Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 11:37 AM EST

PDB ID	:	3WO8
Title	:	Crystal structure of the beta-N-acetylglucosaminidase from Thermotoga maritima
Authors	:	Mine, S.; Kado, Y.; Watanabe, M.; Inoue, T.; Ishikawa, K.
Deposited on	:	2013-12-20
Resolution	:	2.43 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:

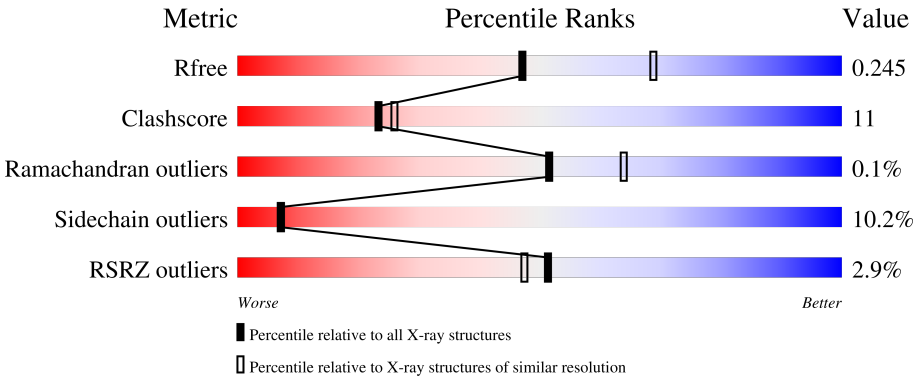
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.43 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	478	3% 69% 21% · 6%
1	B	478	3% 65% 25% · 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7196 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 Beta-N-acetylglucosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3540	2285	575	668	12			
1	B	448	Total	C	N	O	S	0	0	0
			3549	2291	576	670	12			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP Q9WZR6
A	-9	ASN	-	expression tag	UNP Q9WZR6
A	-8	HIS	-	expression tag	UNP Q9WZR6
A	-7	LYS	-	expression tag	UNP Q9WZR6
A	-6	VAL	-	expression tag	UNP Q9WZR6
A	-5	HIS	-	expression tag	UNP Q9WZR6
A	-4	HIS	-	expression tag	UNP Q9WZR6
A	-3	HIS	-	expression tag	UNP Q9WZR6
A	-2	HIS	-	expression tag	UNP Q9WZR6
A	-1	HIS	-	expression tag	UNP Q9WZR6
A	0	HIS	-	expression tag	UNP Q9WZR6
B	-10	MET	-	expression tag	UNP Q9WZR6
B	-9	ASN	-	expression tag	UNP Q9WZR6
B	-8	HIS	-	expression tag	UNP Q9WZR6
B	-7	LYS	-	expression tag	UNP Q9WZR6
B	-6	VAL	-	expression tag	UNP Q9WZR6
B	-5	HIS	-	expression tag	UNP Q9WZR6
B	-4	HIS	-	expression tag	UNP Q9WZR6
B	-3	HIS	-	expression tag	UNP Q9WZR6
B	-2	HIS	-	expression tag	UNP Q9WZR6
B	-1	HIS	-	expression tag	UNP Q9WZR6
B	0	HIS	-	expression tag	UNP Q9WZR6

- Molecule 2 is water.

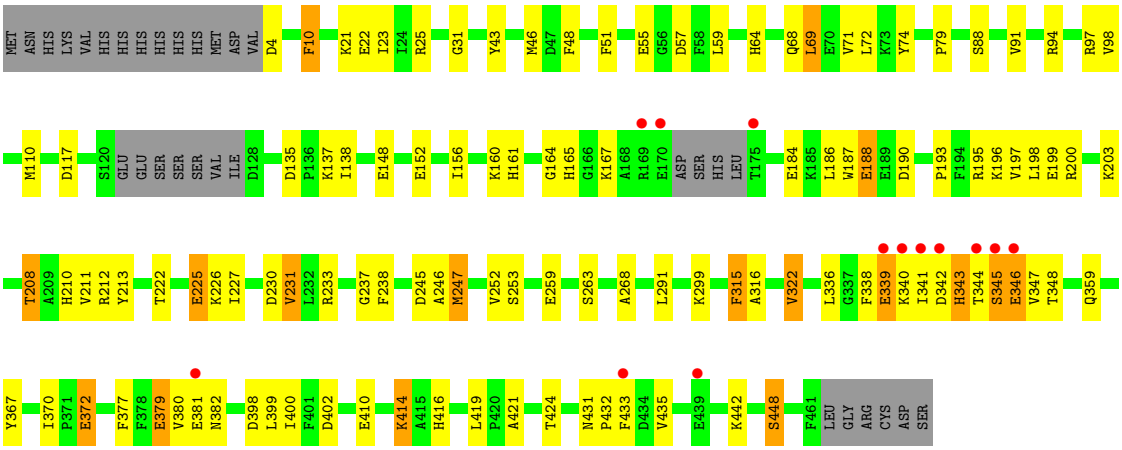
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	60	Total O 60 60	0	0
2	B	47	Total O 47 47	0	0

