



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 12:43 am BST

PDB ID : 2O1E  
Title : Crystal Structure of the Metal-dependent Lipoprotein YcdH from *Bacillus subtilis*, Northeast Structural Genomics Target SR583  
Authors : Forouhar, F.; Zhou, W.; Seetharaman, J.; Chen, C.X.; Fang, Y.; Cunningham, K.; Ma, L.-C.; Janjua, H.; Xiao, R.; Baran, M.C.; Liu, J.; Acton, T.B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2006-11-28  
Resolution : 2.60 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](mailto: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.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

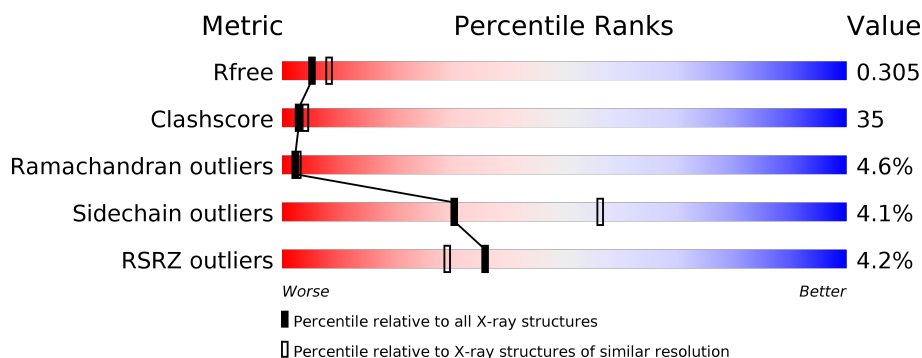
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	312	<div> <div>4%</div> <div> <div></div> <div>37%</div> <div>44%</div> <div>5%</div> <div>15%</div> </div> </div>
1	B	312	<div> <div>4%</div> <div> <div></div> <div>38%</div> <div>41%</div> <div>5%</div> <div>15%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4236 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 YcdH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	Se	0	0	0
			2108	1350	338	414	6			
1	B	264	Total	C	N	O	Se	0	0	0
			2091	1339	334	412	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MSE	-	CLONING ARTIFACT	UNP O34966
A	-3	ALA	-	CLONING ARTIFACT	UNP O34966
A	-2	GLY	-	CLONING ARTIFACT	UNP O34966
A	-1	ASP	-	CLONING ARTIFACT	UNP O34966
A	0	PRO	-	CLONING ARTIFACT	UNP O34966
A	1	MSE	-	CLONING ARTIFACT	UNP O34966
A	26	MSE	MET	MODIFIED RESIDUE	UNP O34966
A	76	MSE	MET	MODIFIED RESIDUE	UNP O34966
A	87	MSE	MET	MODIFIED RESIDUE	UNP O34966
A	104	MSE	MET	MODIFIED RESIDUE	UNP O34966
A	125	MSE	MET	MODIFIED RESIDUE	UNP O34966
A	284	MSE	MET	MODIFIED RESIDUE	UNP O34966
A	300	LEU	-	EXPRESSION TAG	UNP O34966
A	301	GLU	-	EXPRESSION TAG	UNP O34966
A	302	HIS	-	EXPRESSION TAG	UNP O34966
A	303	HIS	-	EXPRESSION TAG	UNP O34966
A	304	HIS	-	EXPRESSION TAG	UNP O34966
A	305	HIS	-	EXPRESSION TAG	UNP O34966
A	306	HIS	-	EXPRESSION TAG	UNP O34966
A	307	HIS	-	EXPRESSION TAG	UNP O34966
B	-4	MSE	-	CLONING ARTIFACT	UNP O34966
B	-3	ALA	-	CLONING ARTIFACT	UNP O34966
B	-2	GLY	-	CLONING ARTIFACT	UNP O34966
B	-1	ASP	-	CLONING ARTIFACT	UNP O34966
B	0	PRO	-	CLONING ARTIFACT	UNP O34966

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MSE	-	CLONING ARTIFACT	UNP O34966
