



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 09:44 PM EDT

PDB ID : 6YV7  
Title : Mannosyltransferase PcManGT from *Pyrobaculum calidifontis*  
Authors : Divne, C.; Rosaria, G.  
Deposited on : 2020-04-28  
Resolution : 2.70 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

<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	:	2.37.1
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)	:	2.37.1

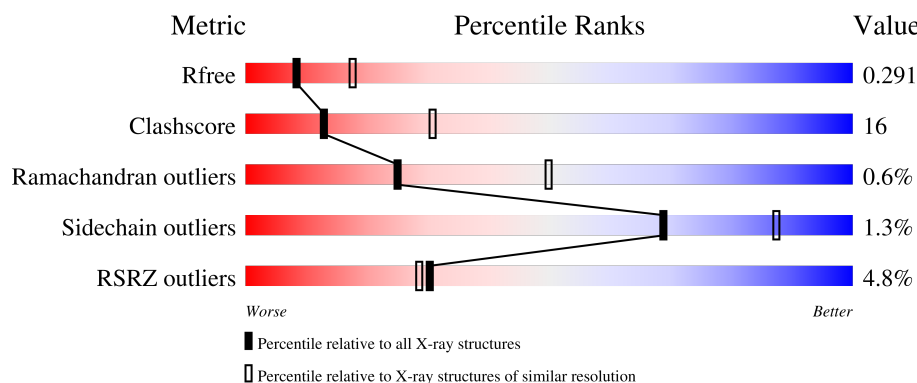
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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	356	<div> <div>5%</div> <div>64%</div> <div>31%</div> <div>..</div> </div>
2	B	355	<div> <div>4%</div> <div>70%</div> <div>26%</div> <div>..</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5386 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 Glycosyl transferase, family 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2697	1739	477	475	6			

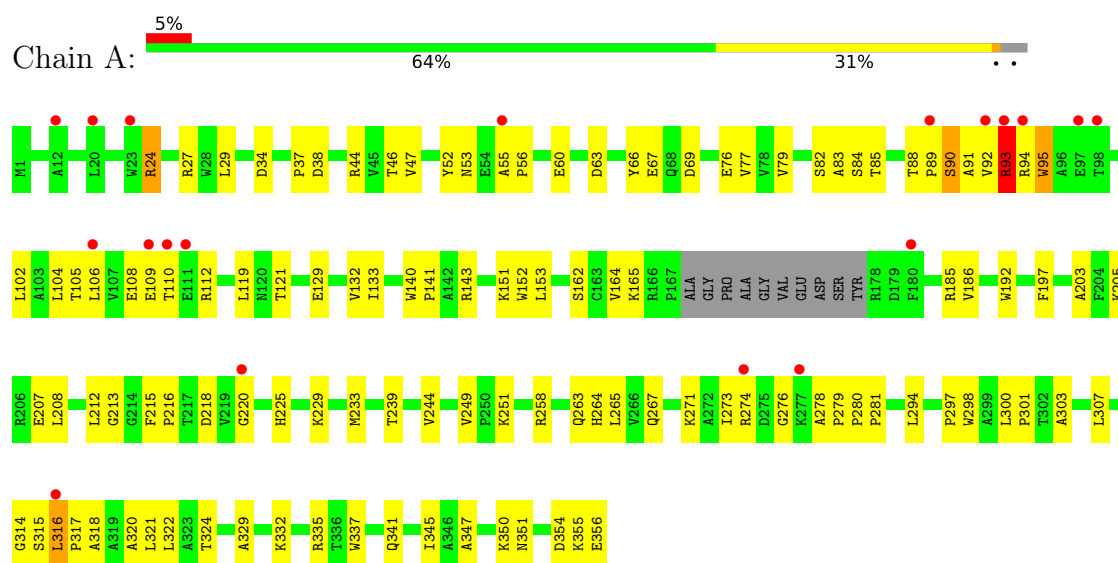
- Molecule 2 is a protein called Glycosyl transferase, family 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	345	Total	C	N	O	S	0	0	0
			2689	1734	476	474	5			

