



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:28 PM UTC

PDB ID : 4J6V / pdb_00004j6v
Title : Crystal Structure of Tyrosinase from Bacillus megaterium N205D mutant
Authors : Kanteev, M.; Goldfeder, M.; Adir, N.; Fishman, A.
Deposited on : 2013-02-12
Resolution : 1.90 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

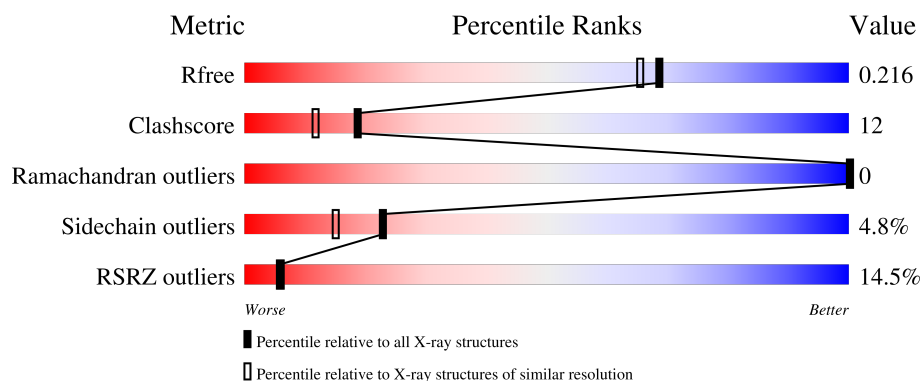
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	303	16% 73% 17% • • 6%
1	B	303	12% 74% 18% • • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5037 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	286	Total	C	N	O	S	0	0	0
			2346	1492	422	424	8			
1	B	287	Total	C	N	O	S	0	0	0
			2354	1498	423	425	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	205	ASP	ASN	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	205	ASP	ASN	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 (CCD ID: CU) (formula: Cu).

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

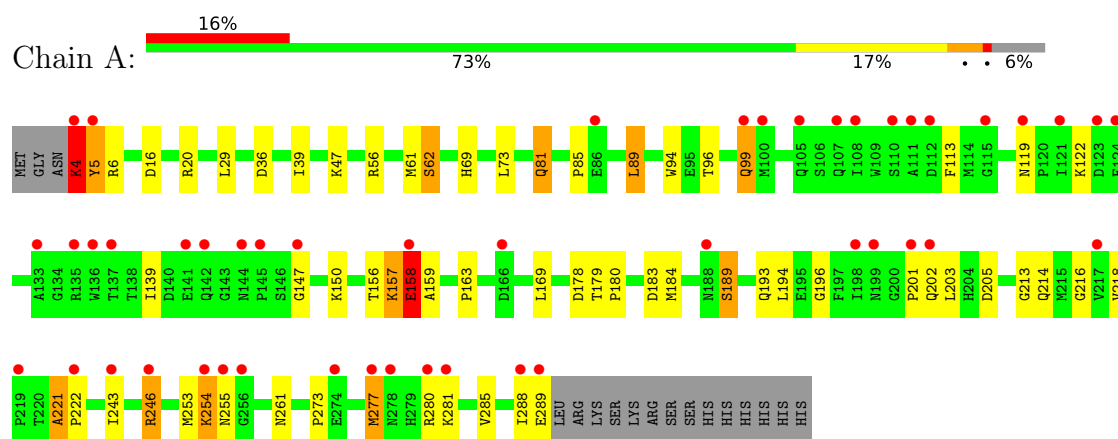
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	165	Total 165	O 165	0	0
3	B	170	Total 170	O 170	0	0

