



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2023 – 11:40 AM EDT

PDB ID : 2ZNY  
Title : Crystal structure of the FFRP  
Authors : Yamada, M.; Suzuki, M.  
Deposited on : 2008-05-02  
Resolution : 2.59 Å(reported)

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

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

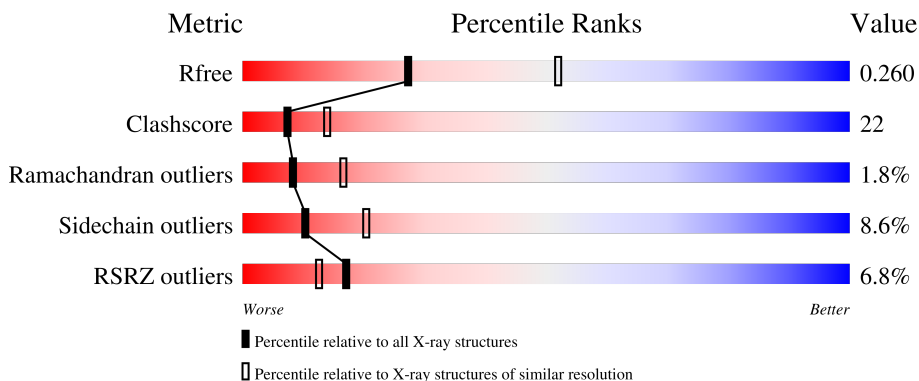
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	171	
1	B	171	
1	C	171	
1	D	171	
1	E	171	

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Mol	Chain	Length	Quality of chain
1	F	171	
1	G	171	
1	H	171	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ARG	A	172	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9491 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 Uncharacterized HTH-type transcriptional regulator PH1519.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	146	1148	736	189	220	3	0	0	0
1	B	146	1148	736	189	220	3	0	0	0
1	C	146	1148	736	189	220	3	0	0	0
1	D	146	1148	736	189	220	3	0	0	0
1	E	146	1148	736	189	220	3	0	0	0
1	F	146	1148	736	189	220	3	0	0	0
1	G	146	1148	736	189	220	3	0	0	0
1	H	146	1148	736	189	220	3	0	0	0

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP O59188
A	2	GLY	-	expression tag	UNP O59188
A	3	SER	-	expression tag	UNP O59188
A	4	SER	-	expression tag	UNP O59188
A	5	HIS	-	expression tag	UNP O59188
A	6	HIS	-	expression tag	UNP O59188
A	7	HIS	-	expression tag	UNP O59188
A	8	HIS	-	expression tag	UNP O59188
A	9	HIS	-	expression tag	UNP O59188
A	10	HIS	-	expression tag	UNP O59188
A	11	SER	-	expression tag	UNP O59188
A	12	SER	-	expression tag	UNP O59188
A	13	GLY	-	expression tag	UNP O59188

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Chain	Residue	Modelled	Actual	Comment	Reference
A	14	LEU	-	expression tag	UNP O59188
A	15	VAL	-	expression tag	UNP O59188
A	16	PRO	-	expression tag	UNP O59188
A	17	ARG	-	expression tag	UNP O59188
A	18	GLY	-	expression tag	UNP O59188
A	19	SER	-	expression tag	UNP O59188
A	20	HIS	-	expression tag	UNP O59188
B	1	MET	-	expression tag	UNP O59188
B	2	GLY	-	expression tag	UNP O59188
B	3	SER	-	expression tag	UNP O59188
B	4	SER	-	expression tag	UNP O59188
B	5	HIS	-	expression tag	UNP O59188
B	6	HIS	-	expression tag	UNP O59188
B	7	HIS	-	expression tag	UNP O59188
B	8	HIS	-	expression tag	UNP O59188
B	9	HIS	-	expression tag	UNP O59188
B	10	HIS	-	expression tag	UNP O59188
B	11	SER	-	expression tag	UNP O59188
B	12	SER	-	expression tag	UNP O59188
B	13	GLY	-	expression tag	UNP O59188
B	14	LEU	-	expression tag	UNP O59188
B	15	VAL	-	expression tag	UNP O59188
B	16	PRO	-	expression tag	UNP O59188
B	17	ARG	-	expression tag	UNP O59188
B	18	GLY	-	expression tag	UNP O59188
B	19	SER	-	expression tag	UNP O59188
B	20	HIS	-	expression tag	UNP O59188
C	1	MET	-	expression tag	UNP O59188
C	2	GLY	-	expression tag	UNP O59188
C	3	SER	-	expression tag	UNP O59188
C	4	SER	-	expression tag	UNP O59188
C	5	HIS	-	expression tag	UNP O59188
C	6	HIS	-	expression tag	UNP O59188
C	7	HIS	-	expression tag	UNP O59188
C	8	HIS	-	expression tag	UNP O59188
C	9	HIS	-	expression tag	UNP O59188
C	10	HIS	-	expression tag	UNP O59188
C	11	SER	-	expression tag	UNP O59188
C	12	SER	-	expression tag	UNP O59188
C	13	GLY	-	expression tag	UNP O59188
C	14	LEU	-	expression tag	UNP O59188
C	15	VAL	-	expression tag	UNP O59188

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Chain	Residue	Modelled	Actual	Comment	Reference
C	16	PRO	-	expression tag	UNP O59188
C	17	ARG	-	expression tag	UNP O59188
C	18	GLY	-	expression tag	UNP O59188
C	19	SER	-	expression tag	UNP O59188
C	20	HIS	-	expression tag	UNP O59188
D	1	MET	-	expression tag	UNP O59188
D	2	GLY	-	expression tag	UNP O59188
D	3	SER	-	expression tag	UNP O59188
D	4	SER	-	expression tag	UNP O59188
D	5	HIS	-	expression tag	UNP O59188
D	6	HIS	-	expression tag	UNP O59188
D	7	HIS	-	expression tag	UNP O59188
D	8	HIS	-	expression tag	UNP O59188
D	9	HIS	-	expression tag	UNP O59188
D	10	HIS	-	expression tag	UNP O59188
D	11	SER	-	expression tag	UNP O59188
D	12	SER	-	expression tag	UNP O59188
D	13	GLY	-	expression tag	UNP O59188
D	14	LEU	-	expression tag	UNP O59188
D	15	VAL	-	expression tag	UNP O59188
D	16	PRO	-	expression tag	UNP O59188
D	17	ARG	-	expression tag	UNP O59188
D	18	GLY	-	expression tag	UNP O59188
D	19	SER	-	expression tag	UNP O59188
D	20	HIS	-	expression tag	UNP O59188
E	1	MET	-	expression tag	UNP O59188
E	2	GLY	-	expression tag	UNP O59188
E	3	SER	-	expression tag	UNP O59188
E	4	SER	-	expression tag	UNP O59188
E	5	HIS	-	expression tag	UNP O59188
E	6	HIS	-	expression tag	UNP O59188
E	7	HIS	-	expression tag	UNP O59188
E	8	HIS	-	expression tag	UNP O59188
E	9	HIS	-	expression tag	UNP O59188
E	10	HIS	-	expression tag	UNP O59188
E	11	SER	-	expression tag	UNP O59188
E	12	SER	-	expression tag	UNP O59188
E	13	GLY	-	expression tag	UNP O59188
E	14	LEU	-	expression tag	UNP O59188
E	15	VAL	-	expression tag	UNP O59188
E	16	PRO	-	expression tag	UNP O59188
E	17	ARG	-	expression tag	UNP O59188