B	26	MSE	MET	MODIFIED RESIDUE	UNP O34966
B	76	MSE	MET	MODIFIED RESIDUE	UNP O34966
B	87	MSE	MET	MODIFIED RESIDUE	UNP O34966
B	104	MSE	MET	MODIFIED RESIDUE	UNP O34966
B	125	MSE	MET	MODIFIED RESIDUE	UNP O34966
B	284	MSE	MET	MODIFIED RESIDUE	UNP O34966
B	300	LEU	-	EXPRESSION TAG	UNP O34966
B	301	GLU	-	EXPRESSION TAG	UNP O34966
B	302	HIS	-	EXPRESSION TAG	UNP O34966
B	303	HIS	-	EXPRESSION TAG	UNP O34966
B	304	HIS	-	EXPRESSION TAG	UNP O34966
B	305	HIS	-	EXPRESSION TAG	UNP O34966
B	306	HIS	-	EXPRESSION TAG	UNP O34966
B	307	HIS	-	EXPRESSION TAG	UNP O34966

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mn 1 1	0	0
2	A	1	Total Mn 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	13	Total O 13 13	0	0
3	B	22	Total O 22 22	0	0



L291	L292	D293	S294	L295	L296	VAL	LYS	SER	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.29Å 54.34Å 62.84Å 103.70° 100.46° 96.75°	Depositor
Resolution (Å)	19.93 – 2.60 39.70 – 2.36	Depositor EDS
% Data completeness (in resolution range)	81.0 (19.93-2.60) 88.3 (39.70-2.36)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.83 (at 2.37Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.223 , 0.290 0.241 , 0.305	Depositor DCC
$R_{free}$ test set	3987 reflections (9.56%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4236	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.45	0/2145	0.57	0/2891
1	B	0.43	0/2127	0.55	0/2866
All	All	0.44	0/4272	0.56	0/5757

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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	24	TYR	Sidechain
1	A	280	TYR	Sidechain
1	B	24	TYR	Sidechain

### 5.2 Too-close contacts [i](#)

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	2108	0	2104	150	0
1	B	2091	0	2088	143	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	13	0	0	1	0
3	B	22	0	0	1	0
All	All	4236	0	4192	292	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 (292) 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:33:ILE:HD11	1:A:147:ILE:HG13	1.42	1.01
1:A:134:VAL:HG11	1:A:201:GLU:OE2	1.64	0.98
1:B:271:LYS:H	1:B:271:LYS:HD2	1.37	0.88
1:A:76:MSE:HE3	1:A:130:TRP:HZ3	1.38	0.88
1:B:264:ASN:HD21	1:B:283:ILE:HG23	1.43	0.83
1:B:191:GLN:HG2	1:B:240:PHE:CD1	2.14	0.82
1:A:253:ALA:O	1:A:257:GLY:HA2	1.80	0.82
1:B:191:GLN:NE2	1:B:241:GLU:H	1.78	0.82
1:A:97:ALA:HB1	1:A:139:GLU:HB3	1.62	0.81
