



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 09:34 PM GMT

PDB ID : 3HN2  
Title : Crystal structure of 2-dehydropantoate 2-reductase FROM *Geobacter metallireducens* GS-15  
Authors : Patskovsky, Y.; Toro, R.; Morano, C.; Rutter, M.; Chang, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2009-05-29  
Resolution : 2.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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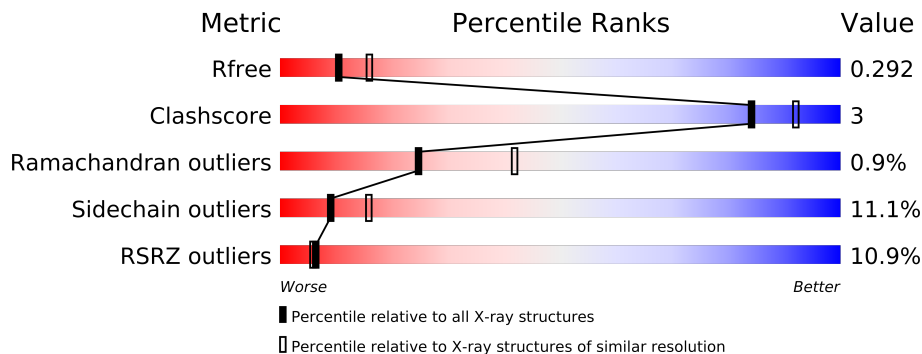
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	312	
1	B	312	
1	C	312	
1	D	312	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9315 atoms, of which 0 are hydrogen and 0 are deuterium.

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 2-dehydropantoate 2-reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2327	1476	409	431	11			
1	B	302	Total	C	N	O	S	0	1	0
			2333	1482	411	429	11			
1	C	302	Total	C	N	O	S	0	0	0
			2326	1477	409	429	11			
1	D	301	Total	C	N	O	S	0	0	0
			2322	1475	408	428	11			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP Q39SB2
A	0	SER	-	EXPRESSION TAG	UNP Q39SB2
A	1	LEU	-	EXPRESSION TAG	UNP Q39SB2
A	303	GLU	-	EXPRESSION TAG	UNP Q39SB2
A	304	GLY	-	EXPRESSION TAG	UNP Q39SB2
A	305	HIS	-	EXPRESSION TAG	UNP Q39SB2
A	306	HIS	-	EXPRESSION TAG	UNP Q39SB2
A	307	HIS	-	EXPRESSION TAG	UNP Q39SB2
A	308	HIS	-	EXPRESSION TAG	UNP Q39SB2
A	309	HIS	-	EXPRESSION TAG	UNP Q39SB2
A	310	HIS	-	EXPRESSION TAG	UNP Q39SB2
B	-1	MET	-	EXPRESSION TAG	UNP Q39SB2
B	0	SER	-	EXPRESSION TAG	UNP Q39SB2
B	1	LEU	-	EXPRESSION TAG	UNP Q39SB2
B	303	GLU	-	EXPRESSION TAG	UNP Q39SB2
B	304	GLY	-	EXPRESSION TAG	UNP Q39SB2
B	305	HIS	-	EXPRESSION TAG	UNP Q39SB2
B	306	HIS	-	EXPRESSION TAG	UNP Q39SB2
B	307	HIS	-	EXPRESSION TAG	UNP Q39SB2
B	308	HIS	-	EXPRESSION TAG	UNP Q39SB2
B	309	HIS	-	EXPRESSION TAG	UNP Q39SB2

