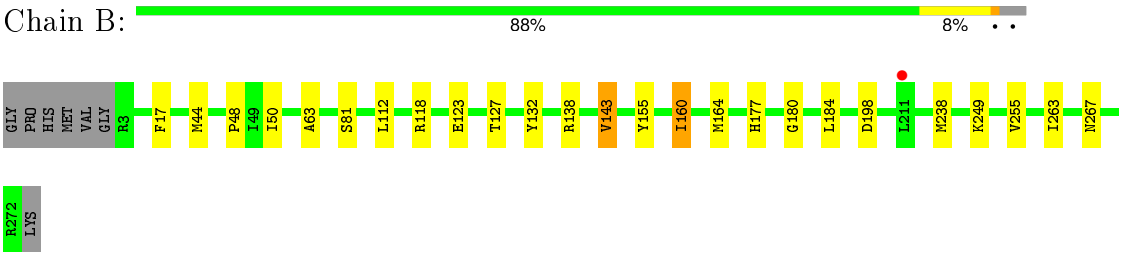
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain A:



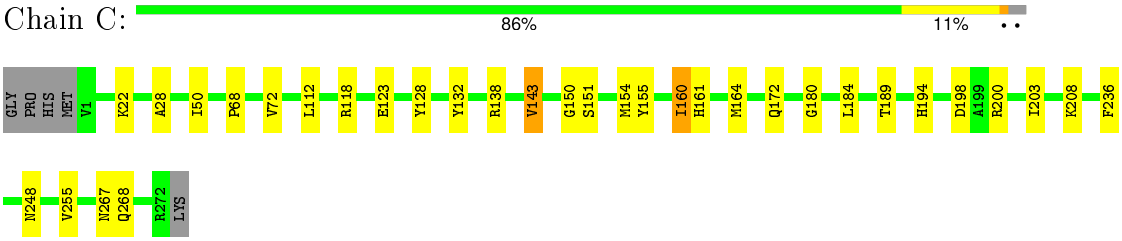
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain B:



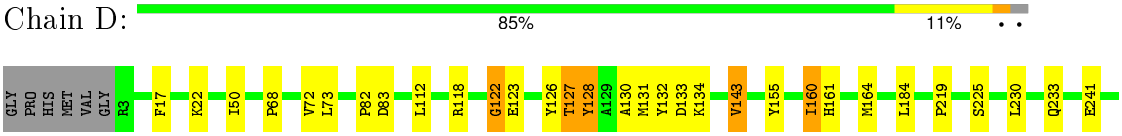
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain C:



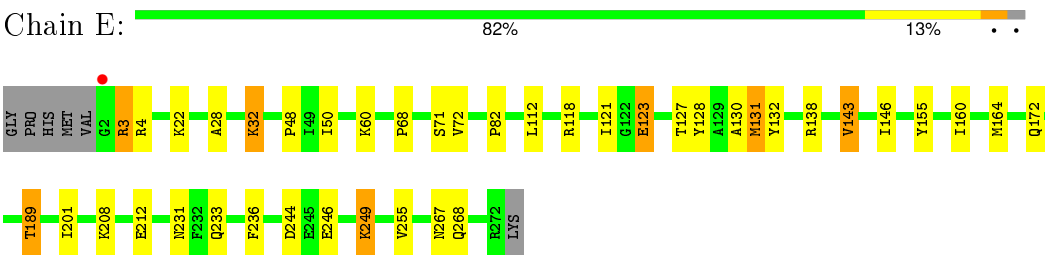
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain D:



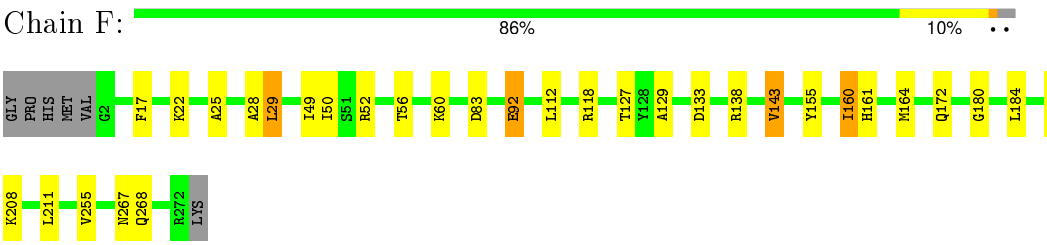
• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain E:



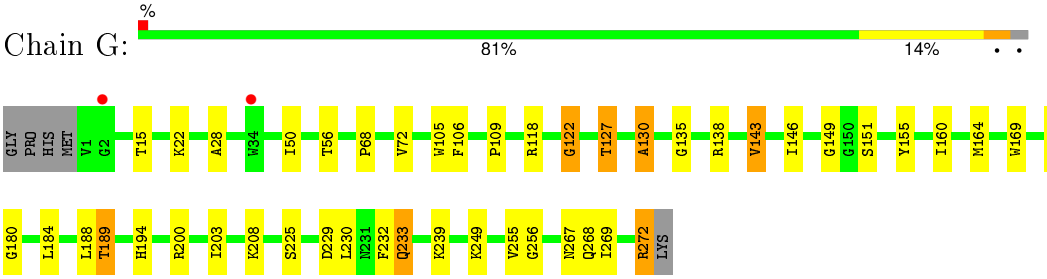
• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain F:



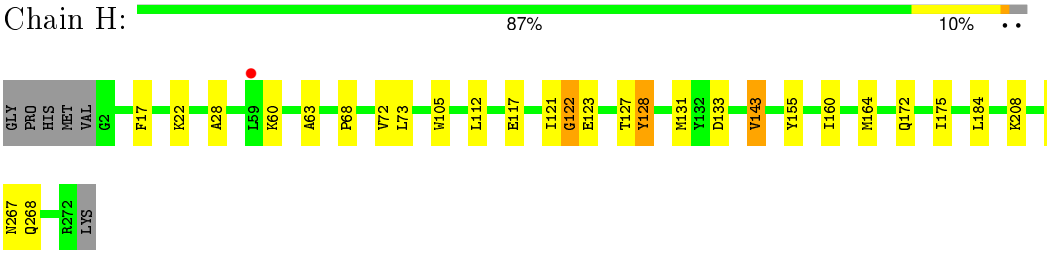
• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain G:



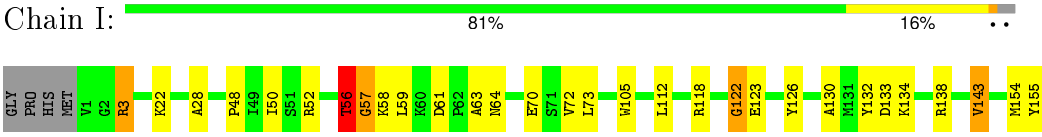
• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

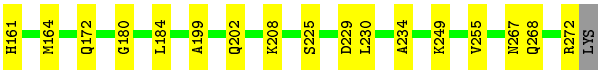
Chain H:



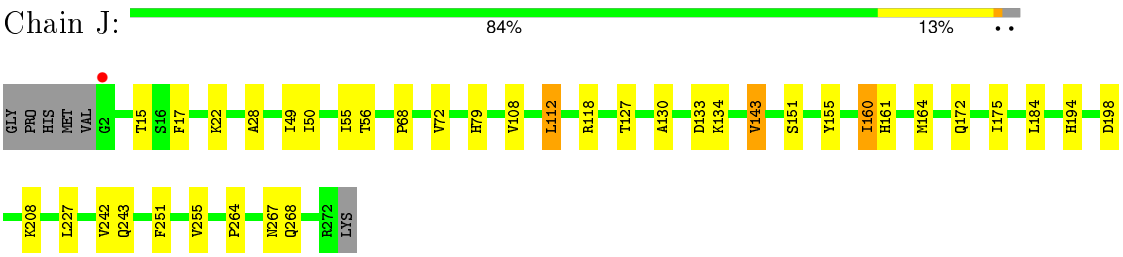
• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain I:

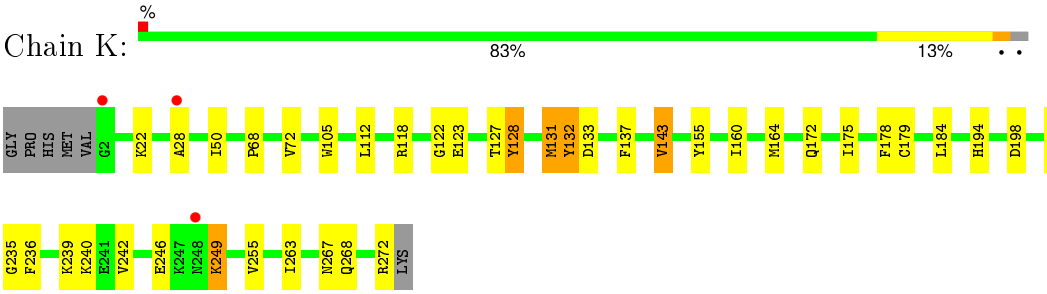




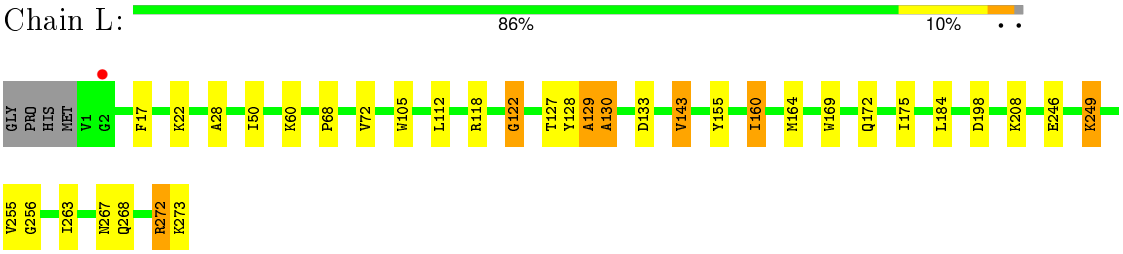
• Molecule 1: NAD(P)H dehydrogenase [quinone] 1



