



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2014 – 03:04 PM GMT

PDB ID : 3NQ5  
Title : Crystal Structure of Tyrosinase from Bacillus megaterium R209H mutant  
Authors : Sendovski, M.; Kanteev, M.; Adir, N.; Fishman, A.  
Deposited on : 2010-06-29  
Resolution : 2.30 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>

---

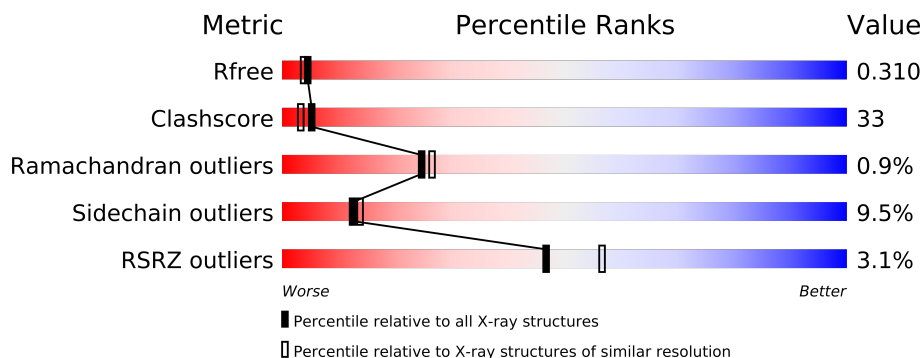
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : trunk22714  
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) : trunk22714

# 1 Overall quality at a glance



The reported resolution of this entry is 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	303	
1	B	303	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	ZN	A	506	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4909 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 Tyrosinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2336	1487	421	420	8			
1	B	282	Total	C	N	O	S	0	0	0
			2311	1474	415	414	8			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	209	HIS	ARG	ENGINEERED MUTATION	UNP B2ZB02
A	298	HIS	-	EXPRESSION TAG	UNP B2ZB02
A	299	HIS	-	EXPRESSION TAG	UNP B2ZB02
A	300	HIS	-	EXPRESSION TAG	UNP B2ZB02
A	301	HIS	-	EXPRESSION TAG	UNP B2ZB02
A	302	HIS	-	EXPRESSION TAG	UNP B2ZB02
A	303	HIS	-	EXPRESSION TAG	UNP B2ZB02
B	209	HIS	ARG	ENGINEERED MUTATION	UNP B2ZB02
B	298	HIS	-	EXPRESSION TAG	UNP B2ZB02
B	299	HIS	-	EXPRESSION TAG	UNP B2ZB02
B	300	HIS	-	EXPRESSION TAG	UNP B2ZB02
B	301	HIS	-	EXPRESSION TAG	UNP B2ZB02
B	302	HIS	-	EXPRESSION TAG	UNP B2ZB02
B	303	HIS	-	EXPRESSION TAG	UNP B2ZB02

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Cu	0	0
			2	2		
2	A	2	Total	Cu	0	0
			2	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total 4	Zn 4	0	0
3	A	6	Total 6	Zn 6	0	0

- Molecule 4 is water.

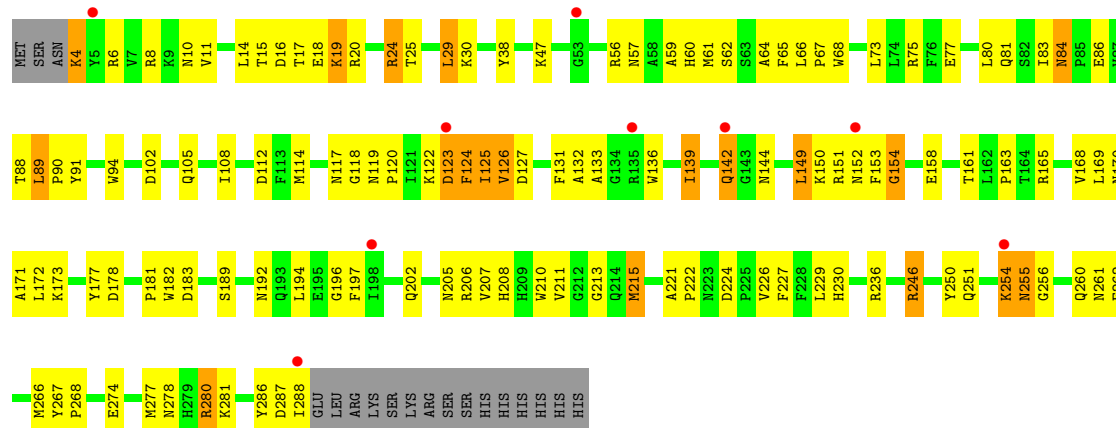
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	116	Total 116	O 116	0	0
4	B	132	Total 132	O 132	0	0

### 3 Residue-property plots

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.

