



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 28, 2022 – 06:20 PM JST

PDB ID : 7W3O
Title : Crystal structure of human CYB5R3
Authors : Noda, N.N.
Deposited on : 2021-11-25
Resolution : 2.46 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

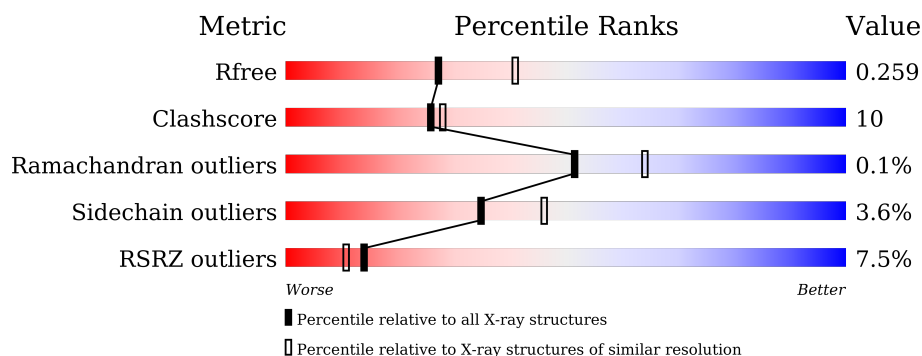
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	278	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 75%, yellow 75%, yellow 99%, grey 99%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 75% 20% .. </div> </div>
1	B	278	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 75%, yellow 75%, yellow 99%, grey 99%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 75% 22% .. </div> </div>
1	C	278	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 5%, orange 5%, orange 75%, yellow 75%, yellow 99%, grey 99%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 5% 75% 20% .. </div> </div>
1	D	278	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 9%, orange 9%, orange 72%, yellow 72%, yellow 99%, grey 99%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 9% 72% 23% .. </div> </div>
1	E	278	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 19%, orange 19%, orange 70%, yellow 70%, yellow 99%, grey 99%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 19% 70% 24% • 5% </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11245 atoms, of which 80 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.

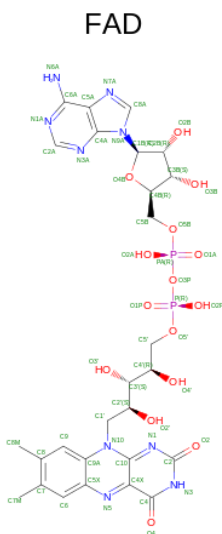
- Molecule 1 is a protein called NADH-cytochrome b5 reductase 3 soluble form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2171	1393	375	391	12			
1	B	272	Total	C	N	O	S	0	0	0
			2170	1393	375	390	12			
1	C	272	Total	C	N	O	S	0	0	0
			2170	1393	375	390	12			
1	D	270	Total	C	N	O	S	0	0	0
			2152	1383	371	386	12			
1	E	264	Total	C	N	O	S	0	0	0
			2098	1347	362	377	12			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P00387
A	-1	PRO	-	expression tag	UNP P00387
A	0	MET	-	expression tag	UNP P00387
B	-2	GLY	-	expression tag	UNP P00387
B	-1	PRO	-	expression tag	UNP P00387
B	0	MET	-	expression tag	UNP P00387
C	-2	GLY	-	expression tag	UNP P00387
C	-1	PRO	-	expression tag	UNP P00387
C	0	MET	-	expression tag	UNP P00387
D	-2	GLY	-	expression tag	UNP P00387
D	-1	PRO	-	expression tag	UNP P00387
D	0	MET	-	expression tag	UNP P00387
E	-2	GLY	-	expression tag	UNP P00387
E	-1	PRO	-	expression tag	UNP P00387
E	0	MET	-	expression tag	UNP P00387

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 73	C 27	H 20	N 9	O 15	P 2	0	1
2	B	1	Total 73	C 27	H 20	N 9	O 15	P 2	0	1
2	C	1	Total 73	C 27	H 20	N 9	O 15	P 2	0	1
2	D	1	Total 73	C 27	H 20	N 9	O 15	P 2	0	1

