



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:09 PM GMT

PDB ID : 4HD6  
Title : Crystal Structure of Tyrosinase from *Bacillus megaterium* V218F mutant soaked in CuSO<sub>4</sub>  
Authors : Goldfeder, M.; Kanteev, M.; Adir, N.; Fishman, A.  
Deposited on : 2012-10-02  
Resolution : 2.00 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

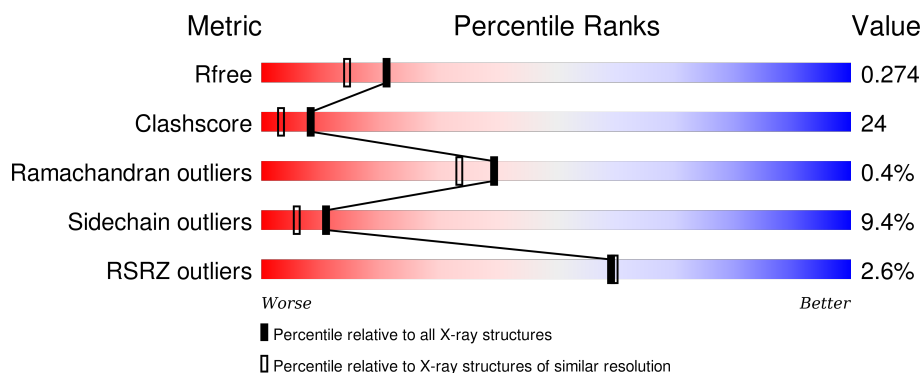
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	303	<div> <div> <div></div> <div>63%</div> <div>28%</div> <div>5%</div> </div> </div>
1	B	303	<div> <div> <div>4%</div> <div>60%</div> <div>27%</div> <div>7%</div> <div>6%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CU	A	402	-	-	-	X
2	CU	B	402	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4966 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 Tyrosinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2358	1502	424	424	8			
1	B	286	Total	C	N	O	S	0	0	0
			2350	1496	423	423	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	SER	ENGINEERED MUTATION	UNP B2ZB02
A	218	PHE	VAL	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	2	GLY	SER	ENGINEERED MUTATION	UNP B2ZB02
B	218	PHE	VAL	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		

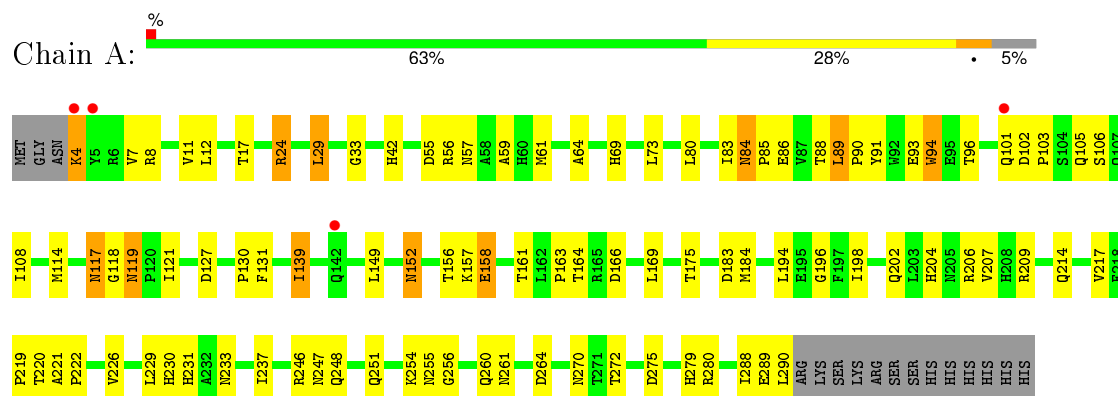
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total 128	O 128	0	0
3	B	126	Total 126	O 126	0	0

