



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:17 AM UTC

PDB ID : 5XFM / pdb_00005xfm
Title : Crystal structure of beta-arabinopyranosidase
Authors : Kato, K.; Okuyama, M.; Yao, M.
Deposited on : 2017-04-10
Resolution : 2.30 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

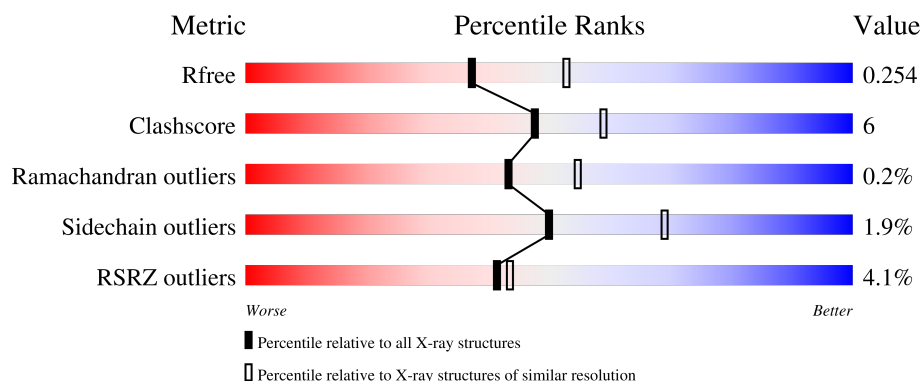
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	642	
1	B	642	
1	C	642	
1	D	642	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21423 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 Alpha-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	632	Total	C	N	O	S	0	0	0
			5056	3204	870	953	29			
1	B	628	Total	C	N	O	S	0	0	0
			5021	3182	864	947	28			
1	C	632	Total	C	N	O	S	0	0	0
			5056	3204	870	953	29			
1	D	629	Total	C	N	O	S	0	0	0
			5029	3188	865	948	28			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	MET	-	expression tag	UNP A0A1H5YQC4
A	7	ASN	-	expression tag	UNP A0A1H5YQC4
A	8	HIS	-	expression tag	UNP A0A1H5YQC4
A	9	LYS	-	expression tag	UNP A0A1H5YQC4
A	10	VAL	-	expression tag	UNP A0A1H5YQC4
A	11	HIS	-	expression tag	UNP A0A1H5YQC4
A	12	HIS	-	expression tag	UNP A0A1H5YQC4
A	13	HIS	-	expression tag	UNP A0A1H5YQC4
A	14	HIS	-	expression tag	UNP A0A1H5YQC4
A	15	HIS	-	expression tag	UNP A0A1H5YQC4
A	16	HIS	-	expression tag	UNP A0A1H5YQC4
A	17	MET	-	expression tag	UNP A0A1H5YQC4
A	18	GLU	-	expression tag	UNP A0A1H5YQC4
A	19	LEU	-	expression tag	UNP A0A1H5YQC4
A	498	LEU	PHE	engineered mutation	UNP A0A1H5YQC4
B	6	MET	-	expression tag	UNP A0A1H5YQC4
B	7	ASN	-	expression tag	UNP A0A1H5YQC4
B	8	HIS	-	expression tag	UNP A0A1H5YQC4
B	9	LYS	-	expression tag	UNP A0A1H5YQC4
B	10	VAL	-	expression tag	UNP A0A1H5YQC4
B	11	HIS	-	expression tag	UNP A0A1H5YQC4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	12	HIS	-	expression tag	UNP A0A1H5YQC4
B	13	HIS	-	expression tag	UNP A0A1H5YQC4
B	14	HIS	-	expression tag	UNP A0A1H5YQC4
B	15	HIS	-	expression tag	UNP A0A1H5YQC4
B	16	HIS	-	expression tag	UNP A0A1H5YQC4
B	17	MET	-	expression tag	UNP A0A1H5YQC4
B	18	GLU	-	expression tag	UNP A0A1H5YQC4
B	19	LEU	-	expression tag	UNP A0A1H5YQC4
B	498	LEU	PHE	engineered mutation	UNP A0A1H5YQC4
C	6	MET	-	expression tag	UNP A0A1H5YQC4
C	7	ASN	-	expression tag	UNP A0A1H5YQC4
C	8	HIS	-	expression tag	UNP A0A1H5YQC4
C	9	LYS	-	expression tag	UNP A0A1H5YQC4
C	10	VAL	-	expression tag	UNP A0A1H5YQC4
C	11	HIS	-	expression tag	UNP A0A1H5YQC4
C	12	HIS	-	expression tag	UNP A0A1H5YQC4
C	13	HIS	-	expression tag	UNP A0A1H5YQC4
C	14	HIS	-	expression tag	UNP A0A1H5YQC4
C	15	HIS	-	expression tag	UNP A0A1H5YQC4
C	16	HIS	-	expression tag	UNP A0A1H5YQC4
C	17	MET	-	expression tag	UNP A0A1H5YQC4
C	18	GLU	-	expression tag	UNP A0A1H5YQC4
C	19	LEU	-	expression tag	UNP A0A1H5YQC4
C	498	LEU	PHE	engineered mutation	UNP A0A1H5YQC4
D	6	MET	-	expression tag	UNP A0A1H5YQC4
D	7	ASN	-	expression tag	UNP A0A1H5YQC4
D	8	HIS	-	expression tag	UNP A0A1H5YQC4
D	9	LYS	-	expression tag	UNP A0A1H5YQC4
D	10	VAL	-	expression tag	UNP A0A1H5YQC4
D	11	HIS	-	expression tag	UNP A0A1H5YQC4
D	12	HIS	-	expression tag	UNP A0A1H5YQC4
D	13	HIS	-	expression tag	UNP A0A1H5YQC4
D	14	HIS	-	expression tag	UNP A0A1H5YQC4
D	15	HIS	-	expression tag	UNP A0A1H5YQC4
D	16	HIS	-	expression tag	UNP A0A1H5YQC4
D	17	MET	-	expression tag	UNP A0A1H5YQC4
D	18	GLU	-	expression tag	UNP A0A1H5YQC4
D	19	LEU	-	expression tag	UNP A0A1H5YQC4
D	498	LEU	PHE	engineered mutation	UNP A0A1H5YQC4

