



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2025 – 01:08 pm BST

PDB ID : 9HTX / pdb_00009htx
Title : Glycosyltransferase C from the *Limosilactobacillus reuteri* accessory secretion system. Apo form.
Authors : Pfalzgraf, H.E.; Griffiths, R.; Juge, N.; Hemmings, A.M.
Deposited on : 2024-12-20
Resolution : 2.00 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

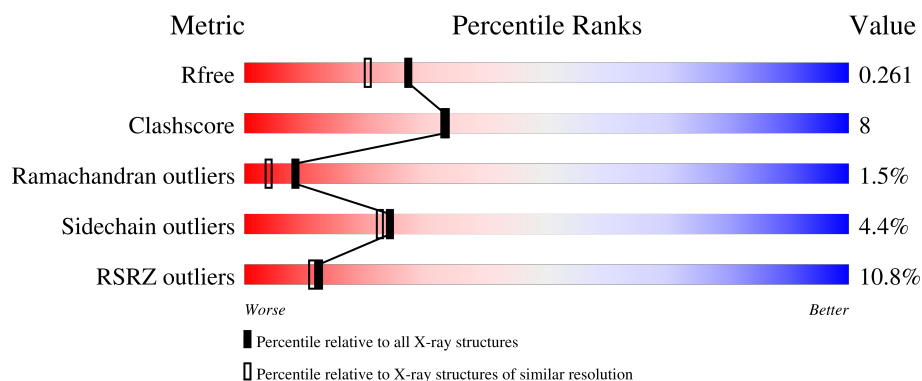
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	354	
1	B	354	
1	C	354	
1	D	354	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11093 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 Glucosyltransferase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2713	1750	451	505	7			
1	B	338	Total	C	N	O	S	0	1	0
			2735	1763	457	508	7			
1	C	339	Total	C	N	O	S	0	0	0
			2736	1764	457	509	6			
1	D	336	Total	C	N	O	S	0	1	0
			2702	1737	454	504	7			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP B3XPQ7
A	-18	GLY	-	expression tag	UNP B3XPQ7
A	-17	SER	-	expression tag	UNP B3XPQ7
A	-16	SER	-	expression tag	UNP B3XPQ7
A	-15	HIS	-	expression tag	UNP B3XPQ7
A	-14	HIS	-	expression tag	UNP B3XPQ7
A	-13	HIS	-	expression tag	UNP B3XPQ7
A	-12	HIS	-	expression tag	UNP B3XPQ7
A	-11	HIS	-	expression tag	UNP B3XPQ7
A	-10	HIS	-	expression tag	UNP B3XPQ7
A	-9	SER	-	expression tag	UNP B3XPQ7
A	-8	SER	-	expression tag	UNP B3XPQ7
A	-7	GLY	-	expression tag	UNP B3XPQ7
A	-6	LEU	-	expression tag	UNP B3XPQ7
A	-5	VAL	-	expression tag	UNP B3XPQ7
A	-4	PRO	-	expression tag	UNP B3XPQ7
A	-3	ARG	-	expression tag	UNP B3XPQ7
A	-2	GLY	-	expression tag	UNP B3XPQ7
A	-1	SER	-	expression tag	UNP B3XPQ7
A	0	HIS	-	expression tag	UNP B3XPQ7
A	1	LEU	-	expression tag	UNP B3XPQ7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP B3XPQ7
B	-18	GLY	-	expression tag	UNP B3XPQ7
B	-17	SER	-	expression tag	UNP B3XPQ7
B	-16	SER	-	expression tag	UNP B3XPQ7
B	-15	HIS	-	expression tag	UNP B3XPQ7
B	-14	HIS	-	expression tag	UNP B3XPQ7
B	-13	HIS	-	expression tag	UNP B3XPQ7
B	-12	HIS	-	expression tag	UNP B3XPQ7
B	-11	HIS	-	expression tag	UNP B3XPQ7
B	-10	HIS	-	expression tag	UNP B3XPQ7
B	-9	SER	-	expression tag	UNP B3XPQ7
B	-8	SER	-	expression tag	UNP B3XPQ7
B	-7	GLY	-	expression tag	UNP B3XPQ7
B	-6	LEU	-	expression tag	UNP B3XPQ7
B	-5	VAL	-	expression tag	UNP B3XPQ7
B	-4	PRO	-	expression tag	UNP B3XPQ7
B	-3	ARG	-	expression tag	UNP B3XPQ7
B	-2	GLY	-	expression tag	UNP B3XPQ7
B	-1	SER	-	expression tag	UNP B3XPQ7
B	0	HIS	-	expression tag	UNP B3XPQ7
B	1	LEU	-	expression tag	UNP B3XPQ7
C	-19	MET	-	initiating methionine	UNP B3XPQ7
C	-18	GLY	-	expression tag	UNP B3XPQ7
C	-17	SER	-	expression tag	UNP B3XPQ7
C	-16	SER	-	expression tag	UNP B3XPQ7
C	-15	HIS	-	expression tag	UNP B3XPQ7
C	-14	HIS	-	expression tag	UNP B3XPQ7
C	-13	HIS	-	expression tag	UNP B3XPQ7
C	-12	HIS	-	expression tag	UNP B3XPQ7
C	-11	HIS	-	expression tag	UNP B3XPQ7
C	-10	HIS	-	expression tag	UNP B3XPQ7
C	-9	SER	-	expression tag	UNP B3XPQ7
C	-8	SER	-	expression tag	UNP B3XPQ7
C	-7	GLY	-	expression tag	UNP B3XPQ7
C	-6	LEU	-	expression tag	UNP B3XPQ7
C	-5	VAL	-	expression tag	UNP B3XPQ7
C	-4	PRO	-	expression tag	UNP B3XPQ7
C	-3	ARG	-	expression tag	UNP B3XPQ7
C	-2	GLY	-	expression tag	UNP B3XPQ7
C	-1	SER	-	expression tag	UNP B3XPQ7
C	0	HIS	-	expression tag	UNP B3XPQ7
C	1	LEU	-	expression tag	UNP B3XPQ7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	initiating methionine	UNP B3XPQ7
D	-18	GLY	-	expression tag	UNP B3XPQ7
D	-17	SER	-	expression tag	UNP B3XPQ7
D	-16	SER	-	expression tag	UNP B3XPQ7
D	-15	HIS	-	expression tag	UNP B3XPQ7
D	-14	HIS	-	expression tag	UNP B3XPQ7
D	-13	HIS	-	expression tag	UNP B3XPQ7
D	-12	HIS	-	expression tag	UNP B3XPQ7
D	-11	HIS	-	expression tag	UNP B3XPQ7
D	-10	HIS	-	expression tag	UNP B3XPQ7
D	-9	SER	-	expression tag	UNP B3XPQ7
D	-8	SER	-	expression tag	UNP B3XPQ7
D	-7	GLY	-	expression tag	UNP B3XPQ7
D	-6	LEU	-	expression tag	UNP B3XPQ7
D	-5	VAL	-	expression tag	UNP B3XPQ7
D	-4	PRO	-	expression tag	UNP B3XPQ7
D	-3	ARG	-	expression tag	UNP B3XPQ7
D	-2	GLY	-	expression tag	UNP B3XPQ7
D	-1	SER	-	expression tag	UNP B3XPQ7
D	0	HIS	-	expression tag	UNP B3XPQ7
D	1	LEU	-	expression tag	UNP B3XPQ7

