



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:15 PM EDT

PDB ID : 6YV7 / pdb_00006yv7
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

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

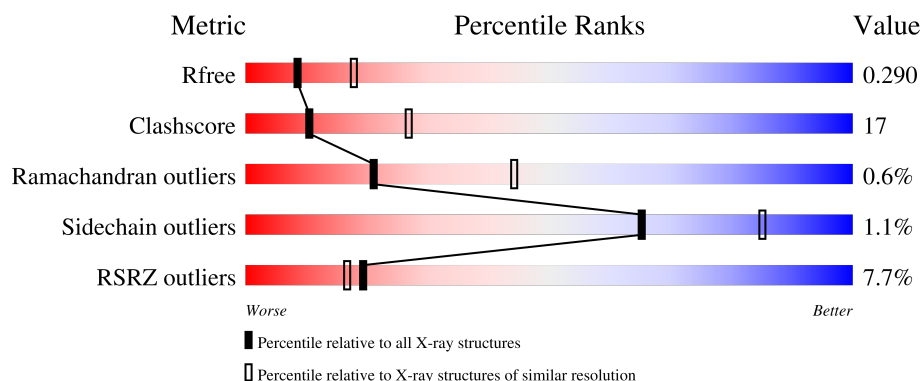
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 ≥ 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	5% 64% 30% • •
2	B	355	10% 69% 27% • •

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			

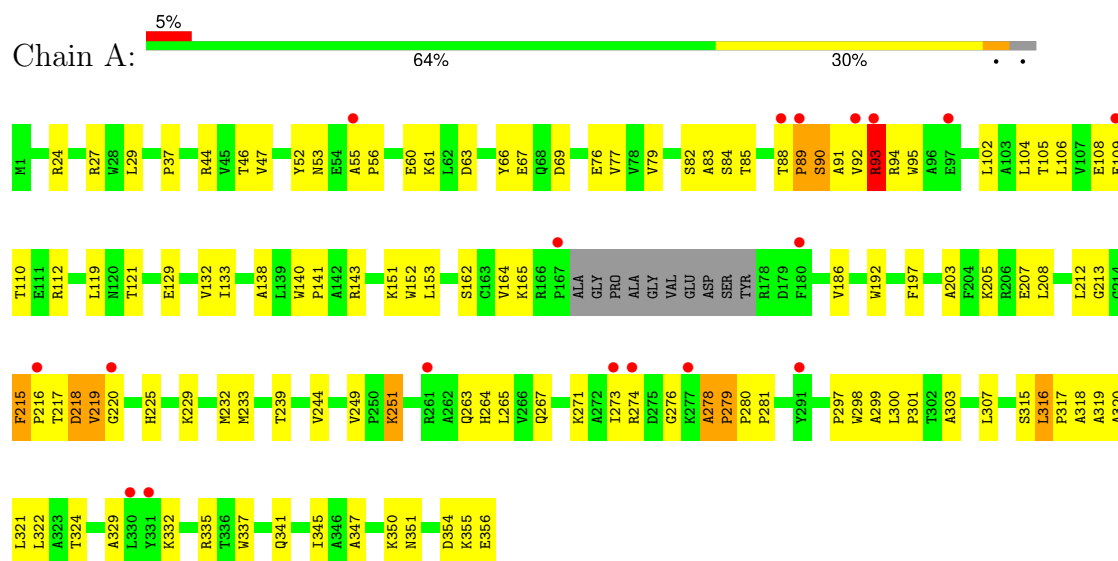
- Molecule 2 is a protein called Glycosyl transferase, family 2.