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

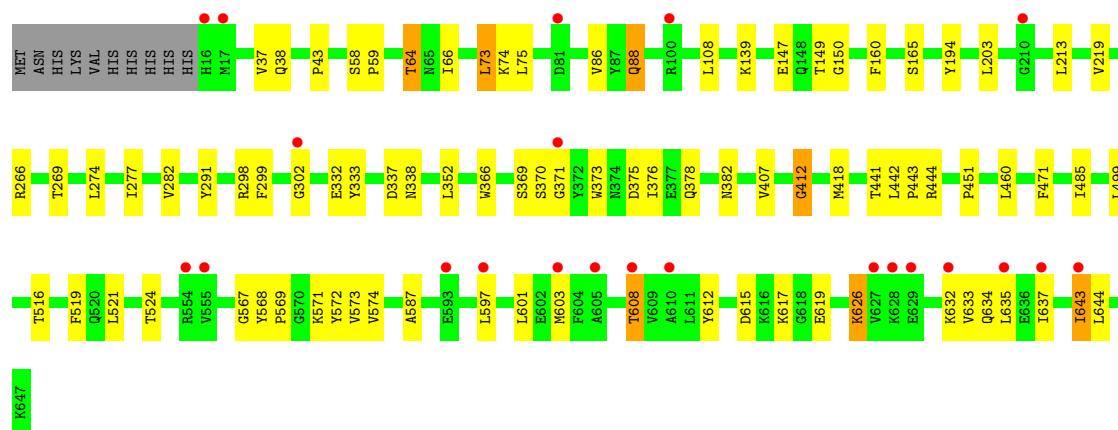
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Ca 1	0	0
2	B	1	Total 1	Ca 1	0	0
2	C	1	Total 1	Ca 1	0	0
2	D	1	Total 1	Ca 1	0	0

- Molecule 3 is water.

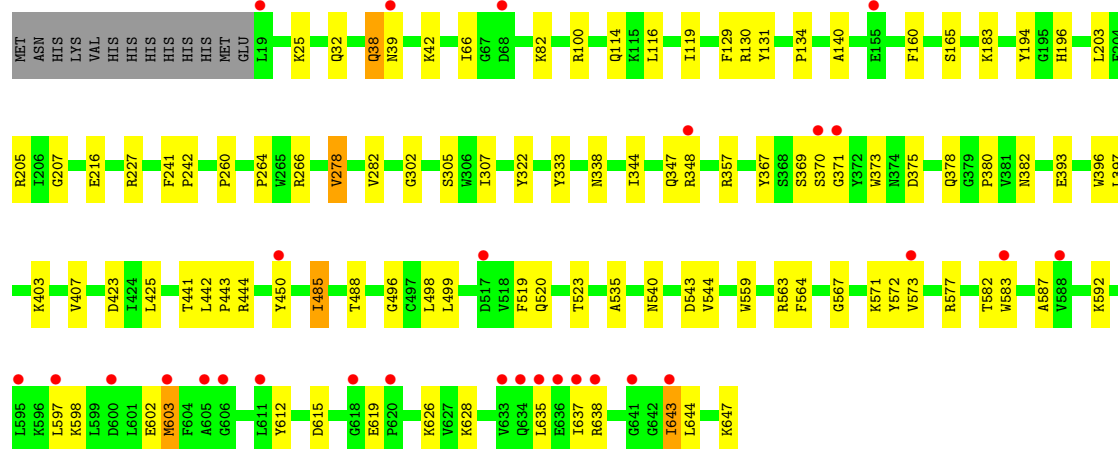
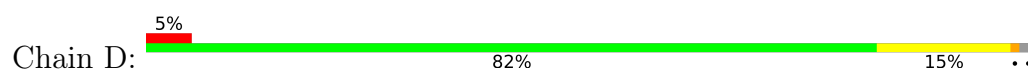
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	333	Total 333	O 333	0	0
3	B	291	Total 291	O 291	0	0
3	C	349	Total 349	O 349	0	0
3	D	284	Total 284	O 284	0	0

