



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:07 am GMT

PDB ID : 4E75  
Title : Structure of LpxD from *Acinetobacter baumannii* at 2.85Å resolution (P21 form)  
Authors : Badger, J.; Chie-Leon, B.; Logan, C.; Sridhar, V.; Sankaran, B.; Zwart, P.H.; Nienaber, V.  
Deposited on : 2012-03-16  
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

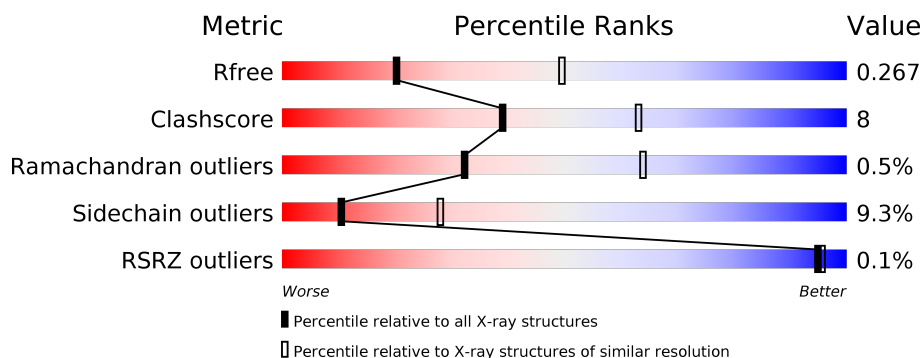
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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))
$R_{free}$	100719	2469 (2.90-2.82)
Clashscore	112137	2749 (2.90-2.82)
Ramachandran outliers	110173	2687 (2.90-2.82)
Sidechain outliers	110143	2690 (2.90-2.82)
RSRZ outliers	101464	2487 (2.90-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	357	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 18%, green 72%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>72%</span> <span>19%</span> <span>• 6%</span> </div> </div>
1	B	357	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 1%, yellow 18%, green 74%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>74%</span> <span>18%</span> <span>• 6%</span> </div> </div>
1	C	357	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 1%, yellow 16%, green 76%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>76%</span> <span>16%</span> <span>• 6%</span> </div> </div>
1	D	357	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 1%, yellow 18%, green 74%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>74%</span> <span>18%</span> <span>• 6%</span> </div> </div>
1	E	357	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 1%, yellow 18%, green 73%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>73%</span> <span>18%</span> <span>• 6%</span> </div> </div>
1	F	357	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 1%, yellow 20%, green 71%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>71%</span> <span>20%</span> <span>• • 6%</span> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15088 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 UDP-3-O-acetylglucosamine N-acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2513	1574	444	487	8			
1	B	337	Total	C	N	O	S	0	0	0
			2515	1575	445	487	8			
1	C	337	Total	C	N	O	S	0	0	0
			2515	1575	445	487	8			
1	D	337	Total	C	N	O	S	0	0	0
			2515	1575	445	487	8			
1	E	337	Total	C	N	O	S	0	0	0
			2515	1575	445	487	8			
1	F	337	Total	C	N	O	S	0	0	0
			2515	1575	445	487	8			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP B0VMV2
A	2	GLY	-	EXPRESSION TAG	UNP B0VMV2
A	3	SER	-	EXPRESSION TAG	UNP B0VMV2
B	1	GLY	-	EXPRESSION TAG	UNP B0VMV2
B	2	GLY	-	EXPRESSION TAG	UNP B0VMV2
B	3	SER	-	EXPRESSION TAG	UNP B0VMV2
C	1	GLY	-	EXPRESSION TAG	UNP B0VMV2
C	2	GLY	-	EXPRESSION TAG	UNP B0VMV2
C	3	SER	-	EXPRESSION TAG	UNP B0VMV2
D	1	GLY	-	EXPRESSION TAG	UNP B0VMV2
D	2	GLY	-	EXPRESSION TAG	UNP B0VMV2
D	3	SER	-	EXPRESSION TAG	UNP B0VMV2
E	1	GLY	-	EXPRESSION TAG	UNP B0VMV2
E	2	GLY	-	EXPRESSION TAG	UNP B0VMV2
E	3	SER	-	EXPRESSION TAG	UNP B0VMV2
F	1	GLY	-	EXPRESSION TAG	UNP B0VMV2
F	2	GLY	-	EXPRESSION TAG	UNP B0VMV2

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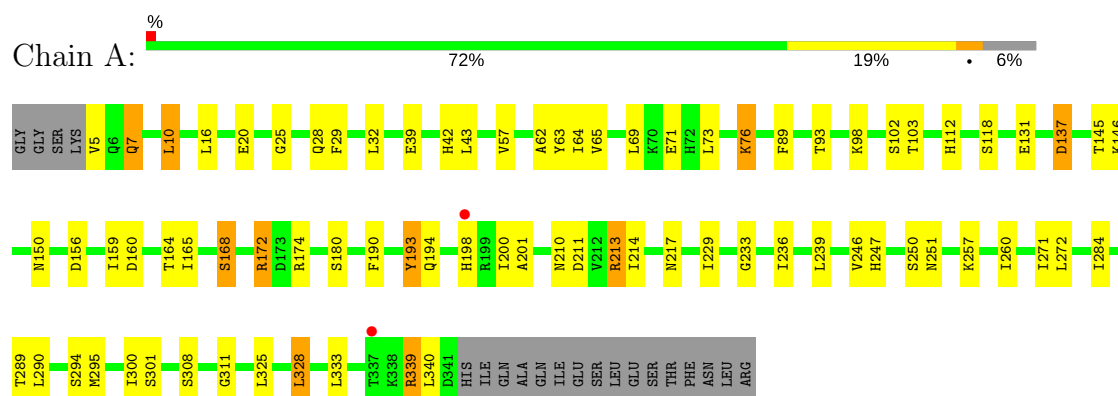
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Chain	Residue	Modelled	Actual	Comment	Reference
F	3	SER	-	EXPRESSION TAG	UNP B0VMV2

