



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2024 – 10:25 PM EST

PDB ID : 4HD7
Title : Crystal Structure of Tyrosinase from *Bacillus megaterium* V218G mutant soaked in CuSO₄
Authors : Goldfeder, M.; Kanteev, M.; Adir, N.; Fishman, A.
Deposited on : 2012-10-02
Resolution : 2.10 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

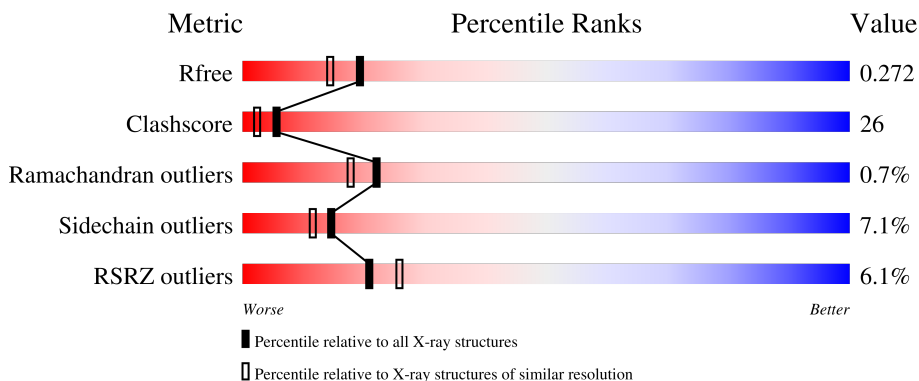
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	
1	B	303	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4914 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
			Total	C	N	O	S			
1	A	286	2353	1495	426	424	8	0	1	0
1	B	286	2343	1489	423	423	8	0	0	0

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	GLY	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	GLY	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	A	2	Total	Cu	0	0
			2	2		
2	B	2	Total	Cu	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	109	Total 109	O 109	0	0
3	B	105	Total 105	O 105	0	0

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.90Å 78.67Å 85.77Å 90.00° 105.91° 90.00°	Depositor
Resolution (Å)	36.21 – 2.10 41.24 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.4 (36.21-2.10) 95.4 (41.24-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.254 , 0.282 0.246 , 0.272	Depositor DCC
R_{free} test set	3431 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtrriage
Anisotropy	0.451	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.039 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4914	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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	0.48	0/2432	0.59	0/3313
1	B	0.43	0/2421	0.61	0/3298
All	All	0.46	0/4853	0.60	0/6611

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 [i](#)

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	2353	0	2227	106	1
1	B	2343	0	2221	131	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	109	0	0	28	0
3	B	105	0	0	34	0
All	All	4914	0	4448	235	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 26.

