



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:20 am GMT

PDB ID : 3WI4  
Title : Crystal structure of wild-type PorB from Neisseria meningitidis serogroup B  
Authors : Kattner, C.; Toussi, D.; Wetzler, L.M.; Ruppel, N.; Massari, P.; Tanabe, M.  
Deposited on : 2013-09-05  
Resolution : 3.32 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

<http://wwpdb.org/validation/2016/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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

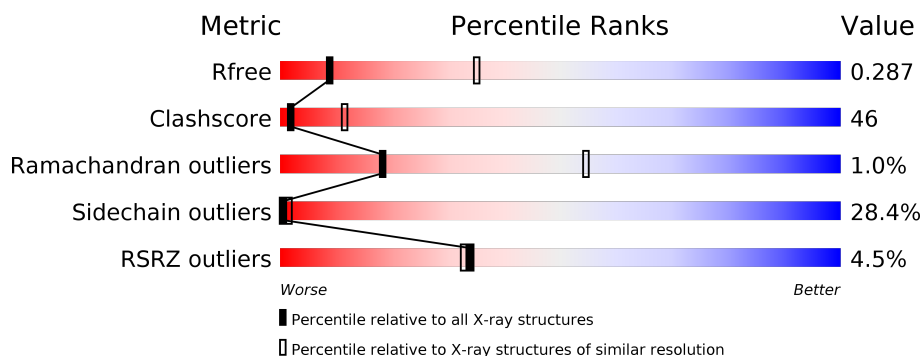
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.32 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))
$R_{free}$	100719	1002 (3.38-3.26)
Clashscore	112137	1066 (3.38-3.26)
Ramachandran outliers	110173	1048 (3.38-3.26)
Sidechain outliers	110143	1047 (3.38-3.26)
RSRZ outliers	101464	1007 (3.38-3.26)

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. 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	313	<div> <div>4%</div> <div>38%</div> <div>44%</div> <div>15%</div> <div>..</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2380 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 Major outer membrane protein P.IB.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	0	1	0
			2380	1487	425	468			

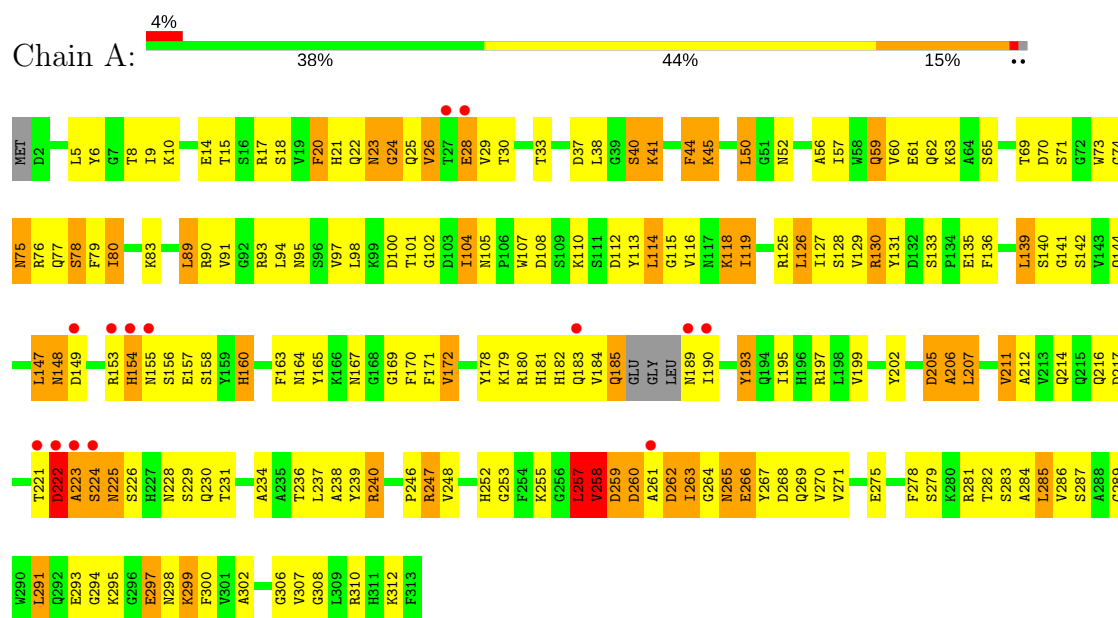
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP P30690

### 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 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: Major outer membrane protein P.IB