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.

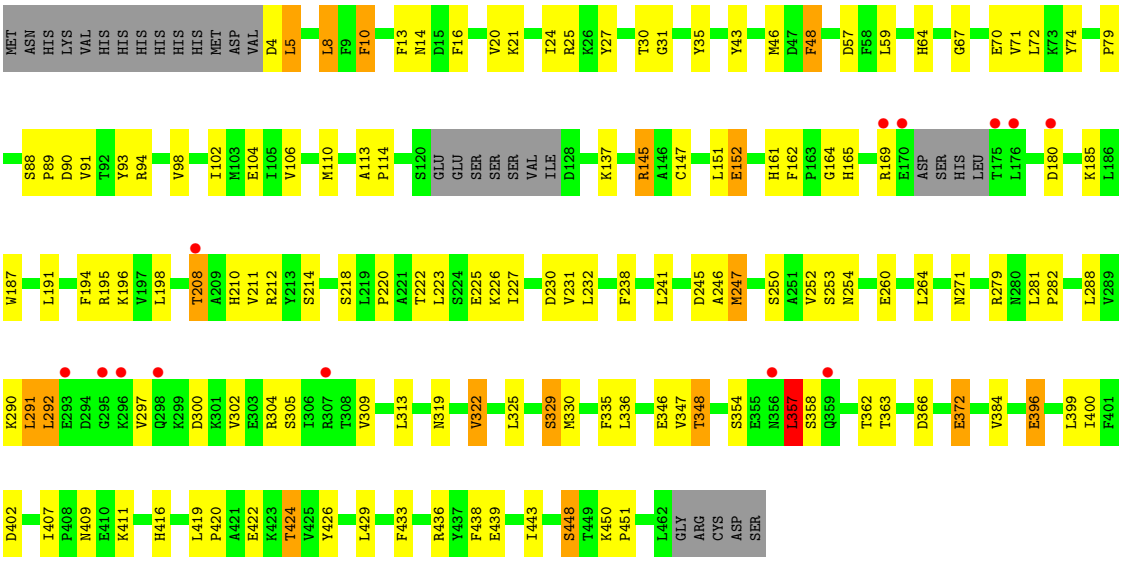
• Molecule 1: Beta-N-acetylglucosaminidase

Chain A:



• Molecule 1: Beta-N-acetylglucosaminidase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	133.46Å 133.46Å 142.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.56 – 2.43 26.56 – 2.43	Depositor EDS
% Data completeness (in resolution range)	92.0 (26.56-2.43) 92.1 (26.56-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.14 (at 2.44Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.194 , 0.246 0.196 , 0.245	Depositor DCC
R_{free} test set	2572 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	40.4	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7196	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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

5.1 Standard geometry

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	0.74	1/3614 (0.0%)	0.88	1/4881 (0.0%)
1	B	0.68	0/3623	0.84	2/4894 (0.0%)
All	All	0.71	1/7237 (0.0%)	0.86	3/9775 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	ASP	CB-CG	5.06	1.62	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	330	MET	CG-SD-CE	5.56	109.09	100.20
1	A	97	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	B	357	LEU	CA-CB-CG	5.22	127.30	115.30

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	3540	0	3548	74	0
1	B	3549	0	3559	90	0
2	A	60	0	0	1	0
2	B	47	0	0	3	0
All	All	7196	0	7107	160	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 11.

