



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2023 – 03:15 PM EDT

PDB ID : 4DYU  
Title : The crystal structure of DNA starvation/stationary phase protection protein Dps from *Yersinia pestis* KIM 10  
Authors : Tan, K.; Gu, M.; Kwon, K.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2012-02-29  
Resolution : 2.75 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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>.

---

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 : 2.35  
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) : 2.35

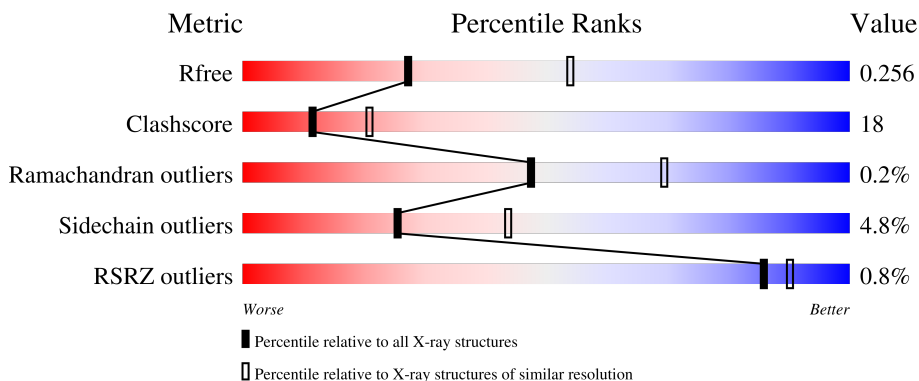
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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.






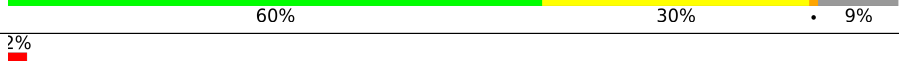
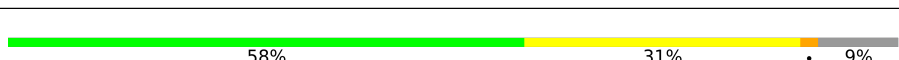

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	170	
1	B	170	
1	C	170	
1	D	170	
1	E	170	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	170	
1	G	170	
1	H	170	
1	I	170	
1	J	170	
1	K	170	
1	L	170	

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
3	SO4	B	202	-	-	X	-
3	SO4	D	202	-	-	X	-
3	SO4	F	202	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15159 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 DNA protection during starvation protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	155	1240	783	216	237	4	0	0	0
1	B	154	1231	778	215	234	4	0	0	0
1	C	154	1231	778	215	234	4	0	0	0
1	D	156	1246	786	217	239	4	0	0	0
1	E	155	1240	783	216	237	4	0	0	0
1	F	154	1231	778	215	234	4	0	0	0
1	G	155	1240	783	216	237	4	0	0	0
1	H	157	1253	791	218	240	4	0	0	0
1	I	155	1240	783	216	237	4	0	0	0
1	J	155	1240	783	216	237	4	0	0	0
1	K	155	1240	783	216	237	4	0	0	0
1	L	155	1240	783	216	237	4	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q7CJ65
A	-1	ASN	-	expression tag	UNP Q7CJ65
A	0	ALA	-	expression tag	UNP Q7CJ65
B	-2	SER	-	expression tag	UNP Q7CJ65
B	-1	ASN	-	expression tag	UNP Q7CJ65

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ALA	-	expression tag	UNP Q7CJ65
C	-2	SER	-	expression tag	UNP Q7CJ65
C	-1	ASN	-	expression tag	UNP Q7CJ65
C	0	ALA	-	expression tag	UNP Q7CJ65
D	-2	SER	-	expression tag	UNP Q7CJ65
D	-1	ASN	-	expression tag	UNP Q7CJ65
D	0	ALA	-	expression tag	UNP Q7CJ65
E	-2	SER	-	expression tag	UNP Q7CJ65
E	-1	ASN	-	expression tag	UNP Q7CJ65
E	0	ALA	-	expression tag	UNP Q7CJ65
F	-2	SER	-	expression tag	UNP Q7CJ65
F	-1	ASN	-	expression tag	UNP Q7CJ65
F	0	ALA	-	expression tag	UNP Q7CJ65
G	-2	SER	-	expression tag	UNP Q7CJ65
G	-1	ASN	-	expression tag	UNP Q7CJ65
G	0	ALA	-	expression tag	UNP Q7CJ65
H	-2	SER	-	expression tag	UNP Q7CJ65
H	-1	ASN	-	expression tag	UNP Q7CJ65
H	0	ALA	-	expression tag	UNP Q7CJ65
I	-2	SER	-	expression tag	UNP Q7CJ65
I	-1	ASN	-	expression tag	UNP Q7CJ65
I	0	ALA	-	expression tag	UNP Q7CJ65
J	-2	SER	-	expression tag	UNP Q7CJ65
J	-1	ASN	-	expression tag	UNP Q7CJ65
J	0	ALA	-	expression tag	UNP Q7CJ65
K	-2	SER	-	expression tag	UNP Q7CJ65
K	-1	ASN	-	expression tag	UNP Q7CJ65
K	0	ALA	-	expression tag	UNP Q7CJ65
L	-2	SER	-	expression tag	UNP Q7CJ65
L	-1	ASN	-	expression tag	UNP Q7CJ65
L	0	ALA	-	expression tag	UNP Q7CJ65

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	2	Total Zn 2 2	0	0
2	F	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0
2	I	1	Total Zn 1 1	0	0
2	J	1	Total Zn 1 1	0	0
2	K	1	Total Zn 1 1	0	0
2	L	1	Total Zn 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		
4	B	20	Total	O	0	0
			20	20		
4	C	18	Total	O	0	0
			18	18		
4	D	24	Total	O	0	0
			24	24		
4	E	15	Total	O	0	0
			15	15		
4	F	22	Total	O	0	0
			22	22		
4	G	14	Total	O	0	0
			14	14		
4	H	19	Total	O	0	0
			19	19		
4	I	16	Total	O	0	0
			16	16		
4	J	13	Total	O	0	0
			13	13		

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	K	21	Total O 21 21	0	0
4	L	10	Total O 10 10	0	0

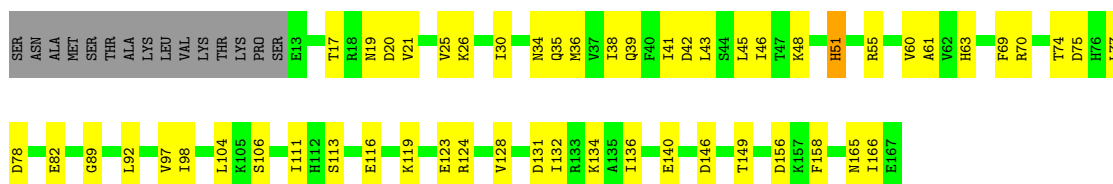


### 3 Residue-property plots

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.

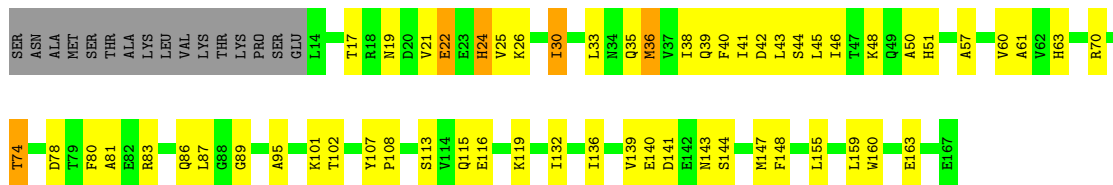
- Molecule 1: DNA protection during starvation protein

Chain A: 



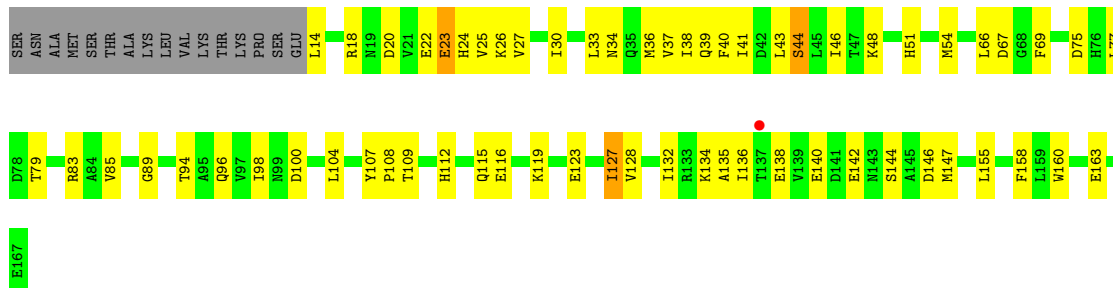
- Molecule 1: DNA protection during starvation protein

Chain B: 



