



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:22 PM UTC

PDB ID : 3NM8 / pdb_00003nm8
Title : Crystal structure of Tyrosinase from *Bacillus megaterium*
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Deposited on : 2010-06-22
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

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

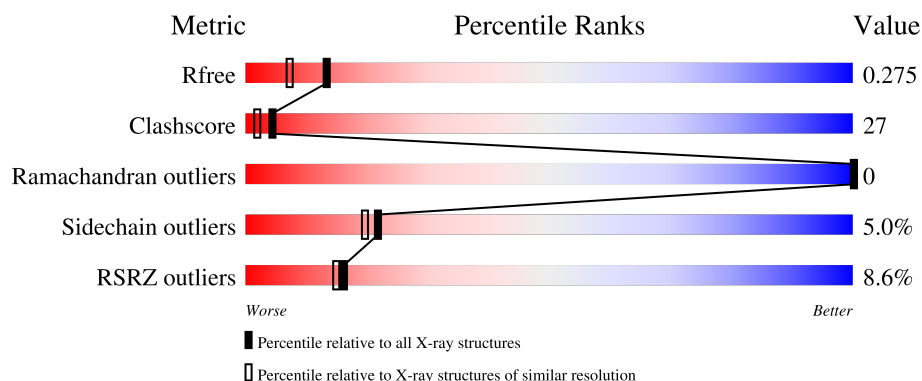
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	8% 58% 32% 6%
1	B	303	8% 56% 34% 5% 6%

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	CL	A	507	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5041 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	285	Total	C	N	O	S	0	1	0
			2348	1493	426	421	8			
1	B	285	Total	C	N	O	S	0	0	0
			2337	1487	422	420	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 (CCD ID: CU) (formula: Cu).

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Cl 2	0	0
4	B	4	Total 4	Cl 4	0	0

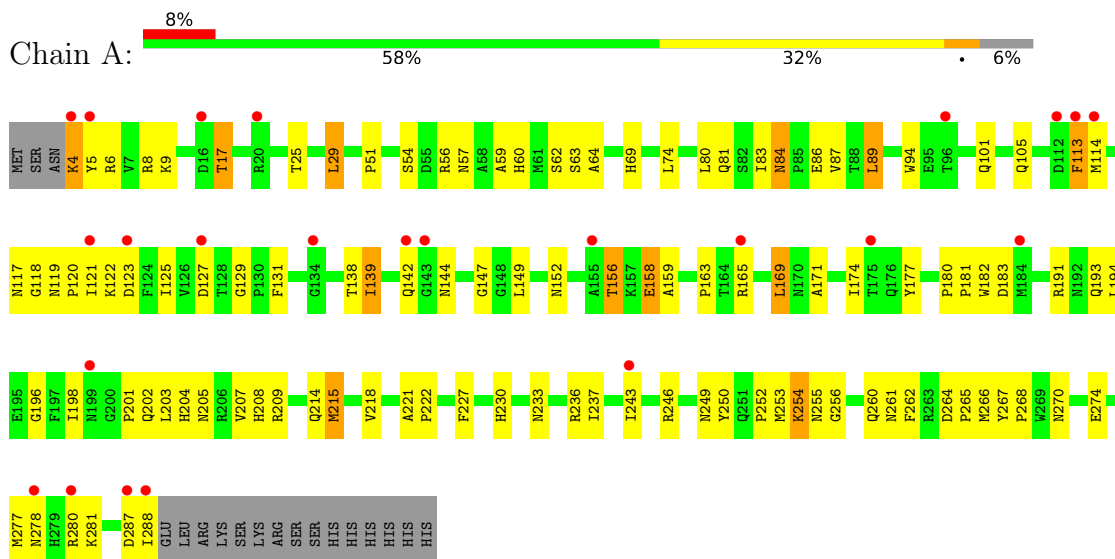
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	187	Total 187	O 187	0	0
5	B	152	Total 152	O 152	0	0