All (160) 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:247:MET:HA	1:B:247:MET:HE2	1.39	1.03
1:A:414:LYS:HA	1:A:414:LYS:HE2	1.50	0.90
1:A:43:TYR:OH	1:A:372:GLU:OE2	1.97	0.82
1:B:402:ASP:OD2	1:B:416:HIS:HD2	1.67	0.78
1:A:210:HIS:CE1	1:A:245:ASP:HB3	2.20	0.76
1:B:5:LEU:HD23	1:B:5:LEU:H	1.51	0.75
1:B:227:ILE:O	1:B:231:VAL:HG12	1.87	0.75
1:B:64:HIS:CD2	1:B:72:LEU:H	2.04	0.74
1:B:407:ILE:HD12	1:B:407:ILE:O	1.89	0.73
1:B:357:LEU:HB2	2:B:515:HOH:O	1.89	0.71
1:A:148:GLU:O	1:A:152:GLU:HG2	1.91	0.70
1:A:347:VAL:O	1:A:380:VAL:O	2.08	0.70
1:A:400:ILE:HB	1:A:424:THR:HG22	1.73	0.70
1:A:46:MET:HG2	1:A:322:VAL:HG13	1.74	0.70
1:A:226:LYS:O	1:A:230:ASP:HB2	1.92	0.69
1:A:64:HIS:HD2	1:A:72:LEU:H	1.40	0.69
1:B:8:LEU:HD12	1:B:271:ASN:O	1.94	0.68
1:B:57:ASP:OD2	1:B:313:LEU:HG	1.94	0.67
1:B:247:MET:HE2	1:B:247:MET:CA	2.17	0.66
1:A:68:GLN:HG2	1:A:69:LEU:HD13	1.76	0.66
1:A:414:LYS:HE2	1:A:414:LYS:CA	2.25	0.66
1:B:64:HIS:CD2	1:B:71:VAL:H	2.13	0.66
1:B:64:HIS:HD2	1:B:72:LEU:H	1.43	0.65
1:A:247:MET:HA	1:A:247:MET:CE	2.27	0.65
1:A:208:THR:HG23	1:A:222:THR:OG1	1.97	0.65
1:B:419:LEU:HB3	1:B:424:THR:HG21	1.78	0.65
1:B:24:ILE:O	1:B:27:TYR:O	2.15	0.64
1:B:227:ILE:HA	1:B:231:VAL:HG12	1.79	0.64
1:A:64:HIS:CD2	1:A:72:LEU:H	2.17	0.61
1:B:407:ILE:O	1:B:407:ILE:CD1	2.48	0.61
1:A:21:LYS:HG2	1:A:51:PHE:CE1	2.35	0.61
1:A:339:GLU:O	1:A:340:LYS:HG3	2.00	0.60
1:A:367:TYR:HA	1:A:370:ILE:HD12	1.83	0.60
1:A:402:ASP:OD2	1:A:416:HIS:HD2	1.85	0.60
1:B:208:THR:HG23	1:B:222:THR:OG1	2.02	0.59
1:A:184:GLU:O	1:A:188:GLU:HG2	2.03	0.59
1:B:363:THR:O	1:B:366:ASP:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:PRO:HB3	1:B:145:ARG:HG3	1.84	0.59
1:B:291:LEU:HD13	1:B:297:VAL:HG23	1.84	0.58
1:B:191:LEU:O	1:B:195:ARG:HG3	2.04	0.58
1:B:211:VAL:O	1:B:220:PRO:HA	2.03	0.57
1:A:59:LEU:HD13	1:A:110:MET:CE	2.34	0.57
1:A:247:MET:HA	1:A:247:MET:HE2	1.85	0.57
1:B:438:PHE:O	1:B:443:ILE:HD11	2.04	0.57
1:A:359:GLN:HE22	1:B:14:ASN:HD21	1.49	0.57
1:B:210:HIS:HD2	1:B:222:THR:OG1	1.88	0.57
1:A:117:ASP:OD2	1:A:161:HIS:HD2	1.88	0.57
1:B:420:PRO:O	1:B:424:THR:HG23	2.04	0.57
1:A:59:LEU:HD13	1:A:110:MET:HE1	1.87	0.57
1:B:43:TYR:OH	1:B:372:GLU:OE2	2.22	0.57
1:B:88:SER:O	1:B:91:VAL:HG22	2.05	0.56
1:B:59:LEU:HD13	1:B:110:MET:CE	2.35	0.56
1:B:433:PHE:CZ	1:B:436:ARG:HD3	2.40	0.56
1:A:348:THR:HG22	1:A:382:ASN:HB2	1.88	0.56
1:B:14:ASN:HD22	1:B:35:TYR:HB2	1.72	0.55
