



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:07 AM UTC

PDB ID : 2JF7 / pdb_00002jf7
Title : Structure of Strictosidine Glucosidase
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Deposited on : 2007-01-26
Resolution : 2.48 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

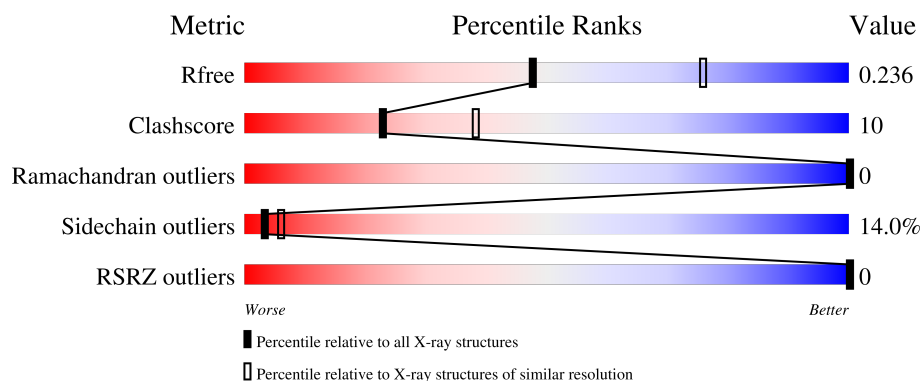
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	532	
1	B	532	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8074 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 STRICTOSIDINE-O-BETA-D-GLUCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	1
			3796	2443	633	705	15			
1	B	467	Total	C	N	O	S	0	0	1
			3788	2438	631	704	15			

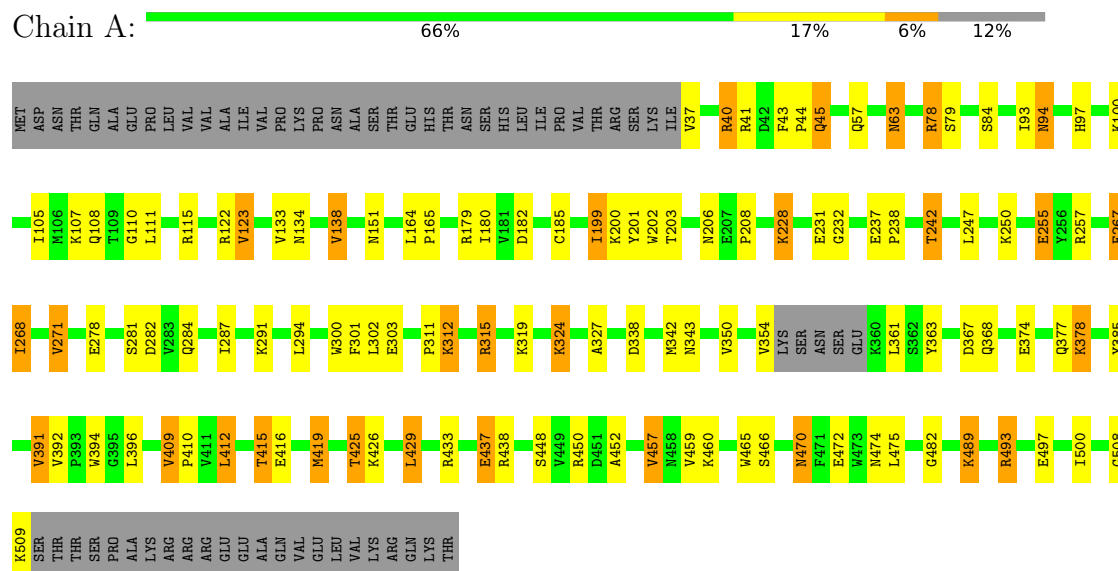
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	245	Total	O	0	0
			245	245		
2	B	245	Total	O	0	0
			245	245		