- Molecule 1: DNA protection during starvation protein

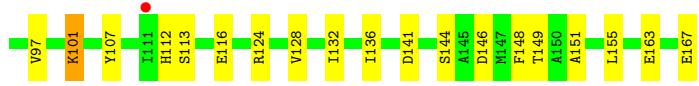
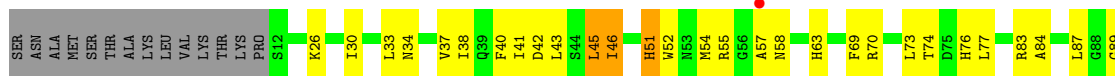
Chain C: 



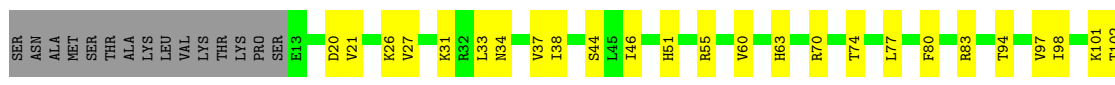
- Molecule 1: DNA protection during starvation protein

Chain D: 

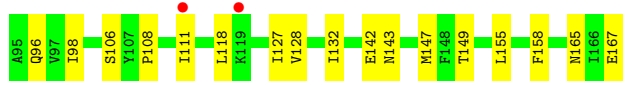
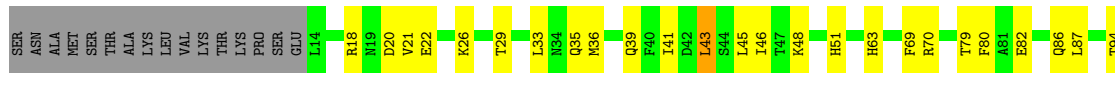




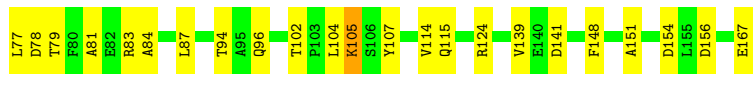
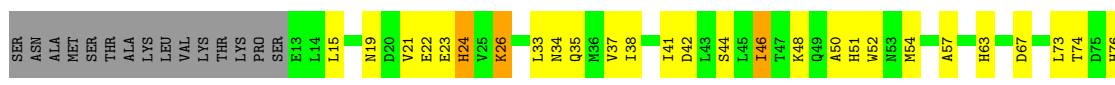
● Molecule 1: DNA protection during starvation protein



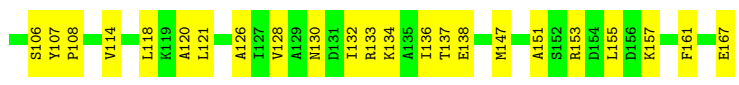
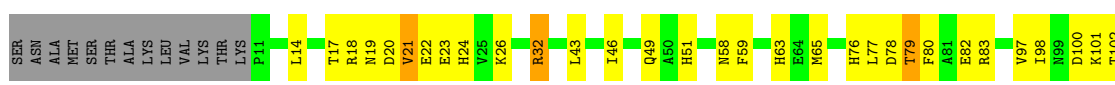
● Molecule 1: DNA protection during starvation protein



● Molecule 1: DNA protection during starvation protein

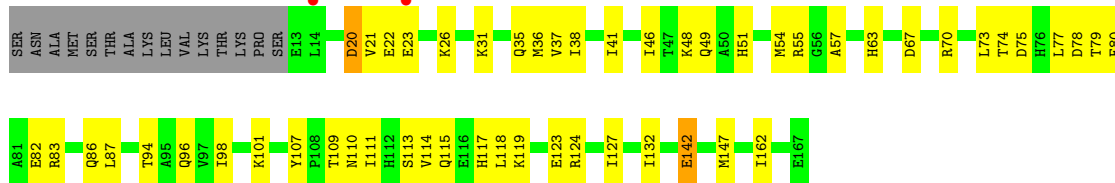


● Molecule 1: DNA protection during starvation protein



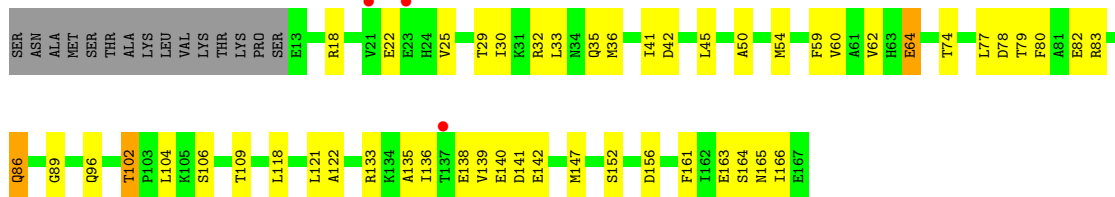
● Molecule 1: DNA protection during starvation protein

Chain I: 



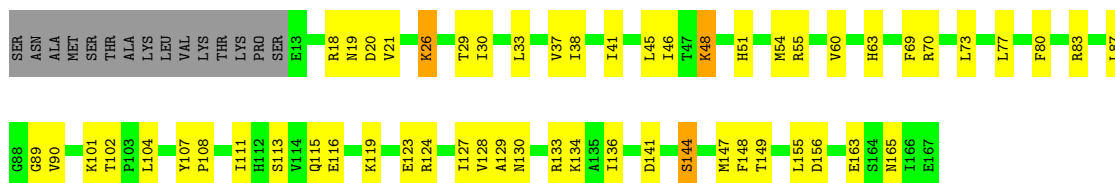
• Molecule 1: DNA protection during starvation protein

Chain J: 



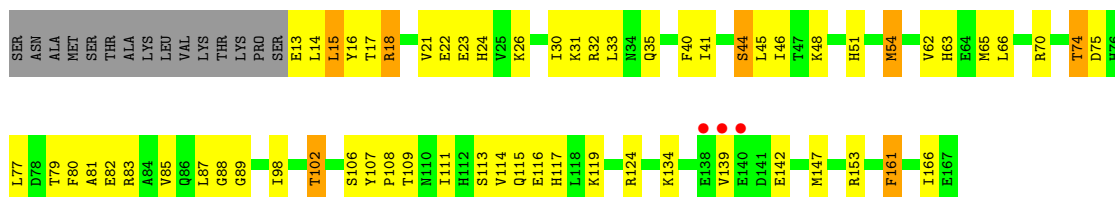
• Molecule 1: DNA protection during starvation protein

Chain K: 



• Molecule 1: DNA protection during starvation protein

Chain L: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.41Å 105.10Å 191.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.19 – 2.75 48.50 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.19-2.75) 99.7 (48.50-2.75)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 2.77Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.179 , 0.269 0.172 , 0.256	Depositor DCC
$R_{free}$ test set	2833 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.0	Xtrriage
Anisotropy	0.207	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.033 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15159	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ZN

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	0.41	0/1261	0.59	0/1707
1	B	0.46	0/1252	0.58	0/1695
1	C	0.44	0/1252	0.56	0/1695
1	D	0.43	0/1267	0.59	0/1715
1	E	0.45	0/1261	0.58	0/1707
1	F	0.43	0/1252	0.56	0/1695
1	G	0.45	0/1261	0.61	0/1707
1	H	0.41	0/1275	0.59	0/1726
1	I	0.45	0/1261	0.60	0/1707
1	J	0.42	0/1261	0.58	0/1707
1	K	0.43	0/1261	0.60	0/1707
1	L	0.41	0/1261	0.58	0/1707
All	All	0.43	0/15125	0.58	0/20475

