



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 12:07 am GMT

PDB ID : 3NQ1  
Title : Crystal Structure of Tyrosinase from *Bacillus megaterium* in complex with inhibitor kojic acid  
Authors : Sendovski, M.; Kanteev, M.; Adir, N.; Fishman, A.  
Deposited on : 2010-06-29  
Resolution : 2.30 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

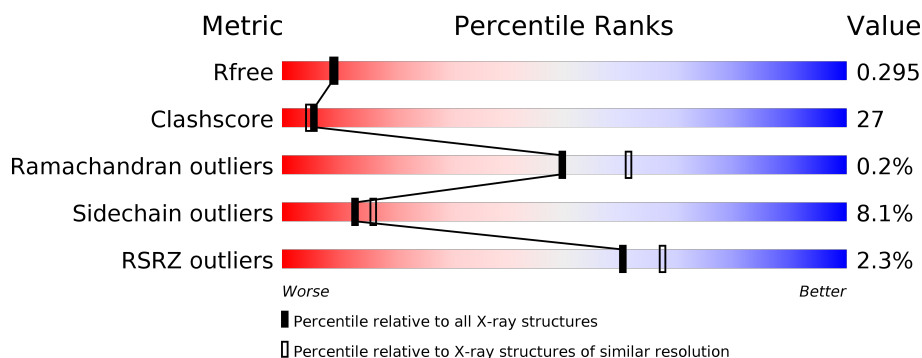
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	111664	4477 (2.30-2.30)
Clashscore	122126	5072 (2.30-2.30)
Ramachandran outliers	120053	5022 (2.30-2.30)
Sidechain outliers	120020	5021 (2.30-2.30)
RSRZ outliers	108989	4374 (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. 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></div> <div>58%</div> <div>29%</div> <div>7%</div> <div>7%</div> </div> </div>
1	B	303	<div> <div>3%</div> <div> <div></div> <div>56%</div> <div>32%</div> <div>6%</div> <div>7%</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
4	KOJ	A	1351	-	-	X	-
4	KOJ	B	1351	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4885 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	283	Total	C	N	O	S	0	0	0
			2321	1477	420	416	8			
1	B	283	Total	C	N	O	S	0	0	0
			2321	1477	420	416	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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

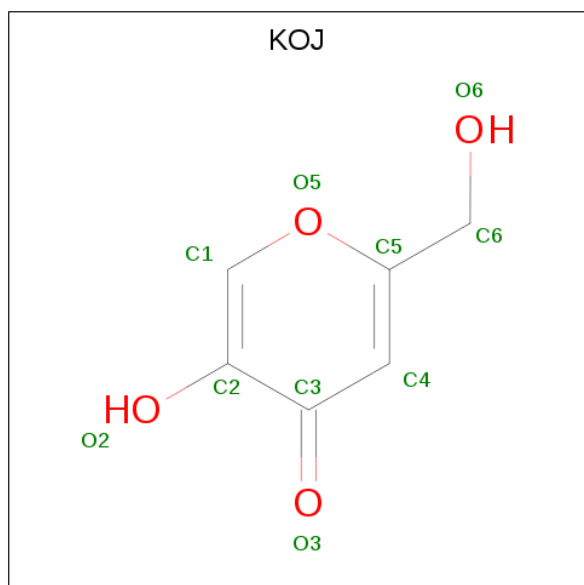
- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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	5	Total	Zn	0	0
			5	5		
3	A	8	Total	Zn	0	0
			8	8		