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.29Å 148.29Å 104.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.32 48.22 – 3.32	Depositor EDS
% Data completeness (in resolution range)	50.0 (50.00-3.32) 82.7 (48.22-3.32)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.80 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.254 , 0.294 0.246 , 0.287	Depositor DCC
$R_{free}$ test set	534 reflections (10.79%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.9	Xtriage
Anisotropy	0.676	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.9	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	0.87	EDS
Total number of atoms	2380	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.26% 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](#)

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	0.68	0/2427	0.93	8/3276 (0.2%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	ALA	CB-CA-C	-15.96	86.16	110.10
1	A	207	LEU	N-CA-CB	12.54	135.47	110.40
1	A	23	ASN	CB-CA-C	-9.22	91.96	110.40
1	A	222	ASP	N-CA-C	7.48	131.20	111.00
1	A	257	LEU	N-CA-C	-6.86	92.48	111.00
1	A	223	ALA	CB-CA-C	-5.83	101.36	110.10
1	A	258	VAL	N-CA-C	-5.79	95.37	111.00
1	A	8	THR	N-CA-C	-5.27	96.76	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	2380	0	2276	214	0
All	All	2380	0	2276	214	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 46.

All (214) 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:281:ARG:HG2	1:A:312:LYS:O	1.32	1.23
1:A:197:ARG:HG2	1:A:214:GLN:HG3	1.18	1.15
1:A:6:TYR:CE2	1:A:45:LYS:HG2	1.82	1.12
1:A:114:LEU:HD23	1:A:287:SER:HB2	1.32	1.06
1:A:37:ASP:O	1:A:110:LYS:HE3	1.56	1.06
1:A:157:GLU:OE1	1:A:157:GLU:N	1.90	1.04
1:A:147:LEU:HD12	1:A:147:LEU:H	1.23	1.00
1:A:133:SER:HB3	1:A:141:GLY:H	1.27	1.00
1:A:197:ARG:CG	1:A:214:GLN:HG3	1.92	0.99
1:A:107:TRP:CZ3	1:A:247:ARG:NH1	2.31	0.98
1:A:20:PHE:CE1	1:A:300:PHE:HD2	1.80	0.97
1:A:60:VAL:HA	1:A:78:SER:HB3	1.48	0.96
1:A:189:ASN:O	1:A:221:THR:HG23	1.68	0.94
1:A:21:HIS:O	1:A:22:GLN:NE2	2.01	0.93
1:A:114:LEU:HD21	1:A:306:GLY:N	1.84	0.93
1:A:89:LEU:HD12	1:A:90:ARG:N	1.81	0.93
1:A:139:LEU:HD23	1:A:164:ASN:O	1.69	0.93
1:A:6:TYR:CD2	1:A:45:LYS:HG2	2.04	0.93
1:A:20:PHE:CE1	1:A:300:PHE:CD2	2.59	0.90
1:A:238:ALA:HB2	1:A:247:ARG:HB2	1.51	0.90
1:A:265:ASN:HB2	1:A:294:GLY:HA2	1.52	0.90
1:A:253:GLY:O	1:A:266:GLU:HB2	1.73	0.88
1:A:185:GLN:OE1	1:A:185:GLN:N	2.08	0.87
1:A:261:ALA:O	1:A:263:ILE:HD12	1.75	0.86
1:A:230:GLN:NE2	1:A:231:THR:O	2.10	0.85
1:A:98:LEU:O	1:A:101:THR:HG23	1.77	0.85
1:A:156:SER:OG	1:A:180:ARG:HB2	1.77	0.84
1:A:114:LEU:HD23	1:A:287:SER:CB	2.06	0.84
1:A:130:ARG:HG2	1:A:144:GLN:HB3	1.59	0.84
1:A:100[B]:ASP:OD2	1:A:130:ARG:NH2	2.11	0.83
