



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:48 AM GMT

PDB ID : 3JQP
Title : Crystal structure of the H286L mutant of Ferredoxin-NADP⁺ reductase from Plasmodium falciparum with 2'P-AMP
Authors : Canevari, G.; Milani, M.; Bolognesi, M.
Deposited on : 2009-09-07
Resolution : 3.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

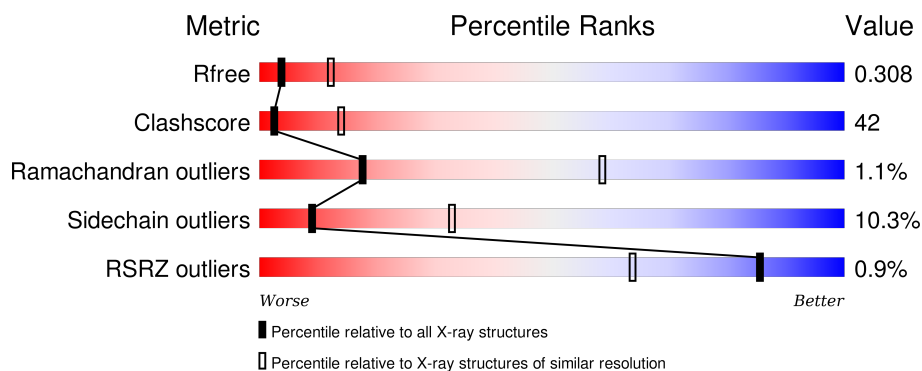
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>44%</div> <div>35%</div> <div>•</div> <div>16%</div> </div>
1	B	316	<div> <div>33%</div> <div>41%</div> <div>9%</div> <div>•</div> <div>16%</div> </div>
1	C	316	<div> <div>49%</div> <div>31%</div> <div>•</div> <div>16%</div> </div>
1	D	316	<div> <div>44%</div> <div>35%</div> <div>5%</div> <div>•</div> <div>15%</div> </div>
1	E	316	<div> <div>3%</div> <div>41%</div> <div>38%</div> <div>•</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	316	<div><div><div>%</div><div><div></div><div>45%</div><div>29%</div><div>7%</div><div>•</div><div>19%</div></div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13874 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.

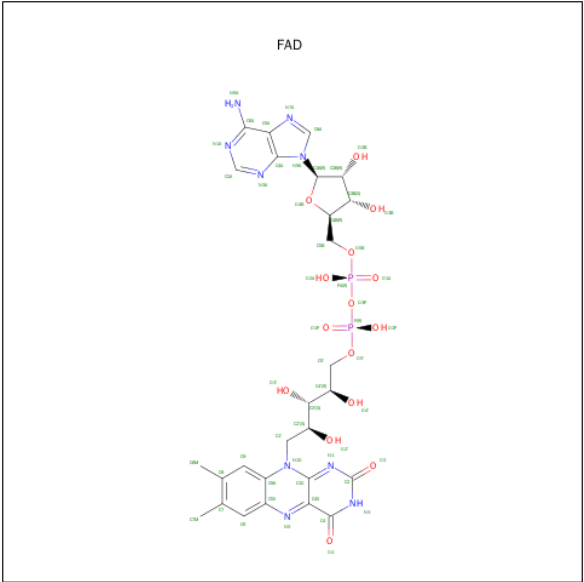
- Molecule 1 is a protein called Ferredoxin NADP reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	5	0	0
			2210	1434	363	404	9			
1	B	266	Total	C	N	O	S	0	0	0
			2231	1451	366	405	9			
1	C	265	Total	C	N	O	S	0	0	0
			2209	1433	361	406	9			
1	D	269	Total	C	N	O	S	0	0	0
			2248	1456	372	411	9			
1	E	261	Total	C	N	O	S	0	0	0
			2190	1425	357	399	9			
1	F	257	Total	C	N	O	S	0	0	0
			2140	1395	349	387	9			

There are 6 discrepancies between the modelled and reference sequences:

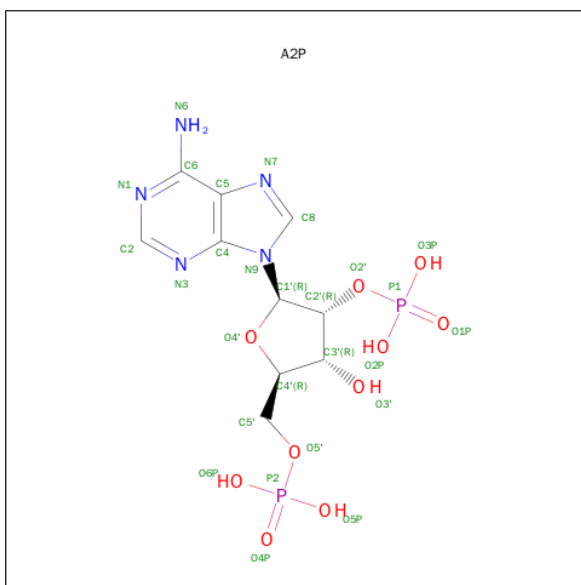
Chain	Residue	Modelled	Actual	Comment	Reference
A	286	LEU	HIS	ENGINEERED	UNP C6KT68
B	286	LEU	HIS	ENGINEERED	UNP C6KT68
C	286	LEU	HIS	ENGINEERED	UNP C6KT68
D	286	LEU	HIS	ENGINEERED	UNP C6KT68
E	286	LEU	HIS	ENGINEERED	UNP C6KT68
F	286	LEU	HIS	ENGINEERED	UNP C6KT68

