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

wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:48 AM GMT

PDB ID	:	3JQQ
Title	:	Crystal structure of the H286K mutant of Ferredoxin-NADP+ reductase from Plasmodium falciparum in complex with 2'P-AMP
Authors	:	Canevari, G.; Milani, M.; Bolognesi, M.
Deposited on	:	2009-09-07
Resolution	:	2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i)) 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 ⓘ

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

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
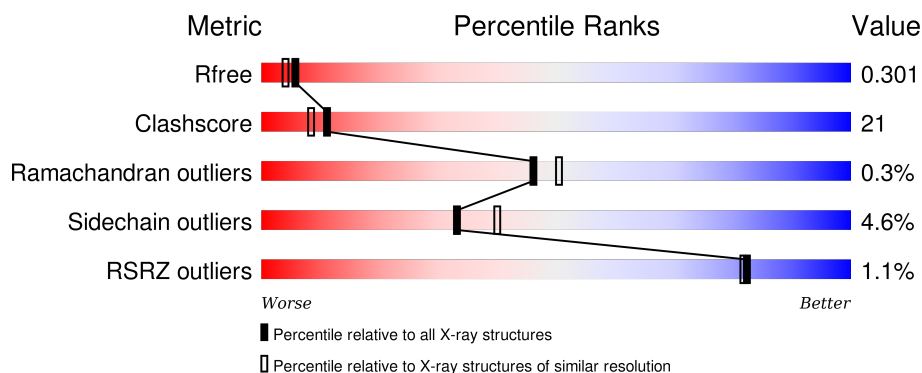
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	316	61% 20% • 17%
1	B	316	62% 19% • 17%
1	C	316	64% 19% • 16%
1	D	316	60% 19% 5% 16%
1	E	316	57% 21% • 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	316	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14736 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	261	Total	C	N	O	S	0	0	0
			2188	1421	360	398	9			
1	B	263	Total	C	N	O	S	0	0	0
			2207	1436	361	401	9			
1	C	267	Total	C	N	O	S	0	0	0
			2227	1443	367	408	9			
1	D	267	Total	C	N	O	S	0	0	0
			2227	1443	366	409	9			
1	E	253	Total	C	N	O	S	0	0	0
			2121	1382	346	384	9			
1	F	254	Total	C	N	O	S	0	0	0
			2126	1382	348	387	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	LYS	HIS	ENGINEERED	UNP C6KT68
B	286	LYS	HIS	ENGINEERED	UNP C6KT68
C	286	LYS	HIS	ENGINEERED	UNP C6KT68
D	286	LYS	HIS	ENGINEERED	UNP C6KT68
E	286	LYS	HIS	ENGINEERED	UNP C6KT68
F	286	LYS	HIS	ENGINEERED	UNP C6KT68

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

FAD

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		

- Molecule 3 is ADENOSINE-2'-5'-DIPHOSPHATE (three-letter code: A2P) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
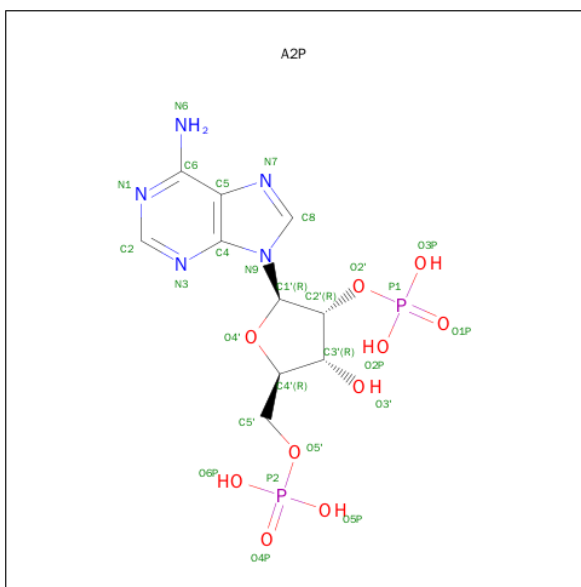
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	F	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	194	Total 194	O 194	0	0
4	B	223	Total 223	O 223	0	0
4	C	221	Total 221	O 221	0	0
4	D	198	Total 198	O 198	0	0
4	E	152	Total 152	O 152	0	0
4	F	172	Total 172	O 172	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 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:

- Molecule 1: Ferredoxin NADP reductase

Chain C:

E220 E228 Y236 V245 Q250 F257 Q260 D261 E262 I263 Y264 K267 N275 K286 K287 S288 I289 M294 S299 HIS ASP GLN PHE D304 E305 K306 K307 K308 K309 Y316

- Molecule 1: Ferredoxin NADP reductase

Chain D:

60%   19%   5%   16%

LYS GLU GLU N4 V12 K13 N14 V27 R28 P29 N30 V35 L45 L49 E50 G51 H52 T53 C54 G55 I56 I57 P58 N61 E62 LEU ASP ASN PRO ASN ASN GLN ILE ILE ASN LYS ASP HIS ASN ILE ILE ASN THR THR ASN HIS THR ASN HIS ASN ASN ILE ALA LEU

SER HIS ILE LYS LYS Q97 R98 C99 L102 M109 N110 M111 L114 S115 V116 K119 Q125 THR GLU ASN ALA PRO ASN I132 I142 L145 K146 I147 L153 H157 G158 Y159 F160 D165 A166 I167 Q168 K169 I174 F175 I176 A177 T180 Y185 F193

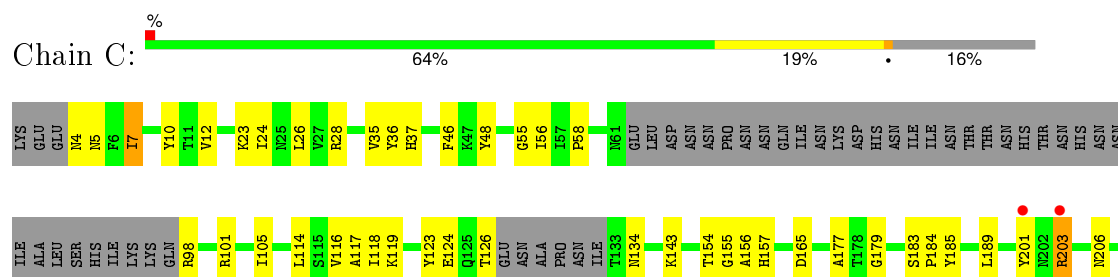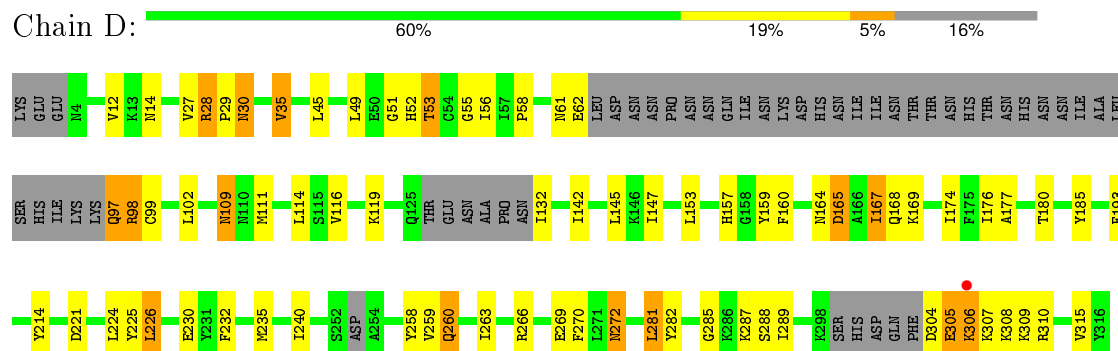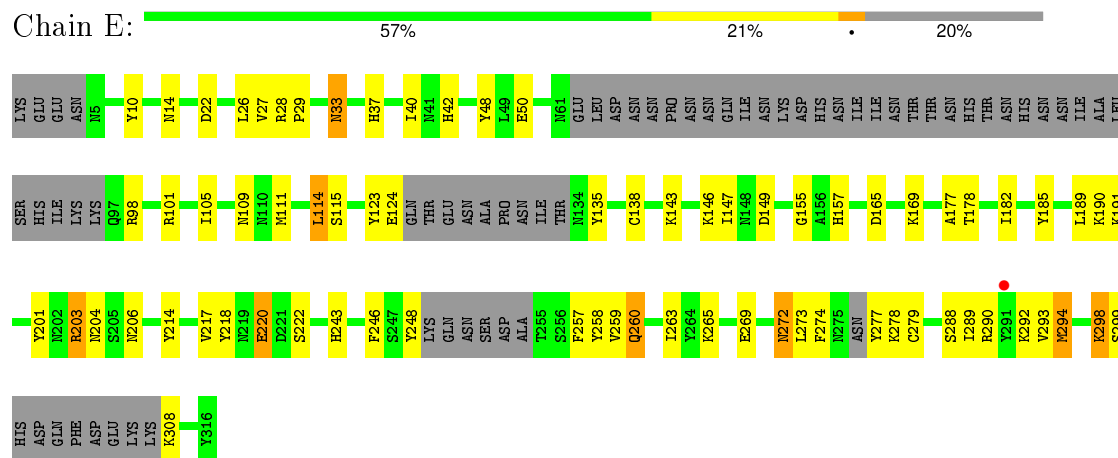Y214 D221 L224 Y225 L226 E230 Y231 F232 M235 I240 S252 ASP A254 Y258 V259 Q260 I263 R266 E269 F270 L271 N272 L281 Y282 G285 K286 K287 S288 I289 K298 SER HIS ASP GLN PHE D304 E305 K306 K307 K308 K309 R310 V315 Y316