1:B:134:VAL:HG13	1:B:135:LEU:HD12	1.60	0.81
1:B:76:MSE:HE3	1:B:130:TRP:HZ3	1.46	0.80
1:A:132:SER:OG	1:A:134:VAL:HG12	1.81	0.80
1:B:76:MSE:HE2	1:B:127:PRO:CG	2.12	0.79
1:A:134:VAL:HG13	1:A:135:LEU:N	1.98	0.78
1:B:97:ALA:HB1	1:B:139:GLU:HB3	1.65	0.77
1:A:76:MSE:HE3	1:A:130:TRP:CZ3	2.18	0.76
1:B:22:THR:HG21	1:B:77:GLU:HG2	1.66	0.76
1:A:264:ASN:HD22	1:A:287:ASN:HD21	1.32	0.76
1:B:26:MSE:HE1	1:B:143:ILE:HD11	1.66	0.76
1:A:264:ASN:H	1:A:287:ASN:HD21	1.34	0.75
1:B:189:ILE:HG23	1:B:209:ILE:HD11	1.70	0.74
1:B:281:ILE:H	1:B:281:ILE:HD12	1.52	0.73
1:B:140:VAL:O	1:B:144:THR:HG22	1.88	0.73
1:B:68:LEU:HD11	1:B:150:GLN:HG2	1.70	0.73
1:B:76:MSE:HE3	1:B:130:TRP:CZ3	2.23	0.73
1:A:22:THR:HG21	1:A:77:GLU:HG2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ILE:HG22	1:B:210:ALA:H	1.53	0.72
1:B:162:SER:O	1:B:166:ILE:HG12	1.89	0.72
1:A:192:HIS:H	1:A:192:HIS:CD2	2.08	0.71
1:A:71:TYR:CZ	1:A:96:ASN:HB3	2.26	0.70
1:B:71:TYR:CZ	1:B:96:ASN:HB3	2.26	0.70
1:A:134:VAL:HG13	1:A:135:LEU:H	1.56	0.70
1:B:23:PHE:H	1:B:23:PHE:HD2	1.40	0.69
1:B:191:GLN:HE21	1:B:241:GLU:H	1.39	0.69
1:A:32:GLN:HG2	1:A:165:TYR:CD2	2.28	0.68
1:B:76:MSE:HE2	1:B:127:PRO:HB2	1.75	0.67
1:A:23:PHE:HD2	1:A:23:PHE:H	1.40	0.67
1:A:32:GLN:HG2	1:A:165:TYR:CG	2.31	0.66
1:B:26:MSE:HE1	1:B:97:ALA:HB2	1.77	0.66
1:A:266:LEU:HD23	1:A:284:MSE:HE3	1.77	0.66
1:A:68:LEU:HD11	1:A:150:GLN:HG2	1.78	0.66
1:B:209:ILE:HG22	1:B:210:ALA:N	2.11	0.65
1:A:191:GLN:HG2	1:A:240:PHE:CD1	2.32	0.65
1:B:128:HIS:HA	1:B:130:TRP:CZ3	2.31	0.65
1:B:76:MSE:HE2	1:B:127:PRO:HG2	1.77	0.65
1:B:176:TYR:CE2	1:B:198:LEU:HD11	2.32	0.65
1:A:134:VAL:CG1	1:A:135:LEU:H	2.08	0.65
1:A:185:LYS:HD2	1:A:187:GLU:HG2	1.79	0.65
1:A:26:MSE:HE1	1:A:143:ILE:HD11	1.79	0.64
1:B:76:MSE:HE2	1:B:127:PRO:CB	2.26	0.64
1:A:64:GLN:HB3	1:A:87:MSE:SE	2.47	0.64
1:B:145:ALA:O	1:B:149:LYS:HG2	1.96	0.64
1:A:134:VAL:CG1	1:A:135:LEU:N	2.61	0.64
1:A:264:ASN:HD22	1:A:264:ASN:H	1.46	0.64
1:A:26:MSE:HE1	1:A:97:ALA:HB2	1.80	0.64
1:B:189:ILE:HD13	1:B:207:VAL:HG13	1.77	0.64
1:A:149:LYS:O	1:A:152:PRO:HD3	1.99	0.63
1:A:145:ALA:O	1:A:148:VAL:HG22	1.97	0.63
1:B:159:GLU:O	1:B:163:LYS:HG2	1.98	0.63
1:B:265:THR:O	1:B:267:GLU:N	2.31	0.62
1:A:151:ASP:O	1:A:151:ASP:OD1	2.16	0.62
1:B:56:THR:HB	1:B:57:PRO:HD2	1.81	0.62
1:A:236:LYS:HD3	1:A:236:LYS:O	1.98	0.62
1:A:162:SER:O	1:A:166:ILE:HG12	2.00	0.62
1:A:56:THR:HB	1:A:57:PRO:HD2	1.81	0.62