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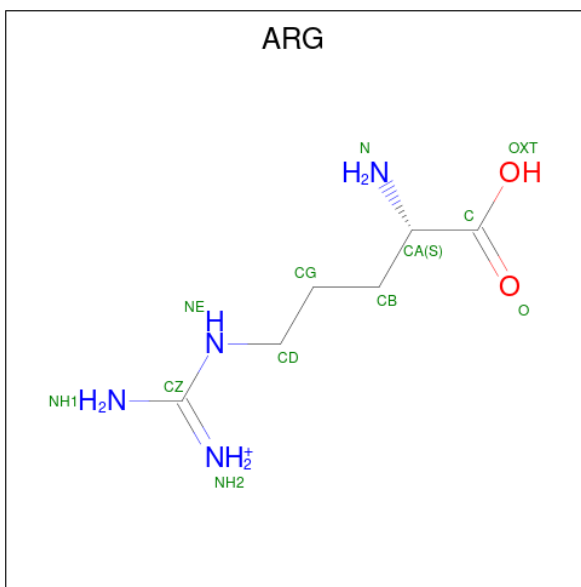
Chain	Residue	Modelled	Actual	Comment	Reference
E	18	GLY	-	expression tag	UNP O59188
E	19	SER	-	expression tag	UNP O59188
E	20	HIS	-	expression tag	UNP O59188
F	1	MET	-	expression tag	UNP O59188
F	2	GLY	-	expression tag	UNP O59188
F	3	SER	-	expression tag	UNP O59188
F	4	SER	-	expression tag	UNP O59188
F	5	HIS	-	expression tag	UNP O59188
F	6	HIS	-	expression tag	UNP O59188
F	7	HIS	-	expression tag	UNP O59188
F	8	HIS	-	expression tag	UNP O59188
F	9	HIS	-	expression tag	UNP O59188
F	10	HIS	-	expression tag	UNP O59188
F	11	SER	-	expression tag	UNP O59188
F	12	SER	-	expression tag	UNP O59188
F	13	GLY	-	expression tag	UNP O59188
F	14	LEU	-	expression tag	UNP O59188
F	15	VAL	-	expression tag	UNP O59188
F	16	PRO	-	expression tag	UNP O59188
F	17	ARG	-	expression tag	UNP O59188
F	18	GLY	-	expression tag	UNP O59188
F	19	SER	-	expression tag	UNP O59188
F	20	HIS	-	expression tag	UNP O59188
G	1	MET	-	expression tag	UNP O59188
G	2	GLY	-	expression tag	UNP O59188
G	3	SER	-	expression tag	UNP O59188
G	4	SER	-	expression tag	UNP O59188
G	5	HIS	-	expression tag	UNP O59188
G	6	HIS	-	expression tag	UNP O59188
G	7	HIS	-	expression tag	UNP O59188
G	8	HIS	-	expression tag	UNP O59188
G	9	HIS	-	expression tag	UNP O59188
G	10	HIS	-	expression tag	UNP O59188
G	11	SER	-	expression tag	UNP O59188
G	12	SER	-	expression tag	UNP O59188
G	13	GLY	-	expression tag	UNP O59188
G	14	LEU	-	expression tag	UNP O59188
G	15	VAL	-	expression tag	UNP O59188
G	16	PRO	-	expression tag	UNP O59188
G	17	ARG	-	expression tag	UNP O59188
G	18	GLY	-	expression tag	UNP O59188
G	19	SER	-	expression tag	UNP O59188

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Chain	Residue	Modelled	Actual	Comment	Reference
G	20	HIS	-	expression tag	UNP O59188
H	1	MET	-	expression tag	UNP O59188
H	2	GLY	-	expression tag	UNP O59188
H	3	SER	-	expression tag	UNP O59188
H	4	SER	-	expression tag	UNP O59188
H	5	HIS	-	expression tag	UNP O59188
H	6	HIS	-	expression tag	UNP O59188
H	7	HIS	-	expression tag	UNP O59188
H	8	HIS	-	expression tag	UNP O59188
H	9	HIS	-	expression tag	UNP O59188
H	10	HIS	-	expression tag	UNP O59188
H	11	SER	-	expression tag	UNP O59188
H	12	SER	-	expression tag	UNP O59188
H	13	GLY	-	expression tag	UNP O59188
H	14	LEU	-	expression tag	UNP O59188
H	15	VAL	-	expression tag	UNP O59188
H	16	PRO	-	expression tag	UNP O59188
H	17	ARG	-	expression tag	UNP O59188
H	18	GLY	-	expression tag	UNP O59188
H	19	SER	-	expression tag	UNP O59188
H	20	HIS	-	expression tag	UNP O59188

- Molecule 2 is ARGinine (three-letter code: ARG) (formula: C<sub>6</sub>H<sub>15</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	12	6	4	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			12	6	4	2		
2	D	1	Total	C	N	O	0	0
			12	6	4	2		
2	F	1	Total	C	N	O	0	0
			12	6	4	2		
2	F	1	Total	C	N	O	0	0
			12	6	4	2		
2	G	1	Total	C	N	O	0	0
			12	6	4	2		

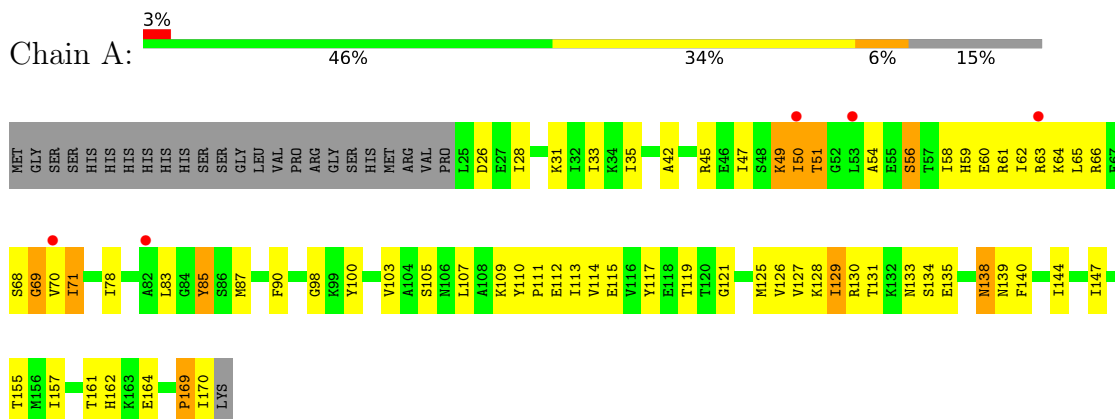
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	18	Total	O	0	0
			18	18		
3	C	57	Total	O	0	0
			57	57		
3	D	29	Total	O	0	0
			29	29		
3	E	36	Total	O	0	0
			36	36		
3	F	34	Total	O	0	0
			34	34		
3	G	22	Total	O	0	0
			22	22		
3	H	19	Total	O	0	0
			19	19		

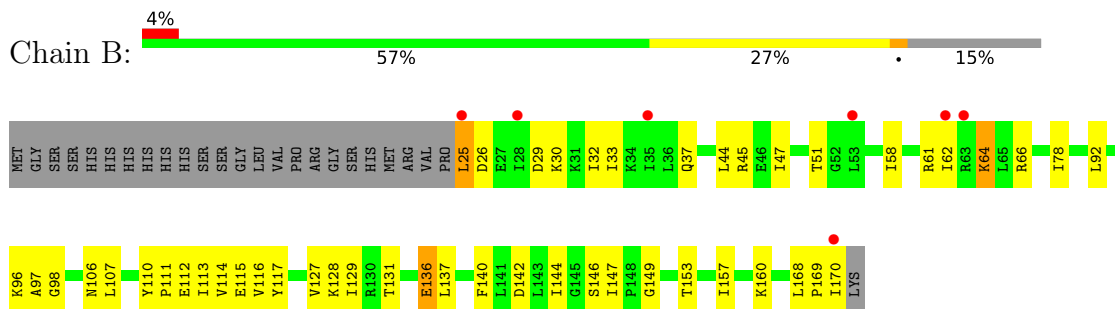
### 3 Residue-property plots [i](#)

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.

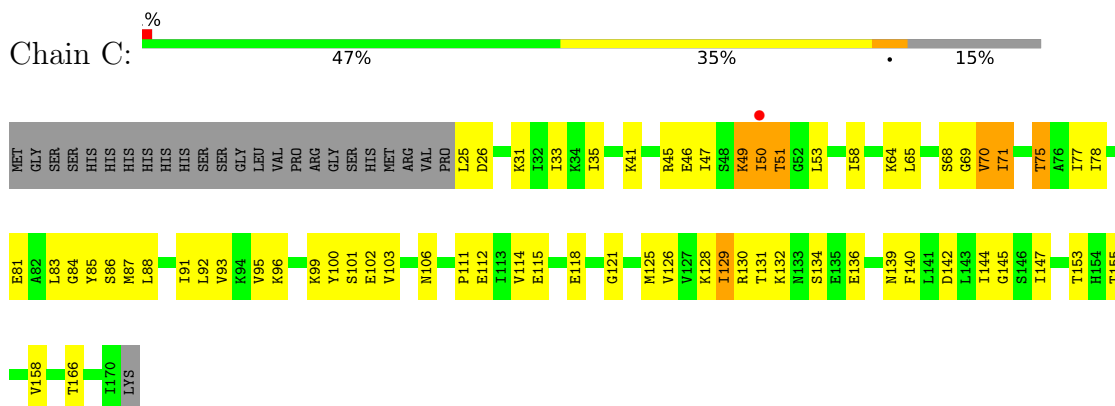
- Molecule 1: Uncharacterized HTH-type transcriptional regulator PH1519



