



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:07 am BST

PDB ID : 4QF6  
Title : Structure of Aldehyde Dehydrogenase from Bacillus cereus, E194S mutant  
Authors : Ngo, H.P.T.; Hong, S.H.; Oh, D.K.; Kang, L.W.  
Deposited on : 2014-05-19  
Resolution : 1.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

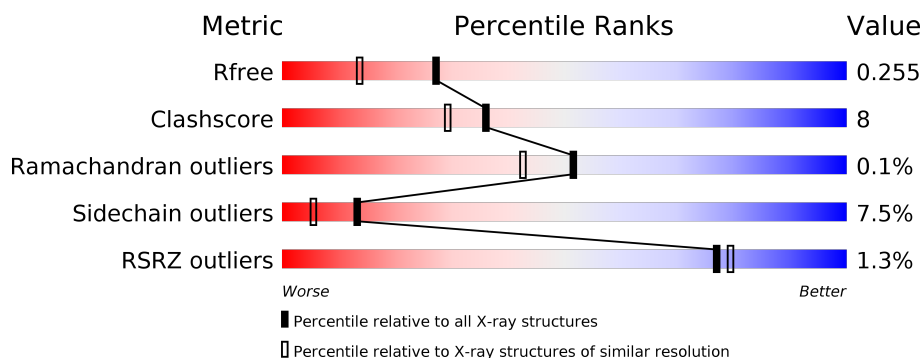
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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	494	<div> <div>81%</div> <div>15%</div> <div>...</div> </div>
1	B	494	<div> <div>%</div> <div>83%</div> <div>13%</div> <div>...</div> </div>
1	C	494	<div> <div>84%</div> <div>13%</div> <div>...</div> </div>
1	D	494	<div> <div>85%</div> <div>12%</div> <div>...</div> </div>
1	E	494	<div> <div>85%</div> <div>12%</div> <div>...</div> </div>
1	F	494	<div> <div>80%</div> <div>17%</div> <div>...</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	494	<div><div>%</div><div><div></div><div>80%</div><div>17%</div><div></div></div><div>...</div></div>
1	H	494	<div><div>%</div><div><div></div><div>80%</div><div>16%</div><div></div></div><div>..</div></div>
1	I	494	<div><div>%</div><div><div></div><div>81%</div><div>16%</div><div></div></div><div>..</div></div>
1	J	494	<div><div>%</div><div><div></div><div>81%</div><div>15%</div><div></div></div><div>..</div></div>
1	K	494	<div><div>4%</div><div><div></div><div>76%</div><div>18%</div><div></div></div><div>..</div></div>
1	L	494	<div><div>5%</div><div><div></div><div>74%</div><div>19%</div><div>5%</div></div><div>.</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 47191 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	1	0
			3791	2414	630	733	14			
1	B	491	Total	C	N	O	S	0	1	0
			3791	2414	630	733	14			
1	C	491	Total	C	N	O	S	0	1	0
			3793	2415	630	734	14			
1	D	489	Total	C	N	O	S	0	3	0
			3787	2413	628	732	14			
1	E	490	Total	C	N	O	S	0	0	0
			3781	2408	629	730	14			
1	F	491	Total	C	N	O	S	0	2	0
			3794	2416	630	734	14			
1	G	490	Total	C	N	O	S	0	0	0
			3781	2408	629	730	14			
1	H	490	Total	C	N	O	S	0	1	0
			3787	2412	629	732	14			
1	I	491	Total	C	N	O	S	0	0	0
			3788	2412	630	732	14			
1	J	491	Total	C	N	O	S	0	0	0
			3788	2412	630	732	14			
1	K	489	Total	C	N	O	S	0	0	0
			3773	2404	627	728	14			
1	L	488	Total	C	N	O	S	0	0	0
			3764	2398	626	726	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217
B	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217
C	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217
D	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217
E	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217
G	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217
H	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217
I	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217
J	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217
K	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217
L	194	SER	GLU	ENGINEERED MUTATION	UNP C2N217

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Na 2 2	0	0
2	J	2	Total Na 2 2	0	0
2	D	2	Total Na 2 2	0	0
2	K	2	Total Na 2 2	0	0
2	E	2	Total Na 2 2	0	0
2	H	2	Total Na 2 2	0	0
2	B	2	Total Na 2 2	0	0
2	I	2	Total Na 2 2	0	0
2	C	2	Total Na 2 2	0	0
2	A	2	Total Na 2 2	0	0
2	L	2	Total Na 2 2	0	0
2	F	2	Total Na 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	255	Total O 255 255	0	0
3	B	123	Total O 123 123	0	0

