



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:23 PM GMT

PDB ID : 1TD5  
Title : Crystal Structure of the Ligand Binding Domain of E. coli IclR.  
Authors : Walker, J.R.; Evdokimova, L.; Zhang, R.-G.; Bochkarev, A.; Joachimiak, A.; Arrowsmith, C.; Edwards, A.; Savchenko, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2004-05-21  
Resolution : 2.30 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

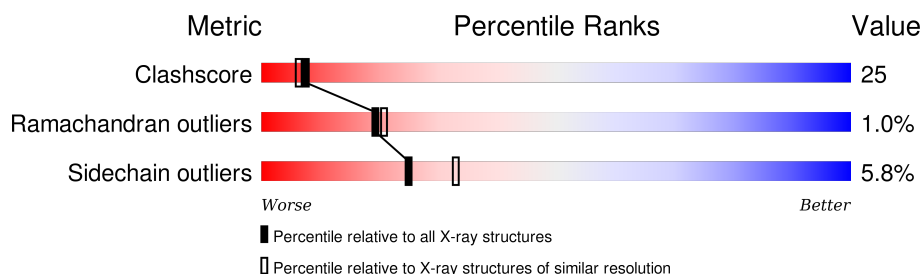
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	202	
1	B	202	
1	C	202	
1	D	202	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5834 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 Acetate operon repressor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	Se	0	0	0
			1373	859	248	255	3	8			
1	B	179	Total	C	N	O	S	Se	0	0	0
			1373	859	248	255	3	8			
1	C	178	Total	C	N	O	S	Se	0	0	0
			1369	857	247	254	3	8			
1	D	180	Total	C	N	O	S	Se	0	0	0
			1384	865	252	256	3	8			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	CLONING ARTIFACT	UNP P16528
A	-18	GLY	-	CLONING ARTIFACT	UNP P16528
A	-17	SER	-	CLONING ARTIFACT	UNP P16528
A	-16	SER	-	CLONING ARTIFACT	UNP P16528
A	-15	HIS	-	CLONING ARTIFACT	UNP P16528
A	-14	HIS	-	CLONING ARTIFACT	UNP P16528
A	-13	HIS	-	CLONING ARTIFACT	UNP P16528
A	-12	HIS	-	CLONING ARTIFACT	UNP P16528
A	-11	HIS	-	CLONING ARTIFACT	UNP P16528
A	-10	HIS	-	CLONING ARTIFACT	UNP P16528
A	-9	SER	-	CLONING ARTIFACT	UNP P16528
A	-8	SER	-	CLONING ARTIFACT	UNP P16528
A	-7	GLY	-	CLONING ARTIFACT	UNP P16528
A	-6	ARG	-	CLONING ARTIFACT	UNP P16528
A	-5	GLU	-	CLONING ARTIFACT	UNP P16528
A	-4	ASN	-	CLONING ARTIFACT	UNP P16528
A	-3	LEU	-	CLONING ARTIFACT	UNP P16528
A	-2	TYR	-	CLONING ARTIFACT	UNP P16528
A	-1	PHE	-	CLONING ARTIFACT	UNP P16528
A	0	GLN	-	CLONING ARTIFACT	UNP P16528
A	1	GLY	-	CLONING ARTIFACT	UNP P16528

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2	HIS	-	CLONING ARTIFACT	UNP P16528
A	3	MSE	-	CLONING ARTIFACT	UNP P16528
A	19	MSE	MET	MODIFIED RESIDUE	UNP P16528
A	28	MSE	MET	MODIFIED RESIDUE	UNP P16528
A	50	MSE	MET	MODIFIED RESIDUE	UNP P16528
A	52	MSE	MET	MODIFIED RESIDUE	UNP P16528
A	62	MSE	MET	MODIFIED RESIDUE	UNP P16528
A	164	MSE	MET	MODIFIED RESIDUE	UNP P16528
A	179	MSE	MET	MODIFIED RESIDUE	UNP P16528
A	181	GLY	-	CLONING ARTIFACT	UNP P16528
A	182	SER	-	CLONING ARTIFACT	UNP P16528
B	-19	MET	-	CLONING ARTIFACT	UNP P16528
B	-18	GLY	-	CLONING ARTIFACT	UNP P16528
B	-17	SER	-	CLONING ARTIFACT	UNP P16528
B	-16	SER	-	CLONING ARTIFACT	UNP P16528
B	-15	HIS	-	CLONING ARTIFACT	UNP P16528
B	-14	HIS	-	CLONING ARTIFACT	UNP P16528
B	-13	HIS	-	CLONING ARTIFACT	UNP P16528
B	-12	HIS	-	CLONING ARTIFACT	UNP P16528
B	-11	HIS	-	CLONING ARTIFACT	UNP P16528
B	-10	HIS	-	CLONING ARTIFACT	UNP P16528
B	-9	SER	-	CLONING ARTIFACT	UNP P16528
B	-8	SER	-	CLONING ARTIFACT	UNP P16528
B	-7	GLY	-	CLONING ARTIFACT	UNP P16528
B	-6	ARG	-	CLONING ARTIFACT	UNP P16528
B	-5	GLU	-	CLONING ARTIFACT	UNP P16528
B	-4	ASN	-	CLONING ARTIFACT	UNP P16528
B	-3	LEU	-	CLONING ARTIFACT	UNP P16528
B	-2	TYR	-	CLONING ARTIFACT	UNP P16528
B	-1	PHE	-	CLONING ARTIFACT	UNP P16528
B	0	GLN	-	CLONING ARTIFACT	UNP P16528
B	1	GLY	-	CLONING ARTIFACT	UNP P16528
B	2	HIS	-	CLONING ARTIFACT	UNP P16528
B	3	MSE	-	CLONING ARTIFACT	UNP P16528
B	19	MSE	MET	MODIFIED RESIDUE	UNP P16528
B	28	MSE	MET	MODIFIED RESIDUE	UNP P16528
B	50	MSE	MET	MODIFIED RESIDUE	UNP P16528
B	52	MSE	MET	MODIFIED RESIDUE	UNP P16528
B	62	MSE	MET	MODIFIED RESIDUE	UNP P16528
B	164	MSE	MET	MODIFIED RESIDUE	UNP P16528
B	179	MSE	MET	MODIFIED RESIDUE	UNP P16528
B	181	GLY	-	CLONING ARTIFACT	UNP P16528

