



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:38 AM GMT

PDB ID : 3KTG  
Title : Structure of ClpP from Bacillus subtilis in monoclinic crystal form  
Authors : Lee, B.-G.; Brotz-Oesterhelt, H.; Song, H.K.  
Deposited on : 2009-11-25  
Resolution : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

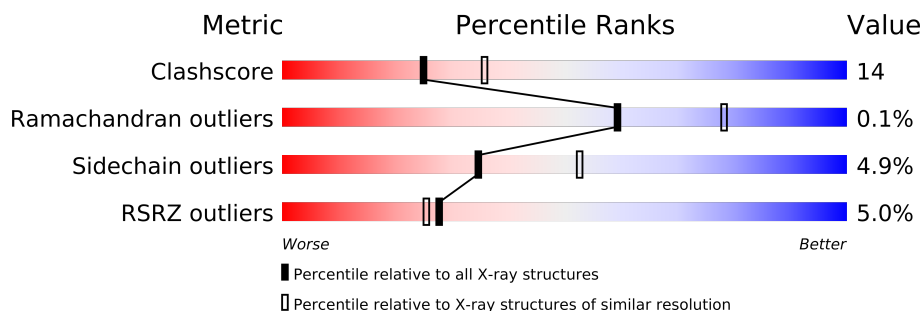
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	199	
1	B	199	
1	C	199	
1	D	199	
1	E	199	
1	F	199	
1	G	199	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10485 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1428	903	245	273	7			
1	B	188	Total	C	N	O	S	0	0	0
			1428	903	245	273	7			
1	C	188	Total	C	N	O	S	0	0	0
			1428	903	245	273	7			
1	D	188	Total	C	N	O	S	0	0	0
			1428	903	245	273	7			
1	E	188	Total	C	N	O	S	0	0	0
			1428	903	245	273	7			
1	F	188	Total	C	N	O	S	0	0	0
			1428	903	245	273	7			
1	G	188	Total	C	N	O	S	0	0	0
			1428	903	245	273	7			

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	LEU	THR	ENGINEERED	UNP P80244
A	194	HIS	ASP	ENGINEERED	UNP P80244
A	195	HIS	LYS	ENGINEERED	UNP P80244
A	196	HIS	LYS	ENGINEERED	UNP P80244
A	197	HIS	-	EXPRESSION TAG	UNP P80244
A	198	HIS	-	EXPRESSION TAG	UNP P80244
A	199	HIS	-	EXPRESSION TAG	UNP P80244
B	192	LEU	THR	ENGINEERED	UNP P80244
B	194	HIS	ASP	ENGINEERED	UNP P80244
B	195	HIS	LYS	ENGINEERED	UNP P80244
B	196	HIS	LYS	ENGINEERED	UNP P80244
B	197	HIS	-	EXPRESSION TAG	UNP P80244
B	198	HIS	-	EXPRESSION TAG	UNP P80244
B	199	HIS	-	EXPRESSION TAG	UNP P80244
C	192	LEU	THR	ENGINEERED	UNP P80244

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	194	HIS	ASP	ENGINEERED	UNP P80244
C	195	HIS	LYS	ENGINEERED	UNP P80244
C	196	HIS	LYS	ENGINEERED	UNP P80244
C	197	HIS	-	EXPRESSION TAG	UNP P80244
C	198	HIS	-	EXPRESSION TAG	UNP P80244
C	199	HIS	-	EXPRESSION TAG	UNP P80244
D	192	LEU	THR	ENGINEERED	UNP P80244
D	194	HIS	ASP	ENGINEERED	UNP P80244
D	195	HIS	LYS	ENGINEERED	UNP P80244
D	196	HIS	LYS	ENGINEERED	UNP P80244
D	197	HIS	-	EXPRESSION TAG	UNP P80244
D	198	HIS	-	EXPRESSION TAG	UNP P80244
D	199	HIS	-	EXPRESSION TAG	UNP P80244
E	192	LEU	THR	ENGINEERED	UNP P80244
E	194	HIS	ASP	ENGINEERED	UNP P80244
E	195	HIS	LYS	ENGINEERED	UNP P80244
E	196	HIS	LYS	ENGINEERED	UNP P80244
E	197	HIS	-	EXPRESSION TAG	UNP P80244
E	198	HIS	-	EXPRESSION TAG	UNP P80244
E	199	HIS	-	EXPRESSION TAG	UNP P80244
F	192	LEU	THR	ENGINEERED	UNP P80244
F	194	HIS	ASP	ENGINEERED	UNP P80244
F	195	HIS	LYS	ENGINEERED	UNP P80244
F	196	HIS	LYS	ENGINEERED	UNP P80244
F	197	HIS	-	EXPRESSION TAG	UNP P80244
F	198	HIS	-	EXPRESSION TAG	UNP P80244
F	199	HIS	-	EXPRESSION TAG	UNP P80244
G	192	LEU	THR	ENGINEERED	UNP P80244
G	194	HIS	ASP	ENGINEERED	UNP P80244
G	195	HIS	LYS	ENGINEERED	UNP P80244
G	196	HIS	LYS	ENGINEERED	UNP P80244
G	197	HIS	-	EXPRESSION TAG	UNP P80244
G	198	HIS	-	EXPRESSION TAG	UNP P80244
G	199	HIS	-	EXPRESSION TAG	UNP P80244

