Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 06:02 PM EST

PDB ID	:	4HD6
Title	:	Crystal Structure of Tyrosinase from Bacillus megaterium V218F mutant soaked in CuSO4
Authors	:	Goldfeder, M.; Kanteev, M.; Adir, N.; Fishman, A.
Deposited on	:	2012-10-02
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

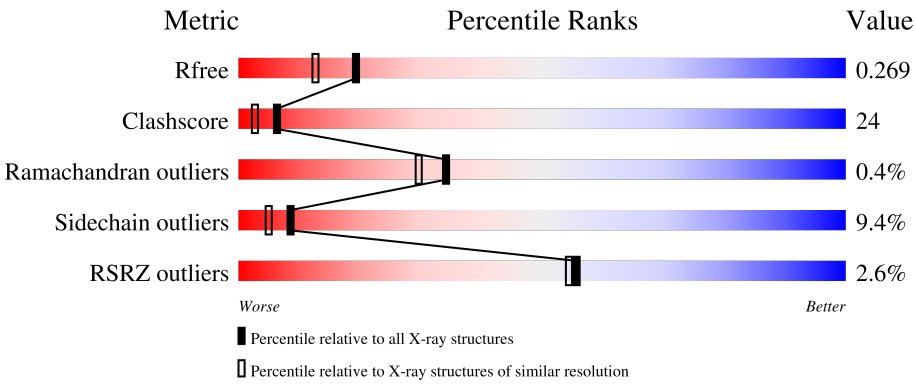
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

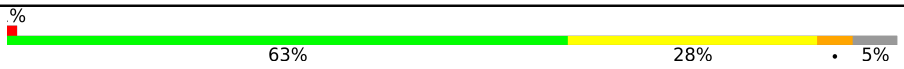
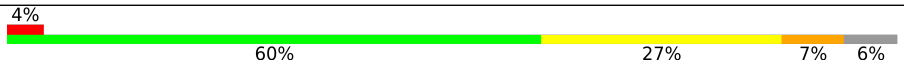
The reported resolution of this entry is 2.00 Å.

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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 4966 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tyrosinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	287	2358	1502	424	424	8	0	0	0
1	B	286	2350	1496	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	PHE	VAL	engineered mutation	UNP B2ZB02
A	298	HIS	-	expression tag	UNP B2ZB02
A	299	HIS	-	expression tag	UNP B2ZB02
A	300	HIS	-	expression tag	UNP B2ZB02
A	301	HIS	-	expression tag	UNP B2ZB02
A	302	HIS	-	expression tag	UNP B2ZB02
A	303	HIS	-	expression tag	UNP B2ZB02
B	2	GLY	SER	engineered mutation	UNP B2ZB02
B	218	PHE	VAL	engineered mutation	UNP B2ZB02
B	298	HIS	-	expression tag	UNP B2ZB02
B	299	HIS	-	expression tag	UNP B2ZB02
B	300	HIS	-	expression tag	UNP B2ZB02
B	301	HIS	-	expression tag	UNP B2ZB02
B	302	HIS	-	expression tag	UNP B2ZB02
B	303	HIS	-	expression tag	UNP B2ZB02

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

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

- Molecule 3 is water.

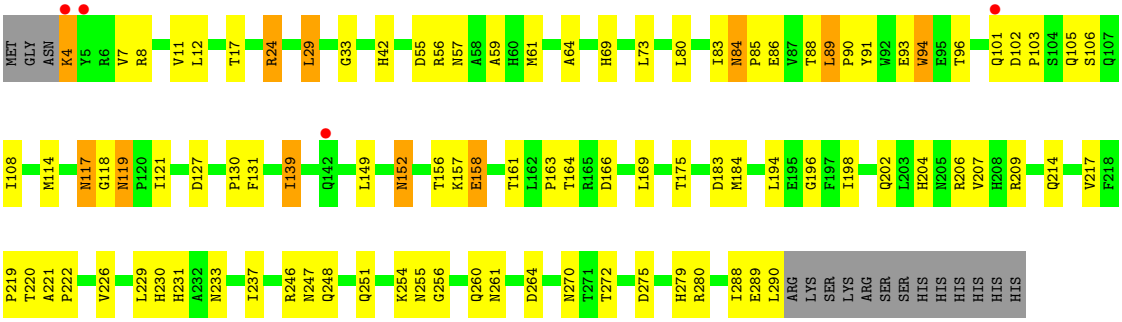
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	128	128	128	0	0
			Total	O		
3	B	126	126	126	0	0

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.