1:A:210:HIS:HD2	1:A:222:THR:OG1	1.88	0.55
1:B:416:HIS:HE1	2:B:509:HOH:O	1.90	0.55
1:A:414:LYS:HA	1:A:414:LYS:CE	2.29	0.54
1:A:347:VAL:HG12	1:A:399:LEU:HB3	1.89	0.54
1:A:74:TYR:HA	1:B:74:TYR:HA	1.91	0.53
1:B:433:PHE:CE1	1:B:436:ARG:CD	2.92	0.53
1:A:167:LYS:HE2	1:A:190:ASP:OD1	2.09	0.52
1:B:180:ASP:HA	1:B:214:SER:OG	2.09	0.52
1:B:220:PRO:HG2	1:B:223:LEU:HD12	1.90	0.52
1:B:5:LEU:HD12	1:B:288:LEU:HD23	1.92	0.52
1:A:227:ILE:HA	1:A:231:VAL:HG13	1.92	0.52
1:A:200:ARG:HH21	1:A:200:ARG:HG3	1.74	0.52
1:A:419:LEU:HB3	1:A:424:THR:HG21	1.92	0.51
1:B:90:ASP:OD1	1:B:145:ARG:NH1	2.44	0.51
1:B:198:LEU:HD22	1:B:238:PHE:CD1	2.45	0.51
1:B:433:PHE:CE1	1:B:436:ARG:NE	2.79	0.51
1:A:64:HIS:CD2	1:A:71:VAL:H	2.29	0.51
1:B:260:GLU:O	1:B:264:LEU:HG	2.11	0.51
1:A:233:ARG:O	1:A:237:GLY:HA2	2.11	0.51
1:B:59:LEU:HD13	1:B:110:MET:HE1	1.93	0.50
1:A:198:LEU:HD22	1:A:238:PHE:CD1	2.47	0.50
1:A:345:SER:O	1:A:379:GLU:HB2	2.11	0.50
1:B:402:ASP:OD2	1:B:416:HIS:CD2	2.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:GLY:O	1:A:213:TYR:OH	2.21	0.50
1:A:346:GLU:HA	1:A:379:GLU:O	2.10	0.50
1:A:187:TRP:CH2	1:A:195:ARG:HD3	2.46	0.49
1:B:250:SER:HB2	1:B:254:ASN:ND2	2.27	0.49
1:A:25:ARG:HG2	1:A:55:GLU:OE1	2.13	0.49
1:A:210:HIS:HE1	1:A:246:ALA:O	1.94	0.49
1:A:344:THR:HG21	1:A:398:ASP:HB3	1.95	0.48
1:B:113:ALA:HB1	1:B:114:PRO:HA	1.95	0.48
1:B:291:LEU:CD1	1:B:297:VAL:HG23	2.44	0.48
1:B:161:HIS:O	1:B:164:GLY:N	2.46	0.48
1:A:343:HIS:NE2	1:A:377:PHE:O	2.46	0.48
1:B:46:MET:HG2	1:B:322:VAL:HG13	1.94	0.48
1:A:79:PRO:O	1:B:448:SER:OG	2.30	0.47
1:B:227:ILE:CA	1:B:231:VAL:HG12	2.44	0.47
1:A:247:MET:HA	1:A:247:MET:HE3	1.95	0.47
1:B:16:PHE:CD1	1:B:48:PHE:CD1	3.03	0.47
1:B:210:HIS:HE1	1:B:246:ALA:O	1.97	0.47
1:A:210:HIS:CD2	1:A:222:THR:OG1	2.68	0.47
1:A:380:VAL:O	1:A:382:ASN:N	2.42	0.47
1:B:64:HIS:HD2	1:B:72:LEU:N	2.09	0.47
1:A:64:HIS:CD2	1:A:72:LEU:HB2	2.49	0.47
1:A:247:MET:HE2	1:A:252:VAL:HG21	1.95	0.47
1:A:341:ILE:HG22	1:A:342:ASP:N	2.29	0.47
1:B:362:THR:OG1	1:B:450:LYS:NZ	2.48	0.46
1:B:102:ILE:O	1:B:106:VAL:HG23	2.15	0.46
1:B:10:PHE:CG	1:B:31:GLY:HA3	2.50	0.46
1:A:156:ILE:CD1	1:A:316:ALA:HB2	2.46	0.46
1:B:208:THR:HG22	1:B:245:ASP:H	1.80	0.45
1:A:135:ASP:HB3	1:A:138:ILE:HD12	1.98	0.45
1:B:433:PHE:CZ	1:B:436:ARG:CD	2.99	0.45
1:A:225:GLU:HA	1:A:268:ALA:HB1	1.97	0.45
1:B:292:LEU:HD11	1:B:302:VAL:HG21	1.98	0.45