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Chain	Residue	Modelled	Actual	Comment	Reference
B	182	SER	-	CLONING ARTIFACT	UNP P16528
C	-19	MET	-	CLONING ARTIFACT	UNP P16528
C	-18	GLY	-	CLONING ARTIFACT	UNP P16528
C	-17	SER	-	CLONING ARTIFACT	UNP P16528
C	-16	SER	-	CLONING ARTIFACT	UNP P16528
C	-15	HIS	-	CLONING ARTIFACT	UNP P16528
C	-14	HIS	-	CLONING ARTIFACT	UNP P16528
C	-13	HIS	-	CLONING ARTIFACT	UNP P16528
C	-12	HIS	-	CLONING ARTIFACT	UNP P16528
C	-11	HIS	-	CLONING ARTIFACT	UNP P16528
C	-10	HIS	-	CLONING ARTIFACT	UNP P16528
C	-9	SER	-	CLONING ARTIFACT	UNP P16528
C	-8	SER	-	CLONING ARTIFACT	UNP P16528
C	-7	GLY	-	CLONING ARTIFACT	UNP P16528
C	-6	ARG	-	CLONING ARTIFACT	UNP P16528
C	-5	GLU	-	CLONING ARTIFACT	UNP P16528
C	-4	ASN	-	CLONING ARTIFACT	UNP P16528
C	-3	LEU	-	CLONING ARTIFACT	UNP P16528
C	-2	TYR	-	CLONING ARTIFACT	UNP P16528
C	-1	PHE	-	CLONING ARTIFACT	UNP P16528
C	0	GLN	-	CLONING ARTIFACT	UNP P16528
C	1	GLY	-	CLONING ARTIFACT	UNP P16528
C	2	HIS	-	CLONING ARTIFACT	UNP P16528
C	3	MSE	-	CLONING ARTIFACT	UNP P16528
C	19	MSE	MET	MODIFIED RESIDUE	UNP P16528
C	28	MSE	MET	MODIFIED RESIDUE	UNP P16528
C	50	MSE	MET	MODIFIED RESIDUE	UNP P16528
C	52	MSE	MET	MODIFIED RESIDUE	UNP P16528
C	62	MSE	MET	MODIFIED RESIDUE	UNP P16528
C	164	MSE	MET	MODIFIED RESIDUE	UNP P16528
C	179	MSE	MET	MODIFIED RESIDUE	UNP P16528
C	181	GLY	-	CLONING ARTIFACT	UNP P16528
C	182	SER	-	CLONING ARTIFACT	UNP P16528
D	-19	MET	-	CLONING ARTIFACT	UNP P16528
D	-18	GLY	-	CLONING ARTIFACT	UNP P16528
D	-17	SER	-	CLONING ARTIFACT	UNP P16528
D	-16	SER	-	CLONING ARTIFACT	UNP P16528
D	-15	HIS	-	CLONING ARTIFACT	UNP P16528
D	-14	HIS	-	CLONING ARTIFACT	UNP P16528
D	-13	HIS	-	CLONING ARTIFACT	UNP P16528
D	-12	HIS	-	CLONING ARTIFACT	UNP P16528
D	-11	HIS	-	CLONING ARTIFACT	UNP P16528

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	HIS	-	CLONING ARTIFACT	UNP P16528
D	-9	SER	-	CLONING ARTIFACT	UNP P16528
D	-8	SER	-	CLONING ARTIFACT	UNP P16528
D	-7	GLY	-	CLONING ARTIFACT	UNP P16528
D	-6	ARG	-	CLONING ARTIFACT	UNP P16528
D	-5	GLU	-	CLONING ARTIFACT	UNP P16528
D	-4	ASN	-	CLONING ARTIFACT	UNP P16528
D	-3	LEU	-	CLONING ARTIFACT	UNP P16528
D	-2	TYR	-	CLONING ARTIFACT	UNP P16528
D	-1	PHE	-	CLONING ARTIFACT	UNP P16528
D	0	GLN	-	CLONING ARTIFACT	UNP P16528
D	1	GLY	-	CLONING ARTIFACT	UNP P16528
D	2	HIS	-	CLONING ARTIFACT	UNP P16528
D	3	MSE	-	CLONING ARTIFACT	UNP P16528
D	19	MSE	MET	MODIFIED RESIDUE	UNP P16528
D	28	MSE	MET	MODIFIED RESIDUE	UNP P16528
D	50	MSE	MET	MODIFIED RESIDUE	UNP P16528
D	52	MSE	MET	MODIFIED RESIDUE	UNP P16528
D	62	MSE	MET	MODIFIED RESIDUE	UNP P16528
D	164	MSE	MET	MODIFIED RESIDUE	UNP P16528
D	179	MSE	MET	MODIFIED RESIDUE	UNP P16528
D	181	GLY	-	CLONING ARTIFACT	UNP P16528
D	182	SER	-	CLONING ARTIFACT	UNP P16528