- Molecule 1: Ferredoxin NADP reductase

Chain E:

57%   21%   •   20%

LYS GLU GLU N5 Y10 N14 D22 L26 V27 R28 P29 N33 H37 I40 N41 H42 Y48 L49 E50 N61 GLU LEU ASP ASN PRO ASN ASN GLN ILE ILE ASN LYS ASP HIS ASN ILE ILE ASN THR THR ASN HIS THR ASN HIS ASN ASN ILE ALA LEU

SER HIS ILE LYS LYS Q97 R98 R101 I105 M109 N110 M111 L114 S115 Y123 E124 GLN THR GLU ASN ALA PRO ASN ILE THR N134 Y135 C138 K143 K146 I147 N143 D149 G155 A156 H157 D165 K169 A177 T178 I182 Y185 L189 K190 K191

Y201 N202 R203 N204 S205 N206 Y214 V217 Y218 N219 E220 D221 S222 E43 F246 S247 Y248 LYS GLN ASN SER ASP ALA T255 S256 F257 Y258 V259 Q260 I263 Y264 K265 E269 N272 L273 F274 N275 ASN Y277 K278 C279 S288 I289 R290 Y291 K292 Y293 M294 K298 S299

HIS ASP GLN PHE ASP GLU LYS K308 Y316

- Molecule 1: Ferredoxin NADP reductase

Chain F:

3%

51%   28%   •   20%

LYS GLU GLU ASN N5 F6 I7 Y10 T11 V12 L26 V27 R28 P29 N30 N33 E34 V35 Y36 H37 F46 L49 E50 G51 H52 T53 C54 G55 E62 LEU ASN ASN PRO ASN ASN GLN ILE LYS ASP HIS ASN ILE ILE ASN THR THR ASN HIS THR ASN HIS ASN

ASN ILE ALA LEU SER HIS ILE LYS LYS Q97 R98 S107 S108 N109 L114 S115 V116 A117 I118 K119 I120 H121 K122 Y123 E124 GLN THR GLU ASN ALA PRO ASN ILE THR N134 Y135 S139 I142 K143 N144 L145 L153 T154 G155 A156 H157 G158 Y159 N164 K169 N172 F173

I174 A177 G181 I182 S183 P184 Y185 I186 N199 L200 Y201 N202 Y214 V217 D221 S222 I223 L224 Y225 L226 E230 Q233 N238 N241 F246 S247 Y248 K249 Q250 ASN SER ASP A254 T255 S256 Q260 D261 E262 I263 Y264 K265 R266 K267 T268 F274 N275 ASN

Y277 K278 C279 E280 L281 Y282 I283 K286 K287 S288 I289 R290 Y291 K292 Y293 M294 D295 ILE LEU LYS SER HIS ASP GLN PHE ASP GLU LYS K307 K308 K309 R310 V315 Y316