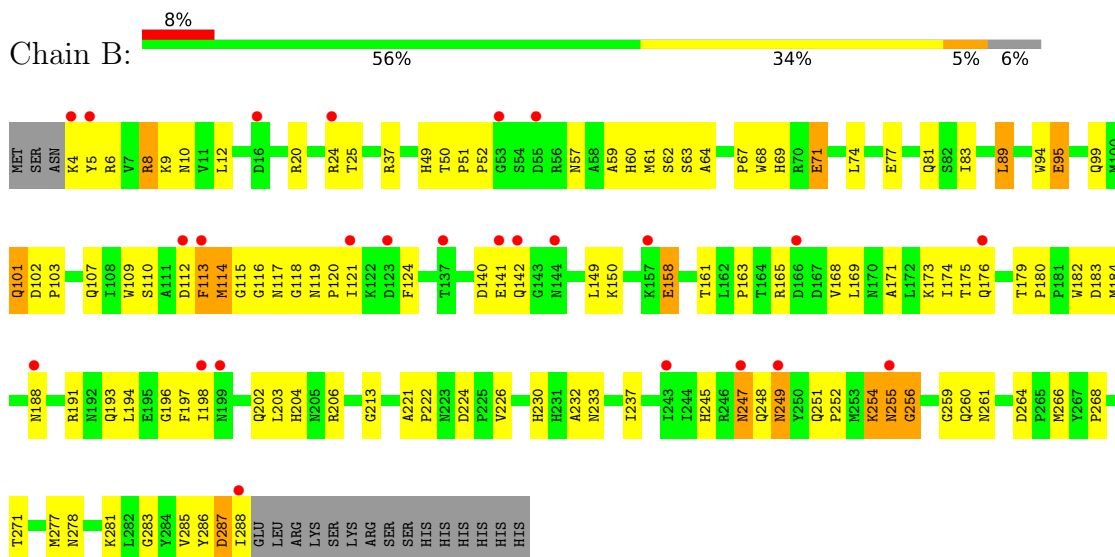
3 Residue-property plots [i](#)

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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.21Å 84.49Å 146.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 50.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.00) 97.8 (50.00-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.00Å)	Xtriage
Refinement program	CNS, REFMAC 5.5.0072	Depositor
R, R_{free}	0.220 , 0.273 0.228 , 0.275	Depositor DCC
R_{free} test set	4281 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5041	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CU, CL

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	0.67	6/2426 (0.2%)	0.99	8/3305 (0.2%)
1	B	0.63	3/2415 (0.1%)	0.97	17/3291 (0.5%)
All	All	0.65	9/4841 (0.2%)	0.98	25/6596 (0.4%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	LEU	C-O	-9.81	1.15	1.24
1	A	5	TYR	N-CA	-7.60	1.36	1.46
1	A	69	HIS	C-O	-6.46	1.15	1.24
1	A	215	MET	SD-CE	-6.25	1.64	1.79
1	B	114	MET	C-O	-6.19	1.16	1.24
1	A	5	TYR	C-O	-5.72	1.16	1.23
1	A	138	THR	C-O	-5.53	1.16	1.23
1	B	109	TRP	C-N	-5.39	1.26	1.33
1	B	140	ASP	C-O	-5.32	1.17	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	113	PHE	N-CA-C	7.33	126.41	110.80
1	A	113	PHE	N-CA-C	6.48	124.60	110.80
1	B	256	GLY	N-CA-C	-6.40	99.28	112.34
1	B	287	ASP	N-CA-C	-6.20	101.50	110.24
1	A	218	VAL	CB-CA-C	-5.88	108.11	113.70
1	A	63	SER	N-CA-C	5.79	118.33	111.33
1	B	124	PHE	N-CA-C	5.75	119.60	112.24
1	B	63	SER	N-CA-C	5.49	117.98	111.33
1	B	259	GLY	N-CA-C	-5.46	107.78	115.32
1	B	256	GLY	CA-C-N	5.38	125.28	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	GLY	C-N-CA	5.38	125.28	119.85
1	A	147	GLY	N-CA-C	5.38	122.20	115.21
1	A	9	LYS	N-CA-C	5.36	118.73	110.42
1	B	116	GLY	N-CA-C	5.32	120.39	112.41
1	B	232	ALA	N-CA-C	-5.28	105.70	111.82
1	B	10	ASN	N-CA-C	-5.24	102.53	110.28
1	B	9	LYS	N-CA-C	5.23	118.25	110.14
1	B	101	GLN	N-CA-C	-5.19	105.51	111.07
1	B	255	ASN	CB-CA-C	-5.19	102.60	111.26
1	B	287	ASP	CA-C-N	-5.19	112.37	121.70
1	B	287	ASP	C-N-CA	-5.19	112.37	121.70
1	A	129	GLY	CA-C-N	5.18	124.85	119.56
1	A	129	GLY	C-N-CA	5.18	124.85	119.56
1	B	115	GLY	N-CA-C	-5.16	105.17	112.81
1	A	177	TYR	N-CA-C	-5.14	105.57	111.07

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	2348	0	2233	124	0
1	B	2337	0	2221	121	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
4	A	2	0	0	4	0
4	B	4	0	0	1	0
5	A	187	0	0	13	0
5	B	152	0	0	14	0
All	All	5041	0	4454	242	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 27.