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	65	Total O 65 65	0	0
2	B	109	Total O 109 109	0	0
2	C	58	Total O 58 58	0	0
2	D	103	Total O 103 103	0	0

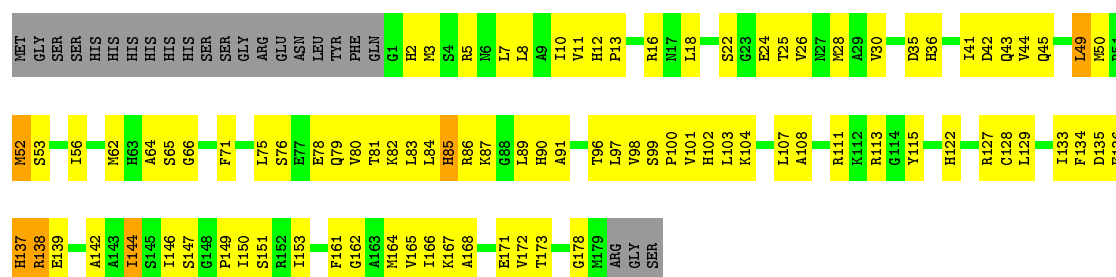
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

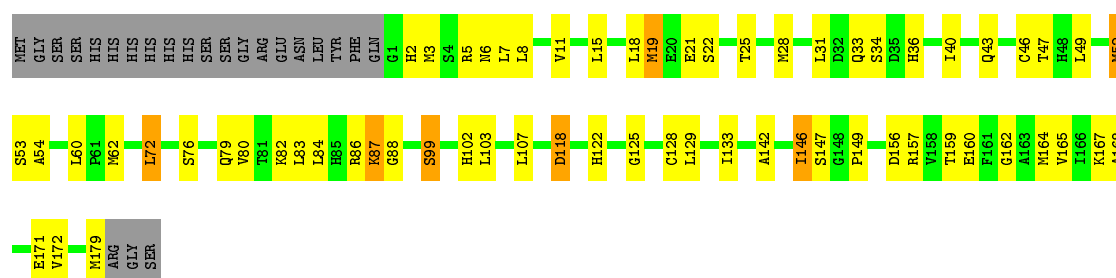
- Molecule 1: Acetate operon repressor

Chain A: 



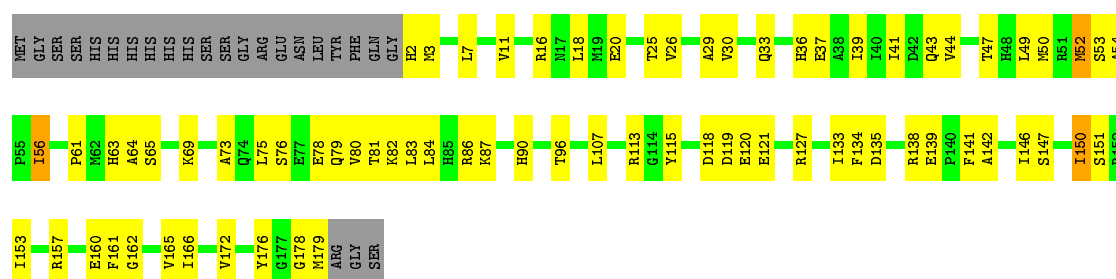
- Molecule 1: Acetate operon repressor

Chain B: 

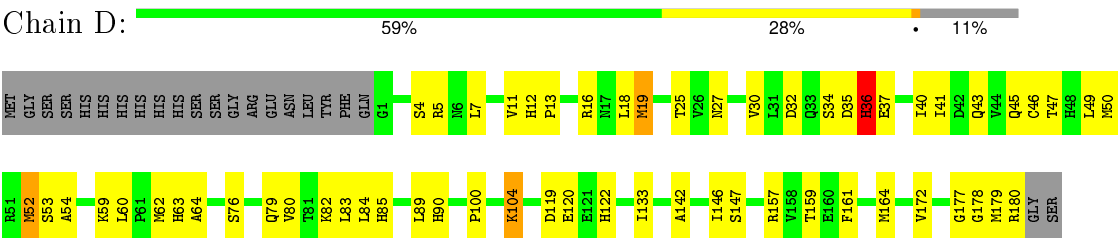


- Molecule 1: Acetate operon repressor

Chain C: 



● Molecule 1: Acetate operon repressor





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.10 Å 82.91 Å 157.32 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.30	Depositor
% Data completeness (in resolution range)	96.1 (19.91-2.30)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.230 , 0.299	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5834	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

## 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	0.60	0/1389	0.74	0/1860
1	B	0.72	0/1389	0.76	0/1860
1	C	0.57	0/1385	0.70	0/1855
1	D	0.70	0/1400	0.77	0/1874
All	All	0.65	0/5563	0.74	0/7449

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1373	0	1382	86	0
1	B	1373	0	1382	69	0
1	C	1369	0	1376	72	0
1	D	1384	0	1395	67	0
2	A	65	0	0	3	0
2	B	109	0	0	5	0
2	C	58	0	0	0	0
2	D	103	0	0	3	0
All	All	5834	0	5535	281	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 25.