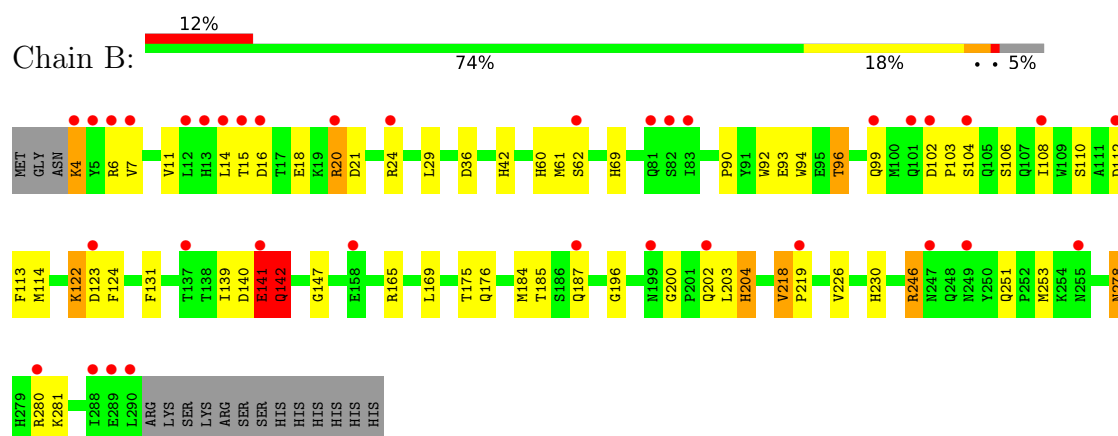
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Tyrosinase



• Molecule 1: Tyrosinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.90Å 78.33Å 82.16Å 90.00° 105.50° 90.00°	Depositor
Resolution (Å)	39.39 – 1.90 39.39 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.3 (39.39-1.90) 97.3 (39.39-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.19 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.7.3 _928	Depositor
R, R_{free}	0.193 , 0.210 0.196 , 0.216	Depositor DCC
R_{free} test set	2619 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5037	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	1.00	19/2424 (0.8%)	0.92	5/3303 (0.2%)
1	B	0.99	13/2432 (0.5%)	0.99	11/3314 (0.3%)
All	All	1.00	32/4856 (0.7%)	0.95	16/6617 (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	A	0	1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	113	PHE	C-O	-7.35	1.14	1.24
1	B	204	HIS	CG-ND1	-7.34	1.30	1.38
1	B	203	LEU	C-O	-7.06	1.17	1.24
1	B	60	HIS	CG-ND1	-6.82	1.30	1.38
1	A	69	HIS	CG-ND1	-6.68	1.30	1.38
1	A	62	SER	C-O	-6.65	1.16	1.23
1	A	157	LYS	C-O	-6.40	1.16	1.24
1	A	218	VAL	C-O	-6.35	1.16	1.24
1	A	180	PRO	C-O	-6.16	1.19	1.25
1	B	42	HIS	CG-ND1	-6.08	1.31	1.38
1	A	113	PHE	C-O	-6.04	1.16	1.24
1	A	69	HIS	CD2-NE2	-6.00	1.31	1.37
1	A	16	ASP	C-O	-5.88	1.17	1.24
1	A	214	GLN	C-O	-5.85	1.17	1.24
1	B	103	PRO	C-N	-5.77	1.26	1.33
1	A	156	THR	C-O	-5.52	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	ILE	C-O	-5.44	1.18	1.24
1	A	159	ALA	C-O	-5.40	1.17	1.23
1	A	158	GLU	C-O	-5.36	1.17	1.24
1	A	20	ARG	C-O	-5.34	1.17	1.24
1	B	69	HIS	CG-ND1	-5.32	1.32	1.38
1	B	218	VAL	C-O	-5.31	1.18	1.24
1	B	175	THR	C-O	-5.23	1.17	1.24
1	B	69	HIS	C-O	-5.23	1.17	1.24
1	B	140	ASP	C-O	-5.22	1.17	1.23
1	A	179	THR	C-O	-5.21	1.18	1.24
1	B	18	GLU	C-O	-5.16	1.18	1.24
1	A	216	GLY	C-O	-5.15	1.17	1.23
1	A	221	ALA	C-O	-5.12	1.19	1.24
1	A	246	ARG	C-O	-5.05	1.17	1.24
1	A	36	ASP	C-O	-5.05	1.17	1.24
1	B	184	MET	C-N	-5.00	1.25	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	GLY	N-CA-C	9.43	128.73	115.43
1	B	16	ASP	N-CA-C	-7.53	103.00	111.14
1	A	180	PRO	O-C-N	7.36	124.70	121.31
1	B	142	GLN	N-CA-C	-7.17	104.56	113.38
1	B	16	ASP	N-CA-CB	-6.51	100.62	110.07
1	B	122	LYS	CA-C-N	-6.22	113.42	122.19
1	B	122	LYS	C-N-CA	-6.22	113.42	122.19
1	B	141	GLU	N-CA-C	6.10	120.45	113.19
1	A	6	ARG	N-CA-C	-6.05	99.79	109.96
1	A	180	PRO	CA-C-O	-5.98	116.60	120.90
1	A	5	TYR	N-CA-CB	5.97	119.55	110.95
1	B	124	PHE	N-CA-C	5.88	119.76	112.24
1	B	20	ARG	N-CA-C	-5.28	105.70	111.82
1	B	218	VAL	O-C-N	5.27	123.81	120.07
1	B	147	GLY	N-CA-C	5.23	122.54	115.32
1	B	15	THR	N-CA-C	-5.13	104.09	110.41