- Molecule 1: Uncharacterized HTH-type transcriptional regulator PH1519

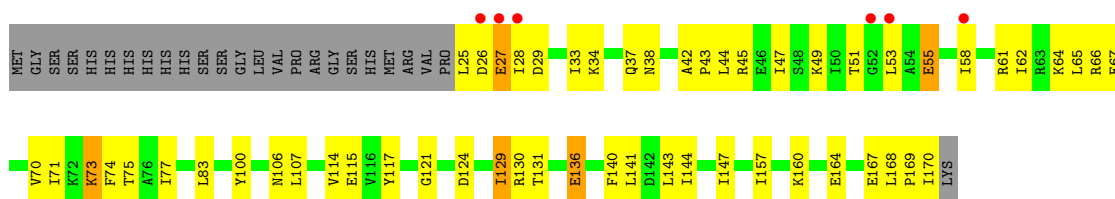


- Molecule 1: Uncharacterized HTH-type transcriptional regulator PH1519



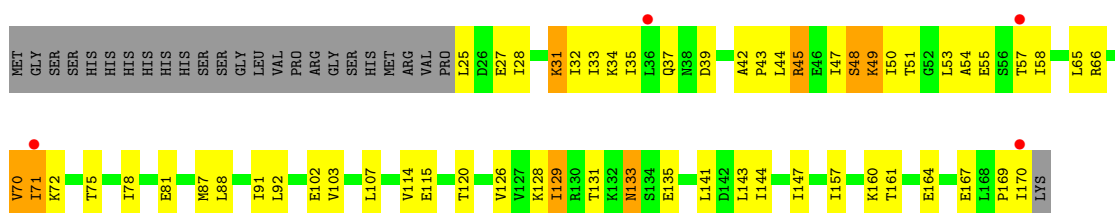
- Molecule 1: Uncharacterized HTH-type transcriptional regulator PH1519

Chain D:



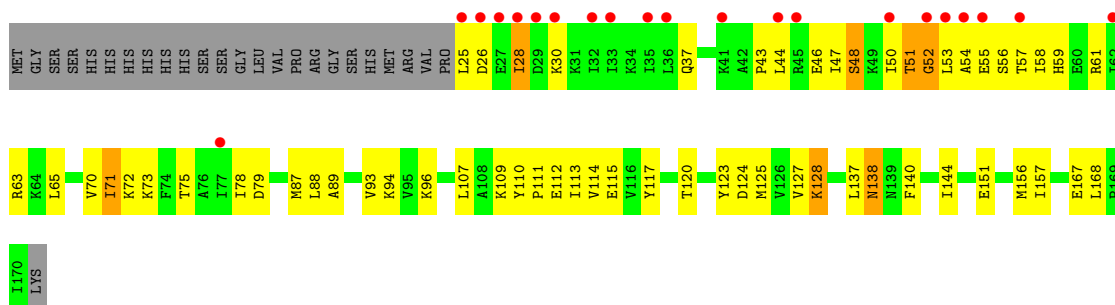
- Molecule 1: Uncharacterized HTH-type transcriptional regulator PH1519

Chain E:



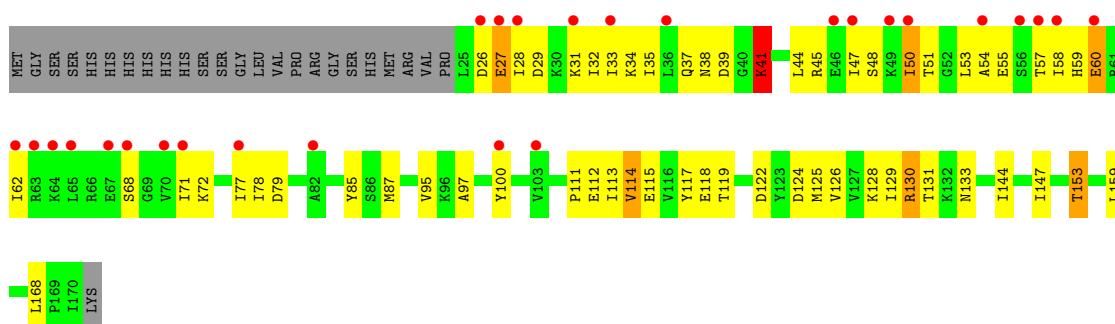
- Molecule 1: Uncharacterized HTH-type transcriptional regulator PH1519

Chain F:

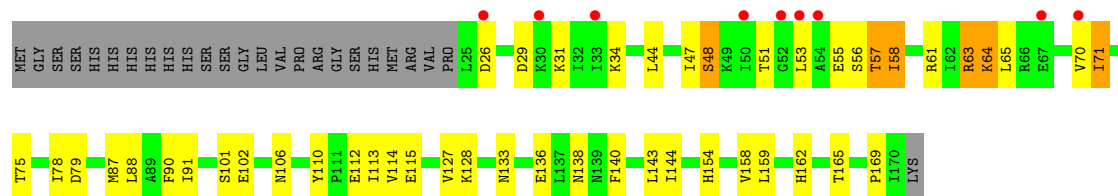


- Molecule 1: Uncharacterized HTH-type transcriptional regulator PH1519

Chain G:



- Molecule 1: Uncharacterized HTH-type transcriptional regulator PH1519



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.31Å 73.50Å 103.06Å 90.00° 98.47° 90.00°	Depositor
Resolution (Å)	50.00 – 2.59 49.53 – 2.59	Depositor EDS
% Data completeness (in resolution range)	95.2 (50.00-2.59) 93.0 (49.53-2.59)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.79 (at 2.58Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.254 , 0.258 0.254 , 0.260	Depositor DCC
$R_{free}$ test set	4561 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.2	Xtrriage
Anisotropy	0.677	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.056 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9491	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.09% 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	0.66	1/1163 (0.1%)	0.72	0/1567
1	B	0.59	0/1163	0.73	1/1567 (0.1%)
1	C	0.67	0/1163	0.79	0/1567
1	D	0.70	0/1163	0.79	0/1567
1	E	0.61	0/1163	0.77	0/1567
1	F	0.60	0/1163	0.72	0/1567
1	G	0.54	0/1163	0.66	0/1567
1	H	0.59	0/1163	0.74	0/1567
All	All	0.62	1/9304 (0.0%)	0.74	1/12536 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	SER	CB-OG	9.69	1.54	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	LEU	CA-CB-CG	5.23	127.34	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1148	0	1209	75	0
1	B	1148	0	1209	40	0
1	C	1148	0	1209	75	0
1	D	1148	0	1209	76	0
1	E	1148	0	1209	51	0
1	F	1148	0	1209	56	0
1	G	1148	0	1209	59	0
1	H	1148	0	1209	43	1
2	A	12	0	12	6	0
2	C	12	0	12	3	0
2	D	12	0	12	5	0
2	F	24	0	24	1	0
2	G	12	0	12	2	0
3	A	20	0	0	6	0
3	B	18	0	0	1	1
3	C	57	0	0	6	0
3	D	29	0	0	1	0
3	E	36	0	0	1	0
3	F	34	0	0	1	0
3	G	22	0	0	4	0
3	H	19	0	0	0	0
All	All	9491	0	9744	424	1

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 22.