- Molecule 1: Alpha-glucosidase





• Molecule 1: Alpha-glucosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.81Å 90.51Å 128.55Å 105.50° 94.80° 96.15°	Depositor
Resolution (Å)	45.78 – 2.30 45.78 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.0 (45.78-2.30) 90.3 (45.78-2.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.207 , 0.253 0.210 , 0.254	Depositor DCC
R_{free} test set	6269 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	21423	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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: CA

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	0.39	0/5180	0.81	2/7022 (0.0%)
1	B	0.37	0/5144	0.80	2/6974 (0.0%)
1	C	0.40	0/5180	0.80	3/7022 (0.0%)
1	D	0.38	0/5152	0.81	2/6985 (0.0%)
All	All	0.39	0/20656	0.80	9/28003 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	282	VAL	CA-C-N	-6.20	113.23	119.56
1	D	282	VAL	C-N-CA	-6.20	113.23	119.56
1	C	282	VAL	CA-C-N	-5.85	112.85	119.28
1	C	282	VAL	C-N-CA	-5.85	112.85	119.28
1	C	412	GLY	N-CA-C	5.78	117.39	111.56
1	A	282	VAL	CA-C-N	-5.75	113.69	119.56
1	A	282	VAL	C-N-CA	-5.75	113.69	119.56
1	B	450	TYR	CA-C-N	5.36	125.17	119.28
1	B	450	TYR	C-N-CA	5.36	125.17	119.28

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	5056	0	4912	62	0
1	B	5021	0	4879	43	0
1	C	5056	0	4912	55	0
1	D	5029	0	4890	65	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	333	0	0	6	0
3	B	291	0	0	7	0
3	C	349	0	0	7	0
3	D	284	0	0	9	0
All	All	21423	0	19593	222	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 6.