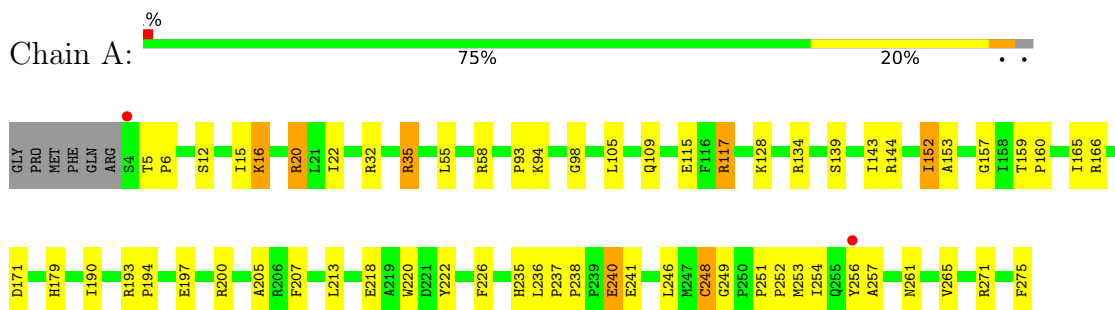
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	81	Total O 81 81	0	0
3	B	36	Total O 36 36	0	0
3	C	37	Total O 37 37	0	0
3	D	21	Total O 21 21	0	0
3	E	17	Total O 17 17	0	0

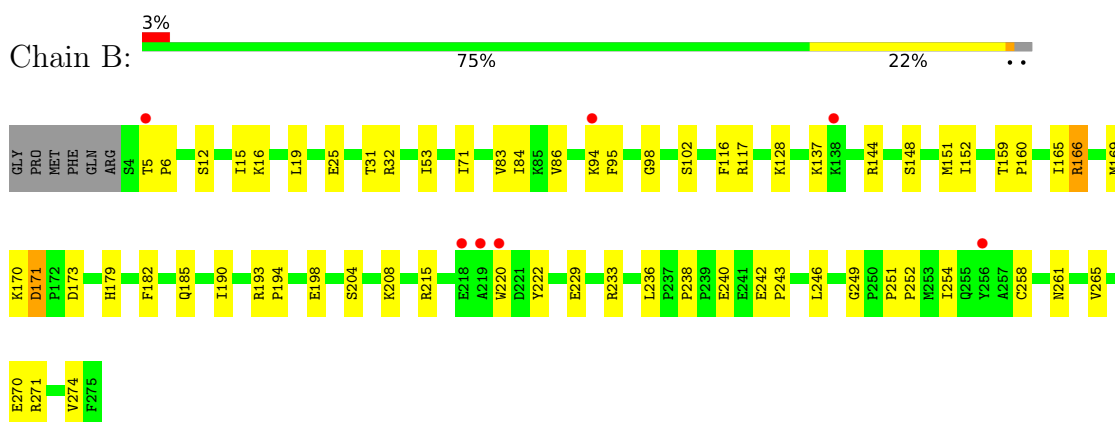
3 Residue-property plots [i](#)

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

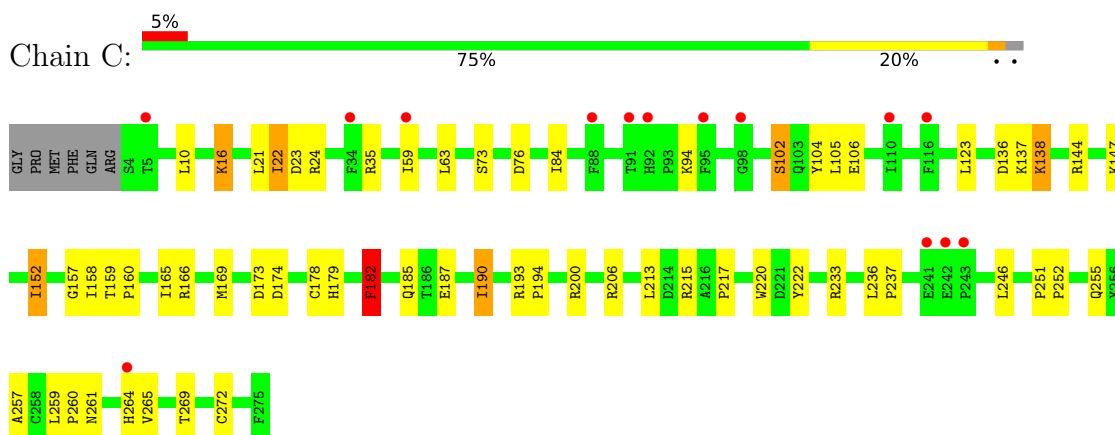
- Molecule 1: NADH-cytochrome b5 reductase 3 soluble form



