



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:13 AM GMT

PDB ID : 3HN2
Title : Crystal structure of 2-dehydropantoate 2-reductase FROM *Geobacter metal-*
lireducens 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 Ge-
nomics (NYSGXRC)
Deposited on : 2009-05-29
Resolution : 2.50 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

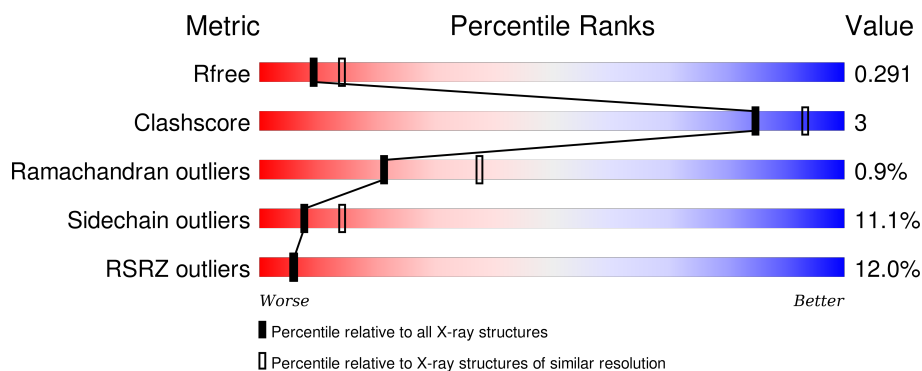
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 ≥ 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	312	<div> <div>5%</div> <div>82%</div> <div>13%</div> <div>..</div> </div>
1	B	312	<div> <div>13%</div> <div>84%</div> <div>11%</div> <div>..</div> </div>
1	C	312	<div> <div>7%</div> <div>79%</div> <div>15%</div> <div>...</div> </div>
1	D	312	<div> <div>21%</div> <div>81%</div> <div>14%</div> <div>..</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9315 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 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

Continued on next page...

Continued from previous page...

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

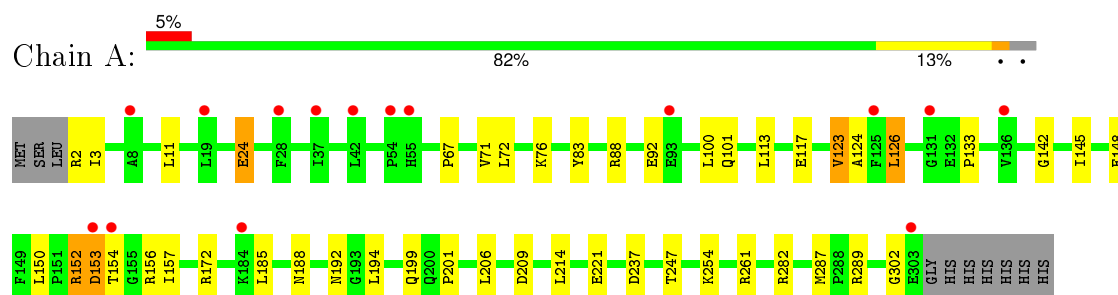
- Molecule 2 is water.

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

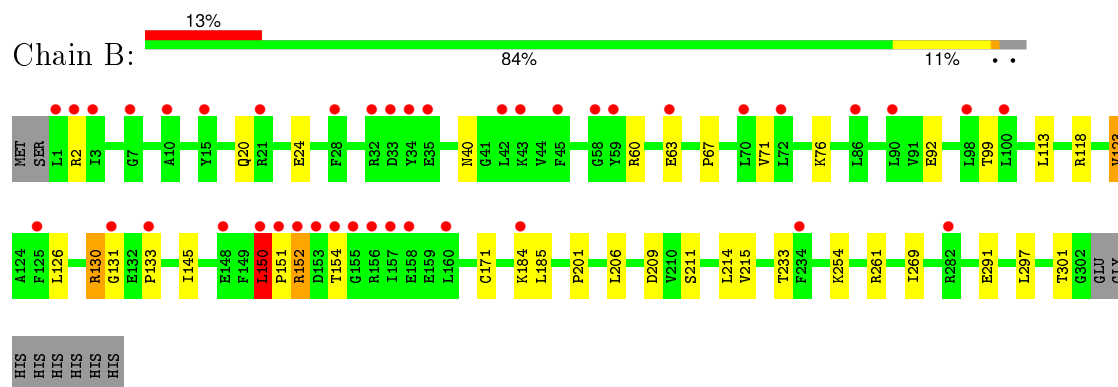
3 Residue-property plots [i](#)

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.