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:C:64:THR:HG22	1:C:66:ILE:H	1.44	0.82
1:A:70:THR:HG22	1:A:71:LYS:HG3	1.62	0.81
1:D:496:GLY:O	3:D:801:HOH:O	1.98	0.80
1:D:583:TRP:O	3:D:802:HOH:O	2.00	0.79
1:D:344:ILE:HA	1:D:348:ARG:HH21	1.48	0.77
1:A:191:ARG:NH1	1:A:192:SER:O	2.16	0.77
1:D:160:PHE:HB2	1:D:203:LEU:HB3	1.68	0.75
1:A:64:THR:HG22	1:A:66:ILE:H	1.52	0.72
1:A:38:GLN:OE1	1:A:75:LEU:N	2.21	0.71
1:D:615:ASP:O	1:D:638:ARG:NH2	2.25	0.70
1:D:338:ASN:HD22	1:D:378:GLN:HE21	1.38	0.69
1:C:38:GLN:OE1	1:C:75:LEU:N	2.23	0.67
1:C:635:LEU:HD23	1:C:643:ILE:HD13	1.80	0.64
1:B:637:ILE:HG12	1:B:643:ILE:HD12	1.80	0.64
1:C:43:PRO:HG3	1:C:73:LEU:HD22	1.79	0.63
1:D:647:LYS:N	3:D:802:HOH:O	2.31	0.63
1:A:637:ILE:HG12	1:A:643:ILE:HD12	1.81	0.63
1:A:338:ASN:ND2	1:A:378:GLN:OE1	2.32	0.63
1:A:441:THR:HB	3:A:803:HOH:O	1.99	0.63
1:A:635:LEU:HD13	1:A:643:ILE:HG21	1.81	0.62
1:B:370:SER:HA	1:B:373:TRP:CZ2	2.34	0.62
1:A:396:TRP:CE3	1:A:397:LEU:HD12	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:LYS:HD2	1:A:629:GLU:H	1.65	0.61
1:A:147:GLU:OE2	1:A:266:ARG:NH2	2.32	0.60
1:A:43:PRO:HG3	1:A:73:LEU:HD22	1.82	0.60
1:D:396:TRP:CE3	1:D:397:LEU:HD12	2.37	0.60
1:D:25:LYS:HG2	1:D:32:GLN:HG2	1.83	0.60
1:C:499:LEU:O	3:C:801:HOH:O	2.16	0.59
1:A:254:ALA:O	3:A:802:HOH:O	2.16	0.59
1:B:56:GLU:OE2	3:B:802:HOH:O	2.17	0.59
1:D:423:ASP:OD1	3:D:803:HOH:O	2.17	0.59
1:C:376:ILE:HG23	1:C:378:GLN:HG2	1.85	0.58
1:A:579:GLN:NE2	3:A:811:HOH:O	2.36	0.58
1:C:637:ILE:HG12	1:C:643:ILE:HD12	1.85	0.58
1:A:73:LEU:HD23	1:A:108:LEU:HD13	1.85	0.57
1:C:370:SER:HA	1:C:373:TRP:CZ2	2.39	0.57
1:A:396:TRP:HE3	1:A:397:LEU:HD12	1.70	0.57
1:A:370:SER:HA	1:A:373:TRP:CZ2	2.39	0.57
1:A:231:VAL:HG22	1:A:237:TYR:CZ	2.39	0.56
1:D:571:LYS:NZ	3:D:817:HOH:O	2.37	0.56
1:B:70:THR:HG23	1:B:148:GLN:OE1	2.05	0.56
1:B:244:ALA:O	1:B:414:LYS:NZ	2.38	0.56
1:A:491:SER:HB3	1:A:529:ASN:ND2	2.20	0.56
1:B:499:LEU:HD13	1:B:544:VAL:HG11	1.89	0.55
1:D:393:GLU:O	1:D:397:LEU:HD13	2.06	0.55
1:A:70:THR:HG23	1:A:148:GLN:OE1	2.07	0.54
1:C:635:LEU:HD23	1:C:643:ILE:HG21	1.90	0.54
1:C:442:LEU:HD12	1:C:443:PRO:HD2	1.89	0.54
1:B:348:ARG:NH1	3:B:827:HOH:O	2.41	0.54
1:A:231:VAL:HG22	1:A:237:TYR:CE2	2.42	0.54
1:C:165:SER:HA	1:C:194:TYR:CD1	2.43	0.53
1:B:378:GLN:NE2	3:B:824:HOH:O	2.40	0.53
1:C:147:GLU:OE2	1:C:266:ARG:NH2	2.38	0.53
1:D:196:HIS:O	1:D:227:ARG:NH1	2.41	0.53
1:B:155:GLU:OE1	3:B:802:HOH:O	2.19	0.53
1:A:191:ARG:HG3	1:A:191:ARG:HH11	1.72	0.53
1:D:370:SER:HA	1:D:373:TRP:CZ2	2.43	0.53
1:D:540:ASN:HA	1:D:543:ASP:OD1	2.09	0.53
1:B:602:GLU:CD	1:B:602:GLU:H	2.17	0.52
1:D:442:LEU:HD12	1:D:443:PRO:HD2	1.91	0.52
1:C:338:ASN:ND2	1:C:378:GLN:HE21	2.08	0.52
1:A:375:ASP:HA	1:B:140:ALA:HB3	1.91	0.52
1:A:412:GLY:O	3:A:803:HOH:O	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:THR:HG21	1:C:266:ARG:HD2	1.91	0.51
1:A:353:VAL:HG22	1:A:363:LEU:HD12	1.91	0.51
1:B:577:ARG:NH2	3:B:831:HOH:O	2.44	0.51
1:C:633:VAL:HG12	1:C:635:LEU:CD1	2.41	0.51
1:C:160:PHE:HB2	1:C:203:LEU:HB3	1.92	0.51
1:A:188:MET:O	1:A:231:VAL:HG21	2.11	0.50
1:D:116:LEU:HD11	1:D:131:TYR:HB3	1.92	0.50
1:D:563:ARG:NH1	1:D:602:GLU:OE2	2.44	0.50
1:D:637:ILE:HG12	1:D:643:ILE:HD12	1.93	0.50
1:B:525:VAL:O	1:B:577:ARG:NH1	2.45	0.50
1:B:47:VAL:HB	1:B:55:LEU:HB2	1.92	0.50
1:D:635:LEU:HD13	1:D:643:ILE:HG21	1.94	0.50
1:B:348:ARG:HG2	1:B:348:ARG:HH11	1.77	0.49
