



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2024 – 12:12 PM JST

PDB ID : 8IXP  
Title : Apo structure of glycosyltransferase LmbT wild type  
Authors : Mori, T.; Sun, X.; Abe, I.  
Deposited on : 2023-04-02  
Resolution : 2.45 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>.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

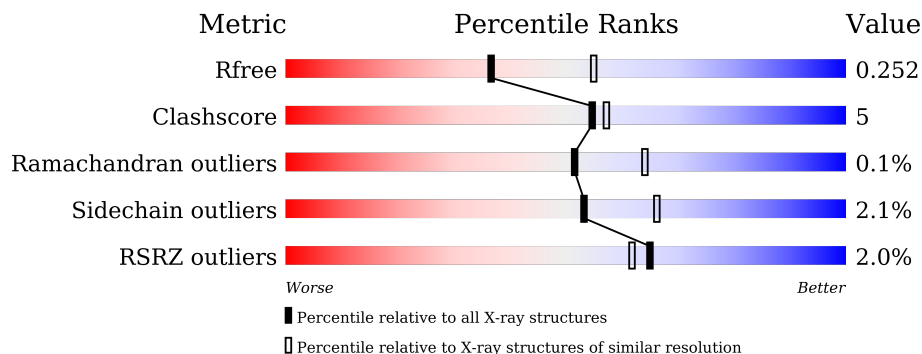
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	451	 2% 83% 12% 5%
1	B	451	 % 80% 15% 5%
1	C	451	 4% 80% 12% 7%
1	D	451	 82% 13% 5%

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 12992 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 Glycosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	429	Total 3205	C 2012	N 590	O 596	S 7	0	0	0
1	B	429	Total 3213	C 2014	N 596	O 596	S 7	0	0	0
1	C	421	Total 3091	C 1944	N 563	O 577	S 7	0	0	0
1	D	428	Total 3206	C 2010	N 594	O 595	S 7	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	437	LYS	-	expression tag	UNP A9Y8T1
A	438	LEU	-	expression tag	UNP A9Y8T1
A	439	ALA	-	expression tag	UNP A9Y8T1
A	440	ALA	-	expression tag	UNP A9Y8T1
A	441	ALA	-	expression tag	UNP A9Y8T1
A	442	LEU	-	expression tag	UNP A9Y8T1
A	443	GLU	-	expression tag	UNP A9Y8T1
A	444	HIS	-	expression tag	UNP A9Y8T1
A	445	HIS	-	expression tag	UNP A9Y8T1
A	446	HIS	-	expression tag	UNP A9Y8T1
A	447	HIS	-	expression tag	UNP A9Y8T1
A	448	HIS	-	expression tag	UNP A9Y8T1
A	449	HIS	-	expression tag	UNP A9Y8T1
A	450	HIS	-	expression tag	UNP A9Y8T1
A	451	HIS	-	expression tag	UNP A9Y8T1
B	437	LYS	-	expression tag	UNP A9Y8T1
B	438	LEU	-	expression tag	UNP A9Y8T1
B	439	ALA	-	expression tag	UNP A9Y8T1
B	440	ALA	-	expression tag	UNP A9Y8T1
B	441	ALA	-	expression tag	UNP A9Y8T1
B	442	LEU	-	expression tag	UNP A9Y8T1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	443	GLU	-	expression tag	UNP A9Y8T1
B	444	HIS	-	expression tag	UNP A9Y8T1
B	445	HIS	-	expression tag	UNP A9Y8T1
B	446	HIS	-	expression tag	UNP A9Y8T1
B	447	HIS	-	expression tag	UNP A9Y8T1
B	448	HIS	-	expression tag	UNP A9Y8T1
B	449	HIS	-	expression tag	UNP A9Y8T1
B	450	HIS	-	expression tag	UNP A9Y8T1
B	451	HIS	-	expression tag	UNP A9Y8T1
C	437	LYS	-	expression tag	UNP A9Y8T1
C	438	LEU	-	expression tag	UNP A9Y8T1
C	439	ALA	-	expression tag	UNP A9Y8T1
C	440	ALA	-	expression tag	UNP A9Y8T1
C	441	ALA	-	expression tag	UNP A9Y8T1
C	442	LEU	-	expression tag	UNP A9Y8T1
C	443	GLU	-	expression tag	UNP A9Y8T1
C	444	HIS	-	expression tag	UNP A9Y8T1
C	445	HIS	-	expression tag	UNP A9Y8T1
C	446	HIS	-	expression tag	UNP A9Y8T1
C	447	HIS	-	expression tag	UNP A9Y8T1
C	448	HIS	-	expression tag	UNP A9Y8T1
C	449	HIS	-	expression tag	UNP A9Y8T1
C	450	HIS	-	expression tag	UNP A9Y8T1
C	451	HIS	-	expression tag	UNP A9Y8T1
D	437	LYS	-	expression tag	UNP A9Y8T1
D	438	LEU	-	expression tag	UNP A9Y8T1
D	439	ALA	-	expression tag	UNP A9Y8T1
D	440	ALA	-	expression tag	UNP A9Y8T1
D	441	ALA	-	expression tag	UNP A9Y8T1
D	442	LEU	-	expression tag	UNP A9Y8T1
D	443	GLU	-	expression tag	UNP A9Y8T1
D	444	HIS	-	expression tag	UNP A9Y8T1
D	445	HIS	-	expression tag	UNP A9Y8T1
D	446	HIS	-	expression tag	UNP A9Y8T1
D	447	HIS	-	expression tag	UNP A9Y8T1
D	448	HIS	-	expression tag	UNP A9Y8T1
D	449	HIS	-	expression tag	UNP A9Y8T1
D	450	HIS	-	expression tag	UNP A9Y8T1
D	451	HIS	-	expression tag	UNP A9Y8T1