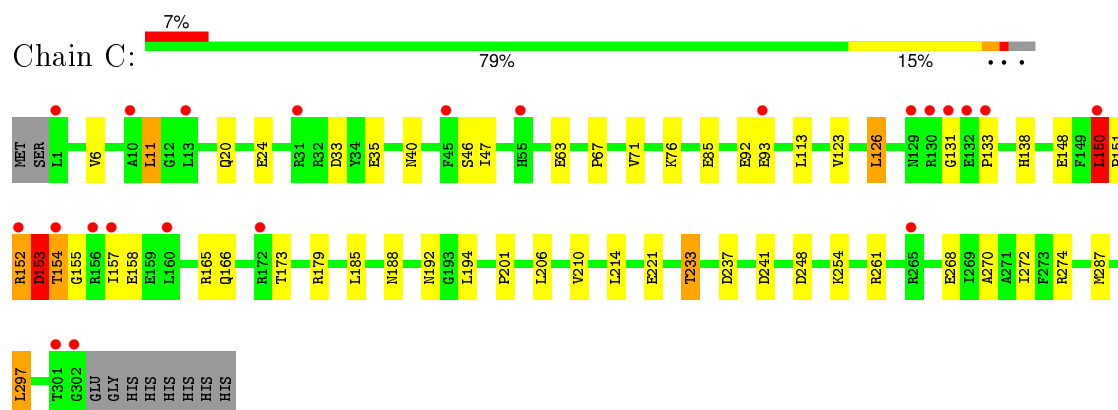
- Molecule 1: 2-dehydropantoate 2-reductase



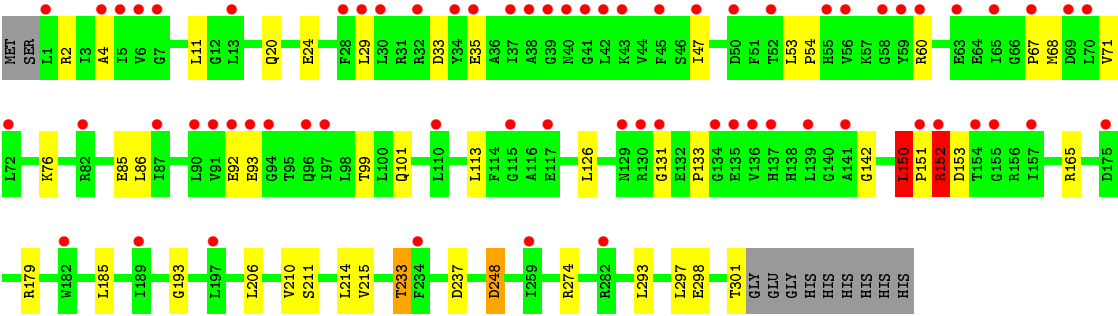
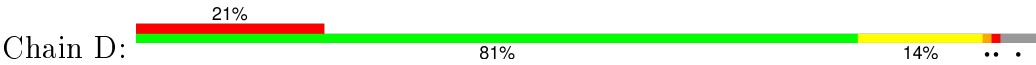
- Molecule 1: 2-dehydropantoate 2-reductase



- Molecule 1: 2-dehydropantoate 2-reductase



- Molecule 1: 2-dehydropantoate 2-reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.243 , 0.292 0.242 , 0.291	Depositor DCC
R_{free} test set	1371 reflections (3.20%)	DCC
Wilson B-factor (Å ²)	58.4	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

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	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

Continued on next page...

Continued from previous page...

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 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	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

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 3.

All (55) 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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:VAL:HG13	1:B:145:ILE:HB	2.02	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	300/312 (96%)	277 (92%)	20 (7%)	3 (1%)	19	34
1	B	301/312 (96%)	285 (95%)	15 (5%)	1 (0%)	46	68
1	C	300/312 (96%)	281 (94%)	16 (5%)	3 (1%)	19	34
1	D	299/312 (96%)	280 (94%)	15 (5%)	4 (1%)	15	26
All	All	1200/1248 (96%)	1123 (94%)	66 (6%)	11 (1%)	21	37

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%)	9	17
1	B	237/245 (97%)	210 (89%)	27 (11%)	7	13
1	C	236/245 (96%)	206 (87%)	30 (13%)	5	10
1	D	236/245 (96%)	212 (90%)	24 (10%)	9	17
All	All	945/980 (96%)	840 (89%)	105 (11%)	8	14

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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 [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](#)