1:A:165:SER:HA	1:A:194:TYR:CD1	2.47	0.49
1:B:601:LEU:HD12	1:B:633:VAL:HG21	1.93	0.49
1:A:406:LYS:HE3	1:A:438:HIS:CD2	2.48	0.49
1:C:516:THR:O	1:C:519:PHE:HB3	2.13	0.49
1:A:219:VAL:HB	1:A:444:ARG:HD3	1.95	0.49
1:C:635:LEU:CD2	1:C:643:ILE:HG21	2.43	0.49
1:A:393:GLU:O	1:A:397:LEU:HD13	2.12	0.49
1:D:603:MET:H	1:D:603:MET:HG3	1.39	0.48
1:A:601:LEU:HD12	1:A:633:VAL:HG21	1.96	0.48
1:C:74:LYS:NZ	3:C:835:HOH:O	2.43	0.48
1:D:378:GLN:HG3	3:D:830:HOH:O	2.14	0.48
1:B:82:LYS:HG2	1:B:102:ASN:OD1	2.14	0.48
1:C:302:GLY:HA2	1:C:333:TYR:O	2.14	0.48
1:D:38:GLN:HA	1:D:38:GLN:OE1	2.14	0.48
1:B:634:GLN:HG2	1:B:635:LEU:N	2.29	0.47
1:C:418:MET:HE1	1:C:441:THR:HG21	1.97	0.47
1:C:298:ARG:HG2	3:C:802:HOH:O	2.13	0.47
1:A:47:VAL:HB	1:A:55:LEU:HB2	1.97	0.47
1:A:371:GLY:HA2	1:A:382:ASN:OD1	2.14	0.47
1:C:338:ASN:HD22	1:C:378:GLN:HE21	1.63	0.47
1:C:568:TYR:CD2	1:C:571:LYS:HD2	2.49	0.47
1:D:498:LEU:N	1:D:520:GLN:OE1	2.41	0.47
1:A:40:GLU:HG3	3:A:801:HOH:O	2.14	0.47
1:B:635:LEU:HD13	1:B:643:ILE:HG21	1.97	0.47
1:D:130:ARG:NH2	3:D:838:HOH:O	2.48	0.47
1:B:442:LEU:HD12	1:B:443:PRO:HD2	1.97	0.47
1:B:302:GLY:HA2	1:B:333:TYR:O	2.15	0.46
1:B:316:TYR:CE2	1:B:352:LEU:HG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:573:VAL:O	1:B:587:ALA:HA	2.16	0.46
1:B:116:LEU:HD11	1:B:131:TYR:HB3	1.97	0.46
1:D:338:ASN:HD22	1:D:378:GLN:NE2	2.09	0.46
1:C:59:PRO:HD2	1:C:150:GLY:HA3	1.97	0.46
1:D:278:VAL:HG11	1:D:564:PHE:CD1	2.51	0.46
1:A:615:ASP:OD2	1:A:619:GLU:HB2	2.16	0.46
1:C:139:LYS:NZ	3:C:815:HOH:O	2.32	0.46
1:D:615:ASP:OD2	1:D:619:GLU:HB2	2.15	0.46
1:A:44:CYS:SG	1:A:57:LYS:HE3	2.56	0.46
1:B:485:ILE:O	1:B:488:THR:HG22	2.16	0.46
1:A:231:VAL:HG23	3:A:907:HOH:O	2.15	0.45
1:D:582:THR:HG22	3:D:802:HOH:O	2.16	0.45
1:A:576:ALA:HB3	1:A:603:MET:HE3	1.98	0.45
1:D:519:PHE:O	1:D:523:THR:HG23	2.16	0.45
1:C:371:GLY:HA2	1:C:382:ASN:OD1	2.16	0.45
1:D:357:ARG:NH1	3:D:836:HOH:O	2.47	0.45
1:D:485:ILE:O	1:D:488:THR:HG22	2.16	0.45
1:A:147:GLU:CD	1:A:266:ARG:HH21	2.24	0.45
1:C:573:VAL:O	1:C:587:ALA:HA	2.17	0.45
1:D:612:TYR:HB2	1:D:644:LEU:HB3	1.98	0.45
1:C:86:VAL:HG12	1:C:88:GLN:HE22	1.82	0.44
1:C:219:VAL:HB	1:C:444:ARG:HD3	1.98	0.44
1:C:612:TYR:HB2	1:C:644:LEU:HB3	1.98	0.44
1:D:602:GLU:HG2	1:D:603:MET:N	2.32	0.44
1:D:367:TYR:O	1:D:407:VAL:HA	2.17	0.44
1:D:216:GLU:OE1	1:D:266:ARG:NH1	2.51	0.44
1:D:425:LEU:HD13	1:D:450:TYR:CG	2.53	0.44
1:C:58:SER:HA	1:C:59:PRO:HD3	1.84	0.44
1:A:568:TYR:CD2	1:A:571:LYS:HD2	2.53	0.44
1:B:556:PRO:HG2	1:B:559:TRP:CH2	2.53	0.44
1:B:567:GLY:HA2	1:B:572:TYR:CE2	2.53	0.44
1:C:412:GLY:HA2	3:C:808:HOH:O	2.16	0.44
1:D:573:VAL:O	1:D:587:ALA:HA	2.17	0.44
1:A:66:ILE:O	1:A:114:GLN:NE2	2.51	0.44
1:B:406:LYS:HE3	1:B:438:HIS:CD2	2.53	0.44
1:B:612:TYR:HB2	1:B:644:LEU:HB3	1.99	0.43
1:D:42:LYS:HB2	1:D:42:LYS:HE3	1.74	0.43
1:B:628:LYS:HG3	1:B:629:GLU:N	2.33	0.43
1:D:396:TRP:HE3	1:D:397:LEU:HD12	1.81	0.43
1:B:603:MET:H	1:B:603:MET:HG2	1.59	0.43
1:D:592:LYS:O	1:D:592:LYS:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:THR:HG23	1:A:343:ARG:HG3	2.00	0.43
1:C:601:LEU:HD12	1:C:633:VAL:HG21	2.00	0.43
1:D:583:TRP:CE3	1:D:603:MET:HE3	2.53	0.43
1:A:216:GLU:OE1	1:A:266:ARG:NH1	2.52	0.43
1:B:167:ALA:HA	1:B:176:PRO:HD3	2.01	0.43
1:A:442:LEU:HD12	1:A:443:PRO:HD2	2.01	0.43
1:B:367:TYR:O	1:B:407:VAL:HA	2.19	0.43
1:C:460:LEU:HD13	1:C:471:PHE:CE1	2.54	0.43
1:D:82:LYS:HD2	1:D:100:ARG:NH2	2.33	0.43
