



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:04 pm GMT

PDB ID : 3O3W  
Title : Crystal Structure of BH2092 protein (residues 14-131) from *Bacillus halodurans*, Northeast Structural Genomics Consortium Target BhR228A  
Authors : Forouhar, F.; Neely, H.; Seetharaman, J.; Sahdev, S.; Xiao, R.; Ciccocanti, C.; Lee, D.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2010-07-26  
Resolution : 2.91 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

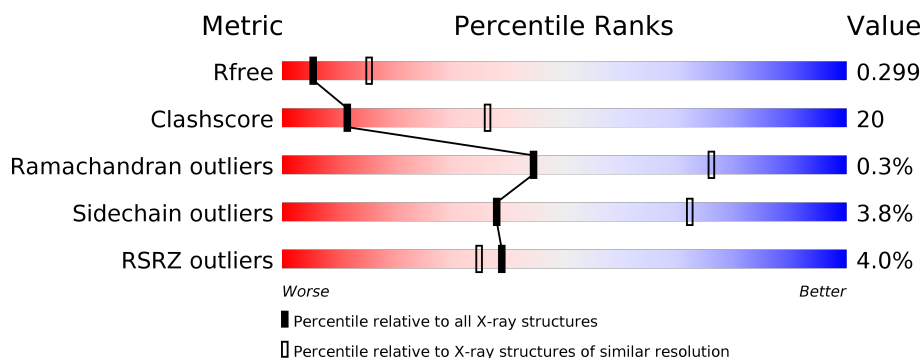
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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	1813 (2.94-2.90)
Clashscore	112137	2045 (2.94-2.90)
Ramachandran outliers	110173	1997 (2.94-2.90)
Sidechain outliers	110143	1999 (2.94-2.90)
RSRZ outliers	101464	1825 (2.94-2.90)

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	126	<div> <div>2%</div> <div> <div></div> <div>63%</div> <div>29%</div> <div>• 6%</div> </div> </div>
1	B	126	<div> <div>2%</div> <div> <div></div> <div>60%</div> <div>31%</div> <div>• 7%</div> </div> </div>
1	C	126	<div> <div>2%</div> <div> <div></div> <div>60%</div> <div>30%</div> <div>• 6%</div> </div> </div>
1	D	126	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>25%</div> <div>• 10%</div> </div> </div>
1	E	126	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>36%</div> <div>•• 6%</div> </div> </div>
1	F	126	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>29%</div> <div>• 6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	126	<p>10% 57% 32% • 10%</p>
1	H	126	<p>6% 66% 25% • 8%</p>
1	I	126	<p>6% 63% 25% • 10%</p>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8353 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 BH2092 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	118	Total	C	N	O	S	Se	0	0	0
			928	591	159	174	3	1			
1	B	117	Total	C	N	O	S	Se	0	0	0
			928	591	158	175	3	1			
1	C	118	Total	C	N	O	S	Se	0	0	0
			933	594	159	176	3	1			
1	D	114	Total	C	N	O	S	Se	0	0	0
			907	578	155	170	3	1			
1	E	118	Total	C	N	O	S	Se	0	0	0
			933	594	159	176	3	1			
1	F	118	Total	C	N	O	S	Se	0	0	0
			929	591	161	173	3	1			
1	G	114	Total	C	N	O	S	Se	0	0	0
			907	578	155	170	3	1			
1	H	116	Total	C	N	O	S	Se	0	0	0
			919	586	157	172	3	1			
1	I	113	Total	C	N	O	S	Se	0	0	0
			890	567	153	166	3	1			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	LEU	-	EXPRESSION TAG	UNP Q9KB42
A	133	GLU	-	EXPRESSION TAG	UNP Q9KB42
A	134	HIS	-	EXPRESSION TAG	UNP Q9KB42
A	135	HIS	-	EXPRESSION TAG	UNP Q9KB42
A	136	HIS	-	EXPRESSION TAG	UNP Q9KB42
A	137	HIS	-	EXPRESSION TAG	UNP Q9KB42
A	138	HIS	-	EXPRESSION TAG	UNP Q9KB42
A	139	HIS	-	EXPRESSION TAG	UNP Q9KB42
B	132	LEU	-	EXPRESSION TAG	UNP Q9KB42
B	133	GLU	-	EXPRESSION TAG	UNP Q9KB42
B	134	HIS	-	EXPRESSION TAG	UNP Q9KB42

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Chain	Residue	Modelled	Actual	Comment	Reference
B	135	HIS	-	EXPRESSION TAG	UNP Q9KB42
B	136	HIS	-	EXPRESSION TAG	UNP Q9KB42
B	137	HIS	-	EXPRESSION TAG	UNP Q9KB42
B	138	HIS	-	EXPRESSION TAG	UNP Q9KB42
B	139	HIS	-	EXPRESSION TAG	UNP Q9KB42
C	132	LEU	-	EXPRESSION TAG	UNP Q9KB42
C	133	GLU	-	EXPRESSION TAG	UNP Q9KB42
C	134	HIS	-	EXPRESSION TAG	UNP Q9KB42
C	135	HIS	-	EXPRESSION TAG	UNP Q9KB42
C	136	HIS	-	EXPRESSION TAG	UNP Q9KB42
C	137	HIS	-	EXPRESSION TAG	UNP Q9KB42
C	138	HIS	-	EXPRESSION TAG	UNP Q9KB42
C	139	HIS	-	EXPRESSION TAG	UNP Q9KB42
D	132	LEU	-	EXPRESSION TAG	UNP Q9KB42
D	133	GLU	-	EXPRESSION TAG	UNP Q9KB42
D	134	HIS	-	EXPRESSION TAG	UNP Q9KB42
D	135	HIS	-	EXPRESSION TAG	UNP Q9KB42
D	136	HIS	-	EXPRESSION TAG	UNP Q9KB42
D	137	HIS	-	EXPRESSION TAG	UNP Q9KB42
D	138	HIS	-	EXPRESSION TAG	UNP Q9KB42
D	139	HIS	-	EXPRESSION TAG	UNP Q9KB42
E	132	LEU	-	EXPRESSION TAG	UNP Q9KB42
E	133	GLU	-	EXPRESSION TAG	UNP Q9KB42
E	134	HIS	-	EXPRESSION TAG	UNP Q9KB42
E	135	HIS	-	EXPRESSION TAG	UNP Q9KB42
E	136	HIS	-	EXPRESSION TAG	UNP Q9KB42
E	137	HIS	-	EXPRESSION TAG	UNP Q9KB42
E	138	HIS	-	EXPRESSION TAG	UNP Q9KB42
E	139	HIS	-	EXPRESSION TAG	UNP Q9KB42
F	132	LEU	-	EXPRESSION TAG	UNP Q9KB42
F	133	GLU	-	EXPRESSION TAG	UNP Q9KB42
F	134	HIS	-	EXPRESSION TAG	UNP Q9KB42
F	135	HIS	-	EXPRESSION TAG	UNP Q9KB42
F	136	HIS	-	EXPRESSION TAG	UNP Q9KB42
F	137	HIS	-	EXPRESSION TAG	UNP Q9KB42
F	138	HIS	-	EXPRESSION TAG	UNP Q9KB42
F	139	HIS	-	EXPRESSION TAG	UNP Q9KB42
G	132	LEU	-	EXPRESSION TAG	UNP Q9KB42
G	133	GLU	-	EXPRESSION TAG	UNP Q9KB42
G	134	HIS	-	EXPRESSION TAG	UNP Q9KB42
G	135	HIS	-	EXPRESSION TAG	UNP Q9KB42
G	136	HIS	-	EXPRESSION TAG	UNP Q9KB42