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	77	Total O 77 77	0	0
2	B	66	Total O 66 66	0	0

*Continued on next page...*

*Continued from previous page...*

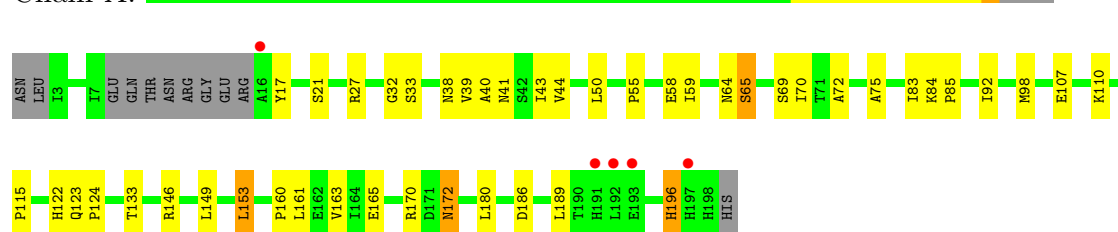
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	67	Total 67	O 67	0	0
2	D	69	Total 69	O 69	0	0
2	E	61	Total 61	O 61	0	0
2	F	71	Total 71	O 71	0	0
2	G	78	Total 78	O 78	0	0

### 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.

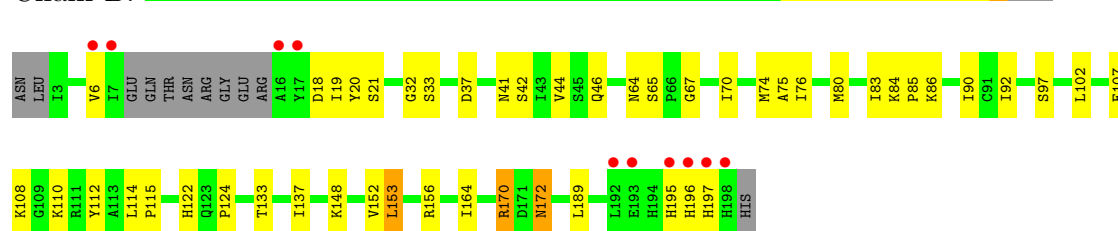
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:



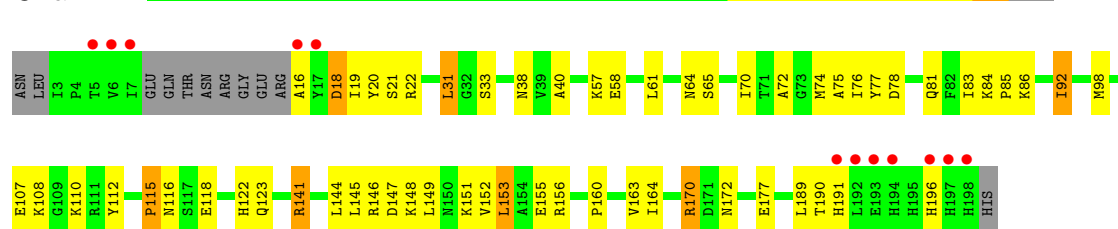
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C:



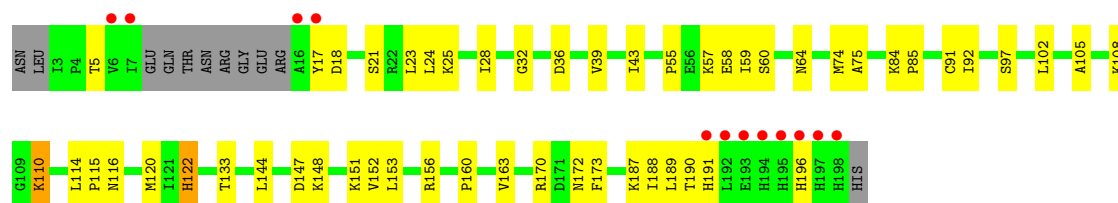
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain D:



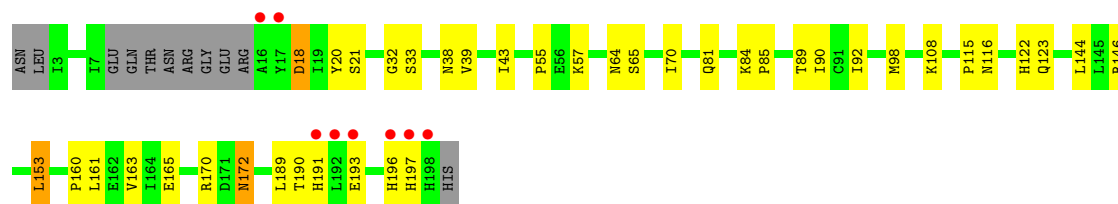
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E:



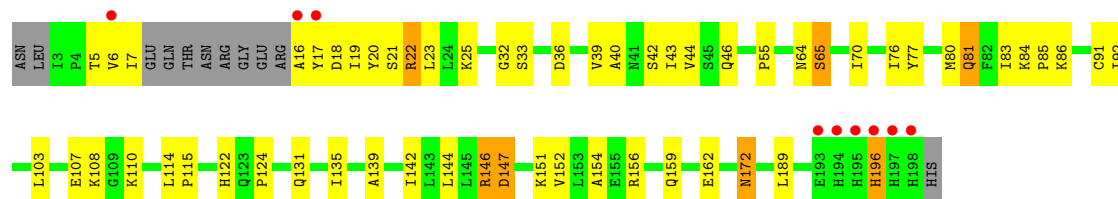
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F:



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.50Å 150.70Å 106.54Å 90.00° 121.65° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 37.29 – 2.39	Depositor EDS
% Data completeness (in resolution range)	89.4 (50.00-2.40) 88.4 (37.29-2.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.79 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.212 , 0.268 0.210 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	36.3	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 32.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	1 of 63498 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10485	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 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	0.35	0/1448	0.57	0/1955
1	B	0.36	0/1448	0.59	0/1955
1	C	0.33	0/1448	0.58	0/1955
1	D	0.35	0/1448	0.56	0/1955
1	E	0.34	0/1448	0.57	0/1955
1	F	0.37	0/1448	0.57	0/1955
1	G	0.36	0/1448	0.56	0/1955
All	All	0.35	0/10136	0.57	0/13685

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1428	0	1438	34	0
1	B	1428	0	1438	38	0
1	C	1428	0	1438	53	0
1	D	1428	0	1438	55	0
1	E	1428	0	1438	38	0
1	F	1428	0	1438	42	0
1	G	1428	0	1438	44	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	77	0	0	1	0
2	B	66	0	0	0	0
2	C	67	0	0	4	0
2	D	69	0	0	3	0
2	E	61	0	0	3	0
2	F	71	0	0	4	0
2	G	78	0	0	3	0
All	All	10485	0	10066	277	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (277) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:77:TYR:HA	1:G:80:MET:HE2	1.48	0.94
1:A:50:LEU:HD13	1:A:59:ILE:HD12	1.49	0.92
1:C:84:LYS:H	1:C:84:LYS:CE	1.84	0.91
1:C:84:LYS:H	1:C:84:LYS:HE3	1.45	0.81
1:C:159:GLN:HB3	1:C:164:ILE:HD11	1.63	0.80
1:E:18:ASP:HB3	1:E:21:SER:OG	1.81	0.79
1:E:115:PRO:HD3	1:E:189:LEU:O	1.84	0.78
1:F:170:ARG:HG3	1:F:170:ARG:HH11	1.48	0.77
1:B:86:LYS:HD3	1:B:107:GLU:HG2	1.67	0.77
1:F:84:LYS:HE2	1:F:85:PRO:HD3	1.68	0.76
1:B:33:SER:O	1:B:65:SER:HB2	1.85	0.75
1:E:152:VAL:O	1:E:156:ARG:HG2	1.85	0.75
1:G:92:ILE:HG22	1:G:114:LEU:HD12	1.70	0.74
1:G:124:PRO:HD2	1:G:146:ARG:HG3	1.71	0.73
1:A:33:SER:O	1:A:65:SER:HB2	1.89	0.72
1:D:141:ARG:HH11	1:D:141:ARG:HG2	1.55	0.71
1:D:84:LYS:NZ	1:D:84:LYS:HB2	2.05	0.71
1:E:191:HIS:HB3	2:E:217:HOH:O	1.90	0.71
1:B:152:VAL:O	1:B:156:ARG:HG2	1.92	0.70
1:B:18:ASP:HB3	1:B:21:SER:OG	1.91	0.70
1:C:98:MET:HA	1:C:98:MET:HE2	1.73	0.68
1:G:139:ALA:O	1:G:142:ILE:HG22	1.93	0.68
1:C:18:ASP:OD1	1:C:21:SER:HB2	1.93	0.68
1:B:44:VAL:HG21	1:C:92:ILE:HD11	1.75	0.68
1:F:123:GLN:HE22	1:F:146:ARG:HH21	1.42	0.68
1:D:160:PRO:HG2	1:D:163:VAL:HG23	1.77	0.67
1:G:81:GLN:HA	1:G:81:GLN:HE21	1.60	0.67
1:C:159:GLN:HG3	1:C:160:PRO:HD2	1.77	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:80:MET:CE	1:B:102:LEU:HD22	2.24	0.66
1:C:28:ILE:HD13	1:C:60:SER:HB2	1.75	0.66
1:C:33:SER:O	1:C:65:SER:HB2	1.95	0.66
1:E:160:PRO:HG2	1:E:163:VAL:HG23	1.77	0.66
1:F:33:SER:O	1:F:65:SER:HB2	1.95	0.66
1:C:84:LYS:H	1:C:84:LYS:HE2	1.61	0.65
1:C:159:GLN:HB3	1:C:164:ILE:CD1	2.25	0.65
1:G:77:TYR:HA	1:G:80:MET:CE	2.27	0.64
1:F:161:LEU:O	1:F:165:GLU:HG3	1.97	0.64
1:D:78:ASP:HB3	1:E:114:LEU:HD13	1.78	0.64
1:G:146:ARG:HH11	1:G:146:ARG:HB3	1.63	0.64
1:D:83:ILE:HB	1:D:85:PRO:HD2	1.79	0.64
1:F:190:THR:HG22	1:F:191:HIS:CD2	2.32	0.64
1:D:123:GLN:HE22	1:D:146:ARG:HH21	1.46	0.64
1:G:86:LYS:HD3	1:G:107:GLU:HG2	1.80	0.64
1:D:151:LYS:O	1:D:155:GLU:HG3	1.98	0.63
1:F:115:PRO:HD3	1:F:189:LEU:O	1.98	0.63
1:A:123:GLN:NE2	1:A:146:ARG:HH21	1.95	0.63