*Continued on next page...*

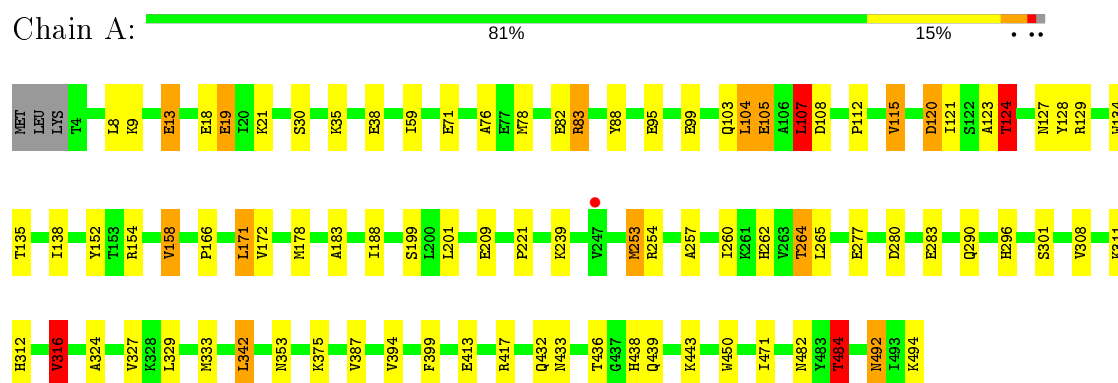
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	197	Total 197	O 197	0	0
3	D	216	Total 216	O 216	0	0
3	E	218	Total 218	O 218	0	0
3	F	124	Total 124	O 124	0	0
3	G	152	Total 152	O 152	0	0
3	H	143	Total 143	O 143	0	0
3	I	109	Total 109	O 109	0	0
3	J	74	Total 74	O 74	0	0
3	K	76	Total 76	O 76	0	0
3	L	62	Total 62	O 62	0	0

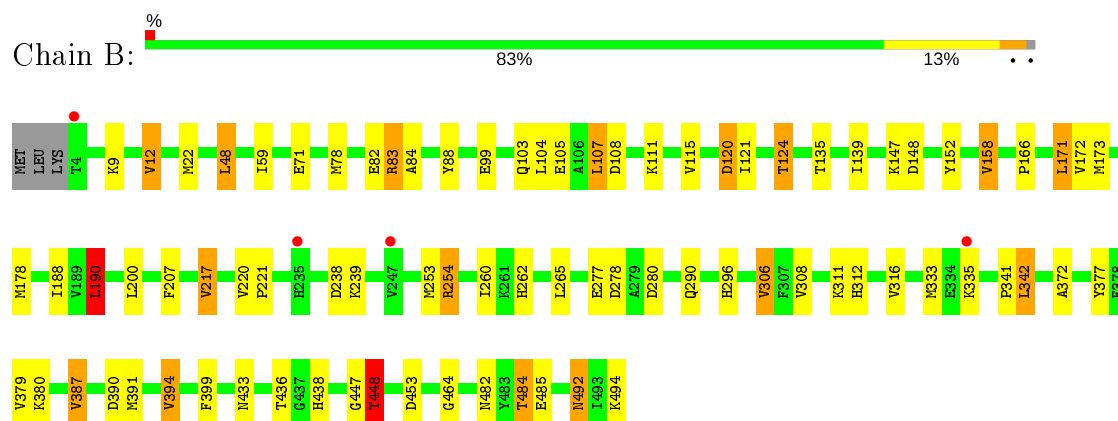
### 3 Residue-property plots

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

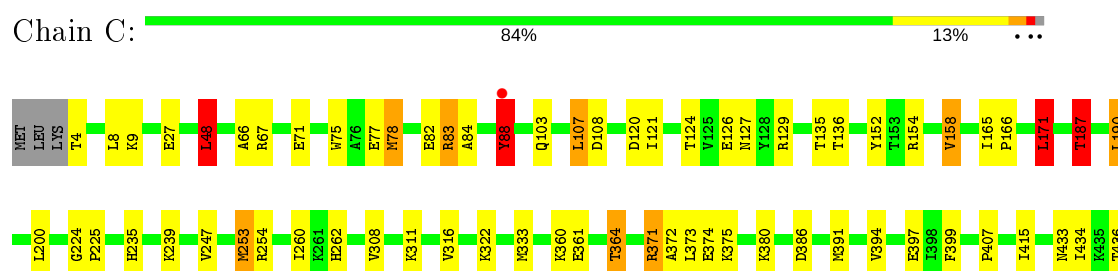
#### • Molecule 1: Aldehyde dehydrogenase