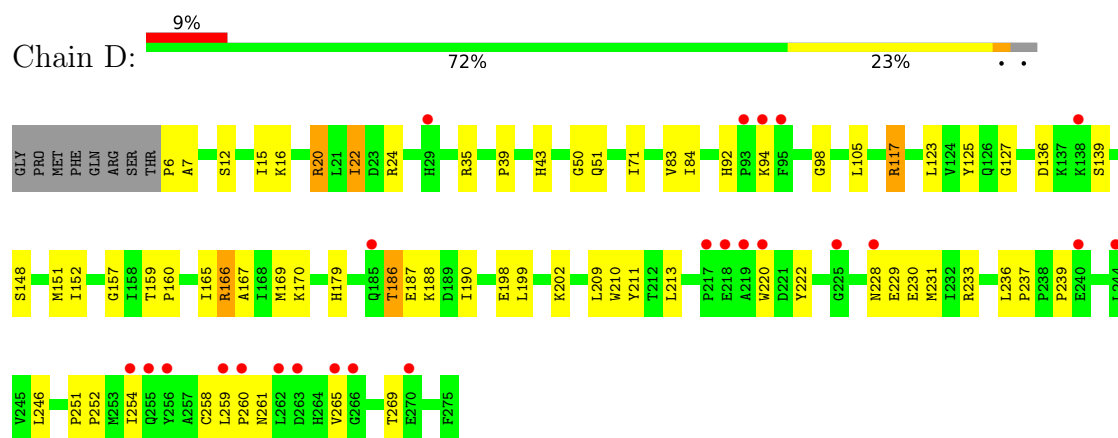
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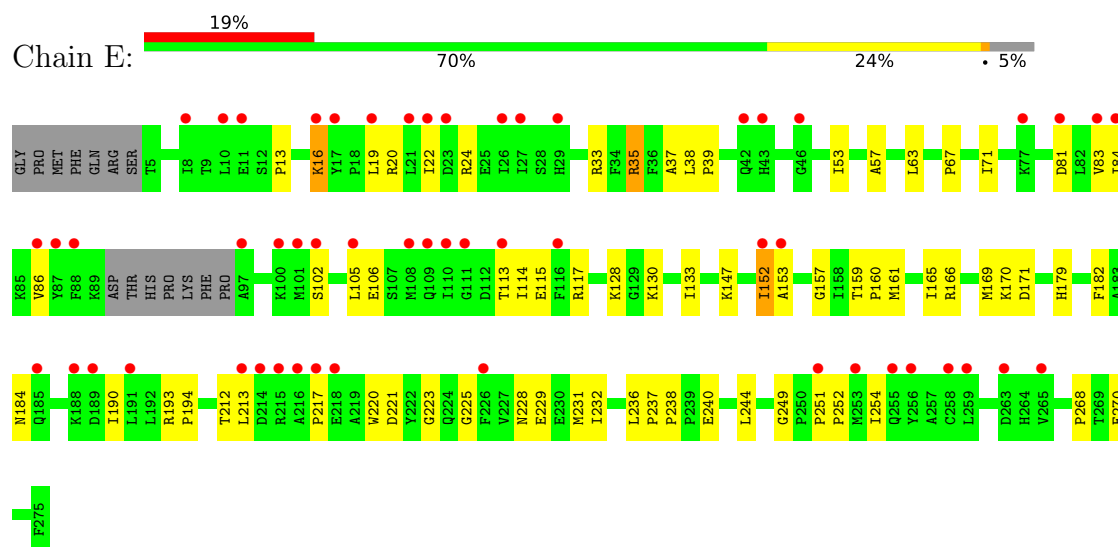
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• Molecule 1: NADH-cytochrome b5 reductase 3 soluble form



• Molecule 1: NADH-cytochrome b5 reductase 3 soluble form



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.36Å 79.92Å 169.40Å 90.00° 98.72° 90.00°	Depositor
Resolution (Å)	49.57 – 2.46 49.56 – 2.46	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.57-2.46) 100.0 (49.56-2.46)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.231 , 0.260 0.231 , 0.259	Depositor DCC
R_{free} test set	4017 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11245	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.83	1/2231 (0.0%)	0.85	6/3028 (0.2%)
1	B	0.66	0/2230	0.70	2/3026 (0.1%)
1	C	0.64	3/2230 (0.1%)	0.70	3/3026 (0.1%)
1	D	0.50	0/2211	0.60	3/2999 (0.1%)
1	E	0.45	0/2152	0.54	1/2917 (0.0%)
All	All	0.63	4/11054 (0.0%)	0.69	15/14996 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	178	CYS	CB-SG	-5.30	1.73	1.81
1	C	272	CYS	CB-SG	-5.28	1.73	1.81
1	C	182	PHE	CE1-CZ	5.11	1.47	1.37
1	A	248	CYS	CB-SG	5.01	1.90	1.82