All (281) 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:A:25:THR:HG21	1:A:52:MSE:HE2	1.32	1.09
1:B:52:MSE:HG2	1:B:147:SER:HB2	1.44	0.96
1:A:76:SER:H	1:A:79:GLN:NE2	1.65	0.94
1:C:52:MSE:HG2	1:C:147:SER:HB2	1.50	0.93
1:D:25:THR:HG21	1:D:52:MSE:HE2	1.47	0.93
1:D:84:LEU:HD22	1:D:89:LEU:HD21	1.51	0.92
1:C:87:LYS:HD2	1:C:87:LYS:H	1.35	0.92
1:A:25:THR:HG21	1:A:52:MSE:CE	2.00	0.92
1:A:25:THR:CG2	1:A:52:MSE:HE2	2.00	0.91
1:D:7:LEU:HD13	1:D:180:ARG:HG2	1.56	0.87
1:D:43:GLN:NE2	1:D:52:MSE:HE1	1.88	0.86
1:C:18:LEU:HG	1:C:146:ILE:HD11	1.55	0.85
1:D:25:THR:CG2	1:D:52:MSE:HE2	2.07	0.84
1:C:25:THR:HG21	1:C:52:MSE:HE2	1.57	0.83
1:D:19:MSE:HE3	1:D:46:CYS:HA	1.61	0.82
1:D:43:GLN:HE21	1:D:52:MSE:HE1	1.43	0.80
1:C:25:THR:CG2	1:C:52:MSE:HE2	2.11	0.80
1:D:25:THR:HG21	1:D:52:MSE:CE	2.12	0.80
1:A:18:LEU:HD11	1:A:146:ILE:HD11	1.64	0.79
1:C:127:ARG:HG3	1:C:150:ILE:HG22	1.64	0.78
1:C:113:ARG:HD2	1:C:115:TYR:CZ	2.18	0.78
1:B:47:THR:HG22	2:B:186:HOH:O	1.82	0.78
1:B:40:ILE:HD11	1:B:60:LEU:HD11	1.67	0.77
1:B:159:THR:HG22	2:B:198:HOH:O	1.83	0.77
1:A:52:MSE:HG2	1:A:147:SER:HB2	1.66	0.76
1:D:47:THR:HG22	2:D:184:HOH:O	1.85	0.76
1:D:52:MSE:HG2	1:D:147:SER:HB2	1.68	0.76
1:D:36:HIS:HB3	1:D:62:MSE:HE3	1.68	0.75
1:B:18:LEU:HD11	1:B:146:ILE:HD11	1.69	0.75
1:A:50:MSE:HE1	1:A:149:PRO:HB3	1.69	0.74
1:A:108:ALA:HA	1:A:111:ARG:NH2	2.02	0.74
1:A:161:PHE:HA	1:A:164:MSE:HE3	1.69	0.74
1:A:83:LEU:HA	1:A:86:ARG:HB3	1.70	0.74
1:C:26:VAL:HG22	1:C:146:ILE:HD13	1.68	0.74
1:A:84:LEU:HD22	1:A:89:LEU:HD11	1.69	0.73
1:C:76:SER:O	1:C:80:VAL:HG23	1.89	0.73
1:B:86:ARG:NH1	1:B:86:ARG:HB3	2.05	0.72
1:C:87:LYS:N	1:C:87:LYS:HD2	2.03	0.72
1:A:3:MSE:SE	1:A:7:LEU:HD12	2.40	0.72
1:D:40:ILE:HD11	1:D:60:LEU:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLU:HG3	1:A:153:ILE:HD11	1.72	0.71
1:D:52:MSE:HG2	1:D:147:SER:CB	2.21	0.71
1:D:52:MSE:HE3	1:D:53:SER:HA	1.73	0.71
1:D:76:SER:H	1:D:79:GLN:HE21	1.39	0.70
1:C:52:MSE:HE3	1:C:53:SER:HA	1.73	0.70
1:D:37:GLU:OE2	1:D:59:LYS:HE2	1.91	0.70
1:A:113:ARG:HD2	1:A:115:TYR:CE1	2.26	0.70
1:A:133:ILE:HB	1:A:142:ALA:HB3	1.73	0.70
1:A:76:SER:O	1:A:80:VAL:HG23	1.91	0.70
1:C:25:THR:HG21	1:C:52:MSE:CE	2.21	0.69
1:D:43:GLN:NE2	1:D:52:MSE:CE	2.55	0.69
1:C:43:GLN:OE1	1:C:52:MSE:HE1	1.94	0.67
1:D:76:SER:O	1:D:80:VAL:HG23	1.94	0.67
1:C:18:LEU:CG	1:C:146:ILE:HD11	2.25	0.66
1:C:73:ALA:HB2	1:C:107:LEU:HD22	1.76	0.66
1:A:85:HIS:HE1	1:C:47:THR:H	1.42	0.66
1:A:3:MSE:HG2	1:A:41:ILE:HD12	1.79	0.65
1:D:7:LEU:HD13	1:D:180:ARG:CG	2.27	0.64
1:B:25:THR:HG21	1:B:52:MSE:HE2	1.79	0.64
1:A:78:GLU:O	1:A:82:LYS:HG2	1.98	0.63
1:B:86:ARG:HH22	1:D:157:ARG:HH22	1.43	0.63
1:D:43:GLN:HE21	1:D:52:MSE:CE	2.11	0.63
1:B:25:THR:HG21	1:B:52:MSE:CE	2.29	0.62
1:A:3:MSE:HG2	1:A:41:ILE:CD1	2.28	0.62
1:D:159:THR:HG22	2:D:224:HOH:O	1.98	0.62
1:C:134:PHE:HB3	1:C:138:ARG:HA	1.80	0.62
1:C:76:SER:OG	1:C:79:GLN:HG3	1.98	0.62
1:B:128:CYS:C	1:B:129:LEU:HD12	2.19	0.62
1:A:97:LEU:HD13	1:A:103:LEU:HA	1.81	0.62