- 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		

- Molecule 3 is ADENOSINE-2'-5'-DIPHOSPHATE (three-letter code: A2P) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		
4	B	29	Total	O	0	0
			29	29		
4	C	29	Total	O	0	0
			29	29		
4	D	30	Total	O	0	0
			30	30		
4	E	22	Total	O	0	0
			22	22		
4	F	27	Total	O	0	0
			27	27		



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	122.57Å 122.57Å 133.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	56.58 – 3.00 56.58 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (56.58-3.00) 99.9 (56.58-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.244 , 0.317 0.244 , 0.308	Depositor DCC
R_{free} test set	2268 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.8	EDS
Estimated twinning fraction	0.012 for -h,-k,l 0.449 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 44961 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13874	wwPDB-VP
Average B, all atoms (Å ²)	55.0	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 33.30 % 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 8.1827e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A2P, 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	0.44	2/2262 (0.1%)	0.55	0/3051
1	B	0.60	0/2283	0.58	1/3078 (0.0%)
1	C	0.45	0/2262	0.54	1/3053 (0.0%)
1	D	0.46	0/2301	0.57	0/3104
1	E	0.36	0/2242	0.56	0/3025
1	F	0.51	0/2191	0.60	2/2954 (0.1%)
All	All	0.48	2/13541 (0.0%)	0.57	4/18265 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	ALA	C-N	-5.06	1.22	1.34
1	A	46	PHE	CD1-CE1	-5.05	1.29	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	297	LEU	CA-CB-CG	-5.64	102.33	115.30
1	F	158	GLY	N-CA-C	5.40	126.60	113.10
1	C	307	LYS	N-CA-C	-5.39	96.46	111.00
1	F	292	LYS	N-CA-C	-5.33	96.60	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	2210	0	2162	173	0
1	B	2231	0	2205	298	0
1	C	2209	0	2150	172	0
1	D	2248	0	2203	179	0
1	E	2190	0	2154	184	0
1	F	2140	0	2096	163	0
2	A	53	0	31	3	0
2	B	53	0	31	3	0
2	C	53	0	31	2	0
2	D	53	0	31	6	0
2	E	53	0	31	3	0
2	F	53	0	31	0	0
3	A	27	0	11	2	0
3	B	27	0	11	3	0
3	C	27	0	11	6	0
3	D	27	0	11	5	0
3	E	27	0	11	2	0
3	F	27	0	11	2	0
4	A	29	0	0	3	0
4	B	29	0	0	4	0
4	C	29	0	0	1	0
4	D	30	0	0	6	0
4	E	22	0	0	2	0
4	F	27	0	0	2	0
All	All	13874	0	13222	1121	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 42.

The worst 5 of 1121 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:203:ARG:HG3	1:B:204:ASN:CA	1.22	1.61
1:E:122:LYS:HE2	1:E:135:TYR:CE2	1.46	1.45
1:C:200:LEU:HD11	1:C:231:TYR:CE1	1.52	1.42
1:F:256:SER:CB	1:F:257:PHE:HB2	1.51	1.39
1:B:96:LYS:HA	1:B:97:GLN:CB	1.43	1.38

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	256/316 (81%)	235 (92%)	20 (8%)	1 (0%)	39	80
1	B	256/316 (81%)	231 (90%)	19 (7%)	6 (2%)	8	36
1	C	255/316 (81%)	238 (93%)	15 (6%)	2 (1%)	24	66
1	D	259/316 (82%)	236 (91%)	20 (8%)	3 (1%)	16	56
1	E	251/316 (79%)	230 (92%)	20 (8%)	1 (0%)	39	80
1	F	245/316 (78%)	219 (89%)	23 (9%)	3 (1%)	16	56
All	All	1522/1896 (80%)	1389 (91%)	117 (8%)	16 (1%)	17	58

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	ALA
1	B	208	THR
1	C	167	ILE
1	D	58	PRO
1	F	293	VAL

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	244/295 (83%)	221 (91%)	23 (9%)	11	39
1	B	248/295 (84%)	211 (85%)	37 (15%)	4	17
1	C	244/295 (83%)	223 (91%)	21 (9%)	13	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	250/295 (85%)	226 (90%)	24 (10%)	10	38
1	E	243/295 (82%)	226 (93%)	17 (7%)	19	55
1	F	235/295 (80%)	206 (88%)	29 (12%)	6	25
All	All	1464/1770 (83%)	1313 (90%)	151 (10%)	9	33