- Molecule 4 is 5-HYDROXY-2-(HYDROXYMETHYL)-4H-PYRAN-4-ONE (three-letter code: KOJ) (formula: C<sub>6</sub>H<sub>6</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	102	Total	O	0	0
			102	102		
5	B	104	Total	O	0	0
			104	104		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.38Å 83.53Å 146.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.09 – 2.30 43.76 – 2.30	Depositor EDS
% Data completeness (in resolution range)	77.1 (42.09-2.30) 83.8 (43.76-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.29Å)	Xtriage
Refinement program	REFMAC, PHENIX 1.6.1_357	Depositor
R, $R_{free}$	0.260 , 0.294 0.264 , 0.295	Depositor DCC
$R_{free}$ test set	1250 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.4	Xtriage
Anisotropy	1.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	4885	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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: ZN, KOJ, 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	0.71	7/2399 (0.3%)	0.73	7/3269 (0.2%)
1	B	0.64	0/2399	0.71	5/3269 (0.2%)
All	All	0.68	7/4798 (0.1%)	0.72	12/6538 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	35	TYR	CD1-CE1	-7.79	1.27	1.39
1	A	35	TYR	CE1-CZ	-6.87	1.29	1.38
1	A	136	TRP	CB-CG	-6.01	1.39	1.50
1	A	136	TRP	CG-CD1	-5.54	1.28	1.36
1	A	35	TYR	CD2-CE2	-5.16	1.31	1.39
1	A	137	THR	C-O	-5.10	1.13	1.23
1	A	8	ARG	CZ-NH1	-5.01	1.26	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	ASN	CB-CA-C	-9.32	91.75	110.40
1	A	261	ASN	CB-CA-C	-7.64	95.11	110.40
1	B	5	TYR	CB-CA-C	-7.34	95.72	110.40
1	B	255	ASN	CB-CA-C	-6.26	97.87	110.40
1	B	113	PHE	N-CA-C	6.13	127.55	111.00
1	B	5	TYR	N-CA-C	6.03	127.27	111.00
1	B	113	PHE	CB-CA-C	-6.01	98.37	110.40
1	A	221	ALA	CB-CA-C	-5.89	101.26	110.10
1	A	113	PHE	N-CA-C	5.84	126.77	111.00
1	A	221	ALA	N-CA-C	5.53	125.94	111.00
1	A	123	ASP	CB-CG-OD2	5.28	123.06	118.30
1	A	5	TYR	CB-CA-C	-5.16	100.07	110.40



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	2321	0	2206	126	1
1	B	2321	0	2206	130	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	8	0	0	0	0
3	B	5	0	0	0	0
4	A	10	0	4	6	0
4	B	10	0	4	6	0
5	A	102	0	0	16	0
5	B	104	0	0	7	0
All	All	4885	0	4420	249	1

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 27.