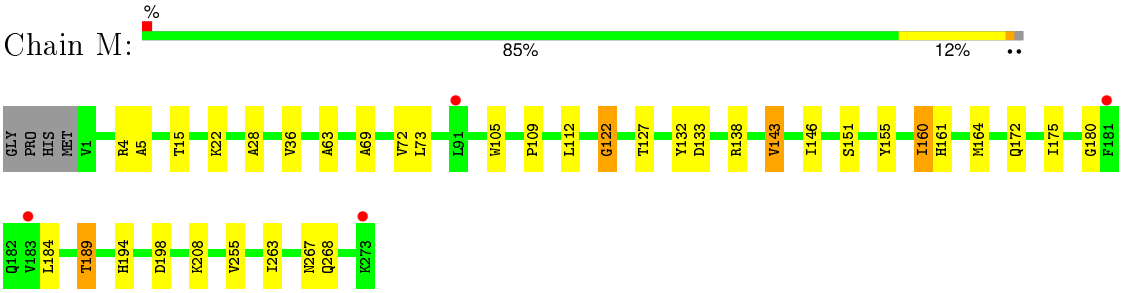
• Molecule 1: NAD(P)H dehydrogenase [quinone] 1



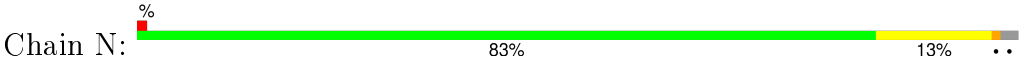
• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

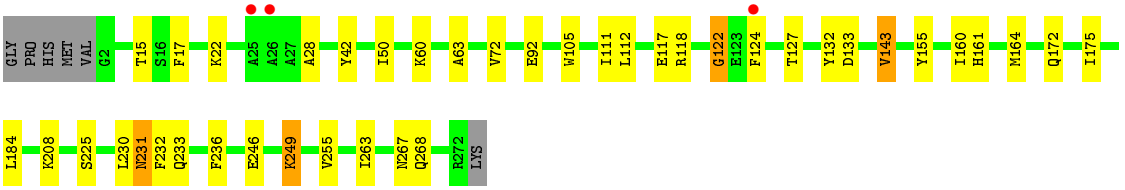


• Molecule 1: NAD(P)H dehydrogenase [quinone] 1



• Molecule 1: NAD(P)H dehydrogenase [quinone] 1




GLY
PRO
HIS
MET
VAL
G2
T15
S16
F17
K22
A25
A26
A27
A28
Y42
I50
K60
A63
V72
E92
W105
I111
L112
E117
R118
G122
E123
F124
T127
Y132
D133
V143
Y155
I160
H161
M164
Q172
I175
L184
K208
S225
L230
N231
F232
Q233
F236
E246
K249
V255
I263
N267
Q268
R272
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.60Å 210.77Å 228.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.67 – 2.90 95.67 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (95.67-2.90) 99.9 (95.67-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.183 , 0.220 0.205 , 0.240	Depositor DCC
R_{free} test set	4972 reflections (5.09%)	DCC
Wilson B-factor (Å^2)	60.8	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 73.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 102741 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	31021	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.04% 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: E6A, 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	0.53	0/2190	0.69	0/2961
1	B	0.50	0/2179	0.68	0/2951
1	C	0.55	0/2219	0.68	0/3000
1	D	0.53	0/2222	0.70	0/3000
1	E	0.55	0/2213	0.69	0/2990
1	F	0.53	0/2210	0.71	2/2987 (0.1%)
1	G	0.52	0/2195	0.73	1/2967 (0.0%)
1	H	0.52	0/2216	0.68	0/2994
1	I	0.52	0/2221	0.71	0/3001
1	J	0.51	0/2205	0.68	0/2979
1	K	0.52	0/2212	0.69	0/2989
1	L	0.54	0/2221	0.73	1/2999 (0.0%)
1	M	0.52	0/2209	0.69	0/2989
1	N	0.53	0/2192	0.70	0/2966
All	All	0.53	0/30904	0.70	4/41773 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	129	ALA	C-N-CA	8.81	143.72	121.70
1	F	92	GLU	CB-CG-CD	5.52	129.12	114.20
1	F	129	ALA	N-CA-C	-5.32	96.64	111.00
1	G	233	GLN	N-CA-C	-5.08	97.29	111.00

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	2134	0	2119	23	0
1	B	2122	0	2085	17	0
1	C	2161	0	2155	21	0
1	D	2164	0	2164	23	0
1	E	2155	0	2150	25	0
1	F	2152	0	2143	24	0
1	G	2139	0	2133	30	0
1	H	2158	0	2154	16	0
1	I	2163	0	2159	31	0
1	J	2148	0	2143	26	0
1	K	2154	0	2148	22	0
1	L	2164	0	2166	20	0
1	M	2151	0	2125	22	0
1	N	2134	0	2108	27	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
2	C	53	0	31	0	0
2	D	53	0	31	1	0
2	E	53	0	31	0	0
2	F	53	0	31	1	0
2	G	53	0	31	0	0
2	H	53	0	31	1	0
2	I	53	0	31	0	0
2	J	53	0	31	1	0
2	K	53	0	31	0	0
2	L	53	0	31	1	0
2	M	53	0	31	0	0
2	N	53	0	31	1	0
3	B	26	0	12	2	0
3	E	26	0	12	2	0
3	H	26	0	12	3	0
3	K	26	0	12	2	0
3	M	26	0	12	2	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	1	0	0	0	0
4	D	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	6	0	0	0	0
4	F	2	0	0	0	0
4	G	1	0	0	0	0
4	H	3	0	0	0	0
4	I	8	0	0	0	0
4	J	4	0	0	0	0
4	K	3	0	0	0	0
4	L	4	0	0	0	0
4	M	3	0	0	0	0
4	N	3	0	0	0	0
All	All	31021	0	30446	278	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 5.

