



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:01 AM UTC

PDB ID : 4DGS / pdb_00004dgs
Title : The crystals structure of dehydrogenase from Rhizobium meliloti
Authors : Zhang, Z.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; Lafleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRG)
Deposited on : 2012-01-26
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

<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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

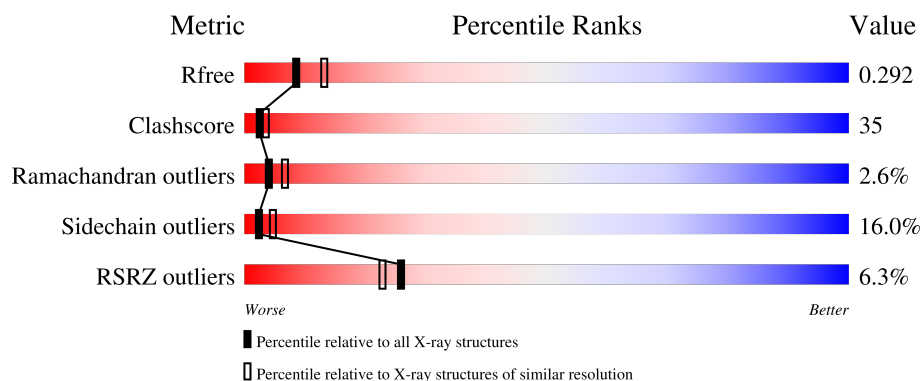
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	340	5% 39% 34% 8% 19%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2113 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 Dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	Se	0	0	0
			2063	1293	381	379	1	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MSE	-	expression tag	UNP Q931A1
A	-21	HIS	-	expression tag	UNP Q931A1
A	-20	HIS	-	expression tag	UNP Q931A1
A	-19	HIS	-	expression tag	UNP Q931A1
A	-18	HIS	-	expression tag	UNP Q931A1
A	-17	HIS	-	expression tag	UNP Q931A1
A	-16	HIS	-	expression tag	UNP Q931A1
A	-15	SER	-	expression tag	UNP Q931A1
A	-14	SER	-	expression tag	UNP Q931A1
A	-13	GLY	-	expression tag	UNP Q931A1
A	-12	VAL	-	expression tag	UNP Q931A1
A	-11	ASP	-	expression tag	UNP Q931A1
A	-10	LEU	-	expression tag	UNP Q931A1
A	-9	GLY	-	expression tag	UNP Q931A1
A	-8	THR	-	expression tag	UNP Q931A1
A	-7	GLU	-	expression tag	UNP Q931A1
A	-6	ASN	-	expression tag	UNP Q931A1
A	-5	LEU	-	expression tag	UNP Q931A1
A	-4	TYR	-	expression tag	UNP Q931A1
A	-3	PHE	-	expression tag	UNP Q931A1
A	-2	GLN	-	expression tag	UNP Q931A1
A	-1	SER	-	expression tag	UNP Q931A1
A	0	MSE	-	expression tag	UNP Q931A1
A	1	LEU	-	expression tag	UNP Q931A1