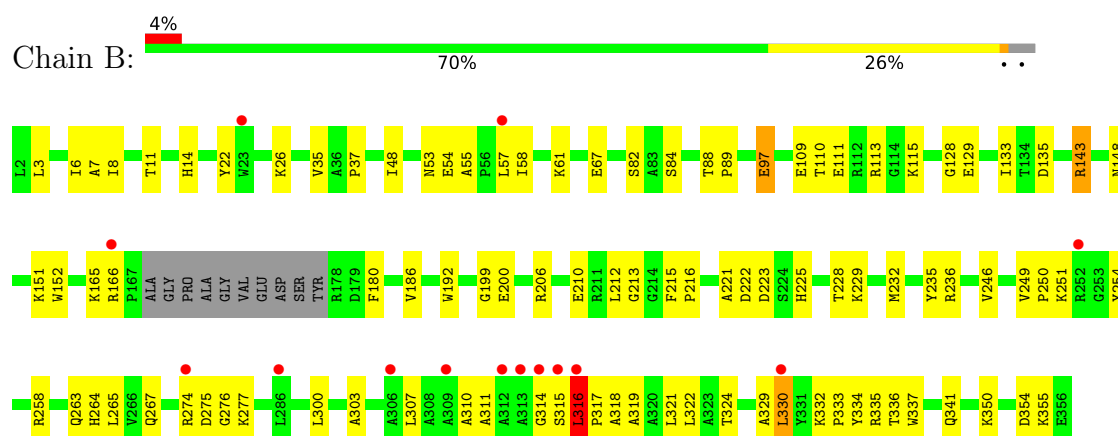
### 3 Residue-property plots [i](#)

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: Glycosyl transferase, family 2



#### • Molecule 2: Glycosyl transferase, family 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.45Å 107.61Å 163.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.08 – 2.70 49.08 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.08-2.70) 100.0 (49.08-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.67 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, $R_{free}$	0.247 , 0.290 0.247 , 0.291	Depositor DCC
$R_{free}$ test set	2000 reflections (7.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.5	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 41.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5386	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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, 0.333 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	0.68	4/2774 (0.1%)	0.89	9/3799 (0.2%)
2	B	0.74	2/2766 (0.1%)	1.06	19/3789 (0.5%)
All	All	0.71	6/5540 (0.1%)	0.98	28/7588 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	129	GLU	CD-OE2	7.96	1.34	1.25
2	B	129	GLU	CD-OE1	7.50	1.33	1.25
1	A	207	GLU	CB-CG	6.79	1.65	1.52
1	A	93	ARG	CG-CD	6.05	1.67	1.51
1	A	95	TRP	CB-CG	-5.84	1.39	1.50
1	A	207	GLU	CG-CD	5.77	1.60	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	ARG	CD-NE-CZ	19.86	151.40	123.60
2	B	330	LEU	CB-CG-CD2	-18.32	79.86	111.00
2	B	330	LEU	CB-CG-CD1	16.42	138.91	111.00
2	B	143	ARG	CB-CG-CD	-13.77	75.80	111.60
2	B	143	ARG	NE-CZ-NH1	-11.15	114.73	120.30
2	B	274	ARG	CA-CB-CG	10.98	137.56	113.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	330	LEU	CA-CB-CG	10.72	139.96	115.30
2	B	355	LYS	CD-CE-NZ	8.46	131.16	111.70
2	B	335	ARG	NE-CZ-NH2	-8.22	116.19	120.30
2	B	335	ARG	CG-CD-NE	-8.18	94.62	111.80
2	B	335	ARG	CB-CG-CD	-7.79	91.34	111.60
1	A	276	GLY	N-CA-C	7.21	131.13	113.10
2	B	129	GLU	CB-CA-C	6.81	124.01	110.40
2	B	330	LEU	CD1-CG-CD2	-6.78	90.16	110.50
2	B	274	ARG	CB-CG-CD	-6.45	94.84	111.60
2	B	314	GLY	N-CA-C	6.21	128.63	113.10
1	A	314	GLY	N-CA-C	5.77	127.52	113.10
1	A	93	ARG	CG-CD-NE	5.62	123.59	111.80
2	B	316	LEU	N-CA-C	5.60	126.13	111.00
2	B	129	GLU	N-CA-CB	-5.58	100.56	110.60
2	B	335	ARG	NE-CZ-NH1	-5.39	117.60	120.30
1	A	90	SER	N-CA-CB	-5.22	102.68	110.50
1	A	185	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	B	335	ARG	NH1-CZ-NH2	5.20	125.12	119.40
2	B	143	ARG	CA-CB-CG	5.19	124.82	113.40
1	A	294	LEU	CB-CG-CD2	-5.09	102.36	111.00
1	A	38	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	90	SER	CA-CB-OG	-5.02	97.65	111.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	93	ARG	Sidechain
2	B	330	LEU	Peptide

## 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	2697	0	2714	92	2
2	B	2689	0	2702	86	2
All	All	5386	0	5416	178	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 16.