All (242) 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:254:LYS:NZ	1:B:255:ASN:HB2	1.56	1.19
1:B:254:LYS:HZ3	1:B:255:ASN:HB2	0.94	1.11
1:B:288:ILE:O	1:B:288:ILE:HG22	1.54	1.05
1:B:287:ASP:O	1:B:288:ILE:HB	1.53	1.04
1:B:64:ALA:H	1:B:260:GLN:NE2	1.58	1.01
1:B:176:GLN:HE21	1:B:251:GLN:HE22	1.00	0.97
1:A:4:LYS:HG3	1:A:280:ARG:HG3	1.43	0.97
1:A:4:LYS:HZ3	1:A:280:ARG:HG2	1.29	0.96
1:A:256:GLY:H	1:A:261:ASN:HD21	1.01	0.92
1:B:95:GLU:HG2	1:B:168:VAL:HG21	1.53	0.90
1:A:156:THR:HG22	1:A:159:ALA:H	1.39	0.87
1:B:247:ASN:HD22	1:B:247:ASN:H	1.22	0.87
1:A:17:THR:HG22	5:A:306:HOH:O	1.73	0.87
1:B:67:PRO:HG2	1:B:266:MET:HE1	1.60	0.84
1:B:8:ARG:HG2	1:B:89:LEU:O	1.77	0.84
1:B:57:ASN:HD21	1:B:60:HIS:HD1	1.25	0.83
1:A:64:ALA:H	1:A:260:GLN:HE22	1.26	0.83
1:B:176:GLN:HE21	1:B:251:GLN:NE2	1.76	0.82
1:B:247:ASN:H	1:B:247:ASN:ND2	1.75	0.82
1:B:256:GLY:H	1:B:261:ASN:HD21	1.28	0.81
1:A:256:GLY:N	1:A:261:ASN:HD21	1.78	0.81
1:A:4:LYS:CG	1:A:280:ARG:HG3	2.11	0.80
1:A:287:ASP:O	1:A:288:ILE:CG1	2.30	0.79
1:A:4:LYS:HG2	1:A:280:ARG:HD2	1.63	0.79
1:A:215:MET:HE1	1:A:227:PHE:HD2	1.47	0.78
1:B:71:GLU:CG	1:B:271:THR:HG21	2.14	0.78
1:A:57:ASN:HD21	1:A:60:HIS:HD1	1.32	0.77
1:B:254:LYS:NZ	1:B:255:ASN:CB	2.46	0.76
1:B:202:GLN:HE21	1:B:202:GLN:HA	1.52	0.74
1:A:287:ASP:O	1:A:288:ILE:CB	2.36	0.74
1:B:64:ALA:H	1:B:260:GLN:HE21	1.36	0.73
1:A:6:ARG:HD3	1:A:81:GLN:OE1	1.89	0.71
1:A:8:ARG:HG2	1:A:89:LEU:O	1.90	0.71
1:B:113:PHE:O	1:B:114:MET:HE2	1.91	0.71
1:A:119:ASN:C	1:A:119:ASN:HD22	1.97	0.70
1:A:74:LEU:HA	5:A:349:HOH:O	1.92	0.70
1:B:249:ASN:HD22	1:B:249:ASN:H	1.39	0.70
1:A:254:LYS:HD3	1:A:255:ASN:ND2	2.06	0.70
1:A:215:MET:HE1	1:A:227:PHE:CD2	2.27	0.69
1:B:64:ALA:H	1:B:260:GLN:HE22	1.38	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LYS:CG	1:A:280:ARG:CG	2.70	0.69
1:A:287:ASP:O	1:A:288:ILE:HG13	1.90	0.69
1:A:215:MET:CE	1:A:227:PHE:HB2	2.24	0.68
1:B:57:ASN:ND2	1:B:60:HIS:H	1.92	0.68
1:B:117:ASN:ND2	1:B:118:GLY:H	1.91	0.67
1:A:193:GLN:HG2	1:A:198:ILE:HG13	1.77	0.67
1:A:165:ARG:HG3	5:A:321:HOH:O	1.94	0.66
1:B:277:MET:HE1	5:B:327:HOH:O	1.94	0.66
1:A:64:ALA:H	1:A:260:GLN:NE2	1.92	0.66
1:A:254:LYS:O	1:A:255:ASN:HB2	1.94	0.66
1:A:4:LYS:NZ	1:A:280:ARG:HG2	2.08	0.66
1:A:94:TRP:CE3	1:A:163:PRO:HG2	2.30	0.65
1:A:142:GLN:HE21	1:A:144:ASN:HD22	1.43	0.65
1:B:69:HIS:NE2	5:B:307:HOH:O	2.27	0.65
1:B:49:HIS:NE2	5:B:312:HOH:O	2.29	0.65
1:A:288:ILE:HD11	4:A:507:CL:CL	2.33	0.65
1:B:57:ASN:HD22	1:B:59:ALA:H	1.45	0.64
1:A:142:GLN:HE21	1:A:144:ASN:ND2	1.96	0.64
1:A:4:LYS:HG2	1:A:280:ARG:CD	2.27	0.64
1:B:57:ASN:ND2	1:B:60:HIS:HD1	1.95	0.64
1:A:105:GLN:HG3	5:A:406:HOH:O	1.98	0.63
1:A:287:ASP:O	1:A:288:ILE:HB	1.97	0.63