All (249) 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:205:ASN:HB3	4:B:1351:KOJ:H4	1.33	1.09
1:A:215:MET:CE	1:A:221:ALA:O	2.03	1.05
1:A:261:ASN:HB2	1:A:264:ASP:OD2	1.58	1.03
1:B:256:GLY:H	1:B:261:ASN:HD21	1.06	0.97
1:B:122:LYS:HE2	1:B:127:ASP:HB3	1.47	0.96
1:A:205:ASN:OD1	4:A:1351:KOJ:H4	1.66	0.94
4:A:1351:KOJ:H1	5:A:335:HOH:O	1.67	0.93
1:A:215:MET:HE3	1:A:221:ALA:O	1.67	0.93
1:A:8:ARG:HG2	1:A:89:LEU:O	1.75	0.86
1:B:205:ASN:CB	4:B:1351:KOJ:H4	2.04	0.86
1:A:278:ASN:HD22	1:A:281:LYS:HD3	1.40	0.86
1:B:57:ASN:HD21	1:B:60:HIS:HD1	1.24	0.86
1:B:246:ARG:HB2	1:B:246:ARG:NH1	1.92	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ASN:HB2	1:A:264:ASP:CG	1.95	0.85
1:A:215:MET:HE3	1:A:227:PHE:HB2	1.60	0.83
1:B:209:ARG:HG2	4:B:1351:KOJ:H6C2	1.62	0.82
1:B:108:ILE:HD11	1:B:229:LEU:HD23	1.63	0.81
1:B:215:MET:HE1	1:B:227:PHE:HD2	1.44	0.80
1:A:64:ALA:H	1:A:260:GLN:HE22	1.29	0.80
1:B:125:ILE:O	1:B:125:ILE:HG22	1.82	0.80
1:B:64:ALA:H	1:B:260:GLN:HE22	1.29	0.79
1:A:215:MET:HE1	1:A:227:PHE:HD2	1.47	0.78
1:B:122:LYS:O	1:B:123:ASP:HB2	1.81	0.77
1:A:215:MET:HE2	1:A:221:ALA:O	1.82	0.77
1:A:57:ASN:OD1	1:A:60:HIS:HD2	1.67	0.77
1:B:256:GLY:N	1:B:261:ASN:HD21	1.81	0.77
1:A:4:LYS:HG2	1:A:280:ARG:HD3	1.68	0.76
1:B:8:ARG:HG2	1:B:89:LEU:O	1.86	0.76
1:B:205:ASN:HB3	4:B:1351:KOJ:C4	2.15	0.75
1:A:4:LYS:HG3	1:A:280:ARG:HG2	1.69	0.74
1:B:122:LYS:HE2	1:B:127:ASP:CB	2.17	0.74
1:A:93:GLU:OE1	1:A:96:THR:HG21	1.88	0.74
1:A:254:LYS:O	1:A:255:ASN:HB2	1.86	0.73
1:B:11:VAL:HG11	1:B:108:ILE:HD12	1.69	0.73
1:B:246:ARG:HB2	1:B:246:ARG:CZ	2.17	0.73
1:A:64:ALA:H	1:A:260:GLN:NE2	1.86	0.72
1:B:278:ASN:HD22	1:B:281:LYS:HD3	1.53	0.72
1:B:215:MET:HE3	1:B:227:PHE:HB2	1.71	0.72
1:B:122:LYS:CE	1:B:127:ASP:HB3	2.20	0.71
1:B:246:ARG:CB	1:B:246:ARG:CZ	2.67	0.71
1:A:119:ASN:HD22	1:A:120:PRO:CD	2.04	0.71
1:B:198:ILE:N	1:B:198:ILE:HD12	2.07	0.70
1:B:119:ASN:HD22	1:B:120:PRO:N	1.90	0.70
1:A:119:ASN:HD22	1:A:119:ASN:C	1.95	0.69
1:A:13:HIS:HB3	5:A:304:HOH:O	1.92	0.69
1:A:198:ILE:N	1:A:198:ILE:HD12	2.07	0.69
1:A:205:ASN:CG	4:A:1351:KOJ:H4	2.13	0.68
1:B:193:GLN:HA	1:B:198:ILE:HD13	1.75	0.68
1:A:119:ASN:ND2	1:A:120:PRO:HD2	2.08	0.68
1:B:94:TRP:CE3	1:B:163:PRO:HG2	2.29	0.68
1:B:119:ASN:ND2	1:B:121:ILE:H	1.91	0.67
1:B:278:ASN:ND2	1:B:281:LYS:HD3	2.09	0.67
1:B:119:ASN:HD22	1:B:119:ASN:C	1.95	0.66
1:A:94:TRP:CE3	1:A:163:PRO:HG2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LYS:HG2	1:A:280:ARG:CD	2.26	0.66
1:A:37:ARG:NH2	1:B:270:ASN:ND2	2.44	0.66
1:A:193:GLN:HA	1:A:198:ILE:HD13	1.76	0.66
1:A:37:ARG:NH2	1:B:270:ASN:HD22	1.94	0.66
1:A:278:ASN:ND2	1:A:281:LYS:HD3	2.09	0.66
1:A:119:ASN:HD22	1:A:120:PRO:HD2	1.58	0.66