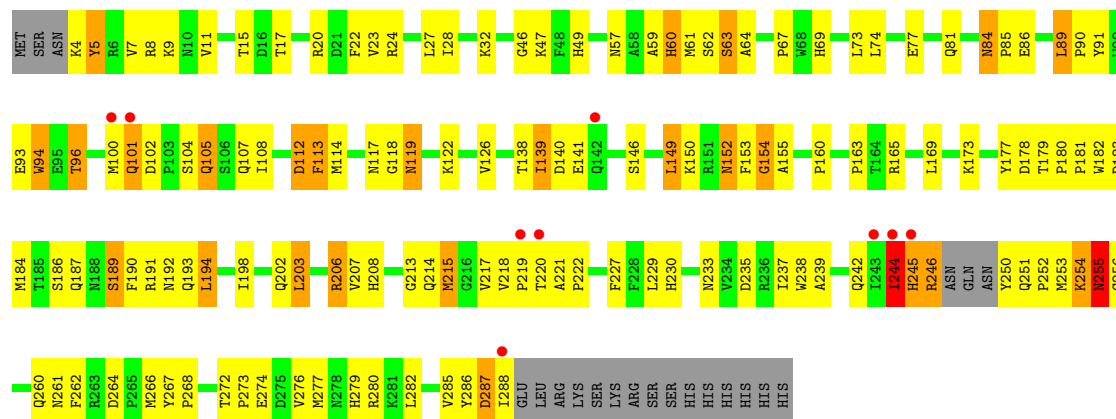
#### • Molecule 1: Tyrosinase

Chain A: 



#### • Molecule 1: Tyrosinase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.13Å 80.85Å 147.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.93 – 2.30 41.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	88.5 (41.93-2.30) 93.6 (41.93-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.217 , 0.304 0.236 , 0.310	Depositor DCC
$R_{free}$ test set	2517 reflections (10.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.9	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 25129 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	4909	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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: ZN, CU

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	0.55	0/2415	0.68	6/3292 (0.2%)
1	B	0.64	3/2389 (0.1%)	0.73	7/3255 (0.2%)
All	All	0.60	3/4804 (0.1%)	0.70	13/6547 (0.2%)

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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	5	TYR	CD2-CE2	-8.67	1.26	1.39
1	B	5	TYR	CD1-CE1	-7.59	1.27	1.39
1	B	5	TYR	CE2-CZ	-7.21	1.29	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	ILE	O-C-N	-14.80	99.02	122.70
1	A	123	ASP	CB-CA-C	-12.40	85.60	110.40
1	B	255	ASN	CB-CA-C	-10.22	89.95	110.40
1	A	255	ASN	CB-CA-C	-8.78	92.85	110.40
1	A	136	TRP	O-C-N	-8.45	109.18	122.70
1	A	124	PHE	N-CA-C	6.53	128.62	111.00
1	A	136	TRP	C-N-CA	6.48	137.90	121.70
1	B	139	ILE	C-N-CA	5.72	136.00	121.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	244	ILE	CB-CA-C	-5.65	100.30	111.60
1	A	136	TRP	CA-C-N	5.61	129.53	117.20
1	B	27	LEU	O-C-N	-5.50	113.90	122.70
1	B	60	HIS	O-C-N	5.47	131.46	122.70
1	B	139	ILE	CA-C-N	5.40	129.07	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	139	ILE	Mainchain

## 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	2336	0	2213	137	0
1	B	2311	0	2194	166	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	6	0	0	0	0
3	B	4	0	0	0	0
4	A	116	0	0	16	0
4	B	132	0	0	17	0
All	All	4909	0	4407	299	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 33.

All (299) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:218:VAL:HG22	4:B:393:HOH:O	1.39	1.22
1:A:246:ARG:CG	1:A:246:ARG:HH11	1.58	1.16
1:A:246:ARG:HH11	1:A:246:ARG:HG3	1.10	1.13
1:B:254:LYS:O	1:B:255:ASN:HB2	1.45	1.12