All (235) 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:A:30:LYS:HE2	3:A:589:HOH:O	1.22	1.35
1:B:288:ILE:H	1:B:289:GLU:CA	1.54	1.20
1:B:288:ILE:N	1:B:289:GLU:HA	1.59	1.15
1:A:81:GLN:HB2	3:A:566:HOH:O	1.44	1.15
1:A:23:VAL:N	3:A:569:HOH:O	1.78	1.14
1:B:278:ASN:ND2	3:B:579:HOH:O	1.84	1.09
1:B:78:ARG:HD2	3:B:569:HOH:O	1.50	1.09
1:B:4:LYS:NZ	3:B:565:HOH:O	1.88	1.04
1:B:287:ASP:O	1:B:288:ILE:HG23	1.60	1.02
1:B:157:LYS:HD3	3:B:510:HOH:O	1.64	0.98
1:B:288:ILE:H	1:B:289:GLU:HA	0.79	0.95
1:B:256:GLY:H	1:B:261:ASN:HD21	1.12	0.95
1:A:77:GLU:O	3:A:566:HOH:O	1.84	0.94
1:A:137:THR:O	3:A:589:HOH:O	1.86	0.93
1:B:156:THR:HG22	1:B:159:ALA:H	1.33	0.93
1:A:18:GLU:OE2	3:A:576:HOH:O	1.86	0.91
1:A:81:GLN:N	3:A:566:HOH:O	2.04	0.91
1:A:281:LYS:O	3:A:571:HOH:O	1.87	0.90
1:A:81:GLN:CB	3:A:566:HOH:O	2.09	0.89
1:B:270:ASN:ND2	3:B:558:HOH:O	2.04	0.88
1:A:251:GLN:OE1	3:A:574:HOH:O	1.93	0.87
1:A:94:TRP:HE1	1:A:230:HIS:HD2	1.20	0.86
1:B:64:ALA:H	1:B:260:GLN:HE22	1.22	0.85
1:A:20:ARG:O	3:A:569:HOH:O	1.97	0.82
1:A:145:PRO:O	3:A:549:HOH:O	1.98	0.82
1:A:8:ARG:HG2	1:A:89:LEU:O	1.80	0.82
1:B:8:ARG:HG2	1:B:89:LEU:O	1.80	0.81
1:A:23:VAL:CA	3:A:569:HOH:O	2.21	0.81
1:A:81:GLN:CA	3:A:566:HOH:O	2.28	0.81
1:B:78:ARG:NH1	3:B:569:HOH:O	1.86	0.81
1:B:287:ASP:O	1:B:288:ILE:CG1	2.29	0.81
1:B:287:ASP:O	1:B:288:ILE:CG2	2.29	0.81
1:A:256:GLY:H	1:A:261:ASN:HD21	1.26	0.80
1:B:157:LYS:CE	3:B:510:HOH:O	2.28	0.80
1:B:51:PRO:O	1:B:54:SER:HB3	1.81	0.80
1:B:156:THR:HB	3:B:557:HOH:O	1.81	0.80
1:A:156:THR:HG22	1:A:159:ALA:H	1.46	0.80
1:B:30:LYS:O	3:B:600:HOH:O	1.99	0.79
1:B:55:ASP:O	3:B:548:HOH:O	1.99	0.79
1:A:94:TRP:CE3	1:A:163:PRO:HG2	2.17	0.78
1:A:79:ASP:O	3:A:568:HOH:O	2.01	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ASN:HD22	1:B:281:LYS:HD3	1.49	0.77
1:A:23:VAL:HB	3:A:569:HOH:O	1.84	0.76
1:B:245:HIS:HB3	1:B:248:GLN:HB2	1.67	0.75
1:B:137:THR:O	3:B:580:HOH:O	2.04	0.75
1:A:173:LYS:HG3	3:A:591:HOH:O	1.86	0.74
1:B:128:THR:OG1	3:B:589:HOH:O	1.89	0.74
1:A:4:LYS:HG3	1:A:280:ARG:HG3	1.68	0.74
1:A:244:ILE:O	3:A:553:HOH:O	2.04	0.73
1:B:30:LYS:NZ	3:B:580:HOH:O	2.17	0.72
1:A:94:TRP:NE1	1:A:230:HIS:HD2	1.89	0.71
1:B:54:SER:O	3:B:560:HOH:O	2.08	0.71
1:B:94:TRP:HE1	1:B:230:HIS:HD2	1.39	0.71
1:B:278:ASN:ND2	1:B:281:LYS:HD3	2.07	0.69
1:A:64:ALA:H	1:A:260:GLN:HE22	1.37	0.69
1:B:64:ALA:H	1:B:260:GLN:NE2	1.91	0.69
1:B:274:GLU:OE1	3:B:518:HOH:O	2.10	0.69
1:B:142:GLN:HE21	1:B:144:ASN:HD22	1.40	0.69
1:B:249:ASN:ND2	3:B:601:HOH:O	1.99	0.69
1:B:135:ARG:NH1	3:B:549:HOH:O	1.82	0.69