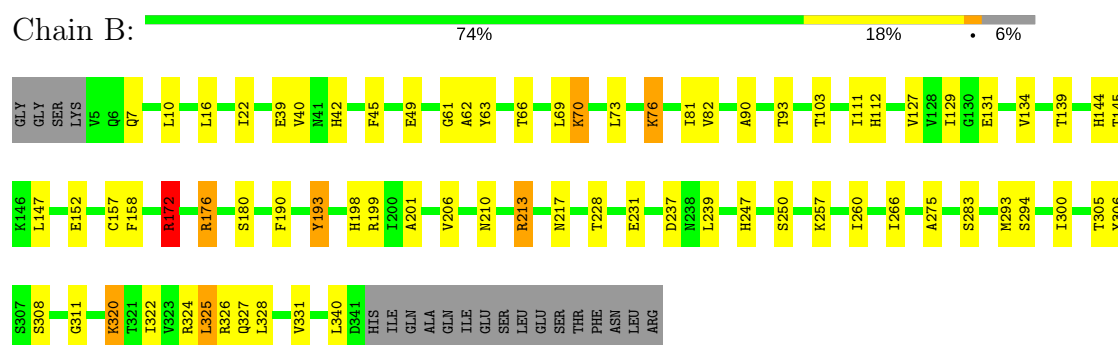
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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.

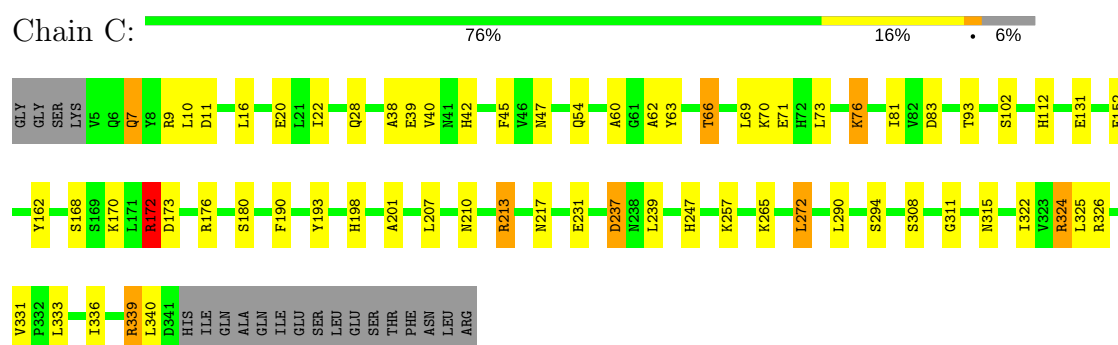
- Molecule 1: UDP-3-O-acylglucosamine N-acyltransferase



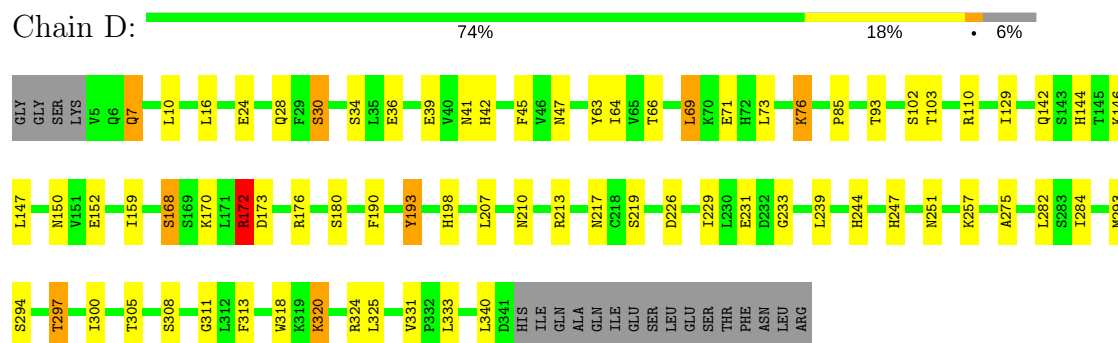
- Molecule 1: UDP-3-O-acylglucosamine N-acyltransferase