All (424) 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:D:65:LEU:HB3	1:D:71:ILE:HD13	1.28	1.10
1:D:33:ILE:HD11	1:D:71:ILE:HD11	1.38	1.04
1:F:96:LYS:HD2	1:F:151:GLU:OE2	1.59	1.01
1:A:35:ILE:HG21	1:A:47:ILE:HD12	1.41	1.01
1:C:77:ILE:HD11	1:D:75:THR:HG22	1.44	1.00
1:A:129:ILE:CD1	1:A:131:THR:HG23	1.92	0.98
1:D:47:ILE:O	1:D:51:THR:HG22	1.64	0.97
1:F:88:LEU:HD11	1:F:128:LYS:HD2	1.48	0.95
1:A:65:LEU:HB3	1:A:71:ILE:HD13	1.49	0.94
1:B:106:ASN:HD22	1:B:147:ILE:HD12	1.32	0.91
1:B:106:ASN:ND2	1:B:147:ILE:HD12	1.87	0.90
1:G:130:ARG:HG3	1:G:130:ARG:HH11	1.33	0.89
1:F:89:ALA:HB2	1:F:157:ILE:HD13	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:ILE:HD13	1:E:31:LYS:HE3	1.55	0.89
1:C:129:ILE:HD12	1:C:131:THR:HG23	1.55	0.88
1:C:129:ILE:HD13	1:C:130:ARG:N	1.89	0.87
1:A:129:ILE:HD11	1:A:131:THR:CG2	2.05	0.87
1:C:35:ILE:HG21	1:C:47:ILE:CD1	2.07	0.84
1:D:65:LEU:HB3	1:D:71:ILE:CD1	2.07	0.84
1:A:110:TYR:HB2	1:A:113:ILE:HD13	1.59	0.83
1:C:129:ILE:CD1	1:C:131:THR:HG23	2.09	0.83
1:C:31:LYS:NZ	1:C:50:ILE:HD11	1.93	0.82
1:A:138:ASN:HD22	1:A:139:ASN:N	1.76	0.82
1:A:70:VAL:HG12	1:A:71:ILE:HD12	1.60	0.81
1:D:25:LEU:N	3:D:173:HOH:O	2.15	0.80
1:H:110:TYR:CB	1:H:113:ILE:HD13	2.13	0.79
2:A:172:ARG:OXT	1:C:155:THR:OG1	2.00	0.79
1:D:51:THR:HG23	1:D:53:LEU:H	1.47	0.78
1:C:35:ILE:HG21	1:C:47:ILE:HD13	1.64	0.78
1:E:55:GLU:HA	1:E:58:ILE:HD12	1.66	0.78
1:D:44:LEU:HA	1:D:47:ILE:HD12	1.63	0.78
1:A:129:ILE:HD11	1:A:131:THR:HG23	1.61	0.78
1:F:115:GLU:HB2	1:F:128:LYS:HB3	1.66	0.78
1:G:113:ILE:HG12	1:G:129:ILE:HD13	1.66	0.77
1:F:87:MET:SD	1:F:157:ILE:HD12	2.24	0.77
1:F:140:PHE:O	1:F:144:ILE:HG12	1.85	0.77
1:E:34:LYS:HE2	1:E:170:ILE:HB	1.65	0.77
1:A:28:ILE:HB	1:A:61:ARG:NH2	2.00	0.76
1:A:65:LEU:O	1:A:70:VAL:O	2.02	0.76
1:F:88:LEU:HD11	1:F:128:LYS:CD	2.15	0.76
1:H:70:VAL:O	1:H:71:ILE:HG12	1.86	0.76
1:C:46:GLU:O	1:C:50:ILE:HG22	1.85	0.75
1:H:63:ARG:CZ	1:H:63:ARG:HB3	2.17	0.74
1:G:113:ILE:CG1	1:G:129:ILE:HD13	2.17	0.74
1:E:33:ILE:HB	1:F:78:ILE:HD11	1.70	0.74
1:D:70:VAL:HG12	1:D:71:ILE:HD12	1.69	0.74
1:G:130:ARG:NH1	3:G:187:HOH:O	2.16	0.73
1:C:65:LEU:O	1:C:70:VAL:O	2.07	0.73
1:H:115:GLU:HB2	1:H:128:LYS:HB3	1.70	0.72
1:A:42:ALA:HB1	1:A:47:ILE:HD11	1.71	0.72
1:A:111:PRO:HB2	1:B:169:PRO:HB3	1.70	0.72
1:A:135:GLU:O	1:A:138:ASN:ND2	2.22	0.72
1:D:129:ILE:HD12	1:D:131:THR:HG23	1.70	0.72
1:E:28:ILE:HG21	1:E:53:LEU:HD21	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:LYS:HE2	3:C:213:HOH:O	1.91	0.71
1:H:110:TYR:HB3	1:H:113:ILE:HD13	1.71	0.71
1:G:57:THR:HA	1:G:60:GLU:HB3	1.73	0.71
1:H:48:SER:OG	1:H:53:LEU:O	2.07	0.71
1:B:110:TYR:HB2	1:B:113:ILE:HD13	1.72	0.70
1:C:78:ILE:HD12	1:D:33:ILE:HD12	1.72	0.70
1:B:140:PHE:O	1:B:144:ILE:HG12	1.91	0.70
1:C:75:THR:HG22	1:D:77:ILE:HD11	1.73	0.70
1:H:51:THR:HG23	1:H:53:LEU:H	1.56	0.70
1:H:48:SER:HA	1:H:51:THR:HG22	1.73	0.70
1:F:89:ALA:HB2	1:F:157:ILE:CD1	2.22	0.69
1:C:92:LEU:CD2	1:C:126:VAL:HG22	2.22	0.69
1:A:71:ILE:N	3:A:183:HOH:O	2.25	0.69
1:A:110:TYR:CB	1:A:113:ILE:HD13	2.22	0.69
1:H:47:ILE:O	1:H:51:THR:HG22	1.93	0.69
1:E:28:ILE:HD13	1:E:31:LYS:CE	2.22	0.68
1:G:29:ASP:OD2	1:G:32:ILE:HD12	1.93	0.68
1:G:59:HIS:O	1:G:62:ILE:HG22	1.92	0.68
1:H:91:ILE:HD13	1:H:144:ILE:HD13	1.75	0.68
1:A:129:ILE:HD13	1:A:129:ILE:C	2.14	0.68
1:B:37:GLN:NE2	1:B:168:LEU:H	1.92	0.68
1:F:47:ILE:O	1:F:51:THR:HG22	1.94	0.68
1:C:111:PRO:HB2	1:D:169:PRO:HB3	1.74	0.68
1:C:131:THR:HB	1:C:136:GLU:HB3	1.76	0.68
1:C:77:ILE:HD11	1:D:75:THR:CG2	2.22	0.67
1:G:27:GLU:OE1	1:G:28:ILE:HD13	1.95	0.67
1:E:45:ARG:NH1	1:E:55:GLU:OE1	2.28	0.67
1:H:110:TYR:HB2	1:H:113:ILE:HD13	1.77	0.67
1:C:31:LYS:HZ3	1:C:50:ILE:HD11	1.59	0.67
1:B:37:GLN:HE22	1:B:168:LEU:H	1.41	0.67
1:F:25:LEU:HD21	1:F:30:LYS:HG3	1.76	0.67
1:D:47:ILE:HD13	1:D:58:ILE:HG21	1.76	0.67
1:G:130:ARG:HG3	3:G:187:HOH:O	1.95	0.66
1:B:137:LEU:HD21	1:B:157:ILE:HD11	1.77	0.66
1:C:85:TYR:OH	1:D:169:PRO:HG2	1.95	0.66
1:D:47:ILE:CD1	1:D:58:ILE:HG21	2.26	0.66
1:A:129:ILE:HD13	1:A:130:ARG:N	2.11	0.66
1:D:44:LEU:HD23	1:D:47:ILE:HD12	1.78	0.66
1:D:107:LEU:CD2	1:D:144:ILE:HD12	2.26	0.66
1:E:129:ILE:HD12	1:E:131:THR:HG23	1.77	0.66
1:D:157:ILE:HG12	1:E:157:ILE:HD12	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:LYS:HZ1	1:C:50:ILE:HD11	1.59	0.65
1:G:35:ILE:HG21	1:G:47:ILE:CD1	2.26	0.65
1:E:28:ILE:CG2	1:E:53:LEU:HD21	2.27	0.65
1:G:115:GLU:HB2	1:G:128:LYS:HB3	1.79	0.64
1:H:48:SER:HA	1:H:51:THR:CG2	2.27	0.64
1:D:106:ASN:CG	1:D:147:ILE:HD12	2.18	0.64
1:C:78:ILE:HG12	1:D:37:GLN:HE21	1.63	0.64
1:C:47:ILE:HG22	1:C:58:ILE:HD13	1.80	0.63
1:A:28:ILE:HB	1:A:61:ARG:HH22	1.62	0.63
1:E:51:THR:HG23	1:E:53:LEU:H	1.62	0.63
1:B:107:LEU:CD2	1:B:144:ILE:HD12	2.28	0.63
1:G:28:ILE:O	1:G:32:ILE:HG13	1.99	0.63
1:C:77:ILE:HD13	1:D:73:LYS:HG3	1.80	0.62
1:F:65:LEU:HB3	1:F:71:ILE:HD13	1.81	0.62
1:G:48:SER:HB2	1:G:55:GLU:HB3	1.82	0.62
1:A:63:ARG:HB3	3:A:179:HOH:O	1.98	0.62
1:A:129:ILE:HD11	1:A:131:THR:HG22	1.82	0.62
1:F:88:LEU:CD1	1:F:128:LYS:HD2	2.26	0.61
1:H:114:VAL:HG12	1:H:115:GLU:HG3	1.81	0.61
1:A:112:GLU:HG2	1:A:140:PHE:CE1	2.35	0.61
1:C:139:ASN:OD1	3:C:211:HOH:O	2.16	0.61
1:D:47:ILE:HD13	1:D:58:ILE:CG2	2.30	0.61
1:A:98:GLY:HA2	3:A:178:HOH:O	1.99	0.61
1:G:85:TYR:OH	1:H:169:PRO:HB2	2.00	0.61
1:A:56:SER:HB3	3:A:186:HOH:O	2.00	0.61
1:C:101:SER:HB2	3:C:199:HOH:O	2.01	0.61
1:D:53:LEU:HB2	1:D:58:ILE:HD11	1.82	0.61
1:C:115:GLU:HB2	1:C:128:LYS:HB3	1.81	0.61
1:F:70:VAL:HG12	1:F:71:ILE:HD12	1.83	0.61
1:D:44:LEU:HD23	1:D:47:ILE:CD1	2.31	0.60
1:E:48:SER:OG	1:E:53:LEU:O	2.17	0.60
1:C:101:SER:CB	3:C:199:HOH:O	2.49	0.60
1:D:121:GLY:O	2:D:172:ARG:N	2.34	0.60
1:H:113:ILE:HD12	1:H:113:ILE:N	2.17	0.60
1:E:47:ILE:O	1:E:51:THR:HG22	2.02	0.60
1:G:97:ALA:HA	1:G:100:TYR:HE1	1.66	0.60
1:A:119:THR:HG21	1:A:126:VAL:HG23	1.83	0.59
1:C:92:LEU:HD23	1:C:126:VAL:HG22	1.84	0.59
1:B:137:LEU:CD2	1:B:157:ILE:HD11	2.33	0.59
1:E:161:THR:HG23	1:F:117:TYR:CE2	2.37	0.58
1:F:138:ASN:HB2	1:G:159:LEU:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:LEU:N	3:C:198:HOH:O	2.35	0.58
1:F:28:ILE:HB	1:F:61:ARG:NH2	2.19	0.58
1:G:122:ASP:H	1:H:154:HIS:CE1	2.21	0.58