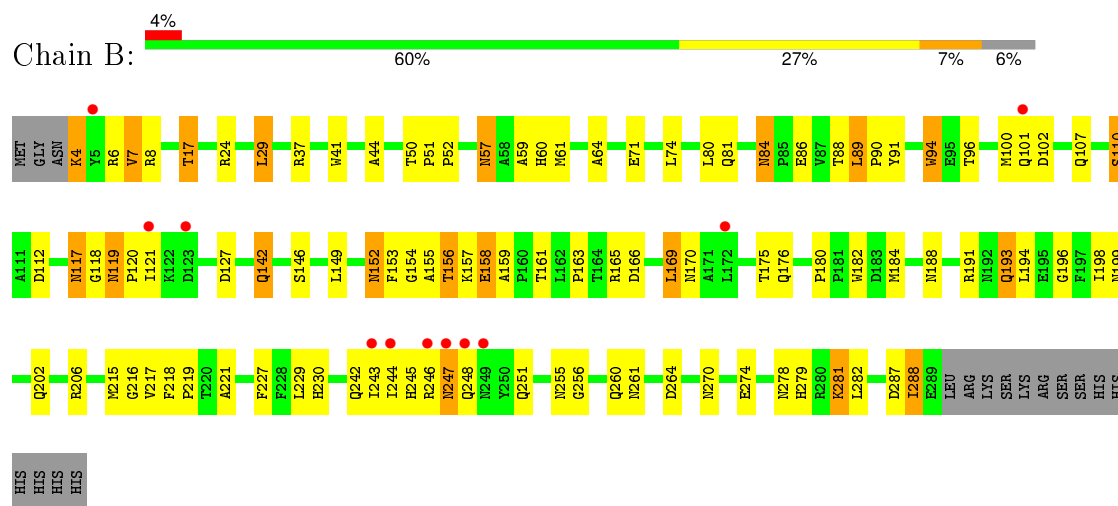
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Tyrosinase



#### • Molecule 1: Tyrosinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.18 Å   78.91 Å   85.81 Å 90.00°   106.13°   90.00°	Depositor
Resolution (Å)	41.22 – 2.00 41.22 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.2 (41.22-2.00) 97.1 (41.22-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.53 (at 2.00 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.245 , 0.277 0.243 , 0.274	Depositor DCC
$R_{free}$ test set	4080 reflections (11.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.3	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.0	EDS
Estimated twinning fraction	0.049 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 40605 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4966	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.45	0/2437	0.63	0/3320
1	B	0.44	0/2429	0.59	0/3309
All	All	0.44	0/4866	0.61	0/6629

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2358	0	2238	107	0
1	B	2350	0	2227	116	3
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	128	0	0	41	3
3	B	126	0	0	33	0
All	All	4966	0	4465	222	3

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 24.