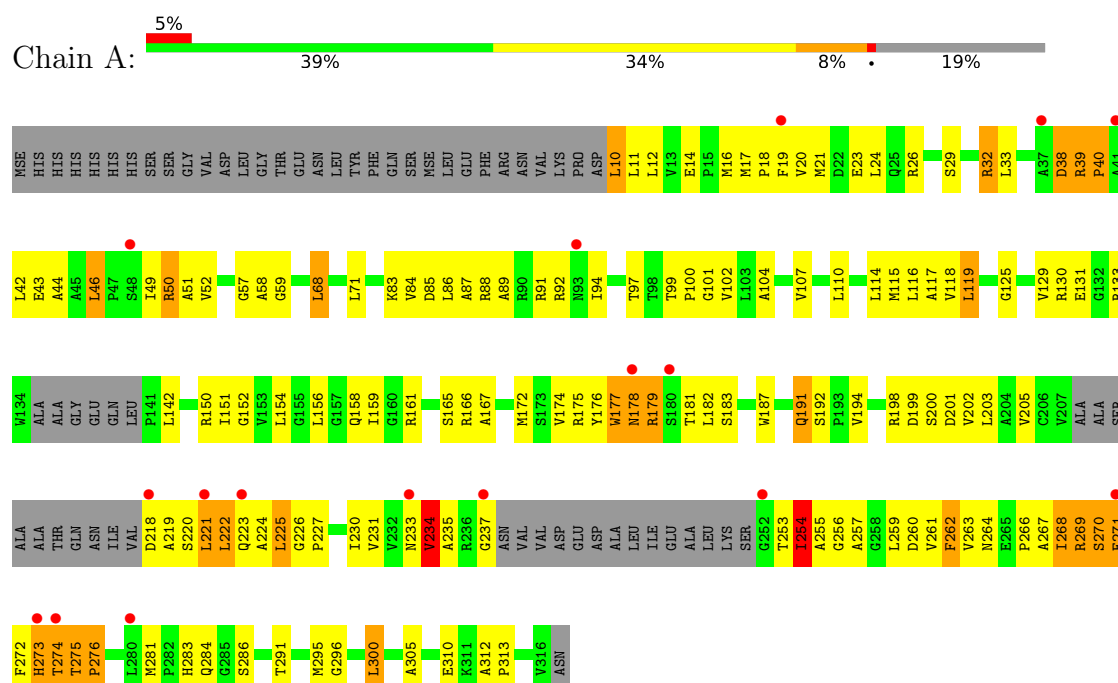
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	50	Total	O	0	0
			50	50		

3 Residue-property plots

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: Dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	79.66Å 71.16Å 55.15Å 90.00° 96.39° 90.00°	Depositor
Resolution (Å)	39.58 – 2.50 39.58 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.2 (39.58-2.50) 99.4 (39.58-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.255 , 0.284 (Not available) , 0.292	Depositor DCC
R_{free} test set	617 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -1/2*h+1/2*k+1,1/2*h-1/2*k+1,1/2*h+1/2*k 0.021 for -1/2*h-1/2*k+1,-1/2*h-1/2*k-1,1/2*h-1/2*k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	2113	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.16% 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

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	0.74	1/2086 (0.0%)	0.97	8/2814 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	267	ALA	CA-CB	-5.09	1.46	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	THR	CA-C-N	7.15	127.11	120.03
1	A	99	THR	C-N-CA	7.15	127.11	120.03
1	A	219	ALA	N-CA-C	-6.72	103.11	112.45
1	A	68	LEU	CA-C-N	6.23	126.13	119.28
1	A	68	LEU	C-N-CA	6.23	126.13	119.28
1	A	226	GLY	CA-C-N	5.52	126.01	120.04
1	A	226	GLY	C-N-CA	5.52	126.01	120.04
1	A	254	ILE	N-CA-C	-5.05	100.52	108.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	TRP	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	2063	0	2102	144	0
2	A	50	0	0	1	0
All	All	2113	0	2102	144	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 35.