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Chain	Residue	Modelled	Actual	Comment	Reference
G	137	HIS	-	EXPRESSION TAG	UNP Q9KB42
G	138	HIS	-	EXPRESSION TAG	UNP Q9KB42
G	139	HIS	-	EXPRESSION TAG	UNP Q9KB42
H	132	LEU	-	EXPRESSION TAG	UNP Q9KB42
H	133	GLU	-	EXPRESSION TAG	UNP Q9KB42
H	134	HIS	-	EXPRESSION TAG	UNP Q9KB42
H	135	HIS	-	EXPRESSION TAG	UNP Q9KB42
H	136	HIS	-	EXPRESSION TAG	UNP Q9KB42
H	137	HIS	-	EXPRESSION TAG	UNP Q9KB42
H	138	HIS	-	EXPRESSION TAG	UNP Q9KB42
H	139	HIS	-	EXPRESSION TAG	UNP Q9KB42
I	132	LEU	-	EXPRESSION TAG	UNP Q9KB42
I	133	GLU	-	EXPRESSION TAG	UNP Q9KB42
I	134	HIS	-	EXPRESSION TAG	UNP Q9KB42
I	135	HIS	-	EXPRESSION TAG	UNP Q9KB42
I	136	HIS	-	EXPRESSION TAG	UNP Q9KB42
I	137	HIS	-	EXPRESSION TAG	UNP Q9KB42
I	138	HIS	-	EXPRESSION TAG	UNP Q9KB42
I	139	HIS	-	EXPRESSION TAG	UNP Q9KB42

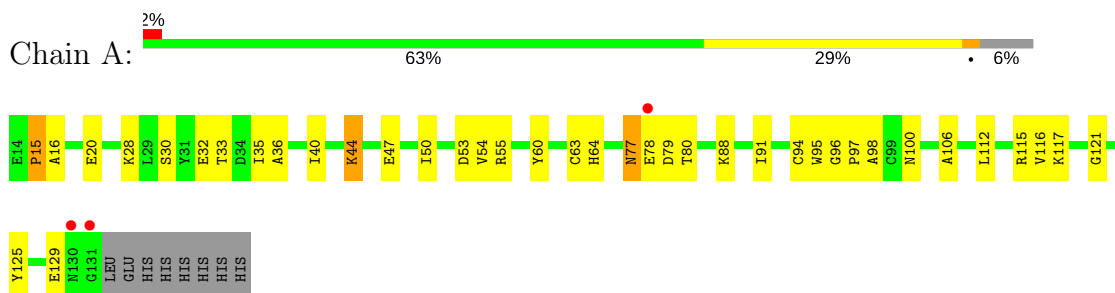
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	14	Total O 14 14	0	0
2	B	9	Total O 9 9	0	0
2	C	6	Total O 6 6	0	0
2	D	10	Total O 10 10	0	0
2	E	11	Total O 11 11	0	0
2	F	7	Total O 7 7	0	0
2	G	10	Total O 10 10	0	0
2	H	2	Total O 2 2	0	0
2	I	10	Total O 10 10	0	0

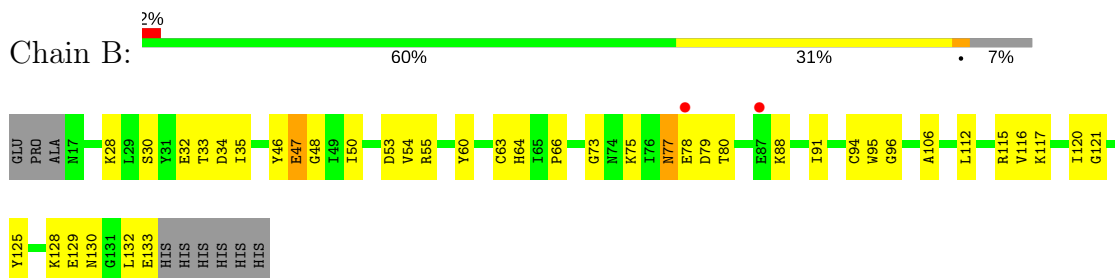
### 3 Residue-property plots [i](#)

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.

