



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:07 PM UTC

PDB ID : 4E75 / pdb\_00004e75  
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

<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 : 4-5-2 with Phenix2.0  
Xtrriage (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

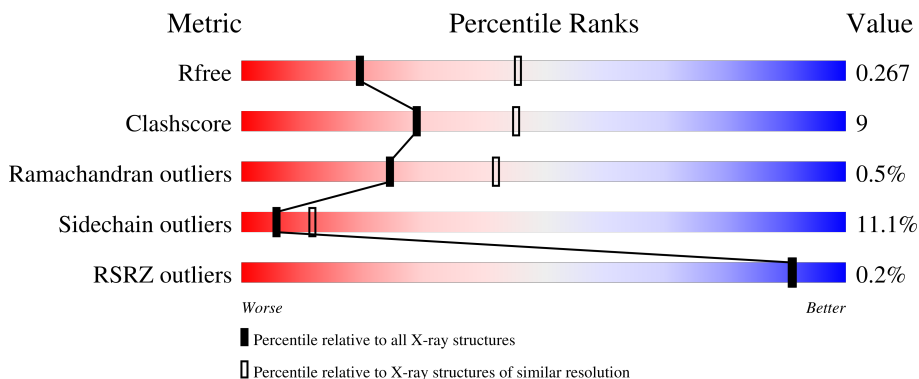
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


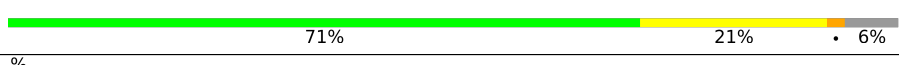

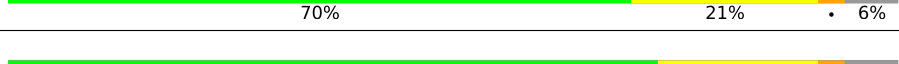
The reported resolution of this entry is 2.85 Å.

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))
$R_{free}$	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	357	 69% 23% • 6%
1	B	357	 71% 21% • 6%
1	C	357	 % 74% 17% • 6%
1	D	357	 70% 21% • 6%
1	E	357	 73% 18% • 6%

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Mol	Chain	Length	Quality of chain
1	F	357	 70% 20% 6%

## 2 Entry composition [i](#)

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-acylglucosamine N-acyltransferase.

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

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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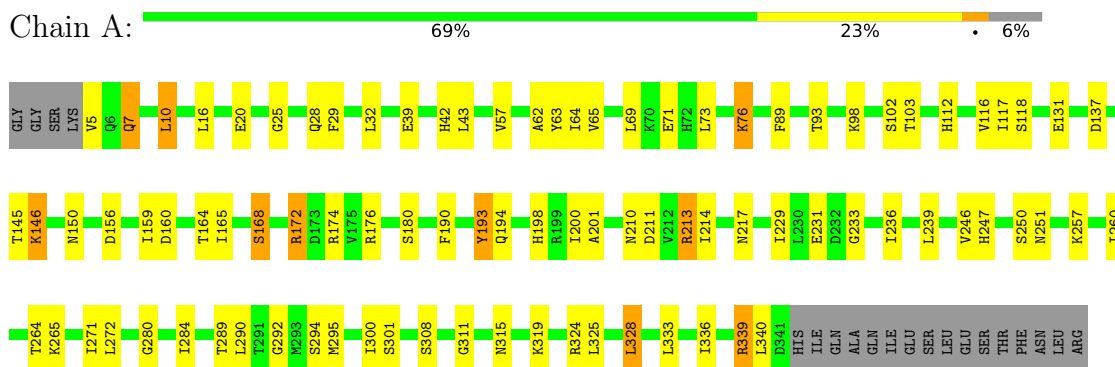
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Chain	Residue	Modelled	Actual	Comment	Reference
F	3	SER	-	expression tag	UNP B0VMV2