#### • Molecule 1: Aldehyde dehydrogenase



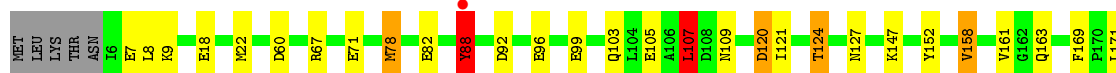
#### • Molecule 1: Aldehyde dehydrogenase





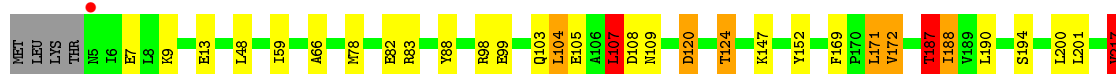
- Molecule 1: Aldehyde dehydrogenase

Chain D: 85% 12% ..



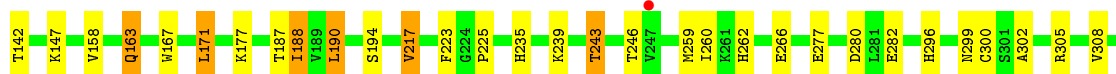
- Molecule 1: Aldehyde dehydrogenase

Chain E: 85% 12% ..



- Molecule 1: Aldehyde dehydrogenase

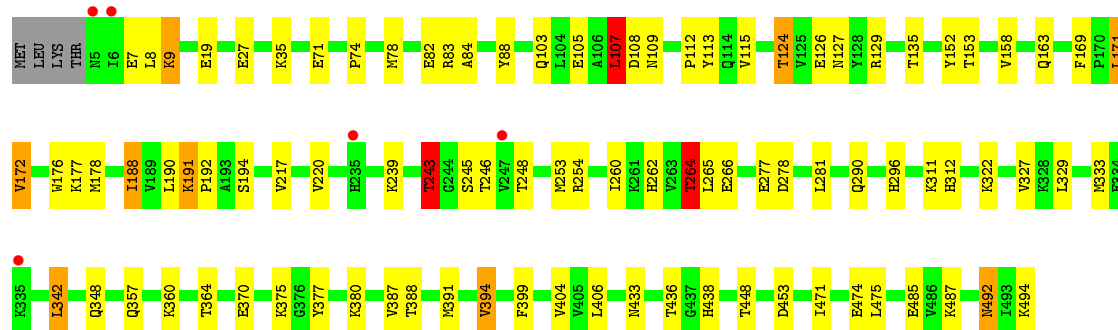
Chain F: 80% 17% ..



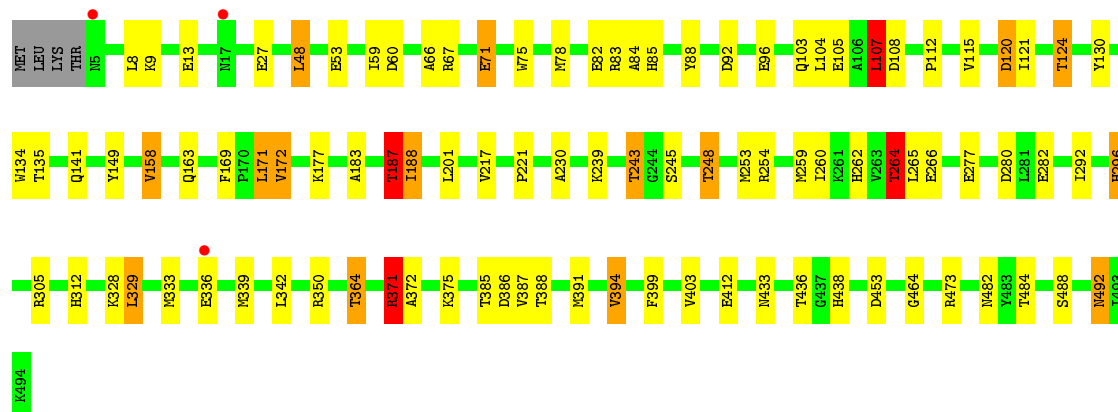
- Molecule 1: Aldehyde dehydrogenase

Chain G: 80% 17% ..

