



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 11:03 PM EDT

PDB ID : 3NY0  
Title : Crystal Structure of UreE from Helicobacter pylori (Ni<sup>2+</sup> bound form)  
Authors : Shi, R.; Munger, C.; Assinas, A.; Matte, A.; Cygler, M.; Montreal-Kingston  
Bacterial Structural Genomics Initiative (BSGI)  
Deposited on : unknown  
Resolution : 3.09 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.

---

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	:	rb-20030345
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)	:	rb-20030345

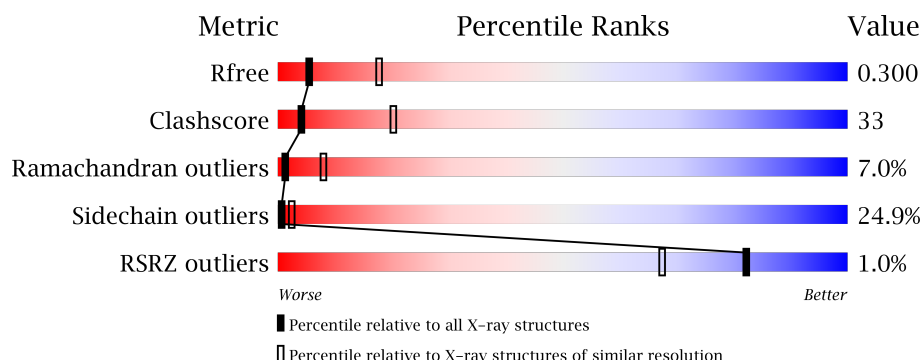
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.09 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	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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	170	
1	B	170	
1	C	170	
1	D	170	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4774 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 Urease accessory protein ureE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	0	0
			1180	756	206	217	1			
1	B	153	Total	C	N	O	S	0	0	0
			1217	777	214	225	1			
1	C	148	Total	C	N	O	S	0	0	0
			1190	761	207	221	1			
1	D	148	Total	C	N	O	S	0	0	0
			1186	759	207	219	1			

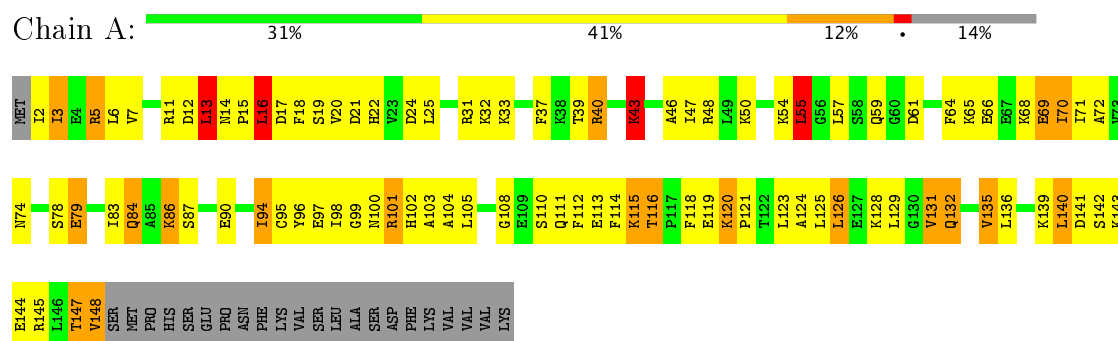
- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ni	0	0
			1	1		

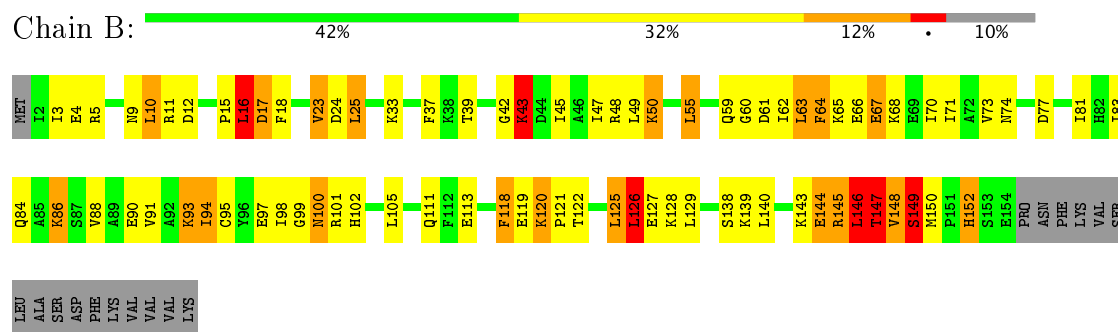
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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.

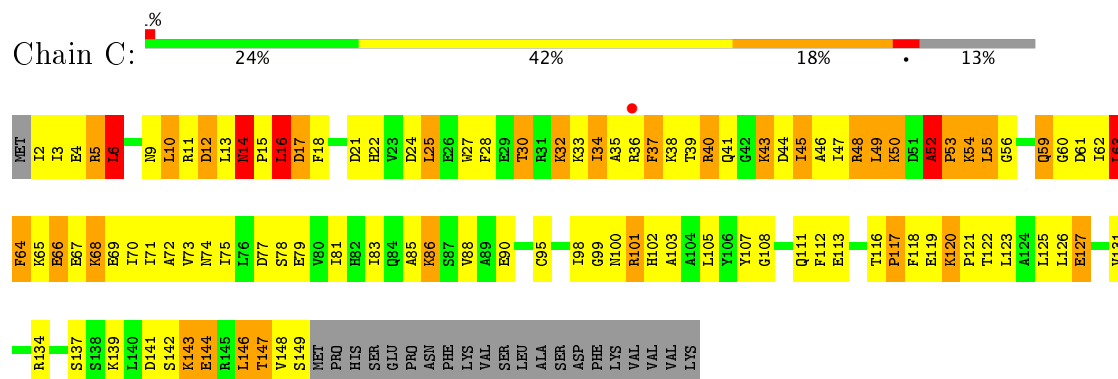
#### • Molecule 1: Urease accessory protein ureE