1:A:199:VAL:HG22	1:A:212:ALA:CB	2.08	0.82
1:A:258:VAL:HG12	1:A:259:ASP:H	1.44	0.81
1:A:267:TYR:CB	1:A:293:GLU:HG2	2.10	0.81
1:A:293:GLU:OE1	1:A:294:GLY:N	2.15	0.80
1:A:189:ASN:O	1:A:221:THR:CG2	2.28	0.80
1:A:65:SER:N	1:A:70:ASP:OD2	2.16	0.79
1:A:129:VAL:O	1:A:144:GLN:HB2	1.83	0.78
1:A:107:TRP:CE3	1:A:247:ARG:NH1	2.51	0.78
1:A:267:TYR:HB3	1:A:293:GLU:HG2	1.65	0.78
1:A:258:VAL:HG12	1:A:259:ASP:N	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ASN:OD1	1:A:221:THR:HG21	1.85	0.77
1:A:114:LEU:CD2	1:A:287:SER:HB2	2.12	0.77
1:A:238:ALA:HB2	1:A:247:ARG:CB	2.15	0.76
1:A:62:GLN:HG3	1:A:74:GLY:H	1.49	0.76
1:A:65:SER:CB	1:A:70:ASP:OD2	2.34	0.76
1:A:183:GLN:NE2	1:A:184:VAL:O	2.19	0.75
1:A:114:LEU:HD22	1:A:306:GLY:HA3	1.66	0.75
1:A:147:LEU:CD1	1:A:147:LEU:H	2.01	0.74
1:A:259:ASP:OD1	1:A:259:ASP:N	2.21	0.74
1:A:97:VAL:HG23	1:A:144:GLN:OE1	1.88	0.74
1:A:104:ILE:HG12	1:A:197:ARG:HH21	1.51	0.74
1:A:104:ILE:HG12	1:A:197:ARG:NH2	2.04	0.72
1:A:98:LEU:C	1:A:101:THR:HG23	2.11	0.70
1:A:89:LEU:HD12	1:A:90:ARG:H	1.54	0.70
1:A:260:ASP:OD1	1:A:260:ASP:N	2.25	0.70
1:A:147:LEU:HD12	1:A:147:LEU:N	2.04	0.69
1:A:107:TRP:CD1	1:A:115:GLY:HA2	2.28	0.68
1:A:165:TYR:HB3	1:A:172:VAL:HG13	1.73	0.67
1:A:156:SER:HB3	1:A:181:HIS:HB2	1.75	0.67
1:A:108:ASP:OD2	1:A:310:ARG:NH1	2.28	0.67
1:A:287:SER:N	1:A:306:GLY:O	2.27	0.67
1:A:104:ILE:HG21	1:A:119:ILE:HG23	1.75	0.67
1:A:75:ASN:O	1:A:93:ARG:NH1	2.27	0.67
1:A:154:HIS:C	1:A:155:ASN:HD22	1.98	0.67
1:A:265:ASN:CB	1:A:294:GLY:HA2	2.25	0.66
1:A:278:PHE:HE2	1:A:284:ALA:HB2	1.61	0.65
1:A:98:LEU:HA	1:A:101:THR:CG2	2.27	0.65
1:A:25:GLN:OE1	1:A:25:GLN:HA	1.97	0.65
1:A:65:SER:HB2	1:A:70:ASP:OD2	1.96	0.64
1:A:98:LEU:HG	1:A:197:ARG:HD3	1.79	0.64
1:A:114:LEU:CD2	1:A:306:GLY:HA3	2.28	0.64
1:A:217:ASP:OD1	1:A:229:SER:HB2	1.98	0.64
1:A:22:GLN:O	1:A:23:ASN:HB2	1.97	0.64
1:A:267:TYR:HB2	1:A:293:GLU:HG2	1.77	0.63
1:A:6:TYR:HE2	1:A:45:LYS:HG2	1.58	0.62
1:A:206:ALA:O	1:A:239:TYR:CE2	2.52	0.62
1:A:199:VAL:HG22	1:A:212:ALA:HB2	1.80	0.61
1:A:133:SER:HB3	1:A:141:GLY:N	2.06	0.61
1:A:199:VAL:HG22	1:A:212:ALA:HB1	1.82	0.61
1:A:114:LEU:HD21	1:A:306:GLY:H	1.62	0.61
1:A:285:LEU:HG	1:A:308:GLY:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLU:OE1	1:A:310:ARG:NH2	2.34	0.60
1:A:94:LEU:O	1:A:125:ARG:HA	2.02	0.60
1:A:238:ALA:HB1	1:A:246:PRO:O	2.01	0.59
1:A:6:TYR:CE2	1:A:45:LYS:CG	2.75	0.59
1:A:105:ASN:OD1	1:A:116:VAL:N	2.36	0.59
1:A:62:GLN:CG	1:A:74:GLY:H	2.16	0.59
1:A:224:SER:O	1:A:225:ASN:C	2.39	0.58
1:A:126:LEU:HD13	1:A:128:SER:HB3	1.85	0.58
1:A:193:TYR:HA	1:A:217:ASP:O	2.03	0.58
1:A:156:SER:HG	1:A:180:ARG:HB2	1.68	0.57
1:A:165:TYR:O	1:A:171:PHE:HA	2.05	0.57
1:A:22:GLN:HA	1:A:22:GLN:NE2	2.18	0.57