1:B:80:VAL:O	1:B:84:LEU:HG	1.99	0.62
1:C:133:ILE:HD13	1:C:172:VAL:HG11	1.81	0.61
1:A:85:HIS:CE1	1:C:47:THR:H	2.19	0.61
1:C:3:MSE:SE	1:C:7:LEU:HD23	2.51	0.61
1:D:19:MSE:HE3	1:D:46:CYS:CA	2.31	0.61
1:A:167:LYS:O	1:A:171:GLU:HG3	2.01	0.61
1:A:128:CYS:C	1:A:129:LEU:HD12	2.22	0.60
1:D:76:SER:OG	1:D:79:GLN:HG3	2.00	0.60
1:B:162:GLY:O	1:B:165:VAL:HG12	2.01	0.60
1:B:125:GLY:O	1:B:149:PRO:HA	2.01	0.60
1:A:64:ALA:O	1:A:122:HIS:HB2	2.02	0.60
1:A:52:MSE:HE3	1:A:53:SER:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:MSE:HE3	1:B:53:SER:HA	1.83	0.59
1:A:76:SER:CB	1:A:79:GLN:HE21	2.14	0.59
1:D:7:LEU:CD1	1:D:180:ARG:HG2	2.31	0.59
1:D:18:LEU:HD11	1:D:146:ILE:HD11	1.83	0.59
1:A:137:HIS:HB2	1:A:139:GLU:HG2	1.85	0.59
1:C:63:HIS:HE1	1:C:90:HIS:O	1.86	0.59
1:C:52:MSE:HG2	1:C:147:SER:CB	2.30	0.58
1:A:162:GLY:O	1:A:166:ILE:HG12	2.01	0.58
1:D:36:HIS:HB3	1:D:62:MSE:CE	2.33	0.58
1:B:79:GLN:HA	1:B:82:LYS:HE3	1.85	0.58
1:A:129:LEU:HD12	1:A:129:LEU:N	2.19	0.58
1:A:84:LEU:CD2	1:A:89:LEU:HD11	2.34	0.58
1:B:33:GLN:HE21	1:B:33:GLN:HA	1.67	0.58
1:B:76:SER:O	1:B:80:VAL:HG23	2.03	0.58
1:C:150:ILE:HD13	1:C:151:SER:N	2.19	0.57
1:B:72:LEU:HD23	1:B:107:LEU:HD11	1.86	0.57
1:D:177:GLY:C	1:D:179:MSE:H	2.07	0.57
1:B:33:GLN:NE2	1:B:33:GLN:HA	2.19	0.57
1:A:30:VAL:HB	1:A:41:ILE:HD13	1.87	0.57
1:B:19:MSE:HE3	1:B:46:CYS:CB	2.34	0.57
1:C:3:MSE:HG2	1:C:41:ILE:HD12	1.87	0.57
1:B:7:LEU:HD13	1:B:179:MSE:SE	2.54	0.57
1:B:25:THR:HB	1:B:52:MSE:HG3	1.87	0.57
1:B:167:LYS:O	1:B:171:GLU:HG3	2.05	0.57
1:C:162:GLY:O	1:C:166:ILE:HG12	2.05	0.56
1:D:100:PRO:O	1:D:104:LYS:HE3	2.05	0.56
1:A:168:ALA:O	1:A:172:VAL:HG23	2.06	0.56
1:B:22:SER:N	1:B:164:MSE:HE1	2.21	0.56
1:B:18:LEU:HD12	1:B:164:MSE:HE2	1.87	0.56
1:A:50:MSE:HE3	1:D:50:MSE:HG2	1.88	0.56
1:B:36:HIS:HB3	1:B:83:LEU:HD11	1.87	0.56
1:B:86:ARG:HH11	1:B:86:ARG:HB3	1.69	0.55
1:A:43:GLN:OE1	1:A:52:MSE:HE1	2.06	0.55
1:D:76:SER:H	1:D:79:GLN:NE2	2.05	0.55
1:C:16:ARG:O	1:C:20:GLU:HG3	2.07	0.55
1:D:84:LEU:CD2	1:D:89:LEU:HD21	2.32	0.55
1:B:11:VAL:HG21	1:B:172:VAL:HG13	1.89	0.55
1:B:43:GLN:OE1	1:B:52:MSE:HE1	2.07	0.54
1:C:11:VAL:HG11	1:C:172:VAL:HG22	1.89	0.54
1:C:157:ARG:HG2	1:C:157:ARG:HH11	1.72	0.54
1:C:16:ARG:HD2	1:C:44:VAL:HG11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:GLY:O	1:D:179:MSE:HB2	2.07	0.54
1:D:82:LYS:O	1:D:85:HIS:HB3	2.07	0.54
1:C:157:ARG:O	1:C:160:GLU:HB3	2.07	0.54
1:D:11:VAL:CG1	1:D:172:VAL:HG22	2.38	0.53
1:B:86:ARG:O	1:B:87:LYS:HE2	2.08	0.53
1:A:127:ARG:HD2	1:A:150:ILE:HG22	1.90	0.53
1:B:25:THR:CG2	1:B:52:MSE:HE2	2.37	0.53
1:C:135:ASP:HA	1:C:176:TYR:CE2	2.45	0.52
1:B:19:MSE:HE3	1:B:46:CYS:HA	1.90	0.52
1:A:82:LYS:O	1:A:86:ARG:HB2	2.09	0.52
1:B:62:MSE:HE2	1:B:72:LEU:HD12	1.91	0.52
1:A:79:GLN:O	1:A:82:LYS:HB2	2.10	0.52
1:C:127:ARG:CG	1:C:150:ILE:HG22	2.36	0.52
1:D:62:MSE:HE1	1:D:83:LEU:HD13	1.91	0.52
1:C:150:ILE:HD13	1:C:151:SER:H	1.75	0.52
1:D:62:MSE:HE1	1:D:83:LEU:HD22	1.92	0.52
1:C:11:VAL:CG1	1:C:172:VAL:HG22	2.39	0.52