1:B:84:ASN:HD22	1:B:86:GLU:H	1.41	0.69
1:B:139:ILE:O	3:B:563:HOH:O	2.11	0.69
1:A:156:THR:HG22	1:A:159:ALA:N	2.08	0.68
1:A:57:ASN:HD22	1:A:59:ALA:H	1.42	0.68
1:A:100:MET:SD	3:A:513:HOH:O	2.51	0.67
1:B:287:ASP:C	1:B:288:ILE:HG13	2.13	0.67
1:A:30:LYS:NZ	3:A:578:HOH:O	1.85	0.67
1:B:74:LEU:HD22	1:B:282:LEU:HD13	1.77	0.67
1:B:178:ASP:O	3:B:522:HOH:O	2.13	0.67
1:A:256:GLY:N	1:A:261:ASN:HD21	1.92	0.67
1:A:84:ASN:HD22	1:A:86:GLU:H	1.42	0.66
1:B:156:THR:HG22	1:B:159:ALA:N	2.09	0.66
1:A:156:THR:HG23	1:A:158:GLU:H	1.61	0.66
1:B:203:LEU:O	1:B:207:VAL:HG23	1.94	0.66
1:A:23:VAL:CB	3:A:569:HOH:O	2.39	0.66
1:A:94:TRP:HE1	1:A:230:HIS:CD2	2.09	0.66
1:B:157:LYS:NZ	3:B:510:HOH:O	2.10	0.66
1:A:64:ALA:H	1:A:260:GLN:NE2	1.95	0.65
1:B:242:GLN:O	1:B:246:ARG:HA	1.96	0.65
1:B:287:ASP:O	1:B:288:ILE:CB	2.43	0.65
1:B:193:GLN:HG2	1:B:198:ILE:HG13	1.77	0.65
1:B:287:ASP:O	1:B:287:ASP:CG	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ASP:OD1	3:A:598:HOH:O	2.14	0.64
1:B:270:ASN:CG	3:B:558:HOH:O	2.34	0.64
1:A:243:ILE:HG23	1:A:246:ARG:NH2	2.13	0.64
1:B:249:ASN:HB3	3:B:528:HOH:O	1.99	0.63
1:B:288:ILE:N	1:B:289:GLU:CA	2.30	0.63
1:A:60[B]:HIS:ND1	1:A:61:MET:HG3	2.13	0.62
1:A:278:ASN:ND2	1:A:281:LYS:HD3	2.14	0.62
1:B:135:ARG:NH2	3:B:549:HOH:O	2.32	0.62
1:B:176:GLN:NE2	1:B:251:GLN:HE22	1.97	0.62
1:B:180:PRO:HD3	1:B:182:TRP:CZ2	2.36	0.61
1:B:287:ASP:C	1:B:288:ILE:CG1	2.68	0.61
1:B:278:ASN:CG	3:B:579:HOH:O	2.30	0.61
1:A:74:LEU:HD22	1:A:282:LEU:HD13	1.82	0.60
1:B:29:LEU:HD22	1:B:80:LEU:HD23	1.84	0.60
1:B:288:ILE:H	1:B:289:GLU:CB	2.15	0.60
1:B:13:HIS:NE2	3:B:594:HOH:O	2.31	0.59
1:A:24:ARG:N	3:A:569:HOH:O	2.27	0.59
1:B:287:ASP:O	1:B:288:ILE:HG12	2.02	0.59
1:A:6:ARG:HD3	1:A:81:GLN:OE1	2.03	0.59
1:B:117:ASN:HD21	1:B:153:PHE:H	1.51	0.59
1:B:256:GLY:N	1:B:261:ASN:HD21	1.92	0.59
1:B:152:ASN:ND2	3:B:576:HOH:O	2.36	0.58
1:A:142:GLN:HE21	1:A:144:ASN:HD22	1.52	0.57
1:B:217:VAL:HG23	1:B:219:PRO:HD2	1.85	0.57
1:B:244:ILE:O	1:B:246:ARG:N	2.37	0.57
1:A:114:MET:HE2	1:A:131:PHE:HE1	1.69	0.57
1:B:122:LYS:HE2	1:B:127:ASP:HB3	1.87	0.56
1:A:158:GLU:HG2	1:A:201:PRO:CD	2.35	0.56
1:A:278:ASN:ND2	1:A:281:LYS:HB2	2.20	0.56
1:B:94:TRP:NE1	1:B:230:HIS:HD2	2.03	0.56
1:B:57:ASN:ND2	1:B:60:HIS:H	2.05	0.55
1:B:142:GLN:NE2	1:B:144:ASN:HD22	2.04	0.55
1:A:119:ASN:ND2	1:A:121:ILE:H	2.03	0.55
1:A:6:ARG:NH1	1:A:77:GLU:OE1	2.40	0.55
1:A:175:THR:O	1:A:248:GLN:HG3	2.06	0.55
1:B:176:GLN:HE22	1:B:251:GLN:HE22	1.53	0.55
1:A:119:ASN:C	1:A:119:ASN:HD22	2.09	0.55