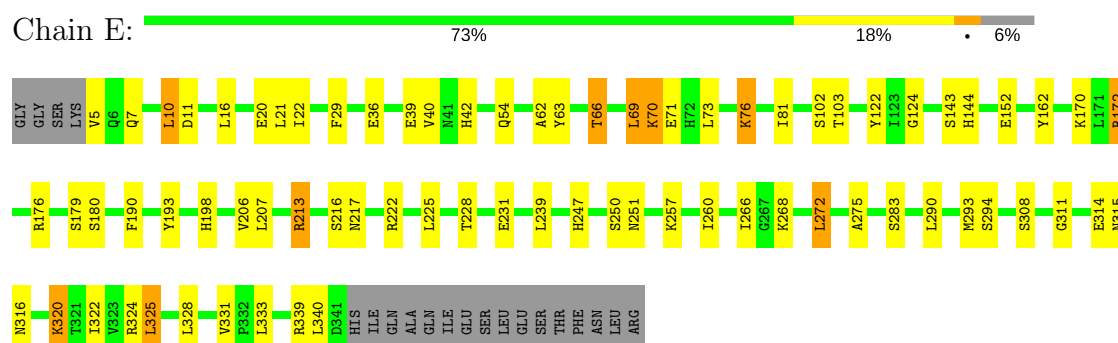
- Molecule 1: UDP-3-O-acylglucosamine N-acyltransferase



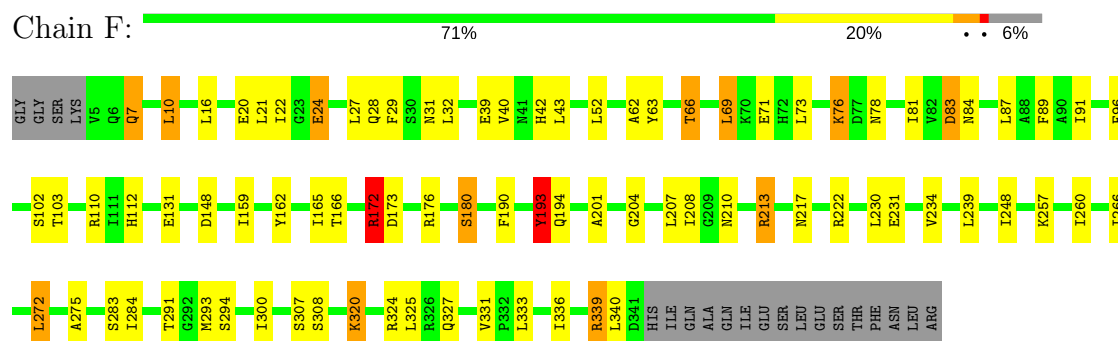
• Molecule 1: UDP-3-O-acylglucosamine N-acyltransferase



• Molecule 1: UDP-3-O-acylglucosamine N-acyltransferase



• Molecule 1: UDP-3-O-acylglucosamine N-acyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.68Å 209.61Å 107.63Å 90.00° 119.23° 90.00°	Depositor
Resolution (Å)	48.15 – 2.85 48.14 – 2.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.15-2.85) 98.1 (48.14-2.85)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.234 , 0.280 0.223 , 0.267	Depositor DCC
$R_{free}$ test set	4743 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.8	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 2.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.070 for -h-l,k,h 0.070 for l,k,-h-l 0.347 for h,-k,-h-l 0.063 for -h-l,-k,l 0.090 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15088	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.87% 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	0.59	0/2552	0.71	0/3467
1	B	0.59	0/2554	0.71	0/3469
1	C	0.61	0/2554	0.73	1/3469 (0.0%)
1	D	0.59	0/2554	0.69	0/3469
1	E	0.60	0/2554	0.71	0/3469
1	F	0.60	0/2554	0.73	1/3469 (0.0%)
All	All	0.60	0/15322	0.71	2/20812 (0.0%)