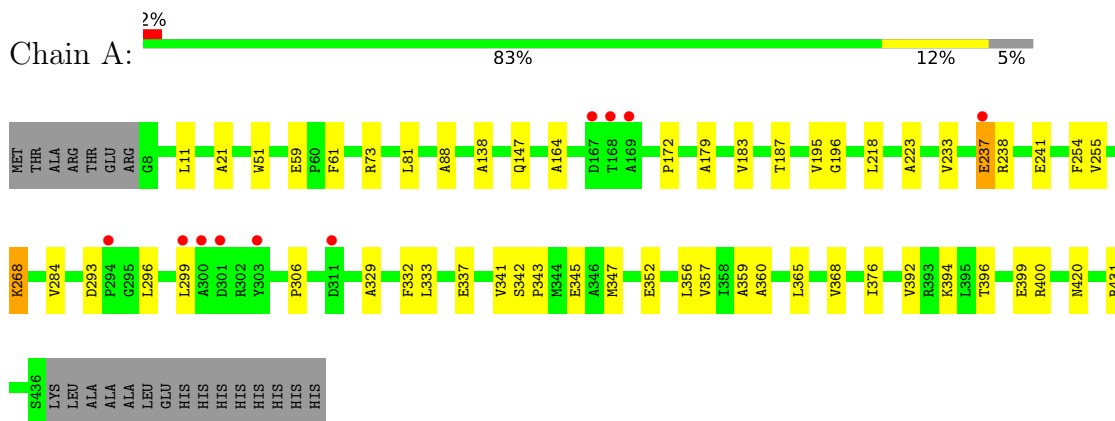
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	73	Total O 73 73	0	0
2	B	61	Total O 61 61	0	0
2	C	50	Total O 50 50	0	0
2	D	93	Total O 93 93	0	0

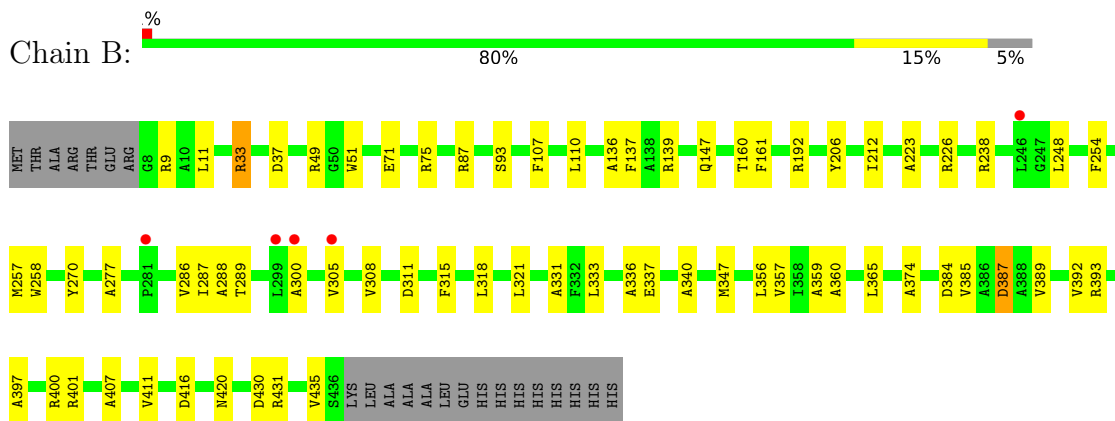
### 3 Residue-property plots [i](#)

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.