1:A:4:LYS:HZ3	1:A:280:ARG:HG2	1.72	0.54
1:B:6:ARG:HD3	1:B:81:GLN:OE1	2.08	0.54
1:B:218:GLY:N	1:B:219:PRO:HD2	2.22	0.54
1:A:117:ASN:HD21	1:A:153:PHE:H	1.56	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LYS:HG3	1:A:280:ARG:CG	2.37	0.54
1:A:117:ASN:HD22	1:A:118:GLY:H	1.57	0.53
1:A:205:ASN:O	1:A:209:ARG:HG2	2.09	0.53
1:B:263:ARG:N	3:B:514:HOH:O	2.22	0.53
1:B:84:ASN:ND2	1:B:86:GLU:H	2.06	0.53
1:A:8:ARG:CG	1:A:89:LEU:O	2.55	0.53
1:A:263:ARG:NH1	1:A:274:GLU:OE2	2.41	0.53
1:A:89:LEU:HD13	1:A:232:ALA:HB2	1.91	0.52
1:A:221:ALA:HB3	1:A:222:PRO:HD3	1.91	0.52
1:A:156:THR:HG23	1:A:158:GLU:N	2.25	0.52
1:B:156:THR:HG23	1:B:158:GLU:H	1.75	0.52
1:A:30:LYS:CE	3:A:589:HOH:O	2.06	0.51
1:B:66:LEU:HB2	1:B:67:PRO:HD3	1.92	0.51
1:A:13:HIS:NE2	3:A:564:HOH:O	2.09	0.51
1:A:11:VAL:HG23	1:A:91:TYR:O	2.11	0.50
1:A:127:ASP:OD1	1:A:127:ASP:N	2.44	0.50
1:A:288:ILE:O	1:A:289:GLU:C	2.49	0.50
1:A:84:ASN:ND2	1:A:86:GLU:H	2.10	0.50
1:B:138:THR:HA	3:B:580:HOH:O	2.10	0.50
1:B:287:ASP:O	1:B:287:ASP:OD1	2.30	0.50
1:B:117:ASN:HD22	1:B:118:GLY:H	1.58	0.50
1:A:117:ASN:ND2	1:A:118:GLY:H	2.09	0.49
1:A:233:ASN:O	1:A:237:ILE:HG12	2.13	0.49
1:B:27:LEU:HB2	3:B:559:HOH:O	2.13	0.49
1:B:156:THR:CG2	1:B:159:ALA:H	2.16	0.49
1:B:204:HIS:CD2	1:B:230:HIS:HE1	2.31	0.49
1:B:57:ASN:HD22	1:B:59:ALA:H	1.61	0.49
1:B:101:GLN:HA	1:B:101:GLN:NE2	2.27	0.49
1:B:233:ASN:O	1:B:237:ILE:HG12	2.13	0.49
1:A:94:TRP:CZ3	1:A:163:PRO:HG2	2.47	0.49
1:B:139:ILE:HG22	3:B:596:HOH:O	2.13	0.49
1:A:7:VAL:HG13	1:A:7:VAL:O	2.12	0.49
1:A:93:GLU:OE1	1:A:96:THR:HG21	2.13	0.49
1:B:69:HIS:CD2	1:B:231:HIS:CE1	3.01	0.48
1:B:286:TYR:O	1:B:289:GLU:HA	2.13	0.48
1:A:150:LYS:O	1:A:213:GLY:HA3	2.14	0.48
1:B:152:ASN:ND2	1:B:155:ALA:HB2	2.29	0.48
1:A:106:SER:OG	1:A:108:ILE:HG22	2.13	0.48
1:A:162:LEU:HB3	1:A:163:PRO:HD2	1.95	0.48
1:B:204:HIS:CD2	1:B:230:HIS:CE1	3.01	0.48
1:B:66:LEU:HB2	1:B:67:PRO:CD	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ASN:HD22	1:B:121:ILE:H	1.61	0.47
1:A:74:LEU:O	1:A:78:ARG:HG3	2.14	0.47
1:B:84:ASN:HD22	1:B:84:ASN:C	2.18	0.47
1:B:84:ASN:HD21	1:B:86:GLU:HB2	1.78	0.47
1:B:198:ILE:O	1:B:199:ASN:HB2	2.15	0.47
1:A:123:ASP:O	1:A:124:PHE:HB2	2.15	0.47
1:B:161:THR:HG23	1:B:206:ARG:NH1	2.29	0.47
1:A:272:THR:O	1:A:275:ASP:HB2	2.15	0.47
1:B:108:ILE:HD11	1:B:229:LEU:HD23	1.97	0.47
1:B:152:ASN:HD22	1:B:152:ASN:C	2.19	0.46
1:B:25:THR:HG23	1:B:83:ILE:HB	1.98	0.46
1:B:4:LYS:HG3	1:B:280:ARG:HG2	1.98	0.46
1:B:157:LYS:CD	3:B:510:HOH:O	2.27	0.46
1:A:204:HIS:CD2	1:A:230:HIS:HE1	2.34	0.46
1:B:182:TRP:CZ2	1:B:252:PRO:HB3	2.51	0.46