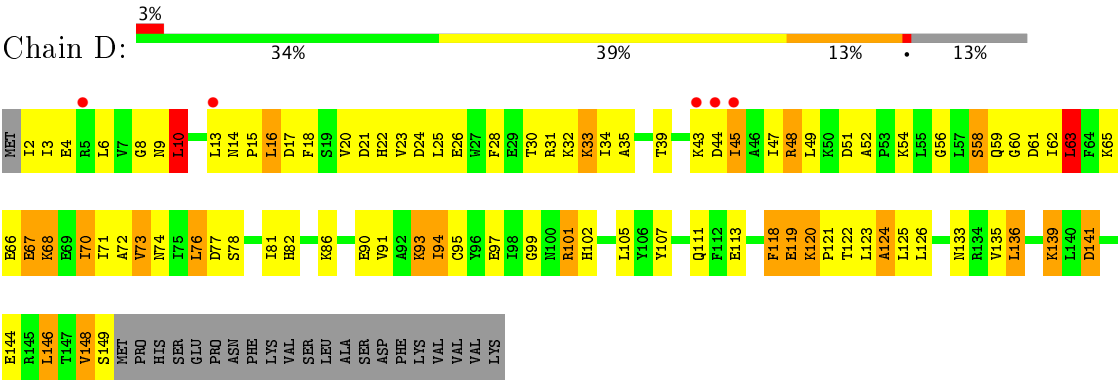
#### • Molecule 1: Urease accessory protein ureE



#### • Molecule 1: Urease accessory protein ureE



#### • Molecule 1: Urease accessory protein ureE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.06 Å 91.06 Å 202.82 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.63 – 3.09 46.63 – 3.09	Depositor EDS
% Data completeness (in resolution range)	86.0 (46.63-3.09) 86.0 (46.63-3.09)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 3.06 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.245 , 0.299 0.240 , 0.300	Depositor DCC
$R_{free}$ test set	695 reflections (5.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.8	Xtriage
Anisotropy	0.738	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 60.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4774	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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

Bond lengths and bond angles in the following residue types are not validated in this section: NI

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	0.85	1/1198 (0.1%)	1.00	5/1611 (0.3%)
1	B	0.82	0/1237	1.01	4/1665 (0.2%)
1	C	0.94	1/1208 (0.1%)	1.09	4/1624 (0.2%)
1	D	0.84	1/1204 (0.1%)	0.89	4/1619 (0.2%)
All	All	0.86	3/4847 (0.1%)	1.00	17/6519 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	2
1	D	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	95	CYS	CB-SG	-7.52	1.69	1.82
1	C	95	CYS	CB-SG	-5.97	1.72	1.81
1	A	95	CYS	CB-SG	-5.54	1.72	1.81

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	48	ARG	NE-CZ-NH1	-8.95	115.83	120.30
1	D	95	CYS	CA-CB-SG	-7.23	100.99	114.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	LEU	CA-CB-CG	-6.99	99.23	115.30
1	D	6	LEU	CA-CB-CG	6.86	131.09	115.30
1	A	140	LEU	CA-CB-CG	6.14	129.43	115.30
1	A	95	CYS	CA-CB-SG	-6.10	103.02	114.00
1	A	14	ASN	N-CA-C	5.83	126.75	111.00
1	B	25	LEU	CA-CB-CG	-5.55	102.53	115.30
1	C	6	LEU	CA-CB-CG	5.52	127.99	115.30
1	B	140	LEU	CA-CB-CG	5.43	127.78	115.30
1	C	63	LEU	CA-CB-CG	5.38	127.68	115.30
1	C	146	LEU	CA-CB-CG	5.38	127.67	115.30
1	B	23	VAL	CB-CA-C	-5.28	101.36	111.40
1	A	94	ILE	CB-CA-C	-5.27	101.07	111.60
1	B	126	LEU	CA-CB-CG	-5.19	103.36	115.30
1	D	136	LEU	CA-CB-CG	5.19	127.23	115.30
1	D	105	LEU	CA-CB-CG	5.15	127.14	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	LEU	Peptide
1	B	147	THR	Peptide
1	B	149	SER	Peptide
1	C	5	ARG	Peptide
1	C	52	ALA	Peptide
1	D	146	LEU	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	1180	0	1219	81	1
1	B	1217	0	1240	73	1
1	C	1190	0	1228	103	1
1	D	1186	0	1224	78	0
2	B	1	0	0	0	0
All	All	4774	0	4911	317	2