All (144) 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:218:ASP:O	1:A:222:LEU:HD22	1.34	1.24
1:A:177:TRP:HA	1:A:178:ASN:ND2	1.54	1.20
1:A:272:PHE:O	1:A:275:THR:HG22	1.46	1.12
1:A:179:ARG:HH11	1:A:179:ARG:HG3	1.20	1.06
1:A:177:TRP:HZ3	1:A:191:GLN:O	1.40	1.03
1:A:179:ARG:HG3	1:A:179:ARG:NH1	1.71	1.00
1:A:177:TRP:CZ3	1:A:192:SER:HA	2.01	0.96
1:A:177:TRP:CA	1:A:178:ASN:ND2	2.29	0.95
1:A:269:ARG:O	1:A:270:SER:HB2	1.65	0.95
1:A:178:ASN:HD22	1:A:178:ASN:N	1.67	0.92
1:A:269:ARG:CG	1:A:271:GLU:HG3	2.01	0.89
1:A:179:ARG:HH11	1:A:179:ARG:CG	1.86	0.88
1:A:269:ARG:HG3	1:A:271:GLU:CG	2.04	0.87
1:A:115:MSE:HE3	1:A:202:VAL:HG11	1.61	0.82
1:A:231:VAL:HG13	1:A:254:ILE:HD11	1.64	0.79
1:A:272:PHE:O	1:A:275:THR:CG2	2.30	0.79
1:A:269:ARG:HG3	1:A:271:GLU:HG3	1.63	0.78
1:A:177:TRP:CZ3	1:A:191:GLN:O	2.33	0.76
1:A:272:PHE:C	1:A:275:THR:HG22	2.10	0.75
1:A:273:HIS:CD2	1:A:273:HIS:C	2.64	0.75
1:A:269:ARG:HG3	1:A:271:GLU:HG2	1.68	0.75
1:A:178:ASN:ND2	1:A:178:ASN:N	2.29	0.73
1:A:269:ARG:HG2	1:A:271:GLU:HG3	1.70	0.73
1:A:178:ASN:C	1:A:179:ARG:HG2	2.15	0.71
1:A:269:ARG:O	1:A:270:SER:CB	2.38	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:PRO:HA	1:A:268:ILE:HD12	1.72	0.71
1:A:266:PRO:HA	1:A:268:ILE:CD1	2.24	0.68
1:A:39:ARG:N	1:A:40:PRO:HD2	2.09	0.66
1:A:177:TRP:CE3	1:A:178:ASN:ND2	2.64	0.66
1:A:17:MSE:HG3	2:A:425:HOH:O	1.94	0.66
1:A:234:VAL:HG13	1:A:234:VAL:O	1.97	0.65
1:A:266:PRO:C	1:A:268:ILE:HD12	2.21	0.65
1:A:269:ARG:CG	1:A:271:GLU:CG	2.68	0.65
1:A:178:ASN:C	1:A:179:ARG:CG	2.67	0.64
1:A:194:VAL:O	1:A:198:ARG:HG3	1.97	0.64
1:A:38:ASP:O	1:A:42:LEU:HB2	1.98	0.63
1:A:115:MSE:HE3	1:A:202:VAL:CG1	2.28	0.62
1:A:194:VAL:HA	1:A:221:LEU:HD11	1.80	0.62
1:A:177:TRP:HA	1:A:178:ASN:HD21	1.54	0.62
1:A:291:THR:O	1:A:295:MSE:HG3	1.99	0.62
1:A:57:GLY:O	1:A:83:LYS:HG3	2.00	0.61
1:A:175:ARG:HH11	1:A:199:ASP:CG	2.08	0.61
1:A:107:VAL:HG11	1:A:159:ILE:HD13	1.83	0.60
1:A:12:LEU:HD11	1:A:14:GLU:O	2.02	0.60
1:A:115:MSE:CE	1:A:172:MSE:HE1	2.32	0.60
1:A:273:HIS:CD2	1:A:274:THR:N	2.70	0.60
1:A:254:ILE:HG23	1:A:256:GLY:H	1.67	0.59
1:A:272:PHE:HA	1:A:275:THR:HG22	1.83	0.59
1:A:296:GLY:O	1:A:300:LEU:HD22	2.02	0.59
1:A:273:HIS:C	1:A:273:HIS:HD2	2.08	0.58
1:A:150:ARG:HB3	1:A:175:ARG:HD2	1.86	0.58
1:A:11:LEU:HB3	1:A:52:VAL:HG22	1.84	0.58
1:A:275:THR:OG1	1:A:276:PRO:CD	2.52	0.58
1:A:194:VAL:CA	1:A:221:LEU:HD11	2.34	0.57
1:A:272:PHE:CA	1:A:275:THR:HG22	2.34	0.57
1:A:178:ASN:O	1:A:179:ARG:CG	2.52	0.57
1:A:266:PRO:CA	1:A:268:ILE:HD12	2.34	0.57
1:A:156:LEU:HD22	1:A:176:TYR:CD2	2.40	0.56
1:A:166:ARG:HG3	1:A:166:ARG:HH11	1.70	0.56
1:A:273:HIS:HD2	1:A:274:THR:N	2.04	0.56
1:A:177:TRP:HA	1:A:178:ASN:CG	2.27	0.56
1:A:59:GLY:HA3	1:A:83:LYS:HB3	1.88	0.55
1:A:178:ASN:HD22	1:A:178:ASN:H	1.52	0.55
1:A:101:GLY:HA2	1:A:158:GLN:HE22	1.71	0.55
1:A:18:PRO:O	1:A:21:MSE:HB2	2.06	0.54
1:A:198:ARG:HG2	1:A:224:ALA:HB1	1.87	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:GLU:O	1:A:275:THR:N	2.35	0.54
1:A:202:VAL:HG22	1:A:230:ILE:HG12	1.89	0.54
1:A:272:PHE:HA	1:A:275:THR:CG2	2.37	0.54
1:A:115:MSE:HE1	1:A:172:MSE:HE1	1.89	0.54
1:A:115:MSE:HE1	1:A:172:MSE:SE	2.58	0.53
1:A:203:LEU:HB2	1:A:225:LEU:HD11	1.90	0.53
1:A:156:LEU:HD22	1:A:176:TYR:CG	2.44	0.52