1:A:123:GLN:HE22	1:A:146:ARG:HH21	1.47	0.62
1:A:41:ASN:HB2	2:A:313:HOH:O	1.99	0.62
1:D:75:ALA:HB1	1:E:92:ILE:HG22	1.81	0.62
1:A:32:GLY:HA2	1:A:64:ASN:O	2.00	0.62
1:C:41:ASN:HB2	2:C:231:HOH:O	1.99	0.61
1:G:146:ARG:HB3	1:G:146:ARG:NH1	2.15	0.61
1:G:6:VAL:O	1:G:17:TYR:HB2	2.01	0.61
1:C:152:VAL:O	1:C:156:ARG:HG2	2.01	0.61
1:E:97:SER:HB3	1:E:122:HIS:NE2	2.15	0.61
1:B:110:LYS:HD2	1:B:196:HIS:CD2	2.36	0.61
1:D:160:PRO:HG2	1:D:163:VAL:CG2	2.30	0.61
1:F:64:ASN:HB2	1:F:92:ILE:HG23	1.83	0.61
1:C:44:VAL:HG21	1:D:92:ILE:HD11	1.83	0.60
1:A:161:LEU:O	1:A:165:GLU:HG3	2.01	0.60
1:C:90:ILE:N	1:C:90:ILE:HD12	2.17	0.60
1:E:91:CYS:O	1:E:92:ILE:HD13	2.02	0.60
1:F:90:ILE:N	1:F:90:ILE:HD12	2.17	0.60
1:C:84:LYS:HE3	1:C:85:PRO:HD3	1.83	0.59
1:E:108:LYS:HE3	1:E:156:ARG:O	2.01	0.59
1:B:76:ILE:HG22	1:B:80:MET:CE	2.32	0.59
1:F:146:ARG:HD2	2:F:203:HOH:O	2.01	0.59
1:A:107:GLU:HG2	1:A:110:LYS:HD2	1.85	0.59
1:A:17:TYR:HB3	1:A:21:SER:HB2	1.85	0.59
1:F:123:GLN:NE2	1:F:146:ARG:HH21	2.00	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:80:MET:HE1	1:B:102:LEU:HD22	1.85	0.58
1:G:33:SER:O	1:G:65:SER:HB2	2.03	0.58
1:F:160:PRO:HG2	1:F:163:VAL:CG2	2.33	0.58
1:E:160:PRO:HG2	1:E:163:VAL:CG2	2.33	0.58
1:F:84:LYS:CE	1:F:84:LYS:H	2.16	0.58
1:B:92:ILE:CD1	1:B:114:LEU:HD23	2.34	0.57
1:D:115:PRO:HD3	1:D:189:LEU:O	2.04	0.57
1:D:21:SER:HB3	1:E:5:THR:O	2.04	0.57
1:F:39:VAL:O	1:F:43:ILE:HD13	2.05	0.57
1:F:32:GLY:HA2	1:F:64:ASN:O	2.05	0.57
1:D:147:ASP:O	1:D:151:LYS:HG2	2.04	0.57
1:G:39:VAL:O	1:G:43:ILE:HG12	2.05	0.56
1:D:148:LYS:HD2	1:E:116:ASN:HD22	1.70	0.56
1:C:109:GLY:C	1:C:110:LYS:HD2	2.26	0.56
1:G:36:ASP:OD2	1:G:39:VAL:HG23	2.05	0.56
1:G:172:ASN:HD22	1:G:172:ASN:C	2.09	0.56
1:G:131:GLN:O	1:G:135:ILE:HG12	2.04	0.56
1:G:16:ALA:HB3	2:G:462:HOH:O	2.05	0.56
1:G:124:PRO:HD2	1:G:146:ARG:CG	2.36	0.55
1:D:146:ARG:HD2	2:D:216:HOH:O	2.06	0.55
1:A:58:GLU:OE1	1:A:196:HIS:HE1	1.89	0.55
1:C:177:GLU:OE2	1:C:177:GLU:N	2.35	0.55
1:A:27:ARG:NH2	1:A:59:ILE:HD11	2.21	0.55
1:D:33:SER:O	1:D:65:SER:HB2	2.06	0.55
1:E:170:ARG:HG3	2:E:440:HOH:O	2.07	0.55
1:B:92:ILE:HD13	1:B:114:LEU:HD23	1.88	0.54
1:G:115:PRO:HD3	1:G:189:LEU:O	2.08	0.54
1:E:32:GLY:HA2	1:E:64:ASN:O	2.08	0.54
1:C:148:LYS:HD2	1:D:116:ASN:HD22	1.72	0.54
1:A:160:PRO:HG2	1:A:163:VAL:HG23	1.90	0.53
1:E:39:VAL:O	1:E:43:ILE:HD13	2.08	0.53
1:C:146:ARG:HD2	2:C:219:HOH:O	2.08	0.53
1:A:27:ARG:HB3	1:A:59:ILE:HD13	1.89	0.53
1:G:7:ILE:HA	2:G:462:HOH:O	2.06	0.53
1:F:55:PRO:HB2	1:F:84:LYS:HD2	1.91	0.53
1:C:123:GLN:HE22	1:C:146:ARG:HH21	1.56	0.53
1:F:160:PRO:HG2	1:F:163:VAL:HG23	1.90	0.52
1:G:152:VAL:O	1:G:156:ARG:HG3	2.08	0.52
1:D:40:ALA:HB2	1:D:72:ALA:HB1	1.92	0.52
1:G:32:GLY:HA2	1:G:64:ASN:O	2.10	0.52
1:D:84:LYS:HZ3	1:D:84:LYS:HB2	1.75	0.52
1:C:84:LYS:HE3	1:C:84:LYS:N	2.21	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:110:LYS:HD2	1:D:196:HIS:CD2	2.45	0.52
1:C:70:ILE:HD11	1:C:124:PRO:HB3	1.92	0.52
1:A:180:LEU:HD11	1:A:186:ASP:O	2.10	0.52
1:C:160:PRO:HG2	1:C:163:VAL:CG2	2.40	0.51
1:D:123:GLN:NE2	1:D:146:ARG:HH21	2.08	0.51
1:C:112:TYR:OH	1:C:196:HIS:HD2	1.93	0.51
1:B:76:ILE:HG22	1:B:80:MET:HE1	1.91	0.51
1:F:108:LYS:HB3	2:F:429:HOH:O	2.10	0.51
1:D:75:ALA:CB	1:E:92:ILE:HG22	2.40	0.51
1:B:75:ALA:HB1	1:C:92:ILE:HG12	1.92	0.51
1:C:133:THR:HG21	1:D:170:ARG:NH1	2.25	0.51
1:G:55:PRO:HA	1:G:85:PRO:HG3	1.93	0.51
1:A:70:ILE:HD11	1:A:124:PRO:HB3	1.93	0.51
1:E:115:PRO:CG	1:E:190:THR:HG22	2.41	0.51