All (222) 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:B:176:GLN:HA	3:B:615:HOH:O	1.27	1.26
1:B:61:MET:SD	3:B:600:HOH:O	1.97	1.19
1:A:101:GLN:CA	3:A:590:HOH:O	1.91	1.16
1:B:96:THR:HG22	1:B:165:ARG:NH2	1.59	1.15
1:A:61:MET:SD	3:A:576:HOH:O	2.02	1.15
1:B:274:GLU:HB3	3:B:571:HOH:O	1.43	1.15
1:A:247:ASN:HB2	3:A:602:HOH:O	1.48	1.11
1:B:206:ARG:NH1	3:B:601:HOH:O	1.83	1.10
1:A:102:ASP:N	3:A:590:HOH:O	1.82	1.08
1:A:101:GLN:HB3	3:A:590:HOH:O	1.55	1.06
1:B:146:SER:O	3:B:521:HOH:O	1.76	1.04
1:B:245:HIS:HB3	1:B:248:GLN:HB2	1.38	0.99
1:B:158:GLU:H	1:B:158:GLU:CD	1.67	0.98
1:B:94:TRP:HE1	1:B:230:HIS:HD2	1.11	0.97
1:B:170:ASN:ND2	3:B:533:HOH:O	1.95	0.97
1:A:183:ASP:HB3	3:A:595:HOH:O	1.64	0.97
1:A:101:GLN:N	3:A:590:HOH:O	1.91	0.96
1:B:157:LYS:HB3	1:B:158:GLU:OE2	1.65	0.96
1:B:193:GLN:HG2	1:B:198:ILE:HG13	1.45	0.96
1:A:219:PRO:O	1:A:220:THR:HG23	1.66	0.94
1:B:270:ASN:ND2	3:B:543:HOH:O	2.03	0.90
1:A:24:ARG:HG3	3:A:599:HOH:O	1.73	0.89
1:B:156:THR:HG22	1:B:159:ALA:H	1.37	0.89
1:B:102:ASP:OD2	3:B:609:HOH:O	1.92	0.88
1:B:96:THR:CG2	1:B:165:ARG:NH2	2.36	0.88
1:A:217:VAL:HG12	1:A:219:PRO:HD2	1.54	0.87
1:B:142:GLN:HA	1:B:142:GLN:OE1	1.75	0.87
1:A:275:ASP:OD1	3:A:569:HOH:O	1.92	0.86
1:B:17:THR:HG22	3:B:587:HOH:O	1.76	0.85
1:A:94:TRP:HE1	1:A:230:HIS:HD2	1.20	0.85
1:A:12:LEU:O	3:A:592:HOH:O	1.93	0.85
1:A:254:LYS:NZ	3:A:603:HOH:O	2.09	0.85
1:A:256:GLY:H	1:A:261:ASN:HD21	1.22	0.85
1:A:56:ARG:CZ	3:A:595:HOH:O	2.24	0.84
1:A:214:GLN:HB3	1:A:220:THR:O	1.77	0.84
1:B:251:GLN:OE1	3:B:528:HOH:O	1.93	0.84
1:A:102:ASP:OD2	3:A:607:HOH:O	1.96	0.83
1:B:96:THR:HG22	1:B:165:ARG:CZ	2.08	0.83
1:A:8:ARG:HG2	1:A:89:LEU:O	1.78	0.82
1:A:169:LEU:HD22	3:A:608:HOH:O	1.78	0.82
1:A:56:ARG:NE	3:A:595:HOH:O	2.11	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:TRP:NE1	1:A:230:HIS:HD2	1.77	0.81
1:B:255:ASN:ND2	3:B:605:HOH:O	2.14	0.81
1:B:215:MET:HE2	1:B:221:ALA:HB1	1.61	0.81
1:A:254:LYS:CE	3:A:603:HOH:O	2.30	0.79
1:A:270:ASN:ND2	3:A:543:HOH:O	2.15	0.79
1:B:256:GLY:H	1:B:261:ASN:HD21	1.31	0.79
1:A:101:GLN:CB	3:A:590:HOH:O	2.05	0.76
1:B:64:ALA:H	1:B:260:GLN:NE2	1.84	0.75
1:A:219:PRO:O	1:A:220:THR:CG2	2.34	0.75
1:B:100:MET:SD	3:B:604:HOH:O	2.45	0.75
1:A:64:ALA:H	1:A:260:GLN:HE22	1.32	0.75
1:B:64:ALA:H	1:B:260:GLN:HE22	1.35	0.74
1:B:119:ASN:HD22	1:B:121:ILE:H	1.33	0.74
1:B:158:GLU:CD	1:B:158:GLU:N	2.39	0.74
1:B:94:TRP:HE1	1:B:230:HIS:CD2	2.00	0.74