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	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	272	LEU	CA-CB-CG	5.60	128.18	115.30
1	C	237	ASP	CB-CG-OD2	-5.28	113.55	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	311	GLY	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	2513	0	2470	49	0
1	B	2515	0	2477	52	0
1	C	2515	0	2477	47	0
1	D	2515	0	2477	49	0
1	E	2515	0	2477	44	0
1	F	2515	0	2477	54	0
All	All	15088	0	14855	253	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 (253) 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:E:193:TYR:CE1	1:E:198:HIS:HB2	2.03	0.94
1:C:152:GLU:HG3	1:C:170:LYS:HE3	1.51	0.93
1:B:190:PHE:HZ	1:C:213:ARG:HD3	1.34	0.90
1:F:66:THR:HG22	1:F:69:LEU:HB2	1.56	0.86
1:F:84:ASN:HD22	1:F:87:LEU:HB3	1.39	0.86
1:E:190:PHE:HZ	1:F:213:ARG:HD3	1.42	0.84
1:D:152:GLU:HG3	1:D:170:LYS:HE3	1.60	0.83
1:D:150:ASN:HB2	1:D:168:SER:HB3	1.60	0.83
1:B:193:TYR:CE1	1:B:198:HIS:HB2	2.13	0.82
1:A:39:GLU:H	1:A:42:HIS:HD2	1.26	0.80
1:E:193:TYR:HE1	1:E:198:HIS:HB2	1.45	0.79
1:F:339:ARG:CG	1:F:339:ARG:HH21	1.96	0.79
1:B:190:PHE:CZ	1:C:213:ARG:HD3	2.18	0.78
1:A:150:ASN:HB2	1:A:168:SER:HB3	1.65	0.77
1:F:7:GLN:HG2	1:F:28:GLN:HB3	1.66	0.77
1:A:39:GLU:H	1:A:42:HIS:CD2	2.04	0.76
1:D:93:THR:HB	1:F:201:ALA:HB3	1.67	0.76
1:F:339:ARG:HG3	1:F:339:ARG:HH21	1.51	0.76
1:C:63:TYR:CE1	1:C:76:LYS:HG2	2.21	0.75
1:C:7:GLN:HG2	1:C:28:GLN:HB3	1.67	0.75
1:A:7:GLN:HG2	1:A:28:GLN:HB3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:TYR:CE1	1:D:198:HIS:HB2	2.22	0.74
1:A:180:SER:OG	1:A:217:ASN:ND2	2.21	0.73
1:F:39:GLU:H	1:F:42:HIS:CD2	2.09	0.71
1:A:201:ALA:HB3	1:B:93:THR:HB	1.73	0.70
1:B:66:THR:CG2	1:B:69:LEU:HD23	2.22	0.69
1:A:190:PHE:HZ	1:B:213:ARG:HD3	1.58	0.69
1:F:159:ILE:HD13	1:F:165:ILE:HD11	1.75	0.69
1:E:190:PHE:CZ	1:F:213:ARG:HD3	2.26	0.68
1:A:257:LYS:O	1:B:257:LYS:HE2	1.94	0.67
1:D:63:TYR:CE1	1:D:76:LYS:HG2	2.29	0.67
1:A:328:LEU:HD13	1:C:324:ARG:HB3	1.75	0.67
1:B:308:SER:HB3	1:C:311:GLY:O	1.95	0.67
1:A:93:THR:HB	1:C:201:ALA:HB3	1.77	0.67
1:A:339:ARG:HH21	1:A:339:ARG:CG	2.09	0.66
1:F:39:GLU:H	1:F:42:HIS:HD2	1.41	0.66
1:F:10:LEU:HG	1:F:29:PHE:HE2	1.61	0.66
1:E:36:GLU:OE2	1:E:54:GLN:NE2	2.30	0.65
1:D:190:PHE:CZ	1:E:213:ARG:HD3	2.32	0.64
1:A:311:GLY:HA3	1:B:326:ARG:NH1	2.13	0.64
1:A:63:TYR:CE1	1:A:76:LYS:HG2	2.32	0.64
1:E:66:THR:HG22	1:E:69:LEU:H	1.63	0.64
1:A:257:LYS:HE2	1:C:257:LYS:O	1.98	0.63
1:C:39:GLU:H	1:C:42:HIS:CD2	2.16	0.63
1:D:229:ILE:HB	1:D:247:HIS:HD2	1.64	0.62
1:A:213:ARG:HD3	1:C:190:PHE:CZ	2.34	0.62
1:F:63:TYR:CE1	1:F:76:LYS:HG2	2.33	0.62
1:E:39:GLU:H	1:E:42:HIS:HD2	1.45	0.62
1:E:275:ALA:O	1:E:293:MET:HA	1.99	0.62
1:B:172:ARG:HB3	1:B:210:ASN:OD1	2.01	0.60
1:C:39:GLU:O	1:C:60:ALA:HA	2.02	0.59
1:D:193:TYR:N	1:D:193:TYR:CD1	2.69	0.59
1:D:180:SER:OG	1:D:217:ASN:ND2	2.34	0.59
1:E:206:VAL:HG22	1:E:228:THR:HB	1.83	0.59
1:D:331:VAL:HG21	1:E:333:LEU:HG	1.85	0.59
1:D:193:TYR:H	1:D:193:TYR:HD1	1.48	0.59
1:D:217:ASN:O	1:D:239:LEU:HA	2.02	0.59
1:F:208:ILE:HG12	1:F:230:LEU:HD12	1.85	0.59
1:D:172:ARG:HB3	1:D:210:ASN:OD1	2.03	0.59
1:A:213:ARG:HD3	1:C:190:PHE:HZ	1.66	0.58
1:A:159:ILE:HD13	1:A:165:ILE:HD11	1.84	0.58
1:B:275:ALA:O	1:B:293:MET:HA	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ALA:C	1:B:63:TYR:CD1	2.78	0.57
1:F:294:SER:HA	1:F:308:SER:OG	2.04	0.57
1:F:84:ASN:ND2	1:F:87:LEU:HB3	2.16	0.57
1:C:45:PHE:CE1	1:C:47:ASN:HB2	2.40	0.57
1:E:331:VAL:HG21	1:F:333:LEU:HG	1.87	0.57
1:B:134:VAL:HB	1:B:152:GLU:HG2	1.87	0.56
1:A:333:LEU:HG	1:C:331:VAL:HG21	1.86	0.56
1:D:193:TYR:HD1	1:D:193:TYR:N	2.02	0.56
1:E:22:ILE:HD12	1:E:81:ILE:HD11	1.87	0.56
1:A:190:PHE:CZ	1:B:213:ARG:HD3	2.39	0.56
1:D:313:PHE:HB2	1:D:318:TRP:HB2	1.86	0.56
1:A:193:TYR:CE1	1:A:198:HIS:HB2	2.41	0.56
1:E:152:GLU:HB2	1:E:170:LYS:HG3	1.87	0.55
1:D:294:SER:HA	1:D:308:SER:OG	2.07	0.55
1:F:10:LEU:HG	1:F:29:PHE:CE2	2.42	0.55
1:C:231:GLU:OE2	1:C:247:HIS:HE1	1.88	0.54