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:4:LYS:HG3	1:A:280:ARG:HG3	1.35	1.07
1:A:246:ARG:NH1	1:A:246:ARG:HB2	1.74	1.02
1:A:256:GLY:H	1:A:261:ASN:ND2	1.62	0.97
1:A:256:GLY:N	1:A:261:ASN:HD21	1.63	0.96
1:A:246:ARG:NH1	1:A:246:ARG:CB	2.30	0.94
1:B:150:LYS:O	1:B:213:GLY:HA3	1.67	0.94
1:A:246:ARG:HH11	1:A:246:ARG:CB	1.81	0.94
1:B:178:ASP:HA	1:B:189:SER:HB2	1.50	0.93
1:B:84:ASN:ND2	1:B:86:GLU:H	1.69	0.90
1:A:178:ASP:HA	1:A:189:SER:HB2	1.54	0.89
1:B:218:VAL:N	1:B:219:PRO:HD2	1.89	0.88
1:A:224:ASP:OD1	1:A:226:VAL:HG23	1.75	0.86
1:A:246:ARG:NH1	1:A:246:ARG:HG3	1.90	0.86
1:A:246:ARG:NH1	1:A:246:ARG:CG	2.30	0.83
1:B:187:GLN:CD	1:B:187:GLN:H	1.81	0.83
1:A:62:SER:HB3	4:A:387:HOH:O	1.77	0.81
1:B:193:GLN:HG2	1:B:198:ILE:HD13	1.62	0.81
1:B:217:VAL:C	1:B:219:PRO:HD2	2.01	0.80
1:B:217:VAL:CG2	1:B:220:THR:OG1	2.30	0.80
1:A:16:ASP:CG	4:A:400:HOH:O	2.21	0.79
1:A:94:TRP:HE1	1:A:230:HIS:HD2	1.31	0.78
1:B:208:HIS:CE1	1:B:215:MET:HE1	2.18	0.78
1:B:84:ASN:HD22	1:B:86:GLU:H	1.30	0.78
1:B:84:ASN:C	1:B:84:ASN:HD22	1.89	0.76
1:B:4:LYS:HE2	1:B:280:ARG:HE	1.50	0.76
1:B:254:LYS:HG3	1:B:255:ASN:N	2.00	0.76
1:B:217:VAL:HG23	1:B:220:THR:OG1	1.85	0.75
1:B:246:ARG:HG2	1:B:246:ARG:O	1.87	0.75
1:A:254:LYS:O	1:A:255:ASN:HB2	1.87	0.74
1:B:4:LYS:HG2	1:B:280:ARG:HE	1.53	0.74
1:B:4:LYS:HE2	1:B:280:ARG:NE	2.02	0.74
1:B:181:PRO:HG2	1:B:183:ASP:OD1	1.87	0.74
1:B:218:VAL:N	1:B:219:PRO:CD	2.50	0.73
1:A:8:ARG:HG3	1:A:89:LEU:O	1.86	0.73
1:B:184:MET:O	1:B:192:ASN:ND2	2.22	0.72
1:B:280:ARG:NH1	4:B:414:HOH:O	2.22	0.71
1:B:49:HIS:NE2	4:B:336:HOH:O	2.20	0.71
1:B:117:ASN:ND2	1:B:153:PHE:H	1.87	0.71
1:B:8:ARG:HG2	1:B:89:LEU:O	1.92	0.70
1:B:117:ASN:HD21	1:B:153:PHE:H	1.39	0.70
1:A:165:ARG:NH1	4:A:399:HOH:O	2.25	0.70
1:B:218:VAL:CG2	4:B:393:HOH:O	2.12	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:57:ASN:HD21	1:B:60:HIS:HD1	1.39	0.69
1:A:114:MET:HE2	1:A:131:PHE:HE1	1.57	0.69
1:A:208:HIS:CE1	1:A:215:MET:HE1	2.27	0.69
1:A:246:ARG:HH11	1:A:246:ARG:HB2	1.46	0.69
1:A:4:LYS:CG	1:A:280:ARG:HG3	2.19	0.69
1:A:133:ALA:HA	4:A:379:HOH:O	1.94	0.68
1:A:67:PRO:HG2	1:A:266:MET:HE1	1.75	0.68
1:B:165:ARG:O	1:B:169:LEU:HD13	1.93	0.68
1:B:208:HIS:HE1	1:B:215:MET:HE1	1.56	0.67
1:B:208:HIS:HD1	1:B:215:MET:HE2	1.58	0.66
1:A:254:LYS:O	1:A:255:ASN:CB	2.42	0.66
4:A:416:HOH:O	1:B:47:LYS:NZ	2.29	0.66
1:B:122:LYS:HE2	4:B:361:HOH:O	1.96	0.66
1:B:102:ASP:HB3	1:B:105:GLN:OE1	1.95	0.65
1:B:215:MET:HE3	1:B:221:ALA:HB1	1.76	0.65
1:A:126:VAL:CG1	1:A:149:LEU:HB3	2.26	0.65
1:B:256:GLY:H	1:B:261:ASN:HD21	1.42	0.65
1:B:245:HIS:CD2	1:B:245:HIS:N	2.63	0.65
1:B:20:ARG:O	1:B:24:ARG:HB2	1.97	0.65
1:B:61:MET:CE	1:B:184:MET:SD	2.85	0.64
1:A:94:TRP:CE3	1:A:163:PRO:HG2	2.31	0.64
1:A:117:ASN:HB2	1:A:153:PHE:CE2	2.33	0.64
1:A:30:LYS:NZ	4:A:315:HOH:O	2.30	0.63
1:B:100:MET:SD	4:B:320:HOH:O	2.56	0.63
1:B:254:LYS:O	1:B:255:ASN:CB	2.29	0.63
1:A:256:GLY:H	1:A:261:ASN:HD21	0.80	0.63
1:B:215:MET:CE	1:B:221:ALA:HB1	2.28	0.63
1:B:221:ALA:HB3	1:B:222:PRO:HD3	1.80	0.63
1:A:221:ALA:HB3	1:A:222:PRO:HD3	1.79	0.63
1:A:8:ARG:CG	1:A:89:LEU:O	2.46	0.62
1:B:126:VAL:CG1	1:B:149:LEU:HB3	2.30	0.62
1:A:59:ALA:O	1:A:65:PHE:HA	1.98	0.62
1:B:94:TRP:HE1	1:B:230:HIS:HD2	1.46	0.62