All (178) 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)
2:B:166:ARG:CG	2:B:246:VAL:HG12	1.89	1.00
1:A:208:LEU:O	1:A:212:LEU:HD13	1.67	0.94
2:B:166:ARG:CD	2:B:246:VAL:HG12	2.06	0.86
1:A:273:ILE:HD12	1:A:274:ARG:N	1.92	0.84
2:B:166:ARG:HD3	2:B:246:VAL:HG12	1.61	0.83
2:B:311:ALA:HB2	2:B:318:ALA:HB3	1.61	0.81
1:A:307:LEU:HB3	1:A:322:LEU:HD21	1.60	0.81
1:A:307:LEU:CB	1:A:322:LEU:HD21	2.11	0.81
1:A:249:VAL:HG13	1:A:249:VAL:O	1.83	0.78
1:A:316:LEU:N	1:A:317:PRO:HD2	1.98	0.78
1:A:273:ILE:HD12	1:A:273:ILE:C	2.04	0.77
2:B:7:ALA:HB1	2:B:307:LEU:CD1	2.15	0.77
2:B:88:THR:OG1	2:B:89:PRO:HD3	1.85	0.76
2:B:54:GLU:H	2:B:88:THR:HG21	1.51	0.76
1:A:267:GLN:HG2	1:A:351:ASN:HD21	1.52	0.75
1:A:90:SER:HA	1:A:93:ARG:H	1.51	0.74
2:B:166:ARG:HD3	2:B:246:VAL:CG1	2.17	0.73
2:B:166:ARG:HG3	2:B:246:VAL:HG12	1.70	0.71
2:B:109:GLU:HB3	2:B:113:ARG:HH21	1.55	0.71
1:A:53:ASN:HD21	1:A:85:THR:HG23	1.54	0.71
2:B:212:LEU:HD22	2:B:229:LYS:HE2	1.73	0.69
1:A:316:LEU:HD23	1:A:316:LEU:O	1.93	0.69
2:B:199:GLY:HA2	2:B:223:ASP:OD2	1.92	0.68
1:A:298:TRP:O	1:A:301:PRO:HD2	1.93	0.67
2:B:22:TYR:CD1	2:B:180:PHE:HD1	2.13	0.67
2:B:165:LYS:NZ	2:B:200:GLU:OE1	2.28	0.66
1:A:329:ALA:O	1:A:335:ARG:HD2	1.96	0.65
1:A:318:ALA:HA	1:A:321:LEU:HD12	1.77	0.65
1:A:119:LEU:HD22	1:A:133:ILE:HD12	1.78	0.64
2:B:61:LYS:NZ	2:B:135:ASP:O	2.31	0.64
2:B:53:ASN:OD1	2:B:84:SER:HB2	1.98	0.63
1:A:316:LEU:N	1:A:317:PRO:CD	2.61	0.63
2:B:115:LYS:HE2	2:B:222:ASP:OD2	1.97	0.63
2:B:350:LYS:NZ	2:B:354:ASP:OD2	2.32	0.63
1:A:220:GLY:HA3	1:A:264:HIS:ND1	2.13	0.62
2:B:115:LYS:CE	2:B:222:ASP:OD2	2.48	0.62
2:B:54:GLU:HB3	2:B:57:LEU:HD13	1.81	0.62