All (278) 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:L:72:VAL:HG22	1:L:122:GLY:HA3	1.36	1.08
3:E:602:E6A:BR	3:E:602:E6A:H5	2.15	1.01
1:G:72:VAL:HG22	1:G:122:GLY:HA3	1.43	0.97
3:B:302:E6A:H5	3:B:302:E6A:BR	2.21	0.95
1:J:108:VAL:HG13	1:J:112:LEU:HB3	1.49	0.91
1:E:60:LYS:HD3	1:K:240:LYS:HB2	1.56	0.87
1:I:72:VAL:HG22	1:I:122:GLY:HA3	1.56	0.86
3:K:602:E6A:BR	3:K:602:E6A:H5	2.33	0.84
1:K:68:PRO:O	1:K:72:VAL:HG23	1.77	0.84
1:D:72:VAL:HG22	1:D:122:GLY:HA3	1.62	0.82
1:G:272:ARG:HH11	1:G:272:ARG:HB3	1.46	0.80
1:J:130:ALA:HB1	1:J:134:LYS:O	1.81	0.79
1:L:127:THR:HB	1:L:130:ALA:HB3	1.67	0.77
1:K:236:PHE:HB3	1:L:160:ILE:HD11	1.68	0.76
1:M:72:VAL:HG22	1:M:122:GLY:HA3	1.68	0.76
1:G:130:ALA:O	1:G:135:GLY:HA2	1.87	0.73
1:E:48:PRO:HG3	1:F:49:ILE:HD11	1.71	0.73
1:J:108:VAL:CG1	1:J:112:LEU:HB3	2.18	0.73
1:H:72:VAL:HG22	1:H:122:GLY:HA3	1.68	0.73
1:G:272:ARG:HB3	1:G:272:ARG:NH1	2.04	0.72
3:E:602:E6A:BR	3:E:602:E6A:C27	2.93	0.70
3:B:302:E6A:BR	3:B:302:E6A:C27	2.94	0.69
1:A:49:ILE:HD11	1:B:48:PRO:HG3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:69:ALA:O	1:M:73:LEU:HD13	1.93	0.68
1:G:188:LEU:HD11	1:G:269:ILE:HG12	1.75	0.67
1:A:128:TYR:N	1:A:128:TYR:CD1	2.62	0.67
1:F:29:LEU:CD1	1:F:211:LEU:HB3	2.24	0.67
1:E:127:THR:HG23	1:E:130:ALA:H	1.60	0.67
1:N:72:VAL:HG22	1:N:122:GLY:HA3	1.76	0.66
1:J:127:THR:HG23	1:J:130:ALA:H	1.61	0.66
3:M:602:E6A:H5	3:M:602:E6A:BR	2.51	0.66
3:H:302:E6A:H5	3:H:302:E6A:BR	2.51	0.66
1:M:161:HIS:HD2	1:N:132:TYR:OH	1.79	0.65
1:F:29:LEU:HD11	1:F:211:LEU:HB3	1.79	0.65
1:C:154:MET:HE1	1:D:128:TYR:HE2	1.63	0.62
1:N:72:VAL:CG2	1:N:122:GLY:HA3	2.29	0.61
1:N:42:TYR:CE1	1:N:111:ILE:HG21	2.36	0.60
1:A:161:HIS:HD2	1:B:132:TYR:OH	1.84	0.60
1:E:71:SER:HB2	1:E:121:ILE:HD12	1.84	0.60
1:A:56:THR:HG23	1:F:83:ASP:HB3	1.83	0.60
1:A:127:THR:HB	1:A:130:ALA:HB3	1.84	0.59
3:K:602:E6A:BR	3:K:602:E6A:C27	3.04	0.59
1:E:231:ASN:OD1	1:E:233:GLN:HB2	2.03	0.59
1:B:138:ARG:HA	1:B:180:GLY:O	2.03	0.58
1:E:131:MET:CE	1:F:160:ILE:HG13	2.34	0.58
1:H:72:VAL:HG13	1:H:123:GLU:H	1.69	0.58
1:D:127:THR:HG23	1:D:130:ALA:HB3	1.86	0.58
1:K:239:LYS:HB2	1:K:242:VAL:HG23	1.84	0.58
1:D:83:ASP:HB3	1:I:56:THR:HG23	1.87	0.57
1:L:155:TYR:HB3	1:L:164:MET:HB2	1.87	0.57
1:D:130:ALA:HB1	1:D:134:LYS:O	2.05	0.57
1:C:132:TYR:OH	1:D:161:HIS:HD2	1.88	0.57
1:H:17:PHE:HB2	2:H:301:FAD:H51A	1.88	0.56
1:M:155:TYR:HB3	1:M:164:MET:HB2	1.88	0.56
1:I:3:ARG:HE	1:I:3:ARG:HA	1.71	0.56
1:L:28:ALA:HB2	1:L:208:LYS:HG2	1.88	0.56
1:H:128:TYR:HA	1:H:131:MET:HG3	1.88	0.55
1:C:28:ALA:HB2	1:C:208:LYS:HG2	1.89	0.55
1:F:28:ALA:HB2	1:F:208:LYS:HG2	1.89	0.55
1:A:236:PHE:HB3	1:B:160:ILE:HG13	1.88	0.55
1:B:155:TYR:HB3	1:B:164:MET:HB2	1.88	0.55
1:N:155:TYR:HB3	1:N:164:MET:HB2	1.89	0.55
1:H:155:TYR:HB3	1:H:164:MET:HB2	1.88	0.54
1:C:160:ILE:HD13	1:D:131:MET:HE1	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:TYR:HB3	1:C:164:MET:HB2	1.90	0.54
1:E:155:TYR:HB3	1:E:164:MET:HB2	1.88	0.54
1:K:155:TYR:HB3	1:K:164:MET:HB2	1.89	0.54
1:I:154:MET:HB3	1:I:161:HIS:CD2	2.42	0.54
1:F:17:PHE:HB2	2:F:301:FAD:H51A	1.90	0.54
1:H:68:PRO:O	1:H:72:VAL:HG23	2.08	0.53
1:J:155:TYR:HB3	1:J:164:MET:HB2	1.89	0.53
1:G:28:ALA:HB2	1:G:208:LYS:HG2	1.91	0.53
1:A:201:ILE:HD12	2:A:601:FAD:H2A	1.90	0.53
1:G:155:TYR:HB3	1:G:164:MET:HB2	1.91	0.53
1:A:82:PRO:HB3	1:F:56:THR:HG22	1.90	0.53
1:G:151:SER:HB2	1:J:194:HIS:HB3	1.90	0.53
1:A:155:TYR:HB3	1:A:164:MET:HB2	1.89	0.53
1:J:28:ALA:HB2	1:J:208:LYS:HG2	1.91	0.53
1:H:28:ALA:HB2	1:H:208:LYS:HG2	1.90	0.53
1:M:255:VAL:HG23	1:M:267:ASN:HD22	1.73	0.53
1:E:28:ALA:HB2	1:E:208:LYS:HG2	1.90	0.53
1:F:155:TYR:HB3	1:F:164:MET:HB2	1.90	0.53
1:H:255:VAL:HG23	1:H:267:ASN:HD22	1.74	0.52
1:I:138:ARG:HA	1:I:180:GLY:O	2.09	0.52
1:G:194:HIS:HB3	1:J:151:SER:HB2	1.91	0.52
1:N:28:ALA:HB2	1:N:208:LYS:HG2	1.91	0.52
1:D:155:TYR:HB3	1:D:164:MET:HB2	1.91	0.52
1:N:17:PHE:HB2	2:N:301:FAD:H51A	1.91	0.52
1:B:17:PHE:HB2	2:B:301:FAD:H51A	1.91	0.52
1:C:255:VAL:HG23	1:C:267:ASN:HD22	1.75	0.52
1:E:138:ARG:HA	1:E:180:GLY:O	2.09	0.52
1:L:17:PHE:HB2	2:L:301:FAD:H51A	1.91	0.52
1:N:143:VAL:HG13	1:N:184:LEU:HB2	1.92	0.52
1:G:164:MET:HG3	1:G:269:ILE:HD11	1.91	0.52
1:E:131:MET:HE3	1:F:160:ILE:HG13	1.92	0.52
1:I:28:ALA:HB2	1:I:208:LYS:HG2	1.91	0.51
1:G:146:ILE:O	1:G:189:THR:HG23	2.10	0.51
1:H:143:VAL:HG13	1:H:184:LEU:HB2	1.91	0.51
1:N:246:GLU:HA	1:N:249:LYS:HG3	1.93	0.51
1:E:132:TYR:OH	1:F:161:HIS:HD2	1.94	0.51
1:L:129:ALA:HB3	1:L:130:ALA:CB	2.41	0.51
1:E:143:VAL:HG13	1:E:184:LEU:HB2	1.93	0.51
1:I:50:ILE:CG2	1:I:118:ARG:HG2	2.40	0.50
1:M:263:ILE:HD11	1:N:263:ILE:HD11	1.93	0.50
1:G:143:VAL:HG13	1:G:184:LEU:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:VAL:HG13	1:B:184:LEU:HB2	1.94	0.50
1:J:255:VAL:HG23	1:J:267:ASN:HD22	1.76	0.50
1:K:143:VAL:HG13	1:K:184:LEU:HB2	1.94	0.50
1:K:246:GLU:HA	1:K:249:LYS:HG3	1.93	0.50
1:L:143:VAL:HG13	1:L:184:LEU:HB2	1.93	0.50
1:J:172:GLN:HB2	1:J:268:GLN:NE2	2.27	0.50
1:I:56:THR:HG22	1:I:57:GLY:N	2.26	0.50
1:A:143:VAL:HG13	1:A:184:LEU:HB2	1.93	0.50
1:I:50:ILE:HG22	1:I:118:ARG:HG2	1.94	0.50
1:C:143:VAL:HG13	1:C:184:LEU:HB2	1.93	0.50
1:N:255:VAL:HG23	1:N:267:ASN:HD22	1.77	0.50
1:C:154:MET:HE3	1:C:160:ILE:HD11	1.94	0.49
1:I:143:VAL:HG13	1:I:184:LEU:HB2	1.94	0.49
1:I:255:VAL:HG23	1:I:267:ASN:HD22	1.76	0.49
1:G:255:VAL:HG23	1:G:267:ASN:HD22	1.76	0.49
1:I:230:LEU:HD21	1:J:160:ILE:HG21	1.94	0.49
1:H:121:ILE:O	1:H:122:GLY:O	2.30	0.49
1:M:28:ALA:HB2	1:M:208:LYS:HG2	1.94	0.49
1:C:236:PHE:HB3	1:D:160:ILE:HG13	1.93	0.49
1:I:155:TYR:HB3	1:I:164:MET:HB2	1.93	0.49
1:F:143:VAL:HG13	1:F:184:LEU:HB2	1.94	0.49
1:I:229:ASP:HB2	1:I:234:ALA:HB1	1.94	0.49
1:M:143:VAL:HG13	1:M:184:LEU:HB2	1.94	0.49
1:C:194:HIS:HB3	1:M:151:SER:HB2	1.94	0.49
1:K:28:ALA:HB2	1:K:208:LYS:HG2	1.94	0.48
1:C:151:SER:HB2	1:M:194:HIS:HB3	1.95	0.48
1:J:143:VAL:HG13	1:J:184:LEU:HB2	1.95	0.48
1:N:92:GLU:HG3	1:N:124:PHE:HE1	1.79	0.48
1:A:130:ALA:O	1:A:135:GLY:HA2	2.12	0.48
1:E:255:VAL:HG23	1:E:267:ASN:HD22	1.77	0.48
1:L:172:GLN:HB2	1:L:268:GLN:NE2	2.28	0.48
1:L:255:VAL:HG23	1:L:267:ASN:HD22	1.78	0.48
1:D:82:PRO:HG2	1:I:56:THR:HG21	1.94	0.48
1:C:161:HIS:HD2	1:D:132:TYR:OH	1.96	0.48
1:E:50:ILE:CG2	1:E:118:ARG:HG2	2.44	0.48
1:G:272:ARG:HH11	1:G:272:ARG:CB	2.22	0.48
1:F:29:LEU:HD11	1:F:211:LEU:HD22	1.95	0.48
1:F:172:GLN:HB2	1:F:268:GLN:NE2	2.28	0.48
1:M:160:ILE:HG13	1:N:236:PHE:HB3	1.95	0.48
3:H:302:E6A:C27	3:H:302:E6A:BR	3.17	0.48
1:I:132:TYR:OH	1:J:161:HIS:HD2	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:PHE:HB2	2:D:301:FAD:H51A	1.94	0.48