The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (317) 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:32:LYS:HE3	1:C:32:LYS:H	1.16	1.10
1:A:126:LEU:HD22	1:A:131:VAL:CG2	1.82	1.09
1:D:3:ILE:HD12	1:D:45:ILE:HG21	1.29	1.09
1:C:49:LEU:HD13	1:C:52:ALA:HA	1.35	1.08
1:A:84:GLN:HA	1:A:84:GLN:HE21	1.12	1.07
1:C:10:LEU:H	1:C:62:ILE:HD11	0.91	1.06
1:C:24:ASP:OD1	1:C:74:ASN:HB3	1.57	1.05
1:A:5:ARG:HH21	1:A:50:LYS:HB2	1.21	1.04
1:C:45:ILE:HD12	1:C:47:ILE:HG23	1.40	1.03
1:C:10:LEU:N	1:C:62:ILE:HD11	1.77	0.97
1:D:2:ILE:HG21	1:D:48:ARG:HG2	1.47	0.94
1:A:84:GLN:NE2	1:A:84:GLN:HA	1.80	0.94
1:B:25:LEU:HD12	1:B:73:VAL:CG1	1.97	0.93
1:B:59:GLN:HE22	1:B:74:ASN:HA	1.35	0.91
1:A:126:LEU:HD22	1:A:131:VAL:HG21	1.53	0.91
1:D:3:ILE:CD1	1:D:45:ILE:HG21	2.01	0.90
1:B:55:LEU:HD12	1:B:55:LEU:H	1.33	0.90
1:D:3:ILE:HG21	1:D:63:LEU:HD23	1.55	0.89
1:C:98:ILE:HD13	1:C:105:LEU:HD13	1.56	0.88
1:B:25:LEU:HD12	1:B:73:VAL:HG13	1.55	0.88
1:A:126:LEU:HD22	1:A:131:VAL:HG23	1.52	0.88
1:A:84:GLN:CA	1:A:84:GLN:HE21	1.88	0.86
1:C:63:LEU:HD23	1:C:72:ALA:HA	1.56	0.86
1:D:16:LEU:HA	1:D:17:ASP:HB2	1.58	0.86
1:C:143:LYS:O	1:C:143:LYS:HG3	1.73	0.85
1:C:3:ILE:HB	1:C:47:ILE:HG22	1.56	0.84
1:B:24:ASP:OD1	1:B:74:ASN:HB3	1.81	0.81
1:D:13:LEU:HA	1:D:14:ASN:HB2	1.63	0.80
1:C:16:LEU:N	1:C:17:ASP:HB2	1.97	0.80
1:C:16:LEU:HA	1:C:17:ASP:HB3	1.63	0.80
1:D:101:ARG:O	1:D:102:HIS:HB2	1.80	0.80
1:C:49:LEU:HD13	1:C:52:ALA:CA	2.12	0.79
1:A:79:GLU:OE2	1:A:79:GLU:HA	1.80	0.79
1:B:100:ASN:OD1	1:C:99:GLY:O	2.02	0.78
1:D:107:TYR:CZ	1:D:146:LEU:HD21	2.19	0.77
1:A:110:SER:OG	1:A:111:GLN:N	2.15	0.77
1:A:118:PHE:HD2	1:A:135:VAL:HG11	1.50	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:LEU:HA	1:C:17:ASP:CB	2.13	0.77
1:C:63:LEU:CD2	1:C:72:ALA:HA	2.15	0.76
1:D:24:ASP:HB3	1:D:76:LEU:HD21	1.68	0.76
1:C:32:LYS:HE3	1:C:32:LYS:N	1.98	0.76
1:A:145:ARG:HH22	1:A:148:VAL:HG22	1.51	0.76
1:C:10:LEU:H	1:C:62:ILE:CD1	1.86	0.76
1:C:16:LEU:CA	1:C:17:ASP:CB	2.64	0.75
1:A:24:ASP:OD1	1:A:74:ASN:HB3	1.87	0.74
1:D:2:ILE:HG21	1:D:48:ARG:CG	2.18	0.74
1:B:128:LYS:HE2	1:C:149:SER:HB3	1.69	0.74
1:C:83:ILE:O	1:C:113:GLU:HA	1.89	0.73
1:A:96:TYR:CE1	1:D:99:GLY:HA2	2.24	0.73
1:C:27:TRP:O	1:C:30:THR:HG23	1.89	0.72
1:B:81:ILE:CD1	1:B:118:PHE:HA	2.19	0.72
1:A:96:TYR:CD1	1:D:99:GLY:CA	2.72	0.72
1:B:90:GLU:O	1:B:94:ILE:HD12	1.89	0.71
1:B:147:THR:HB	1:B:148:VAL:O	1.91	0.71
1:C:45:ILE:HD12	1:C:47:ILE:CG2	2.17	0.70
1:A:118:PHE:CD2	1:A:135:VAL:HG11	2.25	0.70
1:B:37:PHE:HB2	1:B:45:ILE:CG2	2.22	0.70
1:C:25:LEU:CD2	1:C:37:PHE:CE1	2.76	0.69
1:D:34:ILE:HG12	1:D:48:ARG:HH11	1.56	0.69
1:A:96:TYR:CD1	1:D:99:GLY:HA2	2.27	0.69
1:D:65:LYS:HE3	1:D:70:ILE:HD11	1.75	0.68
1:B:3:ILE:HG21	1:B:63:LEU:CD2	2.24	0.68
1:B:3:ILE:HG21	1:B:63:LEU:HD23	1.75	0.68
1:B:86:LYS:N	1:B:90:GLU:OE2	2.28	0.67
1:C:3:ILE:HD13	1:C:45:ILE:HD11	1.76	0.67
1:C:49:LEU:CD1	1:C:52:ALA:HA	2.20	0.67
1:A:39:THR:OG1	1:A:43:LYS:HB2	1.94	0.67
1:D:21:ASP:O	1:D:71:ILE:HA	1.94	0.67
1:B:90:GLU:O	1:B:94:ILE:CD1	2.43	0.67
1:B:81:ILE:HD11	1:B:118:PHE:HA	1.77	0.67
1:C:12:ASP:O	1:C:14:ASN:HB2	1.96	0.66
1:B:144:GLU:HA	1:B:144:GLU:OE2	1.95	0.66
1:A:5:ARG:NH2	1:A:50:LYS:HB2	2.04	0.66
1:B:9:ASN:HB3	1:B:11:ARG:HG2	1.77	0.66
1:B:64:PHE:HB3	1:B:71:ILE:HB	1.77	0.66
1:D:16:LEU:HA	1:D:17:ASP:CB	2.21	0.66
1:B:147:THR:O	1:B:148:VAL:CB	2.44	0.65