1:B:93:GLU:OE1	1:B:96:THR:HG21	2.15	0.46
1:B:161:THR:O	1:B:206:ARG:HD3	2.16	0.46
1:B:66:LEU:HD12	1:B:177:TYR:CE1	2.51	0.45
1:A:119:ASN:HD22	1:A:121:ILE:H	1.64	0.45
1:B:180:PRO:HD3	1:B:182:TRP:CH2	2.51	0.45
1:B:288:ILE:N	1:B:289:GLU:CB	2.77	0.45
1:B:94:TRP:CE3	1:B:163:PRO:HG2	2.51	0.45
1:B:181:PRO:HG2	1:B:183:ASP:CG	2.37	0.45
1:A:246:ARG:HE	1:A:246:ARG:HB2	1.56	0.45
1:A:51:PRO:O	1:A:54:SER:HB3	2.18	0.44
1:A:84:ASN:HD22	1:A:84:ASN:C	2.20	0.44
1:B:119:ASN:HD22	1:B:119:ASN:C	2.21	0.44
1:A:156:THR:CG2	1:A:159:ALA:N	2.79	0.44
1:A:204:HIS:CD2	1:A:230:HIS:CE1	3.05	0.44
1:A:119:ASN:OD1	1:A:122:LYS:HD2	2.18	0.44
1:A:278:ASN:HD22	1:A:281:LYS:HD3	1.80	0.44
1:B:11:VAL:HG23	1:B:91:TYR:O	2.18	0.43
1:B:236:ARG:HD2	1:B:288:ILE:HD11	1.99	0.43
1:B:241:TRP:CD1	1:B:245:HIS:CD2	3.06	0.43
1:A:119:ASN:HD22	1:A:120:PRO:N	2.16	0.43
1:A:60[B]:HIS:HB2	1:A:195:GLU:OE1	2.19	0.43
1:A:4:LYS:HG2	1:A:280:ARG:HD2	2.01	0.43
1:A:4:LYS:NZ	1:A:280:ARG:HG2	2.34	0.42
1:A:152:ASN:ND2	3:A:516:HOH:O	2.51	0.42
1:A:158:GLU:HG2	1:A:201:PRO:HD2	2.01	0.42
1:B:117:ASN:ND2	1:B:153:PHE:H	2.15	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LEU:HB3	1:A:238:TRP:CE3	2.54	0.42
1:A:158:GLU:HG2	1:A:201:PRO:HD3	2.01	0.42
1:B:245:HIS:HB3	1:B:248:GLN:CB	2.44	0.42
1:B:139:ILE:HA	1:B:145:PRO:HA	2.01	0.42
1:A:84:ASN:HB3	1:A:87:VAL:HG23	2.02	0.42
1:A:220:THR:HG22	3:A:577:HOH:O	2.19	0.42
1:B:241:TRP:NE1	1:B:245:HIS:CD2	2.87	0.42
1:B:266:MET:HG3	1:B:273:PRO:HD3	2.01	0.42
1:B:6:ARG:NH1	1:B:77:GLU:OE1	2.52	0.42
1:B:119:ASN:HA	1:B:120:PRO:HD2	1.88	0.42
1:B:243:ILE:N	1:B:243:ILE:HD13	2.34	0.42
1:B:150:LYS:O	1:B:213:GLY:HA3	2.19	0.42
1:A:37:ARG:NH2	1:B:270:ASN:ND2	2.68	0.41
1:A:57:ASN:ND2	1:A:59:ALA:H	2.13	0.41
1:B:59:ALA:HB2	1:B:68:TRP:CE2	2.56	0.41
1:B:71:GLU:CD	1:B:271:THR:HG21	2.40	0.41
1:A:57:ASN:HD21	1:A:60[A]:HIS:HD1	1.68	0.41
1:A:244:ILE:HG22	1:A:245:HIS:CD2	2.54	0.41
1:B:236:ARG:O	1:B:240:VAL:HG23	2.20	0.41
1:A:114:MET:HE2	1:A:131:PHE:CE1	2.53	0.41
1:B:163:PRO:HB3	3:B:554:HOH:O	2.20	0.41
1:B:110:SER:OG	1:B:112:ASP:OD2	2.34	0.41
1:A:37:ARG:NH2	1:B:270:ASN:HD22	2.18	0.41
1:A:254:LYS:O	1:A:255:ASN:HB2	2.21	0.41
1:A:150:LYS:HD2	3:A:525:HOH:O	2.21	0.40
1:A:161:THR:HG23	1:A:206:ARG:NH1	2.36	0.40
1:B:276:VAL:O	1:B:276:VAL:HG23	2.21	0.40
1:B:198:ILE:HG22	1:B:199:ASN:OD1	2.20	0.40
1:B:49:HIS:NE2	3:B:537:HOH:O	1.98	0.40
1:B:184:MET:HB3	3:B:511:HOH:O	2.21	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:101:GLN:CG	1:B:101:GLN:NE2[1_454]	1.95	0.25