1:A:219:PRO:C	1:A:220:THR:HG23	2.06	0.73
1:A:152:ASN:ND2	3:A:555:HOH:O	2.20	0.73
1:B:215:MET:HE1	1:B:227:PHE:HD2	1.52	0.73
1:B:242:GLN:O	1:B:246:ARG:HA	1.89	0.73
1:A:94:TRP:HE1	1:A:230:HIS:CD2	2.06	0.72
1:A:117:ASN:HD22	1:A:118:GLY:H	1.36	0.72
1:B:94:TRP:NE1	1:B:230:HIS:HD2	1.87	0.72
1:B:155:ALA:N	3:B:547:HOH:O	2.22	0.71
1:B:274:GLU:OE1	3:B:531:HOH:O	2.10	0.70
1:B:71:GLU:OE2	3:B:573:HOH:O	2.08	0.70
1:B:215:MET:HE1	1:B:227:PHE:CD2	2.26	0.69
1:B:288:ILE:O	1:B:288:ILE:CG2	2.40	0.69
1:B:81:GLN:NE2	3:B:623:HOH:O	2.24	0.69
1:A:248:GLN:OE1	3:A:580:HOH:O	2.11	0.68
1:A:114:MET:HE2	1:A:131:PHE:HE1	1.58	0.67
1:A:219:PRO:O	1:A:220:THR:CB	2.42	0.67
1:B:6:ARG:HD3	1:B:81:GLN:OE1	1.93	0.67
1:A:24:ARG:HD3	3:A:532:HOH:O	1.95	0.66
1:B:166:ASP:HB2	3:B:568:HOH:O	1.96	0.66
1:B:175:THR:O	3:B:615:HOH:O	2.13	0.66
1:B:206:ARG:CZ	3:B:601:HOH:O	2.34	0.66
1:A:24:ARG:CZ	3:A:532:HOH:O	2.42	0.66
1:A:166:ASP:HA	3:A:608:HOH:O	1.95	0.65
1:B:180:PRO:HD3	1:B:182:TRP:CH2	2.30	0.65
1:A:64:ALA:H	1:A:260:GLN:NE2	1.94	0.65
1:B:84:ASN:C	1:B:84:ASN:HD22	1.99	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LYS:CB	1:B:158:GLU:OE2	2.43	0.65
1:B:117:ASN:HD22	1:B:118:GLY:H	1.44	0.65
1:A:158:GLU:CD	1:A:158:GLU:H	1.98	0.65
1:A:158:GLU:N	1:A:158:GLU:OE2	2.29	0.65
1:A:158:GLU:HG2	1:A:209:ARG:NH2	2.12	0.65
1:B:170:ASN:OD1	3:B:626:HOH:O	2.15	0.65
1:B:287:ASP:OD1	1:B:287:ASP:N	2.29	0.64
1:A:84:ASN:HD22	1:A:86:GLU:H	1.45	0.64
1:B:24:ARG:HG3	1:B:24:ARG:HH11	1.64	0.63
1:B:288:ILE:O	1:B:288:ILE:HG22	1.97	0.63
1:B:37:ARG:NH1	3:B:565:HOH:O	2.00	0.63
1:A:119:ASN:HD22	1:A:121:ILE:H	1.46	0.63
1:B:57:ASN:ND2	1:B:60:HIS:H	1.97	0.62
1:B:215:MET:CE	1:B:227:PHE:HD2	2.11	0.62
1:B:188:ASN:ND2	3:B:539:HOH:O	1.97	0.62
1:B:170:ASN:CG	3:B:533:HOH:O	2.32	0.62
1:A:117:ASN:ND2	1:A:118:GLY:H	1.97	0.62
1:A:158:GLU:HG2	1:A:209:ARG:HH21	1.65	0.62
1:A:103:PRO:HD2	3:A:607:HOH:O	1.98	0.62
1:B:158:GLU:OE2	1:B:158:GLU:N	2.33	0.62
1:A:24:ARG:NH1	3:A:532:HOH:O	2.33	0.62
1:B:245:HIS:O	1:B:248:GLN:N	2.33	0.61
1:B:245:HIS:HB3	1:B:248:GLN:CB	2.24	0.61
1:A:24:ARG:HG3	3:A:625:HOH:O	2.01	0.61
1:B:119:ASN:ND2	1:B:121:ILE:H	1.98	0.61
1:A:33:GLY:O	3:A:623:HOH:O	2.16	0.60
1:B:156:THR:HG22	1:B:159:ALA:N	2.13	0.60
1:A:119:ASN:ND2	1:A:121:ILE:H	1.99	0.59
1:B:96:THR:CG2	1:B:165:ARG:HH22	2.13	0.59
1:B:215:MET:CE	1:B:221:ALA:HB1	2.30	0.59
1:B:84:ASN:HD22	1:B:86:GLU:H	1.50	0.58
