



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:56 AM GMT

PDB ID : 3CQN
Title : Crystal Structure of the Lipocalin domain of Violaxanthin de-epoxidase (VDE) at pH7
Authors : Arnoux, P.; Morosinotto, T.; Pignol, D.
Deposited on : 2008-04-03
Resolution : 2.00 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 ⓘ 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

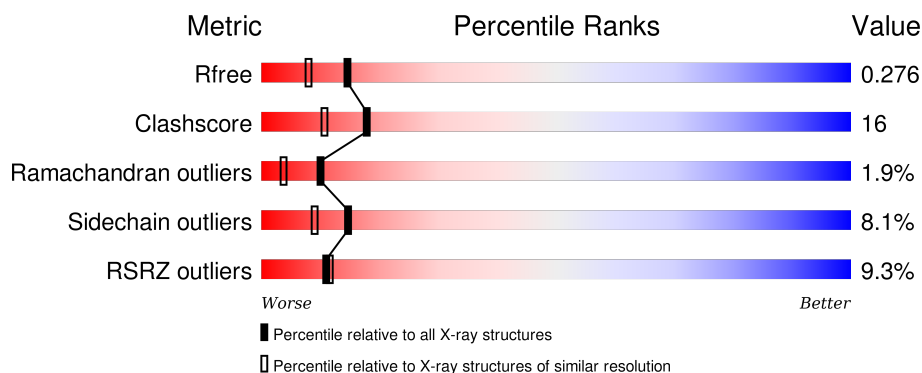
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	185	<div> <div>9%</div> <div> <div></div> <div>63%</div> <div>17%</div> <div>6% •</div> <div>12%</div> </div> </div>
1	B	185	<div> <div>7%</div> <div> <div></div> <div>64%</div> <div>17%</div> <div>5% •</div> <div>13%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2771 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 Violaxanthin de-epoxidase, chloroplast.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1308	837	218	251	2			
1	B	161	Total	C	N	O	S	0	2	0
			1305	835	219	248	3			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	MET	-	INITIATING METHIONINE	UNP Q39249
A	254	ARG	-	EXPRESSION TAG	UNP Q39249
A	255	SER	-	EXPRESSION TAG	UNP Q39249
A	256	HIS	-	EXPRESSION TAG	UNP Q39249
A	257	HIS	-	EXPRESSION TAG	UNP Q39249
A	258	HIS	-	EXPRESSION TAG	UNP Q39249
A	259	HIS	-	EXPRESSION TAG	UNP Q39249
A	260	HIS	-	EXPRESSION TAG	UNP Q39249
A	261	HIS	-	EXPRESSION TAG	UNP Q39249
B	77	MET	-	INITIATING METHIONINE	UNP Q39249
B	254	ARG	-	EXPRESSION TAG	UNP Q39249
B	255	SER	-	EXPRESSION TAG	UNP Q39249
B	256	HIS	-	EXPRESSION TAG	UNP Q39249
B	257	HIS	-	EXPRESSION TAG	UNP Q39249
B	258	HIS	-	EXPRESSION TAG	UNP Q39249
B	259	HIS	-	EXPRESSION TAG	UNP Q39249
B	260	HIS	-	EXPRESSION TAG	UNP Q39249
B	261	HIS	-	EXPRESSION TAG	UNP Q39249

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	82	Total	O	0	0
			82	82		

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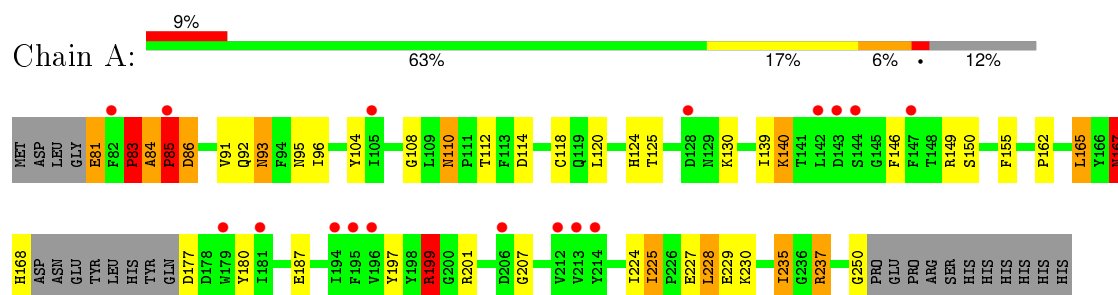
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	76	Total	O	0	0
			76	76		

