



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:57 AM GMT

PDB ID : 2JF7  
Title : Structure of Strictosidine Glucosidase  
Authors : Barleben, L.; Panjikar, S.; Ruppert, M.; Koepke, J.; Stockigt, J.  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

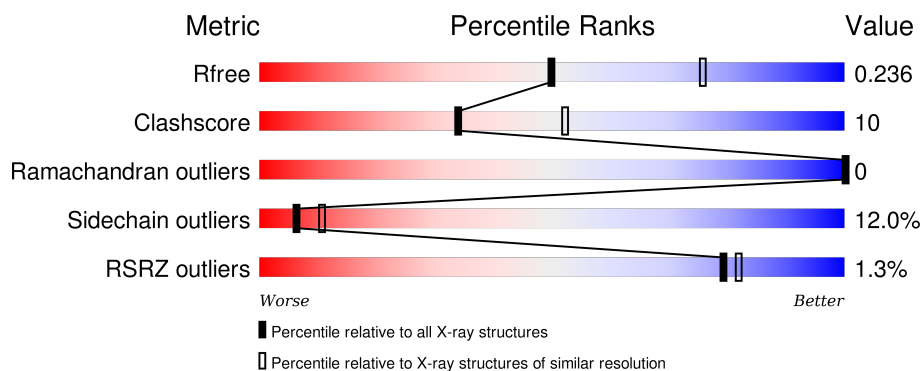
# 1 Overall quality at a glance

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))
$R_{free}$	91344	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div></div> <div>65% 18% 5% 12%</div> </div>
1	B	532	<div> <div></div> <div>64% 20% • 12%</div> </div>

## 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		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.63Å 157.63Å 103.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.48 19.98 – 2.48	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.48) 100.0 (19.98-2.48)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (2.46%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.3	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 28.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	1 of 46616 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8074	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.61	0/3908	0.86	18/5292 (0.3%)
1	B	0.62	0/3900	0.85	19/5283 (0.4%)
All	All	0.61	0/7808	0.85	37/10575 (0.3%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	455	ASP	CB-CG-OD2	8.23	125.70	118.30
1	B	493	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	A	136	ASP	CB-CG-OD2	7.64	125.18	118.30
1	A	508	GLY	O-C-N	-7.61	110.52	122.70
1	B	197	ASP	CB-CG-OD2	7.43	124.99	118.30
1	B	163	ASP	CB-CG-OD2	7.03	124.62	118.30
1	B	182	ASP	CB-CG-OD2	6.99	124.59	118.30
1	B	42	ASP	CB-CG-OD2	6.93	124.54	118.30
1	B	102	ASP	CB-CG-OD2	6.89	124.50	118.30
1	B	328	ASP	CB-CG-OD2	6.70	124.33	118.30
1	A	338	ASP	CB-CG-OD2	6.67	124.30	118.30
1	A	182	ASP	CB-CG-OD2	6.59	124.23	118.30
1	A	163	ASP	CB-CG-OD2	6.55	124.19	118.30
1	B	309	ASP	CB-CG-OD2	6.54	124.19	118.30
1	A	487	ASP	CB-CG-OD2	6.51	124.16	118.30
1	B	233	ASP	CB-CG-OD2	6.47	124.13	118.30
1	A	309	ASP	CB-CG-OD2	6.36	124.03	118.30
1	A	46	ASP	CB-CG-OD2	6.16	123.85	118.30
1	A	197	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	455	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	42	ASP	CB-CG-OD2	5.88	123.59	118.30
1	B	469	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	286	ASP	CB-CG-OD2	5.77	123.49	118.30
1	B	288	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	367	ASP	CB-CG-OD1	5.48	123.24	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	440	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	102	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	288	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	146	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	230	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	493	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	412	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	282	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	183	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	146	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	85	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	367	ASP	CB-CG-OD2	5.02	122.82	118.30