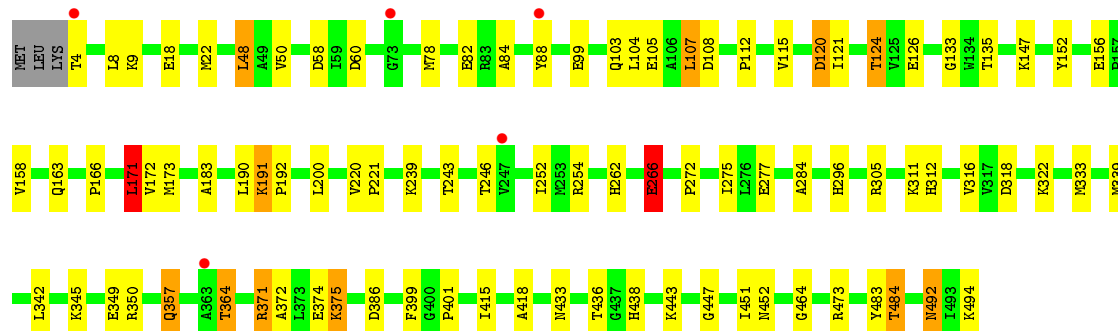
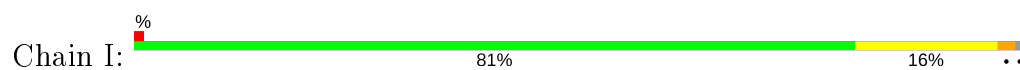




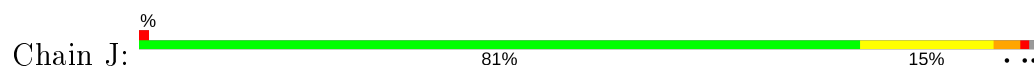
• Molecule 1: Aldehyde dehydrogenase

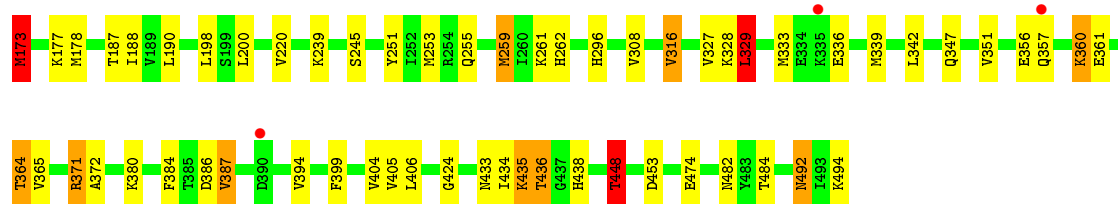


• Molecule 1: Aldehyde dehydrogenase

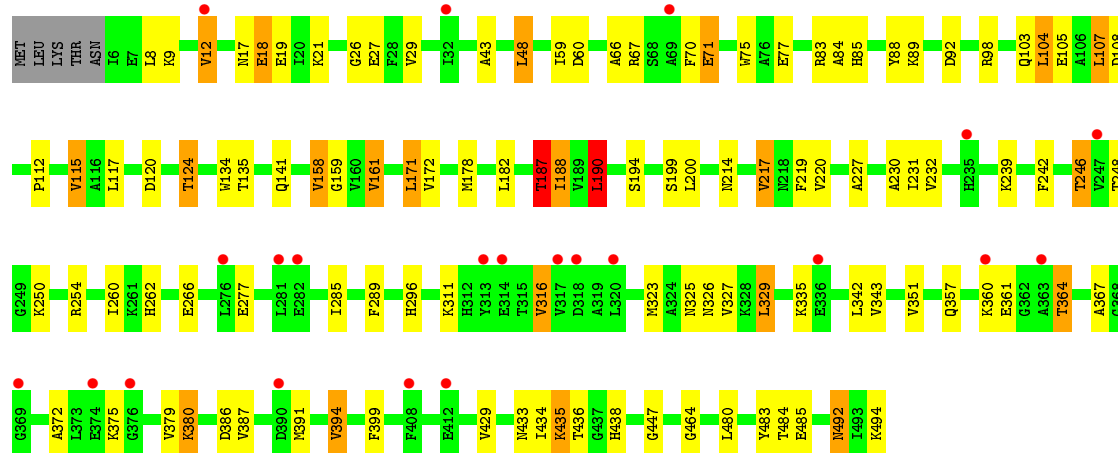
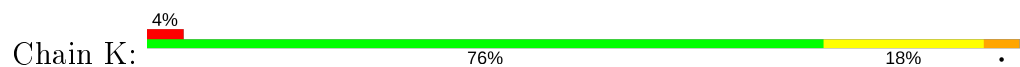