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	1240	0	1228	44	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1231	0	1222	49	0
1	C	1231	0	1222	60	0
1	D	1246	0	1233	34	0
1	E	1240	0	1228	36	0
1	F	1231	0	1222	43	0
1	G	1240	0	1228	44	0
1	H	1253	0	1241	53	0
1	I	1240	0	1228	56	0
1	J	1240	0	1228	48	0
1	K	1240	0	1228	50	0
1	L	1240	0	1228	56	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	10	0	0	0	0
3	B	10	0	0	2	0
3	D	10	0	0	3	0
3	E	5	0	0	1	0
3	F	5	0	0	2	0
3	G	5	0	0	1	0
3	H	5	0	0	1	0
3	J	10	0	0	1	0
3	K	5	0	0	0	0
4	A	18	0	0	1	0
4	B	20	0	0	1	0
4	C	18	0	0	1	0
4	D	24	0	0	0	0
4	E	15	0	0	0	0
4	F	22	0	0	1	0
4	G	14	0	0	0	0
4	H	19	0	0	0	0
4	I	16	0	0	1	0
4	J	13	0	0	1	0
4	K	21	0	0	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	10	0	0	0	0
All	All	15159	0	14736	521	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (521) 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:F:80:PHE:HD1	1:F:147:MET:HE2	1.21	1.00
1:L:80:PHE:HA	1:L:147:MET:HE1	1.50	0.93
1:E:60:VAL:HB	1:L:65:MET:HE3	1.49	0.93
1:H:65:MET:HE2	1:H:161:PHE:HD2	1.33	0.92
1:A:30:ILE:HD13	1:A:89:GLY:HA3	1.53	0.90
1:A:92:LEU:CD2	1:C:109:THR:HG21	2.03	0.88
1:G:102:THR:HG22	1:G:104:LEU:H	1.40	0.87
1:A:17:THR:HG22	1:A:19:ASN:H	1.38	0.86
1:H:65:MET:HE2	1:H:161:PHE:CD2	2.13	0.84
1:K:41:ILE:HG12	1:K:77:LEU:HD11	1.61	0.82
1:H:98:ILE:O	1:H:102:THR:HG23	1.78	0.82
1:F:80:PHE:HD1	1:F:147:MET:CE	1.92	0.82
1:F:80:PHE:CD1	1:F:147:MET:HE2	2.12	0.81
1:J:32:ARG:NH2	1:J:138:GLU:OE2	2.13	0.80
1:H:80:PHE:HD1	1:H:147:MET:CE	1.93	0.80
1:H:80:PHE:HA	1:H:147:MET:HE1	1.63	0.79
1:C:23:GLU:HG3	1:C:24:HIS:N	1.97	0.79
1:K:119:LYS:O	1:K:123:GLU:HG2	1.84	0.78
1:C:144:SER:HA	1:C:147:MET:HE2	1.64	0.78
1:B:136:ILE:HG21	1:L:142:GLU:HG2	1.66	0.77
1:J:102:THR:HG22	1:J:104:LEU:H	1.50	0.76
1:I:41:ILE:HG12	1:I:77:LEU:HD11	1.67	0.76
1:C:33:LEU:O	1:C:37:VAL:HG23	1.86	0.75
1:L:65:MET:HE2	1:L:161:PHE:CD2	2.21	0.75
1:K:51:HIS:CE1	1:K:63:HIS:CE1	2.75	0.75
1:F:36:MET:HE1	1:F:132:ILE:HB	1.67	0.75
1:C:144:SER:HA	1:C:147:MET:CE	2.17	0.74
1:J:60:VAL:O	1:J:64:GLU:HG2	1.88	0.74
1:C:20:ASP:OD2	1:H:134:LYS:NZ	2.22	0.73
1:G:124:ARG:HG3	1:G:124:ARG:HH11	1.53	0.73
1:A:156:ASP:OD2	1:I:83:ARG:NH1	2.22	0.73
1:J:83:ARG:NH2	1:J:141:ASP:OD1	2.21	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:HD23	1:C:109:THR:HG21	1.70	0.72
1:G:105:LYS:NZ	3:G:201:SO4:O1	2.22	0.72
1:I:23:GLU:O	1:I:26:LYS:HB2	1.89	0.72
1:L:80:PHE:HD1	1:L:147:MET:CE	2.02	0.71
1:B:113:SER:OG	1:B:116:GLU:HG3	1.91	0.71
1:F:143:ASN:O	1:F:147:MET:HG2	1.91	0.71
1:B:107:TYR:CG	1:B:108:PRO:HD2	2.26	0.70
1:J:42:ASP:OD2	1:J:102:THR:HG21	1.91	0.70
1:K:21:VAL:HG11	1:K:87:LEU:HD22	1.72	0.70
1:E:70:ARG:NH2	3:E:203:SO4:O2	2.23	0.70
1:F:36:MET:CE	1:F:132:ILE:HB	2.21	0.70
1:H:79:THR:HG23	1:H:147:MET:HE3	1.74	0.70
1:K:128:VAL:HG12	1:K:155:LEU:HD21	1.72	0.70
1:L:31:LYS:O	1:L:35:GLN:HG3	1.92	0.70
1:F:79:THR:HG22	1:F:147:MET:HE3	1.74	0.69
1:J:118:LEU:HB3	1:J:166:ILE:HD11	1.73	0.69
1:C:134:LYS:O	1:C:138:GLU:HG3	1.93	0.69
1:F:79:THR:O	1:F:147:MET:HE1	1.93	0.69
1:H:97:VAL:O	1:H:101:LYS:HB2	1.93	0.69
1:L:18:ARG:HG2	1:L:18:ARG:HH11	1.58	0.69
1:G:139:VAL:HG12	1:G:141:ASP:H	1.58	0.69
1:D:30:ILE:HD13	1:D:89:GLY:HA3	1.73	0.69
1:J:30:ILE:HD13	1:J:89:GLY:HA3	1.75	0.69
1:L:108:PRO:HD3	1:L:124:ARG:NH2	2.08	0.69
1:E:107:TYR:CD2	1:E:108:PRO:HD2	2.26	0.68
1:G:54:MET:HG2	1:G:114:VAL:HG22	1.74	0.68
1:D:132:ILE:O	1:D:136:ILE:HG13	1.93	0.68
1:L:18:ARG:HH11	1:L:18:ARG:CG	2.07	0.68
1:A:70:ARG:O	1:A:74:THR:HG23	1.93	0.68
1:C:136:ILE:HG21	1:J:142:GLU:HG2	1.76	0.68
1:E:46:ILE:HD13	1:E:124:ARG:HD3	1.76	0.68
1:H:78:ASP:O	1:H:82:GLU:HG3	1.94	0.68
3:D:202:SO4:O1	1:I:57:ALA:HB1	1.94	0.67
1:L:98:ILE:O	1:L:102:THR:OG1	2.11	0.67
1:F:21:VAL:O	1:F:26:LYS:HE3	1.95	0.67
1:J:106:SER:HB2	3:J:203:SO4:O4	1.95	0.67
1:E:33:LEU:HD21	1:E:147:MET:HE1	1.77	0.66
1:K:129:ALA:HA	1:K:155:LEU:HD23	1.76	0.66
1:C:48:LYS:O	1:C:51:HIS:HB3	1.96	0.66
1:I:109:THR:HG23	1:K:90:VAL:HG11	1.78	0.66
1:E:119:LYS:O	1:E:123:GLU:HG2	1.95	0.66