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	3796	0	3600	72	0
1	B	3788	0	3591	77	0
2	A	245	0	0	24	2
2	B	245	0	0	14	1
All	All	8074	0	7191	149	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 (149) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:A:367:ASP:OD1	2.07	0.71
1:A:415:THR:CB	2:A:2203:HOH:O	2.39	0.70
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:242:THR:CG2	1:A:300:TRP:CZ2	2.87	0.58
1:A:93:ILE:O	1:A:493:ARG:NH2	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:72:TRP:O	1:B:76:THR:HB	2.08	0.54
1:A:412:LEU:HD23	1:A:457:VAL:HG23	1.89	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
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:H	1:A:63:ASN:HD22	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: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: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:B:202:TRP:O	1:B:268:ILE:HA	2.12	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:378:LYS:NZ	2:A:2191:HOH:O	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:PHE:HB2	2:B:2224:HOH:O	2.14	0.47
1:B:470:ASN:HD22	1:B:470:ASN:C	2.18	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: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:412:LEU:HD23	1:B:457:VAL:HG23	1.98	0.46
1:B:267:GLU:HG2	1:B:338:ASP:HB3	1.98	0.46
1:B:409:VAL:CG2	1:B:412:LEU:HD13	2.43	0.46
1:A:367:ASP:C	1:A:367:ASP:OD1	2.55	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:363:TYR:C	1:A:363:TYR:CD2	2.89	0.45
1:A:228:LYS:HA	2:A:2137:HOH:O	2.17	0.45
1:B:250:LYS:O	1:B:254:GLU:HG3	2.17	0.45
1:B:63:ASN:H	1:B:63:ASN:HD22	1.65	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:343:ASN:CG	1:B:416:GLU:HB2	2.37	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:291:LYS:HG2	1:B:291:LYS:HZ2	1.44	0.44
1:B:199:ILE:O	1:B:199:ILE:HG13	2.14	0.44
1:B:76:THR:HG23	1:B:88:ASN:CB	2.46	0.44
1:A:45:GLN:HA	1:A:45:GLN:HE21	1.82	0.44
1:A:324:LYS:HG2	1:A:324:LYS:H	1.59	0.44
1:A:415:THR:HB	2:A:2203:HOH:O	2.09	0.44
1:B:296:PHE:CG	1:B:367:ASP:HB3	2.53	0.43
1:A:182:ASP:OD1	2:A:2107:HOH:O	2.21	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:B:425:THR:O	1:B:426:LYS:CB	2.47	0.43
1:A:465:TRP:HA	1:A:466:SER:HA	1.77	0.43
1:A:237:GLU:N	1:A:238:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:LYS:NZ	2:A:2237:HOH:O	2.50	0.43
1:A:452:ALA:O	1:A:457:VAL:HG13	2.19	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:B:306:THR:HG21	1:B:407:TYR:HB3	2.02	0.42
1:A:57:GLN:O	1:A:470:ASN:HB2	2.20	0.42
1:A:343:ASN:CG	1:A:416:GLU:HB2	2.40	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:B:367:ASP:C	1:B:367:ASP:OD1	2.58	0.42
1:B:413:TYR:CE2	1:B:460:LYS:HB2	2.54	0.41
1:A:450:ARG:HD2	2:A:2003:HOH:O	2.20	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:202:TRP:O	1:A:268:ILE:HA	2.21	0.41
1:A:185:CYS:SG	1:A:255:GLU:HG2	2.60	0.41
1:B:466:SER:O	1:B:482:GLY:HA2	2.20	0.41
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
1:B:363:TYR:CD2	1:B:363:TYR:C	2.94	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 ⓘ

### 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	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%)	344 (87%)	52 (13%)	5	8
1	B	395/456 (87%)	352 (89%)	43 (11%)	8	13
All	All	791/912 (87%)	696 (88%)	95 (12%)	6	11

All (95) 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	84	SER
1	A	94	ASN
1	A	138	VAL
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

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Mol	Chain	Res	Type
1	A	271	VAL
1	A	282	ASP
1	A	284	GLN
1	A	287	ILE
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	396	LEU
1	A	409	VAL
1	A	412	LEU
1	A	419	MET
1	A	429	LEU
1	A	437	GLU
1	A	448	SER
1	A	457	VAL
1	A	460	LYS
1	A	470	ASN
1	A	474	ASN
1	A	475	LEU
1	A	493	ARG
1	A	502	TYR
1	B	40	ARG
1	B	63	ASN
1	B	76	THR
1	B	93	ILE
1	B	179	ARG
1	B	199	ILE
1	B	228	LYS
1	B	242	THR

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Mol	Chain	Res	Type
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	371	LYS
1	B	375	ARG
1	B	391	VAL
1	B	392	VAL
1	B	396	LEU
1	B	404	LYS
1	B	405	GLU
1	B	409	VAL
1	B	412	LEU
1	B	419	MET
1	B	429	LEU
1	B	457	VAL
1	B	470	ASN
1	B	474	ASN
1	B	475	LEU
1	B	489	LYS
1	B	493	ARG
1	B	502	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	57	GLN
1	A	63	ASN

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Mol	Chain	Res	Type
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	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	284	GLN
1	B	389	GLN
1	B	470	ASN
1	B	474	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	468/532 (87%)	-0.59	5 (1%) 82 84	17, 21, 26, 30	0
1	B	467/532 (87%)	-0.60	7 (1%) 76 79	17, 21, 26, 30	0
All	All	935/1064 (87%)	-0.60	12 (1%) 79 82	17, 21, 26, 30	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	377	GLN	3.5
1	A	377	GLN	3.0
1	B	37	VAL	2.9
1	A	354	VAL	2.8
1	B	283	VAL	2.5
1	A	376	ASN	2.5
1	B	45	GLN	2.4
1	B	354	VAL	2.3
1	B	231	GLU	2.1
1	B	229	GLY	2.0
1	A	41	ARG	2.0
1	A	228	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 carbohydrates 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.