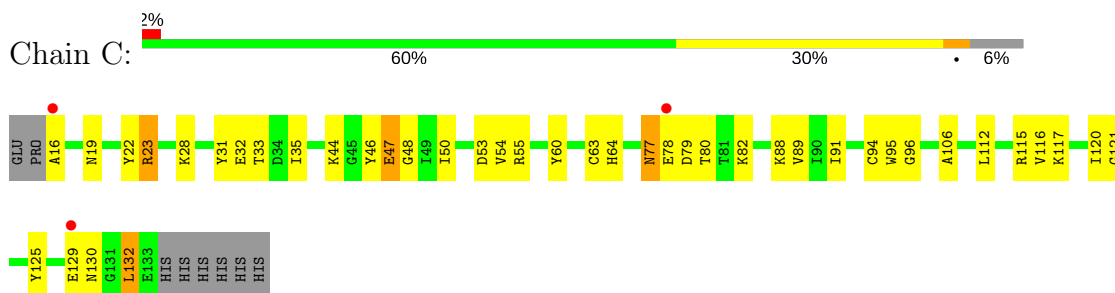
#### • Molecule 1: BH2092 protein



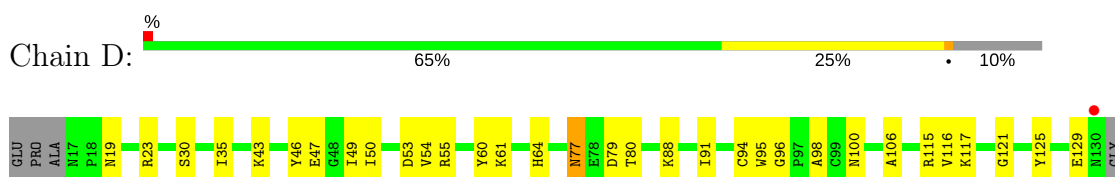
#### • Molecule 1: BH2092 protein



#### • Molecule 1: BH2092 protein



#### • Molecule 1: BH2092 protein



LEU  
GLU  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS

• Molecule 1: BH2092 protein

Chain E:  2% 55% 36% 6%

GLU PRO A16 N17 P18 N19 R23 M26 K27 K28 L29 S30 Y31 E32 T33 D34 I35 A36 K44 E47 I50 D53 V54 R55 Y60 A61 E62 C63 H64 I65 P66 S70 G73 N74 K75 I76 N77 D78 T80 T81 K82 K88 I91 C94 W95 G96 P97

A98 A106 L112 R115 V116 K117 I120 G121 Y125 E129 N130 G131 L132 E133 HIS HIS HIS HIS HIS HIS HIS HIS

• Molecule 1: BH2092 protein

Chain F:  2% 61% 29% 6%

GLU P15 A16 N17 E20 D34 I35 K43 K44 G45 THR G48 I49 I50 D53 V54 R55 Y60 C63 H64 I65 P66 G73 N74 K75 I76 N77 D78 T80 R83 K88 V89 I91 C94 W95 G96 A106 L112 R115 V116 K117 G121

Y125 E129 N130 G131 L132 E133 HIS HIS HIS HIS HIS HIS HIS HIS

• Molecule 1: BH2092 protein

Chain G:  10% 57% 32% 10%

GLU PRO ALA N17 P18 N19 S30 T33 D34 I35 A36 D37 L38 S39 I40 D41 I42 K43 K44 Y46 E47 G48 I49 I50 D53 V54 R55 Y60 K61 E62 C63 H64 I65 P66 G73 N74 K75 I76 N77 D78 T80 T81 S85 K86 E87 K88 V89 I91 C94 W95

G96 M100 A106 R115 V116 K117 I120 G121 Y126 K128 E129 N130 GLY LEU HIS HIS HIS HIS HIS HIS HIS HIS

• Molecule 1: BH2092 protein

Chain H:  6% 66% 25% 8%

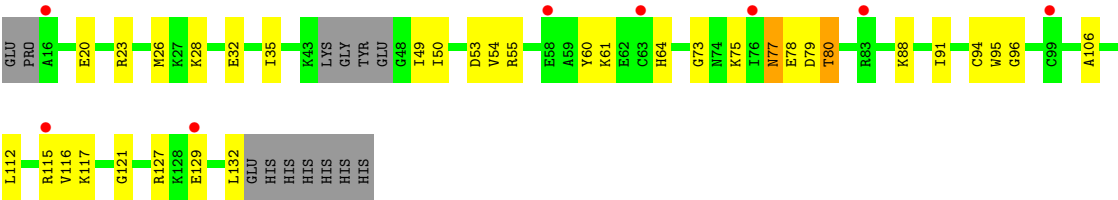
GLU PRO N17 P18 Y31 T35 A36 D37 I40 K44 G45 Y46 E47 I50 D53 V54 R55 Y60 C63 H64 I67 N77 E78 D79 T80 K88 I91 C94 W95 G96 A106 L112 R115 V116 K117 G121 Y125 Y126 R127 K128 E129

L132 GLU HIS HIS HIS HIS HIS HIS HIS HIS

• Molecule 1: BH2092 protein

Chain I:  6% 63% 25% 10%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.24Å 114.24Å 85.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.79 – 2.91 28.56 – 2.91	Depositor EDS
% Data completeness (in resolution range)	93.9 (19.79-2.91) 99.5 (28.56-2.91)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 2.90Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.250 , 0.292 0.261 , 0.299	Depositor DCC
$R_{free}$ test set	2694 reflections (9.91%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.1	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 2.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.098 for -h,-k,l 0.099 for h,-h-k,-l 0.286 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	8353	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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	0.48	0/946	0.61	0/1275
1	B	0.45	0/945	0.58	0/1272
1	C	0.49	0/950	1.26	3/1279 (0.2%)
1	D	0.45	0/924	0.57	0/1244
1	E	0.47	0/950	0.60	0/1279
1	F	0.45	0/946	0.59	0/1272
1	G	0.46	0/924	0.55	0/1244
1	H	0.42	0/936	0.55	0/1260
1	I	0.46	0/905	0.56	0/1218
All	All	0.46	0/8426	0.69	3/11343 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	23	ARG	NE-CZ-NH1	-27.41	106.60	120.30
1	C	23	ARG	NE-CZ-NH2	25.63	133.12	120.30
1	C	23	ARG	CD-NE-CZ	12.99	141.78	123.60

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	928	0	927	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	928	0	930	35	0
1	C	933	0	935	56	1
1	D	907	0	910	41	0
1	E	933	0	935	59	0
1	F	929	0	934	47	1
1	G	907	0	910	35	0
1	H	919	0	924	28	0
1	I	890	0	897	41	0
2	A	14	0	0	1	0
2	B	9	0	0	2	0
2	C	6	0	0	1	0
2	D	10	0	0	1	0
2	E	11	0	0	4	0
2	F	7	0	0	2	0
2	G	10	0	0	4	0
2	H	2	0	0	0	0
2	I	10	0	0	6	0
All	All	8353	0	8302	324	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 20.