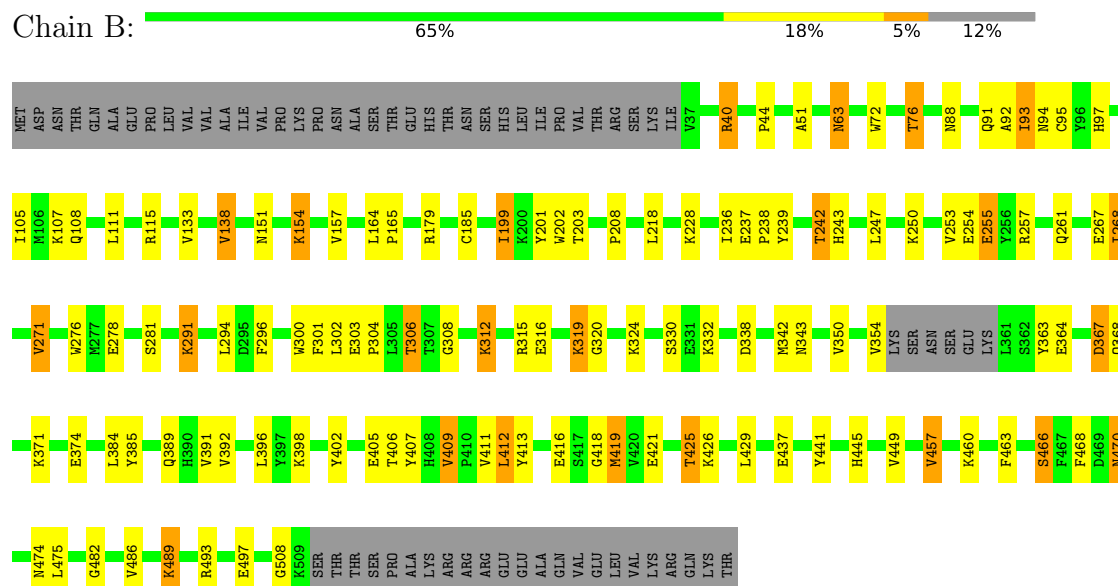
3 Residue-property plots

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: STRICTOSIDINE-O-BETA-D-GLUCOSIDASE



• Molecule 1: STRICTOSIDINE-O-BETA-D-GLUCOSIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	157.63Å 157.63Å 103.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.48 20.00 – 2.48	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.48) 99.7 (20.00-2.48)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.47Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.185 , 0.239 0.184 , 0.236	Depositor DCC
R_{free} test set	1120 reflections (2.40%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8074	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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

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	0.71	4/3908 (0.1%)	0.99	6/5292 (0.1%)
1	B	0.72	3/3900 (0.1%)	1.00	7/5283 (0.1%)
All	All	0.71	7/7808 (0.1%)	1.00	13/10575 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	385	TYR	C-O	-7.01	1.16	1.24
1	A	508	GLY	C-N	-6.87	1.23	1.33
1	B	508	GLY	C-N	-6.25	1.24	1.33
1	B	385	TYR	C-O	-6.20	1.16	1.23
1	B	138	VAL	CA-CB	5.49	1.62	1.54
1	A	391	VAL	CA-CB	5.23	1.59	1.53
1	A	138	VAL	CA-CB	5.10	1.62	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	THR	N-CA-C	-8.84	98.61	110.55
1	A	508	GLY	O-C-N	-7.80	110.52	123.00
1	B	157	VAL	N-CA-C	6.16	116.74	108.11
1	B	425	THR	N-CA-C	-5.95	102.53	110.55
1	A	391	VAL	CB-CA-C	5.60	117.28	111.23
1	A	79	SER	CB-CA-C	-5.57	103.91	111.21
1	B	425	THR	CA-C-N	-5.22	117.23	126.32
1	B	425	THR	C-N-CA	-5.22	117.23	126.32
1	B	418	GLY	N-CA-C	5.18	118.14	110.42
1	A	231	GLU	N-CA-C	5.17	119.67	112.90
1	B	319	LYS	CB-CA-C	-5.10	110.67	116.54
1	B	261	GLN	N-CA-C	5.08	117.21	111.11
1	A	385	TYR	N-CA-C	5.06	117.19	111.02

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	3796	0	3600	74	0
1	B	3788	0	3591	79	0
2	A	245	0	0	23	2
2	B	245	0	0	14	1
All	All	8074	0	7191	153	2

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 10.