1:F:84:LYS:HE2	1:F:84:LYS:H	1.76	0.51
1:A:55:PRO:O	1:A:84:LYS:HG2	2.11	0.51
1:C:115:PRO:HD3	1:C:189:LEU:O	2.11	0.51
1:C:19:ILE:HG23	1:C:20:TYR:N	2.26	0.50
1:A:98:MET:HE3	1:A:149:LEU:HD13	1.93	0.50
1:B:153:LEU:HD12	1:B:164:ILE:HD12	1.92	0.50
1:G:92:ILE:HG22	1:G:114:LEU:CD1	2.39	0.50
1:E:36:ASP:OD2	1:E:39:VAL:HG23	2.11	0.50
1:C:148:LYS:HD2	1:D:116:ASN:ND2	2.25	0.50
1:A:27:ARG:CZ	1:A:59:ILE:HD11	2.42	0.50
1:B:19:ILE:HG23	1:B:20:TYR:N	2.26	0.50
1:D:64:ASN:HB2	1:D:92:ILE:HG23	1.94	0.50
1:C:110:LYS:N	1:C:110:LYS:HD2	2.27	0.49
1:D:141:ARG:NH1	1:D:141:ARG:HG2	2.24	0.49
1:A:172:ASN:HD22	1:A:172:ASN:C	2.15	0.49
1:B:115:PRO:HD3	1:B:189:LEU:O	2.12	0.49
1:G:22:ARG:NE	1:G:25:LYS:HE3	2.28	0.49
1:B:70:ILE:HD11	1:B:124:PRO:HB3	1.94	0.49
1:A:39:VAL:O	1:A:43:ILE:HG12	2.11	0.49
1:F:170:ARG:NH1	2:F:212:HOH:O	2.45	0.49
1:F:55:PRO:CB	1:F:84:LYS:HD2	2.43	0.49
1:F:18:ASP:OD2	1:F:20:TYR:HB2	2.13	0.48
1:E:55:PRO:O	1:E:84:LYS:HB3	2.13	0.48
1:B:112:TYR:OH	1:B:196:HIS:HD2	1.97	0.48
1:F:153:LEU:HA	1:F:153:LEU:HD23	1.65	0.48
1:C:44:VAL:HG11	1:D:92:ILE:HD12	1.96	0.48
1:G:40:ALA:O	1:G:44:VAL:HG23	2.14	0.48
1:C:123:GLN:NE2	1:C:146:ARG:HH21	2.11	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:16:ALA:HB3	2:D:281:HOH:O	2.12	0.48
1:E:28:ILE:HD13	1:E:60:SER:HB2	1.95	0.48
1:C:83:ILE:HB	1:C:85:PRO:HD2	1.94	0.48
1:F:84:LYS:NZ	1:F:84:LYS:H	2.12	0.48
1:E:115:PRO:HG3	1:E:190:THR:HG22	1.94	0.47
1:D:84:LYS:N	1:D:85:PRO:CD	2.77	0.47
1:G:147:ASP:OD2	1:G:151:LYS:HE3	2.14	0.47
1:C:95:ALA:O	1:C:100:ALA:HB2	2.13	0.47
1:E:120:MET:HG3	1:E:173:PHE:CE1	2.49	0.47
1:G:42:SER:O	1:G:46:GLN:HG3	2.14	0.47
1:B:76:ILE:HG22	1:B:80:MET:HE2	1.95	0.47
1:G:64:ASN:HB2	1:G:92:ILE:HG13	1.96	0.47
1:D:84:LYS:HZ2	1:D:84:LYS:HB2	1.78	0.47
1:F:18:ASP:HB3	1:F:21:SER:OG	2.13	0.47
1:F:191:HIS:C	1:F:193:GLU:H	2.18	0.47
1:D:190:THR:HG22	1:D:191:HIS:CD2	2.50	0.47
1:D:177:GLU:N	1:D:177:GLU:OE1	2.40	0.47
1:E:110:LYS:HG3	1:E:196:HIS:HD2	1.79	0.47
1:F:170:ARG:NH1	1:F:170:ARG:HG3	2.23	0.46
1:B:90:ILE:N	1:B:90:ILE:HD12	2.30	0.46
1:F:89:THR:C	1:F:90:ILE:HD12	2.35	0.46
1:C:120:MET:HG3	1:C:173:PHE:CE1	2.50	0.46
1:G:81:GLN:HA	1:G:81:GLN:NE2	2.28	0.46
1:B:84:LYS:N	1:B:85:PRO:CD	2.79	0.46
1:A:84:LYS:HB3	1:A:85:PRO:HD3	1.97	0.46
1:B:172:ASN:C	1:B:172:ASN:HD22	2.19	0.46
1:B:64:ASN:HB2	1:B:92:ILE:HG23	1.98	0.46
1:D:18:ASP:HB3	1:D:21:SER:OG	2.15	0.46
1:C:121:ILE:HA	2:C:200:HOH:O	2.16	0.46
1:C:84:LYS:N	1:C:85:PRO:CD	2.79	0.45
1:E:75:ALA:HB1	1:F:92:ILE:HG12	1.97	0.45
1:B:32:GLY:HA2	1:B:64:ASN:O	2.16	0.45
1:G:22:ARG:HE	1:G:25:LYS:HE3	1.80	0.45
1:C:151:LYS:O	1:C:155:GLU:HG3	2.17	0.45
1:D:145:LEU:O	1:D:149:LEU:HG	2.16	0.45
1:E:74:MET:HE2	1:F:116:ASN:HB3	1.97	0.45
1:A:69:SER:HB3	1:A:72:ALA:HB3	1.98	0.45
1:D:77:TYR:O	1:D:81:GLN:HG2	2.17	0.45
1:F:21:SER:HB3	1:G:5:THR:O	2.17	0.45
1:D:19:ILE:HG23	1:D:20:TYR:N	2.32	0.45
1:C:160:PRO:HG2	1:C:163:VAL:HG23	1.98	0.44
1:A:64:ASN:HB2	1:A:92:ILE:HG13	1.98	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:31:LEU:HB2	1:D:61:LEU:HD11	1.99	0.44
1:G:19:ILE:HG23	1:G:20:TYR:N	2.32	0.44
1:D:75:ALA:HB1	1:E:92:ILE:CG2	2.45	0.44
1:G:76:ILE:O	1:G:80:MET:HG3	2.17	0.44
1:E:148:LYS:HD2	1:F:116:ASN:HD22	1.83	0.44
1:B:67:GLY:HA3	1:B:97:SER:HB3	1.99	0.44
1:C:55:PRO:HB2	1:C:84:LYS:HD2	2.00	0.44
1:C:141:ARG:NE	1:D:118:GLU:OE1	2.50	0.44
1:C:75:ALA:HB1	1:D:92:ILE:CG1	2.47	0.44
1:B:83:ILE:HB	1:B:85:PRO:HD2	1.99	0.44
1:D:152:VAL:O	1:D:156:ARG:HG2	2.18	0.44