1:B:270:ASN:CG	3:B:543:HOH:O	2.39	0.58
1:B:245:HIS:CB	1:B:248:GLN:HB2	2.25	0.58
1:A:73:LEU:HD22	1:A:89:LEU:HD11	1.84	0.58
1:B:24:ARG:HH11	1:B:24:ARG:CG	2.17	0.58
1:A:4:LYS:HG3	1:A:280:ARG:HG2	1.85	0.57
1:A:84:ASN:HD22	1:A:84:ASN:C	2.08	0.56
1:A:233:ASN:O	1:A:237:ILE:HG12	2.05	0.56
1:A:8:ARG:CG	1:A:89:LEU:O	2.53	0.55
1:A:4:LYS:HG3	1:A:280:ARG:CG	2.35	0.55
1:B:198:ILE:O	1:B:199:ASN:CB	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:THR:HB	1:A:158:GLU:OE1	2.07	0.55
1:A:164:THR:HG23	3:A:562:HOH:O	2.07	0.54
1:A:94:TRP:NE1	1:A:230:HIS:CD2	2.67	0.53
1:B:94:TRP:NE1	1:B:230:HIS:CD2	2.70	0.53
1:A:24:ARG:CG	3:A:625:HOH:O	2.56	0.53
1:A:7:VAL:HG13	1:A:7:VAL:O	2.09	0.53
1:A:254:LYS:HD3	3:A:603:HOH:O	2.08	0.53
1:B:57:ASN:HD22	1:B:59:ALA:H	1.55	0.53
1:B:110:SER:OG	1:B:112:ASP:OD2	2.27	0.52
1:B:7:VAL:HG13	3:B:558:HOH:O	2.08	0.52
1:A:94:TRP:CE3	1:A:163:PRO:HG2	2.44	0.52
1:A:184:MET:HG3	3:A:584:HOH:O	2.10	0.52
1:B:119:ASN:HD22	1:B:119:ASN:C	2.13	0.51
1:B:74:LEU:HD22	1:B:282:LEU:HD13	1.93	0.51
1:A:130:PRO:O	3:A:583:HOH:O	2.18	0.50
1:A:93:GLU:HG2	1:A:96:THR:HG23	1.93	0.50
1:A:157:LYS:N	1:A:158:GLU:OE2	2.45	0.50
1:B:88:THR:O	1:B:90:PRO:HD3	2.11	0.50
1:B:196:GLY:HA3	1:B:202:GLN:O	2.12	0.50
1:B:261:ASN:HB2	1:B:264:ASP:OD2	2.11	0.50
1:A:221:ALA:N	1:A:222:PRO:CD	2.75	0.49
1:B:127:ASP:N	1:B:127:ASP:OD1	2.45	0.49
1:A:93:GLU:OE1	1:A:96:THR:HG21	2.12	0.49
1:A:161:THR:HG23	1:A:206:ARG:NH1	2.28	0.49
1:B:161:THR:HG23	3:B:589:HOH:O	2.13	0.49
1:B:278:ASN:ND2	1:B:281:LYS:HD3	2.28	0.49
1:A:119:ASN:HD22	1:A:119:ASN:C	2.16	0.48
1:A:117:ASN:HD22	1:A:118:GLY:N	2.07	0.48
1:B:8:ARG:HG2	1:B:89:LEU:O	2.13	0.48
1:A:272:THR:HG21	3:A:512:HOH:O	2.12	0.48
1:A:106:SER:OG	1:A:108:ILE:HG22	2.14	0.48
1:B:84:ASN:ND2	1:B:86:GLU:H	2.11	0.48
1:B:44:ALA:HA	3:B:607:HOH:O	2.15	0.47
1:B:191:ARG:C	1:B:191:ARG:HD2	2.34	0.47
1:A:127:ASP:N	1:A:127:ASP:OD1	2.48	0.47
1:A:196:GLY:HA3	1:A:202:GLN:O	2.15	0.47
1:A:69:HIS:CD2	1:A:231:HIS:CE1	3.03	0.47
1:B:117:ASN:HD22	1:B:118:GLY:N	2.11	0.46
1:B:161:THR:O	1:B:206:ARG:HD3	2.15	0.46
1:B:218:PHE:N	1:B:219:PRO:HD2	2.31	0.46
1:A:83:ILE:HD13	1:A:83:ILE:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:ASN:HD22	1:B:152:ASN:C	2.18	0.45
1:B:152:ASN:ND2	1:B:155:ALA:HB2	2.32	0.45
1:B:57:ASN:HD21	1:B:60:HIS:H	1.64	0.45
1:A:42:HIS:HB3	3:A:525:HOH:O	2.15	0.45
1:A:156:THR:HB	1:A:158:GLU:CD	2.37	0.45