1:A:243:ILE:HD11	5:A:331:HOH:O	1.98	0.63
1:B:119:ASN:C	1:B:119:ASN:HD22	2.05	0.63
1:B:254:LYS:HZ1	1:B:255:ASN:HB2	1.61	0.63
1:B:61:MET:HE2	5:B:440:HOH:O	1.97	0.63
1:A:278:ASN:ND2	1:A:281:LYS:HD3	2.13	0.63
1:B:71:GLU:HG2	1:B:271:THR:HG21	1.80	0.63
1:B:117:ASN:HD22	1:B:118:GLY:H	1.46	0.63
1:B:67:PRO:HG2	1:B:266:MET:CE	2.29	0.62
1:A:221:ALA:HB3	1:A:222:PRO:HD3	1.81	0.62
1:A:8:ARG:NH1	5:A:349:HOH:O	2.31	0.61
1:A:158:GLU:HG2	1:A:201:PRO:HD3	1.80	0.61
1:A:62:SER:HB3	5:A:328:HOH:O	1.99	0.61
1:A:156:THR:HB	5:A:396:HOH:O	1.99	0.61
1:A:288:ILE:CD1	4:A:507:CL:CL	2.85	0.61
1:A:288:ILE:HG13	4:A:507:CL:CL	2.38	0.61
1:B:94:TRP:HE1	1:B:230:HIS:HD2	1.48	0.61
1:B:94:TRP:CE3	1:B:163:PRO:HG2	2.36	0.60
1:A:4:LYS:HG2	1:A:280:ARG:CG	2.31	0.60
1:B:71:GLU:HG3	1:B:271:THR:HG21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:MET:HE1	1:A:227:PHE:HB2	1.83	0.60
1:B:174:ILE:HD12	1:B:174:ILE:N	2.16	0.60
1:A:156:THR:CG2	1:A:159:ALA:H	2.11	0.60
1:A:233:ASN:O	1:A:237:ILE:HG12	2.02	0.60
1:B:176:GLN:NE2	1:B:251:GLN:HE22	1.85	0.60
1:B:24:ARG:HD3	5:B:317:HOH:O	2.00	0.60
1:B:103:PRO:HG3	5:B:320:HOH:O	2.02	0.59
1:B:64:ALA:N	1:B:260:GLN:NE2	2.41	0.59
1:A:119:ASN:ND2	1:A:121:ILE:H	2.00	0.59
1:B:158:GLU:CD	1:B:158:GLU:H	2.11	0.59
1:A:57:ASN:ND2	1:A:60:HIS:H	1.99	0.59
1:A:278:ASN:HD22	1:A:281:LYS:HB2	1.66	0.59
1:A:119:ASN:HD22	1:A:120:PRO:N	2.01	0.59
1:A:114:MET:HE2	1:A:131:PHE:HE1	1.68	0.59
1:A:4:LYS:HG3	1:A:280:ARG:CG	2.26	0.58
1:B:174:ILE:HD12	1:B:174:ILE:H	1.67	0.58
1:A:278:ASN:HD22	1:A:281:LYS:HD3	1.67	0.58
1:A:117:ASN:ND2	1:A:118:GLY:H	2.01	0.58
1:A:122:LYS:HE2	1:A:127:ASP:HB3	1.85	0.58
1:A:152:ASN:ND2	5:A:367:HOH:O	2.33	0.58
1:B:202:GLN:HA	1:B:202:GLN:NE2	2.18	0.58
1:B:288:ILE:O	1:B:288:ILE:CG2	2.30	0.58
1:B:288:ILE:HG13	4:B:507:CL:CL	2.41	0.58
1:A:156:THR:HG22	1:A:159:ALA:N	2.16	0.57
1:A:84:ASN:HD22	1:A:86:GLU:H	1.52	0.57
1:A:158:GLU:HG2	1:A:201:PRO:CD	2.34	0.57
1:B:248:GLN:HG3	5:B:361:HOH:O	2.04	0.57
1:B:20:ARG:HG3	1:B:20:ARG:HH11	1.68	0.57
1:A:139:ILE:HD11	1:B:52:PRO:HB3	1.87	0.56
1:B:62:SER:HB3	5:B:401:HOH:O	2.04	0.56
1:A:215:MET:HE3	1:A:221:ALA:O	2.05	0.56
1:A:94:TRP:HE1	1:A:230:HIS:HD2	1.54	0.56
1:A:215:MET:HE2	1:A:215:MET:HA	1.87	0.56
1:B:64:ALA:HB1	1:B:266:MET:CE	2.35	0.56
1:B:188:ASN:HB2	5:B:396:HOH:O	2.04	0.55
1:A:84:ASN:HD22	1:A:84:ASN:C	2.14	0.55
1:B:249:ASN:HD22	1:B:249:ASN:N	2.01	0.55
1:A:181:PRO:HG2	1:A:183:ASP:OD2	2.07	0.55
1:A:256:GLY:H	1:A:261:ASN:ND2	1.86	0.54
1:A:202:GLN:HA	1:A:202:GLN:NE2	2.21	0.54
1:B:6:ARG:HB2	1:B:283:GLY:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ASN:ND2	1:B:121:ILE:H	2.06	0.53
1:A:246:ARG:HG3	1:A:246:ARG:HH11	1.73	0.53