1:C:6:LEU:HD21	1:C:61:ASP:CG	2.16	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:PHE:HD1	1:C:68:LYS:HA	1.61	0.64
1:C:45:ILE:CD1	1:C:47:ILE:HG23	2.24	0.64
1:A:84:GLN:NE2	1:A:112:PHE:O	2.30	0.64
1:D:81:ILE:HD11	1:D:118:PHE:HA	1.79	0.64
1:B:120:LYS:N	1:B:121:PRO:HD2	2.13	0.63
1:C:37:PHE:O	1:C:44:ASP:HA	1.99	0.63
1:D:33:LYS:HA	1:D:49:LEU:HD12	1.79	0.63
1:C:14:ASN:N	1:C:15:PRO:HD3	2.14	0.63
1:C:65:LYS:HG3	1:C:70:ILE:HD11	1.82	0.62
1:A:21:ASP:O	1:A:71:ILE:HA	2.00	0.62
1:C:107:TYR:HB2	1:C:144:GLU:HG3	1.81	0.62
1:B:148:VAL:CB	1:B:149:SER:O	2.48	0.62
1:B:145:ARG:O	1:B:146:LEU:HB2	1.99	0.62
1:D:3:ILE:HD12	1:D:45:ILE:CG2	2.17	0.61
1:B:37:PHE:HB2	1:B:45:ILE:HG23	1.82	0.61
1:C:86:LYS:HG2	1:C:90:GLU:OE2	2.01	0.61
1:A:64:PHE:O	1:A:70:ILE:HA	2.00	0.61
1:A:97:GLU:OE2	1:D:148:VAL:HA	2.00	0.61
1:B:118:PHE:C	1:B:118:PHE:CD1	2.73	0.61
1:C:17:ASP:HB3	1:C:18:PHE:CD2	2.35	0.60
1:C:16:LEU:N	1:C:17:ASP:CB	2.64	0.60
1:C:32:LYS:CE	1:C:32:LYS:H	2.04	0.60
1:D:77:ASP:OD1	1:D:139:LYS:HE2	2.00	0.60
1:A:145:ARG:NH2	1:A:148:VAL:HG22	2.17	0.60
1:C:98:ILE:HG23	1:C:103:ALA:HB3	1.84	0.60
1:C:9:ASN:HA	1:C:62:ILE:HG13	1.84	0.59
1:C:141:ASP:O	1:C:144:GLU:N	2.35	0.59
1:A:126:LEU:CD2	1:A:131:VAL:HG21	2.30	0.59
1:C:66:GLU:O	1:C:69:GLU:HB3	2.03	0.59
1:C:36:ARG:HG2	1:C:37:PHE:H	1.67	0.58
1:A:20:VAL:HG13	1:A:70:ILE:CG2	2.33	0.58
1:C:3:ILE:H	1:C:47:ILE:HA	1.68	0.58
1:C:21:ASP:O	1:C:71:ILE:HA	2.02	0.58
1:D:35:ALA:O	1:D:47:ILE:HG12	2.03	0.58
1:D:49:LEU:HD22	1:D:52:ALA:HB2	1.85	0.58
1:D:23:VAL:HG22	1:D:39:THR:HG22	1.85	0.58
1:C:16:LEU:CA	1:C:17:ASP:HB2	2.33	0.58
1:D:3:ILE:CG2	1:D:63:LEU:HD23	2.30	0.57
1:B:98:ILE:HG21	1:B:105:LEU:HD13	1.86	0.57
1:A:16:LEU:HA	1:A:18:PHE:H	1.68	0.57
1:A:57:LEU:O	1:A:142:SER:OG	2.21	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LYS:N	1:A:121:PRO:HD2	2.19	0.56
1:A:12:ASP:O	1:A:13:LEU:O	2.23	0.56
1:D:91:VAL:O	1:D:94:ILE:HB	2.05	0.56
1:A:11:ARG:HG3	1:A:12:ASP:N	2.20	0.56
1:A:84:GLN:HB3	1:A:132:GLN:HB3	1.87	0.56
1:A:11:ARG:CG	1:A:12:ASP:N	2.68	0.56
1:D:118:PHE:C	1:D:118:PHE:CD1	2.78	0.56
1:C:101:ARG:HH21	1:C:121:PRO:HB2	1.71	0.55
1:C:49:LEU:HB3	1:C:52:ALA:HB2	1.88	0.55
1:B:15:PRO:C	1:B:16:LEU:HD12	2.27	0.55
1:B:122:THR:O	1:B:126:LEU:HD12	2.05	0.55
1:B:93:LYS:HE3	1:C:147:THR:OG1	2.07	0.55
1:D:24:ASP:HB3	1:D:76:LEU:CD2	2.35	0.55
1:B:125:LEU:HA	1:B:128:LYS:HB3	1.89	0.55
1:C:59:GLN:HE22	1:C:74:ASN:HA	1.72	0.55
1:A:96:TYR:CD1	1:D:99:GLY:HA3	2.42	0.55
1:C:118:PHE:C	1:C:118:PHE:CD1	2.80	0.55
1:A:147:THR:HG22	1:D:93:LYS:HE3	1.89	0.54
1:A:59:GLN:NE2	1:A:74:ASN:OD1	2.38	0.54
1:A:99:GLY:O	1:A:100:ASN:C	2.42	0.54
1:A:121:PRO:O	1:A:124:ALA:HB3	2.07	0.54
1:B:118:PHE:O	1:B:118:PHE:CD1	2.61	0.54
1:C:122:THR:O	1:C:125:LEU:HB3	2.08	0.54
1:C:120:LYS:N	1:C:121:PRO:HD2	2.23	0.54
1:C:59:GLN:HE22	1:C:75:ILE:H	1.56	0.54
1:A:135:VAL:O	1:A:136:LEU:HD23	2.08	0.53
1:C:33:LYS:HG3	1:C:52:ALA:HB2	1.90	0.53
1:C:53:PRO:O	1:C:54:LYS:C	2.46	0.53
1:A:3:ILE:CD1	1:A:3:ILE:N	2.71	0.53
1:A:126:LEU:CD2	1:A:131:VAL:CG2	2.71	0.53
1:A:33:LYS:O	1:A:47:ILE:HD12	2.09	0.53
1:A:86:LYS:HG3	1:A:87:SER:N	2.23	0.53
1:A:90:GLU:O	1:A:94:ILE:HD12	2.09	0.53
1:C:13:LEU:HA	1:C:14:ASN:CB	2.39	0.53
1:B:81:ILE:HD12	1:B:118:PHE:HA	1.90	0.52
1:D:9:ASN:HA	1:D:60:GLY:O	2.09	0.52
1:C:98:ILE:CD1	1:C:105:LEU:HD13	2.34	0.52
1:C:25:LEU:CD2	1:C:37:PHE:HE1	2.22	0.52
1:A:83:ILE:O	1:A:113:GLU:HA	2.09	0.52
1:A:104:ALA:O	1:A:116:THR:HB	2.08	0.52