1:A:215:MET:CE	1:A:227:PHE:HB2	2.26	0.66
1:B:209:ARG:CG	4:B:1351:KOJ:H6C2	2.25	0.65
1:A:198:ILE:CD1	1:A:198:ILE:N	2.60	0.65
1:B:198:ILE:CD1	1:B:198:ILE:N	2.60	0.65
1:B:221:ALA:HB3	1:B:222:PRO:HD3	1.79	0.65
1:B:4:LYS:HG3	1:B:280:ARG:HG3	1.80	0.64
1:A:4:LYS:CG	1:A:280:ARG:CG	2.76	0.64
1:B:64:ALA:H	1:B:260:GLN:NE2	1.96	0.64
1:A:135:ARG:HB2	5:A:328:HOH:O	1.97	0.63
1:B:215:MET:CE	1:B:227:PHE:HB2	2.27	0.63
1:A:221:ALA:HB3	1:A:222:PRO:HD3	1.79	0.63
1:A:182:TRP:CE3	1:A:252:PRO:HD3	2.34	0.63
1:B:215:MET:HE2	1:B:215:MET:HA	1.81	0.62
1:B:233:ASN:O	1:B:237:ILE:HG12	1.99	0.62
1:A:193:GLN:HG2	1:A:198:ILE:HG12	1.81	0.62
1:A:233:ASN:O	1:A:237:ILE:HG12	1.99	0.62
1:A:123:ASP:OD1	1:A:123:ASP:O	2.18	0.61
1:B:5:TYR:HB2	5:B:356:HOH:O	1.99	0.61
1:B:215:MET:HE1	1:B:227:PHE:CD2	2.30	0.61
1:A:215:MET:HA	1:A:215:MET:HE2	1.83	0.61
1:B:57:ASN:ND2	1:B:60:HIS:H	1.98	0.61
1:B:193:GLN:HG2	1:B:198:ILE:HG12	1.81	0.61
1:A:119:ASN:HD22	1:A:120:PRO:N	1.99	0.60
1:B:198:ILE:H	1:B:198:ILE:CD1	2.14	0.60
1:A:278:ASN:HD22	1:A:281:LYS:HB2	1.67	0.60
1:A:261:ASN:CB	1:A:264:ASP:OD2	2.41	0.60
1:B:176:GLN:NE2	1:B:251:GLN:HE22	2.01	0.59
1:A:198:ILE:CD1	1:A:198:ILE:H	2.14	0.59
1:A:57:ASN:OD1	1:A:60:HIS:CD2	2.53	0.59
1:A:123:ASP:O	1:A:124:PHE:HB2	2.03	0.59
1:A:117:ASN:ND2	1:A:118:GLY:H	2.02	0.58
1:B:198:ILE:HG13	5:B:354:HOH:O	2.03	0.57
1:A:254:LYS:HA	1:A:261:ASN:ND2	2.18	0.57
1:A:6:ARG:NH2	1:A:282:LEU:O	2.37	0.57
1:A:4:LYS:HG3	1:A:280:ARG:CG	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:MET:HE1	1:A:227:PHE:CD2	2.35	0.57
1:B:117:ASN:ND2	1:B:118:GLY:H	2.02	0.56
1:B:119:ASN:CB	1:B:122:LYS:HD3	2.37	0.55
1:B:125:ILE:O	1:B:126:VAL:C	2.44	0.55
1:B:142:GLN:HE21	1:B:144:ASN:HD22	1.54	0.55
1:A:4:LYS:CG	1:A:280:ARG:HG2	2.36	0.55
1:B:119:ASN:HB3	1:B:122:LYS:HD3	1.89	0.55
1:A:253:MET:O	1:A:254:LYS:HG2	2.07	0.55
1:B:4:LYS:HG3	1:B:280:ARG:CG	2.36	0.55
1:B:6:ARG:HD2	1:B:81:GLN:OE1	2.07	0.54
1:A:142:GLN:HE21	1:A:144:ASN:HD22	1.54	0.54
1:B:35:TYR:CE2	1:B:39:ILE:HD11	2.42	0.54
1:B:4:LYS:CG	1:B:280:ARG:HG3	2.37	0.54
1:A:15:THR:OG1	1:A:17:THR:HG23	2.08	0.54
1:A:181:PRO:HG2	1:A:183:ASP:OD2	2.08	0.54
1:A:94:TRP:HE1	1:A:230:HIS:HD2	1.56	0.54
1:B:181:PRO:HG2	1:B:183:ASP:OD2	2.08	0.54
1:A:253:MET:HA	1:A:262:PHE:HB2	1.90	0.54
1:A:142:GLN:HE21	1:A:144:ASN:ND2	2.07	0.53
1:B:261:ASN:HB2	1:B:264:ASP:OD2	2.08	0.53
1:B:39:ILE:HD13	1:B:222:PRO:HB2	1.90	0.53
1:A:39:ILE:HD13	1:A:222:PRO:HB2	1.91	0.53
1:B:84:ASN:C	1:B:84:ASN:HD22	2.11	0.53
1:A:84:ASN:HD22	1:A:84:ASN:C	2.12	0.53
1:B:94:TRP:HE1	1:B:230:HIS:HD2	1.56	0.53
1:B:4:LYS:CG	1:B:280:ARG:CG	2.87	0.53
1:A:84:ASN:HD22	1:A:86:GLU:H	1.56	0.53
1:B:240:VAL:O	1:B:244:ILE:HG12	2.09	0.53