1:D:86:LYS:HD3	1:D:107:GLU:HG2	2.00	0.44
2:E:209:HOH:O	1:F:170:ARG:HD3	2.18	0.43
1:B:37:ASP:HB3	1:C:32:GLY:O	2.18	0.43
1:D:144:LEU:HD13	1:D:144:LEU:O	2.18	0.43
1:B:6:VAL:O	1:B:6:VAL:HG12	2.18	0.43
1:E:133:THR:HG21	1:F:170:ARG:NH1	2.33	0.43
1:B:80:MET:HE3	1:B:102:LEU:HD22	2.00	0.43
1:A:160:PRO:HG2	1:A:163:VAL:CG2	2.47	0.43
1:C:86:LYS:HA	2:C:213:HOH:O	2.18	0.43
1:A:133:THR:HG21	1:B:170:ARG:HD3	2.01	0.43
1:G:84:LYS:N	1:G:85:PRO:CD	2.82	0.43
1:A:83:ILE:HB	1:A:85:PRO:HD2	1.99	0.43
1:E:75:ALA:CB	1:F:92:ILE:HG12	2.49	0.43
1:D:58:GLU:OE1	1:D:196:HIS:CE1	2.72	0.43
1:A:98:MET:CE	1:A:149:LEU:HD13	2.49	0.43
1:F:172:ASN:HD22	1:F:172:ASN:C	2.21	0.43
1:D:19:ILE:O	1:D:22:ARG:HB3	2.19	0.43
1:G:91:CYS:HB2	1:G:103:LEU:HD22	2.01	0.43
1:B:42:SER:O	1:B:46:GLN:HG3	2.18	0.43
1:B:133:THR:O	1:B:137:ILE:HG13	2.18	0.43
1:E:57:LYS:O	1:E:85:PRO:HB3	2.19	0.43
1:G:5:THR:HA	1:G:17:TYR:O	2.18	0.43
1:D:70:ILE:HD12	1:D:98:MET:HE3	2.01	0.43
1:G:70:ILE:HD11	1:G:124:PRO:HB3	2.01	0.43
1:C:32:GLY:HA2	1:C:64:ASN:O	2.18	0.43
1:A:110:LYS:HG2	1:A:196:HIS:CD2	2.54	0.43
1:D:153:LEU:HD13	1:D:164:ILE:HD12	2.00	0.43
1:E:147:ASP:O	1:E:151:LYS:HG3	2.19	0.43
1:G:110:LYS:HG3	1:G:196:HIS:CE1	2.54	0.43
1:G:108:LYS:HG2	2:G:230:HOH:O	2.19	0.42
1:C:82:PHE:HE1	1:D:191:HIS:O	2.02	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:18:ASP:O	1:G:21:SER:N	2.52	0.42
1:G:81:GLN:CA	1:G:81:GLN:HE21	2.25	0.42
1:B:41:ASN:HD21	1:C:30:MET:HB3	1.83	0.42
1:C:64:ASN:HB2	1:C:92:ILE:O	2.19	0.42
1:D:74:MET:HA	1:D:77:TYR:HB3	2.01	0.42
1:E:58:GLU:HG2	1:E:59:ILE:H	1.84	0.42
1:E:144:LEU:HD23	1:E:144:LEU:HA	1.89	0.42
1:F:84:LYS:N	1:F:85:PRO:CD	2.83	0.42
1:D:141:ARG:O	1:D:145:LEU:HG	2.20	0.41
1:F:70:ILE:HG12	1:F:98:MET:CE	2.50	0.41
1:G:154:ALA:HB1	1:G:159:GLN:O	2.20	0.41
1:G:83:ILE:HB	1:G:85:PRO:HD2	2.02	0.41
1:C:55:PRO:CB	1:C:84:LYS:HD2	2.50	0.41
1:D:78:ASP:HB3	1:E:114:LEU:CD1	2.46	0.41
1:C:133:THR:O	1:C:137:ILE:HG13	2.20	0.41
1:D:112:TYR:OH	1:D:196:HIS:HD2	2.03	0.41
1:C:70:ILE:O	1:C:74:MET:HG2	2.21	0.41
1:B:74:MET:HE2	1:B:148:LYS:HE2	2.01	0.41
1:A:50:LEU:HB3	1:A:59:ILE:HD11	2.03	0.41
1:B:112:TYR:OH	1:B:196:HIS:CD2	2.74	0.41
1:B:195:HIS:CE1	1:B:197:HIS:HB2	2.56	0.41
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.95	0.41
1:F:196:HIS:ND1	1:F:197:HIS:N	2.69	0.41
1:D:40:ALA:HA	1:D:76:ILE:HD11	2.03	0.41
1:A:84:LYS:N	1:A:85:PRO:CD	2.84	0.41
1:F:81:GLN:NE2	1:F:81:GLN:HA	2.36	0.41
1:D:57:LYS:HG2	2:D:445:HOH:O	2.21	0.41
1:F:70:ILE:HG12	1:F:98:MET:HE3	2.02	0.41
1:A:40:ALA:O	1:A:44:VAL:HG23	2.21	0.41
1:B:64:ASN:HB2	1:B:92:ILE:O	2.21	0.40
1:D:108:LYS:HB2	1:D:108:LYS:HE2	1.90	0.40
1:E:17:TYR:OH	1:E:25:LYS:HD3	2.21	0.40
1:F:57:LYS:HG3	2:F:400:HOH:O	2.21	0.40
1:C:144:LEU:HD23	1:C:144:LEU:HA	1.92	0.40
1:E:102:LEU:O	1:E:105:ALA:HB3	2.21	0.40
1:A:75:ALA:HB1	1:B:92:ILE:HG13	2.02	0.40
1:G:77:TYR:O	1:G:81:GLN:HG2	2.21	0.40
1:A:115:PRO:HD3	1:A:189:LEU:O	2.21	0.40
1:E:187:LYS:HG3	1:E:188:ILE:N	2.36	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	184/199 (92%)	178 (97%)	6 (3%)	0	100	100
1	B	184/199 (92%)	174 (95%)	10 (5%)	0	100	100
1	C	184/199 (92%)	177 (96%)	7 (4%)	0	100	100
1	D	184/199 (92%)	175 (95%)	8 (4%)	1 (0%)	38	53
1	E	184/199 (92%)	176 (96%)	8 (4%)	0	100	100
1	F	184/199 (92%)	174 (95%)	10 (5%)	0	100	100
1	G	184/199 (92%)	175 (95%)	9 (5%)	0	100	100
All	All	1288/1393 (92%)	1229 (95%)	58 (4%)	1 (0%)	59	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	115	PRO