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:ASP:OD2	1:H:153:ARG:NH1	2.28	0.66
1:D:33:LEU:O	1:D:37:VAL:HG23	1.95	0.66
1:K:37:VAL:O	1:K:41:ILE:HG13	1.96	0.65
1:B:19:ASN:OD1	1:B:21:VAL:HG23	1.96	0.65
1:D:37:VAL:O	1:D:41:ILE:HG13	1.96	0.65
1:D:167:GLU:HG2	1:I:57:ALA:HB2	1.78	0.65
1:I:46:ILE:HD13	1:I:124:ARG:HD3	1.79	0.65
1:A:92:LEU:HD21	1:C:109:THR:HG21	1.76	0.65
1:I:51:HIS:O	1:I:63:HIS:HD2	1.80	0.65
1:I:94:THR:O	1:I:98:ILE:HG12	1.97	0.64
1:L:107:TYR:HA	1:L:124:ARG:HH21	1.62	0.64
1:C:46:ILE:HG23	1:C:107:TYR:CD1	2.32	0.64
1:J:32:ARG:NH1	1:J:36:MET:CE	2.60	0.64
1:K:26:LYS:HG2	1:K:87:LEU:O	1.97	0.64
1:G:94:THR:HG22	1:G:96:GLN:OE1	1.97	0.64
1:L:54:MET:HG2	1:L:114:VAL:HA	1.79	0.63
1:B:115:GLN:O	1:B:119:LYS:HG3	1.99	0.63
1:I:54:MET:HG2	1:I:114:VAL:HG22	1.79	0.63
1:J:32:ARG:NH1	1:J:36:MET:HE3	2.12	0.63
1:H:43:LEU:HG	1:H:128:VAL:HG21	1.81	0.62
1:J:25:VAL:HG13	1:J:140:GLU:HG3	1.81	0.62
1:B:115:GLN:HG2	4:B:314:HOH:O	1.99	0.62
1:G:42:ASP:OD2	1:G:102:THR:HG21	2.00	0.62
1:F:79:THR:HG22	1:F:147:MET:CE	2.29	0.62
1:I:31:LYS:O	1:I:35:GLN:HG3	2.00	0.62
1:J:96:GLN:HG2	1:L:106:SER:OG	2.00	0.62
1:I:75:ASP:HB2	4:I:305:HOH:O	2.00	0.61
1:I:118:LEU:HD22	1:I:162:ILE:HG23	1.81	0.61
1:A:82:GLU:HG2	1:E:160:TRP:CH2	2.35	0.61
1:L:77:LEU:HA	1:L:80:PHE:CD2	2.36	0.61
1:H:83:ARG:NH1	1:J:156:ASP:OD2	2.33	0.61
1:F:96:GLN:OE1	1:F:96:GLN:N	2.27	0.60
1:G:22:GLU:HB3	1:G:24:HIS:CE1	2.36	0.60
1:G:41:ILE:O	1:G:44:SER:HB2	2.02	0.60
1:A:134:LYS:NZ	1:I:20:ASP:OD1	2.23	0.60
1:H:20:ASP:O	1:H:21:VAL:C	2.39	0.60
1:H:80:PHE:HA	1:H:147:MET:CE	2.32	0.60
1:C:79:THR:CG2	1:C:147:MET:HG2	2.32	0.60
1:G:19:ASN:O	1:G:26:LYS:NZ	2.34	0.60
1:C:18:ARG:HB3	1:H:126:ALA:HB1	1.83	0.60
1:C:123:GLU:O	1:C:127:ILE:HG23	2.02	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LEU:HD13	1:A:124:ARG:HB3	1.83	0.60
1:C:79:THR:HG22	1:C:147:MET:HG2	1.84	0.60
1:J:83:ARG:HH21	1:J:141:ASP:CG	2.04	0.60
1:G:33:LEU:O	1:G:37:VAL:HG23	2.02	0.59
1:H:80:PHE:HD1	1:H:147:MET:HE3	1.67	0.59
1:I:79:THR:C	1:I:147:MET:HE3	2.23	0.59
1:K:80:PHE:CE1	1:K:147:MET:HG2	2.36	0.59
1:I:80:PHE:HD1	1:I:147:MET:CE	2.15	0.59
1:H:14:LEU:HD13	1:H:26:LYS:HD3	1.84	0.59
1:H:80:PHE:HZ	1:H:151:ALA:HB2	1.66	0.59
1:K:19:ASN:OD1	1:K:21:VAL:HG12	2.03	0.59
1:C:40:PHE:O	1:C:44:SER:N	2.35	0.59
1:E:33:LEU:CD2	1:E:147:MET:HE1	2.32	0.59
1:F:80:PHE:HA	1:F:147:MET:HE1	1.85	0.59
1:D:51:HIS:CE1	1:D:63:HIS:CE1	2.91	0.59
1:F:106:SER:HB2	3:F:202:SO4:O4	2.02	0.59
1:H:51:HIS:CE1	1:H:63:HIS:CE1	2.91	0.59
1:H:128:VAL:HG12	1:H:155:LEU:HD21	1.83	0.59
1:K:46:ILE:HD13	1:K:124:ARG:HD3	1.83	0.59
1:K:55:ARG:O	1:K:113:SER:HA	2.03	0.59
1:F:82:GLU:O	1:F:86:GLN:HG3	2.02	0.59
1:G:76:HIS:NE2	1:G:154:ASP:OD2	2.25	0.59
1:H:51:HIS:CE1	1:H:63:HIS:NE2	2.71	0.59
1:C:94:THR:O	1:C:98:ILE:HG12	2.03	0.58
1:F:21:VAL:HG12	1:F:26:LYS:HG3	1.86	0.58
1:F:127:ILE:HA	4:F:320:HOH:O	2.02	0.58
1:K:80:PHE:CD1	1:K:147:MET:HG2	2.38	0.58
1:F:94:THR:O	1:F:98:ILE:HG12	2.03	0.58
1:E:83:ARG:HH21	1:E:141:ASP:CG	2.06	0.58
1:L:48:LYS:O	1:L:51:HIS:HB3	2.04	0.58
1:B:60:VAL:HB	1:F:165:ASN:HD21	1.67	0.58
1:F:142:GLU:OE1	1:F:142:GLU:N	2.20	0.58
1:H:65:MET:HE1	1:H:161:PHE:HB3	1.85	0.58
1:A:106:SER:HB2	4:A:315:HOH:O	2.02	0.58
1:F:80:PHE:CD1	1:F:147:MET:CE	2.81	0.58
1:G:26:LYS:HG2	1:G:87:LEU:HD22	1.85	0.58
1:J:135:ALA:HA	1:J:138:GLU:HG2	1.86	0.58
1:E:130:ASN:O	1:E:134:LYS:HD3	2.04	0.58
1:C:128:VAL:HG12	1:C:155:LEU:HD21	1.86	0.57
1:K:130:ASN:HA	1:K:133:ARG:NH1	2.19	0.57
1:H:76:HIS:O	1:H:79:THR:HG22	2.04	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:ARG:NH2	3:D:203:SO4:O2	2.31	0.57
1:H:65:MET:CE	1:H:161:PHE:HB3	2.34	0.57
1:F:51:HIS:CE1	1:F:63:HIS:CE1	2.92	0.57
1:J:161:PHE:O	1:J:165:ASN:ND2	2.38	0.57
1:L:65:MET:CE	1:L:161:PHE:CD2	2.87	0.57
1:E:98:ILE:O	1:E:102:THR:HG22	2.04	0.57
1:L:62:VAL:O	1:L:66:LEU:HG	2.05	0.57
1:A:17:THR:HG23	1:E:163:GLU:OE1	2.04	0.57
1:C:23:GLU:HG3	1:C:24:HIS:H	1.68	0.57
1:G:79:THR:HG21	1:L:153:ARG:NH2	2.20	0.56
1:F:18:ARG:NH1	1:K:163:GLU:HG2	2.20	0.56
1:H:107:TYR:CE1	1:H:120:ALA:HB1	2.39	0.56
1:K:30:ILE:HD13	1:K:89:GLY:HA3	1.87	0.56
1:I:31:LYS:HE2	1:I:35:GLN:HE21	1.70	0.56
1:C:14:LEU:HD11	1:C:27:VAL:HG23	1.87	0.56
1:B:43:LEU:O	1:B:46:ILE:HG12	2.06	0.56
1:H:32:ARG:NH1	1:H:138:GLU:OE1	2.22	0.56
4:J:305:HOH:O	1:L:46:ILE:HD11	2.05	0.56
1:A:25:VAL:HG13	1:A:140:GLU:HB2	1.87	0.56
1:G:124:ARG:HG3	1:G:124:ARG:NH1	2.21	0.56
1:C:79:THR:HG22	1:C:147:MET:SD	2.46	0.55
1:D:34:ASN:O	1:D:38:ILE:HG13	2.06	0.55
1:D:163:GLU:OE2	1:K:18:ARG:NH1	2.36	0.55
1:E:34:ASN:O	1:E:38:ILE:HG13	2.06	0.55
1:E:60:VAL:HB	1:L:65:MET:CE	2.32	0.55
1:K:48:LYS:HD3	1:K:70:ARG:HD2	1.89	0.55
1:I:111:ILE:HG13	1:I:117:HIS:CE1	2.41	0.55
1:I:51:HIS:CE1	1:I:63:HIS:NE2	2.75	0.55
1:A:35:GLN:O	1:A:39:GLN:HG2	2.07	0.55
1:B:30:ILE:HD12	1:B:89:GLY:HA3	1.87	0.55
1:I:46:ILE:O	1:I:49:GLN:HB3	2.07	0.54
1:L:81:ALA:O	1:L:85:VAL:HG23	2.07	0.54
1:L:15:LEU:HD12	1:L:88:GLY:O	2.07	0.54
1:B:22:GLU:OE1	1:B:24:HIS:HB2	2.08	0.54
1:F:80:PHE:HA	1:F:147:MET:CE	2.37	0.54
1:I:21:VAL:O	1:I:22:GLU:C	2.45	0.54
1:A:119:LYS:O	1:A:123:GLU:HG2	2.07	0.54
1:I:46:ILE:HG23	1:I:107:TYR:CD1	2.43	0.54
1:C:30:ILE:HD13	1:C:89:GLY:HA3	1.89	0.54
1:L:51:HIS:O	1:L:63:HIS:HD2	1.90	0.53
1:G:79:THR:HG21	1:L:153:ARG:HH21	1.73	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:102:THR:CG2	1:J:104:LEU:HB2	2.38	0.53
1:B:160:TRP:CH2	1:L:82:GLU:HG2	2.44	0.53
1:C:34:ASN:O	1:C:38:ILE:HG13	2.07	0.53
1:D:54:MET:HA	1:D:112:HIS:O	2.08	0.53
1:A:20:ASP:OD2	1:E:134:LYS:NZ	2.41	0.53
1:B:26:LYS:HD3	1:B:87:LEU:O	2.09	0.53
1:B:74:THR:HG21	3:B:202:SO4:O3	2.08	0.53
1:E:33:LEU:O	1:E:37:VAL:HG23	2.09	0.53
1:H:80:PHE:HZ	1:H:151:ALA:CB	2.21	0.53
1:D:113:SER:HB3	1:D:116:GLU:HB2	1.90	0.53
1:L:111:ILE:HG13	1:L:117:HIS:CE1	2.43	0.53
1:C:109:THR:O	1:C:109:THR:HG22	2.09	0.53
1:E:55:ARG:O	1:E:113:SER:HA	2.08	0.53
1:I:118:LEU:CD2	1:I:162:ILE:HG23	2.39	0.53
1:A:36:MET:SD	1:A:132:ILE:HD12	2.50	0.52
1:I:55:ARG:O	1:I:113:SER:HA	2.09	0.52
1:K:128:VAL:HG12	1:K:155:LEU:CD2	2.37	0.52
1:A:136:ILE:HD11	1:A:149:THR:HA	1.91	0.52
1:J:41:ILE:O	1:J:45:LEU:HD13	2.09	0.52
1:B:57:ALA:HB2	1:F:167:GLU:HG3	1.91	0.52
1:D:30:ILE:HD13	1:D:89:GLY:CA	2.40	0.52
1:A:43:LEU:HD11	1:A:128:VAL:HG21	1.90	0.52
1:G:102:THR:HG22	1:G:104:LEU:N	2.19	0.52
1:I:73:LEU:O	1:I:77:LEU:HB2	2.10	0.52
1:L:16:TYR:CG	1:L:17:THR:N	2.77	0.52
1:H:107:TYR:CD1	1:H:108:PRO:HD2	2.45	0.51