All (153) 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:123:VAL:HA	2:A:2072:HOH:O	1.50	1.12
1:B:306:THR:HG22	2:B:2175:HOH:O	1.58	1.02
1:A:115:ARG:NH1	2:A:2068:HOH:O	2.02	0.92
1:B:368:GLN:HG3	2:B:2181:HOH:O	1.71	0.88
1:B:425:THR:O	1:B:426:LYS:HB2	1.72	0.88
1:A:315:ARG:HG3	2:A:2168:HOH:O	1.75	0.84
1:B:93:ILE:CG1	1:B:486:VAL:HG11	2.08	0.83
1:A:271:VAL:HG11	2:A:2203:HOH:O	1.81	0.81
1:A:415:THR:HG21	2:A:2203:HOH:O	1.80	0.80
1:A:425:THR:O	1:A:426:LYS:HB2	1.81	0.79
1:A:122:ARG:O	2:A:2072:HOH:O	2.00	0.79
1:A:509:LYS:N	2:A:2245:HOH:O	2.15	0.78
1:A:105:ILE:HA	1:A:108:GLN:HE21	1.45	0.77
1:A:37:VAL:HA	2:A:2001:HOH:O	1.85	0.77
1:A:94:ASN:HD21	1:A:97:HIS:HD2	1.31	0.75
1:B:276:TRP:HE1	1:B:278:GLU:HG2	1.51	0.74
1:B:93:ILE:HG12	1:B:486:VAL:HG11	1.69	0.73
1:B:107:LYS:HE2	2:B:2065:HOH:O	1.90	0.72
1:A:367:ASP:OD1	1:A:367:ASP:O	2.07	0.71
1:A:415:THR:CB	2:A:2203:HOH:O	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:THR:HG21	1:A:271:VAL:HG13	1.76	0.68
2:A:2238:HOH:O	1:B:489:LYS:HD3	1.94	0.68
1:B:105:ILE:HA	1:B:108:GLN:HE21	1.58	0.67
1:B:76:THR:HG21	1:B:88:ASN:HB2	1.75	0.67
1:A:40:ARG:NH2	1:A:44:PRO:O	2.26	0.66
1:A:134:ASN:HB3	2:A:2072:HOH:O	1.93	0.66
1:B:276:TRP:NE1	1:B:278:GLU:HG2	2.10	0.66
1:B:409:VAL:HG21	1:B:412:LEU:HD13	1.77	0.65
1:B:306:THR:CG2	2:B:2175:HOH:O	2.28	0.65
1:B:107:LYS:HD2	1:B:151:ASN:HD22	1.62	0.65
1:A:267:GLU:HG2	1:A:338:ASP:HB3	1.77	0.64
1:B:497:GLU:HG3	2:B:2240:HOH:O	1.97	0.63
1:B:243:HIS:N	2:B:2144:HOH:O	2.32	0.63
1:A:242:THR:HG21	1:A:300:TRP:CZ2	2.35	0.61
1:B:201:TYR:HE1	2:B:2132:HOH:O	1.83	0.61
1:A:415:THR:CG2	2:A:2203:HOH:O	2.41	0.61
1:B:201:TYR:CE1	2:B:2132:HOH:O	2.50	0.60
1:A:429:LEU:HD22	1:A:433:ARG:HG3	1.83	0.59
1:A:105:ILE:HA	1:A:108:GLN:NE2	2.17	0.59
1:B:239:TYR:O	2:B:2144:HOH:O	2.17	0.59
1:A:93:ILE:O	1:A:493:ARG:NH2	2.33	0.58
1:A:242:THR:CG2	1:A:300:TRP:CZ2	2.87	0.58
1:B:76:THR:HG23	1:B:88:ASN:HB3	1.84	0.58
1:B:93:ILE:HG13	1:B:486:VAL:HG11	1.83	0.58
1:B:199:ILE:HG12	1:B:202:TRP:CE2	2.39	0.57
1:B:312:LYS:O	1:B:316:GLU:HG3	2.05	0.57
1:B:253:VAL:HG13	1:B:268:ILE:HD13	1.86	0.56
1:B:308:GLY:O	1:B:330:SER:OG	2.22	0.56
1:A:409:VAL:HG21	1:A:412:LEU:HD13	1.87	0.56
1:B:94:ASN:HD21	1:B:97:HIS:HD2	1.54	0.56