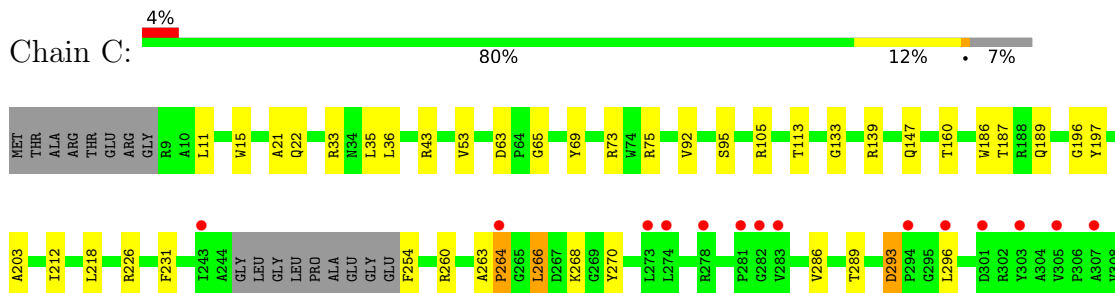
- Molecule 1: Glycosyltransferase

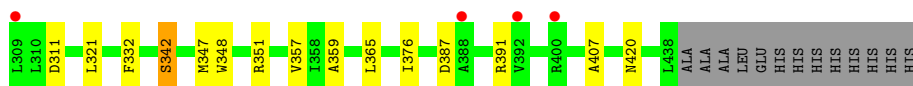


- Molecule 1: Glycosyltransferase

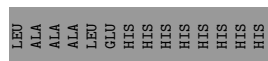
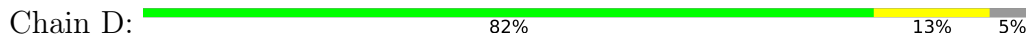


- Molecule 1: Glycosyltransferase





• Molecule 1: Glycosyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.54Å 142.01Å 158.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.77 – 2.45 48.77 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.77-2.45) 100.0 (48.77-2.45)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 2.45Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.203 , 0.254 0.202 , 0.252	Depositor DCC
$R_{free}$ test set	2000 reflections (2.45%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.9	Xtrriage
Anisotropy	0.915	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 36.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12992	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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 [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	0.39	0/3273	0.63	0/4464
1	B	0.39	0/3281	0.62	0/4472
1	C	0.39	0/3156	0.63	1/4313 (0.0%)
1	D	0.40	0/3274	0.64	0/4465
All	All	0.39	0/12984	0.63	1/17714 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	65	GLY	C-N-CA	-5.00	109.20	121.70

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	3205	0	3124	34	0
1	B	3213	0	3132	38	0
1	C	3091	0	2957	31	0
1	D	3206	0	3123	33	0
2	A	73	0	0	1	0
2	B	61	0	0	1	0
2	C	50	0	0	1	0
2	D	93	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12992	0	12336	130	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 5.