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4	LYS	Peptide

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	2346	0	2225	45	0
1	B	2354	0	2236	65	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	165	0	0	5	0
3	B	170	0	0	2	0
All	All	5037	0	4461	109	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 12.

All (109) 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:4:LYS:N	1:B:4:LYS:HD2	1.56	1.17
1:A:158:GLU:N	1:A:158:GLU:OE2	1.79	1.15
1:A:61:MET:SD	1:A:184:MET:CE	2.38	1.11
1:A:4:LYS:N	1:A:4:LYS:HD3	1.50	1.09
1:B:4:LYS:HG3	1:B:280:ARG:HB3	1.30	1.07
1:B:99:GLN:HE22	1:B:165:ARG:NH1	1.50	1.07
1:A:62:SER:HB3	3:A:664:HOH:O	1.61	1.01
1:A:253:MET:SD	3:A:665:HOH:O	2.20	0.96
1:A:4:LYS:N	1:A:4:LYS:CD	2.29	0.95
1:B:99:GLN:NE2	1:B:165:ARG:HD2	1.82	0.95
1:A:61:MET:SD	1:A:184:MET:HE2	2.08	0.92
1:B:4:LYS:N	1:B:4:LYS:CD	2.32	0.88
1:B:253:MET:SD	3:B:580:HOH:O	2.30	0.88
1:B:61:MET:HE3	3:B:669:HOH:O	1.75	0.86
1:A:61:MET:HG2	1:A:184:MET:HE2	1.57	0.85
1:B:99:GLN:HE22	1:B:165:ARG:CZ	1.91	0.84
1:A:61:MET:CG	1:A:184:MET:HE2	2.08	0.83
1:A:158:GLU:H	1:A:158:GLU:CD	1.87	0.82
1:B:99:GLN:HE22	1:B:165:ARG:HH11	1.25	0.82
1:B:122:LYS:O	1:B:123:ASP:HB2	1.83	0.78
1:A:61:MET:SD	1:A:184:MET:HE1	2.22	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:GLN:NE2	1:B:165:ARG:NH1	2.29	0.77
1:B:4:LYS:HG3	1:B:280:ARG:CB	2.15	0.72
1:B:99:GLN:NE2	1:B:165:ARG:CZ	2.52	0.72
1:A:254:LYS:HG2	1:A:255:ASN:H	1.56	0.70
1:B:99:GLN:NE2	1:B:165:ARG:CD	2.54	0.69
1:B:6:ARG:HG3	1:B:6:ARG:HH11	1.57	0.69
1:B:11:VAL:HA	1:B:14:LEU:HD12	1.75	0.69
1:B:278:ASN:HD22	1:B:281:LYS:H	1.41	0.67
1:A:194:LEU:HA	1:A:203:LEU:HD13	1.77	0.67
1:B:142:GLN:N	1:B:142:GLN:NE2	2.42	0.66
1:B:99:GLN:HE22	1:B:165:ARG:HD2	1.62	0.65
1:B:94:TRP:HE1	1:B:230:HIS:HD1	1.46	0.64