1:B:253:MET:O	1:B:261:ASN:HB3	2.00	0.61
1:A:94:TRP:NE1	1:A:230:HIS:HD2	1.96	0.61
1:A:150:LYS:O	1:A:213:GLY:HA3	2.00	0.61
1:B:122:LYS:CE	4:B:361:HOH:O	2.49	0.60
1:B:119:ASN:HD22	1:B:119:ASN:C	2.04	0.60
1:B:287:ASP:O	1:B:288:ILE:HB	2.01	0.60
1:B:187:GLN:CD	1:B:187:GLN:N	2.55	0.59
1:A:173:LYS:NZ	1:A:173:LYS:HB3	2.17	0.59
1:B:208:HIS:CE1	1:B:215:MET:CE	2.86	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:61:MET:HE1	1:B:184:MET:SD	2.43	0.59
1:A:215:MET:HE1	1:A:227:PHE:HD2	1.67	0.59
1:B:214:GLN:HB3	1:B:220:THR:O	2.03	0.59
1:A:280:ARG:NH2	4:A:326:HOH:O	2.36	0.59
1:A:205:ASN:HA	4:A:344:HOH:O	2.02	0.58
1:B:122:LYS:NZ	4:B:361:HOH:O	2.27	0.58
1:B:24:ARG:O	1:B:28:ILE:HD13	2.03	0.58
1:A:84:ASN:HD22	1:A:86:GLU:H	1.51	0.58
1:B:233:ASN:O	1:B:237:ILE:HG12	2.03	0.58
1:B:108:ILE:HD11	1:B:229:LEU:HD23	1.85	0.58
1:A:6:ARG:HD3	1:A:81:GLN:OE1	2.03	0.58
1:B:61:MET:HE2	1:B:184:MET:SD	2.44	0.57
1:B:84:ASN:HD21	1:B:86:GLU:HB2	1.69	0.57
1:A:215:MET:CE	1:A:227:PHE:HD2	2.17	0.56
1:A:14:LEU:HD22	1:A:18:GLU:HB3	1.86	0.56
1:A:4:LYS:HG3	1:A:280:ARG:CG	2.23	0.56
1:A:105:GLN:NE2	4:A:419:HOH:O	2.38	0.56
1:A:181:PRO:HG2	1:A:183:ASP:OD2	2.05	0.56
1:B:117:ASN:HB2	1:B:153:PHE:CD2	2.41	0.56
1:B:126:VAL:HG11	1:B:149:LEU:HD13	1.88	0.55
1:A:47:LYS:NZ	1:B:47:LYS:NZ	2.54	0.55
1:A:67:PRO:HG2	1:A:266:MET:CE	2.36	0.55
1:B:94:TRP:CE3	1:B:163:PRO:HG2	2.41	0.55
1:A:236:ARG:HG3	1:A:286:TYR:CG	2.41	0.55
1:A:208:HIS:HE1	1:A:215:MET:HE1	1.72	0.55
1:B:62:SER:O	1:B:191:ARG:HD3	2.06	0.55
1:A:208:HIS:CE1	1:A:215:MET:CE	2.90	0.55
1:A:215:MET:HE3	1:A:221:ALA:HB1	1.89	0.55
1:A:25:THR:HG23	1:A:83:ILE:HG21	1.88	0.55
1:B:244:ILE:HB	1:B:245:HIS:HD2	1.71	0.55
1:A:246:ARG:CZ	1:A:246:ARG:CB	2.85	0.54
1:B:63:SER:HA	1:B:191:ARG:HG3	1.89	0.54
1:A:196:GLY:HA3	1:A:202:GLN:O	2.06	0.54
1:B:279:HIS:O	1:B:282:LEU:HB2	2.07	0.54
1:B:262:PHE:CE2	1:B:274:GLU:HB2	2.43	0.54
1:B:215:MET:CE	1:B:227:PHE:HD2	2.20	0.54
1:B:4:LYS:HA	1:B:285:VAL:HG13	1.89	0.54
1:A:123:ASP:O	1:A:124:PHE:HB2	2.06	0.54
1:A:125:ILE:HD12	1:A:150:LYS:HE3	1.89	0.54
1:B:46:GLY:HA2	1:B:57:ASN:ND2	2.22	0.54
1:A:47:LYS:HZ1	1:B:47:LYS:NZ	2.06	0.53
1:B:202:GLN:O	1:B:203:LEU:C	2.47	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:250:TYR:HB2	1:B:277:MET:CE	2.38	0.53
1:B:74:LEU:CD2	1:B:282:LEU:HD22	2.38	0.53
1:B:217:VAL:HG21	1:B:220:THR:OG1	2.07	0.53
1:B:254:LYS:HG3	1:B:255:ASN:H	1.73	0.53
1:B:215:MET:HE1	1:B:227:PHE:CD2	2.44	0.53
1:B:94:TRP:CE2	1:B:207:VAL:HG21	2.43	0.53
1:A:117:ASN:HD22	1:A:151:ARG:HB3	1.72	0.53
1:B:235:ASP:HB3	1:B:286:TYR:OH	2.09	0.53
1:B:152:ASN:ND2	1:B:155:ALA:HB2	2.24	0.52
1:A:192:ASN:OD1	1:A:197:PHE:HB2	2.09	0.52
1:A:117:ASN:ND2	1:A:118:GLY:H	2.08	0.52
1:B:287:ASP:O	1:B:288:ILE:CB	2.57	0.52
1:A:182:TRP:CZ3	1:A:251:GLN:HB3	2.44	0.52
1:A:142:GLN:NE2	1:A:144:ASN:HD22	2.07	0.52
1:A:15:THR:O	1:A:19:LYS:HG2	2.08	0.52
1:A:84:ASN:ND2	1:A:86:GLU:H	2.08	0.52
1:B:254:LYS:HE2	4:B:387:HOH:O	2.09	0.52
1:B:117:ASN:HB2	1:B:153:PHE:CE2	2.45	0.52
1:A:25:THR:HG23	1:A:83:ILE:CG2	2.40	0.51
1:A:171:ALA:O	1:A:173:LYS:N	2.44	0.51
1:B:217:VAL:HB	1:B:219:PRO:HD2	1.92	0.51
1:A:168:VAL:HG12	1:A:172:LEU:HD12	1.93	0.51
1:A:125:ILE:CD1	1:A:150:LYS:HE3	2.40	0.51
1:B:169:LEU:O	1:B:173:LYS:HG3	2.11	0.51