1:B:142:GLN:HE21	1:B:144:ASN:ND2	2.07	0.52
1:A:119:ASN:ND2	1:A:121:ILE:H	2.07	0.52
1:B:246:ARG:CB	1:B:246:ARG:NH1	2.66	0.52
1:B:84:ASN:ND2	1:B:86:GLU:H	2.08	0.52
1:A:132:ALA:N	5:A:328:HOH:O	2.41	0.52
1:A:267:TYR:CD1	1:A:268:PRO:HA	2.45	0.52
1:B:215:MET:CE	1:B:221:ALA:O	2.57	0.52
1:B:84:ASN:HD22	1:B:86:GLU:H	1.57	0.51
1:B:11:VAL:HG21	1:B:108:ILE:CD1	2.40	0.51
1:B:267:TYR:CD1	1:B:268:PRO:HA	2.45	0.51
1:B:57:ASN:HD22	1:B:59:ALA:H	1.58	0.51
1:B:57:ASN:ND2	1:B:60:HIS:HD1	2.00	0.51
1:A:171:ALA:O	1:A:174:ILE:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ASN:CG	4:B:1351:KOJ:H4	2.31	0.51
1:A:37:ARG:HH21	1:B:270:ASN:ND2	2.08	0.51
1:A:122:LYS:O	1:A:123:ASP:HB3	2.11	0.51
1:B:119:ASN:OD1	1:B:122:LYS:HD3	2.11	0.51
1:B:254:LYS:O	1:B:255:ASN:HB2	2.12	0.50
1:A:101:GLN:HE21	1:A:101:GLN:HA	1.76	0.50
1:A:269:TRP:HB3	5:A:314:HOH:O	2.11	0.50
1:B:11:VAL:HG21	1:B:108:ILE:HD13	1.92	0.50
1:A:224:ASP:OD1	1:A:226:VAL:HG22	2.12	0.50
1:A:93:GLU:HG2	1:A:96:THR:HG23	1.92	0.50
1:B:101:GLN:HA	1:B:101:GLN:HE21	1.76	0.50
1:B:125:ILE:O	1:B:125:ILE:CG2	2.53	0.50
1:A:205:ASN:HB3	4:A:1351:KOJ:C4	2.42	0.49
1:B:215:MET:HE3	1:B:221:ALA:O	2.12	0.49
1:A:93:GLU:OE1	1:A:96:THR:CG2	2.57	0.49
1:B:101:GLN:HA	1:B:101:GLN:NE2	2.27	0.49
1:B:224:ASP:OD1	1:B:226:VAL:HG22	2.12	0.49
1:A:101:GLN:NE2	1:A:101:GLN:HA	2.27	0.49
1:A:253:MET:C	1:A:254:LYS:CG	2.80	0.49
1:A:262:PHE:CZ	1:A:274:GLU:HG3	2.48	0.49
1:A:265:PRO:HB3	1:A:270:ASN:HA	1.93	0.49
1:B:254:LYS:HD3	1:B:255:ASN:OD1	2.13	0.49
1:A:224:ASP:CG	1:A:226:VAL:HG22	2.34	0.49
1:B:119:ASN:ND2	1:B:119:ASN:C	2.64	0.49
1:A:6:ARG:CZ	5:A:378:HOH:O	2.61	0.48
1:B:265:PRO:HB3	1:B:270:ASN:HA	1.93	0.48
1:B:117:ASN:HD22	1:B:118:GLY:H	1.61	0.48
1:A:253:MET:O	1:A:254:LYS:CG	2.61	0.48
1:B:62:SER:HB3	5:B:386:HOH:O	2.13	0.48
1:A:29:LEU:HD22	1:A:80:LEU:HD23	1.95	0.48
1:A:253:MET:C	1:A:254:LYS:HG3	2.33	0.48
1:B:220:THR:HA	5:B:322:HOH:O	2.14	0.48
1:A:205:ASN:CG	4:A:1351:KOJ:H6C1	2.35	0.47
1:A:84:ASN:ND2	1:A:86:GLU:H	2.11	0.47
1:A:119:ASN:ND2	1:A:119:ASN:C	2.64	0.47
1:B:174:ILE:CD1	1:B:193:GLN:HG3	2.44	0.47
1:B:29:LEU:HD22	1:B:80:LEU:HD23	1.95	0.47
1:B:224:ASP:CG	1:B:226:VAL:HG22	2.34	0.47
1:B:4:LYS:N	1:B:4:LYS:HD2	2.29	0.47
1:B:51:PRO:O	1:B:54:SER:HB3	2.15	0.47
1:A:144:ASN:HA	5:A:346:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ASN:CG	1:B:122:LYS:HD3	2.35	0.47
1:B:107:GLN:HG3	5:B:333:HOH:O	2.15	0.47
1:A:37:ARG:HH22	1:B:270:ASN:HD22	1.63	0.47
1:A:117:ASN:HD22	1:A:118:GLY:H	1.61	0.47
1:A:51:PRO:O	1:A:54:SER:HB3	2.14	0.47
1:B:124:PHE:CE2	1:B:152:ASN:ND2	2.83	0.46
1:B:178:ASP:HA	1:B:189:SER:OG	2.16	0.46
1:A:231:HIS:ND1	5:A:355:HOH:O	2.31	0.46
1:A:8:ARG:CG	1:A:89:LEU:O	2.55	0.46