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	124.24Å 124.24Å 134.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	62.12 – 2.20 62.12 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.12-2.20) 100.0 (62.12-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.256 , 0.308 0.254 , 0.301	Depositor DCC
R_{free} test set	5894 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 32.7	EDS
Estimated twinning fraction	0.000 for -h,-k,l 0.458 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 117660 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14736	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.17 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.4690e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

---

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: A2P, 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	0.36	0/2240	0.47	0/3019
1	B	0.32	0/2258	0.47	0/3039
1	C	0.41	1/2280 (0.0%)	0.48	0/3076
1	D	0.34	0/2279	0.49	0/3073
1	E	0.32	0/2172	0.46	0/2928
1	F	0.34	0/2177	0.47	0/2934
All	All	0.35	1/13406 (0.0%)	0.47	0/18069

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	236	TYR	CD2-CE2	-5.62	1.30	1.39

There are no bond angle outliers.

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	2188	0	2154	73	0
1	B	2207	0	2182	81	0
1	C	2227	0	2183	75	0
1	D	2227	0	2178	101	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2121	0	2083	105	0
1	F	2126	0	2076	134	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
2	C	53	0	31	1	0
2	D	53	0	31	0	0
2	E	53	0	31	0	0
2	F	53	0	31	0	0
3	A	27	0	11	4	0
3	B	27	0	11	4	0
3	C	27	0	11	5	0
3	D	27	0	11	2	0
3	E	27	0	11	7	0
3	F	27	0	11	1	0
4	A	194	0	0	10	0
4	B	223	0	0	22	0
4	C	221	0	0	12	0
4	D	198	0	0	12	0
4	E	152	0	0	17	0
4	F	172	0	0	24	0
All	All	14736	0	13108	556	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 21.

The worst 5 of 556 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:E:294:MET:CE	1:E:294:MET:HA	1.60	1.32
1:D:305:GLU:CG	1:D:307:LYS:HG3	1.66	1.25
1:F:294:MET:O	1:F:295:ASP:OD1	1.65	1.12
1:C:305:GLU:HG2	1:C:306:LYS:N	1.44	1.12
1:D:306:LYS:CG	1:D:309:LYS:HD3	1.79	1.12

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	251/316 (79%)	241 (96%)	8 (3%)	2 (1%)	24	22
1	B	251/316 (79%)	240 (96%)	11 (4%)	0	100	100
1	C	259/316 (82%)	249 (96%)	10 (4%)	0	100	100
1	D	257/316 (81%)	247 (96%)	8 (3%)	2 (1%)	24	22
1	E	241/316 (76%)	236 (98%)	5 (2%)	0	100	100
1	F	242/316 (77%)	231 (96%)	11 (4%)	0	100	100
All	All	1501/1896 (79%)	1444 (96%)	53 (4%)	4 (0%)	46	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	305	GLU
1	A	204	ASN
1	D	306	LYS
1	A	289	ILE

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	243/295 (82%)	234 (96%)	9 (4%)	41	50
1	B	245/295 (83%)	231 (94%)	14 (6%)	25	29
1	C	246/295 (83%)	237 (96%)	9 (4%)	41	50

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	246/295 (83%)	230 (94%)	16 (6%)	21	23
1	E	235/295 (80%)	224 (95%)	11 (5%)	32	39
1	F	234/295 (79%)	226 (97%)	8 (3%)	44	54
All	All	1449/1770 (82%)	1382 (95%)	67 (5%)	33	40

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	287	LYS
1	D	97	GLN
1	F	164	ASN
1	C	309	LYS
1	D	35	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	8	ASN
1	C	241	ASN
1	E	260	GLN
1	C	144	ASN
1	C	206	ASN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