1:A:98:LEU:O	1:A:101:THR:CG2	2.50	0.57
1:A:62:GLN:HG2	1:A:73:TRP:HA	1.86	0.57
1:A:257:LEU:CD1	1:A:262:ASP:OD2	2.53	0.56
1:A:199:VAL:HG13	1:A:212:ALA:HB2	1.87	0.56
1:A:255:LYS:HB3	1:A:264:GLY:O	2.06	0.56
1:A:98:LEU:HA	1:A:101:THR:HG21	1.85	0.56
1:A:118:LYS:HB3	1:A:267:TYR:CZ	2.41	0.56
1:A:239:TYR:CD1	1:A:240:ARG:N	2.74	0.55
1:A:185:GLN:CD	1:A:185:GLN:H	2.02	0.55
1:A:240:ARG:HG3	1:A:240:ARG:O	2.05	0.55
1:A:18:SER:HB2	1:A:300:PHE:CZ	2.41	0.55
1:A:148:ASN:HD22	1:A:148:ASN:C	2.10	0.55
1:A:228:ASN:OD1	1:A:258:VAL:HA	2.06	0.55
1:A:116:VAL:O	1:A:116:VAL:HG12	2.07	0.55
1:A:269:GLN:HB3	1:A:291:LEU:HD12	1.89	0.54
1:A:17:ARG:HE	1:A:29:VAL:HG11	1.73	0.54
1:A:158:SER:HB3	1:A:179:LYS:HD2	1.90	0.54
1:A:295:LYS:O	1:A:299:LYS:HB3	2.08	0.54
1:A:265:ASN:OD1	1:A:265:ASN:N	2.42	0.53
1:A:114:LEU:CD2	1:A:306:GLY:N	2.65	0.53
1:A:45:LYS:HB3	1:A:59:GLN:HB2	1.89	0.53
1:A:50:LEU:HD23	1:A:50:LEU:N	2.23	0.52
1:A:156:SER:OG	1:A:181:HIS:N	2.37	0.52
1:A:160:HIS:N	1:A:160:HIS:CD2	2.77	0.52
1:A:255:LYS:HG2	1:A:264:GLY:O	2.10	0.52
1:A:255:LYS:CG	1:A:264:GLY:O	2.58	0.52
1:A:165:TYR:HB3	1:A:172:VAL:CG1	2.40	0.52
1:A:253:GLY:O	1:A:266:GLU:CB	2.52	0.52
1:A:300:PHE:CD1	1:A:300:PHE:C	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:HD12	1:A:89:LEU:C	2.29	0.51
1:A:107:TRP:CG	1:A:115:GLY:HA2	2.45	0.51
1:A:126:LEU:HD12	1:A:126:LEU:O	2.09	0.51
1:A:169:GLY:HA3	1:A:202:TYR:CE1	2.45	0.51
1:A:193:TYR:C	1:A:193:TYR:CD1	2.84	0.51
1:A:114:LEU:CD2	1:A:306:GLY:CA	2.89	0.51
1:A:107:TRP:CH2	1:A:247:ARG:HG3	2.47	0.50
1:A:129:VAL:O	1:A:144:GLN:CB	2.57	0.50
1:A:286:VAL:HG23	1:A:307:VAL:HG12	1.93	0.50
1:A:23:ASN:N	1:A:298:ASN:HB3	2.26	0.49
1:A:28:GLU:O	1:A:28:GLU:HG2	2.11	0.49
1:A:37:ASP:OD1	1:A:40:SER:OG	2.30	0.49
1:A:230:GLN:HE21	1:A:231:THR:C	2.14	0.49
1:A:163:PHE:C	1:A:163:PHE:CD1	2.85	0.49
1:A:257:LEU:HD12	1:A:262:ASP:HA	1.93	0.49
1:A:44:PHE:CD1	1:A:44:PHE:N	2.80	0.49
1:A:98:LEU:CG	1:A:197:ARG:HD3	2.43	0.49
1:A:118:LYS:HB3	1:A:267:TYR:OH	2.12	0.49
1:A:205:ASP:O	1:A:206:ALA:HB3	2.12	0.49
1:A:230:GLN:NE2	1:A:231:THR:N	2.61	0.48
1:A:23:ASN:OD1	1:A:298:ASN:HB3	2.11	0.48
1:A:255:LYS:CB	1:A:264:GLY:O	2.62	0.48
1:A:20:PHE:HE1	1:A:300:PHE:CD2	2.27	0.48
1:A:20:PHE:CE1	1:A:300:PHE:CE2	3.01	0.48
1:A:216:GLN:O	1:A:229:SER:HB2	2.12	0.48
1:A:197:ARG:HG2	1:A:214:GLN:CG	2.13	0.48
1:A:98:LEU:CA	1:A:101:THR:HG23	2.44	0.47
1:A:182:HIS:ND1	1:A:183:GLN:N	2.62	0.47
1:A:61:GLU:HG2	1:A:76:ARG:HB2	1.95	0.47
1:A:79:PHE:CD1	1:A:90:ARG:HG2	2.49	0.47
1:A:155:ASN:HD22	1:A:155:ASN:N	2.11	0.47
1:A:113:TYR:O	1:A:289:GLY:HA3	2.14	0.47
1:A:156:SER:CB	1:A:180:ARG:HB2	2.45	0.47
1:A:107:TRP:CH2	1:A:247:ARG:CG	2.97	0.47
1:A:189:ASN:O	1:A:221:THR:OG1	2.32	0.47