1:A:25:PRO:HD3	1:A:266:LEU:O	2.00	0.62
1:A:76:MSE:HE2	1:A:127:PRO:CG	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:SER:HB3	1:B:216:GLN:HB3	1.81	0.61
1:B:204:LEU:HD13	1:B:295:LEU:HD21	1.82	0.61
1:B:95:VAL:HB	1:B:146:GLN:HG2	1.83	0.61
1:A:37:LYS:HB2	1:A:157:TYR:CE2	2.34	0.61
1:B:132:SER:OG	1:B:135:LEU:HD13	2.01	0.61
1:A:76:MSE:HE2	1:A:127:PRO:HB2	1.83	0.60
1:A:236:LYS:HD3	1:A:236:LYS:C	2.22	0.60
1:B:230:ALA:HA	1:B:235:VAL:HG23	1.82	0.60
1:B:64:GLN:HB3	1:B:87:MSE:SE	2.52	0.60
1:B:136:ALA:O	1:B:140:VAL:HG23	2.01	0.60
1:A:264:ASN:HD21	1:A:283:ILE:CG2	2.15	0.59
1:A:45:PRO:O	1:A:48:VAL:HG22	2.02	0.59
1:A:266:LEU:HD23	1:A:284:MSE:CE	2.31	0.59
1:B:25:PRO:HD3	1:B:266:LEU:O	2.03	0.59
1:A:177:ARG:HH21	1:A:177:ARG:HG3	1.68	0.59
1:A:144:THR:O	1:A:148:VAL:HG13	2.03	0.58
1:B:191:GLN:HG3	1:B:240:PHE:HA	1.86	0.58
1:A:123:HIS:O	1:A:125:MSE:HE3	2.04	0.58
1:B:191:GLN:HE21	1:B:241:GLU:N	2.01	0.58
1:B:134:VAL:HG13	1:B:135:LEU:CD1	2.33	0.58
1:A:134:VAL:HG11	1:A:201:GLU:CD	2.24	0.58
1:A:76:MSE:HE2	1:A:127:PRO:HG2	1.85	0.57
1:A:209:ILE:HG21	1:A:226:LEU:HD13	1.87	0.57
1:B:45:PRO:O	1:B:48:VAL:HG22	2.04	0.57
1:B:22:THR:CG2	1:B:77:GLU:HG2	2.34	0.57
1:A:276:LYS:HE2	1:B:243:ILE:O	2.05	0.56
1:B:96:ASN:OD1	1:B:99:LYS:HB2	2.05	0.56
1:A:131:LEU:HD22	1:A:284:MSE:HE1	1.87	0.56
1:A:96:ASN:OD1	1:A:99:LYS:HB2	2.06	0.56
1:A:37:LYS:HB2	1:A:157:TYR:HE2	1.71	0.56
1:B:42:LEU:H	1:B:42:LEU:HD23	1.70	0.56
1:B:237:VAL:HG21	1:B:293:ASP:O	2.06	0.55
1:A:239:TYR:HA	1:A:261:GLU:O	2.06	0.55
1:A:133:PRO:O	1:A:137:GLN:HG3	2.05	0.55
1:A:143:ILE:O	1:A:147:ILE:HG12	2.07	0.55
1:B:143:ILE:O	1:B:147:ILE:HG12	2.05	0.55
1:B:101:ILE:HG22	1:B:103:LEU:H	1.72	0.55
1:B:46:SER:HB3	1:B:274:GLN:NE2	2.21	0.55
1:A:185:LYS:HB2	1:A:295:LEU:HA	1.89	0.55
1:A:189:ILE:HA	1:A:207:VAL:HG13	1.87	0.55
1:B:238:ILE:HG22	1:B:240:PHE:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ALA:O	1:A:212:LEU:N	2.40	0.55
1:A:216:GLN:H	1:A:216:GLN:CD	2.10	0.55
1:A:155:LYS:HD2	1:A:156:GLU:OE2	2.07	0.55
1:A:30:THR:O	1:A:33:ILE:HG12	2.06	0.55
1:B:33:ILE:HD11	1:B:147:ILE:HG13	1.87	0.55
1:B:30:THR:O	1:B:33:ILE:HG12	2.07	0.54
1:A:42:LEU:H	1:A:42:LEU:HD23	1.71	0.54
1:B:265:THR:C	1:B:267:GLU:H	2.09	0.54
1:A:76:MSE:HB3	1:A:77:GLU:OE2	2.08	0.54
1:B:177:ARG:HG2	1:B:177:ARG:HH21	1.73	0.54
1:A:253:ALA:O	1:A:257:GLY:CA	2.52	0.54
1:A:80:VAL:N	1:A:81:PRO:HD2	2.23	0.54