All (130) 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:C:263:ALA:HB1	1:C:264:PRO:HD2	1.64	0.79
1:C:286:VAL:HG11	1:C:321:LEU:HD21	1.74	0.67
1:B:49:ARG:NH2	1:B:430:ASP:OD1	2.30	0.65
1:D:46:LEU:HD13	1:D:53:VAL:HG21	1.80	0.63
1:B:147:GLN:HG3	1:D:95:SER:O	1.99	0.63
1:C:359:ALA:HB1	1:C:365:LEU:HB3	1.81	0.62
1:B:400:ARG:NH1	2:B:504:HOH:O	2.32	0.62
1:C:347:MET:HG2	1:C:407:ALA:HB1	1.81	0.62
1:B:347:MET:HG3	1:B:357:VAL:HG21	1.81	0.61
1:A:164:ALA:HB1	1:A:172:PRO:HG2	1.82	0.61
1:D:11:LEU:HB2	1:D:51:TRP:CE3	2.36	0.60
1:D:356:LEU:HD11	1:D:400:ARG:HG3	1.84	0.59
1:A:187:THR:HG21	1:A:195:VAL:HG23	1.85	0.58
1:B:315:PHE:HA	1:B:318:LEU:HD12	1.86	0.58
1:A:284:VAL:HG12	1:A:306:PRO:HG2	1.85	0.57
1:B:270:TYR:HB3	1:B:287:ILE:HD13	1.86	0.57
1:B:359:ALA:HB1	1:B:365:LEU:HB3	1.86	0.57
1:B:226:ARG:HD3	1:B:411:VAL:HG12	1.87	0.56
1:A:431:ARG:NH2	2:A:503:HOH:O	2.38	0.56
1:D:376:ILE:HG13	1:D:392:VAL:HG22	1.86	0.56
1:A:343:PRO:HB2	1:A:368:VAL:HG11	1.88	0.55
1:C:21:ALA:O	1:C:73:ARG:HD2	2.07	0.54
1:D:39:GLN:HG3	1:D:55:PHE:CD2	2.43	0.53
1:B:286:VAL:HG11	1:B:321:LEU:HD21	1.91	0.53
1:C:268:LYS:HB2	1:C:270:TYR:CE2	2.44	0.53
1:B:160:THR:HG23	1:B:161:PHE:CG	2.44	0.53
1:B:257:MET:HG2	1:B:331:ALA:O	2.08	0.53
1:C:260:ARG:NH2	1:C:266:LEU:HD11	2.26	0.51
1:C:332:PHE:HE2	1:C:342:SER:HB3	1.74	0.51
1:C:332:PHE:CE2	1:C:342:SER:HB3	2.46	0.51
1:D:398:ASP:O	1:D:402:ARG:HG3	2.10	0.51
1:B:392:VAL:O	1:B:400:ARG:NH2	2.44	0.50
1:D:289:THR:O	1:D:311:ASP:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:ARG:HB2	2:D:582:HOH:O	2.10	0.50
1:C:187:THR:HG21	1:C:212:ILE:HG23	1.94	0.50
1:C:289:THR:O	1:C:311:ASP:HA	2.12	0.50
1:D:94:ASP:O	1:D:105:ARG:HD2	2.11	0.50
1:B:248:LEU:HD23	1:B:308:VAL:HG21	1.95	0.49
1:D:347:MET:HG2	1:D:407:ALA:HB1	1.93	0.49
1:B:277:ALA:HB3	1:B:305:VAL:HG21	1.94	0.49
1:D:81:LEU:HD12	1:D:88:ALA:HB2	1.95	0.49
1:A:81:LEU:HD12	1:A:88:ALA:HB2	1.95	0.48
1:A:359:ALA:HB1	1:A:365:LEU:HB3	1.95	0.48
1:D:260:ARG:HG3	1:D:266:LEU:HD21	1.94	0.48
1:D:297:ARG:NH2	2:D:508:HOH:O	2.46	0.48
1:A:233:VAL:HG11	1:A:352:GLU:OE1	2.14	0.48
1:B:93:SER:OG	1:D:147:GLN:NE2	2.47	0.48
1:A:396:THR:OG1	1:A:399:GLU:HG3	2.13	0.47
1:B:110:LEU:HG	1:B:137:PHE:CE1	2.48	0.47
1:B:11:LEU:HB2	1:B:51:TRP:CE3	2.49	0.47
1:B:206:TYR:HB3	1:B:212:ILE:HD12	1.97	0.47
1:A:183:VAL:O	1:A:187:THR:HG23	2.15	0.47
1:B:139:ARG:NH2	1:D:94:ASP:OD1	2.48	0.47
1:C:376:ILE:HG23	1:C:391:ARG:NH2	2.30	0.47
1:C:92:VAL:HB	1:C:113:THR:HG21	1.96	0.46
1:B:337:GLU:HG2	1:B:340:ALA:HB2	1.97	0.46
1:B:401:ARG:HH11	1:B:401:ARG:HG3	1.80	0.46
1:D:110:LEU:HG	1:D:137:PHE:CE1	2.51	0.46
1:A:293:ASP:HB3	1:A:296:LEU:HB2	1.98	0.46
1:A:333:LEU:HA	1:A:360:ALA:HB2	1.97	0.46
1:A:254:PHE:CD1	1:A:284:VAL:HG23	2.51	0.46
1:C:15:TRP:CE2	1:C:35:LEU:HD21	2.51	0.46
1:B:107:PHE:CD1	1:B:136:ALA:HA	2.51	0.46
1:C:11:LEU:HD23	1:C:53:VAL:HG22	1.98	0.46
1:C:186:TRP:HA	1:C:189:GLN:HB3	1.97	0.46
1:D:359:ALA:HB1	1:D:365:LEU:HB3	1.98	0.45
1:A:138:ALA:HB3	1:A:179:ALA:HB1	1.98	0.45
1:B:384:ASP:HA	1:B:387:ASP:HB2	1.99	0.45