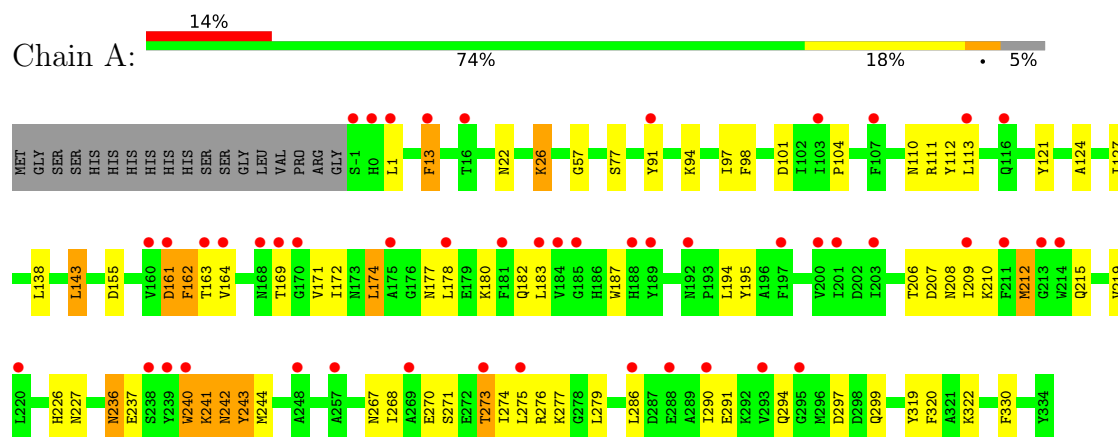
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	36	Total	O	0	0
			36	36		
2	B	83	Total	O	0	0
			83	83		
2	C	69	Total	O	0	0
			69	69		
2	D	19	Total	O	0	0
			19	19		