1:I:80:PHE:HA	1:I:147:MET:HE1	1.91	0.51
1:K:141:ASP:OD2	1:K:144:SER:HB3	2.09	0.51
1:I:37:VAL:O	1:I:41:ILE:HG13	2.10	0.51
1:B:36:MET:HG3	1:B:132:ILE:HD12	1.92	0.51
1:H:107:TYR:CG	1:H:108:PRO:HD2	2.45	0.51
1:J:29:THR:HG22	1:J:33:LEU:HD12	1.92	0.51
1:J:136:ILE:HD11	1:J:152:SER:HB2	1.92	0.51
1:D:136:ILE:HG12	1:D:148:PHE:HB3	1.93	0.51
1:K:123:GLU:O	1:K:127:ILE:HG13	2.09	0.51
1:C:100:ASP:OD2	1:C:100:ASP:N	2.41	0.51
1:F:79:THR:C	1:F:147:MET:HE1	2.31	0.51
1:A:30:ILE:CD1	1:A:89:GLY:HA3	2.34	0.51
1:H:128:VAL:HG12	1:H:155:LEU:CD2	2.41	0.51
1:G:139:VAL:HG21	1:G:148:PHE:HE2	1.76	0.51
1:I:94:THR:HG21	4:K:303:HOH:O	2.11	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:GLU:OE1	1:C:142:GLU:N	2.37	0.51
1:K:128:VAL:CG1	1:K:155:LEU:HD21	2.38	0.51
1:B:70:ARG:HH21	1:D:70:ARG:HH21	1.59	0.50
1:H:80:PHE:CD1	1:H:147:MET:HE3	2.45	0.50
1:K:111:ILE:HB	1:K:116:GLU:HB3	1.92	0.50
1:B:35:GLN:O	1:B:39:GLN:HG2	2.11	0.50
1:E:80:PHE:HD1	1:E:147:MET:HE3	1.77	0.50
1:C:41:ILE:HG13	1:C:77:LEU:HD22	1.93	0.50
1:D:146:ASP:HB2	1:F:149:THR:HG21	1.93	0.50
1:L:13:GLU:O	1:L:14:LEU:HD23	2.11	0.50
1:C:96:GLN:CD	1:C:96:GLN:H	2.14	0.50
1:G:51:HIS:CD2	1:G:63:HIS:CD2	2.99	0.50
1:L:80:PHE:HD1	1:L:147:MET:HE3	1.72	0.50
1:A:61:ALA:HB1	1:K:60:VAL:HG13	1.93	0.50
1:C:96:GLN:O	1:C:100:ASP:OD2	2.30	0.50
1:G:21:VAL:O	1:G:26:LYS:HE2	2.11	0.50
1:C:20:ASP:OD1	1:H:133:ARG:NH1	2.44	0.50
1:L:21:VAL:O	1:L:26:LYS:HE3	2.11	0.50
1:K:107:TYR:CG	1:K:108:PRO:HD2	2.47	0.50
1:I:51:HIS:CD2	1:I:63:HIS:O	2.65	0.49
1:K:41:ILE:HG12	1:K:77:LEU:CD1	2.39	0.49
1:A:165:ASN:HD21	1:K:60:VAL:HB	1.77	0.49
1:F:36:MET:HE2	1:F:132:ILE:HD12	1.94	0.49
1:I:82:GLU:O	1:I:86:GLN:HG3	2.11	0.49
1:E:139:VAL:HG11	1:E:144:SER:HB2	1.95	0.49
1:J:32:ARG:O	1:J:35:GLN:HG2	2.12	0.49
1:L:51:HIS:O	1:L:63:HIS:CD2	2.65	0.49
1:H:114:VAL:O	1:H:118:LEU:HG	2.13	0.49
1:H:80:PHE:HD1	1:H:147:MET:HE2	1.71	0.49
1:L:65:MET:HE2	1:L:161:PHE:HD2	1.75	0.49
1:L:74:THR:HG22	1:L:75:ASP:N	2.28	0.49
1:C:79:THR:HG22	1:C:147:MET:CG	2.42	0.49
1:F:43:LEU:HD22	1:F:128:VAL:HG21	1.95	0.49
1:F:106:SER:HB2	3:F:202:SO4:S	2.52	0.49
1:D:136:ILE:CD1	1:D:149:THR:HA	2.43	0.49
1:H:51:HIS:O	1:H:63:HIS:HD2	1.95	0.49
1:D:69:PHE:O	1:D:73:LEU:HG	2.12	0.49
1:F:35:GLN:O	1:F:39:GLN:HG3	2.13	0.49
1:E:21:VAL:HG12	1:E:26:LYS:HG3	1.95	0.48
1:G:50:ALA:O	1:G:54:MET:HB2	2.12	0.48
1:B:159:LEU:O	1:B:163:GLU:HG3	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:MET:CE	1:C:132:ILE:HB	2.44	0.48
1:C:54:MET:HA	1:C:112:HIS:O	2.13	0.48
1:H:130:ASN:OD1	1:H:133:ARG:NH2	2.44	0.48
1:G:139:VAL:HG21	1:G:148:PHE:CE2	2.48	0.48
1:G:33:LEU:HD11	1:G:83:ARG:HG3	1.94	0.48
1:L:80:PHE:CD1	1:L:147:MET:CE	2.90	0.48
3:B:202:SO4:O1	1:D:74:THR:HG21	2.13	0.48
1:E:139:VAL:HG21	1:E:148:PHE:HE2	1.78	0.48
1:A:60:VAL:HB	1:H:65:MET:HE3	1.96	0.48
1:G:46:ILE:HG12	1:G:107:TYR:CD1	2.49	0.48
1:C:18:ARG:HB3	1:H:126:ALA:CB	2.44	0.48
1:I:51:HIS:HD2	1:I:63:HIS:O	1.97	0.48
1:B:36:MET:HB3	1:B:80:PHE:CD2	2.49	0.48
1:C:26:LYS:O	1:C:30:ILE:HG13	2.14	0.48
1:I:31:LYS:HE2	1:I:35:GLN:NE2	2.29	0.47
1:K:33:LEU:HD23	1:K:148:PHE:CZ	2.48	0.47
1:A:30:ILE:HD13	1:A:89:GLY:CA	2.34	0.47
1:A:41:ILE:O	1:A:45:LEU:HG	2.14	0.47
1:A:41:ILE:HG21	1:A:98:ILE:HD11	1.96	0.47
1:K:21:VAL:HG13	1:K:26:LYS:HD2	1.94	0.47
1:I:36:MET:CE	1:I:132:ILE:HA	2.44	0.47
1:J:32:ARG:CZ	1:J:135:ALA:HB2	2.44	0.47
1:J:78:ASP:OD1	1:L:48:LYS:NZ	2.48	0.47
1:B:26:LYS:O	1:B:30:ILE:HG23	2.15	0.47
1:H:59:PHE:HB3	1:K:165:ASN:OD1	2.14	0.47
1:I:70:ARG:NH2	1:K:70:ARG:HH21	2.13	0.47
1:J:79:THR:HG22	1:J:147:MET:SD	2.55	0.47
1:C:69:PHE:CE2	1:C:158:PHE:HB3	2.49	0.47
1:C:142:GLU:H	1:C:142:GLU:CD	2.16	0.47
1:C:163:GLU:OE2	1:J:18:ARG:HG3	2.15	0.47
1:F:39:GLN:O	1:F:43:LEU:HB2	2.14	0.47
1:H:80:PHE:CD1	1:H:147:MET:CE	2.85	0.47
1:I:79:THR:O	1:I:147:MET:HE3	2.15	0.47
1:I:80:PHE:HA	1:I:147:MET:CE	2.44	0.47
1:J:77:LEU:HD12	1:J:78:ASP:N	2.29	0.47
1:A:55:ARG:HH21	1:C:85:VAL:HG13	1.79	0.47
1:B:139:VAL:HG11	1:B:148:PHE:HE2	1.80	0.47
1:C:39:GLN:O	1:C:43:LEU:HB2	2.15	0.47
1:H:17:THR:C	1:H:19:ASN:H	2.18	0.47
1:L:18:ARG:CG	1:L:18:ARG:NH1	2.71	0.47
1:E:110:ASN:O	1:E:112:HIS:ND1	2.47	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:HIS:CE1	1:A:63:HIS:CE1	3.03	0.47
1:A:119:LYS:CG	1:A:166:ILE:HD13	2.45	0.47
1:B:42:ASP:O	1:B:46:ILE:HG23	2.15	0.47
1:L:40:PHE:O	1:L:44:SER:HB2	2.15	0.47
1:D:26:LYS:HG2	1:D:87:LEU:HB3	1.97	0.46
1:J:82:GLU:O	1:J:86:GLN:HG3	2.14	0.46
1:J:102:THR:HG22	1:J:104:LEU:HB2	1.97	0.46
1:L:33:LEU:HD11	1:L:83:ARG:HG3	1.96	0.46
1:B:81:ALA:CB	1:D:52:TRP:CE2	2.98	0.46
1:C:135:ALA:O	1:C:136:ILE:C	2.52	0.46
1:G:104:LEU:N	1:G:104:LEU:HD12	2.31	0.46
1:K:69:PHE:O	1:K:73:LEU:HG	2.15	0.46
1:C:89:GLY:HA2	4:C:305:HOH:O	2.15	0.46
1:H:18:ARG:NH1	1:J:163:GLU:HG2	2.30	0.46
1:K:46:ILE:HG23	1:K:107:TYR:CD1	2.51	0.46
1:D:33:LEU:HD13	1:D:84:ALA:N	2.30	0.46
1:A:51:HIS:ND1	1:A:63:HIS:O	2.35	0.46
1:B:155:LEU:HD12	1:B:155:LEU:HA	1.77	0.46
1:E:112:HIS:CD2	1:G:15:LEU:HD11	2.51	0.46
1:I:26:LYS:HD3	1:I:87:LEU:O	2.16	0.46
1:B:83:ARG:O	1:B:86:GLN:HB2	2.16	0.46
1:I:51:HIS:O	1:I:63:HIS:CD2	2.66	0.46
1:B:60:VAL:HG13	1:B:61:ALA:N	2.30	0.46
1:B:95:ALA:N	1:D:45:LEU:HD23	2.30	0.46
1:F:70:ARG:NH1	3:H:202:SO4:O1	2.42	0.46
1:L:51:HIS:CE1	1:L:63:HIS:CE1	3.04	0.46
3:D:202:SO4:O4	1:G:57:ALA:HB1	2.15	0.46
1:I:80:PHE:HD1	1:I:147:MET:HE2	1.81	0.46
1:I:118:LEU:HA	1:I:118:LEU:HD23	1.78	0.46
1:E:51:HIS:CE1	1:E:63:HIS:CE1	3.04	0.45
1:G:48:LYS:HG3	1:G:52:TRP:CZ2	2.50	0.45
1:J:96:GLN:H	1:J:96:GLN:CD	2.19	0.45
1:A:38:ILE:CD1	1:A:97:VAL:HG12	2.46	0.45
1:C:40:PHE:O	1:C:44:SER:HB2	2.16	0.45
1:H:19:ASN:O	1:H:26:LYS:NZ	2.48	0.45
1:K:136:ILE:HD11	1:K:149:THR:HA	1.98	0.45
1:L:54:MET:HG2	1:L:114:VAL:HG22	1.98	0.45
1:A:42:ASP:O	1:A:46:ILE:HD13	2.15	0.45
1:B:48:LYS:HA	1:B:51:HIS:HB3	1.99	0.45
1:D:76:HIS:CE1	1:D:151:ALA:HA	2.52	0.45
1:D:136:ILE:HD13	1:D:149:THR:HA	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:115:GLN:NE2	4:K:307:HOH:O	2.32	0.45
1:C:160:TRP:CH2	1:J:82:GLU:HG2	2.51	0.45
1:D:40:PHE:HB3	1:D:77:LEU:HB3	1.99	0.45
1:H:107:TYR:CE1	1:H:120:ALA:CB	2.99	0.45
1:J:29:THR:HG22	1:J:33:LEU:CD1	2.46	0.45
1:F:48:LYS:O	1:F:51:HIS:HB3	2.17	0.45
1:I:36:MET:HE3	1:I:132:ILE:HA	1.99	0.45
1:F:26:LYS:HD3	1:F:87:LEU:O	2.17	0.45
1:J:121:LEU:O	1:J:122:ALA:C	2.56	0.45
1:L:79:THR:HG21	1:L:147:MET:HG2	1.99	0.45
1:C:83:ARG:HG2	1:C:147:MET:HE1	1.99	0.45