1:B:184:MET:HG3	5:B:377:HOH:O	2.09	0.53
1:B:8:ARG:HD2	1:B:77:GLU:OE2	2.08	0.53
1:B:68:TRP:N	1:B:266:MET:HE1	2.23	0.53
1:A:215:MET:CE	1:A:221:ALA:O	2.57	0.53
1:B:101:GLN:HE22	1:B:102:ASP:HB2	1.74	0.52
1:B:179:THR:HB	1:B:180:PRO:HD2	1.92	0.52
1:A:261:ASN:HB2	1:A:264:ASP:OD2	2.09	0.52
1:B:64:ALA:N	1:B:260:GLN:HE21	2.06	0.52
1:B:196:GLY:HA3	1:B:202:GLN:O	2.09	0.52
1:B:278:ASN:OD1	1:B:281:LYS:HG3	2.10	0.51
1:A:101:GLN:HA	1:A:101:GLN:NE2	2.26	0.51
1:A:29:LEU:HD22	1:A:80:LEU:HD23	1.91	0.51
1:B:6:ARG:HD3	1:B:81:GLN:OE1	2.10	0.51
1:B:175:THR:O	1:B:248:GLN:HG2	2.11	0.51
1:A:254:LYS:O	1:A:255:ASN:CB	2.59	0.51
1:B:221:ALA:HB3	1:B:222:PRO:HD3	1.92	0.51
1:A:183:ASP:HB2	5:A:366:HOH:O	2.11	0.51
1:A:265:PRO:HB3	1:A:270:ASN:HA	1.91	0.51
1:B:150:LYS:O	1:B:213:GLY:HA3	2.12	0.50
1:A:215:MET:HE3	1:A:227:PHE:HB2	1.94	0.50
1:B:249:ASN:N	1:B:249:ASN:ND2	2.60	0.50
1:B:165:ARG:HG3	5:B:406:HOH:O	2.12	0.49
1:B:255:ASN:CG	1:B:255:ASN:O	2.54	0.49
1:B:278:ASN:CG	1:B:281:LYS:HG3	2.37	0.49
1:B:286:TYR:O	1:B:287:ASP:C	2.55	0.49
1:B:249:ASN:H	1:B:249:ASN:ND2	2.07	0.49
1:A:57:ASN:HD22	1:A:59:ALA:H	1.61	0.49
1:A:101:GLN:HA	1:A:101:GLN:HE21	1.77	0.49
1:B:57:ASN:ND2	1:B:60:HIS:N	2.59	0.49
1:B:287:ASP:O	1:B:287:ASP:OD1	2.30	0.49
1:A:114:MET:HE2	1:A:131:PHE:CE1	2.48	0.48
1:B:182:TRP:CZ2	1:B:252:PRO:HB3	2.48	0.48
1:A:278:ASN:ND2	1:A:281:LYS:HB2	2.28	0.48
1:A:171:ALA:O	1:A:174:ILE:HG12	2.12	0.48
1:B:101:GLN:NE2	1:B:102:ASP:HB2	2.28	0.48
1:A:180:PRO:HA	1:A:182:TRP:N	2.28	0.48
1:A:119:ASN:HB3	1:A:122:LYS:HD3	1.95	0.48
1:B:57:ASN:HD21	1:B:60:HIS:N	2.11	0.48
1:B:119:ASN:C	1:B:119:ASN:ND2	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ASP:HB2	5:B:377:HOH:O	2.14	0.48
1:B:233:ASN:O	1:B:237:ILE:HG12	2.14	0.48
1:A:84:ASN:ND2	1:A:86:GLU:H	2.11	0.47
1:B:121:ILE:HG22	1:B:121:ILE:O	2.14	0.47
1:B:163:PRO:HB3	5:B:351:HOH:O	2.14	0.47
1:A:288:ILE:CG1	4:A:507:CL:CL	3.00	0.47
1:B:113:PHE:C	1:B:114:MET:HE2	2.39	0.47
1:B:94:TRP:NE1	1:B:230:HIS:HD2	2.13	0.47
1:B:8:ARG:CG	1:B:89:LEU:O	2.56	0.47
1:A:156:THR:HG23	1:A:158:GLU:H	1.80	0.46
1:B:25:THR:HG23	1:B:83:ILE:HB	1.96	0.46
1:A:267:TYR:CD1	1:A:268:PRO:HA	2.50	0.46
1:A:122:LYS:O	1:A:123:ASP:HB2	2.16	0.46
1:A:287:ASP:O	1:A:287:ASP:CG	2.57	0.46
1:B:119:ASN:HD22	1:B:120:PRO:N	2.12	0.46
1:B:117:ASN:HD22	1:B:118:GLY:N	2.13	0.46
1:A:246:ARG:HG3	5:A:327:HOH:O	2.16	0.46
1:B:174:ILE:H	1:B:174:ILE:CD1	2.29	0.46
1:A:165:ARG:NH1	1:A:169:LEU:HD21	2.31	0.46
1:A:182:TRP:CE3	1:A:252:PRO:HD3	2.51	0.46
1:A:215:MET:HE2	1:A:221:ALA:HB1	1.97	0.46
1:A:196:GLY:HA3	1:A:202:GLN:O	2.16	0.45
1:A:209[B]:ARG:HD2	1:A:209[B]:ARG:HA	1.56	0.45
1:B:117:ASN:ND2	1:B:118:GLY:N	2.60	0.45