1:B:215:MET:HE3	1:B:227:PHE:HB2	1.99	0.45
1:A:175:THR:O	1:A:248:GLN:HG3	2.16	0.45
1:A:158:GLU:CD	1:A:158:GLU:N	2.68	0.45
1:B:29:LEU:HD22	1:B:80:LEU:HD23	1.97	0.45
1:A:117:ASN:HD21	1:A:152:ASN:HA	1.82	0.45
1:A:84:ASN:HA	1:A:85:PRO:HD2	1.80	0.44
1:B:216:GLY:HA3	3:B:562:HOH:O	2.16	0.44
1:B:96:THR:HG21	1:B:165:ARG:HH22	1.83	0.44
1:B:180:PRO:HD3	1:B:182:TRP:CZ2	2.53	0.44
1:B:279:HIS:HD2	3:B:518:HOH:O	2.00	0.44
1:A:29:LEU:HD22	1:A:80:LEU:HD23	2.00	0.44
1:B:215:MET:HE3	1:B:221:ALA:O	2.17	0.44
1:B:155:ALA:HB2	3:B:620:HOH:O	2.17	0.44
1:A:219:PRO:C	1:A:220:THR:CG2	2.75	0.44
1:A:24:ARG:NE	3:A:532:HOH:O	2.51	0.44
1:A:196:GLY:HA2	3:A:557:HOH:O	2.16	0.44
1:B:117:ASN:HD21	1:B:153:PHE:H	1.66	0.43
1:B:91:TYR:HE2	1:B:287:ASP:OD1	2.00	0.43
1:A:184:MET:HB3	1:A:184:MET:HE3	1.88	0.43
1:A:166:ASP:OD2	3:A:608:HOH:O	2.20	0.43
1:B:84:ASN:C	1:B:84:ASN:ND2	2.70	0.43
1:A:101:GLN:NE2	1:A:101:GLN:HA	2.34	0.43
1:B:245:HIS:C	1:B:247:ASN:N	2.71	0.43
1:A:73:LEU:HD22	1:A:89:LEU:CD1	2.48	0.43
1:A:279:HIS:HE1	1:A:289:GLU:OE2	2.02	0.43
1:B:169:LEU:HA	1:B:169:LEU:HD12	1.86	0.43
1:A:219:PRO:O	1:A:220:THR:OG1	2.34	0.42
1:B:24:ARG:NH1	1:B:24:ARG:CG	2.77	0.42
1:A:256:GLY:N	1:A:261:ASN:HD21	2.03	0.42
1:B:152:ASN:ND2	3:B:525:HOH:O	2.52	0.42
1:A:24:ARG:CD	3:A:532:HOH:O	2.59	0.42
1:B:243:ILE:HA	1:B:243:ILE:HD13	1.81	0.42
1:B:4:LYS:NZ	3:B:567:HOH:O	2.52	0.42
1:A:88:THR:O	1:A:90:PRO:HD3	2.20	0.42
1:B:175:THR:O	1:B:248:GLN:HG3	2.19	0.42
1:A:139:ILE:HD11	1:B:52:PRO:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ASN:ND2	1:A:86:GLU:H	2.15	0.42
1:B:94:TRP:CE3	1:B:163:PRO:HG2	2.56	0.41
1:A:56:ARG:NH2	3:A:595:HOH:O	2.44	0.41
1:A:261:ASN:HB2	1:A:264:ASP:OD2	2.21	0.41
1:B:4:LYS:HD2	1:B:4:LYS:N	2.36	0.41
1:A:11:VAL:HG23	1:A:91:TYR:O	2.20	0.41
1:B:119:ASN:HA	1:B:120:PRO:HD2	1.86	0.41
1:B:154:GLY:C	3:B:547:HOH:O	2.56	0.41
1:A:57:ASN:HD22	1:A:59:ALA:H	1.69	0.41
1:A:102:ASP:HB3	1:A:105:GLN:HG3	2.03	0.41
1:A:255:ASN:ND2	3:A:603:HOH:O	2.53	0.41
1:B:107:GLN:O	1:B:110:SER:HB3	2.21	0.41
1:B:156:THR:CG2	1:B:159:ALA:H	2.22	0.41
1:B:50:THR:HA	1:B:51:PRO:HA	1.87	0.41
1:A:207:VAL:HG11	1:A:230:HIS:CD2	2.55	0.40
1:A:251:GLN:NE2	3:A:509:HOH:O	2.37	0.40
1:B:101:GLN:HA	1:B:101:GLN:NE2	2.36	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LYS:NZ	3:A:613:HOH:O[2_656]	1.48	0.72
1:B:157:LYS:CE	3:A:613:HOH:O[2_656]	1.54	0.66
1:B:157:LYS:NZ	3:A:543:HOH:O[2_656]	2.07	0.13