• Molecule 1: Aldehyde dehydrogenase

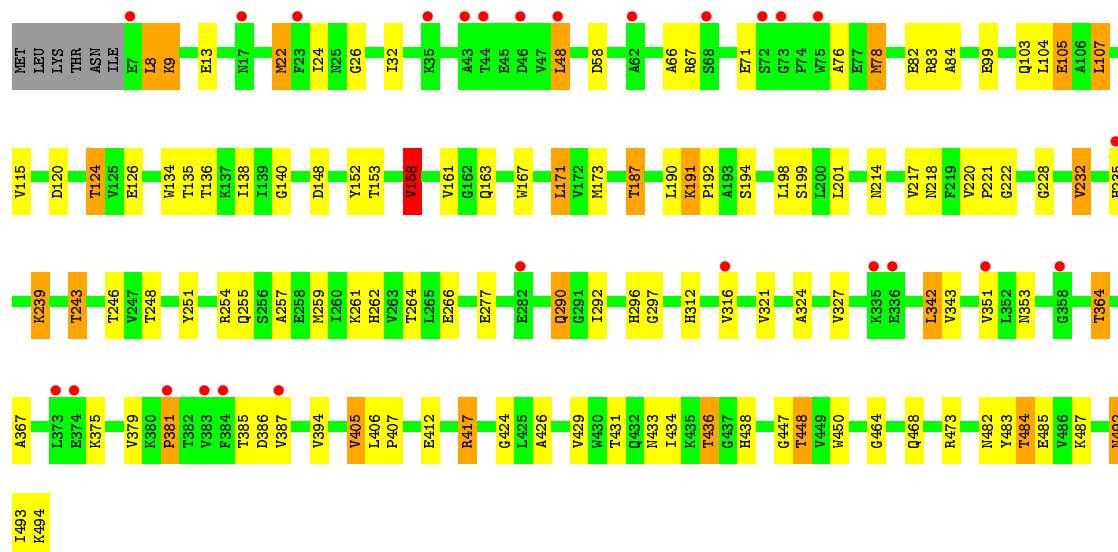
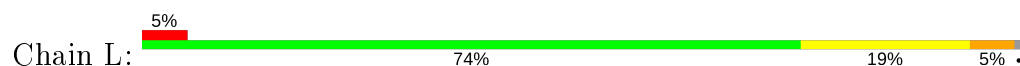




• Molecule 1: Aldehyde dehydrogenase



• Molecule 1: Aldehyde dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.56 Å 93.66 Å 247.85 Å 90.00° 95.55° 90.00°	Depositor
Resolution (Å)	43.56 – 1.90 43.56 – 1.90	Depositor EDS
% Data completeness (in resolution range)	84.9 (43.56-1.90) 84.9 (43.56-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.47 (at 1.89 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.204 , 0.252 0.211 , 0.255	Depositor DCC
$R_{free}$ test set	22144 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.6	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 43.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	47191	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3627e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