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	302/312 (96%)	0.52	15 (4%) 32 37	16, 56, 86, 117	0
1	B	302/312 (96%)	0.83	41 (13%) 4 4	26, 64, 97, 109	0
1	C	302/312 (96%)	0.61	22 (7%) 18 20	31, 61, 100, 120	0
1	D	301/312 (96%)	1.17	67 (22%) 1 1	34, 68, 113, 133	0
All	All	1207/1248 (96%)	0.78	145 (12%) 6 6	16, 62, 103, 133	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	131	GLY	10.3
1	D	35	GLU	9.5
1	D	42	LEU	9.3
1	D	152	ARG	8.2
1	B	155	GLY	6.9
1	D	38	ALA	6.6
1	D	131	GLY	6.6
1	D	41	GLY	5.8
1	B	157	ILE	5.7
1	B	154	THR	5.6
1	D	1	LEU	5.4
1	D	37	ILE	5.4
1	B	1	LEU	5.3
1	D	45	PHE	5.3
1	A	303	GLU	5.2
1	D	39	GLY	5.1
1	C	45	PHE	4.9
1	D	151	PRO	4.8
1	D	58	GLY	4.8
1	B	58	GLY	4.7
1	D	65	ILE	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	63	GLU	4.4
1	B	28	PHE	4.3
1	D	130	ARG	4.2
1	A	42	LEU	4.1
1	D	117	GLU	4.0
1	C	152	ARG	4.0
1	D	59	TYR	3.9
1	D	60	ARG	3.8
1	D	67	PRO	3.8
1	B	45	PHE	3.6
1	B	34	TYR	3.6
1	D	30	LEU	3.6
1	D	5	ILE	3.6
1	A	37	ILE	3.6
1	D	43	LYS	3.5
1	B	151	PRO	3.5
1	D	90	LEU	3.5
1	D	234	PHE	3.5
1	B	63	GLU	3.4
1	D	129	ASN	3.4
1	A	28	PHE	3.4
1	D	137	HIS	3.4
1	D	154	THR	3.3
1	B	152	ARG	3.3
1	B	158	GLU	3.3
1	B	234	PHE	3.3
1	A	154	THR	3.3
1	C	154	THR	3.3
1	C	55	HIS	3.2
1	D	96	GLN	3.2
1	C	129	ASN	3.2
1	D	92	GLU	3.2
1	B	150	LEU	3.1
1	A	54	PRO	3.1
1	B	133	PRO	3.1
1	D	28	PHE	3.1
1	C	133	PRO	3.1
1	D	97	ILE	3.1
1	D	56	VAL	3.1
1	B	90	LEU	3.1
1	D	50	ASP	3.0
1	A	131	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	93	GLU	3.0
1	B	100	LEU	3.0
1	B	86	LEU	3.0
1	B	70	LEU	2.9
1	D	135	GLU	2.9
1	A	55	HIS	2.9
1	D	40	ASN	2.9
1	D	6	VAL	2.9
1	D	55	HIS	2.9
1	C	1	LEU	2.9
1	D	29	LEU	2.8
1	C	130	ARG	2.8
1	D	134	GLY	2.8
1	D	259	ILE	2.8
1	A	93	GLU	2.8
1	C	156	ARG	2.8
1	C	265	ARG	2.7
1	B	32	ARG	2.7
1	C	31	ARG	2.6
1	C	13	LEU	2.6
1	D	87	ILE	2.6
1	B	35	GLU	2.6
1	D	91	VAL	2.6
1	B	15	TYR	2.6
1	D	141	ALA	2.6
1	A	136	VAL	2.5
1	B	42	LEU	2.5
1	B	33	ASP	2.4
1	D	13	LEU	2.4
1	D	70	LEU	2.4
1	B	131	GLY	2.4
1	D	52	THR	2.4
1	D	7	GLY	2.4
1	C	301	THR	2.4
1	A	153	ASP	2.4
1	D	34	TYR	2.4
1	D	136	VAL	2.4
1	D	82	ARG	2.4
1	B	153	ASP	2.3
1	B	43	LYS	2.3
1	D	69	ASP	2.3
1	D	47	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	157	ILE	2.3
1	A	125	PHE	2.3
1	B	98	LEU	2.3
1	A	19	LEU	2.2
1	A	8	ALA	2.2
1	B	10	ALA	2.2
1	D	139	LEU	2.2
1	B	72	LEU	2.2
1	B	160	LEU	2.2
1	C	150	LEU	2.2
1	D	110	LEU	2.2
1	D	32	ARG	2.2
1	D	182	TRP	2.2
1	B	156	ARG	2.2
1	B	3	ILE	2.2
1	C	93	GLU	2.2
1	B	2	ARG	2.2
1	B	184	LYS	2.2
1	D	197	LEU	2.2
1	D	94	GLY	2.1
1	C	157	ILE	2.1
1	D	189	ILE	2.1
1	B	125	PHE	2.1
1	B	148	GLU	2.1
1	C	160	LEU	2.1
1	A	184	LYS	2.1
1	B	282	ARG	2.1
1	D	4	ALA	2.1
1	C	302	GLY	2.1
1	D	282	ARG	2.1
1	D	175	ASP	2.1
1	D	72	LEU	2.0
1	B	21	ARG	2.0
1	C	132	GLU	2.0
1	C	172	ARG	2.0
1	C	10	ALA	2.0
1	B	7	GLY	2.0
1	D	115	GLY	2.0
1	D	155	GLY	2.0
1	B	59	TYR	2.0

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 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.