1:A:62:ILE:O	1:A:66:ARG:HG3	2.04	0.58
1:D:100:TYR:CZ	2:D:172:ARG:HD2	2.39	0.57
1:D:26:ASP:HB3	1:D:29:ASP:OD1	2.04	0.57
1:D:131:THR:HB	1:D:136:GLU:HB3	1.87	0.57
1:D:28:ILE:CG2	1:D:53:LEU:HD11	2.35	0.57
1:B:112:GLU:C	1:B:129:ILE:HD12	2.25	0.57
1:B:112:GLU:O	1:B:129:ILE:HD12	2.05	0.57
1:F:137:LEU:HD22	1:F:157:ILE:HD11	1.86	0.57
1:D:71:ILE:HD12	1:D:71:ILE:N	2.20	0.57
1:E:143:LEU:O	1:E:147:ILE:HD12	2.05	0.57
1:B:115:GLU:HB3	1:B:117:TYR:CE1	2.41	0.56
1:D:157:ILE:HG12	1:E:157:ILE:CD1	2.34	0.56
1:E:169:PRO:C	1:E:170:ILE:HD12	2.26	0.56
1:G:78:ILE:HD13	1:H:71:ILE:HD13	1.86	0.56
1:A:129:ILE:CD1	1:A:131:THR:CG2	2.65	0.56
1:A:162:HIS:HB2	1:B:116:VAL:HG12	1.85	0.56
1:C:130:ARG:HD2	1:D:168:LEU:CD2	2.36	0.56
1:E:28:ILE:O	1:E:32:ILE:HD13	2.06	0.56
1:B:26:ASP:O	1:B:30:LYS:HG3	2.06	0.56
1:D:44:LEU:HA	1:D:47:ILE:CD1	2.35	0.56
1:D:157:ILE:CD1	1:F:120:THR:HG21	2.36	0.56
1:D:157:ILE:CG1	1:E:157:ILE:HD12	2.36	0.56
1:A:113:ILE:N	1:A:113:ILE:HD12	2.20	0.56
1:E:65:LEU:HB3	1:E:71:ILE:HD13	1.86	0.56
1:G:35:ILE:HG21	1:G:47:ILE:HD13	1.88	0.56
1:G:77:ILE:N	1:G:77:ILE:HD12	2.20	0.56
1:F:89:ALA:CB	1:F:157:ILE:HD13	2.32	0.55
1:A:138:ASN:HD22	1:A:139:ASN:H	1.50	0.55
1:E:37:GLN:CD	1:F:78:ILE:HD12	2.27	0.55
1:G:130:ARG:HG3	1:G:130:ARG:NH1	2.12	0.55
1:A:155:THR:HG22	1:A:157:ILE:HD12	1.89	0.55
1:F:109:LYS:NZ	3:F:207:HOH:O	2.34	0.55
1:A:50:ILE:O	1:A:50:ILE:HD13	2.06	0.55
1:F:137:LEU:CD2	1:F:157:ILE:HD11	2.36	0.55
1:G:100:TYR:HB2	3:G:186:HOH:O	2.06	0.55
1:A:35:ILE:CG2	1:A:47:ILE:HD12	2.28	0.55
1:G:153:THR:OG1	2:G:172:ARG:OXT	2.25	0.55
1:H:112:GLU:OE1	1:H:112:GLU:N	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:129:ILE:HD12	1:E:131:THR:CG2	2.36	0.54
1:G:37:GLN:NE2	1:G:168:LEU:H	2.05	0.54
1:E:33:ILE:HB	1:F:78:ILE:CD1	2.37	0.54
1:G:95:VAL:HG21	1:G:125:MET:SD	2.48	0.54
1:E:54:ALA:HB3	1:E:57:THR:HG23	1.89	0.54
1:B:142:ASP:OD1	2:D:172:ARG:NH2	2.42	0.53
1:B:131:THR:HB	1:B:136:GLU:HB3	1.91	0.53
1:A:129:ILE:HD12	1:A:131:THR:HG23	1.85	0.53
1:F:37:GLN:HB3	1:F:167:GLU:HG2	1.90	0.53
1:F:110:TYR:CD1	1:F:113:ILE:HD12	2.43	0.53
1:A:85:TYR:CZ	1:B:169:PRO:HG2	2.43	0.53
1:C:140:PHE:O	1:C:144:ILE:HD13	2.09	0.53
1:A:87:MET:HE2	1:A:133:ASN:HA	1.89	0.53
1:F:28:ILE:N	1:F:28:ILE:HD12	2.23	0.53
1:A:70:VAL:HA	3:A:183:HOH:O	2.08	0.53
1:D:34:LYS:HB3	1:D:170:ILE:HG13	1.90	0.53
1:E:27:GLU:OE1	1:E:31:LYS:HD3	2.08	0.53
1:E:37:GLN:HB3	1:E:167:GLU:HG2	1.90	0.53
1:E:44:LEU:HB3	1:E:55:GLU:HB2	1.91	0.53
1:C:75:THR:CG2	1:D:77:ILE:HD11	2.38	0.53
1:F:44:LEU:HB3	1:F:55:GLU:HB2	1.91	0.53
1:G:77:ILE:CD1	1:H:75:THR:HG22	2.39	0.53
1:H:90:PHE:HA	1:H:127:VAL:O	2.09	0.53
1:C:95:VAL:HG12	1:C:96:LYS:O	2.09	0.52
1:G:130:ARG:HH11	1:G:130:ARG:CG	2.12	0.52
1:A:144:ILE:HA	1:A:147:ILE:CD1	2.39	0.52
1:F:107:LEU:CD2	1:F:144:ILE:HD12	2.39	0.52
1:A:47:ILE:O	1:A:51:THR:HB	2.10	0.52
1:E:25:LEU:N	3:E:187:HOH:O	2.43	0.52
1:B:169:PRO:C	1:B:170:ILE:HD12	2.30	0.52
1:D:77:ILE:HD12	1:D:77:ILE:N	2.25	0.52
1:C:102:GLU:HG2	3:C:201:HOH:O	2.09	0.52
1:A:54:ALA:O	1:A:58:ILE:HD13	2.09	0.52
1:F:28:ILE:HD12	1:F:28:ILE:H	1.75	0.52
1:G:113:ILE:HG13	1:G:129:ILE:HD13	1.93	0.51
1:C:77:ILE:H	1:C:77:ILE:HD12	1.74	0.51
1:E:35:ILE:HD11	1:E:50:ILE:HD13	1.93	0.51
1:G:78:ILE:CD1	1:H:71:ILE:HD13	2.40	0.51
1:C:115:GLU:CD	1:C:128:LYS:HE2	2.31	0.51
1:B:107:LEU:HD23	1:B:144:ILE:HD12	1.92	0.51
1:A:161:THR:HG22	1:A:161:THR:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:GLU:HB2	1:B:128:LYS:HB3	1.93	0.50
1:C:77:ILE:HD12	1:C:77:ILE:N	2.26	0.50
1:E:144:ILE:HA	1:E:147:ILE:HD13	1.94	0.50
1:A:31:LYS:O	1:A:35:ILE:HG12	2.11	0.50
1:B:47:ILE:HG22	1:B:58:ILE:HD13	1.94	0.50
1:G:78:ILE:HG22	1:G:79:ASP:N	2.27	0.50
1:B:92:LEU:O	1:B:153:THR:HA	2.12	0.50
1:C:91:ILE:N	1:C:91:ILE:HD12	2.26	0.50
1:F:47:ILE:HG22	1:F:58:ILE:HD13	1.93	0.50
1:H:26:ASP:HB3	1:H:29:ASP:OD2	2.11	0.50
1:A:33:ILE:HG13	1:A:170:ILE:HD11	1.94	0.49
1:G:54:ALA:O	1:G:58:ILE:HG12	2.11	0.49
1:G:112:GLU:O	1:G:129:ILE:HD12	2.12	0.49
1:G:114:VAL:HG22	1:H:165:THR:O	2.12	0.49
1:F:96:LYS:CD	1:F:151:GLU:OE2	2.46	0.49
1:C:41:LYS:HD3	1:D:74:PHE:CD2	2.47	0.49
1:D:130:ARG:NH2	1:D:164:GLU:OE2	2.45	0.49
1:G:112:GLU:C	1:G:129:ILE:HD12	2.33	0.49
1:G:122:ASP:H	1:H:154:HIS:HE1	1.61	0.49
1:H:113:ILE:N	1:H:113:ILE:CD1	2.75	0.49
1:G:111:PRO:HD2	1:G:112:GLU:OE1	2.11	0.49
1:C:35:ILE:CG2	1:C:47:ILE:CD1	2.88	0.49
1:D:115:GLU:HB3	1:D:117:TYR:CE1	2.48	0.49
1:G:118:GLU:OE1	1:H:162:HIS:HE1	1.96	0.49
1:B:96:LYS:O	1:B:98:GLY:N	2.45	0.49
1:G:51:THR:HG23	1:G:53:LEU:H	1.78	0.49
1:G:119:THR:HG21	1:G:126:VAL:HG23	1.94	0.49
1:D:33:ILE:HD11	1:D:71:ILE:CD1	2.26	0.48
1:F:71:ILE:HD12	1:F:71:ILE:N	2.28	0.48
1:G:55:GLU:HA	1:G:58:ILE:HB	1.95	0.48
1:A:144:ILE:HA	1:A:147:ILE:HD12	1.94	0.48
1:C:70:VAL:O	1:C:71:ILE:HB	2.13	0.48
1:H:87:MET:CE	1:H:133:ASN:HA	2.42	0.48
1:C:118:GLU:HG3	1:D:160:LYS:HB2	1.96	0.48
1:E:115:GLU:CD	1:E:128:LYS:HE3	2.33	0.48
1:G:87:MET:HB3	1:G:131:THR:O	2.14	0.48
1:F:110:TYR:HB2	1:F:113:ILE:HD12	1.95	0.48
1:A:71:ILE:HD12	1:A:71:ILE:N	2.29	0.48
1:F:53:LEU:HD12	1:F:57:THR:HB	1.95	0.48
1:H:56:SER:C	1:H:58:ILE:H	2.17	0.48
1:C:47:ILE:CG2	1:C:58:ILE:HD13	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:GLY:O	1:C:132:LYS:HG2	2.14	0.48
1:F:73:LYS:HE2	1:F:75:THR:HB	1.95	0.47
1:G:50:ILE:HD13	1:G:50:ILE:O	2.14	0.47
1:C:88:LEU:HD11	1:C:128:LYS:HD2	1.96	0.47
1:D:70:VAL:HG12	1:D:71:ILE:CD1	2.43	0.47
1:A:47:ILE:HD13	1:A:47:ILE:N	2.29	0.47
2:A:172:ARG:C	1:C:155:THR:HG1	2.14	0.47
1:F:124:ASP:OD1	2:F:172:ARG:N	2.47	0.47
1:G:71:ILE:HD13	1:H:78:ILE:HG12	1.96	0.47
1:A:78:ILE:HD13	1:B:37:GLN:CG	2.44	0.47
1:E:92:LEU:HD22	1:E:126:VAL:HG22	1.96	0.47
1:F:28:ILE:HB	1:F:61:ARG:HH22	1.79	0.47
1:F:44:LEU:HD11	1:F:59:HIS:HB2	1.97	0.47
1:F:110:TYR:HD1	1:F:113:ILE:HD12	1.80	0.47
1:C:35:ILE:HG21	1:C:47:ILE:HD11	1.94	0.47
1:D:42:ALA:HA	1:D:43:PRO:HD3	1.78	0.47
1:D:47:ILE:HG21	1:D:58:ILE:CG2	2.45	0.47
1:D:107:LEU:HD23	1:D:144:ILE:HD12	1.95	0.47
1:E:170:ILE:HD12	1:E:170:ILE:N	2.30	0.47
1:D:53:LEU:HB2	1:D:58:ILE:CD1	2.45	0.47
1:D:62:ILE:O	1:D:66:ARG:HG3	2.15	0.47
1:A:138:ASN:HD22	1:A:138:ASN:C	2.18	0.46