1:A:332:PHE:HE2	1:A:342:SER:HB3	1.81	0.45
1:A:11:LEU:HB2	1:A:51:TRP:CE3	2.51	0.45
1:A:268:LYS:HE2	1:A:337:GLU:OE2	2.17	0.45
1:B:226:ARG:NE	1:B:416:ASP:OD1	2.43	0.45
1:C:187:THR:CG2	1:C:212:ILE:HG23	2.47	0.45
1:A:347:MET:HG3	1:A:357:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:GLY:HA2	1:D:375:GLY:O	2.18	0.44
1:C:231:PHE:O	1:C:351:ARG:NH2	2.47	0.44
1:D:347:MET:HG3	1:D:357:VAL:HG21	1.99	0.44
1:A:341:VAL:O	1:A:345:GLU:HG3	2.18	0.44
1:D:275:GLU:HG3	1:D:303:TYR:CE2	2.53	0.44
1:A:356:LEU:HD11	1:A:400:ARG:HG3	1.98	0.44
1:B:385:VAL:O	1:B:389:VAL:HG23	2.18	0.44
1:D:412:ARG:NH1	2:D:509:HOH:O	2.49	0.44
1:A:21:ALA:HB3	1:A:59:GLU:OE1	2.18	0.44
1:A:21:ALA:O	1:A:73:ARG:HD2	2.17	0.44
1:C:196:GLY:HA2	1:C:218:LEU:O	2.18	0.43
1:D:332:PHE:HE2	1:D:342:SER:HB3	1.82	0.43
1:A:376:ILE:HG13	1:A:392:VAL:HG22	1.99	0.43
1:D:286:VAL:HG11	1:D:321:LEU:HD11	2.01	0.43
1:A:61:PHE:HB2	1:C:147:GLN:NE2	2.33	0.43
1:A:147:GLN:HG3	1:C:95:SER:O	2.17	0.43
1:A:238:ARG:HD3	1:A:238:ARG:HA	1.90	0.43
1:B:192:ARG:HG2	1:B:435:VAL:HG11	2.01	0.43
1:C:105:ARG:HD3	1:D:104:GLU:OE2	2.18	0.43
1:C:293:ASP:HB3	1:C:296:LEU:HB2	2.01	0.42
1:C:226:ARG:HB2	1:C:348:TRP:CE2	2.54	0.42
1:B:248:LEU:HB3	1:B:254:PHE:CZ	2.53	0.42
1:B:300:ALA:O	1:B:305:VAL:HG12	2.19	0.42
1:D:92:VAL:HB	1:D:113:THR:HG21	2.02	0.42
1:D:378:THR:HB	1:D:388:ALA:HB2	2.01	0.42
1:A:396:THR:HG23	1:A:399:GLU:OE1	2.19	0.42
1:D:107:PHE:CD1	1:D:136:ALA:HA	2.55	0.42
1:D:138:ALA:O	1:D:141:PRO:HD2	2.19	0.42
1:A:254:PHE:HD1	1:A:284:VAL:HG23	1.83	0.42
1:B:258:TRP:HA	1:B:288:ALA:O	2.19	0.42
1:D:238:ARG:HA	1:D:238:ARG:HE	1.83	0.42
1:D:263:ALA:HB1	1:D:264:PRO:HD3	2.02	0.42
1:B:71:GLU:O	1:B:75:ARG:HG3	2.19	0.41
1:B:289:THR:O	1:B:311:ASP:HA	2.19	0.41
1:C:420:ASN:HD22	1:C:420:ASN:HA	1.66	0.41
1:C:347:MET:HG3	1:C:357:VAL:HG21	2.02	0.41
1:A:223:ALA:HB2	1:A:420:ASN:HD22	1.86	0.41
1:C:197:TYR:CD1	1:C:203:ALA:HB2	2.55	0.41
1:D:32:VAL:O	1:D:36:LEU:HG	2.20	0.41
1:B:33:ARG:NH1	1:B:37:ASP:OD2	2.53	0.41
1:B:397:ALA:O	1:B:401:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:LEU:HD23	1:C:36:LEU:HA	1.70	0.41
1:C:139:ARG:HD2	2:C:521:HOH:O	2.20	0.41
1:A:332:PHE:CE2	1:A:342:SER:HB3	2.55	0.41
1:A:196:GLY:HA2	1:A:218:LEU:O	2.21	0.41
1:C:22:GLN:HB3	1:C:69:TYR:CE1	2.55	0.41
1:B:356:LEU:HD11	1:B:400:ARG:HG3	2.03	0.41
1:B:374:ALA:HB1	1:B:407:ALA:HA	2.02	0.41
1:B:333:LEU:HA	1:B:360:ALA:HB2	2.03	0.41
1:C:133:GLY:HA2	1:C:160:THR:O	2.21	0.41
1:D:93:SER:HB2	1:D:106:PHE:CD1	2.55	0.41
1:A:223:ALA:HB2	1:A:420:ASN:ND2	2.36	0.41
1:A:255:VAL:HA	1:A:329:ALA:O	2.20	0.41
1:A:237:GLU:O	1:A:241:GLU:HG3	2.21	0.40
1:B:431:ARG:O	1:B:435:VAL:HG23	2.22	0.40
1:B:223:ALA:HB2	1:B:420:ASN:HD22	1.86	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	427/451 (95%)	413 (97%)	14 (3%)	0	100	100
1	B	427/451 (95%)	409 (96%)	17 (4%)	1 (0%)	47	57
1	C	417/451 (92%)	399 (96%)	17 (4%)	1 (0%)	47	57
1	D	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
All	All	1697/1804 (94%)	1633 (96%)	62 (4%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	336	ALA
1	C	264	PRO