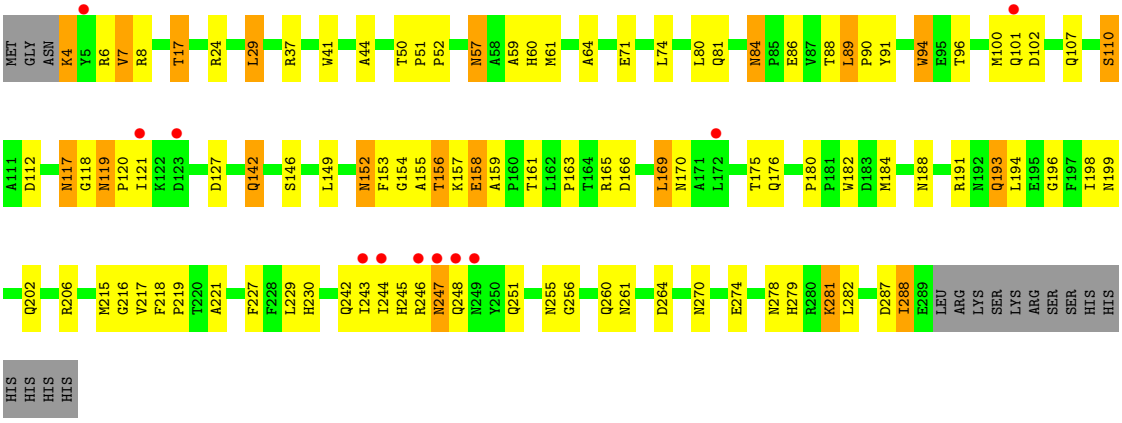
• Molecule 1: Tyrosinase

Chain A:



• Molecule 1: Tyrosinase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.18Å 78.91Å 85.81Å 90.00° 106.13° 90.00°	Depositor
Resolution (Å)	41.22 – 2.00 41.22 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.2 (41.22-2.00) 97.1 (41.22-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.53 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.245 , 0.277 0.238 , 0.269	Depositor DCC
R_{free} test set	4066 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å^2)	22.3	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.049 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4966	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 5.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.45	0/2437	0.63	0/3320
1	B	0.44	0/2429	0.59	0/3309
All	All	0.44	0/4866	0.61	0/6629

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	2358	0	2238	107	0
1	B	2350	0	2227	116	3
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	128	0	0	41	3
3	B	126	0	0	33	0
All	All	4966	0	4465	222	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (222) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:GLN:HA	3:B:615:HOH:O	1.27	1.26
1:B:61:MET:SD	3:B:600:HOH:O	1.97	1.19
1:A:101:GLN:CA	3:A:590:HOH:O	1.91	1.16
1:B:96:THR:HG22	1:B:165:ARG:NH2	1.59	1.15
1:A:61:MET:SD	3:A:576:HOH:O	2.02	1.15
1:B:274:GLU:HB3	3:B:571:HOH:O	1.43	1.15
1:A:247:ASN:HB2	3:A:602:HOH:O	1.48	1.11
1:B:206:ARG:NH1	3:B:601:HOH:O	1.83	1.10
1:A:102:ASP:N	3:A:590:HOH:O	1.82	1.08
1:A:101:GLN:HB3	3:A:590:HOH:O	1.55	1.06
1:B:146:SER:O	3:B:521:HOH:O	1.76	1.04
1:B:245:HIS:HB3	1:B:248:GLN:HB2	1.38	0.99
1:B:158:GLU:H	1:B:158:GLU:CD	1.67	0.98
1:B:94:TRP:HE1	1:B:230:HIS:HD2	1.11	0.97
1:B:170:ASN:ND2	3:B:533:HOH:O	1.95	0.97
1:A:183:ASP:HB3	3:A:595:HOH:O	1.64	0.97
1:A:101:GLN:N	3:A:590:HOH:O	1.91	0.96
1:B:157:LYS:HB3	1:B:158:GLU:OE2	1.65	0.96
1:B:193:GLN:HG2	1:B:198:ILE:HG13	1.45	0.96
1:A:219:PRO:O	1:A:220:THR:HG23	1.66	0.94
1:B:270:ASN:ND2	3:B:543:HOH:O	2.03	0.90
1:A:24:ARG:HG3	3:A:599:HOH:O	1.73	0.89
1:B:156:THR:HG22	1:B:159:ALA:H	1.37	0.89
1:B:102:ASP:OD2	3:B:609:HOH:O	1.92	0.88
1:B:96:THR:CG2	1:B:165:ARG:NH2	2.36	0.88
1:A:217:VAL:HG12	1:A:219:PRO:HD2	1.54	0.87
1:B:142:GLN:HA	1:B:142:GLN:OE1	1.75	0.87
1:A:275:ASP:OD1	3:A:569:HOH:O	1.92	0.86
1:B:17:THR:HG22	3:B:587:HOH:O	1.76	0.85
1:A:12:LEU:O	3:A:592:HOH:O	1.93	0.85
1:A:94:TRP:HE1	1:A:230:HIS:HD2	1.20	0.85
1:A:254:LYS:NZ	3:A:603:HOH:O	2.09	0.85
1:A:256:GLY:H	1:A:261:ASN:HD21	1.22	0.85
1:A:56:ARG:CZ	3:A:595:HOH:O	2.24	0.84
1:A:214:GLN:HB3	1:A:220:THR:O	1.77	0.84
1:B:251:GLN:OE1	3:B:528:HOH:O	1.93	0.84
1:A:102:ASP:OD2	3:A:607:HOH:O	1.96	0.83
1:B:96:THR:HG22	1:B:165:ARG:CZ	2.08	0.83
1:A:8:ARG:HG2	1:A:89:LEU:O	1.78	0.82
1:A:169:LEU:HD22	3:A:608:HOH:O	1.78	0.82
1:A:56:ARG:NE	3:A:595:HOH:O	2.11	0.82