All (324) 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:78:GLU:OE1	1:E:26:MSE:HE2	1.37	1.24
1:I:49:ILE:HD12	1:I:91:ILE:HD12	1.37	1.07
1:E:115:ARG:HH12	1:F:15:PRO:HB2	1.17	1.05
1:D:23:ARG:NH2	1:I:20:GLU:HB2	1.73	1.03
1:G:35:ILE:HG21	1:G:129:GLU:HG3	1.42	0.98
1:B:28:LYS:HD2	2:B:144:HOH:O	1.66	0.96
1:A:16:ALA:N	1:C:115:ARG:HH12	1.65	0.95
1:D:23:ARG:NH2	1:I:20:GLU:CB	2.31	0.92
1:A:15:PRO:C	1:C:115:ARG:HH12	1.79	0.86
1:D:23:ARG:HH21	1:I:20:GLU:CB	1.87	0.86
1:G:100:ASN:HB2	2:G:143:HOH:O	1.75	0.86
1:E:115:ARG:HH22	1:F:15:PRO:C	1.81	0.84
1:E:115:ARG:HH12	1:F:15:PRO:CB	1.91	0.84
1:F:43:LYS:HD3	1:F:44:LYS:N	1.91	0.83
1:B:77:ASN:HD22	1:B:79:ASP:H	1.26	0.83
1:E:94:CYS:HB3	2:E:9:HOH:O	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:ASN:HD22	1:D:79:ASP:H	1.26	0.83
1:C:77:ASN:HD22	1:C:79:ASP:H	1.28	0.82
1:C:35:ILE:HG21	1:C:129:GLU:HG3	1.59	0.82
1:I:77:ASN:HD22	1:I:79:ASP:H	1.28	0.82
1:F:77:ASN:HD22	1:F:79:ASP:H	1.30	0.80
1:B:35:ILE:HG21	1:B:129:GLU:HG3	1.64	0.80
1:E:77:ASN:HD22	1:E:79:ASP:H	1.29	0.79
1:I:35:ILE:HG21	1:I:129:GLU:HG3	1.64	0.79
1:B:129:GLU:HB2	1:B:130:ASN:HD22	1.47	0.78
1:E:35:ILE:HG21	1:E:129:GLU:HG3	1.63	0.78
1:G:77:ASN:HD22	1:G:79:ASP:H	1.30	0.78
1:H:77:ASN:HD22	1:H:79:ASP:H	1.30	0.77
1:A:16:ALA:N	1:C:115:ARG:NH1	2.32	0.77
1:A:77:ASN:HD22	1:A:79:ASP:H	1.31	0.77
1:E:115:ARG:NH1	1:F:15:PRO:HB2	1.98	0.77
1:D:23:ARG:NH2	1:I:20:GLU:CG	2.47	0.76
1:I:26:MSE:HE3	2:I:148:HOH:O	1.84	0.76
1:C:78:GLU:CD	1:E:26:MSE:HE2	2.05	0.76
1:H:35:ILE:HG21	1:H:129:GLU:HG3	1.68	0.74
1:C:82:LYS:NZ	1:E:19:ASN:HD22	1.85	0.73
1:F:129:GLU:HA	2:F:140:HOH:O	1.89	0.73
1:C:78:GLU:OE1	1:E:26:MSE:CE	2.29	0.72
1:D:35:ILE:HG21	1:D:129:GLU:HG3	1.71	0.72
1:E:63:CYS:SG	1:E:132:LEU:HD13	2.29	0.71
1:F:35:ILE:HG21	1:F:129:GLU:HG3	1.72	0.71
1:B:63:CYS:SG	1:B:132:LEU:HD13	2.31	0.71
1:C:82:LYS:HZ1	1:E:19:ASN:HD22	1.37	0.70
1:A:35:ILE:HG21	1:A:129:GLU:HG3	1.72	0.70
1:H:17:ASN:HD22	1:H:18:PRO:HD2	1.55	0.70
1:A:15:PRO:C	1:C:115:ARG:HH22	1.94	0.69
1:I:127:ARG:HG2	1:I:132:LEU:HD21	1.74	0.68
1:H:17:ASN:HD22	1:H:18:PRO:CD	2.07	0.68
1:E:30:SER:O	1:F:15:PRO:HB3	1.92	0.68
1:A:106:ALA:HA	1:A:116:VAL:HG21	1.76	0.68
1:E:44:LYS:HA	1:E:44:LYS:HE3	1.75	0.68
1:C:79:ASP:OD2	1:E:23:ARG:HG2	1.94	0.68
1:I:106:ALA:HA	1:I:116:VAL:HG21	1.76	0.67
1:D:23:ARG:HH21	1:I:20:GLU:HB2	1.51	0.67
1:G:106:ALA:HA	1:G:116:VAL:HG21	1.77	0.67
1:H:47:GLU:O	1:H:88:LYS:HE3	1.95	0.67
1:A:15:PRO:CB	1:C:115:ARG:HH12	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:ALA:HA	1:D:116:VAL:HG21	1.76	0.66
1:E:47:GLU:O	1:E:88:LYS:HE3	1.95	0.66
1:B:106:ALA:HA	1:B:116:VAL:HG21	1.77	0.66
1:H:106:ALA:HA	1:H:116:VAL:HG21	1.77	0.66
1:E:106:ALA:HA	1:E:116:VAL:HG21	1.78	0.66
1:G:47:GLU:O	1:G:88:LYS:HE3	1.95	0.65
1:A:15:PRO:HB2	1:C:115:ARG:HH12	1.61	0.65
1:F:106:ALA:HA	1:F:116:VAL:HG21	1.78	0.65
1:D:23:ARG:NH2	1:I:20:GLU:HG3	2.12	0.65
1:B:77:ASN:HD22	1:B:79:ASP:N	1.95	0.64
1:G:18:PRO:HB2	2:G:147:HOH:O	1.97	0.64
1:A:15:PRO:HG2	1:C:115:ARG:NH1	2.13	0.64
1:A:15:PRO:HB2	1:C:115:ARG:NH1	2.13	0.64
1:A:47:GLU:O	1:A:88:LYS:HE3	1.97	0.64
1:D:77:ASN:HD22	1:D:79:ASP:N	1.95	0.64
1:I:94:CYS:SG	1:I:95:TRP:N	2.70	0.64
1:B:47:GLU:O	1:B:88:LYS:HE3	1.97	0.64
1:C:106:ALA:HA	1:C:116:VAL:HG21	1.80	0.64
1:G:87:GLU:HB2	2:G:142:HOH:O	1.98	0.63
1:C:82:LYS:NZ	1:E:19:ASN:ND2	2.47	0.63
1:C:77:ASN:HD22	1:C:79:ASP:N	1.97	0.62
1:H:77:ASN:HD22	1:H:79:ASP:N	1.98	0.62
1:G:44:LYS:NZ	1:G:44:LYS:HB2	2.15	0.62
1:E:77:ASN:HD22	1:E:79:ASP:N	1.98	0.62
1:E:70:SER:HB3	2:E:141:HOH:O	1.99	0.61
1:B:66:PRO:HA	1:B:133:GLU:OE1	2.01	0.61
1:C:82:LYS:NZ	1:E:23:ARG:NH2	2.49	0.60
1:G:35:ILE:HG21	1:G:129:GLU:CG	2.27	0.60
1:E:66:PRO:HG3	1:E:133:GLU:HB2	1.82	0.60
1:D:77:ASN:ND2	1:D:79:ASP:HB2	2.17	0.60
1:I:77:ASN:HD22	1:I:79:ASP:N	1.98	0.60
1:G:77:ASN:HD22	1:G:79:ASP:N	1.98	0.60
1:E:33:THR:O	1:E:120:ILE:HG12	2.01	0.60
1:A:15:PRO:CB	1:C:115:ARG:NH1	2.65	0.60
1:D:30:SER:O	1:D:117:LYS:HE3	2.02	0.59
1:G:94:CYS:SG	1:G:95:TRP:N	2.74	0.59
1:D:23:ARG:HH21	1:I:20:GLU:CA	2.15	0.59
1:F:77:ASN:HD22	1:F:79:ASP:N	1.99	0.59
1:A:15:PRO:C	1:C:115:ARG:NH1	2.53	0.59
1:C:130:ASN:OD1	2:C:140:HOH:O	2.16	0.59
1:A:77:ASN:HD22	1:A:79:ASP:N	1.99	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:23:ARG:NH1	2:I:146:HOH:O	2.37	0.58
1:A:15:PRO:O	1:C:115:ARG:NH2	2.22	0.57
1:G:77:ASN:ND2	1:G:79:ASP:HB2	2.19	0.57
1:A:77:ASN:ND2	1:A:79:ASP:HB2	2.20	0.57
1:H:77:ASN:ND2	1:H:79:ASP:HB2	2.18	0.57
1:A:30:SER:O	1:A:117:LYS:HE3	2.03	0.57
1:C:132:LEU:C	1:C:132:LEU:HD12	2.26	0.56
1:G:44:LYS:HB2	1:G:44:LYS:HZ2	1.70	0.56
1:C:33:THR:O	1:C:120:ILE:HG12	2.05	0.56