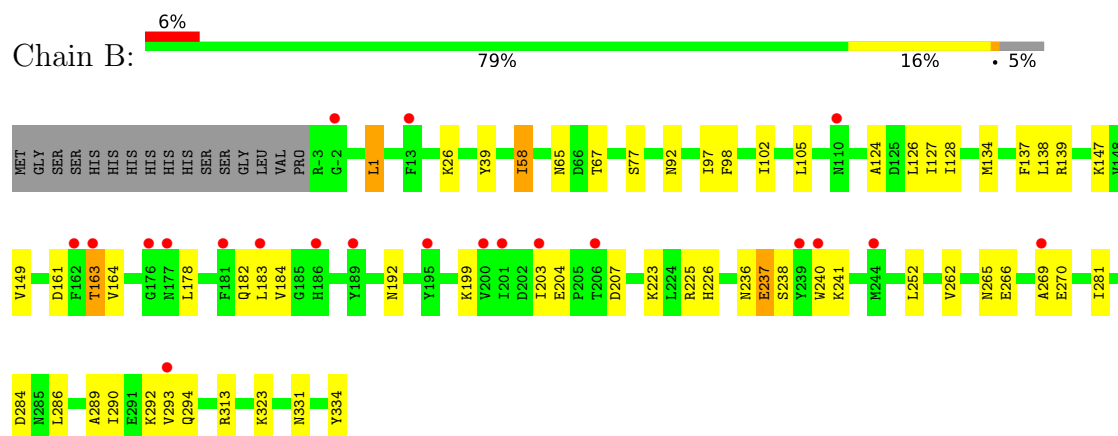
3 Residue-property plots [i](#)

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.

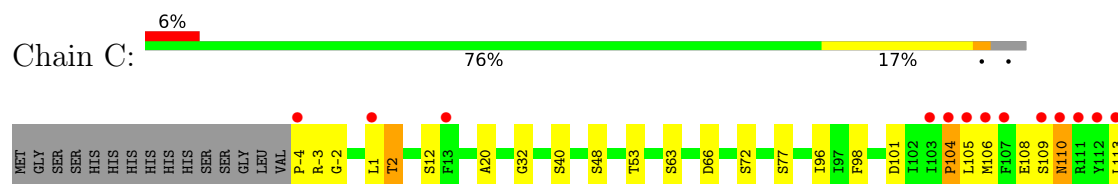
• Molecule 1: Glucosyltransferase 3

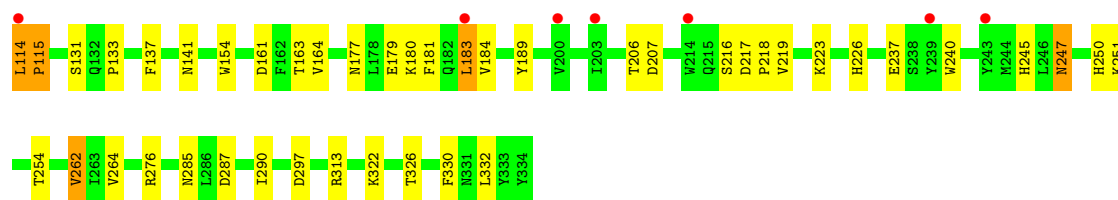


• Molecule 1: Glucosyltransferase 3

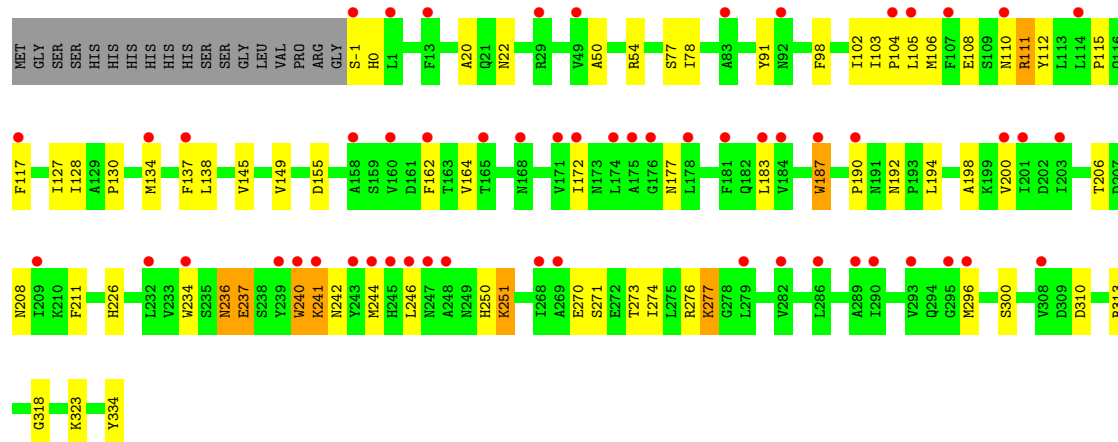
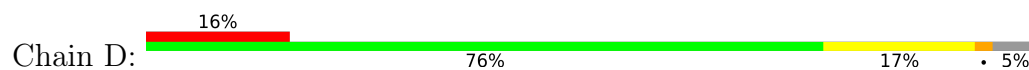