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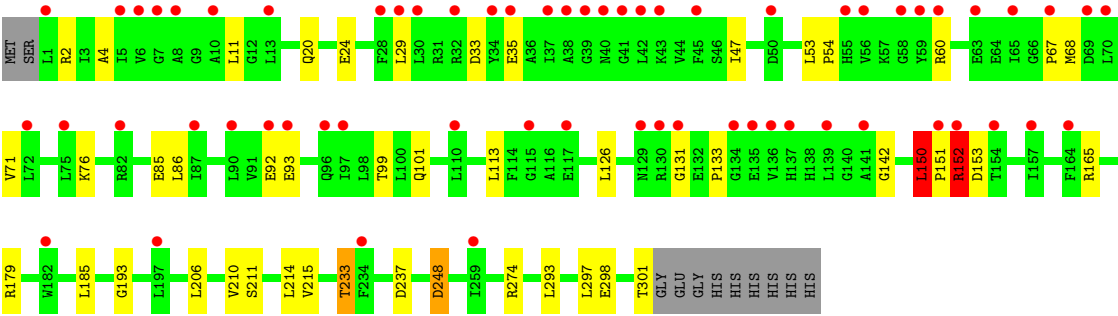
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Chain	Residue	Modelled	Actual	Comment	Reference
B	310	HIS	-	EXPRESSION TAG	UNP Q39SB2
C	-1	MET	-	EXPRESSION TAG	UNP Q39SB2
C	0	SER	-	EXPRESSION TAG	UNP Q39SB2
C	1	LEU	-	EXPRESSION TAG	UNP Q39SB2
C	303	GLU	-	EXPRESSION TAG	UNP Q39SB2
C	304	GLY	-	EXPRESSION TAG	UNP Q39SB2
C	305	HIS	-	EXPRESSION TAG	UNP Q39SB2
C	306	HIS	-	EXPRESSION TAG	UNP Q39SB2
C	307	HIS	-	EXPRESSION TAG	UNP Q39SB2
C	308	HIS	-	EXPRESSION TAG	UNP Q39SB2
C	309	HIS	-	EXPRESSION TAG	UNP Q39SB2
C	310	HIS	-	EXPRESSION TAG	UNP Q39SB2
D	-1	MET	-	EXPRESSION TAG	UNP Q39SB2
D	0	SER	-	EXPRESSION TAG	UNP Q39SB2
D	1	LEU	-	EXPRESSION TAG	UNP Q39SB2
D	303	GLU	-	EXPRESSION TAG	UNP Q39SB2
D	304	GLY	-	EXPRESSION TAG	UNP Q39SB2
D	305	HIS	-	EXPRESSION TAG	UNP Q39SB2
D	306	HIS	-	EXPRESSION TAG	UNP Q39SB2
D	307	HIS	-	EXPRESSION TAG	UNP Q39SB2
D	308	HIS	-	EXPRESSION TAG	UNP Q39SB2
D	309	HIS	-	EXPRESSION TAG	UNP Q39SB2
D	310	HIS	-	EXPRESSION TAG	UNP Q39SB2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total O 3 3	0	0
2	C	4	Total O 4 4	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.32Å 82.18Å 201.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 38.04 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-2.50) 97.8 (38.04-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, $R_{free}$	0.243 , 0.292 0.246 , 0.292	Depositor DCC
$R_{free}$ test set	1377 reflections (3.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.4	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 44287 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9315	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.40	0/2366	0.64	1/3198 (0.0%)
1	B	0.35	0/2376	0.59	0/3212
1	C	0.36	0/2365	0.59	0/3197
1	D	0.34	0/2361	0.59	0/3192
All	All	0.36	0/9468	0.60	1/12799 (0.0%)

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	B	0	4
1	C	0	3
1	D	0	2
All	All	0	9

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	ARG	O-C-N	-5.34	114.16	122.70