1:E:39:GLU:H	1:E:42:HIS:CD2	2.23	0.54
1:B:63:TYR:CE1	1:B:76:LYS:HG2	2.42	0.54
1:D:129:ILE:HG12	1:D:147:LEU:HD22	1.89	0.54
1:C:152:GLU:CG	1:C:170:LYS:HE3	2.33	0.54
1:E:162:TYR:O	1:E:180:SER:HA	2.08	0.53
1:D:219:SER:HG	1:E:216:SER:HG	1.53	0.53
1:C:294:SER:HA	1:C:308:SER:OG	2.09	0.53
1:F:260:ILE:HD12	1:F:266:ILE:HD11	1.90	0.53
1:B:39:GLU:H	1:B:42:HIS:CD2	2.26	0.53
1:A:339:ARG:NH2	1:A:339:ARG:CG	2.72	0.52
1:F:83:ASP:N	1:F:83:ASP:OD2	2.41	0.52
1:D:257:LYS:HE2	1:F:257:LYS:O	2.09	0.52
1:D:39:GLU:H	1:D:42:HIS:CD2	2.27	0.52
1:C:66:THR:HG22	1:C:69:LEU:HB2	1.92	0.52
1:B:112:HIS:CE1	1:B:131:GLU:HG2	2.44	0.52
1:B:63:TYR:N	1:B:63:TYR:CD1	2.78	0.52
1:D:257:LYS:O	1:E:257:LYS:HE2	2.10	0.52
1:D:190:PHE:HZ	1:E:213:ARG:HD3	1.74	0.52
1:D:305:THR:HG22	1:E:315:ASN:HB2	1.91	0.52
1:A:112:HIS:NE2	1:A:131:GLU:HG2	2.24	0.52
1:A:214:ILE:HG12	1:A:236:ILE:HD12	1.91	0.52
1:A:112:HIS:CD2	1:A:131:GLU:HG2	2.45	0.52
1:A:294:SER:HA	1:A:308:SER:OG	2.10	0.52
1:B:127:VAL:HG13	1:B:145:THR:O	2.10	0.51
1:B:294:SER:HA	1:B:308:SER:OG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:SER:HB2	1:E:268:LYS:HG2	1.91	0.51
1:E:260:ILE:HD12	1:E:266:ILE:HD11	1.91	0.51
1:D:30:SER:OG	1:D:41:ASN:ND2	2.43	0.51
1:D:213:ARG:HD3	1:F:190:PHE:HZ	1.76	0.51
1:F:339:ARG:NH2	1:F:339:ARG:HG3	2.22	0.51
1:A:339:ARG:HG3	1:A:339:ARG:NH2	2.24	0.51
1:F:217:ASN:O	1:F:239:LEU:HA	2.10	0.51
1:B:66:THR:HG22	1:B:69:LEU:HD23	1.91	0.51
1:D:150:ASN:CB	1:D:168:SER:HB3	2.36	0.51
1:F:231:GLU:O	1:F:234:VAL:HG23	2.11	0.51
1:A:211:ASP:O	1:A:233:GLY:HA2	2.10	0.51
1:C:39:GLU:H	1:C:42:HIS:HD2	1.59	0.50
1:D:190:PHE:CE1	1:E:213:ARG:HD3	2.47	0.50
1:E:257:LYS:O	1:E:275:ALA:HA	2.10	0.50
1:A:229:ILE:HB	1:A:247:HIS:HD2	1.77	0.50
1:A:339:ARG:HG3	1:A:339:ARG:HH21	1.75	0.50
1:C:239:LEU:O	1:C:257:LYS:HA	2.12	0.50
1:D:34:SER:HB2	1:D:36:GLU:OE1	2.10	0.50
1:B:39:GLU:H	1:B:42:HIS:HD2	1.59	0.50
1:F:284:ILE:HG12	1:F:300:ILE:HD12	1.93	0.50
1:B:322:ILE:O	1:B:326:ARG:HG3	2.12	0.49
1:A:246:VAL:HG11	1:A:260:ILE:HG21	1.94	0.49
1:F:173:ASP:O	1:F:210:ASN:HA	2.12	0.49
1:A:62:ALA:C	1:A:63:TYR:CD1	2.86	0.49
1:B:231:GLU:OE2	1:B:247:HIS:HE1	1.95	0.49
1:D:284:ILE:HG12	1:D:300:ILE:HD12	1.94	0.49
1:C:272:LEU:HD23	1:C:272:LEU:N	2.28	0.49
1:B:22:ILE:HD12	1:B:81:ILE:HD11	1.95	0.49
1:B:331:VAL:HG21	1:C:333:LEU:HG	1.94	0.49
1:D:308:SER:HB3	1:E:311:GLY:O	2.13	0.49
1:C:322:ILE:O	1:C:326:ARG:HG3	2.13	0.48
1:D:64:ILE:HG22	1:D:85:PRO:HB3	1.95	0.48
1:C:193:TYR:CE1	1:C:198:HIS:HB2	2.48	0.48
1:F:172:ARG:HB3	1:F:210:ASN:OD1	2.13	0.48
1:F:62:ALA:C	1:F:63:TYR:CD1	2.86	0.48
1:F:112:HIS:CE1	1:F:131:GLU:HG2	2.47	0.48
1:F:193:TYR:O	1:F:193:TYR:CD1	2.66	0.48
1:B:206:VAL:HG22	1:B:228:THR:HB	1.95	0.48
1:E:63:TYR:CE1	1:E:76:LYS:HG2	2.49	0.48
1:A:295:MET:SD	1:B:293:MET:SD	3.12	0.48
1:A:229:ILE:HB	1:A:247:HIS:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ASN:O	1:B:239:LEU:HA	2.13	0.47
1:C:66:THR:HG22	1:C:69:LEU:H	1.79	0.47
1:D:63:TYR:OH	1:D:76:LYS:HE2	2.13	0.47
1:A:217:ASN:O	1:A:239:LEU:HA	2.14	0.47
1:D:39:GLU:H	1:D:42:HIS:HD2	1.62	0.47
1:F:291:THR:HG1	1:F:307:SER:CB	2.28	0.47
1:A:43:LEU:HD21	1:A:64:ILE:HD11	1.97	0.47
1:E:325:LEU:HD23	1:E:328:LEU:HD12	1.97	0.47
1:F:204:GLY:O	1:F:222:ARG:HD2	2.14	0.47
1:A:233:GLY:O	1:A:251:ASN:HA	2.15	0.47
1:E:320:LYS:HE3	1:E:320:LYS:HB2	1.50	0.47
1:C:336:ILE:HA	1:C:339:ARG:HB2	1.97	0.46
1:A:32:LEU:HD22	1:A:89:PHE:CD2	2.50	0.46
1:B:260:ILE:HD12	1:B:266:ILE:CD1	2.46	0.46
1:C:9:ARG:HB3	1:C:11:ASP:OD1	2.15	0.46
1:D:144:HIS:O	1:E:162:TYR:OH	2.22	0.46
1:F:87:LEU:O	1:F:91:ILE:HG13	2.15	0.46
1:B:201:ALA:HB3	1:C:93:THR:HB	1.97	0.46
1:A:284:ILE:HG12	1:A:300:ILE:HD12	1.98	0.46
1:C:231:GLU:OE2	1:C:247:HIS:CE1	2.69	0.46
1:D:320:LYS:HB2	1:D:320:LYS:HE3	1.67	0.46
1:A:271:ILE:O	1:A:289:THR:HA	2.16	0.46
1:D:213:ARG:HD3	1:F:190:PHE:CZ	2.51	0.46
1:E:62:ALA:C	1:E:63:TYR:CD1	2.90	0.45
1:B:190:PHE:CE2	1:B:199:ARG:HG3	2.50	0.45
1:A:200:ILE:HG22	1:A:201:ALA:O	2.17	0.45