1:A:257:LEU:HD11	1:A:262:ASP:OD2	2.15	0.47
1:A:252:HIS:HE1	1:A:266:GLU:HG3	1.80	0.47
1:A:300:PHE:CE1	1:A:302:ALA:HB2	2.50	0.47
1:A:182:HIS:O	1:A:189:ASN:HB2	2.14	0.47
1:A:105:ASN:OD1	1:A:116:VAL:C	2.53	0.47
1:A:20:PHE:CD1	1:A:300:PHE:CD2	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ASP:O	1:A:223:ALA:HB3	2.16	0.46
1:A:248:VAL:HG23	1:A:271:VAL:O	2.15	0.46
1:A:222:ASP:HB3	1:A:224:SER:H	1.81	0.46
1:A:278:PHE:CE2	1:A:284:ALA:HB2	2.47	0.46
1:A:136:PHE:C	1:A:136:PHE:CD1	2.88	0.45
1:A:26:VAL:CG1	1:A:26:VAL:O	2.64	0.45
1:A:101:THR:OG1	1:A:102:GLY:N	2.49	0.45
1:A:258:VAL:CG1	1:A:259:ASP:N	2.68	0.45
1:A:297:GLU:H	1:A:297:GLU:HG3	1.56	0.45
1:A:10:LYS:NZ	1:A:108:ASP:OD1	2.29	0.44
1:A:131:TYR:O	1:A:142:SER:HA	2.17	0.44
1:A:156:SER:OG	1:A:180:ARG:CB	2.58	0.44
1:A:6:TYR:CD2	1:A:45:LYS:HE2	2.52	0.44
1:A:20:PHE:HE1	1:A:300:PHE:CE2	2.35	0.44
1:A:50:LEU:HD11	1:A:56:ALA:HB2	1.98	0.44
1:A:89:LEU:HD13	1:A:130:ARG:O	2.18	0.44
1:A:222:ASP:O	1:A:223:ALA:CB	2.65	0.44
1:A:95:ASN:OD1	1:A:125:ARG:HD3	2.18	0.44
1:A:14:GLU:HG2	1:A:306:GLY:HA2	1.99	0.44
1:A:37:ASP:O	1:A:110:LYS:HG3	2.18	0.44
1:A:148:ASN:C	1:A:148:ASN:ND2	2.71	0.43
1:A:10:LYS:HD3	1:A:38:LEU:HB2	2.00	0.43
1:A:199:VAL:HA	1:A:212:ALA:HB2	2.00	0.43
1:A:247:ARG:NH2	1:A:275:GLU:OE2	2.48	0.43
1:A:80:ILE:HG23	1:A:80:ILE:O	2.19	0.42
1:A:158:SER:HA	1:A:178:TYR:O	2.19	0.42
1:A:183:GLN:NE2	1:A:184:VAL:C	2.73	0.42
1:A:30:THR:HG22	1:A:30:THR:O	2.19	0.42
1:A:6:TYR:HE1	1:A:61:GLU:OE1	2.01	0.42
1:A:154:HIS:N	1:A:154:HIS:ND1	2.67	0.42
1:A:9:ILE:HA	1:A:40:SER:HB3	2.01	0.42
1:A:57:ILE:HG21	1:A:83:LYS:HE2	2.02	0.42
1:A:230:GLN:HE21	1:A:231:THR:N	2.16	0.42
1:A:148:ASN:O	1:A:148:ASN:ND2	2.53	0.42
1:A:104:ILE:CG1	1:A:197:ARG:NH2	2.79	0.42
1:A:24:GLY:O	1:A:25:GLN:HG2	2.19	0.42
1:A:184:VAL:O	1:A:185:GLN:C	2.59	0.42
1:A:195:ILE:HG13	1:A:216:GLN:HG2	2.00	0.42
1:A:41:LYS:HG2	1:A:41:LYS:O	2.19	0.42
1:A:118:LYS:HB3	1:A:267:TYR:CE2	2.55	0.41
1:A:157:GLU:CD	1:A:180:ARG:HD3	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:VAL:O	1:A:259:ASP:C	2.59	0.41
1:A:270:VAL:O	1:A:270:VAL:HG13	2.20	0.41
1:A:89:LEU:CD1	1:A:130:ARG:O	2.68	0.41
1:A:65:SER:HB3	1:A:70:ASP:OD2	2.19	0.41
1:A:247:ARG:HG2	1:A:247:ARG:NH1	2.36	0.41
1:A:206:ALA:HB1	1:A:239:TYR:CZ	2.56	0.41
1:A:22:GLN:O	1:A:23:ASN:CB	2.64	0.41
1:A:144:GLN:HG2	1:A:160:HIS:HB2	2.02	0.40
1:A:182:HIS:HB3	1:A:190:ILE:HG13	2.04	0.40
1:A:211:VAL:HA	1:A:234:ALA:O	2.22	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	306/313 (98%)	289 (94%)	14 (5%)	3 (1%)	18 54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLY
1	A	207	LEU
1	A	258	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	244/246 (99%)	175 (72%)	69 (28%)	0 2