1:K:33:LEU:HD11	1:K:83:ARG:HG3	1.98	0.45
1:L:40:PHE:HB3	1:L:77:LEU:HB3	1.98	0.45
1:F:20:ASP:OD2	1:K:134:LYS:NZ	2.49	0.45
1:I:48:LYS:O	1:I:51:HIS:HB3	2.15	0.45
1:I:70:ARG:HH21	1:K:70:ARG:HH21	1.64	0.45
1:J:54:MET:SD	1:J:62:VAL:HG12	2.57	0.45
1:L:79:THR:HG22	1:L:147:MET:HE3	1.99	0.45
1:L:113:SER:OG	1:L:116:GLU:HG3	2.17	0.45
1:A:136:ILE:HG21	1:I:142:GLU:HG3	1.98	0.44
1:L:108:PRO:HB2	1:L:111:ILE:HG23	1.98	0.44
1:A:92:LEU:HD23	1:C:109:THR:CG2	2.44	0.44
1:C:119:LYS:O	1:C:123:GLU:HG2	2.18	0.44
1:I:75:ASP:O	1:I:79:THR:HG23	2.18	0.44
1:J:50:ALA:O	1:J:54:MET:HG3	2.16	0.44
1:E:80:PHE:CD1	1:E:147:MET:HE3	2.52	0.44
1:E:105:LYS:O	1:E:106:SER:C	2.55	0.44
1:J:32:ARG:NH2	1:J:135:ALA:HB2	2.32	0.44
1:I:115:GLN:O	1:I:119:LYS:HG3	2.17	0.44
1:B:50:ALA:HB2	1:B:107:TYR:OH	2.17	0.44
1:E:27:VAL:O	1:E:31:LYS:HG3	2.17	0.44
1:B:40:PHE:CZ	1:B:155:LEU:HD22	2.53	0.44
1:J:102:THR:HG22	1:J:104:LEU:N	2.27	0.44
1:C:123:GLU:O	1:C:127:ILE:CG2	2.65	0.44
1:A:119:LYS:HG2	1:A:166:ILE:HD13	1.99	0.44
1:B:83:ARG:NH1	1:B:143:ASN:HD22	2.16	0.44
1:G:46:ILE:HG12	1:G:107:TYR:HB2	1.98	0.44
1:I:54:MET:CE	1:I:63:HIS:HB2	2.48	0.44
1:J:136:ILE:HD11	1:J:152:SER:CB	2.48	0.44
1:L:119:LYS:HG2	1:L:166:ILE:HD13	1.99	0.44
1:G:74:THR:O	1:G:77:LEU:HB3	2.18	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:20:ASP:O	1:H:21:VAL:O	2.36	0.44
1:B:38:ILE:HD13	1:B:101:LYS:HB2	2.00	0.43
1:D:57:ALA:O	1:D:58:ASN:HB3	2.17	0.43
1:G:124:ARG:NH1	1:G:124:ARG:CG	2.81	0.43
1:I:38:ILE:HD13	1:I:101:LYS:HB2	2.00	0.43
1:I:94:THR:HG22	1:I:96:GLN:H	1.82	0.43
1:B:25:VAL:HG13	1:B:140:GLU:HB2	1.99	0.43
1:C:25:VAL:HG12	1:C:140:GLU:HG3	2.00	0.43
1:E:144:SER:HA	1:E:147:MET:HE2	1.99	0.43
1:G:35:GLN:HA	1:G:38:ILE:HD12	2.00	0.43
1:G:73:LEU:O	1:G:77:LEU:HB2	2.18	0.43
1:H:22:GLU:OE1	1:H:24:HIS:HB2	2.19	0.43
1:J:133:ARG:HA	1:J:136:ILE:HD12	2.00	0.43
1:A:43:LEU:CD1	1:A:128:VAL:HG21	2.47	0.43
1:A:111:ILE:HG22	1:A:116:GLU:OE2	2.19	0.43
1:F:108:PRO:HG2	1:F:111:ILE:HD13	2.00	0.43
1:B:163:GLU:OE2	1:L:18:ARG:NH1	2.51	0.43
1:D:155:LEU:HD23	1:D:155:LEU:HA	1.86	0.43
1:E:158:PHE:O	1:E:162:ILE:HG13	2.19	0.43
1:I:123:GLU:O	1:I:127:ILE:HG12	2.19	0.43
1:J:77:LEU:HA	1:J:80:PHE:CD2	2.53	0.43
1:K:38:ILE:HD13	1:K:101:LYS:HB2	1.98	0.43
1:K:133:ARG:NH2	1:K:156:ASP:OD1	2.49	0.43
1:C:46:ILE:HG23	1:C:107:TYR:CE1	2.53	0.43
1:D:33:LEU:HD11	1:D:83:ARG:HG3	2.01	0.43
1:F:69:PHE:CE1	1:F:158:PHE:CD1	3.06	0.43
1:G:81:ALA:O	1:G:84:ALA:HB3	2.18	0.43
1:H:46:ILE:HA	1:H:49:GLN:HB3	2.00	0.43
1:C:104:LEU:HD23	1:C:127:ILE:HD11	1.99	0.43
1:E:51:HIS:CE1	1:E:63:HIS:NE2	2.87	0.43
1:I:70:ARG:HE	1:I:74:THR:HG21	1.84	0.43
1:D:43:LEU:HG	1:D:128:VAL:HG21	2.00	0.43
1:G:26:LYS:HD3	1:G:87:LEU:O	2.18	0.43
1:G:48:LYS:NZ	1:G:67:ASP:OD1	2.51	0.43
1:K:130:ASN:HA	1:K:133:ARG:HH12	1.83	0.43
1:L:44:SER:OG	1:L:70:ARG:HD2	2.19	0.43
1:B:143:ASN:O	1:B:147:MET:HB2	2.19	0.42
1:C:33:LEU:HD13	1:C:83:ARG:HB3	2.01	0.42
1:C:107:TYR:CG	1:C:108:PRO:HD2	2.54	0.42
1:J:102:THR:HG21	1:J:104:LEU:HB2	2.01	0.42
1:L:83:ARG:O	1:L:87:LEU:HG	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:LEU:HD12	1:B:46:ILE:HD11	2.01	0.42
1:F:51:HIS:NE2	1:F:63:HIS:CE1	2.87	0.42
1:G:51:HIS:HD2	1:G:63:HIS:O	2.01	0.42
1:J:133:ARG:NH2	1:J:156:ASP:OD1	2.46	0.42
1:L:40:PHE:CB	1:L:77:LEU:HB3	2.49	0.42
1:C:158:PHE:CD1	1:C:158:PHE:N	2.86	0.42
1:D:46:ILE:HG12	1:D:107:TYR:HB2	2.01	0.42
1:K:21:VAL:HG11	1:K:87:LEU:CD2	2.47	0.42
1:B:33:LEU:CD2	1:B:147:MET:HE1	2.49	0.42
1:B:139:VAL:HG11	1:B:148:PHE:CE2	2.54	0.42
1:B:51:HIS:ND1	1:B:63:HIS:O	2.53	0.42
1:F:29:THR:HG22	1:F:33:LEU:CD1	2.50	0.42
1:J:32:ARG:HD2	1:J:35:GLN:OE1	2.20	0.42
1:K:54:MET:HE1	1:K:63:HIS:N	2.34	0.42
1:E:107:TYR:CG	1:E:108:PRO:HD2	2.54	0.42
1:K:45:LEU:O	1:K:48:LYS:N	2.52	0.42
1:E:55:ARG:CZ	1:G:15:LEU:HD13	2.49	0.42
1:K:102:THR:HG23	1:K:102:THR:O	2.20	0.42
1:B:48:LYS:O	1:B:51:HIS:HB3	2.20	0.42
1:C:36:MET:HE2	1:C:132:ILE:HB	2.02	0.42
1:K:83:ARG:HH21	1:K:141:ASP:CG	2.23	0.42
1:B:41:ILE:O	1:B:45:LEU:HG	2.19	0.41
1:B:102:THR:O	1:B:102:THR:HG23	2.19	0.41
1:J:109:THR:O	1:J:109:THR:CG2	2.67	0.41
1:J:118:LEU:CB	1:J:166:ILE:HD11	2.46	0.41
1:H:80:PHE:CZ	1:H:151:ALA:HB2	2.51	0.41
1:G:76:HIS:CE1	1:G:151:ALA:HA	2.55	0.41
1:H:22:GLU:OE2	1:H:23:GLU:N	2.53	0.41
1:E:94:THR:O	1:E:97:VAL:N	2.54	0.41
1:F:41:ILE:O	1:F:45:LEU:HG	2.19	0.41
1:G:34:ASN:O	1:G:38:ILE:HG13	2.20	0.41
1:C:79:THR:HG21	1:C:147:MET:HG2	2.02	0.41
1:L:22:GLU:OE2	1:L:24:HIS:NE2	2.50	0.41
1:L:41:ILE:O	1:L:45:LEU:HG	2.21	0.41
1:L:134:LYS:HA	1:L:134:LYS:HD3	1.51	0.41
1:A:124:ARG:O	1:A:128:VAL:HG23	2.20	0.41
1:B:141:ASP:HB3	1:B:144:SER:HB2	2.02	0.41
1:C:115:GLN:O	1:C:116:GLU:C	2.57	0.41
1:E:139:VAL:CG1	1:E:141:ASP:H	2.33	0.41
1:G:115:GLN:OE1	1:G:167:GLU:N	2.54	0.41
1:H:132:ILE:O	1:H:136:ILE:HG13	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:VAL:O	1:A:26:LYS:HE3	2.21	0.41
1:A:48:LYS:HG3	1:A:70:ARG:NH1	2.35	0.41
1:F:155:LEU:HD23	1:F:155:LEU:HA	1.84	0.41
1:A:34:ASN:O	1:A:38:ILE:HG12	2.21	0.41
1:G:26:LYS:CD	1:G:87:LEU:O	2.69	0.41
1:B:80:PHE:HA	1:B:147:MET:HE1	2.01	0.41
1:D:83:ARG:HH21	1:D:141:ASP:CG	2.24	0.41
1:D:97:VAL:O	1:D:101:LYS:HB2	2.21	0.41
1:F:118:LEU:HD23	1:F:118:LEU:HA	1.87	0.41
1:G:51:HIS:O	1:G:63:HIS:HD2	2.03	0.41
1:A:60:VAL:CG2	1:H:65:MET:HE3	2.50	0.41
1:B:19:ASN:ND2	1:G:156:ASP:OD2	2.50	0.41
1:D:38:ILE:HD13	1:D:101:LYS:HB3	2.02	0.41
1:E:97:VAL:O	1:E:101:LYS:HB2	2.21	0.41
1:A:146:ASP:OD2	1:E:153:ARG:NH1	2.48	0.40
1:B:33:LEU:HD21	1:B:147:MET:CE	2.51	0.40
1:B:51:HIS:O	1:B:63:HIS:ND1	2.53	0.40
1:I:147:MET:HE2	1:I:147:MET:HB3	1.91	0.40
1:K:46:ILE:HG23	1:K:107:TYR:CE1	2.57	0.40
1:L:107:TYR:CD2	1:L:108:PRO:HD2	2.57	0.40
1:A:69:PHE:CE1	1:A:158:PHE:CD1	3.09	0.40
1:C:66:LEU:N	1:C:66:LEU:HD23	2.35	0.40
1:D:42:ASP:O	1:D:46:ILE:HB	2.21	0.40
1:F:36:MET:HE2	1:F:132:ILE:HB	2.03	0.40
1:K:29:THR:O	1:K:30:ILE:C	2.59	0.40
1:I:48:LYS:HD3	1:I:48:LYS:HA	2.00	0.40
1:I:48:LYS:NZ	1:I:67:ASP:OD1	2.48	0.40
1:I:70:ARG:HE	1:I:74:THR:CG2	2.34	0.40
1:J:77:LEU:HD12	1:J:77:LEU:C	2.42	0.40
1:J:135:ALA:HA	1:J:138:GLU:CG	2.50	0.40
1:B:83:ARG:HH12	1:B:143:ASN:HD22	1.69	0.40
1:B:107:TYR:CD1	1:B:108:PRO:HD2	2.57	0.40
1:H:100:ASP:O	1:H:101:LYS:HD3	2.21	0.40
1:K:104:LEU:HD12	1:K:104:LEU:HA	1.84	0.40
1:H:121:LEU:HA	1:H:121:LEU:HD23	1.76	0.40
1:I:80:PHE:HD1	1:I:147:MET:HE1	1.87	0.40
1:L:30:ILE:HD13	1:L:89:GLY:HA3	2.02	0.40
1:L:111:ILE:CG1	1:L:117:HIS:CE1	3.04	0.40