### 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	149/165 (90%)	142 (95%)	7 (5%)	36	54
1	B	149/165 (90%)	144 (97%)	5 (3%)	49	70
1	C	149/165 (90%)	142 (95%)	7 (5%)	36	54
1	D	149/165 (90%)	140 (94%)	9 (6%)	27	41
1	E	149/165 (90%)	143 (96%)	6 (4%)	42	63
1	F	149/165 (90%)	143 (96%)	6 (4%)	42	63
1	G	149/165 (90%)	138 (93%)	11 (7%)	20	30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1043/1155 (90%)	992 (95%)	51 (5%)	35 53

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	65	SER
1	A	122	HIS
1	A	153	LEU
1	A	170	ARG
1	A	172	ASN
1	A	196	HIS
1	B	108	LYS
1	B	122	HIS
1	B	153	LEU
1	B	170	ARG
1	B	172	ASN
1	C	65	SER
1	C	84	LYS
1	C	92	ILE
1	C	122	HIS
1	C	144	LEU
1	C	153	LEU
1	C	172	ASN
1	D	18	ASP
1	D	31	LEU
1	D	38	ASN
1	D	92	ILE
1	D	122	HIS
1	D	141	ARG
1	D	153	LEU
1	D	170	ARG
1	D	172	ASN
1	E	23	LEU
1	E	24	LEU
1	E	110	LYS
1	E	122	HIS
1	E	153	LEU
1	E	172	ASN
1	F	18	ASP
1	F	38	ASN
1	F	122	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	144	LEU
1	F	153	LEU
1	F	172	ASN
1	G	22	ARG
1	G	23	LEU
1	G	65	SER
1	G	81	GLN
1	G	122	HIS
1	G	144	LEU
1	G	146	ARG
1	G	147	ASP
1	G	162	GLU
1	G	172	ASN
1	G	196	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	116	ASN
1	A	123	GLN
1	A	172	ASN
1	A	191	HIS
1	A	196	HIS
1	B	41	ASN
1	B	123	GLN
1	B	129	GLN
1	B	172	ASN
1	B	196	HIS
1	C	41	ASN
1	C	116	ASN
1	C	123	GLN
1	C	159	GLN
1	C	172	ASN
1	C	196	HIS
1	D	81	GLN
1	D	116	ASN
1	D	123	GLN
1	D	172	ASN
1	D	191	HIS
1	D	196	HIS
1	E	81	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	116	ASN
1	E	123	GLN
1	E	172	ASN
1	F	81	GLN
1	F	116	ASN
1	F	123	GLN
1	F	172	ASN
1	F	191	HIS
1	F	197	HIS
1	G	41	ASN
1	G	81	GLN
1	G	116	ASN
1	G	172	ASN
1	G	191	HIS
1	G	196	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