1:C:129:ILE:CD1	1:C:131:THR:CG2	2.88	0.46
1:A:47:ILE:O	1:A:50:ILE:HG22	2.16	0.46
3:A:183:HOH:O	1:B:78:ILE:HA	2.15	0.46
1:B:113:ILE:HG23	1:B:127:VAL:HG13	1.97	0.46
1:D:64:LYS:HA	1:D:67:GLU:HG3	1.97	0.46
1:D:141:LEU:HD23	1:D:141:LEU:HA	1.79	0.46
1:E:47:ILE:HB	1:E:58:ILE:HD13	1.97	0.46
1:G:77:ILE:HD11	1:H:75:THR:HG22	1.96	0.46
1:A:103:VAL:O	1:A:107:LEU:HG	2.15	0.46
1:E:45:ARG:HG3	1:E:49:LYS:HZ1	1.79	0.46
1:C:65:LEU:CB	1:C:71:ILE:HD12	2.46	0.46
1:C:83:LEU:HD22	1:D:170:ILE:HD13	1.98	0.46
1:F:93:VAL:HB	1:F:125:MET:HB2	1.98	0.46
1:G:113:ILE:HA	1:G:129:ILE:HD12	1.97	0.46
1:C:51:THR:CG2	1:C:53:LEU:HB2	2.46	0.46
1:H:31:LYS:HG3	1:H:34:LYS:HE3	1.97	0.46
1:D:140:PHE:O	1:D:144:ILE:HG12	2.15	0.46
1:E:78:ILE:CD1	1:F:71:ILE:HG13	2.46	0.46
1:G:113:ILE:HG13	1:G:129:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:64:LYS:HG3	1:H:65:LEU:H	1.81	0.45
1:E:120:THR:HA	2:G:172:ARG:O	2.15	0.45
1:G:39:ASP:HB3	3:G:183:HOH:O	2.16	0.45
1:E:133:ASN:HB3	1:E:135:GLU:N	2.31	0.45
1:A:33:ILE:HG22	1:A:71:ILE:HD11	1.98	0.45
1:C:78:ILE:HG12	1:D:37:GLN:NE2	2.30	0.45
1:A:65:LEU:CB	1:A:71:ILE:HD13	2.33	0.45
1:G:33:ILE:HD12	1:G:34:LYS:N	2.31	0.45
1:B:64:LYS:HD2	3:B:179:HOH:O	2.15	0.45
1:C:47:ILE:HG21	1:C:58:ILE:HG21	1.97	0.45
1:C:77:ILE:HD12	1:D:73:LYS:O	2.16	0.45
1:A:85:TYR:OH	1:B:169:PRO:HG2	2.17	0.45
1:A:169:PRO:HB3	1:B:111:PRO:HB2	1.99	0.45
1:B:160:LYS:NZ	1:C:142:ASP:OD2	2.50	0.45
1:C:51:THR:HG23	1:C:53:LEU:H	1.81	0.45
1:H:112:GLU:HG2	1:H:140:PHE:CZ	2.52	0.45
1:E:164:GLU:HG3	1:F:117:TYR:OH	2.17	0.45
1:H:48:SER:HB2	1:H:55:GLU:HB3	1.99	0.45
1:D:47:ILE:HG21	1:D:58:ILE:HG23	1.99	0.45
1:F:94:LYS:HG3	1:F:123:TYR:CE2	2.52	0.45
1:H:64:LYS:HG3	1:H:65:LEU:N	2.31	0.45
1:A:54:ALA:O	1:A:58:ILE:CD1	2.65	0.44
1:D:28:ILE:HG21	1:D:53:LEU:HD11	1.98	0.44
1:G:144:ILE:HA	1:G:147:ILE:HD12	1.99	0.44
1:C:100:TYR:CE2	2:C:172:ARG:HD2	2.51	0.44
1:E:27:GLU:OE1	1:E:31:LYS:CD	2.65	0.44
1:F:112:GLU:OE2	1:F:140:PHE:HZ	2.01	0.44
1:G:29:ASP:O	1:G:33:ILE:HG13	2.17	0.44
1:D:71:ILE:CD1	1:D:71:ILE:N	2.80	0.44
1:A:59:HIS:NE2	1:A:63:ARG:NH1	2.62	0.44
1:D:144:ILE:HA	1:D:147:ILE:HG12	1.99	0.44
1:E:120:THR:O	1:F:156:MET:HG2	2.17	0.44
1:F:53:LEU:HD23	1:F:53:LEU:H	1.82	0.44
1:H:44:LEU:HD23	1:H:58:ILE:HG22	2.00	0.44
1:B:110:TYR:HA	1:B:111:PRO:HD3	1.81	0.44
1:A:45:ARG:O	1:A:49:LYS:HB3	2.18	0.43
1:E:103:VAL:O	1:E:107:LEU:HG	2.17	0.43
1:F:37:GLN:HE22	1:F:168:LEU:H	1.66	0.43
1:B:29:ASP:O	1:B:33:ILE:HG12	2.18	0.43
2:A:172:ARG:HA	1:C:153:THR:O	2.19	0.43
1:D:45:ARG:HG2	1:D:55:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:ILE:O	1:E:37:GLN:HG3	2.18	0.43
1:H:140:PHE:O	1:H:143:LEU:N	2.51	0.43
1:A:58:ILE:HD12	1:A:58:ILE:N	2.34	0.43
1:F:113:ILE:HG23	1:F:127:VAL:HG13	2.01	0.43
1:H:88:LEU:O	1:H:158:VAL:HB	2.18	0.43
1:A:105:SER:O	1:A:109:LYS:HG3	2.19	0.43
1:A:117:TYR:O	1:A:125:MET:HA	2.18	0.43
1:A:68:SER:O	1:A:69:GLY:C	2.56	0.43
1:A:110:TYR:HA	1:A:111:PRO:HD3	1.91	0.43
1:A:112:GLU:HG2	1:A:140:PHE:CZ	2.53	0.43
1:E:87:MET:HG2	1:E:131:THR:OG1	2.19	0.43
1:G:130:ARG:NH1	1:G:130:ARG:CG	2.75	0.43
1:A:26:ASP:OD2	1:A:61:ARG:NH2	2.52	0.43
1:C:103:VAL:HA	1:C:147:ILE:HG21	2.01	0.43
1:D:100:TYR:CE2	2:D:172:ARG:HD2	2.53	0.42
1:E:169:PRO:HG3	1:F:111:PRO:HB2	2.01	0.42
1:C:51:THR:HG23	1:C:53:LEU:HB2	2.01	0.42
1:E:42:ALA:HA	1:E:43:PRO:HD3	1.85	0.42
1:E:91:ILE:HD12	1:E:141:LEU:HD21	2.02	0.42
1:H:91:ILE:HD13	1:H:144:ILE:CD1	2.46	0.42
1:B:32:ILE:CG2	1:B:62:ILE:HD11	2.49	0.42
1:A:129:ILE:CD1	1:A:129:ILE:C	2.83	0.42
1:C:49:LYS:HA	1:C:49:LYS:HE3	2.01	0.42
1:D:77:ILE:HD12	1:D:77:ILE:H	1.84	0.42
1:H:112:GLU:HG2	1:H:140:PHE:CE1	2.55	0.42
1:E:70:VAL:HG12	1:E:71:ILE:H	1.85	0.42
1:B:106:ASN:HD22	1:B:147:ILE:CD1	2.17	0.42
1:C:130:ARG:CD	1:D:168:LEU:CD2	2.97	0.42
1:D:28:ILE:HG21	1:D:53:LEU:HD21	2.01	0.42
1:F:70:VAL:O	1:F:71:ILE:HB	2.19	0.42
1:G:112:GLU:HA	1:H:169:PRO:HG3	2.02	0.42
1:H:102:GLU:O	1:H:106:ASN:HB2	2.20	0.42
1:C:78:ILE:CG1	1:D:37:GLN:NE2	2.83	0.42
1:G:115:GLU:HB3	1:G:117:TYR:CE1	2.55	0.42
1:G:144:ILE:HA	1:G:147:ILE:CD1	2.50	0.41
1:B:47:ILE:O	1:B:51:THR:HG23	2.20	0.41
1:B:168:LEU:O	1:B:170:ILE:HD12	2.19	0.41
1:C:33:ILE:HD11	1:D:83:LEU:HD21	2.02	0.41
1:D:129:ILE:HD12	1:D:131:THR:CG2	2.45	0.41
1:E:45:ARG:HG3	1:E:49:LYS:NZ	2.35	0.41
1:A:87:MET:CE	1:A:133:ASN:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ASP:OD1	1:B:61:ARG:HD2	2.20	0.41
1:A:60:GLU:O	1:A:64:LYS:HG3	2.20	0.41
1:C:112:GLU:HB3	1:C:129:ILE:HD11	2.01	0.41
1:F:48:SER:HA	1:F:51:THR:HG22	2.02	0.41
1:G:41:LYS:NZ	1:G:41:LYS:HB3	2.34	0.41
1:E:88:LEU:HD11	1:E:128:LYS:CD	2.51	0.41
1:G:51:THR:C	1:G:53:LEU:H	2.24	0.41
1:C:35:ILE:CG2	1:C:47:ILE:HD11	2.50	0.41
1:C:65:LEU:HB2	1:C:71:ILE:HD12	2.03	0.41
1:E:161:THR:HG23	1:F:117:TYR:HE2	1.83	0.41
1:A:115:GLU:OE1	1:A:117:TYR:HE1	2.03	0.41
1:A:42:ALA:CB	1:A:47:ILE:HD11	2.44	0.41
1:A:100:TYR:OH	2:A:172:ARG:HD2	2.20	0.41
1:B:96:LYS:HE2	1:B:149:GLY:HA2	2.02	0.41
1:C:99:LYS:O	1:C:103:VAL:HG23	2.21	0.41
1:C:100:TYR:CZ	2:C:172:ARG:HD2	2.55	0.41
1:C:129:ILE:HD11	1:C:131:THR:CG2	2.51	0.41
1:D:70:VAL:C	1:D:71:ILE:HD12	2.41	0.41
1:D:124:ASP:OD1	2:D:172:ARG:N	2.54	0.41
1:F:43:PRO:HG2	1:F:46:GLU:HB3	2.02	0.41
1:G:78:ILE:CG2	1:G:79:ASP:N	2.84	0.41
1:A:113:ILE:N	1:A:113:ILE:CD1	2.84	0.41
1:A:119:THR:HG21	1:A:126:VAL:CG2	2.48	0.41
1:C:121:GLY:O	2:C:172:ARG:N	2.54	0.41
1:D:106:ASN:ND2	1:D:147:ILE:HD12	2.36	0.41
1:G:100:TYR:CE2	1:G:124:ASP:HB3	2.56	0.41
1:C:158:VAL:HG13	1:D:117:TYR:HB3	2.03	0.40
1:A:90:PHE:HA	1:A:127:VAL:O	2.21	0.40
1:D:28:ILE:CG2	1:D:28:ILE:O	2.68	0.40
1:D:37:GLN:HB3	1:D:167:GLU:HG2	2.03	0.40
1:A:121:GLY:O	2:A:172:ARG:N	2.54	0.40
1:C:93:VAL:HB	1:C:125:MET:HB2	2.03	0.40
1:F:51:THR:HG23	1:F:52:GLY:N	2.36	0.40
1:A:115:GLU:HB2	1:A:128:LYS:HB3	2.04	0.40
1:G:26:ASP:OD1	1:G:29:ASP:N	2.42	0.40
1:A:119:THR:O	2:A:172:ARG:HG3	2.21	0.40
1:B:37:GLN:OE1	1:B:170:ILE:HD11	2.21	0.40
1:C:87:MET:HB3	1:C:131:THR:O	2.21	0.40
1:C:129:ILE:HD13	1:C:129:ILE:C	2.40	0.40
1:D:27:GLU:H	1:D:27:GLU:HG3	1.72	0.40
1:F:54:ALA:C	1:F:56:SER:H	2.23	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:61:ARG:HA	1:H:64:LYS:HG2	2.03	0.40