1:A:240:PHE:O	1:A:262:VAL:O	2.26	0.54
1:A:125:MSE:HE2	1:A:125:MSE:HA	1.90	0.53
1:B:76:MSE:CE	1:B:127:PRO:HG2	2.39	0.53
1:B:272:GLU:O	1:B:276:LYS:HG2	2.08	0.53
1:A:101:ILE:HG22	1:A:103:LEU:H	1.74	0.53
1:A:202:TYR:O	1:A:204:LEU:HG	2.09	0.53
1:A:176:TYR:CE2	1:A:198:LEU:HD11	2.44	0.53
1:A:264:ASN:H	1:A:287:ASN:ND2	2.05	0.53
1:B:26:MSE:CE	1:B:143:ILE:HD11	2.35	0.53
1:A:33:ILE:CD1	1:A:147:ILE:HG13	2.27	0.52
1:A:49:GLU:CD	1:A:51:HIS:HB2	2.30	0.52
1:A:140:VAL:O	1:A:144:THR:OG1	2.26	0.52
1:B:198:LEU:HD21	1:B:291:LEU:HD11	1.91	0.52
1:A:192:HIS:H	1:A:192:HIS:HD2	1.56	0.52
1:A:76:MSE:HE2	1:A:127:PRO:CB	2.39	0.52
1:B:159:GLU:HG3	1:B:163:LYS:NZ	2.25	0.52
1:B:37:LYS:HB2	1:B:157:TYR:CE2	2.44	0.52
1:B:68:LEU:CD1	1:B:150:GLN:HG2	2.40	0.52
1:B:263:LEU:HA	1:B:287:ASN:OD1	2.10	0.52
1:B:228:THR:O	1:B:232:GLU:HG2	2.10	0.52
1:A:259:LYS:HE2	1:A:261:GLU:OE1	2.10	0.52
1:A:56:THR:O	1:A:60:ILE:HG12	2.09	0.52
1:A:22:THR:CG2	1:A:77:GLU:HG2	2.39	0.52
1:B:177:ARG:HG2	1:B:177:ARG:NH2	2.25	0.52
1:A:104:MSE:HG2	1:A:105:GLU:H	1.75	0.52
1:B:49:GLU:CD	1:B:51:HIS:HB2	2.30	0.52
1:A:189:ILE:HG12	1:A:207:VAL:HG13	1.91	0.51
1:B:189:ILE:HA	1:B:207:VAL:HG13	1.90	0.51
1:A:262:VAL:O	1:A:263:LEU:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:GLN:O	1:B:173:ASP:HB3	2.10	0.51
1:B:56:THR:O	1:B:60:ILE:HG12	2.11	0.51
1:A:224:ALA:O	1:A:228:THR:HG22	2.10	0.51
1:B:20:VAL:HG23	1:B:66:ALA:HB2	1.91	0.51
1:A:230:ALA:HA	1:A:235:VAL:HG23	1.91	0.51
1:B:26:MSE:HE1	1:B:97:ALA:CB	2.40	0.51
1:A:20:VAL:HG23	1:A:66:ALA:HB2	1.93	0.51
1:A:186:LYS:HA	1:A:204:LEU:HD23	1.91	0.51
1:A:104:MSE:HG2	1:A:105:GLU:N	2.26	0.50
1:B:165:TYR:HE2	1:B:281:ILE:HD11	1.77	0.50
1:B:80:VAL:N	1:B:81:PRO:HD2	2.27	0.50
1:A:283:ILE:HG22	1:A:283:ILE:O	2.10	0.50
1:A:46:SER:O	1:A:47:SER:HB3	2.12	0.50
1:B:185:LYS:HB2	1:B:295:LEU:HA	1.94	0.49
1:A:77:GLU:OE2	1:A:77:GLU:N	2.45	0.49
1:B:77:GLU:N	1:B:77:GLU:OE2	2.45	0.49
1:A:209:ILE:HG22	1:A:210:ALA:N	2.27	0.49
1:A:61:ALA:O	1:A:65:ASP:HB2	2.13	0.49
1:B:46:SER:O	1:B:47:SER:HB3	2.13	0.49
1:A:292:LYS:C	1:A:294:SER:H	2.15	0.49
1:B:76:MSE:HB3	1:B:77:GLU:OE2	2.13	0.49
1:A:215:ASP:HB2	1:A:216:GLN:OE1	2.12	0.48
1:A:128:HIS:HA	1:A:130:TRP:CZ3	2.48	0.48
1:A:265:THR:O	1:A:267:GLU:N	2.44	0.48
1:B:104:MSE:HG2	1:B:105:GLU:H	1.78	0.48
1:B:264:ASN:HD21	1:B:283:ILE:CG2	2.19	0.48
1:A:264:ASN:HD22	1:A:264:ASN:N	2.07	0.48