1:F:32:LEU:HG	1:F:96:PHE:CD1	2.51	0.45
1:B:213:ARG:HH21	1:B:237:ASP:HA	1.82	0.45
1:B:305:THR:HG22	1:C:315:ASN:HB2	1.98	0.45
1:B:40:VAL:O	1:B:61:GLY:HA3	2.16	0.45
1:D:333:LEU:HD23	1:F:327:GLN:HB2	1.98	0.45
1:D:333:LEU:HG	1:F:331:VAL:HG21	1.99	0.45
1:B:193:TYR:N	1:B:193:TYR:CD1	2.85	0.45
1:C:22:ILE:HD12	1:C:81:ILE:HD11	1.98	0.44
1:F:162:TYR:O	1:F:180:SER:HA	2.17	0.44
1:F:32:LEU:HA	1:F:43:LEU:O	2.17	0.44
1:C:62:ALA:C	1:C:63:TYR:CD1	2.91	0.44
1:D:45:PHE:CE1	1:D:47:ASN:HB2	2.52	0.44
1:D:63:TYR:N	1:D:63:TYR:CD1	2.85	0.44
1:E:11:ASP:HB3	1:E:21:LEU:HD22	1.99	0.44
1:B:158:PHE:O	1:B:176:ARG:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:ARG:HB3	1:C:210:ASN:OD1	2.17	0.44
1:C:66:THR:HG22	1:C:69:LEU:N	2.32	0.44
1:F:172:ARG:HB3	1:F:173:ASP:H	1.60	0.44
1:F:231:GLU:HB2	1:F:248:ILE:O	2.17	0.44
1:B:111:ILE:HG12	1:B:129:ILE:HD12	1.99	0.44
1:B:213:ARG:NH2	1:B:237:ASP:HA	2.32	0.44
1:A:93:THR:CB	1:C:201:ALA:HB3	2.46	0.44
1:E:10:LEU:HG	1:E:29:PHE:CE2	2.53	0.44
1:D:233:GLY:O	1:D:251:ASN:HA	2.18	0.44
1:F:21:LEU:O	1:F:22:ILE:HG13	2.18	0.43
1:F:275:ALA:O	1:F:293:MET:HA	2.18	0.43
1:F:39:GLU:N	1:F:42:HIS:HD2	2.11	0.43
1:A:145:THR:OG1	1:A:160:ASP:O	2.32	0.43
1:A:146:LYS:HE3	1:A:164:THR:HG23	1.99	0.43
1:B:139:THR:HG23	1:B:157:CYS:HB2	2.01	0.43
1:C:213:ARG:HH21	1:C:237:ASP:HA	1.84	0.43
1:C:38:ALA:CB	1:C:60:ALA:HB2	2.49	0.43
1:E:322:ILE:HA	1:E:325:LEU:HB2	2.00	0.43
1:B:144:HIS:O	1:C:162:TYR:OH	2.28	0.43
1:C:112:HIS:CE1	1:C:131:GLU:HG2	2.54	0.43
1:C:180:SER:HB3	1:C:217:ASN:ND2	2.33	0.43
1:C:272:LEU:HD13	1:C:290:LEU:HD12	2.01	0.43
1:D:110:ARG:HD3	1:D:110:ARG:HA	1.86	0.43
1:E:143:SER:O	1:E:144:HIS:HB2	2.18	0.43
1:E:294:SER:HA	1:E:308:SER:OG	2.19	0.43
1:B:320:LYS:HE3	1:B:320:LYS:HB2	1.53	0.43
1:C:172:ARG:HB3	1:C:173:ASP:H	1.50	0.43
1:F:148:ASP:HB2	1:F:166:THR:HA	2.01	0.42
1:A:172:ARG:HB3	1:A:210:ASN:OD1	2.20	0.42
1:D:172:ARG:HB3	1:D:173:ASP:H	1.55	0.42
1:B:260:ILE:HD12	1:B:266:ILE:HD11	2.02	0.42
1:E:217:ASN:O	1:E:239:LEU:HA	2.18	0.42
1:F:159:ILE:HD13	1:F:165:ILE:CD1	2.46	0.42
1:A:156:ASP:O	1:A:174:ARG:HA	2.20	0.42
1:A:10:LEU:HG	1:A:29:PHE:HE2	1.84	0.42
1:F:20:GLU:HB3	1:F:81:ILE:HB	2.02	0.42
1:F:320:LYS:HE3	1:F:320:LYS:HB2	1.47	0.42
1:A:118:SER:OG	1:A:137:ASP:HA	2.20	0.42
1:E:206:VAL:HG23	1:E:222:ARG:HA	2.00	0.42
1:E:272:LEU:HD13	1:E:290:LEU:HD12	2.00	0.42
1:F:24:GLU:HB3	1:F:27:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:TYR:CE1	1:F:76:LYS:CG	3.03	0.42
1:E:314:GLU:OE1	1:E:316:ASN:HB2	2.19	0.41
1:B:90:ALA:O	1:B:93:THR:OG1	2.38	0.41
1:D:7:GLN:HG2	1:D:28:GLN:NE2	2.35	0.41
1:E:225:LEU:HD11	1:F:89:PHE:CZ	2.55	0.41
1:B:325:LEU:O	1:B:328:LEU:HB2	2.20	0.41
1:F:31:ASN:HA	1:F:96:PHE:CD2	2.55	0.41
1:A:217:ASN:ND2	1:C:217:ASN:HD22	2.17	0.41
1:A:39:GLU:N	1:A:42:HIS:HD2	2.06	0.41
1:E:231:GLU:OE2	1:E:247:HIS:HE1	2.04	0.41
1:E:250:SER:HB3	1:E:251:ASN:ND2	2.36	0.41
1:D:229:ILE:CB	1:D:247:HIS:HD2	2.32	0.41
1:D:66:THR:HG22	1:D:69:LEU:HB2	2.03	0.41
1:E:70:LYS:HG2	1:E:70:LYS:O	2.21	0.41
1:B:300:ILE:HG21	1:B:306:TYR:CE1	2.55	0.41
1:D:275:ALA:O	1:D:293:MET:HA	2.21	0.41
1:D:282:LEU:HD11	1:D:297:THR:C	2.42	0.41
1:C:217:ASN:O	1:C:239:LEU:HA	2.21	0.40
1:B:311:GLY:HA3	1:C:326:ARG:NH1	2.35	0.40
1:E:122:TYR:CE2	1:E:124:GLY:HA2	2.56	0.40
1:F:22:ILE:O	1:F:78:ASN:HA	2.21	0.40
1:B:69:LEU:O	1:B:70:LYS:C	2.60	0.40
1:B:63:TYR:OH	1:B:76:LYS:HE2	2.22	0.40
1:B:257:LYS:O	1:C:257:LYS:HE2	2.22	0.40
1:B:324:ARG:HA	1:B:327:GLN:OE1	2.21	0.40
1:B:129:ILE:HG12	1:B:147:LEU:HD22	2.04	0.40
1:D:142:GLN:OE1	1:D:142:GLN:HA	2.22	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	335/357 (94%)	318 (95%)	15 (4%)	2 (1%)	28	60
1	B	335/357 (94%)	313 (93%)	21 (6%)	1 (0%)	44	73
1	C	335/357 (94%)	310 (92%)	24 (7%)	1 (0%)	44	73
1	D	335/357 (94%)	311 (93%)	21 (6%)	3 (1%)	20	49
1	E	335/357 (94%)	320 (96%)	14 (4%)	1 (0%)	44	73
1	F	335/357 (94%)	314 (94%)	18 (5%)	3 (1%)	20	49
All	All	2010/2142 (94%)	1886 (94%)	113 (6%)	11 (0%)	32	64