12 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	415	-	48,58,58	1.21	5 (10%)	54,89,89	2.11	6 (11%)
3	A2P	A	416	-	24,29,29	0.94	1 (4%)	29,45,45	1.97	4 (13%)
2	FAD	B	415	-	48,58,58	1.23	5 (10%)	54,89,89	2.13	8 (14%)
3	A2P	B	416	-	24,29,29	0.96	1 (4%)	29,45,45	1.94	4 (13%)
2	FAD	C	415	-	48,58,58	1.21	5 (10%)	54,89,89	2.10	6 (11%)
3	A2P	C	416	-	24,29,29	0.97	1 (4%)	29,45,45	1.93	4 (13%)
2	FAD	D	415	-	48,58,58	1.22	5 (10%)	54,89,89	2.07	7 (12%)
3	A2P	D	416	-	24,29,29	0.99	1 (4%)	29,45,45	1.91	4 (13%)
2	FAD	E	415	-	48,58,58	1.19	5 (10%)	54,89,89	2.07	7 (12%)
3	A2P	E	416	-	24,29,29	0.96	1 (4%)	29,45,45	1.96	5 (17%)
2	FAD	F	415	-	48,58,58	1.19	6 (12%)	54,89,89	2.07	7 (12%)
3	A2P	F	416	-	24,29,29	0.96	1 (4%)	29,45,45	1.94	3 (10%)

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

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	F	415	-	-	0/30/50/50	0/6/6/6
3	A2P	F	416	-	-	0/11/31/31	0/3/3/3

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	415	FAD	C5X-N5	2.03	1.38	1.35
2	E	415	FAD	C1'-N10	2.13	1.50	1.48
2	A	415	FAD	C2A-N1A	2.29	1.38	1.33
2	B	415	FAD	C2A-N1A	2.34	1.38	1.33
2	D	415	FAD	C4-N3	2.36	1.37	1.33

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	415	FAD	N3A-C2A-N1A	-11.54	120.06	128.89
2	C	415	FAD	N3A-C2A-N1A	-11.52	120.08	128.89
2	E	415	FAD	N3A-C2A-N1A	-11.49	120.09	128.89
2	F	415	FAD	N3A-C2A-N1A	-11.30	120.24	128.89
2	B	415	FAD	N3A-C2A-N1A	-11.23	120.29	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	415	FAD	1	0
3	A	416	A2P	4	0
3	B	416	A2P	4	0
2	C	415	FAD	1	0
3	C	416	A2P	5	0
3	D	416	A2P	2	0
3	E	416	A2P	7	0
3	F	416	A2P	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	261/316 (82%)	-0.13	3 (1%)	82	82	17, 27, 47, 56	0
1	B	263/316 (83%)	-0.12	2 (0%)	87	87	17, 30, 53, 67	0
1	C	267/316 (84%)	-0.30	2 (0%)	89	88	14, 25, 44, 54	0
1	D	267/316 (84%)	-0.16	1 (0%)	93	93	14, 27, 52, 67	0
1	E	253/316 (80%)	0.09	1 (0%)	93	93	29, 42, 67, 74	1 (0%)
1	F	254/316 (80%)	0.23	8 (3%)	52	51	35, 48, 68, 77	0
All	All	1565/1896 (82%)	-0.07	17 (1%)	82	82	14, 35, 61, 77	1 (0%)

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	291	TYR	6.8
1	F	254	ALA	3.7
1	B	295	ASP	3.2
1	F	277	TYR	3.2
1	F	291	TYR	2.8

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.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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, 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
3	A2P	A	416	27/27	0.98	0.12	-0.56	17,19,23,23	0
3	A2P	F	416	27/27	0.96	0.12	-0.66	32,33,36,36	0
3	A2P	D	416	27/27	0.98	0.10	-0.67	14,16,20,21	0
2	FAD	D	415	53/53	0.98	0.10	-0.88	11,15,19,20	0
2	FAD	F	415	53/53	0.96	0.12	-0.89	32,34,34,35	0
3	A2P	B	416	27/27	0.98	0.11	-0.90	18,20,24,24	0
2	FAD	A	415	53/53	0.97	0.11	-0.97	9,16,21,22	0
2	FAD	B	415	53/53	0.97	0.10	-0.98	13,17,22,22	0
3	A2P	E	416	27/27	0.96	0.12	-1.02	32,34,38,38	0
2	FAD	C	415	53/53	0.98	0.09	-1.03	9,13,17,18	0
3	A2P	C	416	27/27	0.97	0.09	-1.08	16,17,22,23	0
2	FAD	E	415	53/53	0.97	0.10	-1.14	24,29,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.