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

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	1.18	11/3873 (0.3%)	1.11	22/5254 (0.4%)
1	B	1.03	1/3873 (0.0%)	1.07	11/5254 (0.2%)
1	C	1.08	3/3875 (0.1%)	1.08	14/5257 (0.3%)
1	D	1.07	5/3875 (0.1%)	1.07	19/5256 (0.4%)
1	E	1.13	6/3860 (0.2%)	1.08	17/5236 (0.3%)
1	F	1.06	2/3879 (0.1%)	1.07	14/5262 (0.3%)
1	G	1.05	4/3860 (0.1%)	1.01	7/5236 (0.1%)
1	H	1.02	4/3869 (0.1%)	1.04	12/5248 (0.2%)
1	I	0.98	2/3867 (0.1%)	0.98	8/5246 (0.2%)
1	J	0.94	1/3867 (0.0%)	0.98	4/5246 (0.1%)
1	K	1.02	1/3852 (0.0%)	1.00	7/5225 (0.1%)
1	L	1.01	1/3843 (0.0%)	1.00	3/5214 (0.1%)
All	All	1.05	41/46393 (0.1%)	1.04	138/62934 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	GLU	CD-OE1	8.67	1.35	1.25
1	G	264	THR	CB-CG2	8.24	1.79	1.52
1	D	88	TYR	CE1-CZ	7.98	1.49	1.38
1	C	88	TYR	CE1-CZ	7.86	1.48	1.38
1	H	264	THR	CB-CG2	7.09	1.75	1.52
1	A	484	THR	CB-CG2	-6.64	1.30	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	484	THR	CB-CG2	-6.57	1.30	1.52
1	I	133	GLY	N-CA	6.34	1.55	1.46
1	C	187	THR	CB-CG2	-6.29	1.31	1.52
1	B	448	THR	CB-CG2	-6.20	1.31	1.52
1	I	266	GLU	CD-OE2	6.16	1.32	1.25
1	D	99	GLU	CD-OE1	-6.10	1.19	1.25
1	A	209	GLU	CD-OE1	-6.07	1.19	1.25
1	E	483	TYR	CE1-CZ	-5.95	1.30	1.38
1	D	484	THR	CB-CG2	-5.83	1.33	1.52
1	C	397	GLU	CD-OE1	-5.80	1.19	1.25
1	J	448	THR	CB-CG2	-5.78	1.33	1.52
1	E	412	GLU	CD-OE2	5.76	1.31	1.25
1	A	450	TRP	CZ3-CH2	5.75	1.49	1.40
1	A	99	GLU	CD-OE1	-5.69	1.19	1.25
1	G	113	TYR	CE1-CZ	-5.60	1.31	1.38
1	A	95	GLU	CD-OE1	-5.56	1.19	1.25
1	D	397	GLU	CD-OE1	-5.52	1.19	1.25
1	A	301	SER	CB-OG	-5.48	1.35	1.42
1	K	187	THR	CB-CG2	-5.45	1.34	1.52
1	L	450	TRP	CG-CD1	5.41	1.44	1.36
1	D	88	TYR	CB-CG	-5.35	1.43	1.51
1	G	243	THR	CB-CG2	-5.34	1.34	1.52
1	E	344	SER	CB-OG	5.29	1.49	1.42
1	E	429	VAL	CB-CG1	-5.25	1.41	1.52
1	A	128	TYR	CB-CG	5.24	1.59	1.51
1	E	187	THR	CB-CG2	-5.22	1.35	1.52
1	G	485	GLU	CD-OE2	5.21	1.31	1.25
1	A	413	GLU	CD-OE2	-5.15	1.20	1.25
1	H	134	TRP	CB-CG	5.12	1.59	1.50
1	A	283	GLU	CD-OE2	5.08	1.31	1.25
1	H	53	GLU	CD-OE1	-5.06	1.20	1.25
1	F	163	GLN	C-O	-5.06	1.13	1.23
1	F	466	TYR	CG-CD2	-5.05	1.32	1.39
1	A	450	TRP	CE3-CZ3	-5.03	1.29	1.38
1	H	130	TYR	CG-CD2	-5.03	1.32	1.39