1:A:14:GLU:OE2	1:A:58:ALA:HB2	2.09	0.51
1:A:42:LEU:O	1:A:46:LEU:HD13	2.09	0.51
1:A:17:MSE:O	1:A:21:MSE:HG2	2.10	0.51
1:A:175:ARG:NH1	1:A:199:ASP:OD1	2.43	0.51
1:A:177:TRP:CE3	1:A:192:SER:HA	2.44	0.51
1:A:194:VAL:HA	1:A:221:LEU:CD1	2.41	0.51
1:A:227:PRO:O	1:A:255:ALA:HB2	2.10	0.51
1:A:87:ALA:O	1:A:91:ARG:HG3	2.10	0.51
1:A:125:GLY:O	1:A:129:VAL:HG23	2.11	0.50
1:A:274:THR:O	1:A:275:THR:O	2.30	0.49
1:A:178:ASN:O	1:A:179:ARG:HG3	2.12	0.49
1:A:152:GLY:HA3	1:A:200:SER:OG	2.13	0.49
1:A:161:ARG:HD3	1:A:182:LEU:HD11	1.95	0.49
1:A:49:ILE:CG2	1:A:68:LEU:HD22	2.43	0.49
1:A:177:TRP:C	1:A:178:ASN:ND2	2.71	0.49
1:A:100:PRO:O	1:A:102:VAL:HG23	2.13	0.48
1:A:88:ARG:O	1:A:92:ARG:HG3	2.12	0.48
1:A:19:PHE:O	1:A:23:GLU:HG2	2.14	0.48
1:A:33:LEU:C	1:A:33:LEU:HD23	2.39	0.48
1:A:114:LEU:O	1:A:118:VAL:HG23	2.14	0.48
1:A:259:LEU:HB2	1:A:262:PHE:CE1	2.49	0.48
1:A:174:VAL:HB	1:A:187:TRP:CD1	2.50	0.47
1:A:166:ARG:HG3	1:A:166:ARG:NH1	2.29	0.47
1:A:175:ARG:NH1	1:A:199:ASP:CG	2.73	0.47
1:A:177:TRP:C	1:A:178:ASN:HD22	2.20	0.47
1:A:10:LEU:HB2	1:A:51:ALA:O	2.14	0.46
1:A:32:ARG:H	1:A:32:ARG:HG2	1.57	0.46
1:A:222:LEU:HD12	1:A:222:LEU:HA	1.67	0.46
1:A:97:THR:HG21	1:A:312:ALA:HB1	1.97	0.46
1:A:115:MSE:CE	1:A:151:ILE:HD12	2.46	0.46
1:A:115:MSE:HE1	1:A:151:ILE:HD12	1.99	0.45
1:A:39:ARG:N	1:A:40:PRO:CD	2.79	0.45
1:A:131:GLU:O	1:A:133:ARG:HG3	2.16	0.45
1:A:177:TRP:CA	1:A:178:ASN:HD22	2.19	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASP:O	1:A:222:LEU:CD2	2.30	0.45
1:A:260:ASP:OD1	1:A:284:GLN:N	2.42	0.44
1:A:231:VAL:O	1:A:257:ALA:HA	2.17	0.44
1:A:114:LEU:HD21	1:A:281:MSE:HG2	1.99	0.44
1:A:115:MSE:HE2	1:A:172:MSE:HE1	2.00	0.44
1:A:235:ALA:O	1:A:261:VAL:HG11	2.17	0.44
1:A:167:ALA:O	1:A:172:MSE:HB2	2.18	0.44
1:A:12:LEU:CD1	1:A:14:GLU:O	2.65	0.43
1:A:150:ARG:NH1	1:A:199:ASP:OD1	2.52	0.43
1:A:182:LEU:HD23	1:A:183:SER:O	2.18	0.43
1:A:38:ASP:OD2	1:A:38:ASP:N	2.52	0.43
1:A:154:LEU:HB3	1:A:205:VAL:HA	2.00	0.43
1:A:20:VAL:O	1:A:24:LEU:HG	2.17	0.43
1:A:43:GLU:O	1:A:44:ALA:C	2.62	0.43
1:A:50:ARG:HA	1:A:71:LEU:HA	2.00	0.42
1:A:85:ASP:OD2	1:A:88:ARG:HB2	2.19	0.42
1:A:150:ARG:HD3	1:A:201:ASP:OD2	2.19	0.42
1:A:114:LEU:O	1:A:117:ALA:HB3	2.20	0.42
1:A:115:MSE:HE1	1:A:172:MSE:CE	2.50	0.42
1:A:231:VAL:HG13	1:A:254:ILE:CD1	2.44	0.42
1:A:274:THR:C	1:A:275:THR:O	2.63	0.42
1:A:275:THR:OG1	1:A:276:PRO:HD2	2.20	0.42
1:A:237:GLY:C	1:A:263:VAL:HG22	2.46	0.41
1:A:305:ALA:O	1:A:310:GLU:HG3	2.20	0.41
1:A:275:THR:HA	1:A:276:PRO:HD3	1.91	0.41
1:A:177:TRP:HE3	1:A:178:ASN:HD21	1.69	0.41
1:A:182:LEU:HD23	1:A:183:SER:N	2.35	0.41
1:A:39:ARG:HD3	1:A:39:ARG:HA	1.60	0.41
1:A:115:MSE:HG2	1:A:119:LEU:HD22	2.02	0.41
1:A:260:ASP:O	1:A:283:HIS:HA	2.20	0.41
1:A:233:ASN:ND2	1:A:261:VAL:HG23	2.36	0.41
1:A:312:ALA:HA	1:A:313:PRO:HD3	1.79	0.41
1:A:26:ARG:HG2	1:A:26:ARG:HH11	1.86	0.41
1:A:89:ALA:HB1	1:A:94:ILE:HB	2.02	0.41
1:A:10:LEU:N	1:A:29:SER:O	2.54	0.40
1:A:104:ALA:HA	1:A:159:ILE:HG12	2.03	0.40
1:A:259:LEU:HB2	1:A:262:PHE:HE1	1.85	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	269/340 (79%)	247 (92%)	15 (6%)	7 (3%)	4 7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	ASN
1	A	270	SER
1	A	269	ARG
1	A	276	PRO
1	A	275	THR
1	A	40	PRO
1	A	234	VAL