1:A:47:LYS:HZ1	1:B:47:LYS:HZ1	1.59	0.51
1:B:245:HIS:CD2	1:B:245:HIS:H	2.29	0.51
1:B:208:HIS:ND1	1:B:215:MET:HE2	2.26	0.50
1:B:264:ASP:O	1:B:272:THR:HG22	2.12	0.50
1:B:126:VAL:HG12	1:B:149:LEU:O	2.12	0.50
1:A:56:ARG:HD3	1:A:62:SER:OG	2.11	0.50
1:B:202:GLN:HB2	4:B:314:HOH:O	2.10	0.50
1:B:8:ARG:CG	1:B:89:LEU:O	2.59	0.50
1:B:244:ILE:HD12	1:B:245:HIS:CD2	2.47	0.50
1:B:245:HIS:HD2	1:B:245:HIS:N	2.08	0.50
1:B:84:ASN:HD22	1:B:85:PRO:N	2.09	0.50
1:A:29:LEU:HD22	1:A:80:LEU:HD23	1.94	0.50
1:A:250:TYR:HB2	1:A:277:MET:HE1	1.93	0.49
1:A:168:VAL:HG12	1:A:172:LEU:CD1	2.43	0.49
1:B:215:MET:HE1	1:B:227:PHE:HD2	1.78	0.49
1:A:73:LEU:HD13	1:A:89:LEU:CD1	2.41	0.49
1:B:114:MET:O	4:B:403:HOH:O	2.20	0.49
1:A:57:ASN:O	4:A:387:HOH:O	2.20	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:94:TRP:NE1	1:A:230:HIS:CD2	2.80	0.49
1:B:163:PRO:HB3	4:B:319:HOH:O	2.12	0.49
1:B:94:TRP:HE1	1:B:230:HIS:CD2	2.29	0.49
1:B:242:GLN:O	1:B:246:ARG:HB2	2.13	0.49
1:B:96:THR:HG22	1:B:165:ARG:HH21	1.78	0.49
1:B:276:VAL:HB	1:B:282:LEU:HD11	1.95	0.49
1:A:66:LEU:HB2	1:A:177:TYR:OH	2.13	0.49
1:B:112:ASP:CG	1:B:112:ASP:O	2.51	0.49
1:B:250:TYR:HB2	1:B:277:MET:HE1	1.94	0.48
1:B:94:TRP:CD2	1:B:207:VAL:HG21	2.48	0.48
1:B:74:LEU:HD22	1:B:282:LEU:HD22	1.96	0.48
1:A:88:THR:O	1:A:90:PRO:HD3	2.13	0.48
1:A:47:LYS:NZ	1:B:47:LYS:HZ1	2.10	0.48
1:A:84:ASN:HD22	1:A:84:ASN:C	2.17	0.48
1:A:256:GLY:O	1:A:261:ASN:OD1	2.32	0.48
1:B:153:PHE:O	1:B:154:GLY:C	2.51	0.48
1:A:208:HIS:HD1	1:A:215:MET:HE2	1.79	0.48
1:A:280:ARG:CZ	4:A:326:HOH:O	2.60	0.48
1:A:161:THR:CG2	1:A:206:ARG:NH1	2.76	0.48
1:A:67:PRO:CG	1:A:266:MET:HE1	2.43	0.47
1:B:59:ALA:O	1:B:69:HIS:HE1	1.96	0.47
1:A:108:ILE:HD11	1:A:229:LEU:HD23	1.95	0.47
1:B:178:ASP:OD1	1:B:179:THR:N	2.46	0.47
1:A:8:ARG:HH11	1:A:77:GLU:CD	2.17	0.47
1:B:64:ALA:H	1:B:260:GLN:HE22	1.62	0.47
1:B:4:LYS:CE	1:B:280:ARG:HH21	2.27	0.47
1:B:22:PHE:CE1	1:B:90:PRO:CD	2.98	0.47
1:A:73:LEU:HD13	1:A:89:LEU:HD11	1.96	0.47
1:B:187:GLN:OE1	1:B:187:GLN:N	2.34	0.47
1:B:4:LYS:HE3	1:B:280:ARG:HH21	1.79	0.47
1:B:28:ILE:HD12	1:B:28:ILE:N	2.30	0.47
1:A:64:ALA:H	1:A:260:GLN:HE22	1.62	0.47
1:B:119:ASN:ND2	1:B:119:ASN:C	2.69	0.46
1:A:154:GLY:HA2	4:A:341:HOH:O	2.15	0.46
1:A:215:MET:HE1	1:A:227:PHE:CD2	2.50	0.46
1:B:246:ARG:CG	1:B:246:ARG:O	2.62	0.46
1:B:179:THR:OG1	1:B:187:GLN:O	2.33	0.46
1:B:261:ASN:O	1:B:273:PRO:HG2	2.16	0.46
1:A:125:ILE:HG13	1:A:150:LYS:HG3	1.97	0.46
1:A:102:ASP:HB3	1:A:105:GLN:OE1	2.15	0.46
1:A:142:GLN:HE21	1:A:142:GLN:HB2	1.56	0.46
1:B:9:LYS:HD3	4:B:404:HOH:O	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:64:ALA:H	1:B:260:GLN:NE2	2.13	0.46
1:A:215:MET:CE	1:A:221:ALA:HB1	2.46	0.45
1:A:171:ALA:C	1:A:173:LYS:H	2.18	0.45
1:A:61:MET:O	1:A:183:ASP:HA	2.17	0.45
1:B:160:PRO:HD2	1:B:206:ARG:HH12	1.81	0.45
1:B:104:SER:HB2	1:B:153:PHE:CD2	2.51	0.45
1:A:10:ASN:N	1:A:91:TYR:CE2	2.84	0.45
1:A:126:VAL:HG22	1:A:132:ALA:HA	1.99	0.45
1:B:107:GLN:HG3	4:B:313:HOH:O	2.16	0.45
1:B:67:PRO:HG2	1:B:266:MET:HE1	1.98	0.45
1:B:101:GLN:NE2	4:B:376:HOH:O	2.47	0.45
1:A:267:TYR:CG	1:A:268:PRO:HA	2.51	0.45
1:B:4:LYS:HE2	1:B:280:ARG:CZ	2.46	0.45
1:A:173:LYS:HZ2	1:A:173:LYS:CB	2.30	0.45
1:B:104:SER:HB2	1:B:153:PHE:HD2	1.82	0.45