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	130	ARG	Peptide
1	B	131	GLY	Peptide
1	B	150	LEU	Peptide
1	B	152	ARG	Peptide
1	C	150	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	C	152	ARG	Peptide
1	C	153	ASP	Peptide
1	D	150	LEU	Peptide
1	D	152	ARG	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2327	0	2345	15	0
1	B	2333	0	2360	7	0
1	C	2326	0	2353	21	0
1	D	2322	0	2350	15	0
2	A	3	0	0	0	0
2	C	4	0	0	0	0
All	All	9315	0	9408	55	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (55) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:154:THR:HG23	1:C:155:GLY:H	1.40	0.86
1:A:152:ARG:O	1:A:153:ASP:HB2	1.86	0.75
1:C:155:GLY:HA2	1:C:158:GLU:HB2	1.72	0.69
1:D:150:LEU:HD22	1:D:151:PRO:HD3	1.75	0.68
1:C:148:GLU:HG3	1:C:151:PRO:HA	1.80	0.64
1:A:152:ARG:O	1:A:153:ASP:CB	2.47	0.62
1:C:67:PRO:HB3	1:C:92:GLU:HB2	1.83	0.60
1:C:153:ASP:HB2	1:C:154:THR:HG22	1.85	0.58
1:A:2:ARG:HD2	1:A:24:GLU:HG3	1.86	0.58
1:B:92:GLU:O	1:B:118:ARG:NH1	2.37	0.58
1:C:154:THR:HG23	1:C:155:GLY:N	2.17	0.53
1:B:201:PRO:HB3	1:B:254:LYS:HG2	1.90	0.52
1:C:153:ASP:N	1:C:153:ASP:OD2	2.42	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:221:GLU:OE2	1:A:289:ARG:NH1	2.44	0.50
1:B:67:PRO:HB3	1:B:92:GLU:HB2	1.94	0.49
1:C:165:ARG:HD2	1:D:248:ASP:HB3	1.93	0.49
1:A:117:GLU:O	1:A:156:ARG:NH2	2.45	0.48
1:C:188:ASN:O	1:C:192:ASN:HB2	2.13	0.48
1:C:179:ARG:HD2	1:C:233:THR:HG23	1.96	0.47
1:C:270:ALA:HA	1:C:274:ARG:HB2	1.96	0.47
1:D:85:GLU:HG3	1:D:86:LEU:HG	1.96	0.47
1:D:152:ARG:HD2	1:D:152:ARG:HA	1.67	0.47
1:D:193:GLY:HA3	1:D:293:LEU:HD21	1.97	0.46
1:C:148:GLU:HB3	1:C:157:ILE:HD11	1.96	0.46
1:A:123:VAL:HG13	1:A:145:ILE:HB	1.98	0.46
1:D:53:LEU:HA	1:D:54:PRO:HD3	1.86	0.45
1:D:179:ARG:HD2	1:D:233:THR:HG23	1.99	0.45
1:A:100:LEU:HD22	1:A:124:ALA:HB2	1.97	0.45
1:C:268:GLU:HB2	1:C:272:ILE:HD12	1.98	0.45
1:C:221:GLU:HB3	1:C:287:MET:HG2	1.99	0.44
1:A:201:PRO:HB3	1:A:254:LYS:HG2	2.00	0.44
1:A:152:ARG:HA	1:A:152:ARG:HD2	1.74	0.44
1:C:47:ILE:HB	1:D:47:ILE:HB	1.99	0.44
1:D:4:ALA:HB2	1:D:68:MET:HG3	2.00	0.44
1:B:150:LEU:HA	1:B:151:PRO:HD3	1.75	0.44
1:A:67:PRO:HB3	1:A:92:GLU:HB2	2.00	0.44
1:D:211:SER:O	1:D:215:VAL:HG23	2.19	0.43
1:D:67:PRO:HB3	1:D:92:GLU:HB2	1.99	0.43
1:A:172:ARG:HA	1:A:172:ARG:HD2	1.85	0.43
1:B:123:VAL:HG23	1:B:184:LYS:HD2	2.00	0.43
1:A:221:GLU:HB3	1:A:287:MET:HG2	2.01	0.43
1:A:148:GLU:HB3	1:A:157:ILE:HD11	2.01	0.43
1:B:211:SER:O	1:B:215:VAL:HG23	2.19	0.42
1:D:274:ARG:NH2	1:D:298:GLU:OE2	2.51	0.42
1:C:11:LEU:HD12	1:C:126:LEU:HD12	2.02	0.42
1:A:188:ASN:O	1:A:192:ASN:HB2	2.19	0.42
1:C:201:PRO:HB3	1:C:254:LYS:HG2	2.02	0.41
1:D:29:LEU:HD21	1:D:86:LEU:HD22	2.02	0.41
1:C:248:ASP:HB3	1:D:165:ARG:HD2	2.01	0.41
1:C:297:LEU:HA	1:C:297:LEU:HD12	1.96	0.41
1:C:150:LEU:HA	1:C:150:LEU:HD22	1.96	0.41
1:C:46:SER:HA	1:C:138:HIS:HB3	2.03	0.41
1:A:126:LEU:HG	1:A:142:GLY:HA2	2.03	0.41
1:D:35:GLU:HG2	1:D:35:GLU:H	1.72	0.41
1:B:123:VAL:HG13	1:B:145:ILE:HB	2.02	0.40

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	300/312 (96%)	277 (92%)	20 (7%)	3 (1%)	22	38
1	B	301/312 (96%)	285 (95%)	15 (5%)	1 (0%)	50	73
1	C	300/312 (96%)	281 (94%)	16 (5%)	3 (1%)	22	38
1	D	299/312 (96%)	280 (94%)	15 (5%)	4 (1%)	18	29
All	All	1200/1248 (96%)	1123 (94%)	66 (6%)	11 (1%)	25	42