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:LEU:HD13	2:B:322:LEU:O	2.00	0.62
1:A:332:LYS:HG2	1:A:335:ARG:HH11	1.65	0.61
1:A:44:ARG:HB3	1:A:129:GLU:OE2	2.01	0.61
2:B:166:ARG:HG2	2:B:246:VAL:HG12	1.81	0.59
2:B:249:VAL:CG2	2:B:250:PRO:HD2	2.32	0.59
2:B:7:ALA:HB1	2:B:307:LEU:HD12	1.84	0.59
2:B:225:HIS:CE1	2:B:229:LYS:HD2	2.37	0.59
2:B:263:GLN:O	2:B:267:GLN:HG2	2.03	0.59
1:A:307:LEU:HD13	1:A:322:LEU:CD2	2.33	0.58
1:A:55:ALA:N	1:A:56:PRO:HD2	2.19	0.58
1:A:89:PRO:O	1:A:92:VAL:HG22	2.05	0.57
1:A:212:LEU:N	1:A:213:GLY:HA2	2.19	0.57
1:A:273:ILE:C	1:A:273:ILE:CD1	2.73	0.57
2:B:128:GLY:O	2:B:206:ARG:HD3	2.05	0.57
1:A:249:VAL:O	1:A:249:VAL:CG1	2.50	0.56
2:B:303:ALA:O	2:B:307:LEU:HD12	2.06	0.56
2:B:7:ALA:HB1	2:B:307:LEU:HD11	1.88	0.56
1:A:132:VAL:HG22	1:A:203:ALA:HB2	1.86	0.56
2:B:67:GLU:O	2:B:143:ARG:HB3	2.05	0.56
2:B:275:ASP:OD1	2:B:276:GLY:N	2.38	0.55
2:B:3:LEU:HD11	2:B:310:ALA:HB2	1.87	0.55
1:A:37:PRO:HB2	1:A:151:LYS:HG3	1.87	0.55
1:A:24:ARG:HA	1:A:27:ARG:NH1	2.22	0.54
1:A:186:VAL:HG12	1:A:239:THR:O	2.07	0.54
1:A:316:LEU:H	1:A:317:PRO:HD2	1.69	0.54
2:B:115:LYS:NZ	2:B:222:ASP:OD2	2.40	0.54
1:A:66:TYR:HB2	1:A:95:TRP:HH2	1.73	0.54
2:B:315:SER:C	2:B:317:PRO:HD3	2.28	0.54
2:B:318:ALA:O	2:B:321:LEU:N	2.41	0.54
1:A:79:VAL:HG11	1:A:92:VAL:HG11	1.90	0.53
2:B:3:LEU:CD1	2:B:310:ALA:HB2	2.38	0.53
2:B:263:GLN:OE1	2:B:350:LYS:HD3	2.09	0.53
2:B:337:TRP:O	2:B:341:GLN:HG2	2.09	0.52
1:A:79:VAL:O	1:A:106:LEU:HD12	2.10	0.51
1:A:90:SER:HB3	1:A:93:ARG:CB	2.41	0.51
2:B:329:ALA:HA	2:B:334:TYR:CD2	2.46	0.51
1:A:162:SER:HB2	1:A:197:PHE:CD2	2.46	0.51
2:B:55:ALA:CA	2:B:88:THR:HG22	2.41	0.51
2:B:318:ALA:O	2:B:322:LEU:N	2.41	0.51
2:B:109:GLU:HB3	2:B:113:ARG:NH2	2.25	0.51
2:B:37:PRO:HB2	2:B:151:LYS:HG3	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:VAL:HG21	1:A:106:LEU:HD13	1.93	0.50
2:B:11:THR:HG23	2:B:303:ALA:HB1	1.94	0.50
1:A:307:LEU:HD13	1:A:322:LEU:HD23	1.93	0.50
2:B:318:ALA:O	2:B:321:LEU:HB2	2.12	0.50
1:A:44:ARG:CB	1:A:129:GLU:OE2	2.60	0.50
1:A:104:LEU:HD23	1:A:105:THR:N	2.27	0.50
1:A:355:LYS:O	1:A:356:GLU:HB2	2.11	0.50
1:A:263:GLN:O	1:A:267:GLN:HG3	2.11	0.50
1:A:297:PRO:O	1:A:301:PRO:HD3	2.11	0.50
1:A:332:LYS:HA	1:A:335:ARG:HD3	1.93	0.49
1:A:60:GLU:HA	1:A:63:ASP:HB2	1.94	0.49
2:B:55:ALA:HA	2:B:88:THR:HG22	1.94	0.49
2:B:57:LEU:HD12	2:B:57:LEU:H	1.76	0.49
2:B:110:THR:HB	2:B:111:GLU:OE2	2.13	0.49
2:B:3:LEU:HG	2:B:310:ALA:HB2	1.94	0.48
2:B:22:TYR:CD1	2:B:180:PHE:CD1	2.99	0.48
2:B:148:ASN:O	2:B:151:LYS:HG2	2.14	0.48
2:B:14:HIS:CE1	2:B:300:LEU:HB2	2.48	0.48
2:B:55:ALA:N	2:B:88:THR:HG22	2.28	0.48
2:B:333:PRO:O	2:B:336:THR:OG1	2.26	0.47
2:B:199:GLY:CA	2:B:223:ASP:OD2	2.62	0.47
2:B:206:ARG:O	2:B:210:GLU:HG2	2.13	0.47
2:B:212:LEU:N	2:B:213:GLY:HA2	2.29	0.47
1:A:215:PHE:HA	1:A:216:PRO:HD3	1.70	0.47
2:B:3:LEU:CG	2:B:310:ALA:HB2	2.45	0.47
2:B:316:LEU:HD23	2:B:319:ALA:HB2	1.95	0.47
2:B:8:ILE:HA	2:B:11:THR:OG1	2.15	0.46
2:B:48:ILE:HB	2:B:133:ILE:HD13	1.97	0.46
1:A:66:TYR:HD1	1:A:102:LEU:HD22	1.80	0.46
2:B:3:LEU:HA	2:B:6:ILE:HG13	1.97	0.46
1:A:82:SER:HB2	1:A:112:ARG:HA	1.97	0.46
1:A:320:ALA:O	1:A:321:LEU:C	2.54	0.46