1:A:448:SER:HB2	1:B:79:PRO:O	2.17	0.45
1:B:14:ASN:HD22	1:B:35:TYR:CB	2.30	0.45
1:B:162:PHE:CE2	1:B:232:LEU:HB2	2.52	0.45
1:A:380:VAL:O	1:A:381:GLU:HB3	2.16	0.45
1:B:279:ARG:O	1:B:282:PRO:HD2	2.16	0.45
1:A:421:ALA:O	1:A:442:LYS:HE3	2.17	0.44
1:B:16:PHE:CE1	1:B:48:PHE:CD1	3.06	0.44
1:B:93:TYR:OH	1:B:152:GLU:HG3	2.18	0.44
1:B:400:ILE:HB	1:B:424:THR:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:PHE:CG	1:A:31:GLY:HA3	2.52	0.44
1:B:67:GLY:O	1:B:70:GLU:HG3	2.18	0.44
1:A:341:ILE:CG2	1:A:342:ASP:N	2.81	0.44
1:B:325:LEU:O	1:B:329:SER:OG	2.32	0.44
1:B:194:PHE:O	1:B:198:LEU:HB2	2.18	0.43
1:B:147:CYS:O	1:B:151:LEU:HD12	2.17	0.43
1:B:208:THR:HG21	1:B:222:THR:HG23	2.00	0.43
1:B:416:HIS:O	1:B:426:TYR:OH	2.27	0.43
1:B:335:PHE:HD2	2:B:529:HOH:O	2.00	0.43
1:B:241:LEU:HD11	1:B:309:VAL:HG22	1.99	0.43
1:B:187:TRP:CH2	1:B:195:ARG:HD3	2.53	0.43
1:A:165:HIS:CD2	1:A:165:HIS:O	2.72	0.43
1:A:341:ILE:CG2	1:A:342:ASP:H	2.32	0.43
1:A:203:LYS:HE3	1:A:315:PHE:CG	2.54	0.42
1:A:46:MET:CG	1:A:322:VAL:HG13	2.47	0.42
1:B:227:ILE:O	1:B:231:VAL:CG1	2.64	0.42
1:B:336:LEU:HB2	1:B:443:ILE:HB	2.02	0.42
1:B:210:HIS:CD2	1:B:222:THR:OG1	2.71	0.42
1:A:64:HIS:HD2	1:A:71:VAL:H	1.64	0.42
1:A:263:SER:HB3	1:A:291:LEU:HD13	2.01	0.42
1:A:193:PRO:O	1:A:197:VAL:HG23	2.19	0.42
1:A:208:THR:CG2	1:A:222:THR:OG1	2.68	0.42
1:A:195:ARG:O	1:A:199:GLU:HB3	2.20	0.42
1:B:13:PHE:CD2	1:B:20:VAL:HG13	2.55	0.42
1:A:208:THR:HG21	1:A:222:THR:HG23	2.02	0.41
1:B:8:LEU:HD11	1:B:305:SER:HB3	2.02	0.41
1:B:227:ILE:C	1:B:231:VAL:HG12	2.40	0.41
1:A:64:HIS:HE1	2:A:502:HOH:O	2.03	0.41
1:A:211:VAL:HG12	1:A:212:ARG:N	2.35	0.41
1:B:247:MET:O	1:B:252:VAL:HG23	2.20	0.41
1:B:212:ARG:CD	1:B:218:SER:O	2.68	0.41
1:B:348:THR:HG21	1:B:396:GLU:O	2.20	0.41
1:B:281:LEU:N	1:B:282:PRO:CD	2.83	0.41
1:B:59:LEU:HD13	1:B:110:MET:HE3	2.01	0.41
1:B:226:LYS:O	1:B:230:ASP:HB2	2.21	0.41
1:A:346:GLU:OE1	1:A:381:GLU:HG2	2.21	0.40
1:B:187:TRP:CZ2	1:B:195:ARG:HD3	2.56	0.40
1:B:210:HIS:CE1	1:B:245:ASP:HB3	2.56	0.40
1:A:431:ASN:OD1	1:A:433:PHE:N	2.50	0.40
1:A:432:PRO:O	1:A:435:VAL:HG23	2.20	0.40
1:B:21:LYS:O	1:B:25:ARG:HG3	2.22	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	441/478 (92%)	418 (95%)	22 (5%)	1 (0%)	47 57
1	B	442/478 (92%)	423 (96%)	19 (4%)	0	100 100
All	All	883/956 (92%)	841 (95%)	41 (5%)	1 (0%)	51 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	410	GLU