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

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

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

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

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

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

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	285/303 (94%)	275 (96%)	9 (3%)	1 (0%)	34 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	284/303 (94%)	268 (94%)	15 (5%)	1 (0%)	34	30
All	All	569/606 (94%)	543 (95%)	24 (4%)	2 (0%)	34	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	244	ILE
1	A	198	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	250/265 (94%)	229 (92%)	21 (8%)	11	7
1	B	249/265 (94%)	223 (90%)	26 (10%)	7	4
All	All	499/530 (94%)	452 (91%)	47 (9%)	8	5

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	17	THR
1	A	24	ARG
1	A	29	LEU
1	A	55	ASP
1	A	84	ASN
1	A	89	LEU
1	A	94	TRP
1	A	117	ASN
1	A	119	ASN
1	A	139	ILE
1	A	149	LEU
1	A	152	ASN
1	A	158	GLU

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

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

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

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Mol	Chain	Res	Type
1	A	142	GLN
1	A	152	ASN
1	A	176	GLN
1	A	187	GLN
1	A	202	GLN
1	A	205	ASN
1	A	230	HIS
1	A	247	ASN
1	A	255	ASN
1	A	260	GLN
1	A	261	ASN
1	A	279	HIS
1	B	57	ASN
1	B	84	ASN
1	B	101	GLN
1	B	117	ASN
1	B	119	ASN
1	B	152	ASN
1	B	202	GLN
1	B	205	ASN
1	B	230	HIS
1	B	245	HIS
1	B	247	ASN
1	B	251	GLN
1	B	255	ASN
1	B	260	GLN
1	B	261	ASN
1	B	270	ASN
1	B	279	HIS

5.3.3 RNA (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 (i)

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 (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, 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	287/303 (94%)	0.17	4 (1%)	75	74	12, 21, 48, 85	1 (0%)
1	B	286/303 (94%)	0.28	11 (3%)	40	39	12, 24, 49, 87	0
All	All	573/606 (94%)	0.23	15 (2%)	56	54	12, 23, 49, 87	1 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	247	ASN	11.9
1	B	248	GLN	7.9
1	B	246	ARG	5.4
1	B	244	ILE	5.3
1	A	5	TYR	2.7
1	B	5	TYR	2.6
1	B	243	ILE	2.6
1	A	4	LYS	2.5
1	A	142	GLN	2.5
1	B	249	ASN	2.4
1	A	101	GLN	2.4
1	B	123	ASP	2.3
1	B	121	ILE	2.2
1	B	172	LEU	2.1
1	B	101	GLN	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	0.90	0.29	32,32,32,32	1
2	CU	B	402	1/1	0.94	0.22	35,35,35,35	1
2	CU	A	401	1/1	0.97	0.08	27,27,27,27	0
2	CU	B	401	1/1	0.99	0.07	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.