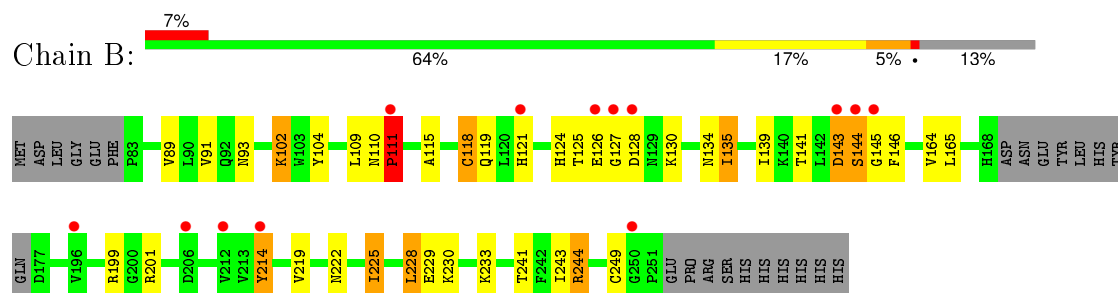
3 Residue-property plots [i](#)

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: Violaxanthin de-epoxidase, chloroplast



- Molecule 1: Violaxanthin de-epoxidase, chloroplast



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	34.63Å 52.46Å 54.60Å 82.52° 75.99° 74.54°	Depositor
Resolution (Å)	30.00 – 2.00 26.42 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.9 (30.00-2.00) 94.5 (26.42-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.272 0.206 , 0.276	Depositor DCC
R_{free} test set	1199 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.7	EDS
Estimated twinning fraction	0.010 for -h,-l,-k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 23469 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2771	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.40% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.01	1/1346 (0.1%)	1.07	6/1830 (0.3%)
1	B	1.07	4/1350 (0.3%)	1.04	4/1836 (0.2%)
All	All	1.04	5/2696 (0.2%)	1.06	10/3666 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	104	TYR	CD1-CE1	8.63	1.52	1.39
1	B	214	TYR	CD2-CE2	6.19	1.48	1.39
1	A	250	GLY	C-O	6.17	1.33	1.23
1	B	118[A]	CYS	CB-SG	-5.86	1.72	1.81
1	B	118[B]	CYS	CB-SG	-5.86	1.72	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	ILE	CG1-CB-CG2	-7.30	95.34	111.40
1	B	228	LEU	CB-CG-CD1	6.88	122.70	111.00
1	A	83	PRO	N-CA-C	6.54	129.10	112.10
1	B	199	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	A	85	PRO	N-CA-C	6.35	128.61	112.10
1	B	201	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	A	237	ARG	NE-CZ-NH1	-5.82	117.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	ASN	CB-CA-C	5.76	121.92	110.40
1	A	86	ASP	N-CA-C	5.72	126.45	111.00
1	A	199	ARG	NE-CZ-NH2	-5.11	117.75	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	PRO	Peptide
1	B	110	ASN	Peptide
1	B	111	PRO	Peptide
1	B	143	ASP	Peptide

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	1308	0	1224	33	0
1	B	1305	0	1231	46	0
2	A	82	0	0	6	0
2	B	76	0	0	6	0
All	All	2771	0	2455	79	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 16.