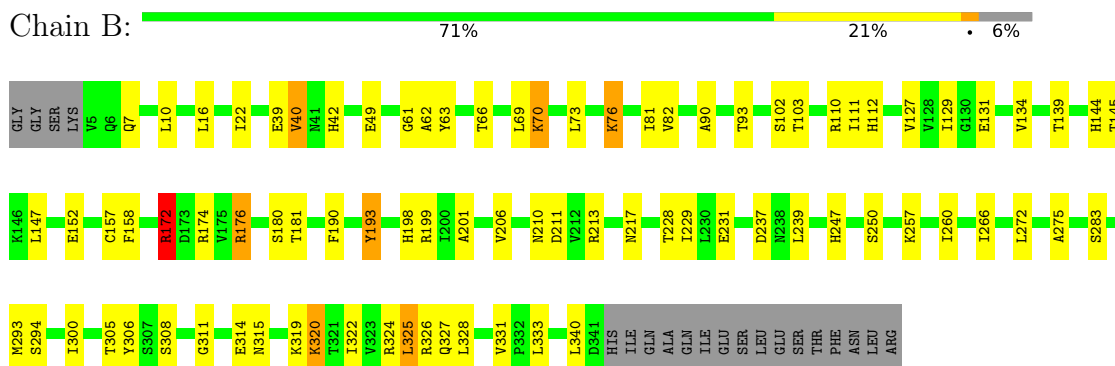
### 3 Residue-property plots [i](#)

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.

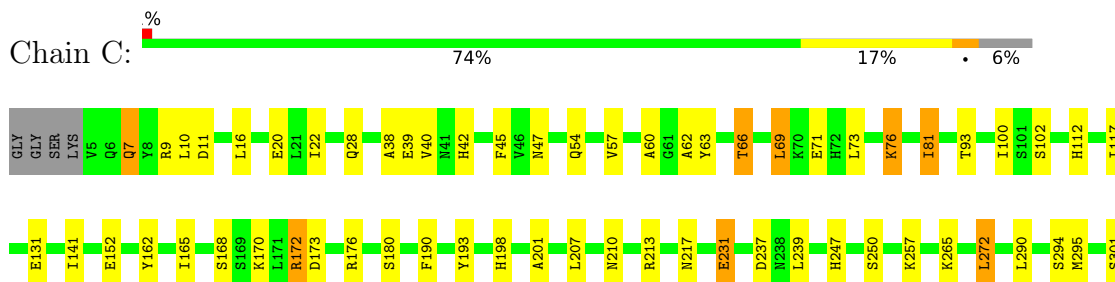
- Molecule 1: UDP-3-O-acylglucosamine N-acyltransferase

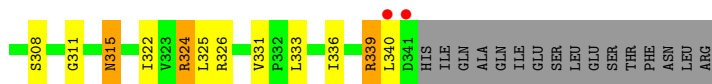


- Molecule 1: UDP-3-O-acylglucosamine N-acyltransferase

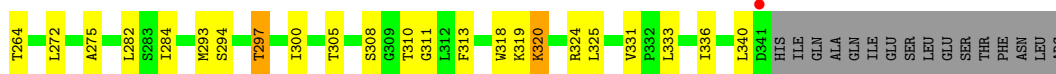
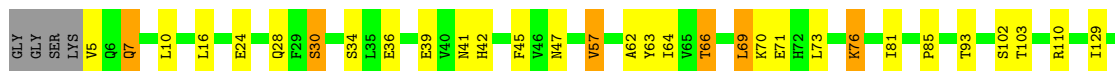


- Molecule 1: UDP-3-O-acylglucosamine N-acyltransferase

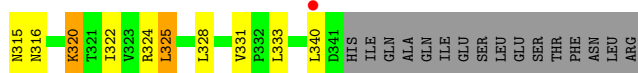
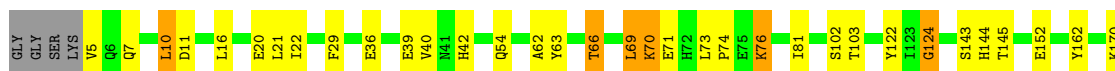




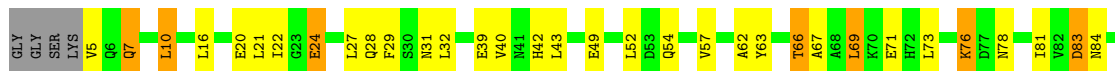
• Molecule 1: UDP-3-O-acylglucosamine N-acyltransferase