1:F:17:ASN:ND2	1:F:20:GLU:HB2	2.20	0.56
1:F:66:PRO:HA	1:F:133:GLU:OE2	2.06	0.56
1:I:77:ASN:ND2	1:I:79:ASP:HB2	2.21	0.56
1:H:31:TYR:OH	1:I:20:GLU:HG2	2.05	0.56
1:H:17:ASN:HD22	1:H:18:PRO:N	2.04	0.56
1:C:47:GLU:O	1:C:88:LYS:HE3	2.06	0.56
1:D:23:ARG:HH22	1:I:20:GLU:CG	2.17	0.55
1:B:77:ASN:ND2	1:B:79:ASP:HB2	2.20	0.55
1:H:63:CYS:SG	1:H:132:LEU:HD13	2.46	0.55
1:H:40:ILE:HG22	1:H:44:LYS:HD2	1.89	0.55
1:F:77:ASN:ND2	1:F:79:ASP:HB2	2.21	0.55
1:F:49:ILE:HG22	1:F:89:VAL:HB	1.89	0.55
1:E:77:ASN:ND2	1:E:79:ASP:HB2	2.22	0.54
1:G:35:ILE:CG2	1:G:129:GLU:HG3	2.27	0.54
1:H:40:ILE:O	1:H:44:LYS:HG3	2.07	0.54
1:D:23:ARG:CZ	1:I:20:GLU:HB2	2.36	0.54
1:A:54:VAL:HG12	1:A:54:VAL:O	2.08	0.54
1:C:77:ASN:ND2	1:C:79:ASP:HB2	2.23	0.53
1:E:115:ARG:HH22	1:F:15:PRO:N	2.07	0.53
1:D:77:ASN:HD21	1:D:79:ASP:HB2	1.72	0.52
1:E:82:LYS:HB2	2:E:146:HOH:O	2.09	0.52
1:H:96:GLY:HA2	1:H:121:GLY:O	2.09	0.52
1:B:128:LYS:HA	2:B:143:HOH:O	2.10	0.52
1:B:77:ASN:HD21	1:B:79:ASP:HB2	1.74	0.52
1:F:116:VAL:HG22	1:F:117:LYS:N	2.24	0.52
1:G:30:SER:O	1:G:117:LYS:HE3	2.10	0.52
1:I:80:THR:CG2	2:I:142:HOH:O	2.57	0.52
1:C:94:CYS:SG	1:C:95:TRP:N	2.81	0.52
1:A:116:VAL:HG22	1:A:117:LYS:N	2.25	0.52
1:D:23:ARG:HH22	1:I:20:GLU:HG3	1.73	0.52
1:F:17:ASN:HD21	1:F:20:GLU:HB2	1.75	0.51
1:I:77:ASN:HD21	1:I:79:ASP:HB2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:THR:O	1:B:120:ILE:HG12	2.10	0.51
1:C:54:VAL:HG12	1:C:54:VAL:O	2.09	0.51
1:H:17:ASN:ND2	1:H:18:PRO:HD2	2.24	0.51
1:A:98:ALA:O	1:B:34:ASP:HB2	2.10	0.51
1:H:116:VAL:HG22	1:H:117:LYS:N	2.25	0.51
1:A:77:ASN:HD21	1:A:79:ASP:HB2	1.75	0.51
1:G:96:GLY:HA2	1:G:121:GLY:O	2.10	0.51
1:H:77:ASN:HD21	1:H:79:ASP:HB2	1.74	0.51
1:H:94:CYS:SG	1:H:95:TRP:N	2.76	0.51
1:C:60:TYR:O	1:C:64:HIS:HD2	1.94	0.51
1:D:47:GLU:O	1:D:88:LYS:HE3	2.10	0.51
1:E:117:LYS:NZ	1:F:15:PRO:HG3	2.26	0.51
1:F:77:ASN:HD21	1:F:79:ASP:HB2	1.75	0.51
1:G:53:ASP:OD1	1:G:55:ARG:HD3	2.11	0.51
1:E:53:ASP:OD1	1:E:55:ARG:HD3	2.11	0.50
1:E:115:ARG:HH12	1:F:16:ALA:H	1.58	0.50
1:B:116:VAL:HG22	1:B:117:LYS:N	2.27	0.50
1:I:116:VAL:HG22	1:I:117:LYS:N	2.26	0.50
1:E:94:CYS:SG	1:E:95:TRP:N	2.78	0.50
1:F:53:ASP:OD1	1:F:55:ARG:HD3	2.12	0.50
1:I:53:ASP:OD1	1:I:55:ARG:HD3	2.12	0.50
1:F:94:CYS:SG	1:F:95:TRP:N	2.75	0.49
1:G:33:THR:O	1:G:120:ILE:HG12	2.12	0.49
1:I:26:MSE:CE	2:I:148:HOH:O	2.51	0.49
1:C:116:VAL:HG22	1:C:117:LYS:N	2.28	0.49
1:C:77:ASN:HD21	1:C:79:ASP:HB2	1.77	0.49
1:D:94:CYS:SG	1:D:95:TRP:N	2.80	0.49
1:D:96:GLY:HA2	1:D:121:GLY:O	2.13	0.49
1:G:77:ASN:HD21	1:G:79:ASP:HB2	1.77	0.49
1:A:15:PRO:CG	1:C:115:ARG:NH1	2.75	0.49
1:E:115:ARG:NH1	1:F:16:ALA:H	2.11	0.49
1:G:116:VAL:HG22	1:G:117:LYS:N	2.28	0.48
1:G:50:ILE:HD11	1:G:88:LYS:HD2	1.95	0.48
1:E:60:TYR:O	1:E:64:HIS:HD2	1.96	0.48
1:E:115:ARG:NH1	1:F:16:ALA:N	2.61	0.48
1:D:43:LYS:NZ	1:D:43:LYS:HB3	2.28	0.48
1:C:64:HIS:O	1:C:132:LEU:HB2	2.13	0.48
1:C:78:GLU:HG2	1:C:112:LEU:HD22	1.96	0.48
1:D:60:TYR:O	1:D:64:HIS:HD2	1.95	0.48
1:B:60:TYR:O	1:B:64:HIS:HD2	1.96	0.48
1:E:115:ARG:HH22	1:F:15:PRO:CA	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:17:ASN:HD22	1:H:17:ASN:C	2.17	0.48
1:H:53:ASP:OD1	1:H:55:ARG:HD3	2.13	0.48
1:E:54:VAL:O	1:E:54:VAL:HG12	2.13	0.48
1:H:60:TYR:O	1:H:64:HIS:HD2	1.96	0.48
1:I:96:GLY:HA2	1:I:121:GLY:O	2.14	0.48
1:E:116:VAL:HG22	1:E:117:LYS:N	2.29	0.47
1:F:60:TYR:O	1:F:64:HIS:HD2	1.97	0.47
1:A:40:ILE:O	1:A:44:LYS:HG3	2.14	0.47
1:A:15:PRO:CA	1:C:115:ARG:HH12	2.27	0.47
1:I:54:VAL:HG12	1:I:54:VAL:O	2.13	0.47
1:E:77:ASN:HD21	1:E:79:ASP:HB2	1.78	0.47
1:F:43:LYS:HD3	1:F:44:LYS:H	1.76	0.47
1:F:50:ILE:HD11	1:F:88:LYS:HD2	1.95	0.47
1:A:15:PRO:C	1:C:115:ARG:NH2	2.65	0.47
1:D:116:VAL:HG22	1:D:117:LYS:N	2.30	0.47
1:E:30:SER:HB2	1:F:15:PRO:HA	1.96	0.47
1:E:115:ARG:HH12	1:F:16:ALA:N	2.12	0.47
1:E:115:ARG:NH2	1:F:15:PRO:C	2.59	0.47
1:E:98:ALA:O	1:F:34:ASP:HB2	2.15	0.47
1:B:30:SER:O	1:B:117:LYS:HE3	2.14	0.47
1:B:54:VAL:O	1:B:54:VAL:HG12	2.14	0.47
1:G:54:VAL:O	1:G:54:VAL:HG12	2.15	0.47
1:A:60:TYR:O	1:A:64:HIS:HD2	1.97	0.47
1:B:115:ARG:HG3	1:B:115:ARG:HH11	1.80	0.47
1:E:50:ILE:HD11	1:E:88:LYS:HD2	1.97	0.47
1:F:94:CYS:HB3	2:F:142:HOH:O	2.15	0.46
1:G:91:ILE:HA	1:G:117:LYS:O	2.16	0.46
1:I:60:TYR:O	1:I:64:HIS:HD2	1.98	0.46
1:D:19:ASN:HB2	2:D:6:HOH:O	2.15	0.46
1:B:66:PRO:HG3	1:B:133:GLU:HB2	1.98	0.46
1:I:115:ARG:HH11	1:I:115:ARG:HG3	1.80	0.46
1:A:53:ASP:OD1	1:A:55:ARG:HD3	2.16	0.46
1:A:16:ALA:O	1:C:115:ARG:NH1	2.49	0.46
1:C:46:TYR:CZ	1:C:48:GLY:HA3	2.51	0.46
1:F:54:VAL:O	1:F:54:VAL:HG12	2.15	0.46
1:D:49:ILE:HD12	1:D:49:ILE:O	2.16	0.45
1:E:115:ARG:NH2	1:F:15:PRO:N	2.64	0.45