There are no symmetry-related clashes.

## 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	153/170 (90%)	150 (98%)	3 (2%)	0	100	100
1	B	152/170 (89%)	146 (96%)	6 (4%)	0	100	100
1	C	152/170 (89%)	144 (95%)	8 (5%)	0	100	100
1	D	154/170 (91%)	145 (94%)	9 (6%)	0	100	100
1	E	153/170 (90%)	144 (94%)	9 (6%)	0	100	100
1	F	152/170 (89%)	147 (97%)	5 (3%)	0	100	100
1	G	153/170 (90%)	143 (94%)	10 (6%)	0	100	100
1	H	155/170 (91%)	144 (93%)	10 (6%)	1 (1%)	25	42
1	I	153/170 (90%)	145 (95%)	8 (5%)	0	100	100
1	J	153/170 (90%)	140 (92%)	11 (7%)	2 (1%)	12	21
1	K	153/170 (90%)	142 (93%)	11 (7%)	0	100	100
1	L	153/170 (90%)	141 (92%)	12 (8%)	0	100	100
All	All	1836/2040 (90%)	1731 (94%)	102 (6%)	3 (0%)	47	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	21	VAL
1	J	86	GLN
1	J	59	PHE

### 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	133/146 (91%)	127 (96%)	6 (4%)	27	46
1	B	132/146 (90%)	124 (94%)	8 (6%)	18	33
1	C	132/146 (90%)	126 (96%)	6 (4%)	27	46
1	D	134/146 (92%)	128 (96%)	6 (4%)	27	46
1	E	133/146 (91%)	126 (95%)	7 (5%)	22	38
1	F	132/146 (90%)	129 (98%)	3 (2%)	50	69
1	G	133/146 (91%)	127 (96%)	6 (4%)	27	46
1	H	135/146 (92%)	127 (94%)	8 (6%)	19	34
1	I	133/146 (91%)	129 (97%)	4 (3%)	41	61
1	J	133/146 (91%)	127 (96%)	6 (4%)	27	46
1	K	133/146 (91%)	129 (97%)	4 (3%)	41	61
1	L	133/146 (91%)	121 (91%)	12 (9%)	9	16
All	All	1596/1752 (91%)	1520 (95%)	76 (5%)	25	44