1:B:367:ASP:O	1:B:367:ASP:OD1	2.23	0.56
1:B:291:LYS:NZ	1:B:402:TYR:OH	2.38	0.56
1:A:208:PRO:HB2	1:A:301:PHE:CE1	2.41	0.55
1:A:409:VAL:CG2	1:A:412:LEU:HD13	2.35	0.55
1:A:312:LYS:HD3	2:A:2166:HOH:O	2.06	0.55
1:B:208:PRO:HB2	1:B:301:PHE:CE1	2.41	0.55
1:A:232:GLY:HA3	2:A:2140:HOH:O	2.07	0.54
1:A:412:LEU:HD23	1:A:457:VAL:HG23	1.89	0.54
1:B:72:TRP:O	1:B:76:THR:HB	2.08	0.54
1:A:107:LYS:HD2	1:A:151:ASN:HD22	1.73	0.54
1:B:76:THR:CG2	1:B:88:ASN:HB2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:GLU:HB3	1:A:311:PRO:HD3	1.91	0.53
1:B:242:THR:HG21	1:B:300:TRP:CZ2	2.43	0.53
1:A:63:ASN:HD22	1:A:63:ASN:H	1.57	0.53
1:B:242:THR:CG2	1:B:300:TRP:CZ2	2.92	0.52
1:A:203:THR:CG2	1:A:271:VAL:HG13	2.39	0.52
1:B:154:LYS:HE2	2:B:2096:HOH:O	2.10	0.52
1:A:327:ALA:HB3	2:A:2174:HOH:O	2.09	0.52
1:B:470:ASN:HD22	1:B:470:ASN:C	2.18	0.52
1:B:76:THR:CG2	1:B:88:ASN:CB	2.88	0.52
1:A:281:SER:HA	2:A:2157:HOH:O	2.09	0.51
1:A:312:LYS:NZ	2:A:2168:HOH:O	2.39	0.51
1:A:206:ASN:HA	1:A:271:VAL:HG22	1.93	0.51
1:A:94:ASN:HD21	1:A:97:HIS:CD2	2.19	0.51
1:A:303:GLU:OE2	1:A:303:GLU:HA	2.10	0.51
1:A:271:VAL:CG1	2:A:2203:HOH:O	2.51	0.50
1:A:94:ASN:ND2	1:A:97:HIS:HD2	2.05	0.50
1:A:367:ASP:OD1	1:A:367:ASP:C	2.55	0.50
1:B:303:GLU:HB3	1:B:304:PRO:HD3	1.94	0.50
1:A:242:THR:HG21	1:A:300:TRP:CH2	2.46	0.50
1:A:363:TYR:CD2	1:A:363:TYR:C	2.89	0.50
1:B:202:TRP:O	1:B:268:ILE:HA	2.12	0.49
1:B:343:ASN:CG	1:B:416:GLU:HB2	2.37	0.49
1:A:278:GLU:HG3	1:A:394:TRP:HH2	1.77	0.49
1:B:115:ARG:HG3	1:B:463:PHE:CD2	2.48	0.49
1:B:242:THR:HG21	1:B:300:TRP:CH2	2.47	0.49
1:A:78:ARG:CG	1:A:78:ARG:HH21	2.25	0.48
1:A:312:LYS:HA	1:A:312:LYS:HD2	1.61	0.48
1:B:253:VAL:HG13	1:B:268:ILE:CD1	2.43	0.47
1:A:470:ASN:ND2	1:A:472:GLU:OE1	2.46	0.47
1:B:468:PHE:HB2	2:B:2224:HOH:O	2.14	0.47
1:A:199:ILE:HD12	1:A:201:TYR:H	1.79	0.47
1:B:107:LYS:CE	2:B:2065:HOH:O	2.56	0.47
1:B:199:ILE:HG12	1:B:202:TRP:CZ2	2.50	0.47
1:B:237:GLU:N	1:B:238:PRO:CD	2.78	0.47
1:A:164:LEU:HD12	1:A:165:PRO:HD2	1.97	0.47
1:A:343:ASN:CG	1:A:416:GLU:HB2	2.40	0.46
1:B:367:ASP:OD1	1:B:367:ASP:C	2.58	0.46
1:B:218:LEU:HD21	1:B:364:GLU:HG3	1.97	0.46
1:B:115:ARG:NH2	1:B:203:THR:OG1	2.48	0.46
1:B:267:GLU:HG2	1:B:338:ASP:HB3	1.98	0.46