1:D:13:LEU:HA	1:D:14:ASN:CB	2.34	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:LEU:HA	1:B:18:PHE:N	2.25	0.51
1:A:124:ALA:O	1:A:125:LEU:C	2.48	0.51
1:A:20:VAL:HG13	1:A:70:ILE:HG22	1.93	0.51
1:B:10:LEU:HG	1:B:60:GLY:O	2.11	0.51
1:B:62:ILE:HG21	1:B:65:LYS:HB2	1.92	0.51
1:C:25:LEU:HD23	1:C:37:PHE:CE1	2.46	0.51
1:B:25:LEU:CD1	1:B:73:VAL:HG13	2.33	0.51
1:B:94:ILE:HG22	1:B:95:CYS:N	2.24	0.51
1:A:65:LYS:HG3	1:A:70:ILE:HD12	1.92	0.50
1:B:47:ILE:HB	1:B:49:LEU:CD2	2.41	0.50
1:B:94:ILE:HD12	1:B:94:ILE:H	1.76	0.50
1:B:37:PHE:HB2	1:B:45:ILE:HG22	1.93	0.50
1:C:123:LEU:O	1:C:126:LEU:N	2.44	0.50
1:A:128:LYS:NZ	1:D:149:SER:HB3	2.26	0.50
1:B:86:LYS:HG2	1:B:90:GLU:OE2	2.11	0.50
1:C:105:LEU:HD12	1:C:116:THR:HB	1.94	0.50
1:A:2:ILE:HD12	1:A:46:ALA:HB3	1.92	0.50
1:C:62:ILE:HA	1:C:72:ALA:HB2	1.94	0.50
1:B:99:GLY:O	1:C:100:ASN:HA	2.12	0.49
1:C:3:ILE:O	1:C:48:ARG:O	2.29	0.49
1:B:100:ASN:O	1:C:102:HIS:HE1	1.96	0.49
1:D:18:PHE:HD1	1:D:68:LYS:HA	1.76	0.49
1:D:33:LYS:O	1:D:34:ILE:HG13	2.12	0.49
1:D:24:ASP:OD1	1:D:74:ASN:HB3	2.12	0.49
1:A:99:GLY:O	1:A:101:ARG:N	2.45	0.49
1:B:55:LEU:CD1	1:B:55:LEU:H	2.06	0.49
1:C:111:GLN:C	1:C:112:PHE:HD1	2.15	0.49
1:C:18:PHE:HB3	1:C:68:LYS:O	2.12	0.49
1:C:48:ARG:HB2	1:C:50:LYS:HZ1	1.78	0.49
1:D:124:ALA:O	1:D:125:LEU:C	2.50	0.49
1:A:61:ASP:O	1:A:72:ALA:HA	2.12	0.49
1:B:149:SER:HA	1:B:150:MET:O	2.12	0.49
1:A:25:LEU:HD21	1:A:37:PHE:CE2	2.47	0.49
1:A:84:GLN:HE22	1:A:112:PHE:C	2.16	0.49
1:C:22:HIS:HD2	1:C:74:ASN:HB2	1.78	0.49
1:C:59:GLN:NE2	1:C:74:ASN:HA	2.28	0.48
1:D:121:PRO:O	1:D:124:ALA:HB3	2.13	0.48
1:B:138:SER:OG	1:B:139:LYS:N	2.47	0.47
1:B:9:ASN:HD22	1:B:61:ASP:CG	2.17	0.47
1:D:120:LYS:HG2	1:D:121:PRO:HD3	1.96	0.47
1:C:9:ASN:ND2	1:C:11:ARG:HH12	2.12	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ARG:CG	1:C:37:PHE:H	2.27	0.47
1:C:90:GLU:OE1	1:C:131:VAL:HG22	2.14	0.47
1:C:3:ILE:CD1	1:C:45:ILE:HD11	2.45	0.47
1:B:9:ASN:O	1:B:62:ILE:HD11	2.15	0.47
1:C:59:GLN:HE21	1:C:59:GLN:HA	1.80	0.47
1:B:64:PHE:C	1:B:64:PHE:CD2	2.87	0.47
1:B:128:LYS:HE2	1:C:149:SER:CB	2.42	0.47
1:C:125:LEU:HD12	1:C:125:LEU:C	2.35	0.47
1:B:105:LEU:HD23	1:B:146:LEU:HG	1.97	0.46
1:B:90:GLU:O	1:B:91:VAL:C	2.53	0.46
1:A:96:TYR:HD1	1:D:99:GLY:CA	2.25	0.46
1:C:17:ASP:HB3	1:C:18:PHE:CE2	2.51	0.46
1:D:31:ARG:HG3	1:D:56:GLY:HA2	1.96	0.46
1:B:25:LEU:HD12	1:B:73:VAL:HG11	1.93	0.46
1:D:44:ASP:O	1:D:45:ILE:HG12	2.16	0.46
1:C:123:LEU:HG	1:C:127:GLU:OE2	2.15	0.46
1:C:112:PHE:CD1	1:C:112:PHE:N	2.84	0.46
1:D:14:ASN:N	1:D:15:PRO:HD3	2.31	0.46
1:D:18:PHE:HB3	1:D:68:LYS:O	2.16	0.46
1:C:22:HIS:HB2	1:C:40:ARG:NH1	2.30	0.46
1:B:102:HIS:NE2	1:C:102:HIS:CE1	2.83	0.45
1:D:82:HIS:CE1	1:D:136:LEU:HD12	2.51	0.45
1:A:98:ILE:HD13	1:A:105:LEU:HD13	1.98	0.45
1:A:11:ARG:CG	1:A:12:ASP:H	2.29	0.45
1:B:119:GLU:HB3	1:B:121:PRO:HD2	1.98	0.45
1:B:88:VAL:HG13	1:C:88:VAL:HG13	1.98	0.45
1:D:23:VAL:HG23	1:D:72:ALA:O	2.16	0.45
1:C:143:LYS:O	1:C:143:LYS:CG	2.57	0.45
1:D:3:ILE:CG1	1:D:45:ILE:HG21	2.47	0.45
1:D:59:GLN:HB3	1:D:141:ASP:OD1	2.17	0.45
1:A:108:GLY:HA3	1:A:113:GLU:HB3	1.99	0.45
1:B:149:SER:HB2	1:C:100:ASN:HD21	1.81	0.45
1:D:16:LEU:HB2	1:D:18:PHE:H	1.81	0.45
1:D:16:LEU:HB2	1:D:18:PHE:O	2.17	0.45
1:A:22:HIS:ND1	1:A:40:ARG:NH1	2.64	0.45
1:A:64:PHE:CE2	1:A:66:GLU:HB2	2.52	0.45
1:C:49:LEU:HD13	1:C:52:ALA:CB	2.47	0.45
1:D:123:LEU:O	1:D:124:ALA:C	2.53	0.45