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	PRO
1	A	153	ASP
1	B	133	PRO
1	C	133	PRO
1	D	133	PRO
1	C	93	GLU
1	C	131	GLY
1	D	93	GLU
1	A	302	GLY
1	D	131	GLY
1	D	142	GLY

### 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	236/245 (96%)	212 (90%)	24 (10%)	11	19
1	B	237/245 (97%)	210 (89%)	27 (11%)	8	15
1	C	236/245 (96%)	206 (87%)	30 (13%)	6	11
1	D	236/245 (96%)	212 (90%)	24 (10%)	11	19
All	All	945/980 (96%)	840 (89%)	105 (11%)	9	16

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	11	LEU
1	A	24	GLU
1	A	71	VAL
1	A	72	LEU
1	A	76	LYS
1	A	83	TYR
1	A	88	ARG
1	A	101	GLN
1	A	113	LEU
1	A	123	VAL
1	A	126	LEU
1	A	150	LEU
1	A	154	THR
1	A	185	LEU
1	A	194	LEU
1	A	199	GLN
1	A	206	LEU
1	A	209	ASP
1	A	214	LEU
1	A	237	ASP
1	A	247	THR
1	A	261	ARG
1	A	282	ARG
1	B	2	ARG
1	B	20	GLN
1	B	24	GLU
1	B	40	ASN
1	B	60	ARG
1	B	63	GLU
1	B	71	VAL
1	B	76	LYS
1	B	99	THR

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Mol	Chain	Res	Type
1	B	113	LEU
1	B	123	VAL
1	B	126	LEU
1	B	130	ARG
1	B	150	LEU
1	B	152	ARG
1	B	154	THR
1	B	171	CYS
1	B	185	LEU
1	B	206	LEU
1	B	209	ASP
1	B	214	LEU
1	B	233	THR
1	B	261	ARG
1	B	269	ILE
1	B	291	GLU
1	B	297	LEU
1	B	301	THR
1	C	6	VAL
1	C	11	LEU
1	C	20	GLN
1	C	24	GLU
1	C	33	ASP
1	C	35	GLU
1	C	40	ASN
1	C	63	GLU
1	C	71	VAL
1	C	76	LYS
1	C	85	GLU
1	C	113	LEU
1	C	123	VAL
1	C	126	LEU
1	C	150	LEU
1	C	152	ARG
1	C	153	ASP
1	C	154	THR
1	C	166	GLN
1	C	173	THR
1	C	185	LEU
1	C	194	LEU
1	C	206	LEU
1	C	210	VAL