1:A:255:VAL:HG23	1:A:267:ASN:HD22	1.78	0.48
1:E:246:GLU:HA	1:E:249:LYS:HG3	1.94	0.48
1:E:172:GLN:HB2	1:E:268:GLN:NE2	2.28	0.48
1:I:225:SER:HB2	1:I:230:LEU:HD11	1.96	0.47
1:N:225:SER:HB2	1:N:230:LEU:HD11	1.95	0.47
1:A:236:PHE:HB3	1:B:160:ILE:CG1	2.43	0.47
1:F:50:ILE:CG2	1:F:118:ARG:HG2	2.44	0.47
1:K:236:PHE:HB3	1:L:160:ILE:CD1	2.40	0.47
1:B:50:ILE:CG2	1:B:118:ARG:HG2	2.44	0.47
1:F:255:VAL:HG23	1:F:267:ASN:HD22	1.79	0.47
1:F:25:ALA:O	1:F:29:LEU:HD22	2.15	0.47
1:C:50:ILE:CG2	1:C:118:ARG:HG2	2.44	0.47
1:J:17:PHE:HB2	2:J:301:FAD:H51A	1.94	0.47
1:G:105:TRP:HB3	1:H:175:ILE:HG12	1.97	0.47
1:C:172:GLN:HB2	1:C:268:GLN:NE2	2.29	0.47
1:K:255:VAL:HG23	1:K:267:ASN:HD22	1.78	0.47
1:K:50:ILE:CG2	1:K:118:ARG:HG2	2.45	0.47
1:A:50:ILE:CG2	1:A:118:ARG:HG2	2.44	0.47
1:L:272:ARG:O	1:L:273:LYS:HG3	2.15	0.47
1:A:28:ALA:HB2	1:A:208:LYS:HG2	1.96	0.47
1:D:225:SER:HB2	1:D:230:LEU:HD11	1.97	0.47
1:D:241:GLU:HG3	1:N:60:LYS:HG2	1.97	0.47
1:K:172:GLN:HB2	1:K:268:GLN:NE2	2.29	0.47
1:D:143:VAL:HG13	1:D:184:LEU:HB2	1.96	0.47
1:B:132:TYR:HA	1:B:177:HIS:O	2.16	0.46
1:A:263:ILE:HD11	1:B:263:ILE:HD11	1.96	0.46
1:N:231:ASN:HB2	1:N:233:GLN:HB2	1.96	0.46
1:K:105:TRP:HB3	1:L:175:ILE:HG12	1.98	0.46
1:G:229:ASP:OD2	1:G:239:LYS:HG2	2.16	0.46
1:I:3:ARG:NE	1:I:3:ARG:HA	2.30	0.46
1:G:175:ILE:HG12	1:H:105:TRP:HB3	1.98	0.46
1:F:194:HIS:NE2	1:K:235:GLY:HA2	2.30	0.46
1:N:172:GLN:HB2	1:N:268:GLN:NE2	2.30	0.46
1:A:172:GLN:HB2	1:A:268:GLN:NE2	2.31	0.46
1:I:154:MET:HB3	1:I:161:HIS:HD2	1.79	0.46
1:B:255:VAL:HG23	1:B:267:ASN:HD22	1.81	0.46
1:D:255:VAL:HG23	1:D:267:ASN:HD22	1.81	0.46
1:C:138:ARG:HA	1:C:180:GLY:O	2.16	0.46
1:E:32:LYS:HD3	1:E:212:GLU:HG2	1.97	0.46
1:I:132:TYR:O	1:I:180:GLY:HA2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:172:GLN:HB2	1:I:268:GLN:NE2	2.31	0.45
1:E:68:PRO:O	1:E:72:VAL:HG23	2.15	0.45
1:L:246:GLU:HA	1:L:249:LYS:HG3	1.99	0.45
1:F:138:ARG:HA	1:F:180:GLY:O	2.16	0.45
1:E:3:ARG:HA	1:E:3:ARG:HE	1.81	0.45
1:I:130:ALA:HB1	1:I:134:LYS:O	2.16	0.45
1:J:50:ILE:CG2	1:J:118:ARG:HG2	2.47	0.45
1:I:105:TRP:HB3	1:J:175:ILE:HG12	1.98	0.45
1:G:172:GLN:HB2	1:G:268:GLN:NE2	2.32	0.45
1:A:246:GLU:HA	1:A:249:LYS:HG3	1.98	0.45
1:J:251:PHE:CD2	1:J:264:PRO:HA	2.52	0.45
1:G:50:ILE:CG2	1:G:118:ARG:HG2	2.47	0.45
1:G:68:PRO:O	1:G:72:VAL:HG23	2.17	0.45
1:G:188:LEU:CD1	1:G:269:ILE:HG12	2.45	0.45
1:C:154:MET:CE	1:D:128:TYR:HE2	2.28	0.45
1:E:236:PHE:HB3	1:F:160:ILE:HD11	1.98	0.45
1:M:172:GLN:HB2	1:M:268:GLN:NE2	2.32	0.45
1:M:63:ALA:O	1:N:15:THR:HG21	2.17	0.45
1:L:68:PRO:O	1:L:72:VAL:HG23	2.18	0.44
1:M:132:TYR:OH	1:N:161:HIS:HD2	2.00	0.44
1:M:138:ARG:HA	1:M:180:GLY:O	2.16	0.44
1:D:127:THR:CG2	1:D:130:ALA:HB3	2.48	0.44
1:G:138:ARG:HA	1:G:180:GLY:O	2.18	0.44
1:H:172:GLN:HB2	1:H:268:GLN:NE2	2.32	0.44
1:G:15:THR:HG21	1:H:63:ALA:O	2.17	0.44
1:G:169:TRP:CZ2	1:G:256:GLY:HA3	2.52	0.44
1:M:175:ILE:HG12	1:N:105:TRP:HB3	1.98	0.44
3:M:602:E6A:BR	3:M:602:E6A:C27	3.20	0.44
1:G:106:PHE:N	1:G:106:PHE:CD1	2.85	0.44
1:N:50:ILE:CG2	1:N:118:ARG:HG2	2.47	0.44
1:L:127:THR:HB	1:L:130:ALA:CB	2.43	0.43
1:A:50:ILE:HG22	1:A:118:ARG:HG2	2.00	0.43
1:D:72:VAL:CG2	1:D:122:GLY:HA3	2.42	0.43
1:I:56:THR:HG22	1:I:57:GLY:H	1.82	0.43
1:M:146:ILE:O	1:M:189:THR:HG23	2.17	0.43
1:G:109:PRO:HA	1:H:117:GLU:OE2	2.18	0.43
1:I:58:LYS:HE3	1:I:59:LEU:O	2.19	0.43
1:I:48:PRO:HG3	1:J:49:ILE:HD11	2.00	0.43
1:H:127:THR:O	1:H:128:TYR:HB2	2.18	0.43
1:D:68:PRO:O	1:D:72:VAL:HG23	2.19	0.43
1:E:50:ILE:HG22	1:E:118:ARG:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:251:PHE:HD2	1:J:264:PRO:HA	1.84	0.43
1:B:123:GLU:HA	1:B:127:THR:HG22	2.00	0.43
1:M:5:ALA:HB3	1:M:36:VAL:HG22	2.01	0.43
1:I:199:ALA:HA	1:I:202:GLN:HE21	1.83	0.42
1:K:194:HIS:N	1:K:194:HIS:CD2	2.88	0.42
1:D:50:ILE:CG2	1:D:118:ARG:HG2	2.49	0.42
1:I:122:GLY:O	1:I:126:TYR:O	2.37	0.42
1:M:161:HIS:CD2	1:N:132:TYR:OH	2.67	0.42
1:B:50:ILE:HG22	1:B:118:ARG:HG2	2.00	0.42
1:F:52:ARG:HG2	1:F:52:ARG:H	1.72	0.42
1:B:44:MET:HA	1:E:82:PRO:HG2	2.02	0.42
1:E:146:ILE:O	1:E:189:THR:HG23	2.19	0.42
1:K:50:ILE:HG22	1:K:118:ARG:HG2	2.01	0.42
1:D:122:GLY:HA2	1:D:126:TYR:CZ	2.54	0.42
1:J:55:ILE:HG23	1:J:79:HIS:CD2	2.54	0.42
1:M:105:TRP:HB3	1:N:175:ILE:HG12	2.01	0.42
1:E:132:TYR:OH	1:F:161:HIS:CD2	2.73	0.41
1:G:50:ILE:HG22	1:G:118:ARG:HG2	2.02	0.41
1:K:128:TYR:HA	1:K:131:MET:HG2	2.02	0.41
1:K:263:ILE:HD11	1:L:263:ILE:HD11	2.01	0.41
1:K:132:TYR:CD1	1:K:178:PHE:HA	2.55	0.41
1:M:109:PRO:HA	1:N:117:GLU:OE2	2.20	0.41
1:M:15:THR:HG21	1:N:63:ALA:O	2.20	0.41
1:G:149:GLY:HA3	3:H:302:E6A:BR	2.74	0.41
1:N:50:ILE:HG22	1:N:118:ARG:HG2	2.03	0.41
1:A:15:THR:HG21	1:B:63:ALA:O	2.20	0.41
1:I:158:GLN:HG2	1:J:243:GLN:OE1	2.20	0.41
1:C:50:ILE:HG22	1:C:118:ARG:HG2	2.01	0.41
1:E:72:VAL:HG13	1:E:123:GLU:HB2	2.03	0.41
1:J:50:ILE:HG22	1:J:118:ARG:HG2	2.02	0.41
1:A:161:HIS:CD2	1:B:132:TYR:OH	2.69	0.41
1:A:52:ARG:HG2	1:A:52:ARG:H	1.68	0.41
1:C:160:ILE:HG21	1:D:230:LEU:HD21	2.02	0.41
1:F:50:ILE:HG22	1:F:118:ARG:HG2	2.02	0.41
1:L:50:ILE:CG2	1:L:118:ARG:HG2	2.49	0.41
1:C:200:ARG:HA	1:C:203:ILE:HD12	2.03	0.41
1:J:68:PRO:O	1:J:72:VAL:HG23	2.20	0.41
1:K:175:ILE:HG12	1:L:105:TRP:HB3	2.04	0.40
1:J:227:LEU:HB3	1:J:242:VAL:HG11	2.02	0.40
1:I:63:ALA:O	1:J:15:THR:HG21	2.21	0.40
1:G:225:SER:HB2	1:G:230:LEU:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:56:THR:HB	1:J:79:HIS:HB2	2.04	0.40
1:G:200:ARG:HA	1:G:203:ILE:HD12	2.03	0.40
1:I:61:ASP:OD2	1:I:64:ASN:HB3	2.21	0.40
1:K:72:VAL:HG13	1:K:123:GLU:H	1.86	0.40
1:K:137:PHE:CD2	1:K:179:CYS:HB3	2.56	0.40
1:C:68:PRO:O	1:C:72:VAL:HG23	2.21	0.40
1:C:150:GLY:HA2	1:N:232:PHE:HE2	1.85	0.40
1:A:56:THR:CG2	1:F:83:ASP:HB3	2.49	0.40
1:L:169:TRP:CZ2	1:L:256:GLY:HA3	2.56	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	268/277 (97%)	254 (95%)	14 (5%)	0	100	100
1	B	268/277 (97%)	256 (96%)	12 (4%)	0	100	100
1	C	270/277 (98%)	259 (96%)	10 (4%)	1 (0%)	39	74
1	D	269/277 (97%)	255 (95%)	12 (4%)	2 (1%)	26	63
1	E	269/277 (97%)	255 (95%)	12 (4%)	2 (1%)	26	63
1	F	269/277 (97%)	259 (96%)	10 (4%)	0	100	100
1	G	270/277 (98%)	249 (92%)	16 (6%)	5 (2%)	10	35
1	H	269/277 (97%)	253 (94%)	14 (5%)	2 (1%)	26	63
1	I	270/277 (98%)	260 (96%)	7 (3%)	3 (1%)	17	51
1	J	269/277 (97%)	253 (94%)	16 (6%)	0	100	100
1	K	269/277 (97%)	256 (95%)	11 (4%)	2 (1%)	26	63
1	L	271/277 (98%)	255 (94%)	12 (4%)	4 (2%)	13	42
1	M	271/277 (98%)	260 (96%)	10 (4%)	1 (0%)	39	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	N	269/277 (97%)	251 (93%)	17 (6%)	1 (0%)	39 74
All	All	3771/3878 (97%)	3575 (95%)	173 (5%)	23 (1%)	30 67