1:D:25:LEU:HD12	1:D:73:VAL:CG1	2.46	0.45
1:C:34:ILE:HG23	1:C:47:ILE:O	2.17	0.45
1:A:55:LEU:HG	1:A:55:LEU:H	1.28	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:TYR:CE1	1:D:146:LEU:HD21	2.51	0.45
1:A:97:GLU:HG3	1:A:125:LEU:HD21	1.99	0.45
1:A:99:GLY:O	1:A:102:HIS:N	2.44	0.44
1:C:22:HIS:O	1:C:40:ARG:HB2	2.18	0.44
1:D:107:TYR:CZ	1:D:146:LEU:CD2	2.96	0.44
1:C:101:ARG:HH11	1:C:101:ARG:CG	2.30	0.44
1:B:4:GLU:O	1:B:49:LEU:HA	2.17	0.44
1:D:28:PHE:C	1:D:30:THR:H	2.20	0.44
1:A:141:ASP:HB3	1:A:143:LYS:HG2	2.00	0.44
1:B:67:GLU:HB2	1:B:68:LYS:H	1.54	0.44
1:D:81:ILE:CD1	1:D:118:PHE:HA	2.46	0.44
1:D:8:GLY:O	1:D:62:ILE:N	2.38	0.44
1:A:15:PRO:C	1:A:16:LEU:HD12	2.38	0.44
1:A:98:ILE:HG23	1:A:103:ALA:HB3	2.00	0.44
1:C:38:LYS:HA	1:C:43:LYS:O	2.18	0.44
1:C:53:PRO:O	1:C:56:GLY:N	2.40	0.44
1:A:120:LYS:N	1:A:121:PRO:CD	2.81	0.43
1:C:112:PHE:HD1	1:C:112:PHE:N	2.16	0.43
1:A:123:LEU:O	1:A:124:ALA:C	2.56	0.43
1:C:13:LEU:HA	1:C:14:ASN:HB3	2.00	0.43
1:A:83:ILE:N	1:A:114:PHE:O	2.51	0.43
1:B:61:ASP:O	1:B:73:VAL:HG23	2.19	0.43
1:C:141:ASP:OD2	1:C:143:LYS:HB3	2.19	0.43
1:D:45:ILE:HA	1:D:45:ILE:HD13	1.86	0.43
1:D:58:SER:N	1:D:61:ASP:OD1	2.52	0.43
1:A:19:SER:HB3	1:A:69:GLU:OE1	2.19	0.43
1:A:98:ILE:O	1:A:99:GLY:C	2.54	0.43
1:B:39:THR:CG2	1:B:43:LYS:HB2	2.49	0.43
1:C:108:GLY:HA3	1:C:113:GLU:O	2.19	0.43
1:D:48:ARG:O	1:D:49:LEU:HD23	2.19	0.43
1:D:31:ARG:HD3	1:D:54:LYS:O	2.18	0.42
1:D:49:LEU:HA	1:D:49:LEU:HD23	1.75	0.42
1:B:121:PRO:HG2	1:B:122:THR:H	1.85	0.42
1:B:148:VAL:HA	1:B:149:SER:CB	2.49	0.42
1:B:60:GLY:N	1:B:73:VAL:O	2.40	0.42
1:D:119:GLU:HB3	1:D:121:PRO:HD2	2.00	0.42
1:B:64:PHE:C	1:B:64:PHE:HD2	2.22	0.42
1:D:122:THR:CG2	1:D:126:LEU:HD11	2.49	0.42
1:D:146:LEU:HD23	1:D:146:LEU:HA	1.80	0.42
1:B:4:GLU:HA	1:B:48:ARG:O	2.20	0.42
1:D:82:HIS:O	1:D:133:ASN:HA	2.19	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:PHE:CD2	1:C:71:ILE:HD12	2.54	0.42
1:D:122:THR:O	1:D:123:LEU:C	2.55	0.42
1:D:33:LYS:HE3	1:D:33:LYS:H	1.84	0.42
1:D:32:LYS:HD3	1:D:35:ALA:CB	2.50	0.42
1:A:16:LEU:CA	1:A:17:ASP:CB	2.98	0.41
1:A:16:LEU:HA	1:A:18:PHE:HD2	1.84	0.41
1:B:83:ILE:O	1:B:113:GLU:HA	2.20	0.41
1:A:115:LYS:HE3	1:A:139:LYS:O	2.20	0.41
1:C:25:LEU:HD22	1:C:37:PHE:HE1	1.85	0.41
1:A:47:ILE:C	1:A:48:ARG:HG3	2.41	0.41
1:A:112:PHE:CD1	1:A:112:PHE:N	2.88	0.41
1:A:18:PHE:CD2	1:A:18:PHE:N	2.87	0.41
1:B:16:LEU:HA	1:B:17:ASP:C	2.41	0.41
1:B:86:LYS:HG2	1:B:90:GLU:CD	2.40	0.41
1:D:10:LEU:HD23	1:D:62:ILE:HG12	2.02	0.41
1:C:85:ALA:O	1:C:112:PHE:CB	2.69	0.41
1:D:122:THR:O	1:D:126:LEU:HD12	2.21	0.41
1:A:20:VAL:HA	1:A:70:ILE:HG22	2.02	0.41
1:C:60:GLY:H	1:C:73:VAL:HB	1.85	0.41
1:B:50:LYS:HD3	1:B:50:LYS:HA	1.88	0.41
1:B:90:GLU:O	1:B:94:ILE:HD13	2.20	0.41
1:D:122:THR:HG22	1:D:126:LEU:HD11	2.01	0.41
1:D:86:LYS:HG2	1:D:90:GLU:OE2	2.21	0.41
1:A:125:LEU:HD12	1:A:125:LEU:HA	1.70	0.41
1:B:47:ILE:CG2	1:B:63:LEU:HD21	2.52	0.40
1:C:14:ASN:ND2	1:C:18:PHE:HE2	2.19	0.40
1:A:6:LEU:HD13	1:A:61:ASP:HB3	2.03	0.40
1:C:65:LYS:HG3	1:C:70:ILE:CD1	2.49	0.40
1:A:147:THR:CG2	1:D:93:LYS:HE3	2.51	0.40
1:C:36:ARG:NH2	1:C:46:ALA:HB2	2.36	0.40
1:D:35:ALA:H	1:D:47:ILE:HG12	1.86	0.40
1:D:61:ASP:HB2	1:D:73:VAL:HG21	2.03	0.40
1:B:70:ILE:CG2	1:B:71:ILE:N	2.84	0.40
1:D:118:PHE:CD1	1:D:118:PHE:O	2.74	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:PHE:O	1:A:110:SER:OG[7_555]	2.11	0.09
1:B:77:ASP:OD2	1:C:77:ASP:OD2[4_454]	2.12	0.08