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	393/423 (93%)	359 (91%)	34 (9%)	10 11
1	B	394/423 (93%)	348 (88%)	46 (12%)	5 4
All	All	787/846 (93%)	707 (90%)	80 (10%)	7 7

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	PHE
1	A	22	GLU

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Mol	Chain	Res	Type
1	A	23	ILE
1	A	48	PHE
1	A	57	ASP
1	A	69	LEU
1	A	88	SER
1	A	91	VAL
1	A	94	ARG
1	A	98	VAL
1	A	137	LYS
1	A	160	LYS
1	A	186	LEU
1	A	188	GLU
1	A	196	LYS
1	A	208	THR
1	A	225	GLU
1	A	231	VAL
1	A	247	MET
1	A	253	SER
1	A	259	GLU
1	A	299	LYS
1	A	315	PHE
1	A	322	VAL
1	A	336	LEU
1	A	338	PHE
1	A	339	GLU
1	A	343	HIS
1	A	345	SER
1	A	346	GLU
1	A	372	GLU
1	A	379	GLU
1	A	414	LYS
1	A	448	SER
1	B	4	ASP
1	B	5	LEU
1	B	8	LEU
1	B	10	PHE
1	B	30	THR
1	B	48	PHE
1	B	94	ARG
1	B	98	VAL
1	B	104	GLU
1	B	137	LYS

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Mol	Chain	Res	Type
1	B	145	ARG
1	B	152	GLU
1	B	165	HIS
1	B	169	ARG
1	B	185	LYS
1	B	196	LYS
1	B	208	THR
1	B	225	GLU
1	B	247	MET
1	B	253	SER
1	B	290	LYS
1	B	291	LEU
1	B	292	LEU
1	B	300	ASP
1	B	304	ARG
1	B	319	ASN
1	B	322	VAL
1	B	329	SER
1	B	346	GLU
1	B	347	VAL
1	B	348	THR
1	B	354	SER
1	B	357	LEU
1	B	358	SER
1	B	372	GLU
1	B	384	VAL
1	B	396	GLU
1	B	399	LEU
1	B	409	ASN
1	B	411	LYS
1	B	422	GLU
1	B	424	THR
1	B	429	LEU
1	B	439	GLU
1	B	448	SER
1	B	451	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	64	HIS

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Mol	Chain	Res	Type
1	A	142	HIS
1	A	161	HIS
1	A	165	HIS
1	A	210	HIS
1	A	254	ASN
1	A	298	GLN
1	A	416	HIS
1	B	14	ASN
1	B	64	HIS
1	B	210	HIS
1	B	254	ASN
1	B	319	ASN
1	B	343	HIS
1	B	416	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 95^{th} 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	447/478 (93%)	-0.34	13 (2%) 51 47	25, 42, 89, 141	0
1	B	448/478 (93%)	-0.26	13 (2%) 51 47	28, 50, 85, 108	0
All	All	895/956 (93%)	-0.30	26 (2%) 51 47	25, 47, 87, 141	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	345	SER	8.4
1	A	433	PHE	8.1
1	A	339	GLU	5.2
1	A	340	LYS	4.6
1	B	169	ARG	3.9
1	A	381	GLU	3.9
1	B	356	ASN	3.7
1	B	170	GLU	3.4
1	A	344	THR	3.3
1	B	359	GLN	3.2
1	A	170	GLU	3.1
1	A	341	ILE	2.9
1	A	169	ARG	2.8
1	A	175	THR	2.6
1	B	298	GLN	2.4
1	B	176	LEU	2.4
1	B	175	THR	2.4
1	A	342	ASP	2.3
1	A	439	GLU	2.3
1	B	293	GLU	2.2
1	A	346	GLU	2.1
1	B	296	LYS	2.1
1	B	295	GLY	2.0
1	B	180	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	208	THR	2.0
1	B	307	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.