1:B:14:LEU:HD11	1:B:90:PRO:HB3	1.80	0.63
1:A:61:MET:CG	1:A:184:MET:CE	2.74	0.63
1:B:278:ASN:ND2	1:B:281:LYS:H	1.98	0.62
1:B:20:ARG:O	1:B:20:ARG:HD3	2.01	0.61
1:A:243:ILE:HD12	3:A:561:HOH:O	2.02	0.59
1:B:20:ARG:HD3	1:B:20:ARG:C	2.27	0.58
1:B:114:MET:HE2	1:B:131:PHE:HE1	1.67	0.58
1:B:218:VAL:N	1:B:219:PRO:HD2	2.18	0.57
1:B:4:LYS:CG	1:B:280:ARG:HB3	2.21	0.57
1:A:288:ILE:O	1:A:289:GLU:C	2.47	0.57
1:B:93:GLU:HG2	1:B:96:THR:HG23	1.86	0.57
1:A:150:LYS:O	1:A:213:GLY:HA3	2.04	0.57
1:A:4:LYS:O	1:A:285:VAL:HG22	2.04	0.56
1:A:254:LYS:HG2	1:A:255:ASN:N	2.18	0.56
1:B:99:GLN:HE22	1:B:165:ARG:CD	2.18	0.56
1:B:108:ILE:HG12	1:B:108:ILE:O	2.06	0.56
1:A:94:TRP:CE3	1:A:163:PRO:HG2	2.41	0.56
1:B:278:ASN:ND2	1:B:281:LYS:HG3	2.21	0.56
1:B:196:GLY:HA3	1:B:202:GLN:O	2.07	0.54
1:B:99:GLN:HE21	1:B:165:ARG:HD2	1.70	0.54
1:A:4:LYS:HD3	1:A:280:ARG:HH21	1.73	0.54
1:B:99:GLN:OE1	1:B:165:ARG:CZ	2.57	0.53
1:B:96:THR:HB	1:B:165:ARG:HH21	1.74	0.53
1:B:102:ASP:OD1	1:B:104:SER:HB3	2.08	0.52
1:B:61:MET:O	1:B:62:SER:HB2	2.09	0.52
1:B:93:GLU:OE1	1:B:96:THR:HG21	2.09	0.52
1:B:142:GLN:N	1:B:142:GLN:HE21	2.08	0.52
1:B:110:SER:OG	1:B:112:ASP:OD1	2.26	0.50
1:B:196:GLY:CA	1:B:202:GLN:O	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ILE:CD1	3:A:561:HOH:O	2.56	0.50
1:B:99:GLN:NE2	1:B:165:ARG:NE	2.59	0.50
1:B:20:ARG:C	1:B:20:ARG:CD	2.85	0.49
1:B:36:ASP:OD2	1:B:139:ILE:HD13	2.13	0.49
1:B:14:LEU:HD11	1:B:90:PRO:CB	2.42	0.49
1:B:99:GLN:CD	1:B:165:ARG:CZ	2.85	0.49
1:B:106:SER:OG	1:B:108:ILE:HG22	2.13	0.49
1:A:119:ASN:HD22	1:A:122:LYS:HE3	1.79	0.48
1:A:39:ILE:HG12	1:A:222:PRO:HB2	1.96	0.48
1:A:81:GLN:HG3	1:A:85:PRO:HA	1.96	0.47
1:A:196:GLY:CA	1:A:202:GLN:O	2.62	0.47
1:A:4:LYS:HE3	1:A:280:ARG:HE	1.80	0.47
1:A:273:PRO:O	1:A:277:MET:HE2	2.16	0.47
1:B:185:THR:O	1:B:187:GLN:HG2	2.15	0.46