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

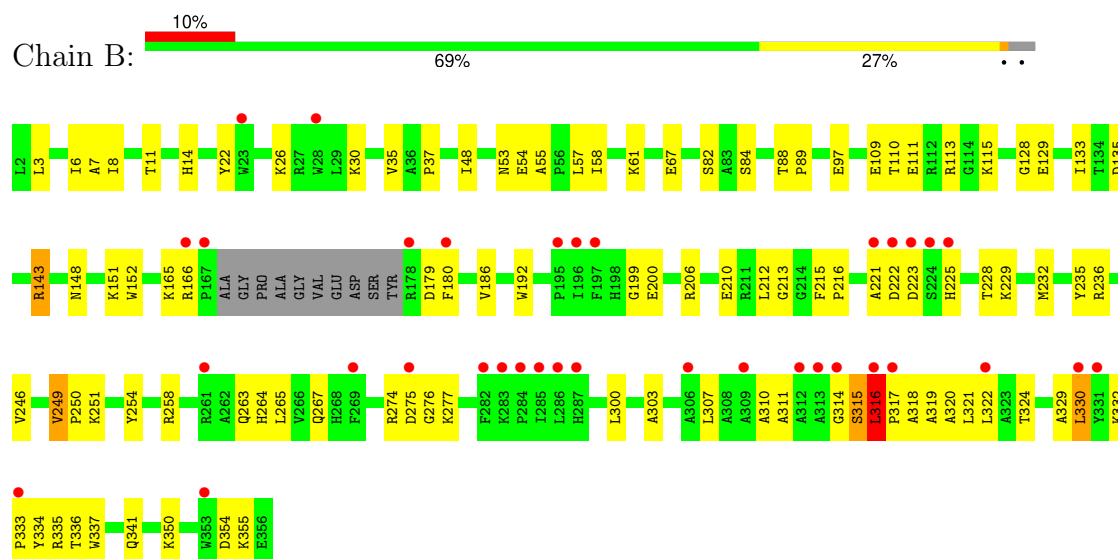
3 Residue-property plots

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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.247 , 0.290 0.247 , 0.290	Depositor DCC
R_{free} test set	2000 reflections (7.77%)	wwPDB-VP
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

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	0.73	1/2774 (0.0%)	1.11	18/3799 (0.5%)
2	B	0.76	1/2766 (0.0%)	1.14	28/3789 (0.7%)
All	All	0.75	2/5540 (0.0%)	1.12	46/7588 (0.6%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	335	ARG	CD-NE	-5.35	1.38	1.46
1	A	279	PRO	C-O	-5.05	1.20	1.25

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	ARG	CD-NE-CZ	19.29	151.40	124.40
2	B	143	ARG	CB-CG-CD	-15.44	75.80	111.30
1	A	276	GLY	N-CA-C	15.33	131.13	112.73
2	B	274	ARG	CA-CB-CG	11.73	137.56	114.10
2	B	330	LEU	CB-CG-CD2	-10.28	79.86	110.70
1	A	278	ALA	CA-C-N	9.59	126.66	119.66
1	A	278	ALA	C-N-CA	9.59	126.66	119.66
2	B	330	LEU	CB-CG-CD1	9.40	138.91	110.70
2	B	330	LEU	CD1-CG-CD2	-9.38	90.16	110.80
2	B	249	VAL	CA-C-N	8.95	128.61	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	249	VAL	C-N-CA	8.95	128.61	118.85
2	B	335	ARG	CB-CG-CD	-8.68	91.34	111.30
2	B	320	ALA	N-CA-C	-8.46	102.06	111.28
2	B	335	ARG	CG-CD-NE	-7.90	94.62	112.00
2	B	315	SER	N-CA-C	7.70	119.67	111.28
2	B	316	LEU	N-CA-C	7.38	126.13	109.81
2	B	274	ARG	CB-CG-CD	-7.16	94.84	111.30
2	B	129	GLU	CB-CA-C	7.14	124.01	109.67
1	A	299	ALA	CA-C-N	-6.96	111.39	120.44
1	A	299	ALA	C-N-CA	-6.96	111.39	120.44
1	A	215	PHE	CA-C-N	6.79	126.55	119.76
1	A	215	PHE	C-N-CA	6.79	126.55	119.76
2	B	143	ARG	NE-CZ-NH1	-6.77	114.73	121.50
2	B	330	LEU	CA-CB-CG	6.76	139.96	116.30
1	A	207	GLU	CB-CG-CD	6.76	124.09	112.60
1	A	90	SER	CA-CB-OG	-6.73	97.65	111.10
2	B	314	GLY	N-CA-C	6.52	128.63	113.18
2	B	129	GLU	N-CA-CB	-6.51	100.56	110.33
1	A	89	PRO	CA-C-N	-6.25	112.65	122.65
1	A	89	PRO	C-N-CA	-6.25	112.65	122.65
1	A	207	GLU	N-CA-CB	6.20	119.37	110.06
2	B	355	LYS	CD-CE-NZ	6.02	131.16	111.90
2	B	355	LYS	CG-CD-CE	-6.01	97.48	111.30
1	A	219	VAL	N-CA-C	5.94	117.15	108.53
2	B	355	LYS	CB-CG-CD	5.72	124.45	111.30
1	A	218	ASP	N-CA-C	5.68	117.47	111.28
2	B	30	LYS	CA-C-N	5.58	131.54	120.94
2	B	30	LYS	C-N-CA	5.58	131.54	120.94
1	A	93	ARG	CB-CG-CD	5.50	123.95	111.30
2	B	179	ASP	CA-C-N	5.49	127.64	120.28
2	B	179	ASP	C-N-CA	5.49	127.64	120.28
1	A	90	SER	N-CA-CB	-5.40	102.68	110.56
2	B	143	ARG	CA-CB-CG	5.36	124.82	114.10
1	A	93	ARG	CG-CD-NE	5.27	123.59	112.00
2	B	316	LEU	CA-C-N	-5.20	113.34	119.84
2	B	316	LEU	C-N-CA	-5.20	113.34	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	93	ARG	Sidechain

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Mol	Chain	Res	Type	Group
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	95	2
2	B	2689	0	2702	87	2
All	All	5386	0	5416	182	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 17.