## 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	285/303 (94%)	275 (96%)	9 (3%)	1 (0%)	39 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	284/303 (94%)	268 (94%)	15 (5%)	1 (0%)	39	33
All	All	569/606 (94%)	543 (95%)	24 (4%)	2 (0%)	39	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	244	ILE
1	A	198	ILE

### 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	250/265 (94%)	229 (92%)	21 (8%)	14	8
1	B	249/265 (94%)	223 (90%)	26 (10%)	9	4
All	All	499/530 (94%)	452 (91%)	47 (9%)	11	6

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	24	ARG
1	A	29	LEU
1	A	55	ASP
1	A	84	ASN
1	A	89	LEU
1	A	94	TRP
1	A	117	ASN
1	A	119	ASN
1	A	139	ILE
1	A	149	LEU
1	A	152	ASN
1	A	158	GLU

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Mol	Chain	Res	Type
1	A	194	LEU
1	A	204	HIS
1	A	226	VAL
1	A	229	LEU
1	A	246	ARG
1	A	288	ILE
1	A	290	LEU
1	B	4	LYS
1	B	7	VAL
1	B	17	THR
1	B	29	LEU
1	B	41	TRP
1	B	57	ASN
1	B	84	ASN
1	B	89	LEU
1	B	94	TRP
1	B	110	SER
1	B	117	ASN
1	B	119	ASN
1	B	142	GLN
1	B	149	LEU
1	B	152	ASN
1	B	156	THR
1	B	158	GLU
1	B	169	LEU
1	B	184	MET
1	B	193	GLN
1	B	194	LEU
1	B	217	VAL
1	B	229	LEU
1	B	247	ASN
1	B	281	LYS
1	B	288	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	84	ASN
1	A	101	GLN
1	A	117	ASN
1	A	119	ASN

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Mol	Chain	Res	Type
1	A	142	GLN
1	A	152	ASN
1	A	176	GLN
1	A	187	GLN
1	A	202	GLN
1	A	205	ASN
1	A	230	HIS
1	A	247	ASN
1	A	255	ASN
1	A	260	GLN
1	A	261	ASN
1	A	279	HIS
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	202	GLN
1	B	205	ASN
1	B	230	HIS
1	B	245	HIS
1	B	247	ASN
1	B	251	GLN
1	B	255	ASN
1	B	260	GLN
1	B	261	ASN
1	B	270	ASN
1	B	279	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 4 ligands modelled in this entry, 4 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

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	287/303 (94%)	0.24	4 (1%) 78 78	12, 21, 48, 85	1 (0%)
1	B	286/303 (94%)	0.35	11 (3%) 44 45	12, 24, 49, 87	0
All	All	573/606 (94%)	0.29	15 (2%) 59 60	12, 23, 49, 87	1 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	247	ASN	12.2
1	B	248	GLN	8.1
1	B	244	ILE	5.7
1	B	246	ARG	5.5
1	A	5	TYR	2.9
1	B	5	TYR	2.8
1	B	243	ILE	2.8
1	A	4	LYS	2.7
1	A	142	GLN	2.6
1	B	249	ASN	2.5
1	A	101	GLN	2.5
1	B	123	ASP	2.4
1	B	121	ILE	2.4
1	B	172	LEU	2.3
1	B	101	GLN	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 [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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CU	A	402	1/1	0.90	0.29	7.59	32,32,32,32	1
2	CU	B	402	1/1	0.94	0.22	4.02	35,35,35,35	1
2	CU	B	401	1/1	0.99	0.07	-2.97	34,34,34,34	0
2	CU	A	401	1/1	0.97	0.08	-3.83	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.