1:B:256:GLY:H	1:B:261:ASN:ND2	1.91	0.46
1:B:35:TYR:HE2	1:B:39:ILE:HD11	1.77	0.46
1:B:11:VAL:HG11	1:B:108:ILE:CD1	2.40	0.46
1:A:270:ASN:HD22	1:B:37:ARG:NH2	2.14	0.45
1:B:119:ASN:HA	1:B:120:PRO:HD2	1.86	0.45
1:A:135:ARG:NE	5:A:328:HOH:O	2.49	0.45
1:A:270:ASN:ND2	1:B:37:ARG:NH2	2.64	0.45
1:B:123:ASP:O	1:B:124:PHE:HB2	2.16	0.45
1:B:188:ASN:HB3	5:B:397:HOH:O	2.16	0.45
1:A:69:HIS:O	1:A:73:LEU:HG	2.17	0.45
1:A:117:ASN:HD21	1:A:153:PHE:H	1.65	0.44
1:A:271:THR:HB	5:A:364:HOH:O	2.17	0.44
1:B:180:PRO:HA	1:B:182:TRP:N	2.33	0.44
1:A:182:TRP:CZ2	1:A:252:PRO:HB3	2.53	0.44
1:B:279:HIS:HB2	1:B:284:TYR:CZ	2.52	0.44
1:A:253:MET:HA	1:A:262:PHE:CB	2.47	0.43
1:A:59:ALA:HB2	1:A:68:TRP:CD2	2.53	0.43
1:B:262:PHE:CZ	1:B:274:GLU:HG3	2.52	0.43
1:B:278:ASN:HD22	1:B:281:LYS:HB2	1.83	0.43
1:B:279:HIS:HA	1:B:282:LEU:HD12	1.99	0.43
1:B:28:ILE:CG2	1:B:32:LYS:HE2	2.48	0.43
1:A:180:PRO:HA	1:A:182:TRP:N	2.33	0.43
1:A:231:HIS:HB3	5:A:355:HOH:O	2.17	0.43
1:B:117:ASN:HD21	1:B:153:PHE:H	1.65	0.43
1:B:250:TYR:HB2	1:B:277:MET:CE	2.49	0.43
1:A:258:PHE:CZ	1:B:34:ILE:CD1	3.02	0.43
4:A:1351:KOJ:C6	5:A:356:HOH:O	2.66	0.43
1:A:250:TYR:HB2	1:A:277:MET:CE	2.49	0.43
1:B:246:ARG:CG	1:B:246:ARG:HH11	2.32	0.43
1:A:246:ARG:HH11	1:A:246:ARG:HG3	1.84	0.43
1:A:145:PRO:HD3	1:B:53:GLY:N	2.34	0.43
1:A:180:PRO:HA	1:A:182:TRP:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ILE:CG2	1:A:32:LYS:HE2	2.48	0.43
1:A:254:LYS:CA	1:A:261:ASN:ND2	2.81	0.42
1:A:278:ASN:HD22	1:A:281:LYS:CD	2.21	0.42
1:B:119:ASN:HB3	1:B:122:LYS:HB2	2.00	0.42
1:B:144:ASN:HA	5:B:323:HOH:O	2.19	0.42
1:B:96:THR:HG22	1:B:165:ARG:CZ	2.49	0.42
1:B:50:THR:HA	1:B:51:PRO:HA	1.89	0.42
1:B:109:TRP:CZ3	1:B:226:VAL:HG11	2.55	0.42
1:A:191:ARG:C	1:A:191:ARG:HD2	2.40	0.42
1:A:109:TRP:CZ3	1:A:226:VAL:HG11	2.55	0.42
1:A:279:HIS:HA	1:A:282:LEU:HD12	2.00	0.42
1:A:278:ASN:ND2	1:A:281:LYS:HB2	2.33	0.42
1:B:180:PRO:HA	1:B:182:TRP:H	1.84	0.42
1:B:96:THR:HG22	1:B:165:ARG:NH1	2.35	0.42
1:A:19:LYS:HG2	1:A:113:PHE:CE1	2.55	0.41
1:A:215:MET:HE1	1:A:221:ALA:HB1	2.03	0.41
1:A:71:GLU:HG2	1:A:271:THR:HG21	2.03	0.41
1:B:191:ARG:C	1:B:191:ARG:HD2	2.40	0.41
1:A:158:GLU:HB2	5:A:391:HOH:O	2.20	0.41
1:A:101:GLN:HB3	5:A:372:HOH:O	2.20	0.41
1:A:258:PHE:HZ	1:B:34:ILE:HD11	1.85	0.41
1:B:207:VAL:HB	1:B:230:HIS:CE1	2.56	0.41
1:B:6:ARG:HH22	1:B:74:LEU:CD1	2.34	0.41
1:A:175:THR:O	1:A:248:GLN:HG3	2.21	0.41
1:B:73:LEU:HD22	1:B:89:LEU:HD11	2.02	0.41
1:A:24:ARG:HG3	5:A:383:HOH:O	2.21	0.41
1:A:108:ILE:HD11	1:A:229:LEU:HD23	2.02	0.41
1:B:150:LYS:O	1:B:213:GLY:HA3	2.21	0.41
1:A:39:ILE:CD1	1:A:222:PRO:HB2	2.51	0.40
1:B:71:GLU:HG2	1:B:271:THR:HG21	2.03	0.40
1:A:13:HIS:CB	5:A:304:HOH:O	2.59	0.40