• Molecule 1: Glucosyltransferase 3





• Molecule 1: Glucosyltransferase 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.44Å 140.49Å 145.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.66 – 2.00 72.66 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (72.66-2.00) 88.8 (72.66-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.12 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.228 , 0.265 0.226 , 0.261	Depositor DCC
R_{free} test set	5106 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11093	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.47% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.35	0/2786	0.57	0/3797
1	B	0.51	0/2811	0.64	2/3827 (0.1%)
1	C	0.48	0/2811	0.66	1/3829 (0.0%)
1	D	0.37	0/2775	0.56	0/3782
All	All	0.44	0/11183	0.61	3/15235 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	ILE	CG1-CB-CG2	-6.61	96.86	111.40
1	B	1	LEU	CA-CB-CG	5.21	127.28	115.30
1	C	297	ASP	CB-CG-OD1	5.05	122.85	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	2713	0	2630	46	0
1	B	2735	0	2659	39	0
1	C	2736	0	2644	42	0
1	D	2702	0	2622	50	0
2	A	36	0	0	1	0
2	B	83	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	69	0	0	0	0
2	D	19	0	0	1	0
All	All	11093	0	10555	165	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 8.

All (165) 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:D:251:LYS:H	1:D:251:LYS:HD2	1.33	0.92
1:D:20:ALA:HB2	1:D:250:HIS:HE1	1.37	0.87
1:B:334:TYR:OXT	1:C:276:ARG:NH2	2.11	0.84
1:B:139:ARG:NH1	2:B:403:HOH:O	2.17	0.77
1:B:225:ARG:NH2	2:B:404:HOH:O	2.17	0.77
1:D:134:MET:HA	1:D:246:LEU:HD12	1.72	0.72
1:B:223:LYS:HE3	1:B:223:LYS:HA	1.74	0.69
1:C:-3:ARG:HG3	1:C:-3:ARG:HH11	1.57	0.68
1:A:22:ASN:O	1:A:26:LYS:HE2	1.96	0.66
1:B:182:GLN:O	1:B:236:ASN:ND2	2.29	0.65
1:A:161:ASP:OD1	1:A:163:THR:HG22	1.97	0.65
1:B:39:TYR:OH	2:B:401:HOH:O	2.14	0.64
1:C:262:VAL:HG13	1:C:264:VAL:HG13	1.79	0.64
1:C:1:LEU:HD22	1:C:32:GLY:O	1.99	0.63
1:C:20:ALA:HB1	1:C:154:TRP:CH2	2.34	0.63
1:D:187:TRP:HH2	1:D:192:ASN:O	1.83	0.62
1:B:164:VAL:HG21	1:B:226:HIS:NE2	2.16	0.61
1:A:195:TYR:HB3	1:A:212:MET:HE3	1.81	0.61
1:C:53:THR:HG21	1:D:50:ALA:O	2.00	0.61
1:A:178:LEU:HD21	1:A:209:ILE:HD13	1.82	0.60
1:A:104:PRO:HB3	1:A:111:ARG:HA	1.83	0.60
1:A:273:THR:HA	1:A:276:ARG:HB2	1.83	0.60
1:C:105:LEU:N	1:C:110:ASN:OD1	2.35	0.59
1:A:240:TRP:O	1:A:242:ASN:N	2.37	0.58
1:A:138:LEU:HB2	1:A:143:LEU:HD12	1.86	0.57
1:C:251:LYS:N	1:C:251:LYS:HD2	2.19	0.57
1:C:114:LEU:HD13	1:C:141:ASN:ND2	2.19	0.57
1:A:169:THR:HG23	1:A:171:VAL:H	1.70	0.57
1:D:-1:SER:HB2	2:D:410:HOH:O	2.05	0.57
1:D:276:ARG:HG3	1:D:277:LYS:HG2	1.86	0.56
1:C:251:LYS:HD2	1:C:251:LYS:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:LEU:HD13	1:D:313:ARG:HD3	1.88	0.56
1:C:216:SER:HB3	1:C:219:VAL:HG12	1.87	0.56
1:C:114:LEU:HD13	1:C:141:ASN:HD22	1.71	0.56