1:A:117:ASN:HD22	1:A:118:GLY:H	1.63	0.45
1:B:161:THR:O	1:B:206:ARG:HD3	2.17	0.45
1:A:204:HIS:NE2	1:A:208:HIS:CD2	2.84	0.45
1:B:64:ALA:HB1	1:B:266:MET:HE2	1.98	0.45
1:B:261:ASN:HB2	1:B:264:ASP:OD2	2.17	0.45
1:A:191:ARG:C	1:A:191:ARG:HD2	2.42	0.44
1:A:253:MET:HE1	1:A:262:PHE:CD2	2.52	0.44
1:B:95:GLU:HG2	1:B:168:VAL:CG2	2.36	0.44
1:B:169:LEU:O	1:B:173:LYS:HG3	2.17	0.44
1:A:51:PRO:O	1:A:54:SER:HB3	2.16	0.44
1:B:249:ASN:HB2	5:B:404:HOH:O	2.18	0.44
1:B:113:PHE:HB3	1:B:114:MET:H	1.70	0.44
1:A:57:ASN:ND2	1:A:60:HIS:HD1	2.08	0.43
1:A:25:THR:HG23	1:A:83:ILE:HB	2.00	0.43
1:B:224:ASP:OD1	1:B:226:VAL:HG12	2.17	0.43
1:B:4:LYS:HA	1:B:285:VAL:HG13	2.01	0.43
1:B:191:ARG:HD2	1:B:191:ARG:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:GLN:HA	1:B:198:ILE:HD13	2.01	0.43
1:A:56:ARG:HB3	1:A:62:SER:HB2	2.01	0.43
1:A:246:ARG:HG3	1:A:246:ARG:NH1	2.34	0.43
1:B:202:GLN:HE21	1:B:202:GLN:CA	2.19	0.43
1:A:214:GLN:O	1:A:221:ALA:HA	2.19	0.42
1:B:99:GLN:OE1	1:B:165:ARG:NH2	2.52	0.42
1:B:184:MET:HE3	1:B:197:PHE:CE1	2.55	0.42
1:A:207:VAL:HB	1:A:230:HIS:CE1	2.53	0.42
1:B:110:SER:C	1:B:112:ASP:H	2.28	0.42
1:B:245:HIS:HA	1:B:247:ASN:HD21	1.84	0.42
1:A:250:TYR:HB2	1:A:277:MET:CE	2.50	0.42
1:A:87:VAL:HG22	5:A:395:HOH:O	2.19	0.42
1:A:139:ILE:HD11	1:B:52:PRO:CB	2.48	0.42
1:B:20:ARG:HG3	1:B:20:ARG:NH1	2.33	0.42
1:B:158:GLU:CD	1:B:158:GLU:N	2.76	0.42
1:A:236:ARG:NH1	5:A:451:HOH:O	2.53	0.42
1:A:287:ASP:C	1:A:288:ILE:HG13	2.44	0.42
1:B:224:ASP:CG	1:B:226:VAL:HG12	2.45	0.42
1:B:71:GLU:OE1	1:B:74:LEU:HD23	2.20	0.41
1:B:50:THR:HA	1:B:51:PRO:HA	1.92	0.41
1:B:12:LEU:HD22	1:B:107:GLN:CG	2.51	0.41
1:A:119:ASN:HD22	1:A:120:PRO:CD	2.33	0.41
1:A:119:ASN:HD22	1:A:121:ILE:H	1.69	0.41
1:A:57:ASN:ND2	1:A:60:HIS:N	2.69	0.41
1:A:249:ASN:OD1	1:A:277:MET:HE2	2.21	0.41
1:A:113:PHE:HB3	1:A:114:MET:H	1.71	0.41
1:A:202:GLN:HA	1:A:202:GLN:HE21	1.83	0.41
1:A:266:MET:O	1:A:267:TYR:C	2.64	0.41
1:B:203:LEU:O	1:B:204:HIS:C	2.64	0.41
1:A:262:PHE:CZ	1:A:274:GLU:HG3	2.56	0.41
1:A:204:HIS:HD1	1:A:205:ASN:ND2	2.18	0.41
1:B:141:GLU:HG2	1:B:142:GLN:NE2	2.36	0.41
1:B:247:ASN:ND2	1:B:247:ASN:N	2.53	0.41
1:A:142:GLN:NE2	1:A:144:ASN:HD22	2.15	0.40
1:A:182:TRP:CZ2	1:A:252:PRO:HB3	2.55	0.40
1:A:270:ASN:HD22	1:B:37:ARG:NH2	2.20	0.40
1:B:198:ILE:HD12	1:B:198:ILE:N	2.37	0.40
1:B:171:ALA:O	1:B:174:ILE:HD13	2.22	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	284/303 (94%)	275 (97%)	9 (3%)	0	100	100
1	B	283/303 (93%)	276 (98%)	7 (2%)	0	100	100
All	All	567/606 (94%)	551 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	249/266 (94%)	236 (95%)	13 (5%)	21	18
1	B	248/266 (93%)	236 (95%)	12 (5%)	23	21
All	All	497/532 (93%)	472 (95%)	25 (5%)	22	20