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	147	ILE
1	D	35	VAL
1	F	203	ARG
1	C	170	ASN
1	C	272	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	134	ASN
1	D	14	ASN
1	F	148	ASN
1	C	206	ASN
1	D	134	ASN

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

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	1.45	5 (10%)	54,89,89	1.86	8 (14%)
3	A2P	A	416	-	24,29,29	0.90	1 (4%)	29,45,45	2.20	5 (17%)
2	FAD	B	415	-	48,58,58	1.44	6 (12%)	54,89,89	1.81	8 (14%)
3	A2P	B	416	-	24,29,29	0.96	1 (4%)	29,45,45	1.98	5 (17%)
2	FAD	C	415	-	48,58,58	1.47	5 (10%)	54,89,89	1.91	7 (12%)
3	A2P	C	416	-	24,29,29	0.96	1 (4%)	29,45,45	1.91	4 (13%)
2	FAD	D	415	-	48,58,58	1.49	5 (10%)	54,89,89	1.89	7 (12%)
3	A2P	D	416	-	24,29,29	0.99	1 (4%)	29,45,45	1.84	3 (10%)
2	FAD	E	415	-	48,58,58	1.46	5 (10%)	54,89,89	1.86	9 (16%)
3	A2P	E	416	-	24,29,29	0.97	1 (4%)	29,45,45	1.97	5 (17%)
2	FAD	F	415	-	48,58,58	1.42	6 (12%)	54,89,89	1.83	8 (14%)
3	A2P	F	416	-	24,29,29	0.99	1 (4%)	29,45,45	1.76	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

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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 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	415	FAD	C10-N10	2.00	1.41	1.39
2	F	415	FAD	C10-N10	2.04	1.41	1.39
2	F	415	FAD	O4B-C1B	2.65	1.44	1.41
2	B	415	FAD	C5X-N5	2.65	1.39	1.35
2	E	415	FAD	C5X-N5	2.77	1.39	1.35

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	415	FAD	N3A-C2A-N1A	-9.91	121.31	128.89
2	A	415	FAD	N3A-C2A-N1A	-9.86	121.34	128.89
2	E	415	FAD	N3A-C2A-N1A	-9.50	121.62	128.89
2	D	415	FAD	N3A-C2A-N1A	-9.40	121.69	128.89
2	F	415	FAD	N3A-C2A-N1A	-9.03	121.98	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	415	FAD	3	0
3	A	416	A2P	2	0
2	B	415	FAD	3	0
3	B	416	A2P	3	0
2	C	415	FAD	2	0
3	C	416	A2P	6	0
2	D	415	FAD	6	0
3	D	416	A2P	5	0
2	E	415	FAD	3	0
3	E	416	A2P	2	0
3	F	416	A2P	2	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 ⓘ

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	265/316 (83%)	-0.21	1 (0%) 93 80	22, 42, 74, 89	0
1	B	266/316 (84%)	-0.22	0 100 100	26, 46, 79, 88	0
1	C	265/316 (83%)	-0.30	1 (0%) 93 80	21, 38, 72, 85	0
1	D	269/316 (85%)	-0.22	1 (0%) 93 80	23, 44, 78, 87	0
1	E	261/316 (82%)	0.05	8 (3%) 52 24	50, 68, 99, 104	0
1	F	257/316 (81%)	0.11	3 (1%) 81 55	58, 78, 97, 101	0
All	All	1583/1896 (83%)	-0.13	14 (0%) 85 64	21, 56, 90, 104	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	205	SER	3.6
1	F	238	ASN	3.2
1	F	117	ALA	2.8
1	E	168	GLN	2.7
1	E	203	ARG	2.3

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 [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	0.96	0.20	-0.26	31,34,41,42	0
2	FAD	F	415	53/53	0.94	0.23	-0.32	66,72,79,81	0
2	FAD	C	415	53/53	0.98	0.20	-0.35	15,22,34,35	0
2	FAD	D	415	53/53	0.97	0.19	-0.48	15,30,34,36	0
2	FAD	B	415	53/53	0.97	0.19	-0.56	23,34,39,40	0
2	FAD	A	415	53/53	0.97	0.19	-0.56	31,35,39,40	0
3	A2P	C	416	27/27	0.98	0.18	-0.67	20,30,42,44	0
2	FAD	E	415	53/53	0.96	0.21	-0.93	41,58,74,75	0
3	A2P	D	416	27/27	0.98	0.18	-1.06	27,29,35,37	0
3	A2P	F	416	27/27	0.93	0.17	-1.19	56,69,73,73	0
3	A2P	E	416	27/27	0.96	0.16	-1.48	55,60,67,69	0
3	A2P	B	416	27/27	0.97	0.15	-1.70	29,38,43,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.