All (1) 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:A:112:ASP:OD2	1:B:16:ASP:OD1[2_455]	2.16	0.04



## 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	281/303 (93%)	272 (97%)	9 (3%)	0	100	100
1	B	281/303 (93%)	270 (96%)	10 (4%)	1 (0%)	36	45
All	All	562/606 (93%)	542 (96%)	19 (3%)	1 (0%)	49	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	126	VAL

### 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	246/266 (92%)	226 (92%)	20 (8%)	13	16
1	B	246/266 (92%)	226 (92%)	20 (8%)	13	16
All	All	492/532 (92%)	452 (92%)	40 (8%)	13	16

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	17	THR
1	A	29	LEU
1	A	55	ASP
1	A	84	ASN

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Mol	Chain	Res	Type
1	A	89	LEU
1	A	94	TRP
1	A	117	ASN
1	A	119	ASN
1	A	122	LYS
1	A	149	LEU
1	A	152	ASN
1	A	169	LEU
1	A	189	SER
1	A	194	LEU
1	A	198	ILE
1	A	254	LYS
1	A	268	PRO
1	A	271	THR
1	A	281	LYS
1	B	4	LYS
1	B	17	THR
1	B	29	LEU
1	B	55	ASP
1	B	84	ASN
1	B	89	LEU
1	B	94	TRP
1	B	117	ASN
1	B	119	ASN
1	B	123	ASP
1	B	139	ILE
1	B	149	LEU
1	B	152	ASN
1	B	169	LEU
1	B	194	LEU
1	B	198	ILE
1	B	246	ARG
1	B	268	PRO
1	B	271	THR
1	B	281	LYS