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	271	ALA
1	E	131	MET
1	G	130	ALA
1	H	122	GLY
1	I	56	THR
1	L	272	ARG
1	D	122	GLY
1	G	122	GLY
1	G	233	GLN
1	H	128	TYR
1	I	57	GLY
1	I	122	GLY
1	K	122	GLY
1	L	122	GLY
1	L	128	TYR
1	L	130	ALA
1	G	127	THR
1	G	232	PHE
1	C	123	GLU
1	E	32	LYS
1	K	132	TYR
1	N	122	GLY
1	M	122	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	221/230 (96%)	212 (96%)	9 (4%)	37 73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	218/230 (95%)	211 (97%)	7 (3%)	46 81
1	C	225/230 (98%)	217 (96%)	8 (4%)	42 78
1	D	226/230 (98%)	214 (95%)	12 (5%)	28 63
1	E	224/230 (97%)	212 (95%)	12 (5%)	27 62
1	F	224/230 (97%)	214 (96%)	10 (4%)	34 70
1	G	220/230 (96%)	212 (96%)	8 (4%)	42 78
1	H	225/230 (98%)	217 (96%)	8 (4%)	42 78
1	I	225/230 (98%)	212 (94%)	13 (6%)	25 58
1	J	223/230 (97%)	217 (97%)	6 (3%)	52 84
1	K	224/230 (97%)	212 (95%)	12 (5%)	27 62
1	L	225/230 (98%)	217 (96%)	8 (4%)	42 78
1	M	221/230 (96%)	212 (96%)	9 (4%)	37 73
1	N	220/230 (96%)	212 (96%)	8 (4%)	42 78
All	All	3121/3220 (97%)	2991 (96%)	130 (4%)	36 73