1:B:3:MSE:HE3	1:B:28:MSE:SE	2.60	0.52
1:A:83:LEU:HA	1:A:86:ARG:CB	2.39	0.51
1:A:36:HIS:HB2	1:A:87:LYS:HE3	1.91	0.51
1:B:86:ARG:HH22	1:D:157:ARG:NH2	2.08	0.51
1:C:69:LYS:NZ	1:C:121:GLU:OE2	2.32	0.51
1:B:15:LEU:HD11	1:B:28:MSE:HE2	1.92	0.51
1:A:76:SER:HB3	1:A:79:GLN:HE21	1.75	0.51
1:B:11:VAL:HG21	1:B:172:VAL:HG22	1.93	0.51
1:C:25:THR:HG22	1:C:52:MSE:HE2	1.92	0.50
1:A:136:GLU:H	1:A:136:GLU:CD	2.14	0.50
1:D:161:PHE:HA	1:D:164:MSE:HE3	1.92	0.50
1:C:79:GLN:O	1:C:83:LEU:HG	2.11	0.50
1:B:18:LEU:CD1	1:B:146:ILE:HD11	2.41	0.50
1:A:35:ASP:O	1:A:87:LYS:HE3	2.12	0.50
1:A:49:LEU:O	1:D:52:MSE:HA	2.11	0.49
1:A:129:LEU:HD22	1:A:161:PHE:HB3	1.94	0.49
1:B:160:GLU:HG2	2:B:213:HOH:O	2.10	0.49
1:D:5:ARG:HG2	2:D:189:HOH:O	2.10	0.49
1:B:156:ASP:OD2	1:B:157:ARG:HG3	2.11	0.49
1:D:63:HIS:HE1	1:D:90:HIS:O	1.94	0.49
1:B:129:LEU:N	1:B:129:LEU:HD12	2.26	0.49
1:C:52:MSE:HE3	1:C:53:SER:CA	2.40	0.49
1:B:21:GLU:CG	1:B:164:MSE:HE3	2.43	0.49
1:D:64:ALA:O	1:D:122:HIS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:MSE:HG2	1:C:41:ILE:CD1	2.41	0.49
1:C:26:VAL:HG22	1:C:146:ILE:CD1	2.41	0.48
1:B:86:ARG:NH2	1:D:157:ARG:HH22	2.11	0.48
1:C:7:LEU:O	1:C:11:VAL:HG23	2.13	0.48
1:B:99:SER:HB3	1:B:102:HIS:CD2	2.48	0.48
1:C:153:ILE:HG12	1:C:161:PHE:HE1	1.78	0.48
1:A:134:PHE:O	1:A:173:THR:HG23	2.13	0.48
1:B:43:GLN:OE1	1:B:52:MSE:CE	2.61	0.48
1:A:28:MSE:HB3	1:A:42:ASP:HB3	1.95	0.48
1:A:76:SER:H	1:A:79:GLN:CD	2.16	0.48
1:B:19:MSE:HE3	1:B:46:CYS:HB2	1.96	0.48
1:A:127:ARG:CD	1:A:150:ILE:HG22	2.44	0.48
1:D:12:HIS:HB3	1:D:13:PRO:HD3	1.96	0.48
1:C:113:ARG:HD2	1:C:115:TYR:CE1	2.47	0.48
1:A:135:ASP:OD1	1:A:139:GLU:HB2	2.14	0.47
1:A:104:LYS:HA	1:A:107:LEU:HD12	1.96	0.47
1:D:11:VAL:HG12	1:D:11:VAL:O	2.15	0.47
1:C:36:HIS:CD2	1:C:83:LEU:HD21	2.50	0.47
1:B:86:ARG:NH2	1:D:157:ARG:NH2	2.62	0.47
1:D:133:ILE:HB	1:D:142:ALA:HB3	1.96	0.47
1:C:37:GLU:HG3	1:C:39:ILE:HD11	1.96	0.47
1:B:11:VAL:CG2	1:B:172:VAL:HG22	2.45	0.47
1:B:133:ILE:HB	1:B:142:ALA:HB3	1.97	0.47
1:A:101:VAL:HG13	2:A:191:HOH:O	2.15	0.47
1:C:118:ASP:OD1	1:C:121:GLU:HB2	2.14	0.46
1:C:61:PRO:HG2	1:C:65:SER:HB3	1.96	0.46
1:C:82:LYS:O	1:C:86:ARG:HG2	2.15	0.46
1:B:168:ALA:O	1:B:172:VAL:HG23	2.16	0.46
1:C:64:ALA:HB2	1:C:96:THR:HG23	1.96	0.46
1:A:35:ASP:O	1:A:87:LYS:NZ	2.46	0.46
1:D:4:SER:H	1:D:180:ARG:NH2	2.13	0.46
1:B:8:LEU:HD23	1:B:8:LEU:HA	1.71	0.46
1:B:62:MSE:HE2	1:B:72:LEU:CD1	2.45	0.46
1:A:75:LEU:N	1:A:75:LEU:HD23	2.31	0.46
1:C:56:ILE:N	1:C:56:ILE:CD1	2.79	0.46
1:D:11:VAL:HG11	1:D:172:VAL:HG22	1.96	0.46
1:B:84:LEU:HD11	1:B:103:LEU:HD23	1.96	0.46
1:C:33:GLN:HA	1:C:33:GLN:NE2	2.31	0.46
1:C:29:ALA:HA	1:C:39:ILE:O	2.17	0.45
1:A:16:ARG:HA	1:A:44:VAL:HG11	1.98	0.45
1:D:43:GLN:HE22	1:D:54:ALA:H	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLU:C	1:A:138:ARG:H	2.19	0.45
1:C:157:ARG:HG2	1:C:157:ARG:NH1	2.31	0.45
1:A:62:MSE:HE1	1:A:71:PHE:CB	2.47	0.45
1:B:118:ASP:C	1:B:118:ASP:OD1	2.55	0.45
1:D:16:ARG:HG3	1:D:16:ARG:HH11	1.82	0.45