All (1) 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:H:56:SER:OG	3:B:175:HOH:O[2_545]	2.17	0.03

## 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	144/171 (84%)	134 (93%)	7 (5%)	3 (2%)	7	13
1	B	144/171 (84%)	138 (96%)	3 (2%)	3 (2%)	7	13
1	C	144/171 (84%)	133 (92%)	7 (5%)	4 (3%)	5	7
1	D	144/171 (84%)	135 (94%)	8 (6%)	1 (1%)	22	43
1	E	144/171 (84%)	135 (94%)	6 (4%)	3 (2%)	7	13
1	F	144/171 (84%)	129 (90%)	12 (8%)	3 (2%)	7	13
1	G	144/171 (84%)	133 (92%)	10 (7%)	1 (1%)	22	43
1	H	144/171 (84%)	128 (89%)	13 (9%)	3 (2%)	7	13
All	All	1152/1368 (84%)	1065 (92%)	66 (6%)	21 (2%)	8	16

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	70	VAL
1	E	70	VAL
1	E	71	ILE
1	H	71	ILE

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Mol	Chain	Res	Type
1	A	85	TYR
1	B	97	ALA
1	D	55	GLU
1	F	51	THR
1	A	69	GLY
1	C	145	GLY
1	G	41	LYS
1	B	64	LYS
1	H	57	THR
1	A	71	ILE
1	B	66	ARG
1	E	39	ASP
1	F	71	ILE
1	C	71	ILE
1	C	69	GLY
1	F	52	GLY
1	H	58	ILE

### 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	129/151 (85%)	119 (92%)	10 (8%)	12	25
1	B	129/151 (85%)	123 (95%)	6 (5%)	26	50
1	C	129/151 (85%)	115 (89%)	14 (11%)	6	11
1	D	129/151 (85%)	120 (93%)	9 (7%)	15	30
1	E	129/151 (85%)	116 (90%)	13 (10%)	7	14
1	F	129/151 (85%)	119 (92%)	10 (8%)	12	25
1	G	129/151 (85%)	115 (89%)	14 (11%)	6	11
1	H	129/151 (85%)	120 (93%)	9 (7%)	15	30
All	All	1032/1208 (85%)	947 (92%)	85 (8%)	10	22