1:A:161:THR:HG22	1:A:206:ARG:NH1	2.32	0.45
1:A:287:ASP:OD1	1:A:288:ILE:N	2.49	0.45
1:A:171:ALA:C	1:A:173:LYS:N	2.70	0.44
1:B:28:ILE:O	1:B:32:LYS:HG3	2.17	0.44
1:B:190:PHE:CZ	1:B:194:LEU:HD12	2.53	0.43
1:A:170:ASN:ND2	4:A:408:HOH:O	2.43	0.43
1:B:11:VAL:HG11	1:B:108:ILE:CD1	2.48	0.43
1:B:63:SER:HB3	1:B:177:TYR:HE2	1.83	0.43
1:B:74:LEU:HD22	1:B:282:LEU:HD13	2.00	0.43
1:A:8:ARG:HD2	1:A:77:GLU:OE2	2.19	0.43
1:B:215:MET:HA	1:B:215:MET:CE	2.47	0.43
1:A:173:LYS:NZ	1:A:173:LYS:CB	2.80	0.43
1:A:139:ILE:HG21	1:A:139:ILE:HD13	1.68	0.43
1:A:20:ARG:O	1:A:24:ARG:HB2	2.18	0.43
1:B:252:PRO:HG3	1:B:256:GLY:HA3	2.00	0.43
1:A:142:GLN:HE21	1:A:144:ASN:HD22	1.66	0.43
1:B:208:HIS:ND1	1:B:215:MET:CE	2.82	0.43
1:A:38:TYR:OH	1:A:75:ARG:C	2.57	0.43
1:A:11:VAL:HG23	1:A:91:TYR:O	2.18	0.43
1:A:112:ASP:OD1	1:A:112:ASP:C	2.55	0.43
1:A:262:PHE:CE2	1:A:274:GLU:HB2	2.54	0.43
1:B:239:ALA:O	1:B:242:GLN:HB2	2.20	0.42
1:A:67:PRO:CB	1:A:266:MET:HE1	2.49	0.42
1:A:181:PRO:C	1:A:182:TRP:CD1	2.93	0.42
1:B:8:ARG:NH1	1:B:77:GLU:OE1	2.53	0.42
1:A:207:VAL:O	1:A:211:VAL:HG23	2.20	0.42
1:B:96:THR:CG2	1:B:165:ARG:HH21	2.32	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:242:GLN:O	1:B:246:ARG:CB	2.68	0.42
1:A:89:LEU:HD22	1:A:90:PRO:O	2.20	0.42
1:B:11:VAL:HG11	1:B:108:ILE:HD12	2.00	0.42
1:B:267:TYR:CG	1:B:268:PRO:HA	2.55	0.42
1:A:119:ASN:HA	1:A:120:PRO:HD2	1.78	0.42
1:B:190:PHE:HE2	1:B:238:TRP:CD1	2.37	0.42
1:B:93:GLU:HG2	1:B:96:THR:HG23	2.01	0.42
1:B:100:MET:HG2	4:B:400:HOH:O	2.19	0.42
1:A:29:LEU:HD22	1:A:80:LEU:CD2	2.49	0.42
1:B:23:VAL:HG21	1:B:113:PHE:HA	2.02	0.42
1:A:170:ASN:O	1:A:173:LYS:HB3	2.19	0.42
1:A:81:GLN:NE2	4:A:348:HOH:O	2.53	0.42
1:A:10:ASN:OD1	1:A:11:VAL:N	2.53	0.42
1:A:64:ALA:O	1:A:68:TRP:HB2	2.19	0.42
1:A:117:ASN:ND2	1:A:118:GLY:N	2.67	0.41
1:A:281:LYS:O	1:A:281:LYS:HD2	2.20	0.41
1:B:138:THR:OG1	1:B:146:SER:OG	2.35	0.41
1:B:182:TRP:CZ3	1:B:251:GLN:HB3	2.55	0.41
1:B:4:LYS:HG2	1:B:280:ARG:NE	2.27	0.41
1:A:117:ASN:HB2	1:A:153:PHE:CD2	2.55	0.41
1:A:165:ARG:HG3	4:A:381:HOH:O	2.20	0.41
1:B:9:LYS:O	1:B:91:TYR:CD2	2.73	0.41
1:B:9:LYS:CD	4:B:404:HOH:O	2.68	0.41
1:B:267:TYR:CD1	1:B:268:PRO:HA	2.56	0.41
1:B:149:LEU:HD23	1:B:150:LYS:N	2.36	0.41
1:B:11:VAL:HG21	1:B:108:ILE:HD13	2.03	0.41
1:A:67:PRO:HB2	1:A:266:MET:HE1	2.03	0.41
1:B:15:THR:OG1	1:B:17:THR:HG22	2.21	0.41
1:A:127:ASP:HA	1:A:132:ALA:HB1	2.03	0.41
1:B:64:ALA:HA	1:B:67:PRO:HG2	2.03	0.41
1:A:57:ASN:HD21	1:A:60:HIS:HB2	1.86	0.41
1:B:238:TRP:O	1:B:239:ALA:C	2.60	0.41
1:B:272:THR:O	1:B:273:PRO:C	2.59	0.41
1:A:154:GLY:N	1:A:210:TRP:O	2.49	0.41
1:B:180:PRO:HA	1:B:182:TRP:N	2.36	0.41
1:A:158:GLU:OE1	4:A:360:HOH:O	2.22	0.41
1:B:73:LEU:HD22	1:B:89:LEU:HD11	2.02	0.40
1:A:182:TRP:CH2	1:A:251:GLN:HB3	2.56	0.40
1:B:117:ASN:ND2	1:B:118:GLY:H	2.19	0.40
1:A:250:TYR:HB2	1:A:277:MET:CE	2.50	0.40
1:A:288:ILE:HG13	1:A:288:ILE:O	2.21	0.40
1:B:150:LYS:O	1:B:213:GLY:CA	2.54	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:256:GLY:N	1:B:261:ASN:HD21	2.16	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	283/303 (93%)	267 (94%)	15 (5%)	1 (0%)	43	52
1	B	278/303 (92%)	256 (92%)	18 (6%)	4 (1%)	16	15
All	All	561/606 (93%)	523 (93%)	33 (6%)	5 (1%)	25	26