1:A:90:SER:HB3	1:A:93:ARG:HB3	1.97	0.46
2:B:332:LYS:N	2:B:333:PRO:HD2	2.30	0.46
1:A:153:LEU:O	1:A:205:LYS:NZ	2.49	0.45
2:B:249:VAL:HG22	2:B:250:PRO:HD2	1.97	0.45
1:A:321:LEU:O	1:A:324:THR:OG1	2.28	0.45
1:A:307:LEU:CD1	1:A:322:LEU:HD21	2.47	0.45
2:B:221:ALA:HB2	2:B:264:HIS:HB3	1.98	0.45
2:B:165:LYS:HZ1	2:B:200:GLU:CD	2.18	0.45
1:A:37:PRO:HD3	1:A:152:TRP:CH2	2.52	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:THR:O	2:B:232:MET:HG2	2.17	0.44
1:A:88:THR:OG1	1:A:89:PRO:HD3	2.17	0.44
1:A:52:TYR:HE1	1:A:83:ALA:O	2.00	0.44
1:A:53:ASN:OD1	1:A:84:SER:HB2	2.18	0.44
1:A:337:TRP:O	1:A:341:GLN:HG2	2.17	0.44
2:B:254:TYR:OH	2:B:258:ARG:NH1	2.51	0.44
1:A:91:ALA:HA	1:A:94:ARG:HE	1.83	0.44
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.80	0.43
1:A:66:TYR:HB2	1:A:95:TRP:CH2	2.54	0.43
1:A:164:VAL:O	1:A:244:VAL:HA	2.18	0.43
2:B:82:SER:HA	2:B:109:GLU:HB2	2.00	0.43
2:B:321:LEU:O	2:B:324:THR:HB	2.18	0.43
1:A:44:ARG:H	1:A:129:GLU:CD	2.22	0.43
1:A:37:PRO:CB	1:A:151:LYS:HG3	2.49	0.43
1:A:263:GLN:HA	1:A:347:ALA:HB1	2.01	0.43
2:B:222:ASP:N	2:B:222:ASP:OD1	2.50	0.43
1:A:47:VAL:HB	1:A:77:VAL:HG22	2.01	0.43
1:A:225:HIS:NE2	1:A:229:LYS:HD2	2.34	0.43
1:A:303:ALA:O	1:A:307:LEU:HG	2.19	0.42
2:B:35:VAL:HG13	2:B:236:ARG:NH1	2.33	0.42
1:A:218:ASP:OD2	1:A:271:LYS:NZ	2.52	0.42
1:A:279:PRO:HA	1:A:280:PRO:HD3	1.92	0.42
1:A:89:PRO:HB3	1:A:108:GLU:OE1	2.19	0.42
1:A:300:LEU:HB3	1:A:301:PRO:HD3	2.02	0.42
2:B:303:ALA:O	2:B:307:LEU:CD1	2.67	0.42
2:B:265:LEU:HD23	2:B:265:LEU:HA	1.81	0.42
1:A:307:LEU:HD13	1:A:322:LEU:HD21	2.01	0.42
1:A:307:LEU:CD1	1:A:322:LEU:CD2	2.97	0.42
2:B:249:VAL:O	2:B:249:VAL:HG13	2.20	0.42
1:A:165:LYS:HE3	1:A:165:LYS:HB2	1.74	0.42
2:B:88:THR:HG1	2:B:89:PRO:HD3	1.79	0.42
2:B:318:ALA:HA	2:B:321:LEU:HB2	2.01	0.42
1:A:95:TRP:CZ3	1:A:102:LEU:HD23	2.55	0.42
1:A:278:ALA:HA	1:A:279:PRO:HD3	1.82	0.41
1:A:162:SER:HB3	1:A:239:THR:HG22	2.01	0.41
1:A:29:LEU:HD11	1:A:186:VAL:HG23	2.01	0.41
1:A:119:LEU:HD22	1:A:133:ILE:CD1	2.46	0.41
1:A:208:LEU:HD22	1:A:233:MET:HE1	2.02	0.41
1:A:95:TRP:HZ3	1:A:102:LEU:HD23	1.84	0.41
2:B:263:GLN:HE22	2:B:350:LYS:NZ	2.19	0.41
2:B:277:LYS:HB3	2:B:277:LYS:HE2	1.90	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ARG:O	1:A:129:GLU:N	2.54	0.41
1:A:109:GLU:CD	1:A:121:THR:HG21	2.41	0.41
1:A:132:VAL:HG22	1:A:203:ALA:CB	2.49	0.41
1:A:307:LEU:HB2	1:A:322:LEU:HD21	1.98	0.41
2:B:249:VAL:HG23	2:B:250:PRO:HD2	2.02	0.41
1:A:67:GLU:O	1:A:143:ARG:NH1	2.50	0.41
2:B:215:PHE:HA	2:B:216:PRO:HD3	1.82	0.40
1:A:140:TRP:HA	1:A:141:PRO:HD3	1.96	0.40
1:A:280:PRO:HB2	1:A:281:PRO:HD3	2.04	0.40
2:B:88:THR:N	2:B:89:PRO:CD	2.84	0.40
1:A:46:THR:HG23	1:A:76:GLU:HG3	2.02	0.40
1:A:315:SER:OG	1:A:317:PRO:HG2	2.21	0.40
2:B:26:LYS:HE2	2:B:26:LYS:HB2	1.81	0.40
2:B:37:PRO:HD3	2:B:152:TRP:CZ3	2.55	0.40
2:B:329:ALA:HA	2:B:334:TYR:CE2	2.56	0.40
2:B:55:ALA:O	2:B:58:ILE:HG22	2.22	0.40
1:A:345:ILE:HD13	1:A:345:ILE:HA	1.88	0.40
1:A:350:LYS:NZ	1:A:354:ASP:OD2	2.54	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)
1:A:251:LYS:NZ	2:B:97:GLU:OE1[4_455]	1.51	0.69
1:A:69:ASP:OD2	2:B:235:TYR:OH[2_564]	2.08	0.12