• 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 48.15 – 2.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.15-2.85) 98.5 (48.15-2.85)	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)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.234 , 0.280 0.223 , 0.267	Depositor DCC
$R_{free}$ test set	4744 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.8	Xtrriage
Anisotropy	0.102	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 11.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
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	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15088	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage'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 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	0.75	1/2552 (0.0%)	0.99	3/3467 (0.1%)
1	B	0.76	0/2554	0.99	4/3469 (0.1%)
1	C	0.78	0/2554	0.99	3/3469 (0.1%)
1	D	0.75	0/2554	0.97	5/3469 (0.1%)
1	E	0.75	0/2554	1.00	1/3469 (0.0%)
1	F	0.75	0/2554	1.02	1/3469 (0.0%)
All	All	0.75	1/15322 (0.0%)	0.99	17/20812 (0.1%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	VAL	CA-CB	5.12	1.59	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	310	THR	N-CA-C	-7.50	98.84	110.17
1	C	100	ILE	N-CA-C	6.31	112.96	106.21
1	B	315	ASN	N-CA-C	6.07	117.89	111.28
1	B	229	ILE	N-CA-C	5.88	116.33	107.75
1	A	280	GLY	N-CA-C	5.76	118.67	112.33
1	B	314	GLU	N-CA-C	-5.74	102.55	110.35
1	E	124	GLY	N-CA-C	5.71	118.61	112.33
1	D	57	VAL	CB-CA-C	5.69	116.23	110.65
1	C	250	SER	N-CA-C	5.43	117.96	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	LYS	N-CA-C	5.41	118.22	109.40
1	B	102	SER	N-CA-C	5.35	117.63	110.35
1	D	248	ILE	CA-C-N	5.35	125.06	119.92
1	D	248	ILE	C-N-CA	5.35	125.06	119.92
1	D	249	GLY	N-CA-C	5.12	117.35	111.36
1	C	315	ASN	N-CA-C	5.09	116.51	111.07
1	F	179	SER	N-CA-C	5.01	117.31	110.24
1	A	315	ASN	N-CA-C	5.00	116.73	111.28

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 [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	2513	0	2470	50	0
1	B	2515	0	2477	53	0
1	C	2515	0	2477	48	0
1	D	2515	0	2477	52	0
1	E	2515	0	2477	45	0
1	F	2515	0	2477	54	0
All	All	15088	0	14855	259	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 9.

All (259) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH21	1:F:339:ARG:CG	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:HH21	1:F:339:ARG:HG3	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:GLU:H	1:C:42:HIS:CD2	2.16	0.63
1:B:62:ALA:C	1:B:63:TYR:CD1	2.78	0.62
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:HD1	1:D:193:TYR:H	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
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:N	1:D:193:TYR:HD1	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:A:62:ALA:C	1:A:63:TYR:CD1	2.86	0.54
1:F:62:ALA:C	1:F:63:TYR:CD1	2.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:TYR:O	1:E:180:SER:HA	2.08	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:D:219:SER:HG	1:E:216:SER:HG	1.54	0.53
1:B:39:GLU:H	1:B:42:HIS:CD2	2.26	0.53
1:A:339:ARG:CG	1:A:339:ARG:NH2	2.72	0.52
1:F:83:ASP:OD2	1:F:83:ASP:N	2.41	0.52
1:D:39:GLU:H	1:D:42:HIS:CD2	2.27	0.52
1:D:257:LYS:HE2	1:F:257:LYS:O	2.09	0.52
1:C:66:THR:HG22	1:C:69:LEU:HB2	1.92	0.52
1:B:63:TYR:CD1	1:B:63:TYR:N	2.78	0.52
1:B:112:HIS:CE1	1:B:131:GLU:HG2	2.44	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
1:E:250:SER:HB2	1:E:268:LYS:HG2	1.91	0.51