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	166	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	C	166	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	A	32	ARG	NE-CZ-NH2	-8.31	116.14	120.30
1	C	206	ARG	NE-CZ-NH1	-7.66	116.47	120.30
1	A	166	ARG	NE-CZ-NH2	-7.39	116.60	120.30

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	2171	0	2178	46	0
1	B	2170	0	2177	39	0
1	C	2170	0	2177	50	0
1	D	2152	0	2161	52	0
1	E	2098	0	2107	54	0
2	A	53	20	0	0	0
2	B	53	20	0	0	0
2	C	53	20	0	0	0
2	D	53	20	0	0	0
3	A	81	0	0	6	0
3	B	36	0	0	3	1
3	C	37	0	0	12	1
3	D	21	0	0	12	0
3	E	17	0	0	3	0
All	All	11165	80	10800	229	1

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 10.

The worst 5 of 229 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:THR:HB	1:A:6:PRO:HD3	1.33	1.07
1:D:20:ARG:NH1	3:D:1401:HOH:O	1.84	0.97
1:B:152:ILE:HD11	1:B:236:LEU:HD11	1.49	0.93
1:D:50:GLY:O	3:D:1403:HOH:O	1.92	0.88
1:C:174:ASP:OD2	3:C:1401:HOH:O	1.92	0.86

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1412:HOH:O	3:C:1434:HOH:O[3_545]	2.17	0.03

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	270/278 (97%)	259 (96%)	11 (4%)	0	100	100
1	B	270/278 (97%)	263 (97%)	7 (3%)	0	100	100
1	C	270/278 (97%)	262 (97%)	7 (3%)	1 (0%)	34	41
1	D	268/278 (96%)	261 (97%)	7 (3%)	0	100	100
1	E	260/278 (94%)	254 (98%)	6 (2%)	0	100	100
All	All	1338/1390 (96%)	1299 (97%)	38 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	190	ILE

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	241/246 (98%)	230 (95%)	11 (5%)	27	35
1	B	241/246 (98%)	233 (97%)	8 (3%)	38	49
1	C	241/246 (98%)	231 (96%)	10 (4%)	30	40
1	D	238/246 (97%)	228 (96%)	10 (4%)	30	39
1	E	231/246 (94%)	227 (98%)	4 (2%)	60	73
All	All	1192/1230 (97%)	1149 (96%)	43 (4%)	35	46

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	246	LEU
1	D	188	LYS
1	D	16	LYS
1	D	117	ARG
1	D	246	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	179	HIS
1	D	261	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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(Å ²)	Q<0.9
1	A	272/278 (97%)	-0.07	2 (0%) 87 88	28, 43, 79, 133	0
1	B	272/278 (97%)	-0.04	7 (2%) 56 52	32, 57, 97, 138	0
1	C	272/278 (97%)	0.22	14 (5%) 28 25	35, 63, 98, 129	0
1	D	270/278 (97%)	0.35	24 (8%) 9 6	45, 73, 113, 146	0
1	E	264/278 (94%)	1.13	54 (20%) 1 0	54, 97, 117, 138	0
All	All	1350/1390 (97%)	0.31	101 (7%) 14 11	28, 66, 112, 146	0

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	256	TYR	9.3
1	D	256	TYR	8.8
1	E	86	VAL	7.3
1	A	4	SER	7.0
1	E	88	PHE	6.0

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 monosaccharides 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. 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	B-factors(Å ²)	Q<0.9
2	FAD	C	1301[A]	53/53	0.81	0.21	52,85,108,113	1
2	FAD	C	1301[B]	53/53	0.81	0.21	52,85,108,113	1
2	FAD	D	1301[A]	53/53	0.93	0.17	52,67,83,90	1
2	FAD	D	1301[B]	53/53	0.93	0.17	52,67,83,90	1
2	FAD	B	1301[A]	53/53	0.95	0.15	34,52,76,83	1
2	FAD	B	1301[B]	53/53	0.95	0.15	34,52,76,83	1
2	FAD	A	1301[A]	53/53	0.96	0.17	31,51,75,84	1
2	FAD	A	1301[B]	53/53	0.96	0.17	31,51,75,84	1

6.5 Other polymers ⓘ

There are no such residues in this entry.