All (182) 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
1:A:273:ILE:HD12	1:A:273:ILE:C	2.04	0.82
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:322:LEU:HD13	2:B:322:LEU:O	2.00	0.62
1:A:273:ILE:C	1:A:273:ILE:CD1	2.73	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
2:B:315:SER:C	2:B:317:PRO:HD3	2.28	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
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
1:A:232:MET:HE1	1:A:278:ALA:HB2	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:320:ALA:O	1:A:321:LEU:C	2.54	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
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: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
2:B:165:LYS:HZ1	2:B:200:GLU:CD	2.17	0.50
1:A:332:LYS:HA	1:A:335:ARG:HD3	1.93	0.49
1:A:355:LYS:O	1:A:356:GLU:HB2	2.11	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
1:A:44:ARG:H	1:A:129:GLU:CD	2.22	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
1:A:321:LEU:O	1:A:324:THR:OG1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:109:GLU:CD	1:A:121:THR:HG21	2.41	0.45
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:61:LYS:NZ	1:A:138:ALA:O	2.50	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
1:A:37:PRO:HD3	1:A:152:TRP:CH2	2.52	0.44
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
2:B:88:THR:HG1	2:B:89:PRO:HD3	1.77	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:318:ALA:O	1:A:319:ALA:C	2.61	0.43
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: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:165:LYS:NZ	2:B:200:GLU:CD	2.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:44:ARG:O	1:A:129:GLU:N	2.54	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%)	21	44
2	B	341/355 (96%)	329 (96%)	10 (3%)	2 (1%)	21	44
All	All	683/711 (96%)	658 (96%)	21 (3%)	4 (1%)	21	44

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 [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	268/274 (98%)	264 (98%)	4 (2%)	57	81
2	B	267/273 (98%)	265 (99%)	2 (1%)	76	90
All	All	535/547 (98%)	529 (99%)	6 (1%)	65	85

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	217	THR
1	A	219	VAL
1	A	251	LYS
1	A	316	LEU
2	B	186	VAL
2	B	251	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	GLN
1	A	267	GLN
1	A	351	ASN
2	B	68	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 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 ⓘ

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	346/356 (97%)	0.60	18 (5%) 33 29	50, 70, 107, 120	0
2	B	345/355 (97%)	0.64	35 (10%) 12 10	48, 67, 117, 132	0
All	All	691/711 (97%)	0.62	53 (7%) 19 17	48, 69, 109, 132	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	312	ALA	6.7
2	B	286	LEU	4.7
1	A	55	ALA	4.2
2	B	223	ASP	4.0
2	B	313	ALA	3.8
1	A	167	PRO	3.8
2	B	309	ALA	3.7
1	A	274	ARG	3.5
1	A	89	PRO	3.3
2	B	221	ALA	3.3
2	B	331	TYR	3.3
2	B	330	LEU	3.2
1	A	180	PHE	3.2
2	B	275	ASP	3.1
2	B	314	GLY	3.1
2	B	178	ARG	3.0
2	B	222	ASP	3.0
2	B	269	PHE	2.9
2	B	167	PRO	2.9
2	B	306	ALA	2.9
2	B	322	LEU	2.9
2	B	285	ILE	2.9
1	A	331	TYR	2.8
2	B	225	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	291	TYR	2.6
2	B	196	ILE	2.6
2	B	180	PHE	2.5
1	A	273	ILE	2.5
2	B	353	TRP	2.5
1	A	92	VAL	2.5
2	B	316	LEU	2.4
2	B	317	PRO	2.4
2	B	224	SER	2.4
1	A	93	ARG	2.4
1	A	220	GLY	2.3
1	A	330	LEU	2.3
2	B	287	HIS	2.3
2	B	23	TRP	2.2
1	A	88	THR	2.2
2	B	283	LYS	2.2
1	A	97	GLU	2.1
1	A	216	PRO	2.1
2	B	195	PRO	2.1
2	B	333	PRO	2.1
2	B	282	PHE	2.1
2	B	261	ARG	2.1
2	B	197	PHE	2.1
1	A	261	ARG	2.1
2	B	166	ARG	2.1
2	B	28	TRP	2.1
1	A	109	GLU	2.0
1	A	277	LYS	2.0
2	B	284	PRO	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](#)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.