1:B:180:ALA:HB1	1:B:204:LEU:HD21	1.95	0.48
1:A:154:ASN:HA	3:A:403:HOH:O	2.13	0.48
1:A:195:PHE:HB2	1:A:206:GLN:OE1	2.14	0.48
1:A:228:THR:HA	1:A:231:LYS:HD3	1.95	0.48
1:B:133:PRO:O	1:B:137:GLN:HG3	2.14	0.48
1:B:190:THR:O	1:B:208:PRO:HA	2.13	0.47
1:A:177:ARG:HG3	1:A:177:ARG:NH2	2.29	0.47
1:A:199:ALA:HB1	1:A:204:LEU:O	2.15	0.47
1:B:37:LYS:HB2	1:B:157:TYR:HE2	1.80	0.47
1:B:61:ALA:O	1:B:65:ASP:HB2	2.14	0.47
1:B:104:MSE:HG2	1:B:105:GLU:N	2.30	0.47
1:A:259:LYS:HB3	1:A:259:LYS:NZ	2.29	0.47
1:B:191:GLN:HE22	1:B:241:GLU:HB2	1.78	0.47
1:B:271:LYS:N	1:B:271:LYS:HD2	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:MSE:CE	1:A:143:ILE:HD11	2.44	0.47
1:B:264:ASN:ND2	1:B:283:ILE:HG23	2.21	0.47
1:B:189:ILE:CG2	1:B:209:ILE:HD11	2.43	0.47
1:A:265:THR:C	1:A:267:GLU:H	2.18	0.46
1:B:240:PHE:O	1:B:262:VAL:O	2.33	0.46
1:A:76:MSE:CE	1:A:127:PRO:HG2	2.45	0.46
1:A:189:ILE:HG23	1:A:209:ILE:HD11	1.98	0.46
1:B:151:ASP:OD1	1:B:154:ASN:ND2	2.49	0.46
1:B:18:HIS:CD2	1:B:66:ALA:HA	2.49	0.46
1:A:106:GLY:HA3	1:A:124:ALA:O	2.16	0.46
1:B:270:SER:OG	1:B:273:GLU:HG3	2.16	0.46
1:B:269:LEU:CB	1:B:274:GLN:HE22	2.28	0.46
1:B:46:SER:CB	1:B:274:GLN:NE2	2.79	0.45
1:A:133:PRO:HG2	1:A:202:TYR:OH	2.16	0.45
1:A:106:GLY:HA2	1:A:126:ASP:HB2	1.98	0.45
1:B:134:VAL:HG11	1:B:201:GLU:CD	2.37	0.45
1:B:236:LYS:HD3	1:B:236:LYS:O	2.17	0.45
1:A:18:HIS:CD2	1:A:66:ALA:HA	2.51	0.45
1:A:264:ASN:HD21	1:A:283:ILE:HG22	1.80	0.45
1:B:26:MSE:HE2	1:B:70:VAL:HG12	1.99	0.45
1:A:95:VAL:HB	1:A:146:GLN:HG2	1.99	0.45
1:B:46:SER:HB3	1:B:274:GLN:HE21	1.82	0.45
1:A:133:PRO:CG	1:A:202:TYR:OH	2.65	0.45
1:B:133:PRO:HG2	1:B:202:TYR:OH	2.17	0.45
1:B:138:LYS:HA	1:B:138:LYS:HD2	1.89	0.45
1:A:237:VAL:HG12	1:A:238:ILE:N	2.32	0.44
1:B:23:PHE:N	1:B:23:PHE:CD2	2.83	0.44
1:B:190:THR:O	1:B:209:ILE:HG12	2.18	0.44
1:B:98:SER:HA	1:B:101:ILE:HD12	1.99	0.44
1:A:26:MSE:HE1	1:A:97:ALA:CB	2.46	0.44
1:B:252:LEU:O	1:B:256:ILE:HB	2.18	0.44
1:A:209:ILE:O	1:A:210:ALA:O	2.35	0.44
1:A:28:GLU:O	1:A:32:GLN:HB2	2.17	0.44
1:A:131:LEU:HD12	1:A:194:ALA:O	2.17	0.44
1:A:101:ILE:C	1:A:103:LEU:H	2.21	0.44
1:B:33:ILE:HD12	1:B:144:THR:HA	1.99	0.44
1:A:46:SER:OG	1:A:269:LEU:N	2.51	0.44
1:A:259:LYS:HD2	1:A:260:THR:N	2.33	0.43
1:B:101:ILE:C	1:B:103:LEU:H	2.21	0.43
1:B:191:GLN:HB2	1:B:212:LEU:O	2.18	0.43
1:B:45:PRO:O	1:B:47:SER:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLN:HG2	1:B:165:TYR:CD2	2.54	0.43