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	145/170 (85%)	113 (78%)	26 (18%)	6 (4%)	3	19
1	B	151/170 (89%)	118 (78%)	21 (14%)	12 (8%)	1	6
1	C	146/170 (86%)	115 (79%)	17 (12%)	14 (10%)	1	4
1	D	146/170 (86%)	113 (77%)	24 (16%)	9 (6%)	2	10
All	All	588/680 (86%)	459 (78%)	88 (15%)	41 (7%)	1	8

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	55	LEU
1	B	94	ILE
1	B	145	ARG
1	B	146	LEU
1	B	147	THR
1	B	148	VAL
1	C	6	LEU
1	C	10	LEU
1	C	14	ASN
1	C	35	ALA
1	C	52	ALA
1	C	55	LEU
1	C	67	GLU
1	D	16	LEU
1	D	111	GLN
1	B	16	LEU
1	B	111	GLN
1	B	149	SER
1	C	16	LEU
1	C	54	LYS
1	D	63	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	94	ILE
1	D	148	VAL
1	A	16	LEU
1	C	43	LYS
1	C	53	PRO
1	D	10	LEU
1	D	67	GLU
1	A	32	LYS
1	A	43	LYS
1	B	143	LYS
1	B	152	HIS
1	C	17	ASP
1	B	43	LYS
1	C	148	VAL
1	D	93	LYS
1	D	124	ALA
1	C	117	PRO
1	A	7	VAL
1	B	42	GLY