1:G:60:TYR:O	1:G:64:HIS:HD2	1.98	0.45
1:A:94:CYS:SG	1:A:95:TRP:N	2.81	0.45
1:B:129:GLU:CB	1:B:130:ASN:HD22	2.24	0.45
1:C:115:ARG:HG3	1:C:115:ARG:HH11	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:GLY:HA3	1:C:125:TYR:CD2	2.52	0.45
1:C:91:ILE:HA	1:C:117:LYS:O	2.16	0.45
1:D:115:ARG:HG3	1:D:115:ARG:HH11	1.81	0.45
1:D:53:ASP:OD1	1:D:55:ARG:HD3	2.17	0.45
1:E:17:ASN:H	1:E:18:PRO:CD	2.29	0.45
1:I:78:GLU:HG2	1:I:112:LEU:HD22	1.99	0.45
1:E:36:ALA:N	2:E:143:HOH:O	2.45	0.45
1:F:115:ARG:HH11	1:F:115:ARG:HG3	1.82	0.44
1:A:115:ARG:HH11	1:A:115:ARG:HG3	1.81	0.44
1:C:63:CYS:HB2	1:C:132:LEU:CD1	2.47	0.44
1:A:91:ILE:HA	1:A:117:LYS:O	2.18	0.44
1:C:96:GLY:HA2	1:C:121:GLY:O	2.16	0.44
1:D:50:ILE:HD11	1:D:88:LYS:HD2	1.99	0.44
1:F:78:GLU:HG2	1:F:112:LEU:HD22	2.00	0.44
1:D:121:GLY:HA3	1:D:125:TYR:CD2	2.53	0.44
1:G:48:GLY:HA2	1:G:88:LYS:HG2	2.00	0.44
1:H:54:VAL:O	1:H:54:VAL:HG12	2.17	0.44
1:G:115:ARG:HH11	1:G:115:ARG:HG3	1.82	0.44
1:B:96:GLY:HA2	1:B:121:GLY:O	2.18	0.44
1:A:50:ILE:HD11	1:A:88:LYS:HD2	1.98	0.44
1:A:96:GLY:HA2	1:A:121:GLY:O	2.17	0.44
1:H:115:ARG:HG3	1:H:115:ARG:HH11	1.83	0.44
1:H:91:ILE:HA	1:H:117:LYS:O	2.17	0.44
1:B:115:ARG:NH1	1:C:16:ALA:N	2.66	0.44
1:B:77:ASN:ND2	1:B:79:ASP:H	2.05	0.44
1:D:91:ILE:HA	1:D:117:LYS:O	2.18	0.44
1:E:28:LYS:O	1:E:32:GLU:HG2	2.17	0.44
1:E:78:GLU:HG2	1:E:112:LEU:HD22	1.99	0.43
1:F:96:GLY:HA2	1:F:121:GLY:O	2.18	0.43
1:G:38:LEU:HD12	1:G:126:TRP:CZ3	2.53	0.43
1:G:129:GLU:O	1:G:130:ASN:C	2.55	0.43
1:B:94:CYS:SG	1:B:95:TRP:N	2.81	0.43
1:F:43:LYS:HE2	1:F:43:LYS:HB2	1.69	0.43
1:A:28:LYS:O	1:A:32:GLU:HG2	2.17	0.43
1:B:46:TYR:CE2	1:B:48:GLY:HA3	2.54	0.43
1:D:43:LYS:NZ	1:D:43:LYS:CB	2.81	0.43
1:B:28:LYS:O	1:B:32:GLU:HG2	2.18	0.43
1:B:91:ILE:HA	1:B:117:LYS:O	2.18	0.43
1:C:125:TYR:O	1:C:129:GLU:HG2	2.19	0.43
1:C:53:ASP:OD1	1:C:55:ARG:HD3	2.19	0.43
1:C:89:VAL:HG13	1:C:115:ARG:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:ARG:NH1	1:E:17:ASN:OD1	2.52	0.43
1:G:89:VAL:HG13	1:G:115:ARG:O	2.19	0.43
1:C:50:ILE:HD11	1:C:88:LYS:HD2	2.00	0.43
1:I:77:ASN:ND2	1:I:79:ASP:H	2.07	0.43
1:D:98:ALA:O	1:E:34:ASP:HB2	2.19	0.42
1:E:62:GLU:O	1:E:63:CYS:HB3	2.19	0.42
1:B:50:ILE:HD11	1:B:88:LYS:HD2	2.01	0.42
1:F:91:ILE:HA	1:F:117:LYS:O	2.19	0.42
1:D:23:ARG:HH21	1:I:20:GLU:HA	1.84	0.42
1:A:97:PRO:HB2	1:B:125:TYR:CE2	2.55	0.42
1:E:73:GLY:C	1:E:75:LYS:H	2.23	0.42
1:D:54:VAL:HG12	1:D:54:VAL:O	2.19	0.42
1:E:115:ARG:HH11	1:E:115:ARG:HG3	1.85	0.42
1:E:30:SER:HB2	1:F:15:PRO:CA	2.49	0.42
1:A:125:TYR:O	1:A:129:GLU:HG2	2.18	0.42
1:B:115:ARG:HH12	1:C:16:ALA:N	2.17	0.42
1:F:63:CYS:SG	1:F:132:LEU:HD22	2.59	0.42
1:G:73:GLY:C	1:G:75:LYS:H	2.23	0.42
1:D:77:ASN:ND2	1:D:79:ASP:H	2.05	0.42
1:E:91:ILE:HA	1:E:117:LYS:O	2.19	0.42
1:D:115:ARG:CZ	1:E:17:ASN:OD1	2.68	0.42
1:H:50:ILE:HD11	1:H:88:LYS:HD2	2.01	0.42
1:I:50:ILE:HD11	1:I:88:LYS:HD2	2.01	0.42
1:A:100:ASN:HA	1:A:100:ASN:HD22	1.62	0.42
1:A:54:VAL:O	1:A:54:VAL:CG1	2.68	0.42
1:B:121:GLY:HA3	1:B:125:TYR:CD2	2.55	0.42
1:C:19:ASN:HB3	1:C:23:ARG:NH1	2.35	0.42
1:I:91:ILE:HA	1:I:117:LYS:O	2.20	0.42
1:G:127:ARG:O	1:G:130:ASN:HB2	2.20	0.41
1:G:44:LYS:CB	1:G:44:LYS:NZ	2.82	0.41
1:B:78:GLU:HG2	1:B:112:LEU:HD22	2.02	0.41
1:D:125:TYR:O	1:D:129:GLU:HG2	2.20	0.41
1:D:46:TYR:HD2	1:D:49:ILE:HG13	1.85	0.41
1:G:36:ALA:O	1:G:40:ILE:HG12	2.20	0.41
1:I:61:LYS:HB2	1:I:61:LYS:HE3	1.87	0.41
1:F:73:GLY:C	1:F:75:LYS:H	2.23	0.41
1:H:127:ARG:HG2	1:H:132:LEU:HD11	2.02	0.41
1:I:75:LYS:HE3	2:I:142:HOH:O	2.21	0.41
1:F:121:GLY:HA3	1:F:125:TYR:CD2	2.56	0.41
1:G:19:ASN:OD1	2:G:147:HOH:O	2.21	0.41
1:I:28:LYS:O	1:I:32:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ALA:O	1:A:40:ILE:HG12	2.21	0.41
1:C:77:ASN:ND2	1:C:79:ASP:H	2.06	0.41
1:D:61:LYS:HB2	1:D:61:LYS:HE3	1.90	0.41
1:E:121:GLY:HA3	1:E:125:TYR:CD2	2.56	0.41
1:E:96:GLY:HA2	1:E:121:GLY:O	2.21	0.41
1:I:54:VAL:HG13	1:I:73:GLY:CA	2.51	0.41
1:A:20:GLU:HG2	1:C:31:TYR:OH	2.21	0.41
1:C:28:LYS:O	1:C:32:GLU:HG2	2.21	0.41
1:H:121:GLY:HA3	1:H:125:TYR:CD2	2.56	0.41
1:I:80:THR:HG23	2:I:142:HOH:O	2.20	0.41
1:A:78:GLU:HG2	1:A:112:LEU:HD22	2.02	0.40
1:C:19:ASN:HB3	1:C:23:ARG:HH12	1.86	0.40
1:H:78:GLU:HG2	1:H:112:LEU:HD22	2.03	0.40
1:G:65:ILE:HA	1:G:66:PRO:HD3	1.99	0.40
1:I:53:ASP:OD2	1:I:55:ARG:NH1	2.53	0.40
1:A:33:THR:HA	2:A:11:HOH:O	2.20	0.40
1:F:77:ASN:ND2	1:F:79:ASP:H	2.09	0.40
1:B:73:GLY:C	1:B:75:LYS:H	2.25	0.40
1:E:115:ARG:NH2	1:F:16:ALA:N	2.70	0.40
1:B:53:ASP:OD1	1:B:55:ARG:HD3	2.21	0.40
1:D:100:ASN:HD22	1:D:100:ASN:HA	1.64	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:C:22:TYR:OH	1:F:83:ARG:NH1[2_455]	2.11	0.09