1:D:134:PRO:HA	1:D:260:PRO:HB3	2.01	0.43
1:C:521:LEU:O	1:C:524:THR:OG1	2.36	0.43
1:D:559:TRP:CE2	1:D:577:ARG:HD3	2.54	0.43
1:D:369:SER:HB3	1:D:407:VAL:HG12	2.01	0.43
1:B:225:GLY:O	1:B:242:PRO:HD3	2.19	0.43
1:C:37:VAL:HG11	1:C:108:LEU:HD22	2.01	0.43
1:B:370:SER:HB3	1:B:374:ASN:HD21	1.83	0.42
1:C:139:LYS:HA	1:D:375:ASP:OD1	2.19	0.42
1:C:337:ASP:HA	1:C:366:TRP:HB2	2.00	0.42
1:D:119:ILE:O	1:D:129:PHE:HA	2.19	0.42
1:D:307:ILE:HG21	1:D:535:ALA:HA	2.01	0.42
1:D:205:ARG:NH1	1:D:207:GLY:O	2.52	0.42
1:D:302:GLY:HA2	1:D:333:TYR:O	2.19	0.42
1:D:635:LEU:HD13	1:D:643:ILE:HD13	2.00	0.42
1:A:305:SER:HA	1:A:322:TYR:CZ	2.54	0.42
1:C:634:GLN:C	1:C:635:LEU:HD12	2.44	0.42
1:A:191:ARG:HH11	1:A:191:ARG:CG	2.32	0.42
1:A:567:GLY:HA2	1:A:572:TYR:CE2	2.55	0.42
1:B:241:PHE:HB3	1:B:242:PRO:HD2	2.01	0.42
1:C:615:ASP:OD2	1:C:619:GLU:HB2	2.19	0.42
1:B:130:ARG:NH1	3:B:812:HOH:O	2.31	0.42
1:C:603:MET:H	1:C:603:MET:HG2	1.69	0.42
1:D:371:GLY:HA2	1:D:382:ASN:OD1	2.20	0.42
1:B:119:ILE:O	1:B:129:PHE:HA	2.20	0.42
1:C:213:LEU:HB3	1:C:269:THR:HB	2.02	0.42
1:C:375:ASP:HA	1:D:140:ALA:HB3	2.02	0.42
1:D:441:THR:OG1	1:D:444:ARG:NH1	2.46	0.42
1:C:567:GLY:HA2	1:C:572:TYR:CE2	2.55	0.42
1:D:403:LYS:HA	1:D:403:LYS:HD2	1.81	0.42
1:C:299:PHE:O	3:C:802:HOH:O	2.22	0.41
1:D:165:SER:HA	1:D:194:TYR:CD1	2.54	0.41
1:D:305:SER:HA	1:D:322:TYR:CZ	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ILE:O	1:A:488:THR:HG22	2.20	0.41
1:A:464:ASN:HB3	1:A:471:PHE:CD2	2.55	0.41
1:B:554:ARG:NH2	3:B:838:HOH:O	2.49	0.41
1:C:269:THR:HG22	1:C:277:ILE:HD13	2.03	0.41
1:C:568:TYR:HA	1:C:569:PRO:HD3	1.88	0.41
1:C:608:THR:CG2	1:C:626:LYS:HG3	2.50	0.41
1:D:241:PHE:HB3	1:D:242:PRO:HD2	2.02	0.41
1:D:567:GLY:HA2	1:D:572:TYR:CE2	2.55	0.41
1:C:73:LEU:HD23	1:C:108:LEU:HD13	2.02	0.41
1:D:499:LEU:HD13	1:D:544:VAL:HG11	2.03	0.41
1:A:16:HIS:HB3	1:A:17:MET:H	1.55	0.41
1:A:367:TYR:OH	1:A:397:LEU:HD11	2.21	0.41
1:A:201:PRO:HB2	1:A:213:LEU:HD11	2.02	0.41
1:A:455:GLY:HA3	1:A:529:ASN:HD21	1.86	0.41
1:B:42:LYS:HB2	1:B:42:LYS:HE3	1.73	0.41
1:A:367:TYR:CD2	1:A:380:PRO:HG2	2.56	0.41
1:B:441:THR:OG1	1:B:444:ARG:NH1	2.43	0.41
1:C:291:TYR:CE2	1:C:451:PRO:HD2	2.56	0.41
1:C:352:LEU:HA	1:C:352:LEU:HD23	1.86	0.41
1:A:119:ILE:O	1:A:129:PHE:HA	2.21	0.41
1:A:572:TYR:CD2	1:A:595:LEU:HD21	2.56	0.41
1:A:615:ASP:OD1	1:A:619:GLU:N	2.50	0.41
1:C:369:SER:HB3	1:C:407:VAL:HG12	2.03	0.41
1:D:378:GLN:HG3	1:D:378:GLN:H	1.69	0.41
1:A:291:TYR:CE2	1:A:451:PRO:HD2	2.56	0.40
1:D:367:TYR:CD2	1:D:380:PRO:HG2	2.56	0.40
1:B:155:GLU:H	1:B:155:GLU:CD	2.23	0.40
1:C:332:GLU:HG2	3:C:802:HOH:O	2.20	0.40
1:A:248:ASN:HB2	1:A:373:TRP:O	2.21	0.40
1:C:574:VAL:HG13	1:C:587:ALA:HB2	2.03	0.40
1:D:66:ILE:O	1:D:114:GLN:NE2	2.55	0.40
1:D:264:PRO:HB2	1:D:266:ARG:HH12	1.86	0.40
1:A:302:GLY:HA2	1:A:333:TYR:O	2.21	0.40
1:A:241:PHE:HB3	1:A:242:PRO:HD2	2.04	0.40
1:A:573:VAL:O	1:A:587:ALA:HA	2.21	0.40
1:B:351:SER:HA	1:B:354:GLU:OE1	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	630/642 (98%)	600 (95%)	29 (5%)	1 (0%)	43	55
1	B	626/642 (98%)	601 (96%)	23 (4%)	2 (0%)	36	46
1	C	630/642 (98%)	602 (96%)	27 (4%)	1 (0%)	43	55
1	D	627/642 (98%)	600 (96%)	26 (4%)	1 (0%)	43	55
All	All	2513/2568 (98%)	2403 (96%)	105 (4%)	5 (0%)	43	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	605	ALA
1	A	485	ILE
1	B	485	ILE
1	C	485	ILE
1	D	485	ILE