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	278	ASP	CB-CG-OD1	11.71	128.84	118.30
1	G	108	ASP	CB-CG-OD2	-10.16	109.16	118.30
1	I	108	ASP	CB-CG-OD2	-9.77	109.51	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	254	ARG	NE-CZ-NH1	9.27	124.94	120.30
1	D	158	VAL	CB-CA-C	-9.20	93.92	111.40
1	K	108	ASP	CB-CG-OD2	-9.18	110.04	118.30
1	C	171	LEU	CB-CG-CD2	8.84	126.03	111.00
1	A	254	ARG	NE-CZ-NH1	8.65	124.62	120.30
1	E	278	ASP	CB-CG-OD2	-8.33	110.81	118.30
1	E	83	ARG	NE-CZ-NH1	-8.13	116.24	120.30
1	E	108	ASP	CB-CG-OD2	-8.12	110.99	118.30
1	D	78	MET	CG-SD-CE	-8.12	87.21	100.20
1	A	158	VAL	CB-CA-C	-8.09	96.02	111.40
1	A	171	LEU	CB-CG-CD2	8.07	124.72	111.00
1	G	108	ASP	CB-CG-OD1	8.02	125.51	118.30
1	H	108	ASP	CB-CG-OD2	-7.93	111.17	118.30
1	B	108	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	E	98	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	F	371	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	B	108	ASP	CB-CG-OD1	7.41	124.97	118.30
1	A	316	VAL	CG1-CB-CG2	7.39	122.72	110.90
1	E	107	LEU	CB-CG-CD1	7.27	123.36	111.00
1	H	305	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	E	83	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	G	278	ASP	CB-CG-OD1	7.26	124.83	118.30
1	A	280	ASP	CB-CG-OD1	7.21	124.79	118.30
1	F	305	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	G	342	LEU	CB-CG-CD1	7.16	123.17	111.00
1	D	190	LEU	CB-CG-CD1	7.13	123.13	111.00
1	F	371	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	D	88	TYR	CB-CG-CD2	-7.07	116.76	121.00
1	D	329	LEU	CA-CB-CG	7.02	131.45	115.30
1	C	83	ARG	NE-CZ-NH1	-7.01	116.79	120.30
1	E	217	VAL	CG1-CB-CG2	7.00	122.10	110.90
1	F	300	CYS	CA-CB-SG	-6.96	101.47	114.00
1	C	254	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	H	254	ARG	NE-CZ-NH1	-6.82	116.89	120.30
1	D	107	LEU	CB-CG-CD1	6.77	122.51	111.00
1	E	187	THR	OG1-CB-CG2	6.76	125.56	110.00
1	E	217	VAL	CA-CB-CG1	6.76	121.04	110.90
1	C	253	MET	CG-SD-CE	-6.73	89.43	100.20
1	E	108	ASP	CB-CG-OD1	6.69	124.32	118.30
1	J	173	MET	CG-SD-CE	6.68	110.89	100.20
1	B	171	LEU	CB-CG-CD2	6.67	122.34	111.00
1	A	108	ASP	CB-CG-OD2	-6.57	112.38	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	187	THR	N-CA-CB	-6.55	97.86	110.30
1	K	92	ASP	CB-CG-OD2	-6.53	112.43	118.30
1	F	473	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	I	350	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	K	108	ASP	CB-CG-OD1	6.40	124.06	118.30
1	D	217	VAL	CA-CB-CG1	6.36	120.43	110.90
1	F	104	LEU	CB-CG-CD1	6.33	121.76	111.00
1	A	129	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	D	238	ASP	CB-CG-OD2	6.26	123.93	118.30
1	A	83	ARG	NE-CZ-NH2	6.25	123.42	120.30
1	B	280	ASP	CB-CG-OD1	6.20	123.88	118.30
1	F	473	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	C	108	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	H	254	ARG	NE-CZ-NH2	6.15	123.37	120.30
1	J	108	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	D	217	VAL	CG1-CB-CG2	6.08	120.63	110.90
1	L	417	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	D	60	ASP	CB-CG-OD1	6.07	123.77	118.30
1	E	327	VAL	CA-CB-CG1	6.01	119.92	110.90
1	H	107	LEU	CA-CB-CG	5.99	129.07	115.30
1	C	154	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	K	104	LEU	CB-CG-CD1	5.96	121.13	111.00
1	A	104	LEU	CB-CG-CD1	5.95	121.11	111.00
1	J	171	LEU	CB-CG-CD2	5.93	121.09	111.00
1	F	217	VAL	CG1-CB-CG2	5.91	120.35	110.90
1	C	78	MET	CA-CB-CG	5.86	123.26	113.30
1	G	254	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	124	THR	OG1-CB-CG2	5.82	123.38	110.00
1	A	254	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	I	350	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	F	305	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	I	305	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	115	VAL	CG1-CB-CG2	5.71	120.03	110.90
1	D	371	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	394	VAL	CG1-CB-CG2	5.64	119.92	110.90
1	H	371	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	306	VAL	CG1-CB-CG2	5.62	119.90	110.90