1:D:240:TRP:O	1:D:244:MET:HG3	2.05	0.56
1:D:251:LYS:H	1:D:251:LYS:CD	2.13	0.56
1:C:108:GLU:C	1:C:110:ASN:H	2.10	0.55
1:C:131:SER:HB2	1:C:133:PRO:HD2	1.88	0.55
1:C:219:VAL:HG22	1:C:223:LYS:HD2	1.89	0.55
1:D:273:THR:HA	1:D:276:ARG:HG2	1.88	0.55
1:A:241:LYS:O	1:A:243:TYR:N	2.37	0.55
1:D:127:ILE:HG13	1:D:145:VAL:HG11	1.89	0.55
1:D:270:GLU:O	1:D:273:THR:N	2.40	0.54
1:A:319:TYR:HA	1:A:322:LYS:HB2	1.90	0.54
1:D:105:LEU:HD22	1:D:137:PHE:CE2	2.43	0.54
1:D:274:ILE:H	1:D:274:ILE:HD12	1.72	0.54
1:B:97:ILE:HG13	1:B:124:ALA:HB2	1.89	0.54
1:C:247:ASN:H	1:C:247:ASN:HD22	1.55	0.54
1:C:53:THR:HG22	1:D:54:ARG:HB2	1.90	0.53
1:C:240:TRP:CE2	1:C:245:HIS:HE1	2.27	0.53
1:D:187:TRP:HZ3	1:D:208:ASN:HB3	1.73	0.53
1:C:53:THR:CG2	1:D:54:ARG:HB2	2.40	0.52
1:D:236:ASN:O	1:D:237:GLU:HB2	2.09	0.52
1:A:97:ILE:HG13	1:A:124:ALA:HB2	1.92	0.52
1:C:-3:ARG:HG3	1:C:-3:ARG:NH1	2.22	0.51
1:A:101:ASP:OD1	1:A:243:TYR:OH	2.23	0.51
1:D:190:PRO:HA	1:D:208:ASN:HD22	1.75	0.51
1:B:269:ALA:O	1:B:270:GLU:HB2	2.10	0.51
1:A:286:LEU:HB3	1:A:290:ILE:HD11	1.93	0.50
1:D:164:VAL:HG21	1:D:226:HIS:CE1	2.46	0.50
1:A:177:ASN:N	1:A:177:ASN:OD1	2.45	0.49
1:C:164:VAL:HG11	1:C:226:HIS:NE2	2.26	0.49
1:D:103:ILE:HA	1:D:106:MET:HG3	1.95	0.49
1:A:57:GLY:O	1:B:58:ILE:HG22	2.13	0.49
1:B:147:LYS:HE2	1:B:331:ASN:O	2.13	0.49
1:A:215:GLN:HB3	1:A:219:VAL:HG23	1.95	0.48
1:A:242:ASN:O	1:A:243:TYR:HB2	2.13	0.48
1:B:289:ALA:O	1:B:293:VAL:HG23	2.14	0.48
1:D:112:TYR:O	1:D:115:PRO:HD2	2.13	0.48
1:A:208:ASN:OD1	1:A:210:LYS:NZ	2.46	0.48
1:D:91:TYR:CD1	1:D:91:TYR:N	2.82	0.48
1:D:296:MET:HG3	1:D:300:SER:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-4:PRO:HG3	1:C:66:ASP:OD1	2.14	0.48
1:D:102:ILE:CD1	1:D:138:LEU:HD21	2.43	0.47
1:D:187:TRP:CZ2	1:D:194:LEU:HB2	2.48	0.47
1:A:286:LEU:O	1:A:290:ILE:HG13	2.13	0.47
1:B:313:ARG:HG2	2:B:474:HOH:O	2.14	0.47
1:C:240:TRP:CZ2	1:C:245:HIS:HE1	2.32	0.47
1:B:1:LEU:HD11	1:B:67:THR:OG1	2.14	0.47
1:A:162:PHE:HE1	1:D:-1:SER:C	2.18	0.47
1:D:102:ILE:HD11	1:D:138:LEU:HD11	1.96	0.47
1:B:281:ILE:HD13	1:B:292:LYS:HB3	1.96	0.47
1:B:286:LEU:O	1:B:290:ILE:HG12	2.14	0.47
1:D:164:VAL:HG21	1:D:226:HIS:NE2	2.29	0.47
1:C:285:ASN:OD1	1:C:287:ASP:HB2	2.15	0.47
1:B:1:LEU:HB2	1:C:313:ARG:HG2	1.97	0.47
1:D:241:LYS:HD3	1:D:242:ASN:H	1.80	0.46
1:A:291:GLU:HA	1:A:294:GLN:OE1	2.15	0.46
1:B:164:VAL:HG21	1:B:226:HIS:CE1	2.50	0.46
1:A:169:THR:HG21	1:A:227:ASN:O	2.16	0.46
1:D:271:SER:HA	1:D:274:ILE:HD13	1.97	0.46
1:B:252:LEU:HD12	1:B:262:VAL:HG11	1.96	0.46
1:D:130:PRO:HD2	1:D:134:MET:SD	2.56	0.46
1:D:187:TRP:CH2	1:D:192:ASN:O	2.68	0.46
1:D:104:PRO:HD3	1:D:117:PHE:CE2	2.51	0.46
1:A:138:LEU:CB	1:A:143:LEU:HD12	2.45	0.46
1:C:161:ASP:OD1	1:C:163:THR:HG23	2.16	0.46
1:C:96:ILE:HD11	1:C:332:LEU:HD22	1.98	0.46
1:A:277:LYS:HB2	1:A:279:LEU:HG	1.99	0.45
1:B:290:ILE:O	1:B:294:GLN:HG3	2.17	0.45