1:B:412:LEU:HD23	1:B:457:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:VAL:CG2	1:B:412:LEU:HD13	2.43	0.46
1:A:433:ARG:NH1	1:A:497:GLU:OE2	2.48	0.46
1:B:445:HIS:O	1:B:449:VAL:HG23	2.16	0.45
1:B:154:LYS:CE	2:B:2096:HOH:O	2.63	0.45
1:B:384:LEU:HD12	1:B:389:GLN:HG2	1.98	0.45
1:A:228:LYS:HA	2:A:2137:HOH:O	2.17	0.45
1:A:419:MET:HE2	1:A:438:ARG:HB2	1.98	0.45
1:B:63:ASN:HD22	1:B:63:ASN:H	1.65	0.45
1:B:250:LYS:O	1:B:254:GLU:HG3	2.17	0.45
1:A:378:LYS:HE3	1:A:378:LYS:HB3	1.56	0.45
1:B:419:MET:SD	1:B:437:GLU:HG2	2.57	0.45
1:B:363:TYR:CD2	1:B:363:TYR:C	2.94	0.45
1:B:276:TRP:CD1	1:B:278:GLU:HG2	2.52	0.45
1:B:411:VAL:HG13	1:B:460:LYS:HG3	1.98	0.45
1:B:51:ALA:HB3	1:B:111:LEU:HD21	1.98	0.45
1:B:199:ILE:O	1:B:199:ILE:HG13	2.14	0.44
1:A:419:MET:HE1	1:A:437:GLU:HB3	2.00	0.44
1:B:76:THR:HG23	1:B:88:ASN:CB	2.46	0.44
1:A:45:GLN:HE21	1:A:45:GLN:HA	1.82	0.44
1:A:324:LYS:H	1:A:324:LYS:HG2	1.59	0.44
1:A:415:THR:HB	2:A:2203:HOH:O	2.09	0.44
1:A:182:ASP:OD1	2:A:2107:HOH:O	2.21	0.43
1:B:296:PHE:CG	1:B:367:ASP:HB3	2.53	0.43
1:B:203:THR:HG21	1:B:271:VAL:HG13	1.99	0.43
1:A:40:ARG:HH21	1:A:43:PHE:HB2	1.84	0.43
1:B:164:LEU:HD12	1:B:165:PRO:HD2	2.01	0.43
1:A:110:GLY:O	1:A:111:LEU:C	2.61	0.43
1:A:465:TRP:HA	1:A:466:SER:HA	1.77	0.43
1:B:425:THR:O	1:B:426:LYS:CB	2.47	0.43
1:A:237:GLU:N	1:A:238:PRO:CD	2.82	0.43
1:A:452:ALA:O	1:A:457:VAL:HG13	2.19	0.42
1:A:489:LYS:NZ	2:A:2237:HOH:O	2.50	0.42
1:B:95:CYS:HB3	2:B:2062:HOH:O	2.19	0.42
1:A:242:THR:HG23	1:A:300:TRP:CZ2	2.54	0.42
1:A:466:SER:O	1:A:482:GLY:HA2	2.20	0.42
1:A:199:ILE:HD11	1:A:202:TRP:CD1	2.55	0.42
1:A:57:GLN:O	1:A:470:ASN:HB2	2.20	0.42
1:B:306:THR:HG21	1:B:407:TYR:HB3	2.02	0.42
1:A:409:VAL:HA	1:A:410:PRO:HD3	1.91	0.42
1:B:40:ARG:NH2	1:B:44:PRO:O	2.53	0.42
1:A:450:ARG:HD2	2:A:2003:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:TYR:CE2	1:B:460:LYS:HB2	2.54	0.41
1:B:242:THR:HG23	1:B:300:TRP:CZ2	2.55	0.41
1:B:185:CYS:SG	1:B:255:GLU:HG2	2.61	0.41
1:A:185:CYS:SG	1:A:255:GLU:HG2	2.60	0.41
1:A:202:TRP:O	1:A:268:ILE:HA	2.21	0.41
1:B:419:MET:HE1	1:B:437:GLU:HG2	2.02	0.41
1:B:466:SER:O	1:B:482:GLY:HA2	2.20	0.41
1:B:91:GLN:O	1:B:92:ALA:C	2.65	0.40
1:B:319:LYS:HB3	1:B:320:GLY:H	1.65	0.40
1:B:441:TYR:CZ	1:B:445:HIS:CE1	3.10	0.40