1:D:30:VAL:HG13	1:D:41:ILE:HD13	1.98	0.45
1:B:5:ARG:HG3	1:B:6:ASN:N	2.32	0.45
1:A:25:THR:HB	1:A:52:MSE:HG3	1.98	0.45
1:D:27:ASN:ND2	1:D:43:GLN:HB2	2.32	0.45
1:A:81:THR:HA	1:A:84:LEU:HG	1.98	0.45
1:A:113:ARG:HG2	1:A:115:TYR:H	1.82	0.45
1:A:113:ARG:HD2	1:A:115:TYR:CZ	2.52	0.45
1:A:56:ILE:N	1:A:56:ILE:HD12	2.31	0.45
1:A:76:SER:N	1:A:79:GLN:NE2	2.49	0.44
1:D:27:ASN:HD21	1:D:43:GLN:HE21	1.65	0.44
1:B:125:GLY:O	1:C:50:MSE:HE2	2.16	0.44
1:C:178:GLY:O	1:C:179:MSE:HB2	2.16	0.44
1:A:18:LEU:CD1	1:A:146:ILE:HD11	2.42	0.44
1:A:49:LEU:HD22	2:A:214:HOH:O	2.16	0.44
1:D:45:GLN:OE1	1:D:53:SER:HB2	2.17	0.44
1:A:50:MSE:HE1	1:D:50:MSE:SE	2.68	0.44
1:B:33:GLN:CA	1:B:33:GLN:HE21	2.29	0.44
1:C:81:THR:O	1:C:84:LEU:HB3	2.18	0.44
1:A:76:SER:CB	1:A:79:GLN:NE2	2.81	0.44
1:D:52:MSE:HG2	1:D:147:SER:HB3	1.96	0.44
1:B:31:LEU:HB3	2:B:220:HOH:O	2.18	0.44
1:C:52:MSE:HE1	1:C:54:ALA:H	1.83	0.43
1:B:21:GLU:C	1:B:164:MSE:HE1	2.38	0.43
1:A:26:VAL:CG1	1:A:144:ILE:HD11	2.49	0.43
1:B:19:MSE:HE2	1:B:19:MSE:O	2.18	0.43
1:A:91:ALA:HB2	1:A:98:VAL:HG11	2.00	0.43
1:A:10:ILE:O	1:A:13:PRO:HD2	2.18	0.43
1:A:43:GLN:NE2	1:A:45:GLN:HE21	2.17	0.43
1:A:161:PHE:HA	1:A:164:MSE:CE	2.45	0.43
1:C:39:ILE:HD12	1:C:39:ILE:N	2.34	0.43
1:A:66:GLY:HA3	1:A:128:CYS:SG	2.58	0.43
1:A:7:LEU:HD13	1:A:7:LEU:C	2.39	0.43
1:B:3:MSE:SE	1:B:7:LEU:HD23	2.68	0.43
1:D:11:VAL:HG13	1:D:172:VAL:HG22	2.01	0.43
1:B:21:GLU:CD	1:B:164:MSE:HE3	2.39	0.43
1:D:37:GLU:HG2	1:D:60:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:ARG:CD	1:C:150:ILE:HG22	2.49	0.42
1:A:89:LEU:HD11	1:A:100:PRO:HG3	2.01	0.42
1:C:127:ARG:HD2	1:C:150:ILE:HG22	2.00	0.42
1:B:149:PRO:HB3	1:C:50:MSE:SE	2.69	0.42
1:B:19:MSE:HE3	1:B:46:CYS:CA	2.50	0.42
1:A:136:GLU:OE2	1:A:136:GLU:N	2.52	0.42
1:A:62:MSE:HE1	1:A:71:PHE:HB2	2.01	0.42
1:B:160:GLU:CG	2:B:213:HOH:O	2.67	0.42
1:B:164:MSE:HB3	1:B:164:MSE:HE2	1.89	0.42
1:B:54:ALA:HB2	1:C:49:LEU:HD22	2.01	0.42
1:C:25:THR:HB	1:C:52:MSE:HG3	2.00	0.42
1:D:19:MSE:HE3	1:D:46:CYS:CB	2.49	0.42
1:A:22:SER:HB2	1:A:161:PHE:CE1	2.54	0.42
1:A:11:VAL:O	1:A:12:HIS:C	2.55	0.42
1:C:133:ILE:HB	1:C:142:ALA:HB3	2.02	0.42
1:A:90:HIS:CD2	1:A:91:ALA:H	2.37	0.42
1:A:8:LEU:HD22	1:A:42:ASP:OD2	2.20	0.41
1:A:64:ALA:HB2	1:A:96:THR:HG23	2.02	0.41
1:C:150:ILE:N	1:C:150:ILE:HD13	2.35	0.41
1:A:133:ILE:CB	1:A:142:ALA:HB3	2.44	0.41
1:C:43:GLN:OE1	1:C:52:MSE:CE	2.64	0.41
1:B:72:LEU:HD21	1:B:80:VAL:HG13	2.03	0.41
1:C:11:VAL:HG12	1:C:11:VAL:O	2.21	0.41
1:A:98:VAL:HB	2:A:206:HOH:O	2.19	0.41
1:D:119:ASP:O	1:D:120:GLU:HB2	2.21	0.41
1:D:179:MSE:O	1:D:180:ARG:HB2	2.21	0.41
1:C:3:MSE:SE	1:C:7:LEU:CD2	3.18	0.41
1:D:18:LEU:CD1	1:D:146:ILE:HD11	2.48	0.41
1:C:86:ARG:HA	1:C:86:ARG:HD3	1.90	0.41
1:B:122:HIS:CD2	1:B:122:HIS:O	2.73	0.41
1:A:76:SER:HB3	1:A:79:GLN:NE2	2.36	0.41
1:C:134:PHE:HD1	1:C:139:GLU:C	2.25	0.41
1:D:177:GLY:C	1:D:179:MSE:N	2.73	0.40
1:A:149:PRO:HB3	1:D:50:MSE:SE	2.71	0.40
1:D:32:ASP:HB3	1:D:35:ASP:O	2.21	0.40
1:C:119:ASP:O	1:C:120:GLU:HB2	2.22	0.40