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Mol	Chain	Res	Type
1	C	214	LEU
1	C	233	THR
1	C	237	ASP
1	C	241	ASP
1	C	261	ARG
1	C	297	LEU
1	D	2	ARG
1	D	11	LEU
1	D	20	GLN
1	D	24	GLU
1	D	33	ASP
1	D	60	ARG
1	D	71	VAL
1	D	76	LYS
1	D	99	THR
1	D	101	GLN
1	D	113	LEU
1	D	126	LEU
1	D	150	LEU
1	D	152	ARG
1	D	153	ASP
1	D	185	LEU
1	D	206	LEU
1	D	210	VAL
1	D	214	LEU
1	D	233	THR
1	D	237	ASP
1	D	248	ASP
1	D	297	LEU
1	D	301	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	B	40	ASN
1	B	200	GLN
1	B	229	GLN
1	C	40	ASN
1	C	192	ASN
1	D	40	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	302/312 (96%)	0.45	10 (3%) 44 45	16, 56, 86, 117	0
1	B	302/312 (96%)	0.81	36 (11%) 5 5	26, 64, 97, 109	0
1	C	302/312 (96%)	0.58	23 (7%) 14 13	31, 61, 100, 120	0
1	D	301/312 (96%)	1.13	62 (20%) 1 1	34, 68, 113, 133	0
All	All	1207/1248 (96%)	0.74	131 (10%) 6 6	16, 62, 103, 133	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	42	LEU	10.5
1	C	131	GLY	8.6
1	D	35	GLU	8.4
1	D	152	ARG	7.1
1	B	155	GLY	6.4
1	D	38	ALA	6.0
1	D	131	GLY	5.9
1	B	157	ILE	5.9
1	D	37	ILE	5.8
1	A	303	GLU	5.8
1	B	1	LEU	5.6
1	D	41	GLY	5.6
1	B	154	THR	5.2
1	D	39	GLY	4.9
1	D	1	LEU	4.8
1	D	130	ARG	4.8
1	D	45	PHE	4.2
1	D	151	PRO	4.2
1	D	63	GLU	4.0
1	C	45	PHE	4.0
1	D	154	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	150	LEU	3.9
1	D	234	PHE	3.9
1	D	40	ASN	3.8
1	D	134	GLY	3.8
1	C	152	ARG	3.8
1	D	65	ILE	3.8
1	D	58	GLY	3.8
1	B	151	PRO	3.8
1	B	28	PHE	3.8
1	B	45	PHE	3.7
1	D	137	HIS	3.7
1	D	67	PRO	3.6
1	D	129	ASN	3.6
1	A	42	LEU	3.6
1	C	55	HIS	3.6
1	D	43	LYS	3.5
1	A	28	PHE	3.4
1	D	136	VAL	3.3
1	D	60	ARG	3.3
1	D	59	TYR	3.3
1	A	37	ILE	3.3
1	D	135	GLU	3.2
1	D	30	LEU	3.2
1	B	32	ARG	3.2
1	C	129	ASN	3.2
1	B	160	LEU	3.2
1	D	92	GLU	3.1
1	B	133	PRO	3.1
1	B	100	LEU	3.1
1	C	154	THR	3.1
1	A	154	THR	3.1
1	B	15	TYR	3.0
1	D	55	HIS	3.0
1	B	58	GLY	3.0
1	B	158	GLU	3.0
1	C	31	ARG	2.9
1	D	117	GLU	2.9
1	B	63	GLU	2.9
1	B	70	LEU	2.9
1	D	13	LEU	2.9
1	C	133	PRO	2.8
1	A	131	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	8	ALA	2.8
1	D	93	GLU	2.8
1	C	13	LEU	2.8
1	B	125	PHE	2.8
1	C	156	ARG	2.8
1	B	156	ARG	2.7
1	C	42	LEU	2.7
1	B	34	TYR	2.7
1	D	96	GLN	2.7
1	B	152	ARG	2.7
1	C	1	LEU	2.7
1	B	234	PHE	2.6
1	D	139	LEU	2.6
1	B	148	GLU	2.6
1	D	34	TYR	2.6
1	B	72	LEU	2.6
1	D	90	LEU	2.6
1	D	7	GLY	2.6
1	C	130	ARG	2.5
1	A	54	PRO	2.5
1	D	5	ILE	2.5
1	D	97	ILE	2.5
1	D	87	ILE	2.5
1	A	93	GLU	2.5
1	D	50	ASP	2.5
1	C	37	ILE	2.5
1	C	265	ARG	2.4
1	D	32	ARG	2.4
1	D	29	LEU	2.4
1	D	28	PHE	2.4
1	D	82	ARG	2.4
1	C	302	GLY	2.4
1	D	10	ALA	2.4
1	B	90	LEU	2.4
1	B	98	LEU	2.4
1	D	72	LEU	2.4
1	A	136	VAL	2.4
1	D	141	ALA	2.4
1	B	42	LEU	2.4
1	C	10	ALA	2.4
1	C	301	THR	2.3
1	D	56	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	75	LEU	2.3
1	D	69	ASP	2.3
1	B	131	GLY	2.3
1	B	96	GLN	2.3
1	C	93	GLU	2.3
1	B	55[A]	HIS	2.3
1	C	153	ASP	2.3
1	D	259	ILE	2.3
1	D	115	GLY	2.2
1	B	35	GLU	2.2
1	A	55	HIS	2.2
1	B	93	GLU	2.2
1	D	164	PHE	2.1
1	C	160	LEU	2.1
1	C	52	THR	2.1
1	B	86	LEU	2.1
1	D	70	LEU	2.1
1	D	110	LEU	2.1
1	D	182	TRP	2.1
1	B	33	ASP	2.1
1	D	6	VAL	2.1
1	B	159	GLU	2.1
1	B	3	ILE	2.1
1	D	197	LEU	2.0
1	D	157	ILE	2.0
1	C	150	LEU	2.0

## 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 ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.