1:A:104:MSE:HB2	1:A:197:TYR:CE2	2.52	0.43
1:A:123:HIS:C	1:A:125:MSE:HE3	2.39	0.43
1:A:191:GLN:CG	1:A:240:PHE:HA	2.48	0.43
1:A:26:MSE:HE2	1:A:70:VAL:HG12	2.00	0.43
1:A:185:LYS:HG3	1:A:294:SER:O	2.18	0.43
1:A:98:SER:HA	1:A:101:ILE:HD12	1.99	0.43
1:B:59:ASP:O	1:B:63:ILE:HG13	2.18	0.43
1:A:45:PRO:O	1:A:47:SER:N	2.52	0.43
1:B:189:ILE:HD11	1:B:229:TYR:HE2	1.84	0.43
1:B:259:LYS:HG2	1:B:260:THR:H	1.84	0.43
1:B:20:VAL:HG23	1:B:66:ALA:CB	2.49	0.43
1:B:212:LEU:HD21	1:B:238:ILE:HG21	2.01	0.43
1:B:130:TRP:C	1:B:132:SER:H	2.23	0.42
1:B:132:SER:OG	1:B:134:VAL:HG12	2.19	0.42
1:B:28:GLU:O	1:B:32:GLN:HB2	2.19	0.42
1:B:265:THR:C	1:B:267:GLU:N	2.71	0.42
1:A:138:LYS:HE3	1:A:142:ASN:HD21	1.85	0.42
1:B:137:GLN:NE2	1:B:170:GLN:HG3	2.33	0.42
1:A:202:TYR:O	1:A:203:GLY:C	2.58	0.42
1:A:266:LEU:HD21	1:A:283:ILE:HB	2.02	0.42
1:A:292:LYS:O	1:A:294:SER:N	2.47	0.42
1:B:124:ALA:O	1:B:125:MSE:HE2	2.20	0.42
1:B:24:TYR:OH	1:B:279:GLY:HA2	2.20	0.42
1:B:262:VAL:HB	1:B:263:LEU:H	1.74	0.42
1:A:76:MSE:HB2	1:A:127:PRO:HB2	2.02	0.42
1:A:20:VAL:HG22	1:A:41:ASP:OD1	2.20	0.41
1:B:209:ILE:CG2	1:B:210:ALA:H	2.19	0.41
1:A:185:LYS:HZ3	1:A:187:GLU:CD	2.23	0.41
1:B:135:LEU:O	1:B:139:GLU:HG3	2.20	0.41
1:B:224:ALA:HA	1:B:227:LYS:HB2	2.02	0.41
1:B:264:ASN:HB2	3:B:415:HOH:O	2.19	0.41
1:A:103:LEU:HD13	1:A:125:MSE:CG	2.50	0.41
1:B:155:LYS:HE2	1:B:159:GLU:OE1	2.20	0.41
1:B:18:HIS:O	1:B:67:ASP:HB2	2.21	0.41
1:B:229:TYR:HA	1:B:232:GLU:CG	2.51	0.41
1:A:264:ASN:ND2	1:A:287:ASN:HD21	2.08	0.41
1:B:97:ALA:HB2	1:B:143:ILE:HD11	2.03	0.41
1:B:209:ILE:HG13	1:B:212:LEU:HD22	2.02	0.41
1:A:139:GLU:O	1:A:143:ILE:HG13	2.21	0.41
1:A:33:ILE:HD12	1:A:144:THR:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD23	1:A:42:LEU:N	2.36	0.41
1:B:134:VAL:HG13	1:B:135:LEU:N	2.36	0.41
1:B:202:TYR:HB2	1:B:204:LEU:HG	2.03	0.41
1:B:46:SER:OG	1:B:274:GLN:NE2	2.53	0.41
1:A:138:LYS:HG3	1:A:142:ASN:HD21	1.86	0.41
1:A:262:VAL:O	1:A:263:LEU:CB	2.69	0.41
1:A:59:ASP:O	1:A:63:ILE:HG13	2.21	0.41
1:B:193:THR:HA	1:B:206:GLN:NE2	2.36	0.41
1:A:19:VAL:HG22	1:A:68:LEU:HD13	2.03	0.40
1:A:246:SER:O	1:A:247:LYS:C	2.60	0.40
1:A:288:LEU:HA	1:A:291:LEU:HD12	2.02	0.40
1:B:188:PHE:N	1:B:188:PHE:CD1	2.89	0.40
1:A:17:LEU:HD11	1:A:68:LEU:HD11	2.03	0.40
1:B:67:ASP:CB	1:B:68:LEU:HD12	2.51	0.40
1:B:129:VAL:HB	1:B:135:LEU:HD23	2.03	0.40
1:B:42:LEU:N	1:B:42:LEU:HD23	2.34	0.40