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	140	ASP
1	B	154	GLY
1	B	203	LEU
1	B	113	PHE
1	A	154	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	248/266 (93%)	227 (92%)	21 (8%)	15	18
1	B	245/266 (92%)	219 (89%)	26 (11%)	10	10
All	All	493/532 (93%)	446 (90%)	47 (10%)	12	14



All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	17	THR
1	A	19	LYS
1	A	24	ARG
1	A	29	LEU
1	A	84	ASN
1	A	89	LEU
1	A	122	LYS
1	A	125	ILE
1	A	126	VAL
1	A	139	ILE
1	A	142	GLN
1	A	149	LEU
1	A	152	ASN
1	A	169	LEU
1	A	194	LEU
1	A	215	MET
1	A	246	ARG
1	A	254	LYS
1	A	278	ASN
1	A	280	ARG
1	B	5	TYR
1	B	7	VAL
1	B	63	SER
1	B	81	GLN
1	B	84	ASN
1	B	89	LEU
1	B	94	TRP
1	B	96	THR
1	B	101	GLN
1	B	105	GLN
1	B	112	ASP
1	B	119	ASN
1	B	141	GLU
1	B	149	LEU
1	B	152	ASN
1	B	186	SER
1	B	189	SER
1	B	194	LEU
1	B	206	ARG
1	B	215	MET
1	B	244	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	245	HIS
1	B	246	ARG
1	B	254	LYS
1	B	255	ASN
1	B	287	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	84	ASN
1	A	117	ASN
1	A	142	GLN
1	A	152	ASN
1	A	202	GLN
1	A	205	ASN
1	A	209	HIS
1	A	230	HIS
1	A	260	GLN
1	A	261	ASN
1	A	270	ASN
1	B	57	ASN
1	B	84	ASN
1	B	101	GLN
1	B	117	ASN
1	B	119	ASN
1	B	152	ASN
1	B	205	ASN
1	B	230	HIS
1	B	245	HIS
1	B	260	GLN
1	B	261	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 ⓘ