1:B:246:ARG:HA	1:B:246:ARG:HD2	1.53	0.46
1:B:6:ARG:HG3	1:B:6:ARG:NH1	2.29	0.46
1:B:20:ARG:HG2	1:B:20:ARG:HH11	1.79	0.46
1:B:94:TRP:NE1	1:B:230:HIS:HD1	2.11	0.46
1:A:4:LYS:O	1:A:285:VAL:CG2	2.63	0.46
1:B:204:HIS:HD2	1:B:230:HIS:NE2	2.14	0.46
1:A:254:LYS:O	1:A:261:ASN:CG	2.60	0.45
1:B:93:GLU:OE1	1:B:96:THR:CG2	2.65	0.45
1:A:56:ARG:HD3	1:A:62:SER:OG	2.17	0.45
1:B:99:GLN:HE22	1:B:165:ARG:NE	2.15	0.45
1:B:122:LYS:O	1:B:123:ASP:CB	2.48	0.44
1:A:96:THR:O	1:A:99:GLN:HG2	2.17	0.44
1:B:92:TRP:CG	1:B:108:ILE:CD1	3.01	0.44
1:A:178:ASP:HA	1:A:189:SER:HB2	1.99	0.44
1:A:196:GLY:HA3	1:A:202:GLN:O	2.17	0.43
1:A:183:ASP:HB2	3:A:520:HOH:O	2.19	0.43
1:B:200:GLY:HA2	1:B:202:GLN:HG2	2.00	0.43
1:A:61:MET:SD	1:A:184:MET:HE3	2.48	0.42
1:B:278:ASN:HD22	1:B:278:ASN:C	2.28	0.42
1:B:122:LYS:O	1:B:123:ASP:C	2.58	0.42
1:B:176:GLN:NE2	1:B:251:GLN:HE22	2.17	0.42
1:A:73:LEU:HD22	1:A:89:LEU:HD11	2.00	0.42
1:A:47:LYS:HE3	1:B:141:GLU:O	2.19	0.42
1:A:201:PRO:HB3	1:A:205:ASP:OD2	2.20	0.42
1:B:21:ASP:OD1	1:B:24:ARG:NH2	2.52	0.42
1:B:141:GLU:C	1:B:142:GLN:NE2	2.78	0.42
1:A:119:ASN:ND2	1:A:122:LYS:HE3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:VAL:N	1:B:219:PRO:CD	2.82	0.41
1:A:221:ALA:N	1:A:222:PRO:CD	2.84	0.41
1:A:280:ARG:HG2	1:A:285:VAL:HG12	2.01	0.41
1:A:202:GLN:O	1:A:203:LEU:HB2	2.21	0.41
1:A:196:GLY:HA2	1:A:202:GLN:O	2.21	0.41
1:A:193:GLN:O	1:A:203:LEU:HD12	2.20	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	284/303 (94%)	272 (96%)	12 (4%)	0	100	100
1	B	285/303 (94%)	277 (97%)	8 (3%)	0	100	100
All	All	569/606 (94%)	549 (96%)	20 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	249/265 (94%)	235 (94%)	14 (6%)	19	11
1	B	250/265 (94%)	240 (96%)	10 (4%)	28	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	499/530 (94%)	475 (95%)	24 (5%)	23	15