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	172	ARG
1	D	24	GLU
1	F	172	ARG
1	A	25	GLY
1	A	98	LYS
1	B	172	ARG
1	D	172	ARG
1	E	172	ARG
1	D	226	ASP
1	F	193	TYR
1	F	24	GLU

### 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	267/295 (90%)	240 (90%)	27 (10%)	9	24
1	B	268/295 (91%)	248 (92%)	20 (8%)	16	39
1	C	268/295 (91%)	244 (91%)	24 (9%)	11	29
1	D	268/295 (91%)	244 (91%)	24 (9%)	11	29
1	E	268/295 (91%)	242 (90%)	26 (10%)	9	26
1	F	268/295 (91%)	239 (89%)	29 (11%)	7	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1607/1770 (91%)	1457 (91%)	150 (9%)	10	28

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	7	GLN
1	A	10	LEU
1	A	16	LEU
1	A	20	GLU
1	A	57	VAL
1	A	65	VAL
1	A	69	LEU
1	A	71	GLU
1	A	73	LEU
1	A	76	LYS
1	A	102	SER
1	A	103	THR
1	A	137	ASP
1	A	168	SER
1	A	172	ARG
1	A	193	TYR
1	A	194	GLN
1	A	213	ARG
1	A	250	SER
1	A	272	LEU
1	A	290	LEU
1	A	301	SER
1	A	325	LEU
1	A	328	LEU
1	A	339	ARG
1	A	340	LEU
1	B	7	GLN
1	B	10	LEU
1	B	16	LEU
1	B	45	PHE
1	B	49	GLU
1	B	70	LYS
1	B	73	LEU
1	B	76	LYS
1	B	82	VAL
1	B	103	THR