1:B:126:LEU:HD23	1:B:127:ILE:N	2.32	0.45
1:B:192:ASN:OD1	1:B:294:GLN:NE2	2.48	0.45
1:B:313:ARG:H	1:B:313:ARG:HG3	1.54	0.45
1:C:250:HIS:O	1:C:254:THR:HG23	2.15	0.45
1:B:58:ILE:HD13	1:B:58:ILE:HG21	1.49	0.45
1:B:241:LYS:HE3	1:B:265:ASN:HD21	1.81	0.45
1:A:94:LYS:NZ	2:A:402:HOH:O	2.48	0.45
1:B:102:ILE:HD12	1:B:134:MET:SD	2.57	0.45
1:D:187:TRP:CH2	1:D:194:LEU:HB2	2.52	0.45
1:D:270:GLU:O	1:D:274:ILE:HD12	2.17	0.45
1:A:172:ILE:HG22	1:A:194:LEU:HD12	2.00	0.45
1:D:200:VAL:HG13	1:D:211:PHE:CD2	2.52	0.44
1:B:105:LEU:HD11	1:B:137:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:THR:HG22	1:B:164:VAL:HG23	2.00	0.44
1:D:91:TYR:H	1:D:91:TYR:HD1	1.65	0.44
1:D:242:ASN:HB3	1:D:246:LEU:HD23	2.00	0.44
1:A:121:TYR:HB3	1:A:127:ILE:HD11	1.99	0.44
1:A:273:THR:HB	1:A:276:ARG:HH21	1.83	0.44
1:C:189:TYR:CD2	1:C:290:ILE:HD13	2.53	0.43
1:A:271:SER:HA	1:A:274:ILE:HG13	2.00	0.43
1:B:204:GLU:HG3	1:B:207:ASP:OD2	2.18	0.43
1:B:323:LYS:HD2	1:C:330:PHE:CG	2.54	0.43
1:C:181:PHE:O	1:C:183:LEU:N	2.51	0.43
1:D:155:ASP:CG	1:D:318:GLY:HA2	2.39	0.43
1:A:270:GLU:OE1	1:D:334:TYR:OH	2.35	0.43
1:C:114:LEU:N	1:C:115:PRO:HD2	2.32	0.43
1:C:217:ASP:HB3	1:C:218:PRO:HD3	2.00	0.43
1:A:297:ASP:OD1	1:A:299:GLN:N	2.51	0.43
1:D:172:ILE:HG22	1:D:194:LEU:HD12	2.00	0.43
1:A:212:MET:HE2	1:A:212:MET:HB2	1.53	0.43
1:A:237:GLU:O	1:A:240:TRP:HB3	2.19	0.43
1:B:102:ILE:HD13	1:B:138:LEU:HD21	2.00	0.43
1:C:322:LYS:O	1:C:326:THR:HG23	2.18	0.43
1:D:78:ILE:HD13	1:D:117:PHE:CE1	2.54	0.43
1:B:65:ASN:HA	1:B:92:ASN:O	2.18	0.42
1:A:174:LEU:HB2	1:A:194:LEU:HD11	2.01	0.42
1:B:128:ILE:HA	1:B:149:VAL:O	2.19	0.42
1:A:290:ILE:HG13	1:A:290:ILE:H	1.63	0.42
1:C:114:LEU:HD21	1:C:137:PHE:CE2	2.55	0.42
1:A:244:MET:HB3	1:A:268:ILE:HG12	2.01	0.42
1:A:330:PHE:CG	1:D:323:LYS:HD2	2.55	0.42
1:B:265:ASN:OD1	1:B:266:GLU:N	2.52	0.42
1:C:-4:PRO:HG2	1:C:2:THR:OG1	2.19	0.42
1:B:178:LEU:HD11	1:B:183:LEU:HD11	2.02	0.42
1:C:104:PRO:HA	1:C:110:ASN:CG	2.40	0.42
1:B:184:VAL:HG22	1:B:203:ILE:HG22	2.01	0.42
1:D:177:ASN:HA	1:D:198:ALA:HB2	2.02	0.42
1:A:182:GLN:HB3	1:A:236:ASN:HB3	2.02	0.41
1:C:237:GLU:HB3	1:C:240:TRP:HB2	2.02	0.41
1:D:128:ILE:HA	1:D:149:VAL:O	2.20	0.41
1:A:13:PHE:CD1	1:A:13:PHE:N	2.86	0.41
1:B:92:ASN:HB2	2:B:449:HOH:O	2.20	0.41
1:A:241:LYS:HE2	1:A:267:ASN:ND2	2.35	0.41
1:A:291:GLU:HG2	1:A:294:GLN:NE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:ASN:OD1	1:C:180:LYS:HB2	2.21	0.41
1:D:108:GLU:HA	1:D:111:ARG:HB2	2.03	0.41
1:A:112:TYR:CZ	1:A:113:LEU:HG	2.56	0.40
1:A:155:ASP:OD1	1:A:320:PHE:HB2	2.21	0.40
1:B:139:ARG:HA	1:B:139:ARG:HD3	1.79	0.40
1:A:163:THR:HG23	1:A:164:VAL:HG13	2.02	0.40
1:B:237:GLU:CD	1:B:241:LYS:HD3	2.42	0.40
1:C:184:VAL:O	1:C:207:ASP:OD2	2.38	0.40
1:C:-4:PRO:HB3	1:C:63:SER:HB2	2.03	0.40
1:C:-2:GLY:HA2	1:D:22:ASN:OD1	2.21	0.40
1:D:20:ALA:HB2	1:D:250:HIS:CE1	2.30	0.40