All (25) 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	84	ASN
1	A	89	LEU
1	A	125	ILE
1	A	139	ILE
1	A	149	LEU

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Mol	Chain	Res	Type
1	A	156	THR
1	A	158	GLU
1	A	169	LEU
1	A	194	LEU
1	A	254	LYS
1	B	5	TYR
1	B	8	ARG
1	B	71	GLU
1	B	89	LEU
1	B	95	GLU
1	B	149	LEU
1	B	158	GLU
1	B	194	LEU
1	B	247	ASN
1	B	249	ASN
1	B	254	LYS
1	B	268	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) 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
1	A	142	GLN
1	A	144	ASN
1	A	152	ASN
1	A	176	GLN
1	A	188	ASN
1	A	202	GLN
1	A	205	ASN
1	A	255	ASN
1	A	260	GLN
1	A	261	ASN
1	A	270	ASN
1	A	278	ASN
1	B	57	ASN
1	B	84	ASN
1	B	101	GLN
1	B	105	GLN

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Mol	Chain	Res	Type
1	B	117	ASN
1	B	119	ASN
1	B	142	GLN
1	B	144	ASN
1	B	152	ASN
1	B	202	GLN
1	B	205	ASN
1	B	230	HIS
1	B	247	ASN
1	B	249	ASN
1	B	251	GLN
1	B	260	GLN
1	B	261	ASN
1	B	270	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 17 ligands modelled in this entry, 17 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, 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	285/303 (94%)	0.52	24 (8%) 17 15	8, 27, 56, 101	2 (0%)
1	B	285/303 (94%)	0.51	25 (8%) 15 14	15, 29, 56, 92	0
All	All	570/606 (94%)	0.51	49 (8%) 16 15	8, 28, 58, 101	2 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	288	ILE	7.1
1	A	5	TYR	6.2
1	B	255	ASN	6.0
1	A	287	ASP	4.6
1	B	5	TYR	4.4
1	B	166	ASP	4.4
1	A	142	GLN	4.3
1	A	16	ASP	4.0
1	A	199	ASN	4.0
1	B	4	LYS	3.8
1	A	113	PHE	3.7
1	B	247	ASN	3.6
1	B	53	GLY	3.6
1	B	112	ASP	3.5
1	B	55	ASP	3.4
1	A	280	ARG	3.3
1	A	243	ILE	3.1
1	B	198	ILE	3.1
1	B	288	ILE	3.1
1	A	165	ARG	2.9
1	A	4	LYS	2.7
1	B	142	GLN	2.7
1	A	121	ILE	2.6
1	A	114	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	123	ASP	2.6
1	B	243	ILE	2.5
1	B	249	ASN	2.5
1	A	143	GLY	2.5
1	B	121	ILE	2.5
1	B	141	GLU	2.5
1	A	278	ASN	2.5
1	B	113	PHE	2.4
1	A	175	THR	2.4
1	A	20	ARG	2.2
1	A	184	MET	2.2
1	B	137	THR	2.2
1	A	134	GLY	2.2
1	B	157	LYS	2.2
1	B	188	ASN	2.2
1	A	155	ALA	2.1
1	B	24	ARG	2.1
1	A	96	THR	2.1
1	A	127	ASP	2.1
1	B	16	ASP	2.1
1	B	123	ASP	2.1
1	B	144	ASN	2.0
1	B	199	ASN	2.0
1	A	112	ASP	2.0
1	B	176	GLN	2.0