Of 14 ligands modelled in this entry, 14 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.

## 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	285/303 (94%)	0.23	9 (3%) 45 55	12, 26, 43, 71	0
1	B	282/303 (93%)	0.16	9 (3%) 45 55	11, 23, 44, 86	0
All	All	567/606 (93%)	0.19	18 (3%) 47 55	11, 24, 44, 86	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	244	ILE	5.8
1	A	152	ASN	5.5
1	A	288	ILE	3.3
1	B	288	ILE	2.8
1	A	135	ARG	2.7
1	B	220	THR	2.6
1	A	53	GLY	2.6
1	A	5	TYR	2.5
1	B	100	MET	2.5
1	A	198	ILE	2.4
1	B	243	ILE	2.3
1	B	142	GLN	2.3
1	B	101	GLN	2.3
1	A	123	ASP	2.2
1	B	219	PRO	2.2
1	A	142	GLN	2.2
1	B	245	HIS	2.1
1	A	254	LYS	2.1

### 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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	A	506	1/1	0.22	6.68	82,82,82,82	0
2	CU	B	502	1/1	0.13	0.39	24,24,24,24	0
2	CU	B	501	1/1	0.12	-0.62	28,28,28,28	0
3	ZN	B	506	1/1	0.05	-0.99	36,36,36,36	0
3	ZN	B	503	1/1	0.09	-1.37	23,23,23,23	0
3	ZN	A	503	1/1	0.07	-1.40	28,28,28,28	0
2	CU	A	501	1/1	0.10	-1.42	31,31,31,31	0
3	ZN	A	505	1/1	0.06	-1.51	59,59,59,59	1
2	CU	A	502	1/1	0.10	-1.55	22,22,22,22	0
3	ZN	B	505	1/1	0.07	-1.65	54,54,54,54	0
3	ZN	B	504	1/1	0.10	-2.06	61,61,61,61	0
3	ZN	A	508	1/1	0.04	-2.35	47,47,47,47	0
3	ZN	A	507	1/1	0.09	-2.41	46,46,46,46	1
3	ZN	A	504	1/1	0.04	-3.47	50,50,50,50	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.