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	60	HIS
1	A	84	ASN
1	A	101	GLN

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Mol	Chain	Res	Type
1	A	117	ASN
1	A	119	ASN
1	A	142	GLN
1	A	144	ASN
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	260	GLN
1	A	261	ASN
1	A	270	ASN
1	A	278	ASN
1	B	49	HIS
1	B	57	ASN
1	B	84	ASN
1	B	101	GLN
1	B	117	ASN
1	B	119	ASN
1	B	142	GLN
1	B	144	ASN
1	B	152	ASN
1	B	176	GLN
1	B	202	GLN
1	B	205	ASN
1	B	230	HIS
1	B	260	GLN
1	B	261	ASN
1	B	270	ASN
1	B	278	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 17 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	KOJ	A	1351	-	8,10,10	3.61	4 (50%)	6,13,13	1.42	1 (16%)
4	KOJ	B	1351	-	8,10,10	3.58	4 (50%)	6,13,13	1.41	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	KOJ	A	1351	-	-	0/1/2/2	0/1/1/1
4	KOJ	B	1351	-	-	0/1/2/2	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1351	KOJ	O5-C5	-7.70	1.25	1.35
4	B	1351	KOJ	O5-C5	-7.55	1.25	1.35
4	B	1351	KOJ	C6-C5	-2.22	1.48	1.50
4	A	1351	KOJ	C6-C5	-2.19	1.48	1.50
4	B	1351	KOJ	C4-C5	2.09	1.39	1.35
4	A	1351	KOJ	C4-C5	2.20	1.39	1.35
4	A	1351	KOJ	O3-C3	5.24	1.32	1.23
4	B	1351	KOJ	O3-C3	5.27	1.32	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1351	KOJ	O6-C6-C5	2.89	118.69	112.18
4	A	1351	KOJ	O6-C6-C5	2.92	118.77	112.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1351	KOJ	6	0
4	B	1351	KOJ	6	0

## 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	283/303 (93%)	0.13	4 (1%) 75 80	8, 18, 34, 52	0
1	B	283/303 (93%)	0.24	9 (3%) 47 55	11, 18, 38, 64	0
All	All	566/606 (93%)	0.18	13 (2%) 60 67	8, 18, 37, 64	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	255	ASN	5.1
1	B	5	TYR	4.7
1	A	5	TYR	4.6
1	B	4	LYS	3.3
1	A	24	ARG	2.9
1	B	198	ILE	2.7
1	A	20	ARG	2.6
1	B	147	GLY	2.6
1	A	255	ASN	2.4
1	B	20	ARG	2.3
1	B	125	ILE	2.2
1	B	246	ARG	2.2
1	B	187	GLN	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](#)

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
3	ZN	A	508	1/1	0.74	0.12	64,64,64,64	0
3	ZN	B	506	1/1	0.80	0.13	77,77,77,77	0
3	ZN	B	504	1/1	0.81	0.11	60,60,60,60	0
4	KOJ	B	1351	10/10	0.84	0.19	14,32,36,43	0
3	ZN	A	510	1/1	0.86	0.11	43,43,43,43	0
3	ZN	A	506	1/1	0.86	0.17	27,27,27,27	0
4	KOJ	A	1351	10/10	0.87	0.27	15,30,36,47	0
3	ZN	B	505	1/1	0.87	0.12	30,30,30,30	0
3	ZN	A	503	1/1	0.88	0.11	22,22,22,22	0
3	ZN	A	505	1/1	0.89	0.10	42,42,42,42	0
3	ZN	B	503	1/1	0.95	0.13	18,18,18,18	0
3	ZN	A	504	1/1	0.96	0.07	57,57,57,57	0
3	ZN	A	507	1/1	0.96	0.06	48,48,48,48	0
3	ZN	B	507	1/1	0.97	0.09	34,34,34,34	0
3	ZN	A	509	1/1	0.98	0.08	41,41,41,41	0
2	CU	A	501	1/1	0.98	0.13	22,22,22,22	0
2	CU	B	501	1/1	0.99	0.11	14,14,14,14	0
2	CU	B	502	1/1	0.99	0.08	16,16,16,16	0
2	CU	A	502	1/1	1.00	0.07	14,14,14,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.