## 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	342/356 (96%)	329 (96%)	11 (3%)	2 (1%)	25 50

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	341/355 (96%)	329 (96%)	10 (3%)	2 (1%)	25	50
All	All	683/711 (96%)	658 (96%)	21 (3%)	4 (1%)	25	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	TRP
2	B	192	TRP
2	B	316	LEU
1	A	110	THR

### 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	268/274 (98%)	264 (98%)	4 (2%)	65	86
2	B	267/273 (98%)	264 (99%)	3 (1%)	73	90
All	All	535/547 (98%)	528 (99%)	7 (1%)	69	87

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	34	ASP
1	A	258	ARG
1	A	316	LEU
2	B	97	GLU
2	B	186	VAL
2	B	251	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	GLN
2	B	225	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](#)

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 ⓘ

### 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<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	346/356 (97%)	0.36	19 (5%) 25 24	50, 70, 107, 120	0
2	B	345/355 (97%)	0.18	14 (4%) 37 36	48, 67, 117, 132	0
All	All	691/711 (97%)	0.27	33 (4%) 30 28	48, 69, 109, 132	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	313	ALA	4.7
2	B	312	ALA	4.6
1	A	89	PRO	4.3
2	B	314	GLY	4.2
1	A	274	ARG	4.1
2	B	316	LEU	3.9
1	A	93	ARG	3.9
1	A	110	THR	3.7
1	A	109	GLU	3.4
1	A	220	GLY	3.4
1	A	97	GLU	3.4
1	A	55	ALA	3.3
2	B	57	LEU	2.9
2	B	309	ALA	2.6
1	A	92	VAL	2.5
1	A	111	GLU	2.5
1	A	12	ALA	2.5
2	B	315	SER	2.5
1	A	180	PHE	2.5
2	B	286	LEU	2.4
1	A	94	ARG	2.3
1	A	23	TRP	2.3
1	A	277	LYS	2.3
1	A	316	LEU	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	274	ARG	2.2
2	B	330	LEU	2.2
1	A	106	LEU	2.2
1	A	98	THR	2.2
2	B	23	TRP	2.2
2	B	252	ARG	2.2
2	B	166	ARG	2.1
1	A	20	LEU	2.1
2	B	306	ALA	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.