There are no symmetry-related clashes.

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	334/354 (94%)	315 (94%)	14 (4%)	5 (2%)	8 4
1	B	337/354 (95%)	319 (95%)	13 (4%)	5 (2%)	8 4
1	C	337/354 (95%)	319 (95%)	12 (4%)	6 (2%)	7 3
1	D	335/354 (95%)	315 (94%)	16 (5%)	4 (1%)	11 6
All	All	1343/1416 (95%)	1268 (94%)	55 (4%)	20 (2%)	8 4

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	SER
1	A	243	TYR
1	B	77	SER
1	C	77	SER

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Mol	Chain	Res	Type
1	A	161	ASP
1	A	241	LYS
1	A	242	ASN
1	B	240	TRP
1	C	104	PRO
1	C	110	ASN
1	D	236	ASN
1	D	240	TRP
1	B	161	ASP
1	B	238	SER
1	C	109	SER
1	D	77	SER
1	B	237	GLU
1	C	106	MET
1	D	237	GLU
1	C	115	PRO

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	293/309 (95%)	274 (94%)	19 (6%)	14	11
1	B	295/309 (96%)	289 (98%)	6 (2%)	50	55
1	C	294/309 (95%)	280 (95%)	14 (5%)	21	19
1	D	291/309 (94%)	278 (96%)	13 (4%)	23	21
All	All	1173/1236 (95%)	1121 (96%)	52 (4%)	24	22

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	PHE
1	A	26	LYS
1	A	91	TYR
1	A	98	PHE
1	A	110	ASN

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Mol	Chain	Res	Type
1	A	143	LEU
1	A	162	PHE
1	A	174	LEU
1	A	180	LYS
1	A	183	LEU
1	A	187	TRP
1	A	206	THR
1	A	207	ASP
1	A	212	MET
1	A	226	HIS
1	A	236	ASN
1	A	240	TRP
1	A	273	THR
1	A	275	LEU
1	B	26[A]	LYS
1	B	26[B]	LYS
1	B	98	PHE
1	B	163	THR
1	B	199	LYS
1	B	284	ASP
1	C	2	THR
1	C	12	SER
1	C	40	SER
1	C	48	SER
1	C	72	SER
1	C	98	PHE
1	C	101	ASP
1	C	113	LEU
1	C	114	LEU
1	C	179	GLU
1	C	183	LEU
1	C	206	THR
1	C	247	ASN
1	C	262	VAL
1	D	0	HIS
1	D	98	PHE
1	D	110	ASN
1	D	111	ARG
1	D	162	PHE
1	D	183	LEU
1	D	187	TRP
1	D	206	THR

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Mol	Chain	Res	Type
1	D	234	TRP
1	D	241	LYS
1	D	251	LYS
1	D	277	LYS
1	D	310	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	132	GLN
1	B	22	ASN
1	B	110	ASN
1	B	227	ASN
1	C	167	GLN
1	C	182	GLN
1	C	245	HIS
1	C	247	ASN
1	D	215	GLN
1	D	250	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 [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	336/354 (94%)	1.02	48 (14%) 7 6	39, 80, 132, 163	0
1	B	338/354 (95%)	0.50	21 (6%) 28 26	27, 54, 103, 154	1 (0%)
1	C	339/354 (95%)	0.52	20 (5%) 29 27	34, 52, 91, 178	0
1	D	336/354 (94%)	1.17	57 (16%) 5 4	29, 87, 138, 157	1 (0%)
All	All	1349/1416 (95%)	0.80	146 (10%) 12 11	27, 65, 130, 178	2 (0%)