There are no symmetry-related clashes.

## 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	177/202 (88%)	165 (93%)	10 (6%)	2 (1%)	17	18
1	B	177/202 (88%)	169 (96%)	6 (3%)	2 (1%)	17	18
1	C	176/202 (87%)	158 (90%)	17 (10%)	1 (1%)	30	36
1	D	178/202 (88%)	167 (94%)	9 (5%)	2 (1%)	17	18
All	All	708/808 (88%)	659 (93%)	42 (6%)	7 (1%)	19	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	34	SER
1	B	88	GLY
1	C	75	LEU
1	D	36	HIS
1	A	178	GLY
1	A	137	HIS
1	B	34	SER

### 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	146/158 (92%)	134 (92%)	12 (8%)	14	17
1	B	146/158 (92%)	137 (94%)	9 (6%)	23	30
1	C	146/158 (92%)	138 (94%)	8 (6%)	27	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	147/158 (93%)	142 (97%)	5 (3%)	44	59
All	All	585/632 (93%)	551 (94%)	34 (6%)	25	33

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	5	ARG
1	A	49	LEU
1	A	52	MSE
1	A	65	SER
1	A	85	HIS
1	A	99	SER
1	A	102	HIS
1	A	138	ARG
1	A	144	ILE
1	A	151	SER
1	A	165	VAL
1	B	2	HIS
1	B	19	MSE
1	B	49	LEU
1	B	52	MSE
1	B	72	LEU
1	B	87	LYS
1	B	99	SER
1	B	118	ASP
1	B	146	ILE
1	C	2	HIS
1	C	30	VAL
1	C	52	MSE
1	C	56	ILE
1	C	78	GLU
1	C	141	PHE
1	C	150	ILE
1	C	165	VAL
1	D	19	MSE
1	D	36	HIS
1	D	49	LEU
1	D	52	MSE
1	D	104	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	6	ASN
1	A	48	HIS
1	A	79	GLN
1	A	85	HIS
1	A	90	HIS
1	A	122	HIS
1	B	6	ASN
1	B	33	GLN
1	B	36	HIS
1	B	102	HIS
1	B	122	HIS
1	C	17	ASN
1	C	33	GLN
1	C	36	HIS
1	C	63	HIS
1	C	74	GLN
1	C	122	HIS
1	D	6	ASN
1	D	43	GLN
1	D	63	HIS
1	D	79	GLN
1	D	109	GLN
1	D	122	HIS

### 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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.