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	548/558 (98%)	532 (97%)	16 (3%)	37	55
1	B	544/558 (98%)	539 (99%)	5 (1%)	70	84
1	C	548/558 (98%)	538 (98%)	10 (2%)	51	70
1	D	545/558 (98%)	534 (98%)	11 (2%)	48	67
All	All	2185/2232 (98%)	2143 (98%)	42 (2%)	50	69

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	THR
1	A	73	LEU
1	A	191	ARG
1	A	270	VAL
1	A	378	GLN
1	A	395	LYS
1	A	493	GLU
1	A	523	THR
1	A	592	LYS
1	A	597	LEU
1	A	598	LYS
1	A	616	LYS
1	A	617	LYS
1	A	632	LYS
1	A	643	ILE
1	A	644	LEU
1	B	191	ARG
1	B	592	LYS
1	B	597	LEU
1	B	632	LYS
1	B	643	ILE
1	C	64	THR
1	C	73	LEU
1	C	88	GLN
1	C	274	LEU
1	C	597	LEU
1	C	608	THR
1	C	617	LYS
1	C	626	LYS
1	C	632	LYS
1	C	643	ILE
1	D	38	GLN
1	D	39	ASN
1	D	183	LYS
1	D	278	VAL
1	D	347	GLN
1	D	597	LEU
1	D	598	LYS
1	D	603	MET
1	D	626	LYS
1	D	628	LYS
1	D	643	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	273	HIS
1	A	464	ASN
1	A	529	ASN
1	B	38	GLN
1	B	88	GLN
1	B	338	ASN
1	B	378	GLN
1	B	464	ASN
1	C	338	ASN
1	C	464	ASN
1	D	338	ASN
1	D	464	ASN
1	D	579	GLN
1	D	640	GLN