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Mol	Chain	Res	Type
1	B	172	ARG
1	B	176	ARG
1	B	180	SER
1	B	193	TYR
1	B	213	ARG
1	B	250	SER
1	B	283	SER
1	B	320	LYS
1	B	325	LEU
1	B	340	LEU
1	C	7	GLN
1	C	10	LEU
1	C	16	LEU
1	C	20	GLU
1	C	40	VAL
1	C	54	GLN
1	C	66	THR
1	C	70	LYS
1	C	71	GLU
1	C	73	LEU
1	C	76	LYS
1	C	83	ASP
1	C	102	SER
1	C	168	SER
1	C	172	ARG
1	C	176	ARG
1	C	207	LEU
1	C	213	ARG
1	C	265	LYS
1	C	272	LEU
1	C	324	ARG
1	C	325	LEU
1	C	339	ARG
1	C	340	LEU
1	D	7	GLN
1	D	10	LEU
1	D	16	LEU
1	D	30	SER
1	D	69	LEU
1	D	71	GLU
1	D	73	LEU
1	D	76	LYS

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Mol	Chain	Res	Type
1	D	102	SER
1	D	103	THR
1	D	146	LYS
1	D	159	ILE
1	D	168	SER
1	D	172	ARG
1	D	176	ARG
1	D	193	TYR
1	D	207	LEU
1	D	231	GLU
1	D	244	HIS
1	D	297	THR
1	D	320	LYS
1	D	324	ARG
1	D	325	LEU
1	D	340	LEU
1	E	5	VAL
1	E	7	GLN
1	E	10	LEU
1	E	16	LEU
1	E	20	GLU
1	E	40	VAL
1	E	66	THR
1	E	69	LEU
1	E	70	LYS
1	E	71	GLU
1	E	73	LEU
1	E	76	LYS
1	E	102	SER
1	E	103	THR
1	E	172	ARG
1	E	176	ARG
1	E	179	SER
1	E	207	LEU
1	E	213	ARG
1	E	272	LEU
1	E	283	SER
1	E	320	LYS
1	E	324	ARG
1	E	325	LEU
1	E	339	ARG
1	E	340	LEU

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Mol	Chain	Res	Type
1	F	7	GLN
1	F	10	LEU
1	F	16	LEU
1	F	40	VAL
1	F	52	LEU
1	F	66	THR
1	F	69	LEU
1	F	71	GLU
1	F	73	LEU
1	F	76	LYS
1	F	83	ASP
1	F	102	SER
1	F	103	THR
1	F	110	ARG
1	F	172	ARG
1	F	176	ARG
1	F	180	SER
1	F	193	TYR
1	F	194	GLN
1	F	207	LEU
1	F	213	ARG
1	F	272	LEU
1	F	283	SER
1	F	320	LYS
1	F	324	ARG
1	F	325	LEU
1	F	336	ILE
1	F	339	ARG
1	F	340	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	47	ASN
1	A	51	HIS
1	A	54	GLN
1	A	84	ASN
1	A	217	ASN
1	A	247	HIS
1	B	42	HIS
1	B	47	ASN

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Mol	Chain	Res	Type
1	B	72	HIS
1	B	247	HIS
1	C	42	HIS
1	C	217	ASN
1	C	247	HIS
1	D	28	GLN
1	D	41	ASN
1	D	42	HIS
1	D	47	ASN
1	D	51	HIS
1	D	54	GLN
1	D	72	HIS
1	D	217	ASN
1	E	42	HIS
1	E	51	HIS
1	E	54	GLN
1	E	72	HIS
1	E	217	ASN
1	E	247	HIS
1	E	251	ASN
1	F	7	GLN
1	F	42	HIS
1	F	47	ASN
1	F	54	GLN
1	F	84	ASN
1	F	251	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	337/357 (94%)	-0.27	2 (0%) 89 88	26, 52, 82, 120	0
1	B	337/357 (94%)	-0.26	0 100 100	33, 48, 79, 116	0
1	C	337/357 (94%)	-0.24	0 100 100	31, 48, 74, 114	0
1	D	337/357 (94%)	-0.21	0 100 100	32, 51, 83, 124	0
1	E	337/357 (94%)	-0.27	0 100 100	29, 47, 75, 115	0
1	F	337/357 (94%)	-0.29	0 100 100	28, 48, 76, 117	0
All	All	2022/2142 (94%)	-0.26	2 (0%) 95 95	26, 49, 79, 124	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	337	THR	2.3
1	A	198	HIS	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.