All (79) 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:121[B]:HIS:CE1	1:B:135:ILE:HG22	1.72	1.24
1:B:121[B]:HIS:CE1	1:B:135:ILE:CG2	2.32	1.11
1:B:111:PRO:HG2	1:B:243:ILE:HD12	1.45	0.95
1:B:121[B]:HIS:ND1	1:B:135:ILE:HG22	1.83	0.92
1:B:121[B]:HIS:NE2	1:B:135:ILE:CG2	2.37	0.86
1:B:121[B]:HIS:CG	1:B:135:ILE:HG22	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:PRO:HG2	1:B:243:ILE:CD1	2.07	0.85
1:A:95:ASN:HB2	2:A:307:HOH:O	1.74	0.85
1:B:121[B]:HIS:NE2	1:B:135:ILE:HG22	1.92	0.82
1:B:109:LEU:O	1:B:111:PRO:HD2	1.79	0.82
1:A:167:ASN:HB3	1:A:177:ASP:O	1.81	0.81
1:A:168:HIS:O	2:A:282:HOH:O	1.99	0.80
1:B:121[B]:HIS:CD2	1:B:135:ILE:HG22	2.16	0.79
1:A:104:TYR:CE1	1:A:120:LEU:HD21	2.18	0.78
1:B:111:PRO:CG	1:B:243:ILE:HD12	2.13	0.77
1:A:140:LYS:HE2	1:A:146:PHE:HB3	1.64	0.77
1:B:118[A]:CYS:SG	2:B:278:HOH:O	2.32	0.70
1:A:104:TYR:CD1	1:A:120:LEU:HD21	2.28	0.69
1:A:118:CYS:HB2	2:A:302:HOH:O	1.94	0.67
1:B:134:ASN:HB2	2:B:295:HOH:O	1.94	0.67
1:A:96:ILE:HD11	1:A:165:LEU:HD11	1.78	0.66
1:B:118[B]:CYS:CB	1:B:249:CYS:HG	2.10	0.65
1:B:111:PRO:HG3	1:B:115:ALA:HB2	1.78	0.64
1:B:125:THR:CG2	1:B:127:GLY:O	2.45	0.64
1:B:135:ILE:O	1:B:135:ILE:HG13	1.98	0.64
1:B:121[B]:HIS:NE2	1:B:135:ILE:HG21	2.14	0.63
1:B:241:THR:HG22	1:B:241:THR:O	1.98	0.62
1:A:91:VAL:CG1	1:A:93:ASN:O	2.47	0.62
1:B:124:HIS:HE1	2:B:304:HOH:O	1.83	0.62
1:B:222:ASN:O	1:B:225:ILE:HG23	2.00	0.62
1:B:125:THR:HG22	1:B:127:GLY:O	2.00	0.61
1:B:121[B]:HIS:CD2	1:B:135:ILE:CG2	2.84	0.61
1:B:121[B]:HIS:CE1	1:B:135:ILE:HG23	2.35	0.60
1:B:91:VAL:HG13	1:B:93:ASN:O	2.02	0.60
1:B:165:LEU:HD12	1:B:165:LEU:N	2.18	0.58
1:B:229:GLU:O	1:B:233:LYS:HG2	2.04	0.58
1:A:124:HIS:HD2	2:A:273:HOH:O	1.87	0.58
1:B:244:ARG:HG2	1:B:244:ARG:HH11	1.70	0.57
1:A:110:ASN:C	1:A:110:ASN:HD22	2.09	0.55
1:B:111:PRO:HB2	2:B:273:HOH:O	2.07	0.54
1:A:96:ILE:CD1	1:A:165:LEU:HD11	2.37	0.53
1:A:110:ASN:HD22	1:A:112:THR:H	1.57	0.53
1:A:91:VAL:HG11	2:A:333:HOH:O	2.09	0.52
1:A:91:VAL:HG12	1:A:93:ASN:O	2.09	0.52
1:B:164:VAL:C	1:B:165:LEU:HD12	2.30	0.51
1:B:141:THR:HG22	1:B:145:GLY:C	2.30	0.51
1:A:230:LYS:HE3	2:A:305:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118[A]:CYS:SG	1:B:249:CYS:HA	2.51	0.50
1:B:124:HIS:HD2	2:B:282:HOH:O	1.93	0.50
1:A:155:PHE:HB3	1:A:165:LEU:HB3	1.94	0.48
1:B:244:ARG:HG2	1:B:244:ARG:NH1	2.27	0.48
1:A:110:ASN:ND2	1:A:112:THR:H	2.13	0.47
1:A:108:GLY:HA3	1:A:114:ASP:HB3	1.96	0.47
1:A:104:TYR:CD1	1:A:120:LEU:CD2	2.96	0.46
1:A:139:ILE:O	1:A:146:PHE:HA	2.16	0.46
1:A:83:PRO:HB3	1:A:199:ARG:HD2	1.98	0.45
1:B:111:PRO:HG2	1:B:243:ILE:CG1	2.46	0.44
1:B:139:ILE:O	1:B:146:PHE:HA	2.18	0.44
1:B:102:LYS:HE2	1:B:102:LYS:HB3	1.60	0.44
1:B:143:ASP:O	1:B:144:SER:HB2	2.14	0.44
1:B:111:PRO:HG3	1:B:115:ALA:CB	2.46	0.43
1:B:165:LEU:N	1:B:165:LEU:CD1	2.81	0.43
1:A:139:ILE:CD1	1:A:149:ARG:HG3	2.48	0.43
1:A:140:LYS:CE	1:A:146:PHE:HB3	2.42	0.42
1:A:93:ASN:HD22	1:A:93:ASN:H	1.66	0.42
1:B:126:GLU:O	1:B:130:LYS:HB2	2.20	0.41
1:B:135:ILE:HG21	1:B:135:ILE:HD13	1.60	0.41
1:A:92:GLN:O	1:A:162:PRO:HG2	2.20	0.41
1:A:197:TYR:CD1	1:A:235:ILE:HD13	2.55	0.41
1:A:224:ILE:HG13	1:A:228:LEU:HD22	2.01	0.41
1:A:81:GLU:HB2	1:A:237:ARG:HH22	1.84	0.41
1:B:119:GLN:HB3	1:B:121[A]:HIS:NE2	2.35	0.41
1:A:225:ILE:HD11	1:A:229:GLU:OE2	2.21	0.41
1:B:141:THR:HG22	1:B:145:GLY:O	2.20	0.41
1:A:84:ALA:HA	1:A:85:PRO:HD3	1.79	0.41
1:A:85:PRO:HB3	1:A:180:TYR:CE1	2.55	0.40
1:B:230:LYS:NZ	2:B:312:HOH:O	2.54	0.40
1:A:201:ARG:HA	1:A:207:GLY:HA2	2.03	0.40
1:B:121[B]:HIS:HD2	1:B:214:TYR:OH	2.04	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	158/185 (85%)	151 (96%)	3 (2%)	4 (2%)	7	2
1	B	159/185 (86%)	148 (93%)	9 (6%)	2 (1%)	15	7
All	All	317/370 (86%)	299 (94%)	12 (4%)	6 (2%)	10	4