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	5	TYR
1	A	29	LEU
1	A	81	GLN
1	A	89	LEU
1	A	99	GLN
1	A	157	LYS
1	A	158	GLU
1	A	169	LEU
1	A	189	SER
1	A	246	ARG
1	A	254	LYS
1	A	277	MET
1	A	281	LYS
1	B	4	LYS
1	B	7	VAL
1	B	29	LEU
1	B	96	THR
1	B	141	GLU
1	B	142	GLN
1	B	169	LEU
1	B	226	VAL
1	B	246	ARG
1	B	278	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	144	ASN
1	A	193	GLN
1	A	199	ASN
1	A	270	ASN
1	B	99	GLN
1	B	142	GLN
1	B	176	GLN

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Mol	Chain	Res	Type
1	B	204	HIS
1	B	278	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	286/303 (94%)	0.82	47 (16%) 4 4	10, 22, 46, 96	1 (0%)
1	B	287/303 (94%)	0.67	36 (12%) 8 8	8, 21, 45, 104	1 (0%)
All	All	573/606 (94%)	0.75	83 (14%) 6 6	8, 21, 47, 104	2 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	288	ILE	8.1
1	A	254	LYS	7.4
1	A	5	TYR	7.1
1	A	255	ASN	7.1
1	B	5	TYR	6.9
1	A	256	GLY	6.7
1	B	289	GLU	6.3
1	B	7	VAL	5.8
1	B	290	LEU	5.1
1	A	110	SER	5.1
1	B	158	GLU	4.7
1	B	15	THR	4.4
1	A	121	ILE	4.3
1	B	255	ASN	4.3
1	B	101	GLN	4.0
1	B	16	ASP	4.0
1	B	102	ASP	4.0
1	B	108	ILE	3.8
1	B	62	SER	3.7
1	A	123	ASP	3.7
1	B	247	ASN	3.7
1	B	14	LEU	3.6
1	A	86	GLU	3.6
1	A	201	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	82	SER	3.5
1	A	278	ASN	3.5
1	A	202	GLN	3.5
1	A	133	ALA	3.5
1	A	280	ARG	3.5
1	B	199	ASN	3.4
1	B	24	ARG	3.4
1	A	4	LYS	3.3
1	B	141	GLU	3.3
1	A	277	MET	3.3
1	A	119	ASN	3.3
1	A	135	ARG	3.2
1	B	4	LYS	3.1
1	B	99	GLN	3.1
1	A	112	ASP	3.1
1	A	166	ASP	3.0
1	B	123	ASP	3.0
1	A	99	GLN	2.9
1	B	81	GLN	2.9
1	A	188	ASN	2.8
1	A	107	GLN	2.8
1	A	217	VAL	2.8
1	B	20	ARG	2.8
1	A	137	THR	2.8
1	A	158	GLU	2.7
1	B	288	ILE	2.7
1	A	136	TRP	2.7
1	B	12	LEU	2.7
1	B	6	ARG	2.6
1	A	142	GLN	2.6
1	A	222	PRO	2.6
1	A	243	ILE	2.6
1	A	115	GLY	2.6
1	A	147	GLY	2.6
1	A	274	GLU	2.5
1	A	111	ALA	2.5
1	B	112	ASP	2.5
1	B	249	ASN	2.4
1	B	219	PRO	2.3
1	A	199	ASN	2.3
1	A	105	GLN	2.2
1	B	187	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	202	GLN	2.2
1	B	13	HIS	2.2
1	B	280	ARG	2.2
1	A	145	PRO	2.2
1	A	246	ARG	2.2
1	A	281	LYS	2.2
1	A	124	PHE	2.1
1	A	108	ILE	2.1
1	B	83	ILE	2.1
1	B	137	THR	2.1
1	A	141	GLU	2.1
1	A	100	MET	2.1
1	A	198	ILE	2.1
1	B	104	SER	2.1
1	A	289	GLU	2.1
1	A	219	PRO	2.1
1	A	144	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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(Å ²)	Q<0.9
2	CU	A	401	1/1	0.86	0.11	27,27,27,27	1
2	CU	B	401	1/1	0.93	0.11	33,33,33,33	1

6.5 Other polymers [i](#)

There are no such residues in this entry.