## 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	116/126 (92%)	108 (93%)	7 (6%)	1 (1%)	20	53
1	B	115/126 (91%)	109 (95%)	6 (5%)	0	100	100
1	C	116/126 (92%)	108 (93%)	7 (6%)	1 (1%)	20	53
1	D	112/126 (89%)	108 (96%)	4 (4%)	0	100	100
1	E	116/126 (92%)	109 (94%)	6 (5%)	1 (1%)	20	53
1	F	114/126 (90%)	106 (93%)	8 (7%)	0	100	100
1	G	112/126 (89%)	103 (92%)	9 (8%)	0	100	100
1	H	114/126 (90%)	105 (92%)	9 (8%)	0	100	100
1	I	109/126 (86%)	102 (94%)	7 (6%)	0	100	100
All	All	1024/1134 (90%)	958 (94%)	63 (6%)	3 (0%)	44	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	17	ASN
1	A	15	PRO
1	C	132	LEU

### 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	96/104 (92%)	92 (96%)	4 (4%)	34	68
1	B	97/104 (93%)	94 (97%)	3 (3%)	45	79
1	C	97/104 (93%)	93 (96%)	4 (4%)	35	69
1	D	95/104 (91%)	93 (98%)	2 (2%)	59	85
1	E	97/104 (93%)	91 (94%)	6 (6%)	21	51
1	F	97/104 (93%)	91 (94%)	6 (6%)	21	51
1	G	95/104 (91%)	92 (97%)	3 (3%)	44	78
1	H	96/104 (92%)	93 (97%)	3 (3%)	45	79
1	I	93/104 (89%)	91 (98%)	2 (2%)	57	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	863/936 (92%)	830 (96%)	33 (4%)	38	72