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	75	ASP
1	A	77	LEU
1	A	78	ASP
1	A	113	SER
1	A	131	ASP
1	B	17	THR
1	B	22	GLU
1	B	24	HIS
1	B	30	ILE
1	B	36	MET
1	B	44	SER
1	B	74	THR
1	B	78	ASP
1	C	22	GLU
1	C	23	GLU
1	C	44	SER
1	C	67	ASP
1	C	75	ASP
1	C	127	ILE
1	D	45	LEU
1	D	46	ILE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	51	HIS
1	D	55	ARG
1	D	101	LYS
1	D	144	SER
1	E	20	ASP
1	E	44	SER
1	E	74	THR
1	E	77	LEU
1	E	108	PRO
1	E	110	ASN
1	E	142	GLU
1	F	22	GLU
1	F	43	LEU
1	F	46	ILE
1	G	23	GLU
1	G	24	HIS
1	G	26	LYS
1	G	46	ILE
1	G	78	ASP
1	G	105	LYS
1	H	32	ARG
1	H	58	ASN
1	H	77	LEU
1	H	79	THR
1	H	106	SER
1	H	137	THR
1	H	157	LYS
1	H	167	GLU
1	I	20	ASP
1	I	78	ASP
1	I	110	ASN
1	I	142	GLU
1	J	22	GLU
1	J	64	GLU
1	J	74	THR
1	J	102	THR
1	J	139	VAL
1	J	164	SER
1	K	20	ASP
1	K	26	LYS
1	K	48	LYS
1	K	144	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	L	15	LEU
1	L	18	ARG
1	L	23	GLU
1	L	32	ARG
1	L	44	SER
1	L	54	MET
1	L	74	THR
1	L	102	THR
1	L	109	THR
1	L	115	GLN
1	L	139	VAL
1	L	161	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	D	51	HIS
1	E	51	HIS
1	G	51	HIS
1	G	63	HIS
1	H	51	HIS
1	H	58	ASN
1	H	63	HIS
1	I	51	HIS
1	I	63	HIS
1	L	63	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

Of 25 ligands modelled in this entry, 12 are monoatomic - leaving 13 for Mogul analysis.

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
3	SO4	B	203	-	4,4,4	0.18	0	6,6,6	0.10	0
3	SO4	D	202	-	4,4,4	0.13	0	6,6,6	0.17	0
3	SO4	A	202	-	4,4,4	0.14	0	6,6,6	0.10	0
3	SO4	G	201	-	4,4,4	0.13	0	6,6,6	0.39	0
3	SO4	B	202	-	4,4,4	0.19	0	6,6,6	0.25	0
3	SO4	K	202	-	4,4,4	0.12	0	6,6,6	0.34	0
3	SO4	E	203	-	4,4,4	0.11	0	6,6,6	0.25	0
3	SO4	D	203	-	4,4,4	0.13	0	6,6,6	0.26	0
3	SO4	H	202	-	4,4,4	0.09	0	6,6,6	0.30	0
3	SO4	J	203	-	4,4,4	0.16	0	6,6,6	0.14	0
3	SO4	J	202	-	4,4,4	0.15	0	6,6,6	0.14	0
3	SO4	F	202	-	4,4,4	0.13	0	6,6,6	0.10	0
3	SO4	A	203	-	4,4,4	0.16	0	6,6,6	0.11	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	202	SO4	2	0
3	G	201	SO4	1	0
3	B	202	SO4	2	0
3	E	203	SO4	1	0
3	D	203	SO4	1	0
3	H	202	SO4	1	0
3	J	203	SO4	1	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	202	SO4	2	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	155/170 (91%)	-0.23	0 100 100	22, 36, 57, 78	0
1	B	154/170 (90%)	-0.35	0 100 100	18, 36, 52, 67	0
1	C	154/170 (90%)	-0.05	1 (0%) 89 92	23, 40, 61, 74	0
1	D	156/170 (91%)	-0.14	2 (1%) 77 84	15, 33, 54, 97	0
1	E	155/170 (91%)	-0.05	2 (1%) 77 84	17, 33, 55, 75	0
1	F	154/170 (90%)	-0.11	2 (1%) 77 84	17, 33, 53, 66	0
1	G	155/170 (91%)	-0.22	0 100 100	15, 34, 57, 82	0
1	H	157/170 (92%)	-0.23	0 100 100	17, 38, 59, 108	0
1	I	155/170 (91%)	-0.19	2 (1%) 77 84	17, 31, 58, 77	0
1	J	155/170 (91%)	-0.20	3 (1%) 66 75	23, 36, 57, 80	0
1	K	155/170 (91%)	-0.17	0 100 100	20, 34, 51, 69	0
1	L	155/170 (91%)	-0.03	3 (1%) 66 75	18, 36, 59, 80	0
All	All	1860/2040 (91%)	-0.16	15 (0%) 86 90	15, 35, 57, 108	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	139	VAL	3.6
1	I	14	LEU	3.3
1	E	134	LYS	3.2
1	J	21	VAL	3.1
1	I	23	GLU	2.8
1	F	111	ILE	2.6
1	L	140	GLU	2.6
1	J	23	GLU	2.6
1	E	139	VAL	2.6
1	C	137	THR	2.3
1	D	57	ALA	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	L	138	GLU	2.2
1	D	111	ILE	2.1
1	J	137	THR	2.0
1	F	119	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
3	SO4	D	203	5/5	0.90	0.31	74,78,79,82	5
3	SO4	F	202	5/5	0.91	0.17	79,82,83,84	5
2	ZN	I	201	1/1	0.93	0.08	82,82,82,82	0
3	SO4	A	203	5/5	0.93	0.18	85,87,91,92	0
3	SO4	B	203	5/5	0.94	0.32	78,79,82,83	0
3	SO4	H	202	5/5	0.94	0.15	86,92,94,94	0
3	SO4	J	202	5/5	0.95	0.20	77,80,84,85	0
2	ZN	B	201	1/1	0.96	0.09	81,81,81,81	0
2	ZN	J	201	1/1	0.96	0.15	98,98,98,98	0
3	SO4	K	202	5/5	0.96	0.13	63,68,69,70	0
2	ZN	L	201	1/1	0.97	0.08	68,68,68,68	0
3	SO4	E	203	5/5	0.97	0.15	80,81,82,84	0
3	SO4	A	202	5/5	0.97	0.13	75,80,83,85	0
2	ZN	H	201	1/1	0.97	0.07	81,81,81,81	0
3	SO4	B	202	5/5	0.97	0.17	61,65,68,68	0
2	ZN	K	201	1/1	0.97	0.12	80,80,80,80	0
2	ZN	E	201	1/1	0.98	0.09	73,73,73,73	0
2	ZN	F	201	1/1	0.98	0.07	71,71,71,71	0
3	SO4	G	201	5/5	0.98	0.14	29,37,40,55	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	A	201	1/1	0.98	0.06	81,81,81,81	0
3	SO4	D	202	5/5	0.98	0.20	60,68,69,71	0
2	ZN	C	201	1/1	0.98	0.11	73,73,73,73	0
2	ZN	D	201	1/1	0.99	0.05	68,68,68,68	0
3	SO4	J	203	5/5	0.99	0.13	37,43,47,53	0
2	ZN	E	202	1/1	0.99	0.08	72,72,72,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.