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	22	LYS
1	A	52	ARG
1	A	112	LEU
1	A	128	TYR
1	A	133	ASP
1	A	143	VAL
1	A	160	ILE
1	A	248	ASN
1	B	81	SER
1	B	112	LEU
1	B	143	VAL
1	B	160	ILE
1	B	198	ASP
1	B	238	MET
1	B	249	LYS
1	C	22	LYS
1	C	112	LEU
1	C	128	TYR

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Mol	Chain	Res	Type
1	C	143	VAL
1	C	160	ILE
1	C	189	THR
1	C	198	ASP
1	C	248	ASN
1	D	22	LYS
1	D	73	LEU
1	D	112	LEU
1	D	123	GLU
1	D	127	THR
1	D	128	TYR
1	D	133	ASP
1	D	143	VAL
1	D	160	ILE
1	D	219	PRO
1	D	233	GLN
1	D	248	ASN
1	E	3	ARG
1	E	4	ARG
1	E	22	LYS
1	E	112	LEU
1	E	123	GLU
1	E	128	TYR
1	E	143	VAL
1	E	160	ILE
1	E	189	THR
1	E	201	ILE
1	E	244	ASP
1	E	249	LYS
1	F	22	LYS
1	F	29	LEU
1	F	60	LYS
1	F	92	GLU
1	F	112	LEU
1	F	127	THR
1	F	133	ASP
1	F	143	VAL
1	F	160	ILE
1	F	198	ASP
1	G	22	LYS
1	G	56	THR
1	G	127	THR

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Mol	Chain	Res	Type
1	G	143	VAL
1	G	160	ILE
1	G	189	THR
1	G	249	LYS
1	G	272	ARG
1	H	22	LYS
1	H	60	LYS
1	H	73	LEU
1	H	112	LEU
1	H	133	ASP
1	H	143	VAL
1	H	160	ILE
1	H	248	ASN
1	I	3	ARG
1	I	22	LYS
1	I	52	ARG
1	I	56	THR
1	I	70	GLU
1	I	73	LEU
1	I	112	LEU
1	I	123	GLU
1	I	133	ASP
1	I	143	VAL
1	I	160	ILE
1	I	249	LYS
1	I	272	ARG
1	J	22	LYS
1	J	112	LEU
1	J	133	ASP
1	J	143	VAL
1	J	160	ILE
1	J	198	ASP
1	K	22	LYS
1	K	112	LEU
1	K	127	THR
1	K	128	TYR
1	K	131	MET
1	K	133	ASP
1	K	143	VAL
1	K	160	ILE
1	K	198	ASP
1	K	230	LEU