### 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	307/335 (92%)	303 (99%)	4 (1%)	69 79
1	B	307/335 (92%)	301 (98%)	6 (2%)	55 67
1	C	288/335 (86%)	279 (97%)	9 (3%)	40 52
1	D	307/335 (92%)	301 (98%)	6 (2%)	55 67
All	All	1209/1340 (90%)	1184 (98%)	25 (2%)	53 66

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	GLU
1	A	268	LYS
1	A	299	LEU
1	A	394	LYS
1	B	9	ARG
1	B	33	ARG
1	B	87	ARG
1	B	238	ARG
1	B	387	ASP
1	B	393	ARG
1	C	33	ARG
1	C	43	ARG
1	C	63	ASP
1	C	75	ARG
1	C	254	PHE
1	C	266	LEU
1	C	293	ASP
1	C	342	SER
1	C	387	ASP
1	D	33	ARG

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Mol	Chain	Res	Type
1	D	63	ASP
1	D	170	HIS
1	D	241	GLU
1	D	260	ARG
1	D	317	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	420	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 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	429/451 (95%)	-0.07	10 (2%) 60 56	30, 45, 70, 86	0
1	B	429/451 (95%)	0.04	5 (1%) 79 77	32, 47, 73, 82	0
1	C	421/451 (93%)	0.20	18 (4%) 35 32	29, 48, 83, 94	0
1	D	428/451 (94%)	-0.18	1 (0%) 95 95	30, 41, 56, 72	0
All	All	1707/1804 (94%)	-0.00	34 (1%) 65 62	29, 45, 74, 94	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	305	VAL	5.8
1	C	303	TYR	4.1
1	C	264	PRO	3.9
1	C	307	ALA	3.7
1	B	305	VAL	3.6
1	A	168	THR	3.6
1	C	283	VAL	3.5
1	A	294	PRO	3.5
1	A	167	ASP	3.5
1	B	299	LEU	3.3
1	A	300	ALA	3.1
1	C	274	LEU	3.0
1	C	294	PRO	2.7
1	C	243	ILE	2.7
1	C	278	ARG	2.6
1	A	303	TYR	2.6
1	C	388	ALA	2.5
1	B	246	LEU	2.5
1	B	300	ALA	2.5
1	A	301	ASP	2.4
1	A	311	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	392	VAL	2.4
1	D	264	PRO	2.4
1	B	281	PRO	2.4
1	C	400	ARG	2.3
1	A	169	ALA	2.3
1	C	273	LEU	2.3
1	C	281	PRO	2.2
1	C	282	GLY	2.2
1	C	296	LEU	2.2
1	A	237	GLU	2.1
1	C	301	ASP	2.1
1	A	299	LEU	2.0
1	C	309	LEU	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.