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 oligosaccharides 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. 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($\text{\AA}^2$)	Q<0.9
3	ZN	B	506	1/1	0.81	0.33	30,30,30,30	0
3	ZN	A	505	1/1	0.84	0.33	30,30,30,30	0
4	CL	B	509	1/1	0.92	0.19	30,30,30,30	1
3	ZN	A	304	1/1	0.95	0.10	30,30,30,30	1
4	CL	B	508	1/1	0.97	0.06	30,30,30,30	0
2	CU	B	501	1/1	0.98	0.06	27,27,27,27	0
2	CU	B	502	1/1	0.98	0.06	22,22,22,22	0
4	CL	A	507	1/1	0.98	0.05	30,30,30,30	0
4	CL	B	507	1/1	0.98	0.12	30,30,30,30	1
3	ZN	A	504	1/1	0.98	0.04	31,31,31,31	1
2	CU	A	501	1/1	0.98	0.05	25,25,25,25	0
4	CL	B	510	1/1	0.98	0.08	30,30,30,30	1
3	ZN	B	504	1/1	0.99	0.03	31,31,31,31	1
3	ZN	A	503	1/1	0.99	0.03	31,31,31,31	0
4	CL	A	506	1/1	0.99	0.04	30,30,30,30	0
3	ZN	B	503	1/1	0.99	0.06	31,31,31,31	0
2	CU	A	502	1/1	1.00	0.02	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.