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Mol	Chain	Res	Type
1	K	249	LYS
1	K	272	ARG
1	L	22	LYS
1	L	60	LYS
1	L	112	LEU
1	L	133	ASP
1	L	143	VAL
1	L	160	ILE
1	L	198	ASP
1	L	249	LYS
1	M	4	ARG
1	M	22	LYS
1	M	112	LEU
1	M	127	THR
1	M	133	ASP
1	M	143	VAL
1	M	160	ILE
1	M	189	THR
1	M	198	ASP
1	N	22	LYS
1	N	112	LEU
1	N	127	THR
1	N	133	ASP
1	N	143	VAL
1	N	160	ILE
1	N	231	ASN
1	N	249	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	HIS
1	A	172	GLN
1	A	267	ASN
1	A	268	GLN
1	B	79	HIS
1	B	172	GLN
1	B	267	ASN
1	B	268	GLN
1	C	79	HIS
1	C	161	HIS
1	C	172	GLN

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Mol	Chain	Res	Type
1	C	267	ASN
1	C	268	GLN
1	D	88	GLN
1	D	161	HIS
1	D	267	ASN
1	D	268	GLN
1	E	79	HIS
1	E	172	GLN
1	E	267	ASN
1	E	268	GLN
1	F	79	HIS
1	F	161	HIS
1	F	172	GLN
1	F	194	HIS
1	F	267	ASN
1	F	268	GLN
1	G	172	GLN
1	G	231	ASN
1	G	267	ASN
1	G	268	GLN
1	H	172	GLN
1	H	267	ASN
1	H	268	GLN
1	I	172	GLN
1	I	202	GLN
1	I	267	ASN
1	I	268	GLN
1	J	79	HIS
1	J	161	HIS
1	J	194	HIS
1	J	267	ASN
1	J	268	GLN
1	K	79	HIS
1	K	172	GLN
1	K	194	HIS
1	K	267	ASN
1	K	268	GLN
1	L	172	GLN
1	L	267	ASN
1	L	268	GLN
1	M	161	HIS
1	M	172	GLN

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Mol	Chain	Res	Type
1	M	194	HIS
1	M	267	ASN
1	M	268	GLN
1	N	161	HIS
1	N	267	ASN
1	N	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

19 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	-	52,58,58	1.15	5 (9%)	52,89,89	2.45	5 (9%)
2	FAD	B	301	-	52,58,58	1.10	5 (9%)	52,89,89	2.40	5 (9%)
3	E6A	B	302	-	26,29,29	2.46	5 (19%)	34,44,44	2.43	10 (29%)
2	FAD	C	601	-	52,58,58	1.12	5 (9%)	52,89,89	2.37	6 (11%)
2	FAD	D	301	-	52,58,58	1.17	5 (9%)	52,89,89	2.39	6 (11%)
2	FAD	E	601	-	52,58,58	1.10	5 (9%)	52,89,89	2.41	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	E6A	E	602	-	26,29,29	2.59	5 (19%)	34,44,44	2.20	12 (35%)
2	FAD	F	301	-	52,58,58	1.16	4 (7%)	52,89,89	2.34	5 (9%)
2	FAD	G	601	-	52,58,58	1.04	5 (9%)	52,89,89	2.43	5 (9%)
2	FAD	H	301	-	52,58,58	1.22	5 (9%)	52,89,89	2.38	5 (9%)
3	E6A	H	302	-	26,29,29	2.55	4 (15%)	34,44,44	2.50	14 (41%)
2	FAD	I	601	-	52,58,58	1.14	5 (9%)	52,89,89	2.38	5 (9%)
2	FAD	J	301	-	52,58,58	1.04	4 (7%)	52,89,89	2.39	5 (9%)
2	FAD	K	601	-	52,58,58	1.12	5 (9%)	52,89,89	2.39	6 (11%)
3	E6A	K	602	-	26,29,29	2.43	4 (15%)	34,44,44	2.43	11 (32%)
2	FAD	L	301	-	52,58,58	1.15	5 (9%)	52,89,89	2.39	5 (9%)
2	FAD	M	601	-	52,58,58	1.06	5 (9%)	52,89,89	2.36	5 (9%)
3	E6A	M	602	-	26,29,29	2.64	6 (23%)	34,44,44	2.65	13 (38%)
2	FAD	N	301	-	52,58,58	1.18	5 (9%)	52,89,89	2.37	5 (9%)

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	-	-	0/30/50/50	0/6/6/6
2	FAD	B	301	-	-	0/30/50/50	0/6/6/6
3	E6A	B	302	-	-	0/4/44/44	0/4/4/4
2	FAD	C	601	-	-	0/30/50/50	0/6/6/6
2	FAD	D	301	-	-	0/30/50/50	0/6/6/6
2	FAD	E	601	-	-	0/30/50/50	0/6/6/6
3	E6A	E	602	-	-	0/4/44/44	0/4/4/4
2	FAD	F	301	-	-	0/30/50/50	0/6/6/6
2	FAD	G	601	-	-	0/30/50/50	0/6/6/6
2	FAD	H	301	-	-	0/30/50/50	0/6/6/6
3	E6A	H	302	-	-	0/4/44/44	0/4/4/4
2	FAD	I	601	-	-	0/30/50/50	0/6/6/6
2	FAD	J	301	-	-	0/30/50/50	0/6/6/6
2	FAD	K	601	-	-	0/30/50/50	0/6/6/6
3	E6A	K	602	-	-	0/4/44/44	0/4/4/4
2	FAD	L	301	-	-	0/30/50/50	0/6/6/6
2	FAD	M	601	-	-	0/30/50/50	0/6/6/6
3	E6A	M	602	-	-	0/4/44/44	0/4/4/4
2	FAD	N	301	-	-	0/30/50/50	0/6/6/6

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	602	E6A	C25-C26	2.05	1.52	1.48
3	B	302	E6A	C24-C23	2.08	1.52	1.48
2	G	601	FAD	C4-C4X	2.09	1.45	1.41
2	A	601	FAD	C4-C4X	2.09	1.45	1.41
3	K	602	E6A	C25-C26	2.12	1.52	1.48
2	B	301	FAD	C9A-N10	2.17	1.41	1.38
3	M	602	E6A	C24-C23	2.21	1.52	1.48
3	B	302	E6A	BR-C5	2.24	2.05	1.97
3	E	602	E6A	C24-C23	2.33	1.52	1.48
2	B	301	FAD	C4-C4X	2.33	1.46	1.41
2	J	301	FAD	C5X-N5	2.37	1.39	1.35
3	M	602	E6A	BR-C5	2.40	2.05	1.97
3	H	302	E6A	C24-C23	2.58	1.53	1.48
2	L	301	FAD	C5X-N5	2.59	1.39	1.35
2	L	301	FAD	C4-C4X	2.61	1.46	1.41
2	C	601	FAD	C4-C4X	2.64	1.46	1.41
2	E	601	FAD	C9A-N10	2.70	1.42	1.38
2	J	301	FAD	C9A-N10	2.72	1.42	1.38
2	M	601	FAD	C9A-N10	2.74	1.42	1.38
2	G	601	FAD	C5X-N5	2.74	1.39	1.35
2	M	601	FAD	C4-C4X	2.76	1.46	1.41
2	D	301	FAD	C4-C4X	2.77	1.46	1.41
2	C	601	FAD	C5X-N5	2.79	1.39	1.35
3	E	602	E6A	C25-C26	2.79	1.53	1.48
2	I	601	FAD	C4-C4X	2.81	1.47	1.41
2	G	601	FAD	C9A-N10	2.82	1.42	1.38
2	K	601	FAD	C4X-C10	2.84	1.46	1.40
2	M	601	FAD	C4X-C10	2.86	1.46	1.40
2	N	301	FAD	C4-C4X	2.87	1.47	1.41
2	G	601	FAD	C4X-C10	2.87	1.46	1.40
2	H	301	FAD	C4-C4X	2.93	1.47	1.41
2	D	301	FAD	C5X-N5	2.95	1.40	1.35
2	K	601	FAD	C5X-N5	2.96	1.40	1.35
2	E	601	FAD	C4-N3	2.98	1.38	1.33
2	N	301	FAD	C5X-N5	2.98	1.40	1.35
2	N	301	FAD	C9A-N10	2.99	1.43	1.38
2	A	601	FAD	C5X-N5	3.01	1.40	1.35
2	E	601	FAD	C5X-N5	3.02	1.40	1.35
2	C	601	FAD	C9A-N10	3.02	1.43	1.38
2	E	601	FAD	C4X-C10	3.10	1.46	1.40
2	M	601	FAD	C5X-N5	3.11	1.40	1.35
2	B	301	FAD	C5X-N5	3.13	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	301	FAD	C5X-N5	3.17	1.40	1.35
2	M	601	FAD	C4-N3	3.17	1.38	1.33
2	C	601	FAD	C4X-C10	3.21	1.46	1.40
2	I	601	FAD	C4X-C10	3.22	1.46	1.40
2	J	301	FAD	C4X-C10	3.22	1.46	1.40
2	F	301	FAD	C5X-N5	3.26	1.40	1.35
2	B	301	FAD	C4-N3	3.27	1.38	1.33
2	D	301	FAD	C4-N3	3.27	1.38	1.33
2	K	601	FAD	C9A-N10	3.29	1.43	1.38
2	I	601	FAD	C5X-N5	3.29	1.40	1.35
2	A	601	FAD	C4-N3	3.34	1.39	1.33
2	G	601	FAD	C4-N3	3.35	1.39	1.33
2	K	601	FAD	C4-N3	3.36	1.39	1.33
2	F	301	FAD	C9A-N10	3.37	1.43	1.38
2	K	601	FAD	C4-C4X	3.37	1.48	1.41
2	L	301	FAD	C9A-N10	3.38	1.43	1.38
2	I	601	FAD	C9A-N10	3.41	1.43	1.38
2	F	301	FAD	C4-N3	3.42	1.39	1.33
2	D	301	FAD	C4X-C10	3.43	1.47	1.40
2	L	301	FAD	C4-N3	3.44	1.39	1.33
2	A	601	FAD	C9A-N10	3.44	1.43	1.38
2	E	601	FAD	C4-C4X	3.54	1.48	1.41
2	H	301	FAD	C4-N3	3.54	1.39	1.33
2	C	601	FAD	C4-N3	3.56	1.39	1.33
2	I	601	FAD	C4-N3	3.57	1.39	1.33
2	L	301	FAD	C4X-C10	3.57	1.47	1.40
2	H	301	FAD	C4X-C10	3.62	1.47	1.40
2	N	301	FAD	C4-N3	3.66	1.39	1.33
2	J	301	FAD	C4-N3	3.66	1.39	1.33
2	B	301	FAD	C4X-C10	3.68	1.47	1.40
2	D	301	FAD	C9A-N10	3.69	1.44	1.38
2	N	301	FAD	C4X-C10	3.72	1.47	1.40
2	H	301	FAD	C9A-N10	3.76	1.44	1.38
2	A	601	FAD	C4X-C10	3.85	1.48	1.40
2	F	301	FAD	C4X-C10	3.85	1.48	1.40
3	B	302	E6A	C13-C18	4.09	1.47	1.40
3	H	302	E6A	C13-C18	4.16	1.47	1.40
3	E	602	E6A	C13-C18	4.45	1.47	1.40
3	M	602	E6A	C13-C18	4.72	1.47	1.40
3	K	602	E6A	C13-C18	4.79	1.48	1.40
3	K	602	E6A	C24-C25	5.51	1.49	1.40
3	H	302	E6A	C24-C25	5.59	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	602	E6A	C24-C25	5.84	1.49	1.40
3	B	302	E6A	C24-C25	5.88	1.49	1.40
3	E	602	E6A	C24-C25	6.41	1.50	1.40
3	K	602	E6A	C6-C5	8.71	1.63	1.53
3	B	302	E6A	C6-C5	8.86	1.63	1.53
3	E	602	E6A	C6-C5	8.94	1.63	1.53
3	H	302	E6A	C6-C5	9.68	1.64	1.53
3	M	602	E6A	C6-C5	9.80	1.64	1.53