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	109	SER	4.8
1	A	184	VAL	4.8
1	C	105	LEU	4.5
1	C	114	LEU	4.5
1	A	178	LEU	4.5
1	D	209	ILE	4.4
1	C	107	PHE	4.3
1	D	239	TYR	4.3
1	A	203	ILE	4.2
1	D	183	LEU	4.2
1	A	181	PHE	4.1
1	D	29[A]	ARG	4.0
1	A	183	LEU	3.9
1	C	113	LEU	3.9
1	D	178	LEU	3.9
1	A	240	TRP	3.9
1	D	243	TYR	3.9
1	A	290	ILE	3.8
1	D	181	PHE	3.7
1	D	295	GLY	3.6
1	D	240	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	201	ILE	3.5
1	C	110	ASN	3.5
1	D	184	VAL	3.4
1	B	-2	GLY	3.4
1	C	106	MET	3.4
1	C	-4	PRO	3.4
1	D	190	PRO	3.3
1	B	240	TRP	3.3
1	D	160	VAL	3.3
1	A	1	LEU	3.3
1	D	289	ALA	3.2
1	A	188	HIS	3.2
1	D	104	PRO	3.2
1	B	13	PHE	3.1
1	D	13	PHE	3.1
1	C	239	TYR	3.1
1	A	175	ALA	3.1
1	D	105	LEU	3.1
1	A	103	ILE	3.1
1	D	286	LEU	3.1
1	D	83	ALA	3.1
1	A	16	THR	3.1
1	A	163	THR	3.1
1	D	117	PHE	3.0
1	A	0	HIS	3.0
1	C	13	PHE	3.0
1	A	211	PHE	3.0
1	D	1	LEU	2.9
1	D	162	PHE	2.9
1	A	209	ILE	2.9
1	D	168	ASN	2.9
1	C	104	PRO	2.8
1	A	160	VAL	2.8
1	A	13	PHE	2.8
1	D	290	ILE	2.8
1	C	214	TRP	2.8
1	B	239	TYR	2.8
1	D	234	TRP	2.8
1	D	293	VAL	2.8
1	A	-1	SER	2.8
1	A	239	TYR	2.7
1	A	275	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	113	LEU	2.6
1	B	162	PHE	2.6
1	A	295	GLY	2.6
1	D	203	ILE	2.6
1	C	200	VAL	2.5
1	D	49	VAL	2.5
1	D	308	VAL	2.5
1	A	189	TYR	2.5
1	A	288	GLU	2.5
1	D	187	TRP	2.5
1	B	110	ASN	2.5
1	A	197	PHE	2.5
1	D	246	LEU	2.5
1	C	103	ILE	2.4
1	A	214	TRP	2.4
1	A	269	ALA	2.4
1	D	247	ASN	2.4
1	B	183	LEU	2.4
1	D	165	THR	2.4
1	C	112	TYR	2.4
1	D	171	VAL	2.4
1	C	1	LEU	2.3
1	D	114	LEU	2.3
1	D	279	LEU	2.3
1	B	186	HIS	2.3
1	B	206	THR	2.3
1	D	-1	SER	2.3
1	D	172	ILE	2.3
1	D	245	HIS	2.3
1	A	286	LEU	2.3
1	A	257	ALA	2.3
1	A	107	PHE	2.3
1	A	192	ASN	2.3
1	D	201	ILE	2.2
1	D	268	ILE	2.2
1	D	134	MET	2.2
1	D	174	LEU	2.2
1	B	269	ALA	2.2
1	D	269	ALA	2.2
1	B	293	VAL	2.2
1	D	244	MET	2.2
1	A	213	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	168	ASN	2.2
1	D	92	ASN	2.2
1	C	203	ILE	2.2
1	D	175	ALA	2.2
1	D	248	ALA	2.2
1	A	185	GLY	2.2
1	C	111	ARG	2.2
1	A	220	LEU	2.1
1	A	238	SER	2.1
1	C	243	TYR	2.1
1	A	116	GLN	2.1
1	A	200	VAL	2.1
1	D	200	VAL	2.1
1	D	282	VAL	2.1
1	D	241	LYS	2.1
1	B	163	THR	2.1
1	A	170	GLY	2.1
1	B	195	TYR	2.1
1	A	293	VAL	2.1
1	B	200	VAL	2.1
1	B	181	PHE	2.1
1	C	183	LEU	2.1
1	A	273	THR	2.1
1	A	248	ALA	2.1
1	B	244	MET	2.1
1	D	296	MET	2.1
1	D	110	ASN	2.1
1	A	161	ASP	2.1
1	D	232	LEU	2.1
1	A	169	THR	2.1
1	B	201	ILE	2.1
1	B	203	ILE	2.1
1	D	137	PHE	2.1
1	D	158	ALA	2.0
1	B	189	TYR	2.0
1	A	164	VAL	2.0
1	D	107	PHE	2.0
1	B	176	GLY	2.0
1	B	177	ASN	2.0
1	D	176	GLY	2.0
1	A	91	TYR	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.