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	PRO
1	A	86	ASP
1	B	144	SER
1	A	83	PRO
1	B	111	PRO
1	A	84	ALA

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	143/165 (87%)	128 (90%)	15 (10%)	8	4
1	B	144/165 (87%)	136 (94%)	8 (6%)	26	20
All	All	287/330 (87%)	264 (92%)	23 (8%)	15	9

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	GLU
1	A	93	ASN
1	A	110	ASN
1	A	125	THR
1	A	130	LYS
1	A	140	LYS

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Mol	Chain	Res	Type
1	A	150	SER
1	A	165	LEU
1	A	167	ASN
1	A	187	GLU
1	A	199	ARG
1	A	225	ILE
1	A	227	GLU
1	A	228	LEU
1	A	235	ILE
1	B	89	VAL
1	B	102	LYS
1	B	111	PRO
1	B	128	ASP
1	B	219	VAL
1	B	225	ILE
1	B	228	LEU
1	B	244	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	93	ASN
1	A	110	ASN
1	A	124	HIS
1	A	161	GLN
1	A	167	ASN
1	B	124	HIS
1	B	161	GLN
1	B	167	ASN
1	B	168	HIS

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	162/185 (87%)	0.56	17 (10%) 8 9	22, 33, 47, 57	0
1	B	161/185 (87%)	0.49	13 (8%) 15 15	21, 33, 46, 52	0
All	All	323/370 (87%)	0.53	30 (9%) 11 11	21, 33, 47, 57	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	LEU	5.2
1	A	144	SER	5.0
1	B	143	ASP	4.2
1	A	206	ASP	3.9
1	B	144	SER	3.8
1	A	82	PHE	3.6
1	B	111	PRO	3.5
1	A	147	PHE	3.4
1	A	143	ASP	3.4
1	A	212	VAL	3.4
1	B	206	ASP	3.4
1	A	214	TYR	3.2
1	A	196	VAL	3.2
1	B	128	ASP	3.2
1	B	196	VAL	3.1
1	A	213	VAL	3.1
1	B	145	GLY	3.1
1	B	126	GLU	2.7
1	B	121[A]	HIS	2.5
1	A	194	ILE	2.5
1	B	250	GLY	2.5
1	A	85	PRO	2.4
1	B	214	TYR	2.4
1	B	127	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	179	TRP	2.3
1	A	195	PHE	2.3
1	A	105	ILE	2.2
1	A	181	ILE	2.2
1	B	212	VAL	2.2
1	A	128	ASP	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.