1:D:144:HIS:O	1:E:162:TYR:OH	2.22	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:HG3	1:F:339:ARG:NH2	2.22	0.51
1:A:339:ARG:NH2	1:A:339:ARG:HG3	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:HH21	1:A:339:ARG:HG3	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:E:62:ALA:C	1:E:63:TYR:CD1	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:62:ALA:C	1:C:63:TYR:CD1	2.91	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: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
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: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:145:THR:OG1	1:A:160:ASP:O	2.32	0.47
1:A:233:GLY:O	1:A:251:ASN:HA	2.15	0.47
1:E:320:LYS:HB2	1:E:320:LYS:HE3	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:LYS:HE3	1:D:320:LYS:HB2	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:B:190:PHE:CE2	1:B:199:ARG:HG3	2.50	0.45
1:D:145:THR:OG1	1:D:160:ASP:O	2.34	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:69:LEU:O	1:B:70:LYS:C	2.60	0.45
1:B:144:HIS:O	1:C:162:TYR:OH	2.28	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:282:LEU:HD11	1:D:297:THR:C	2.42	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:D:45:PHE:CE1	1:D:47:ASN:HB2	2.52	0.44
1:D:63:TYR:CD1	1:D:63:TYR:N	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
1:C:66:THR:HG22	1:C:69:LEU:N	2.32	0.44
1:C:172:ARG:HB3	1:C:210:ASN:OD1	2.17	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:A:93:THR:CB	1:C:201:ALA:HB3	2.46	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: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:39:GLU:N	1:F:42:HIS:HD2	2.11	0.43
1:F:275:ALA:O	1:F:293:MET:HA	2.18	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:38:ALA:CB	1:C:60:ALA:HB2	2.49	0.43
1:C:213:ARG:HH21	1:C:237:ASP:HA	1.84	0.43
1:E:322:ILE:HA	1:E:325:LEU:HB2	2.00	0.43
1:C:112:HIS:CE1	1:C:131:GLU:HG2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:D:110:ARG:HD3	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:E:74:PRO:C	1:E:76:LYS:H	2.28	0.42
1:F:159:ILE:HD13	1:F:165:ILE:CD1	2.46	0.42
1:A:10:LEU:HG	1:A:29:PHE:HE2	1.84	0.42
1:A:156:ASP:O	1:A:174:ARG:HA	2.20	0.42
1:F:20:GLU:HB3	1:F:81:ILE:HB	2.02	0.42
1:D:69:LEU:O	1:D:70:LYS:C	2.62	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
1:F:63:TYR:CE1	1:F:76:LYS:CG	3.03	0.42
1:D:62:ALA:C	1:D:63:TYR:CD1	2.98	0.41
1:B:174:ARG:HE	1:B:211:ASP:CG	2.28	0.41
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:39:GLU:N	1:A:42:HIS:HD2	2.06	0.41
1:A:217:ASN:ND2	1:C:217:ASN:HD22	2.17	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:A:292:GLY:HA3	1:C:295:MET:HE2	2.02	0.41
1:D:66:THR:HG22	1:D:69:LEU:HB2	2.03	0.41
1:D:229:ILE:CB	1:D:247:HIS:HD2	2.32	0.41
1:E:70:LYS:O	1:E:70:LYS:HG2	2.21	0.41
1:B:300:ILE:HG21	1:B:306:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:ALA:O	1:D:293:MET:HA	2.21	0.41
1:F:67:ALA:C	1:F:69:LEU:H	2.29	0.41
1:B:311:GLY:HA3	1:C:326:ARG:NH1	2.35	0.40
1:C:217:ASN:O	1:C:239:LEU:HA	2.21	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: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%)	21	38
1	B	335/357 (94%)	313 (93%)	21 (6%)	1 (0%)	36	54
1	C	335/357 (94%)	310 (92%)	24 (7%)	1 (0%)	36	54
1	D	335/357 (94%)	311 (93%)	21 (6%)	3 (1%)	14	28
1	E	335/357 (94%)	320 (96%)	14 (4%)	1 (0%)	36	54
1	F	335/357 (94%)	314 (94%)	18 (5%)	3 (1%)	14	28
All	All	2010/2142 (94%)	1886 (94%)	113 (6%)	11 (0%)	24	42