### 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	188/199 (94%)	-0.24	5 (2%) 52 49	26, 36, 68, 106	0
1	B	188/199 (94%)	-0.27	10 (5%) 25 23	24, 36, 69, 108	0
1	C	188/199 (94%)	-0.05	10 (5%) 25 23	27, 39, 66, 110	0
1	D	188/199 (94%)	-0.25	12 (6%) 19 17	25, 36, 73, 109	0
1	E	188/199 (94%)	-0.06	12 (6%) 19 17	27, 40, 69, 110	0
1	F	188/199 (94%)	-0.29	8 (4%) 34 32	23, 33, 70, 107	0
1	G	188/199 (94%)	-0.22	9 (4%) 29 27	24, 36, 69, 109	0
All	All	1316/1393 (94%)	-0.20	66 (5%) 28 25	23, 37, 71, 110	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	196	HIS	8.8
1	E	192	LEU	7.5
1	E	194	HIS	6.7
1	E	195	HIS	6.6
1	C	192	LEU	6.4
1	E	193	GLU	6.4
1	D	16	ALA	6.4
1	G	16	ALA	6.1
1	D	193	GLU	5.9
1	C	16	ALA	5.7
1	C	197	HIS	5.7
1	G	197	HIS	5.6
1	E	198	HIS	5.4
1	E	16	ALA	5.4
1	A	191	HIS	5.3
1	E	197	HIS	5.2
1	C	198	HIS	5.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	197	HIS	5.0
1	B	198	HIS	5.0
1	F	197	HIS	4.8
1	B	196	HIS	4.7
1	E	6	VAL	4.6
1	C	193	GLU	4.5
1	D	197	HIS	4.4
1	D	194	HIS	4.2
1	F	17	TYR	4.0
1	D	192	LEU	3.9
1	F	193	GLU	3.9
1	A	193	GLU	3.8
1	G	17	TYR	3.8
1	G	196	HIS	3.8
1	C	6	VAL	3.7
1	A	192	LEU	3.7
1	B	17	TYR	3.7
1	B	16	ALA	3.6
1	D	7	ILE	3.6
1	G	6	VAL	3.5
1	C	196	HIS	3.4
1	G	198	HIS	3.4
1	D	6	VAL	3.4
1	G	194	HIS	3.4
1	B	193	GLU	3.3
1	F	16	ALA	3.2
1	G	193	GLU	3.1
1	C	194	HIS	3.1
1	D	17	TYR	3.0
1	A	197	HIS	3.0
1	D	196	HIS	3.0
1	F	196	HIS	3.0
1	D	198	HIS	3.0
1	B	6	VAL	2.9
1	E	7	ILE	2.8
1	F	198	HIS	2.8
1	E	17	TYR	2.7
1	D	191	HIS	2.6
1	E	191	HIS	2.6
1	A	16	ALA	2.6
1	C	7	ILE	2.6
1	C	191	HIS	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	192	LEU	2.5
1	D	5	THR	2.5
1	B	195	HIS	2.4
1	G	195	HIS	2.3
1	B	192	LEU	2.3
1	F	191	HIS	2.1
1	B	7	ILE	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.