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	15	THR
1	A	20	PHE
1	A	26	VAL
1	A	28	GLU
1	A	33	THR
1	A	40	SER
1	A	41	LYS
1	A	44	PHE
1	A	45	LYS
1	A	50	LEU
1	A	52	ASN
1	A	59	GLN
1	A	63	LYS
1	A	69	THR
1	A	71	SER
1	A	75	ASN
1	A	77	GLN
1	A	78	SER
1	A	80	ILE
1	A	89	LEU
1	A	91	VAL
1	A	104	ILE
1	A	112	ASP
1	A	114	LEU
1	A	118	LYS
1	A	119	ILE
1	A	126	LEU
1	A	127	ILE
1	A	130	ARG
1	A	135	GLU
1	A	139	LEU
1	A	140	SER
1	A	147	LEU
1	A	148	ASN
1	A	149	ASP

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Mol	Chain	Res	Type
1	A	153	ARG
1	A	154	HIS
1	A	160	HIS
1	A	167	ASN
1	A	170	PHE
1	A	172	VAL
1	A	185	GLN
1	A	193	TYR
1	A	205	ASP
1	A	211	VAL
1	A	222	ASP
1	A	224	SER
1	A	225	ASN
1	A	226	SER
1	A	236	THR
1	A	237	LEU
1	A	240	ARG
1	A	247	ARG
1	A	257	LEU
1	A	259	ASP
1	A	260	ASP
1	A	262	ASP
1	A	263	ILE
1	A	265	ASN
1	A	266	GLU
1	A	268	ASP
1	A	279	SER
1	A	282	THR
1	A	283	SER
1	A	285	LEU
1	A	291	LEU
1	A	297	GLU
1	A	299	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	148	ASN
1	A	155	ASN
1	A	160	HIS
1	A	181	HIS

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Mol	Chain	Res	Type
1	A	225	ASN
1	A	230	GLN
1	A	252	HIS

### 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 [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, 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	309/313 (98%)	0.17	14 (4%) 34 33	32, 49, 97, 141	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	ASP	7.3
1	A	154	HIS	4.7
1	A	189	ASN	4.0
1	A	224	SER	3.5
1	A	223	ALA	3.1
1	A	149	ASP	3.1
1	A	221	THR	2.6
1	A	183	GLN	2.6
1	A	28	GLU	2.6
1	A	153	ARG	2.5
1	A	27	THR	2.5
1	A	155	ASN	2.4
1	A	261	ALA	2.2
1	A	190	ILE	2.2

### 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.