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	172	ARG

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Mol	Chain	Res	Type
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 [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	267/295 (90%)	233 (87%)	34 (13%)	4 8
1	B	268/295 (91%)	244 (91%)	24 (9%)	9 19
1	C	268/295 (91%)	240 (90%)	28 (10%)	7 14
1	D	268/295 (91%)	236 (88%)	32 (12%)	5 10
1	E	268/295 (91%)	242 (90%)	26 (10%)	8 17
1	F	268/295 (91%)	233 (87%)	35 (13%)	4 7
All	All	1607/1770 (91%)	1428 (89%)	179 (11%)	6 12

All (179) 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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	71	GLU
1	A	73	LEU
1	A	76	LYS
1	A	102	SER
1	A	103	THR
1	A	117	ILE
1	A	168	SER
1	A	172	ARG
1	A	176	ARG
1	A	193	TYR
1	A	194	GLN
1	A	213	ARG
1	A	231	GLU
1	A	250	SER
1	A	264	THR
1	A	265	LYS
1	A	272	LEU
1	A	290	LEU
1	A	301	SER
1	A	319	LYS
1	A	324	ARG
1	A	325	LEU
1	A	328	LEU
1	A	336	ILE
1	A	339	ARG
1	A	340	LEU
1	B	7	GLN
1	B	10	LEU
1	B	16	LEU
1	B	40	VAL
1	B	49	GLU
1	B	70	LYS
1	B	73	LEU
1	B	76	LYS
1	B	82	VAL
1	B	103	THR
1	B	110	ARG
1	B	172	ARG
1	B	176	ARG
1	B	180	SER
1	B	181	THR
1	B	193	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	250	SER
1	B	272	LEU
1	B	283	SER
1	B	319	LYS
1	B	320	LYS
1	B	325	LEU
1	B	333	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	57	VAL
1	C	66	THR
1	C	69	LEU
1	C	71	GLU
1	C	73	LEU
1	C	76	LYS
1	C	81	ILE
1	C	102	SER
1	C	117	ILE
1	C	141	ILE
1	C	165	ILE
1	C	168	SER
1	C	176	ARG
1	C	207	LEU
1	C	231	GLU
1	C	265	LYS
1	C	272	LEU
1	C	301	SER
1	C	324	ARG
1	C	325	LEU
1	C	339	ARG
1	C	340	LEU
1	D	5	VAL
1	D	7	GLN
1	D	10	LEU
1	D	16	LEU
1	D	30	SER
1	D	57	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	66	THR
1	D	69	LEU
1	D	71	GLU
1	D	73	LEU
1	D	76	LYS
1	D	81	ILE
1	D	102	SER
1	D	103	THR
1	D	146	LYS
1	D	147	LEU
1	D	159	ILE
1	D	168	SER
1	D	176	ARG
1	D	193	TYR
1	D	207	LEU
1	D	220	ILE
1	D	231	GLU
1	D	264	THR
1	D	272	LEU
1	D	297	THR
1	D	319	LYS
1	D	320	LYS
1	D	324	ARG
1	D	325	LEU
1	D	336	ILE
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	145	THR
1	E	172	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	176	ARG
1	E	179	SER
1	E	181	THR
1	E	207	LEU
1	E	213	ARG
1	E	272	LEU
1	E	320	LYS
1	E	324	ARG
1	E	325	LEU
1	E	340	LEU
1	F	5	VAL
1	F	7	GLN
1	F	10	LEU
1	F	16	LEU
1	F	40	VAL
1	F	49	GLU
1	F	52	LEU
1	F	54	GLN
1	F	57	VAL
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	87	LEU
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	231	GLU
1	F	272	LEU
1	F	283	SER
1	F	320	LYS
1	F	324	ARG
1	F	325	LEU

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Mol	Chain	Res	Type
1	F	336	ILE
1	F	339	ARG
1	F	340	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) 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	217	ASN
1	A	247	HIS
1	B	6	GLN
1	B	28	GLN
1	B	42	HIS
1	B	47	ASN
1	B	138	ASN
1	B	194	GLN
1	B	247	HIS
1	C	42	HIS
1	C	47	ASN
1	C	51	HIS
1	C	84	ASN
1	C	132	ASN
1	C	150	ASN
1	C	217	ASN
1	C	227	ASN
1	C	247	HIS
1	C	251	ASN
1	D	28	GLN
1	D	41	ASN
1	D	42	HIS
1	D	47	ASN
1	D	54	GLN
1	D	72	HIS
1	D	138	ASN
1	D	202	GLN
1	D	217	ASN
1	D	227	ASN
1	D	247	HIS
1	D	327	GLN

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Mol	Chain	Res	Type
1	E	28	GLN
1	E	42	HIS
1	E	47	ASN
1	E	78	ASN
1	E	217	ASN
1	E	247	HIS
1	E	251	ASN
1	F	28	GLN
1	F	42	HIS
1	F	47	ASN
1	F	54	GLN
1	F	78	ASN
1	F	84	ASN
1	F	198	HIS
1	F	251	ASN
1	F	327	GLN

### 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 [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%)	-1.47	0 <a href="#">100</a> <a href="#">100</a>	26, 52, 82, 120	0
1	B	337/357 (94%)	-1.46	0 <a href="#">100</a> <a href="#">100</a>	33, 48, 79, 116	0
1	C	337/357 (94%)	-1.41	2 (0%) <a href="#">85</a> <a href="#">82</a>	31, 48, 74, 114	0
1	D	337/357 (94%)	-1.40	1 (0%) <a href="#">90</a> <a href="#">89</a>	32, 51, 83, 124	0
1	E	337/357 (94%)	-1.49	1 (0%) <a href="#">90</a> <a href="#">89</a>	29, 47, 75, 115	0
1	F	337/357 (94%)	-1.46	1 (0%) <a href="#">90</a> <a href="#">89</a>	28, 48, 76, 117	0
All	All	2022/2142 (94%)	-1.45	5 (0%) <a href="#">91</a> <a href="#">91</a>	26, 49, 79, 124	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	341	ASP	3.3
1	D	341	ASP	3.0
1	C	341	ASP	2.8
1	C	340	LEU	2.5
1	E	340	LEU	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 oligosaccharides 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.