### 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	128/152 (84%)	100 (78%)	28 (22%)	1	5
1	B	131/152 (86%)	100 (76%)	31 (24%)	1	3
1	C	130/152 (86%)	89 (68%)	41 (32%)	0	1
1	D	129/152 (85%)	100 (78%)	29 (22%)	1	4
All	All	518/608 (85%)	389 (75%)	129 (25%)	1	2

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	5	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	16	LEU
1	A	31	ARG
1	A	40	ARG
1	A	43	LYS
1	A	54	LYS
1	A	55	LEU
1	A	68	LYS
1	A	69	GLU
1	A	70	ILE
1	A	78	SER
1	A	79	GLU
1	A	84	GLN
1	A	86	LYS
1	A	101	ARG
1	A	115	LYS
1	A	116	THR
1	A	119	GLU
1	A	120	LYS
1	A	129	LEU
1	A	131	VAL
1	A	132	GLN
1	A	135	VAL
1	A	140	LEU
1	A	144	GLU
1	A	147	THR
1	A	148	VAL
1	B	5	ARG
1	B	10	LEU
1	B	12	ASP
1	B	16	LEU
1	B	17	ASP
1	B	23	VAL
1	B	33	LYS
1	B	43	LYS
1	B	50	LYS
1	B	55	LEU
1	B	63	LEU
1	B	64	PHE
1	B	66	GLU
1	B	67	GLU
1	B	84	GLN
1	B	86	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	93	LYS
1	B	97	GLU
1	B	100	ASN
1	B	101	ARG
1	B	118	PHE
1	B	120	LYS
1	B	125	LEU
1	B	126	LEU
1	B	127	GLU
1	B	129	LEU
1	B	144	GLU
1	B	146	LEU
1	B	147	THR
1	B	149	SER
1	B	152	HIS
1	C	2	ILE
1	C	4	GLU
1	C	5	ARG
1	C	12	ASP
1	C	14	ASN
1	C	16	LEU
1	C	25	LEU
1	C	28	PHE
1	C	30	THR
1	C	32	LYS
1	C	34	ILE
1	C	37	PHE
1	C	39	THR
1	C	40	ARG
1	C	41	GLN
1	C	45	ILE
1	C	49	LEU
1	C	50	LYS
1	C	55	LEU
1	C	59	GLN
1	C	63	LEU
1	C	64	PHE
1	C	66	GLU
1	C	68	LYS
1	C	78	SER
1	C	79	GLU
1	C	81	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	86	LYS
1	C	101	ARG
1	C	117	PRO
1	C	119	GLU
1	C	120	LYS
1	C	127	GLU
1	C	134	ARG
1	C	137	SER
1	C	139	LYS
1	C	142	SER
1	C	143	LYS
1	C	144	GLU
1	C	146	LEU
1	C	147	THR
1	D	4	GLU
1	D	10	LEU
1	D	20	VAL
1	D	22	HIS
1	D	26	GLU
1	D	33	LYS
1	D	43	LYS
1	D	45	ILE
1	D	48	ARG
1	D	51	ASP
1	D	58	SER
1	D	63	LEU
1	D	66	GLU
1	D	67	GLU
1	D	68	LYS
1	D	70	ILE
1	D	73	VAL
1	D	76	LEU
1	D	78	SER
1	D	97	GLU
1	D	101	ARG
1	D	113	GLU
1	D	118	PHE
1	D	119	GLU
1	D	120	LYS
1	D	135	VAL
1	D	139	LYS
1	D	141	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	144	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	A	84	GLN
1	B	84	GLN
1	C	9	ASN
1	C	22	HIS
1	C	59	GLN
1	C	133	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 ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	147/170 (86%)	-0.41	0	100 100	42, 77, 109, 116	0
1	B	153/170 (90%)	-0.27	0	100 100	43, 83, 126, 136	0
1	C	148/170 (87%)	-0.22	1 (0%)	87 75	50, 85, 147, 166	0
1	D	148/170 (87%)	0.06	5 (3%)	46 23	46, 105, 175, 187	0
All	All	596/680 (87%)	-0.21	6 (1%)	82 67	42, 85, 163, 187	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	13	LEU	2.9
1	D	45	ILE	2.7
1	D	5	ARG	2.5
1	C	36	ARG	2.4
1	D	44	ASP	2.1
1	D	43	LYS	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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron



density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NI	B	171	1/1	0.99	0.14	-1.01	63,63,63,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.