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LYS
1	A	63	CYS
1	A	77	ASN
1	A	80	THR
1	B	47	GLU
1	B	77	ASN
1	B	80	THR
1	C	44	LYS
1	C	47	GLU
1	C	77	ASN
1	C	80	THR
1	D	77	ASN
1	D	80	THR
1	E	17	ASN
1	E	44	LYS
1	E	77	ASN
1	E	80	THR
1	E	130	ASN
1	E	133	GLU
1	F	43	LYS
1	F	77	ASN
1	F	80	THR
1	F	130	ASN
1	F	132	LEU
1	F	133	GLU
1	G	77	ASN
1	G	80	THR
1	G	130	ASN
1	H	17	ASN
1	H	77	ASN
1	H	80	THR
1	I	77	ASN
1	I	80	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	100	ASN
1	A	111	GLN
1	B	17	ASN
1	B	77	ASN
1	B	100	ASN
1	B	111	GLN
1	B	130	ASN
1	C	17	ASN
1	C	77	ASN
1	C	100	ASN
1	C	111	GLN
1	D	19	ASN
1	D	77	ASN
1	D	100	ASN
1	D	111	GLN
1	D	130	ASN
1	E	19	ASN
1	E	77	ASN
1	E	100	ASN
1	E	111	GLN
1	F	77	ASN
1	F	100	ASN
1	F	111	GLN
1	F	134	HIS
1	G	77	ASN
1	G	100	ASN
1	G	111	GLN
1	G	130	ASN
1	H	17	ASN
1	H	77	ASN
1	H	100	ASN
1	H	111	GLN
1	I	77	ASN
1	I	100	ASN
1	I	111	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [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	117/126 (92%)	0.19	3 (2%) 56 52	12, 25, 46, 55	0
1	B	116/126 (92%)	0.17	2 (1%) 70 68	6, 25, 47, 52	0
1	C	117/126 (92%)	0.28	3 (2%) 56 52	11, 24, 44, 52	0
1	D	113/126 (89%)	0.18	1 (0%) 84 83	10, 27, 47, 54	0
1	E	117/126 (92%)	0.22	2 (1%) 70 68	5, 23, 46, 55	0
1	F	117/126 (92%)	0.29	2 (1%) 70 68	9, 26, 46, 52	0
1	G	113/126 (89%)	0.71	13 (11%) 5 4	22, 38, 57, 66	0
1	H	115/126 (91%)	0.46	7 (6%) 22 18	24, 37, 55, 69	0
1	I	112/126 (88%)	0.64	8 (7%) 17 13	25, 38, 55, 62	0
All	All	1037/1134 (91%)	0.35	41 (3%) 39 35	5, 31, 51, 69	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	83	ARG	4.5
1	G	115	ARG	4.2
1	G	130	ASN	3.9
1	H	47	GLU	3.4
1	A	131	GLY	3.4
1	I	16	ALA	3.3
1	A	130	ASN	3.0
1	G	43	LYS	3.0
1	G	78	GLU	2.9
1	I	58	GLU	2.8
1	I	76	ILE	2.8
1	I	115	ARG	2.8
1	C	129	GLU	2.7
1	G	42	ILE	2.7
1	H	17	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	130	ASN	2.7
1	I	99	CYS	2.6
1	E	16	ALA	2.6
1	E	129	GLU	2.6
1	G	85	SER	2.6
1	I	129	GLU	2.5
1	H	67	THR	2.5
1	G	44	LYS	2.4
1	G	81	THR	2.4
1	H	129	GLU	2.4
1	F	15	PRO	2.3
1	G	34	ASP	2.3
1	H	121	GLY	2.2
1	I	63	CYS	2.2
1	B	78	GLU	2.2
1	G	62	GLU	2.2
1	H	46	TYR	2.1
1	B	87	GLU	2.1
1	A	78	GLU	2.1
1	F	129	GLU	2.1
1	C	78	GLU	2.1
1	G	79	ASP	2.1
1	H	37	ASP	2.1
1	G	45	GLY	2.0
1	G	60	TYR	2.0
1	C	16	ALA	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.