All (2) 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)
2:A:2074:HOH:O	2:A:2216:HOH:O[3_655]	1.72	0.48
2:A:2047:HOH:O	2:B:2110:HOH:O[3_655]	1.97	0.23

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	464/532 (87%)	444 (96%)	20 (4%)	0	100	100
1	B	463/532 (87%)	443 (96%)	20 (4%)	0	100	100
All	All	927/1064 (87%)	887 (96%)	40 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	396/456 (87%)	335 (85%)	61 (15%)	2	4
1	B	395/456 (87%)	345 (87%)	50 (13%)	4	8
All	All	791/912 (87%)	680 (86%)	111 (14%)	3	6

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	41	ARG
1	A	45	GLN
1	A	63	ASN
1	A	78	ARG
1	A	84	SER
1	A	94	ASN
1	A	100	LYS
1	A	123	VAL
1	A	133	VAL
1	A	138	VAL
1	A	179	ARG
1	A	180	ILE
1	A	199	ILE
1	A	200	LYS
1	A	228	LYS
1	A	242	THR
1	A	247	LEU
1	A	250	LYS
1	A	255	GLU
1	A	257	ARG
1	A	267	GLU
1	A	268	ILE
1	A	271	VAL
1	A	282	ASP
1	A	284	GLN
1	A	287	ILE

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Mol	Chain	Res	Type
1	A	291	LYS
1	A	294	LEU
1	A	302	LEU
1	A	312	LYS
1	A	315	ARG
1	A	319	LYS
1	A	324	LYS
1	A	342	MET
1	A	350	VAL
1	A	354	VAL
1	A	361	LEU
1	A	368	GLN
1	A	374	GLU
1	A	377	GLN
1	A	378	LYS
1	A	391	VAL
1	A	392	VAL
1	A	396	LEU
1	A	409	VAL
1	A	412	LEU
1	A	415	THR
1	A	419	MET
1	A	429	LEU
1	A	437	GLU
1	A	448	SER
1	A	457	VAL
1	A	459	VAL
1	A	460	LYS
1	A	470	ASN
1	A	474	ASN
1	A	475	LEU
1	A	489	LYS
1	A	493	ARG
1	A	500	ILE
1	B	40	ARG
1	B	63	ASN
1	B	76	THR
1	B	93	ILE
1	B	133	VAL
1	B	138	VAL
1	B	154	LYS
1	B	179	ARG

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Mol	Chain	Res	Type
1	B	199	ILE
1	B	228	LYS
1	B	236	ILE
1	B	242	THR
1	B	247	LEU
1	B	255	GLU
1	B	257	ARG
1	B	268	ILE
1	B	271	VAL
1	B	281	SER
1	B	291	LYS
1	B	294	LEU
1	B	302	LEU
1	B	306	THR
1	B	312	LYS
1	B	315	ARG
1	B	324	LYS
1	B	332	LYS
1	B	342	MET
1	B	350	VAL
1	B	354	VAL
1	B	367	ASP
1	B	371	LYS
1	B	374	GLU
1	B	391	VAL
1	B	392	VAL
1	B	396	LEU
1	B	398	LYS
1	B	405	GLU
1	B	406	THR
1	B	409	VAL
1	B	412	LEU
1	B	419	MET
1	B	421	GLU
1	B	429	LEU
1	B	457	VAL
1	B	466	SER
1	B	470	ASN
1	B	474	ASN
1	B	475	LEU
1	B	489	LYS
1	B	493	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	57	GLN
1	A	63	ASN
1	A	66	ASN
1	A	77	GLN
1	A	94	ASN
1	A	97	HIS
1	A	108	GLN
1	A	151	ASN
1	A	178	HIS
1	A	214	ASN
1	A	264	GLN
1	A	470	ASN
1	A	474	ASN
1	A	504	ASN
1	B	45	GLN
1	B	57	GLN
1	B	63	ASN
1	B	77	GLN
1	B	94	ASN
1	B	97	HIS
1	B	108	GLN
1	B	151	ASN
1	B	214	ASN
1	B	264	GLN
1	B	389	GLN
1	B	470	ASN
1	B	474	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	468/532 (87%)	-0.61	0 100 100	17, 21, 26, 30	0
1	B	467/532 (87%)	-0.50	0 100 100	17, 21, 26, 30	0
All	All	935/1064 (87%)	-0.56	0 100 100	17, 21, 26, 30	0

There are no RSRZ outliers to report.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.