5.3.2 Protein sidechains [i](#)

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	213/254 (84%)	179 (84%)	34 (16%)	2 5

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	16	MSE
1	A	32	ARG
1	A	38	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	39	ARG
1	A	46	LEU
1	A	50	ARG
1	A	84	VAL
1	A	86	LEU
1	A	110	LEU
1	A	116	LEU
1	A	119	LEU
1	A	130	ARG
1	A	142	LEU
1	A	165	SER
1	A	178	ASN
1	A	179	ARG
1	A	181	THR
1	A	191	GLN
1	A	220	SER
1	A	221	LEU
1	A	222	LEU
1	A	223	GLN
1	A	225	LEU
1	A	234	VAL
1	A	253	THR
1	A	254	ILE
1	A	262	PHE
1	A	268	ILE
1	A	271	GLU
1	A	273	HIS
1	A	274	THR
1	A	286	SER
1	A	300	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	HIS
1	A	158	GLN
1	A	178	ASN
1	A	223	GLN
1	A	273	HIS
1	A	284	GLN

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 oligosaccharides 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 [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	268/340 (78%)	0.64	17 (6%) 26 23	22, 40, 54, 63	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	THR	4.3
1	A	273	HIS	3.9
1	A	252	GLY	3.9
1	A	218	ASP	3.4
1	A	178	ASN	3.3
1	A	280	LEU	2.8
1	A	19	PHE	2.8
1	A	41	ALA	2.7
1	A	271	GLU	2.5
1	A	221	LEU	2.4
1	A	37	ALA	2.4
1	A	180	SER	2.3
1	A	223	GLN	2.3
1	A	233	ASN	2.2
1	A	93	ASN	2.2
1	A	48	SER	2.2
1	A	237	GLY	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 oligosaccharides 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.