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	601	FAD	C4X-C4-N3	-7.49	113.73	123.52
2	M	601	FAD	C4X-C4-N3	-7.14	114.18	123.52
2	B	301	FAD	C4X-C4-N3	-7.14	114.19	123.52
2	A	601	FAD	C4X-C4-N3	-7.11	114.22	123.52
2	J	301	FAD	C4X-C4-N3	-7.08	114.27	123.52
2	G	601	FAD	C4X-C4-N3	-7.07	114.27	123.52
2	L	301	FAD	C4X-C4-N3	-7.06	114.30	123.52
2	H	301	FAD	C4X-C4-N3	-7.02	114.35	123.52
2	I	601	FAD	C4X-C4-N3	-6.99	114.38	123.52
2	N	301	FAD	C4X-C4-N3	-6.99	114.39	123.52
2	K	601	FAD	C4X-C4-N3	-6.97	114.41	123.52
2	C	601	FAD	C4X-C4-N3	-6.94	114.44	123.52
2	F	301	FAD	C4X-C4-N3	-6.93	114.47	123.52
2	D	301	FAD	C4X-C4-N3	-6.86	114.55	123.52
3	M	602	E6A	C18-C13-C1	-6.07	114.12	120.65
3	B	302	E6A	C13-C18-C4	-5.67	114.55	120.65
2	L	301	FAD	C4X-C10-N10	-5.57	116.47	120.52
3	K	602	E6A	C18-C13-C1	-5.50	114.73	120.65
2	N	301	FAD	C4X-C10-N10	-5.47	116.55	120.52
2	J	301	FAD	C4X-C10-N10	-5.44	116.56	120.52
2	D	301	FAD	C4X-C10-N10	-5.41	116.58	120.52
2	A	601	FAD	C4X-C10-N10	-5.37	116.62	120.52
2	H	301	FAD	C4X-C10-N10	-5.31	116.66	120.52
2	C	601	FAD	C4X-C10-N10	-5.29	116.68	120.52
3	M	602	E6A	C13-C18-C4	-5.27	114.99	120.65
2	B	301	FAD	C4X-C10-N10	-5.24	116.72	120.52
3	B	302	E6A	C18-C13-C1	-5.19	115.06	120.65
2	K	601	FAD	C4X-C10-N10	-5.06	116.84	120.52
2	F	301	FAD	C4X-C10-N10	-5.03	116.87	120.52
3	E	602	E6A	C13-C18-C4	-5.00	115.27	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	601	FAD	N3-C2-N1	-4.99	119.29	127.69
2	M	601	FAD	C4X-C10-N10	-4.95	116.92	120.52
2	I	601	FAD	C4X-C10-N10	-4.93	116.94	120.52
2	K	601	FAD	N3-C2-N1	-4.92	119.40	127.69
2	H	301	FAD	N3-C2-N1	-4.92	119.41	127.69
2	L	301	FAD	N3-C2-N1	-4.90	119.44	127.69
2	G	601	FAD	C4X-C10-N10	-4.89	116.96	120.52
2	D	301	FAD	N3-C2-N1	-4.86	119.50	127.69
2	A	601	FAD	N3-C2-N1	-4.86	119.50	127.69
2	E	601	FAD	C4X-C10-N10	-4.85	116.99	120.52
2	J	301	FAD	N3-C2-N1	-4.79	119.63	127.69
2	F	301	FAD	N3-C2-N1	-4.78	119.65	127.69
2	N	301	FAD	N3-C2-N1	-4.77	119.65	127.69
2	I	601	FAD	N3-C2-N1	-4.76	119.68	127.69
2	B	301	FAD	N3-C2-N1	-4.76	119.68	127.69
2	M	601	FAD	N3-C2-N1	-4.62	119.91	127.69
3	H	302	E6A	C13-C18-C4	-4.59	115.71	120.65
3	H	302	E6A	C18-C13-C1	-4.59	115.72	120.65
2	C	601	FAD	N3-C2-N1	-4.54	120.05	127.69
3	K	602	E6A	C13-C18-C4	-4.52	115.79	120.65
2	E	601	FAD	N3-C2-N1	-4.45	120.20	127.69
3	E	602	E6A	C18-C13-C1	-4.25	116.08	120.65
2	G	601	FAD	C4-C4X-C10	-4.12	117.31	119.94
2	A	601	FAD	C4-C4X-C10	-4.03	117.36	119.94
2	H	301	FAD	C4-C4X-C10	-3.99	117.39	119.94
2	D	301	FAD	C4-C4X-C10	-3.94	117.42	119.94
2	L	301	FAD	C4-C4X-C10	-3.94	117.42	119.94
2	J	301	FAD	C4-C4X-C10	-3.93	117.42	119.94
2	K	601	FAD	C4-C4X-C10	-3.90	117.45	119.94
2	C	601	FAD	C4-C4X-C10	-3.88	117.46	119.94
2	I	601	FAD	C4-C4X-C10	-3.84	117.48	119.94
2	B	301	FAD	C4-C4X-C10	-3.84	117.48	119.94
2	N	301	FAD	C4-C4X-C10	-3.83	117.49	119.94
2	E	601	FAD	C4-C4X-C10	-3.82	117.50	119.94
2	M	601	FAD	C4-C4X-C10	-3.78	117.52	119.94
3	H	302	E6A	O40-C23-C24	-3.59	116.56	121.88
2	F	301	FAD	C4-C4X-C10	-3.46	117.73	119.94
3	H	302	E6A	O20-C4-C18	-3.46	116.75	121.88
3	E	602	E6A	O40-C23-C24	-3.31	116.98	121.88
3	B	302	E6A	O40-C23-C24	-3.01	117.42	121.88
3	K	602	E6A	O20-C4-C18	-2.80	117.74	121.88
3	E	602	E6A	O20-C4-C18	-2.74	117.82	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	302	E6A	C24-C25-C26	-2.67	117.78	120.65
3	E	602	E6A	O38-C26-C27	-2.54	116.98	119.91
3	M	602	E6A	C24-C25-C26	-2.54	117.92	120.65
3	K	602	E6A	O40-C23-C24	-2.52	118.15	121.88
3	H	302	E6A	O38-C26-C25	-2.50	118.18	121.88
3	K	602	E6A	C25-C24-C23	-2.34	118.13	120.65
3	E	602	E6A	O41-C27-C26	-2.33	106.01	111.64
3	M	602	E6A	O41-C27-C26	-2.26	106.17	111.64
3	B	302	E6A	O19-C1-C13	-2.23	118.58	121.88
3	H	302	E6A	O41-C27-C26	-2.21	106.31	111.64
3	E	602	E6A	O19-C1-C13	-2.19	118.63	121.88
3	M	602	E6A	O20-C4-C18	-2.19	118.64	121.88
3	B	302	E6A	C24-C25-C26	-2.09	118.41	120.65
3	M	602	E6A	C25-C24-C23	-2.03	118.47	120.65
3	M	602	E6A	O40-C23-C24	-2.02	118.89	121.88
2	K	601	FAD	O5B-PA-O1A	2.00	117.42	109.21
2	C	601	FAD	O5B-PA-O1A	2.01	117.43	109.21
2	D	301	FAD	O5B-PA-O1A	2.02	117.47	109.21
3	H	302	E6A	C34-C25-C26	2.12	122.95	119.83
2	E	601	FAD	O5B-PA-O1A	2.22	118.30	109.21
3	M	602	E6A	C25-C26-C27	2.26	119.83	116.14
3	M	602	E6A	C34-C25-C26	2.33	123.27	119.83
3	H	302	E6A	C17-C18-C4	2.47	123.47	119.83
3	H	302	E6A	C18-C4-C5	2.48	121.76	116.78
3	E	602	E6A	C17-C18-C4	2.53	123.56	119.83
3	B	302	E6A	C25-C26-C27	2.64	120.44	116.14
3	K	602	E6A	C6-C22-C27	2.64	118.40	112.41
3	K	602	E6A	C18-C4-C5	2.93	122.66	116.78
3	E	602	E6A	C14-C13-C1	3.04	124.31	119.83
3	H	302	E6A	C14-C13-C1	3.05	124.32	119.83
3	E	602	E6A	C25-C26-C27	3.06	121.14	116.14
3	K	602	E6A	C17-C18-C4	3.15	124.47	119.83
3	H	302	E6A	C25-C26-C27	3.27	121.48	116.14
3	E	602	E6A	C6-C22-C27	3.35	120.01	112.41
3	K	602	E6A	C25-C26-C27	3.51	121.88	116.14
3	B	302	E6A	C6-C22-C27	3.66	120.71	112.41
3	M	602	E6A	C14-C13-C1	3.81	125.44	119.83
3	B	302	E6A	C17-C18-C4	3.82	125.45	119.83
3	K	602	E6A	C14-C13-C1	3.89	125.56	119.83
3	M	602	E6A	C17-C18-C4	3.96	125.67	119.83
3	B	302	E6A	C14-C13-C1	4.52	126.48	119.83
3	E	602	E6A	BR-C5-C6	4.71	115.05	109.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	302	E6A	C6-C22-C27	4.77	123.24	112.41
3	M	602	E6A	C6-C22-C27	5.12	124.03	112.41
3	B	302	E6A	BR-C5-C6	6.36	117.06	109.28
3	H	302	E6A	BR-C5-C6	6.95	117.78	109.28
3	K	602	E6A	BR-C5-C6	7.54	118.52	109.28
3	M	602	E6A	BR-C5-C6	8.03	119.11	109.28
2	N	301	FAD	C4-N3-C2	12.73	125.78	115.16
2	H	301	FAD	C4-N3-C2	12.73	125.78	115.16
2	F	301	FAD	C4-N3-C2	12.78	125.82	115.16
2	M	601	FAD	C4-N3-C2	12.79	125.83	115.16
2	D	301	FAD	C4-N3-C2	12.79	125.83	115.16
2	K	601	FAD	C4-N3-C2	12.80	125.84	115.16
2	C	601	FAD	C4-N3-C2	12.82	125.86	115.16
2	I	601	FAD	C4-N3-C2	12.86	125.88	115.16
2	L	301	FAD	C4-N3-C2	12.86	125.89	115.16
2	J	301	FAD	C4-N3-C2	12.89	125.91	115.16
2	E	601	FAD	C4-N3-C2	12.96	125.97	115.16
2	B	301	FAD	C4-N3-C2	12.99	126.00	115.16
2	G	601	FAD	C4-N3-C2	13.00	126.00	115.16
2	A	601	FAD	C4-N3-C2	13.07	126.06	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	1	0
2	B	301	FAD	1	0
3	B	302	E6A	2	0
2	D	301	FAD	1	0
3	E	602	E6A	2	0
2	F	301	FAD	1	0
2	H	301	FAD	1	0
3	H	302	E6A	3	0
2	J	301	FAD	1	0
3	K	602	E6A	2	0
2	L	301	FAD	1	0
3	M	602	E6A	2	0
2	N	301	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, 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	270/277 (97%)	-0.11	0 100 100	47, 66, 90, 104	13 (4%)
1	B	269/277 (97%)	-0.07	1 (0%) 93 92	52, 74, 100, 114	17 (6%)
1	C	271/277 (97%)	-0.14	0 100 100	39, 62, 86, 109	13 (4%)
1	D	271/277 (97%)	-0.07	1 (0%) 93 92	44, 69, 99, 113	16 (5%)
1	E	271/277 (97%)	-0.08	1 (0%) 93 92	42, 62, 91, 109	16 (5%)
1	F	270/277 (97%)	-0.08	0 100 100	45, 69, 96, 108	14 (5%)
1	G	272/277 (98%)	-0.06	2 (0%) 89 88	47, 78, 103, 134	21 (7%)
1	H	271/277 (97%)	0.04	1 (0%) 93 92	44, 71, 98, 112	23 (8%)
1	I	272/277 (98%)	-0.07	0 100 100	46, 67, 92, 102	9 (3%)
1	J	270/277 (97%)	-0.12	1 (0%) 93 92	45, 67, 95, 102	14 (5%)
1	K	271/277 (97%)	-0.01	3 (1%) 82 80	52, 76, 101, 116	20 (7%)
1	L	272/277 (98%)	-0.06	1 (0%) 93 92	46, 72, 101, 117	17 (6%)
1	M	272/277 (98%)	0.01	4 (1%) 76 74	52, 79, 101, 119	19 (6%)
1	N	271/277 (97%)	0.08	3 (1%) 82 80	50, 75, 103, 112	15 (5%)
All	All	3793/3878 (97%)	-0.05	18 (0%) 91 90	39, 71, 99, 134	227 (5%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	2	GLY	3.9
1	E	2	GLY	3.5
1	M	181	PHE	2.8
1	J	2	GLY	2.6
1	G	34	TRP	2.5
1	M	273	LYS	2.5
1	K	248	ASN	2.5
1	M	91	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	2	GLY	2.4
1	H	59	LEU	2.3
1	B	211	LEU	2.3
1	K	28	ALA	2.3
1	M	183	VAL	2.2
1	N	25	ALA	2.2
1	K	2	GLY	2.2
1	D	273	LYS	2.1
1	N	124	PHE	2.1
1	N	26	ALA	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	E6A	B	302	26/26	0.89	0.25	1.71	90,98,109,120	4
3	E6A	M	602	26/26	0.85	0.26	1.68	98,111,115,126	4
3	E6A	K	602	26/26	0.92	0.29	1.55	81,94,99,108	4
3	E6A	H	302	26/26	0.93	0.24	1.21	81,87,97,104	4
3	E6A	E	602	26/26	0.89	0.26	0.89	74,87,99,106	4
2	FAD	J	301	53/53	0.96	0.17	-0.41	52,67,84,90	0
2	FAD	M	601	53/53	0.95	0.17	-0.45	57,76,102,106	0
2	FAD	K	601	53/53	0.96	0.16	-0.47	56,75,89,97	0
2	FAD	H	301	53/53	0.95	0.17	-0.49	59,69,79,81	0
2	FAD	B	301	53/53	0.94	0.17	-0.64	48,75,107,110	0
2	FAD	C	601	53/53	0.96	0.16	-0.67	50,59,84,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FAD	F	301	53/53	0.96	0.16	-0.71	50,60,88,93	0
2	FAD	N	301	53/53	0.96	0.16	-0.74	61,69,79,80	0
2	FAD	G	601	53/53	0.96	0.16	-0.77	49,67,90,95	0
2	FAD	A	601	53/53	0.96	0.18	-0.82	56,68,91,92	0
2	FAD	D	301	53/53	0.96	0.15	-0.87	41,63,103,103	0
2	FAD	L	301	53/53	0.96	0.16	-0.88	50,69,94,101	0
2	FAD	E	601	53/53	0.96	0.16	-1.03	47,62,86,87	0
2	FAD	I	601	53/53	0.96	0.16	-1.23	56,70,85,86	0

6.5 Other polymers

There are no such residues in this entry.