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	50	ILE
1	A	51	THR
1	A	83	LEU
1	A	114	VAL
1	A	129	ILE
1	A	134	SER
1	A	138	ASN
1	A	164	GLU
1	A	169	PRO
1	B	25	LEU
1	B	44	LEU
1	B	45	ARG
1	B	114	VAL
1	B	136	GLU
1	B	146	SER
1	C	26	ASP
1	C	45	ARG
1	C	49	LYS
1	C	50	ILE
1	C	51	THR
1	C	68	SER
1	C	75	THR
1	C	81	GLU
1	C	86	SER
1	C	106	ASN
1	C	114	VAL
1	C	129	ILE
1	C	134	SER
1	C	166	THR
1	D	27	GLU
1	D	38	ASN
1	D	49	LYS
1	D	61	ARG
1	D	73	LYS
1	D	114	VAL
1	D	129	ILE
1	D	136	GLU
1	D	143	LEU
1	E	31	LYS
1	E	45	ARG
1	E	48	SER
1	E	49	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	66	ARG
1	E	72	LYS
1	E	75	THR
1	E	81	GLU
1	E	102	GLU
1	E	114	VAL
1	E	129	ILE
1	E	133	ASN
1	E	160	LYS
1	F	26	ASP
1	F	28	ILE
1	F	48	SER
1	F	50	ILE
1	F	63	ARG
1	F	72	LYS
1	F	79	ASP
1	F	114	VAL
1	F	128	LYS
1	F	138	ASN
1	G	27	GLU
1	G	31	LYS
1	G	38	ASN
1	G	41	LYS
1	G	44	LEU
1	G	45	ARG
1	G	50	ILE
1	G	60	GLU
1	G	68	SER
1	G	72	LYS
1	G	114	VAL
1	G	130	ARG
1	G	133	ASN
1	G	153	THR
1	H	48	SER
1	H	57	THR
1	H	63	ARG
1	H	64	LYS
1	H	79	ASP
1	H	101	SER
1	H	136	GLU
1	H	138	ASN
1	H	159	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	139	ASN
1	B	37	GLN
1	B	106	ASN
1	C	106	ASN
1	C	162	HIS
1	D	37	GLN
1	E	133	ASN
1	E	139	ASN
1	F	37	GLN
1	F	139	ASN
1	F	154	HIS
1	G	37	GLN
1	G	38	ASN
1	G	133	ASN
1	G	139	ASN
1	H	37	GLN
1	H	139	ASN
1	H	154	HIS
1	H	162	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ARG	D	172	-	10,11,11	0.92	0	11,13,13	0.81	0
2	ARG	A	172	-	10,11,11	0.69	0	11,13,13	1.44	2 (18%)
2	ARG	F	172	-	10,11,11	0.70	0	11,13,13	1.14	1 (9%)
2	ARG	G	172	-	10,11,11	0.97	1 (10%)	11,13,13	1.38	1 (9%)
2	ARG	F	173	-	10,11,11	0.84	1 (10%)	11,13,13	0.91	0
2	ARG	C	172	-	10,11,11	0.77	0	11,13,13	1.13	1 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ARG	D	172	-	-	2/11/11/11	-
2	ARG	A	172	-	-	2/11/11/11	-
2	ARG	F	172	-	-	0/11/11/11	-
2	ARG	G	172	-	-	4/11/11/11	-
2	ARG	F	173	-	-	1/11/11/11	-
2	ARG	C	172	-	-	3/11/11/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	172	ARG	OXT-C	-2.58	1.22	1.30
2	F	173	ARG	OXT-C	-2.13	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	172	ARG	OXT-C-O	-3.62	115.86	124.09
2	A	172	ARG	O-C-CA	-3.29	110.53	122.14
2	C	172	ARG	OXT-C-O	-2.92	117.45	124.09
2	A	172	ARG	OXT-C-O	2.45	129.64	124.09
2	F	172	ARG	OXT-C-O	-2.22	119.05	124.09

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	172	ARG	N-CA-CB-CG
2	A	172	ARG	C-CA-CB-CG
2	C	172	ARG	N-CA-CB-CG
2	D	172	ARG	NE-CD-CG-CB
2	C	172	ARG	NE-CD-CG-CB
2	G	172	ARG	NE-CD-CG-CB
2	F	173	ARG	CA-CB-CG-CD
2	C	172	ARG	C-CA-CB-CG
2	G	172	ARG	C-CA-CB-CG
2	G	172	ARG	N-CA-CB-CG
2	G	172	ARG	CG-CD-NE-CZ
2	D	172	ARG	C-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	172	ARG	5	0
2	A	172	ARG	6	0
2	F	172	ARG	1	0
2	G	172	ARG	2	0
2	C	172	ARG	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	146/171 (85%)	0.43	5 (3%) 45 38	36, 49, 63, 67	0
1	B	146/171 (85%)	0.34	7 (4%) 30 24	34, 51, 67, 77	1 (0%)
1	C	146/171 (85%)	0.10	1 (0%) 87 86	26, 40, 52, 57	0
1	D	146/171 (85%)	0.31	6 (4%) 37 30	24, 42, 63, 70	0
1	E	146/171 (85%)	0.35	4 (2%) 54 48	30, 46, 68, 71	0
1	F	146/171 (85%)	0.70	21 (14%) 2 1	30, 47, 87, 90	0
1	G	146/171 (85%)	0.91	27 (18%) 1 0	37, 59, 101, 106	0
1	H	146/171 (85%)	0.55	9 (6%) 20 15	40, 55, 83, 86	0
All	All	1168/1368 (85%)	0.46	80 (6%) 17 12	24, 48, 83, 106	1 (0%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	50	ILE	6.7
1	G	57	THR	6.5
1	G	58	ILE	5.8
1	F	26	ASP	4.9
1	G	28	ILE	4.9
1	F	53	LEU	4.7
1	G	68	SER	3.8
1	F	32	ILE	3.5
1	F	50	ILE	3.5
1	E	170	ILE	3.5
1	G	33	ILE	3.4
1	E	36	LEU	3.3
1	F	52	GLY	3.3
1	G	47	ILE	3.3
1	B	62	ILE	3.2
1	A	82	ALA	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	52	GLY	3.1
1	D	28	ILE	3.0
1	H	50	ILE	3.0
1	H	52	GLY	3.0
1	H	70	VAL	3.0
1	G	64	LYS	3.0
1	F	25	LEU	3.0
1	F	45	ARG	2.9
1	G	71	ILE	2.9
1	B	63	ARG	2.9
1	F	44	LEU	2.9
1	G	103	VAL	2.9
1	D	26	ASP	2.8
1	F	55	GLU	2.8
1	G	82	ALA	2.7
1	E	57	THR	2.7
1	F	77	ILE	2.7
1	H	67	GLU	2.7
1	B	25	LEU	2.7
1	H	33	ILE	2.7
1	H	30	LYS	2.6
1	F	28	ILE	2.6
1	G	65	LEU	2.6
1	G	27	GLU	2.6
1	F	54	ALA	2.6
1	F	30	LYS	2.6
1	H	53	LEU	2.5
1	C	50	ILE	2.5
1	G	54	ALA	2.5
1	E	71	ILE	2.5
1	F	57	THR	2.5
1	H	54	ALA	2.4
1	A	50	ILE	2.4
1	G	49	LYS	2.3
1	B	28	ILE	2.3
1	D	58	ILE	2.3
1	G	36	LEU	2.3
1	F	29	ASP	2.3
1	B	53	LEU	2.3
1	B	170	ILE	2.3
1	G	60	GLU	2.3
1	G	31	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	62	ILE	2.3
1	G	77	ILE	2.2
1	G	67	GLU	2.2
1	A	53	LEU	2.2
1	D	27	GLU	2.2
1	G	26	ASP	2.2
1	F	27	GLU	2.2
1	A	63	ARG	2.1
1	H	26	ASP	2.1
1	G	63	ARG	2.1
1	F	33	ILE	2.1
1	G	62	ILE	2.1
1	D	53	LEU	2.1
1	B	35	ILE	2.1
1	G	56	SER	2.1
1	A	70	VAL	2.1
1	G	70	VAL	2.1
1	G	100	TYR	2.1
1	G	46	GLU	2.1
1	F	35	ILE	2.0
1	F	36	LEU	2.0
1	F	41	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 monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	ARG	D	172	12/12	0.91	0.21	40,40,46,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ARG	C	172	12/12	0.92	0.16	30,31,44,44	0
2	ARG	G	172	12/12	0.92	0.19	44,45,50,50	0
2	ARG	A	172	12/12	0.93	0.20	39,40,43,50	0
2	ARG	F	173	12/12	0.95	0.17	27,29,39,41	0
2	ARG	F	172	12/12	0.96	0.13	39,40,50,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.