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 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

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	632/642 (98%)	0.48	20 (3%)	50	52	14, 24, 46, 68	0
1	B	628/642 (97%)	0.65	33 (5%)	32	34	17, 29, 50, 68	0
1	C	632/642 (98%)	0.51	22 (3%)	47	49	14, 25, 46, 67	0
1	D	629/642 (97%)	0.68	29 (4%)	37	39	18, 31, 56, 77	0
All	All	2521/2568 (98%)	0.58	104 (4%)	41	43	14, 27, 50, 77	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	603	MET	4.6
1	A	605	ALA	4.4
1	D	371	GLY	4.0
1	C	371	GLY	3.9
1	B	644	LEU	3.8
1	C	554	ARG	3.7
1	D	603	MET	3.7
1	D	595	LEU	3.6
1	D	635	LEU	3.5
1	A	16	HIS	3.5
1	B	605	ALA	3.4
1	C	16	HIS	3.4
1	A	81	ASP	3.3
1	C	629	GLU	3.3
1	C	608	THR	3.3
1	D	634	GLN	3.3
1	D	600	ASP	3.3
1	C	635	LEU	3.1
1	B	633	VAL	3.1
1	C	605	ALA	3.1
1	B	39	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	603	MET	3.0
1	B	610	ALA	2.9
1	A	80	VAL	2.9
1	C	100	ARG	2.9
1	A	542	LYS	2.9
1	B	518	VAL	2.9
1	B	155	GLU	2.9
1	B	595	LEU	2.8
1	D	605	ALA	2.8
1	B	321	ARG	2.8
1	A	261	GLY	2.8
1	A	135	HIS	2.7
1	A	600	ASP	2.7
1	B	623	THR	2.7
1	B	631	GLY	2.7
1	D	643	ILE	2.7
1	D	618	GLY	2.7
1	C	610	ALA	2.6
1	B	489	VAL	2.6
1	B	647	LYS	2.6
1	D	583	TRP	2.6
1	C	302	GLY	2.6
1	A	555	VAL	2.6
1	D	19	LEU	2.5
1	D	611	LEU	2.5
1	D	39	ASN	2.5
1	B	628	LYS	2.5
1	B	646	ILE	2.5
1	B	355	TYR	2.5
1	D	637	ILE	2.5
1	A	628	LYS	2.5
1	D	370	SER	2.4
1	B	499	LEU	2.4
1	D	588	VAL	2.4
1	B	630	ASN	2.4
1	C	210	GLY	2.4
1	B	632	LYS	2.4
1	B	603	MET	2.4
1	D	68	ASP	2.3
1	D	638	ARG	2.3
1	A	66	ILE	2.3
1	D	636	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	620	PRO	2.3
1	B	370	SER	2.3
1	C	627	VAL	2.3
1	B	592	LYS	2.3
1	D	517	ASP	2.3
1	A	262	ALA	2.3
1	B	357	ARG	2.3
1	B	634	GLN	2.3
1	D	606	GLY	2.2
1	A	633	VAL	2.2
1	D	633	VAL	2.2
1	B	345	GLY	2.2
1	D	155	GLU	2.2
1	A	378	GLN	2.2
1	A	64	THR	2.2
1	A	643	ILE	2.2
1	A	632	LYS	2.2
1	D	641	GLY	2.2
1	B	266	ARG	2.1
1	D	450	TYR	2.1
1	C	637	ILE	2.1
1	C	17	MET	2.1
1	B	127	VAL	2.1
1	C	555	VAL	2.1
1	D	348	ARG	2.1
1	C	643	ILE	2.1
1	D	597	LEU	2.1
1	C	81	ASP	2.1
1	D	573	VAL	2.1
1	B	597	LEU	2.1
1	C	597	LEU	2.1
1	B	160	PHE	2.1
1	B	617	LYS	2.1
1	C	632	LYS	2.1
1	C	593	GLU	2.1
1	B	206	ILE	2.1
1	A	361	VAL	2.1
1	A	466	VAL	2.1
1	B	581	ASP	2.0
1	B	626	LYS	2.0
1	C	628	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	701	1/1	0.98	0.02	20,20,20,20	0
2	CA	D	701	1/1	0.98	0.02	25,25,25,25	0
2	CA	C	701	1/1	0.99	0.04	21,21,21,21	0
2	CA	B	701	1/1	0.99	0.04	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.