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%)	10 (4%)	0	100	100
1	B	284/303 (94%)	266 (94%)	14 (5%)	4 (1%)	11	6
All	All	569/606 (94%)	541 (95%)	24 (4%)	4 (1%)	22	18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	288	ILE
1	B	203	LEU
1	B	245	HIS
1	B	244	ILE

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	249/264 (94%)	232 (93%)	17 (7%)	16	13
1	B	248/264 (94%)	230 (93%)	18 (7%)	14	11
All	All	497/528 (94%)	462 (93%)	35 (7%)	14	12

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	17	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	55	ASP
1	A	84	ASN
1	A	89	LEU
1	A	94	TRP
1	A	101	GLN
1	A	117	ASN
1	A	119	ASN
1	A	149	LEU
1	A	152	ASN
1	A	156	THR
1	A	194	LEU
1	A	226	VAL
1	A	246	ARG
1	A	281	LYS
1	A	288	ILE
1	B	4	LYS
1	B	17	THR
1	B	54	SER
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	149	LEU
1	B	152	ASN
1	B	156	THR
1	B	169	LEU
1	B	194	LEU
1	B	244	ILE
1	B	247	ASN
1	B	288	ILE
1	B	289	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	84	ASN
1	A	117	ASN
1	A	119	ASN
1	A	142	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	152	ASN
1	A	176	GLN
1	A	202	GLN
1	A	205	ASN
1	A	230	HIS
1	A	251	GLN
1	A	255	ASN
1	A	260	GLN
1	A	261	ASN
1	A	270	ASN
1	B	57	ASN
1	B	84	ASN
1	B	101	GLN
1	B	117	ASN
1	B	119	ASN
1	B	142	GLN
1	B	152	ASN
1	B	176	GLN
1	B	187	GLN
1	B	202	GLN
1	B	205	ASN
1	B	230	HIS
1	B	245	HIS
1	B	247	ASN
1	B	260	GLN
1	B	261	ASN
1	B	270	ASN
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 monosaccharides 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, 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%)	0.65	14 (4%) 29 35	11, 21, 45, 82	1 (0%)
1	B	286/303 (94%)	0.86	21 (7%) 15 19	13, 26, 50, 86	1 (0%)
All	All	572/606 (94%)	0.75	35 (6%) 21 26	11, 23, 49, 86	2 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	247	ASN	10.7
1	A	5	TYR	8.4
1	B	248	GLN	8.0
1	B	5	TYR	7.6
1	B	246	ARG	7.2
1	B	245	HIS	4.1
1	A	20	ARG	3.9
1	B	111	ALA	3.9
1	B	288	ILE	3.8
1	A	4	LYS	3.6
1	A	142	GLN	3.6
1	B	249	ASN	3.3
1	A	198	ILE	3.3
1	B	122	LYS	3.2
1	A	17	THR	3.0
1	B	123	ASP	2.9
1	B	24	ARG	2.9
1	A	101	GLN	2.9
1	B	20	ARG	2.9
1	B	145	PRO	2.9
1	A	15	THR	2.7
1	A	255	ASN	2.7
1	A	86	GLU	2.7
1	A	24	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	244	ILE	2.6
1	B	121	ILE	2.4
1	B	198	ILE	2.4
1	B	188	ASN	2.3
1	B	142	GLN	2.3
1	A	68	TRP	2.2
1	B	287	ASP	2.2
1	B	102	ASP	2.1
1	B	116	GLY	2.1
1	A	103	PRO	2.1
1	A	246	ARG	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 monosaccharides 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	402	1/1	0.69	0.11	48,48,48,48	1
2	CU	B	402	1/1	0.90	0.09	48,48,48,48	1
2	CU	B	401	1/1	0.97	0.05	34,34,34,34	1
2	CU	A	401	1/1	0.98	0.06	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.