1:A:225:LYS:O	1:A:228:THR:HG23	2.22	0.40
1:A:26:MSE:CE	1:A:70:VAL:HG12	2.51	0.40
1:A:67:ASP:HB2	1:A:68:LEU:HD12	2.04	0.40
1:B:17:LEU:HD11	1:B:68:LEU:HD11	2.03	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	262/312 (84%)	220 (84%)	31 (12%)	11 (4%)	3	3
1	B	260/312 (83%)	220 (85%)	27 (10%)	13 (5%)	2	2
All	All	522/624 (84%)	440 (84%)	58 (11%)	24 (5%)	2	3

All (24) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	47	SER
1	A	210	ALA
1	B	47	SER
1	B	294	SER
1	A	211	GLY
1	B	22	THR
1	B	209	ILE
1	B	266	LEU
1	A	22	THR
1	A	46	SER
1	A	102	ASP
1	B	46	SER
1	B	227	LYS
1	A	193	THR
1	A	293	ASP
1	B	102	ASP
1	B	128	HIS
1	B	262	VAL
1	A	87	MSE
1	B	87	MSE
1	A	294	SER
1	B	293	ASP
1	A	262	VAL
1	B	268	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	231/262 (88%)	220 (95%)	11 (5%)	25	49
1	B	229/262 (87%)	221 (96%)	8 (4%)	36	62
All	All	460/524 (88%)	441 (96%)	19 (4%)	30	56

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	PHE
1	A	146	GLN
1	A	149	LYS
1	A	184	GLU
1	A	192	HIS
1	A	216	GLN
1	A	228	THR
1	A	234	ASN
1	A	242	GLU
1	A	259	LYS
1	A	264	ASN
1	B	23	PHE
1	B	146	GLN
1	B	168	LYS
1	B	175	LEU
1	B	192	HIS
1	B	216	GLN
1	B	264	ASN
1	B	271	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	137	GLN
1	A	142	ASN
1	A	154	ASN
1	A	170	GLN
1	A	191	GLN
1	A	192	HIS
1	A	233	HIS
1	A	264	ASN
1	A	287	ASN
1	B	89	GLN
1	B	137	GLN
1	B	170	GLN
1	B	191	GLN
1	B	192	HIS
1	B	216	GLN
1	B	264	ASN
1	B	274	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

### 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	260/312 (83%)	0.17	11 (4%) 36 29	30, 60, 81, 96	0
1	B	258/312 (82%)	0.21	11 (4%) 35 28	31, 61, 96, 107	0
All	All	518/624 (83%)	0.19	22 (4%) 36 29	30, 60, 88, 107	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	GLY	8.6
1	B	221	ALA	5.6
1	B	230	ALA	5.1
1	A	124	ALA	4.6
1	A	105	GLU	4.6
1	A	123	HIS	4.4
1	B	224	ALA	3.2
1	A	89	GLN	3.2
1	B	227	LYS	3.1
1	A	256	ILE	2.9
1	B	235	VAL	2.6
1	A	147	ILE	2.5
1	B	88	GLY	2.5
1	B	222	SER	2.3
1	B	228	THR	2.2
1	A	297	VAL	2.2
1	B	180	ALA	2.2
1	A	234	ASN	2.2
1	A	229	TYR	2.1
1	B	90	GLY	2.1
1	A	296	LEU	2.1
1	B	231	LYS	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](#)

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	MN	B	401	1/1	0.98	0.19	50,50,50,50	0
2	MN	A	401	1/1	0.99	0.13	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.