1	F	190	LEU	CA-CB-CG	5.60	128.18	115.30
1	L	158	VAL	CB-CA-C	-5.59	100.79	111.40
1	A	417	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	D	158	VAL	CA-CB-CG2	5.54	119.20	110.90
1	E	98	ARG	NE-CZ-NH2	-5.53	117.53	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	ARG	NE-CZ-NH2	5.53	123.07	120.30
1	B	254	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	I	171	LEU	CB-CG-CD2	5.52	120.39	111.00
1	E	254	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	I	58	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	A	253	MET	CG-SD-CE	-5.50	91.40	100.20
1	D	158	VAL	CG1-CB-CG2	5.49	119.69	110.90
1	D	88	TYR	OH-CZ-CE2	-5.48	105.30	120.10
1	I	108	ASP	CB-CG-OD1	5.47	123.23	118.30
1	C	371	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	342	LEU	CB-CG-CD1	5.45	120.26	111.00
1	B	190	LEU	CB-CG-CD2	5.44	120.25	111.00
1	H	158	VAL	CB-CA-C	-5.43	101.08	111.40
1	D	385	THR	N-CA-CB	-5.42	99.99	110.30
1	A	108	ASP	CB-CG-OD1	5.40	123.16	118.30
1	D	88	TYR	CE1-CZ-OH	5.40	134.69	120.10
1	A	417	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	D	318	ASP	CB-CG-OD1	5.38	123.14	118.30
1	K	190	LEU	CA-CB-CG	5.37	127.65	115.30
1	C	48	LEU	CB-CG-CD2	5.35	120.10	111.00
1	F	107	LEU	CA-CB-CG	5.34	127.57	115.30
1	B	278	ASP	CB-CG-OD1	5.32	123.09	118.30
1	J	329	LEU	CA-CB-CG	5.30	127.50	115.30
1	I	318	ASP	CB-CG-OD1	5.29	123.06	118.30
1	H	280	ASP	CB-CG-OD1	5.27	123.04	118.30
1	B	173	MET	CG-SD-CE	5.26	108.62	100.20
1	A	158	VAL	CA-CB-CG2	5.26	118.78	110.90
1	A	154	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	G	107	LEU	CA-CB-CG	5.25	127.37	115.30
1	C	187	THR	OG1-CB-CG2	5.24	122.04	110.00
1	H	108	ASP	CB-CG-OD1	5.23	123.00	118.30
1	E	371	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	G	158	VAL	CB-CA-C	-5.20	101.51	111.40
1	D	217	VAL	CB-CA-C	5.20	121.28	111.40
1	D	217	VAL	N-CA-CB	-5.19	100.08	111.50
1	H	60	ASP	CB-CG-OD1	5.18	122.96	118.30
1	E	48	LEU	CB-CG-CD2	-5.17	102.20	111.00
1	A	107	LEU	CA-CB-CG	5.17	127.18	115.30
1	C	190	LEU	CB-CG-CD2	5.15	119.76	111.00
1	F	129	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	C	187	THR	N-CA-CB	-5.12	100.56	110.30
1	K	107	LEU	CA-CB-CG	5.12	127.08	115.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	148	ASP	CB-CG-OD2	5.12	122.91	118.30
1	H	305	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	C	158	VAL	CB-CA-C	-5.09	101.72	111.40
1	A	115	VAL	CA-CB-CG2	5.09	118.53	110.90
1	E	104	LEU	CB-CG-CD1	5.09	119.65	111.00
1	B	238	ASP	CB-CG-OD2	5.06	122.86	118.30
1	F	481	ASP	CB-CG-OD2	5.05	122.84	118.30
1	F	350	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	K	48	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	493	ILE	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3791	0	3743	61	0
1	B	3791	0	3743	57	0
1	C	3793	0	3742	53	0
1	D	3787	0	3742	54	0
1	E	3781	0	3731	53	0
1	F	3794	0	3748	75	0
1	G	3781	0	3731	73	0
1	H	3787	0	3737	74	0
1	I	3788	0	3738	66	0
1	J	3788	0	3738	65	0
1	K	3773	0	3725	83	0
1	L	3764	0	3714	89	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	255	0	0	11	0
3	B	123	0	0	3	0
3	C	197	0	0	3	0
3	D	216	0	0	5	0
3	E	218	0	0	1	0
3	F	124	0	0	2	0
3	G	152	0	0	4	0
3	H	143	0	0	3	0
3	I	109	0	0	1	0
3	J	74	0	0	4	0
3	K	76	0	0	3	0
3	L	62	0	0	4	0
All	All	47191	0	44832	720	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 8.

All (720) 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:H:264:THR:CG2	1:H:264:THR:CB	1.75	1.63
1:G:264:THR:CB	1:G:264:THR:CG2	1.79	1.58
1:L:448:THR:HG23	3:L:627:HOH:O	1.60	1.02
1:D:88:TYR:CE2	3:D:689:HOH:O	2.12	1.01
1:I:173:MET:HE1	1:I:243:THR:HG21	1.48	0.92
1:L:32:ILE:HD12	1:L:58:ASP:OD1	1.70	0.91
1:F:127:ASN:HB3	3:F:716:HOH:O	1.69	0.91
1:L:327:VAL:HG11	1:L:381:PRO:HG2	1.53	0.89
1:J:357:GLN:O	1:J:361:GLU:HG3	1.73	0.88
1:G:243:THR:HB	1:G:266:GLU:HB2	1.57	0.86
1:A:443:LYS:HE2	3:A:740:HOH:O	1.77	0.84
1:C:9:LYS:H	1:C:103:GLN:HE22	1.25	0.83
1:C:66:ALA:HB1	1:C:187:THR:HG23	1.60	0.83
1:H:239:LYS:HZ3	1:H:262:HIS:HD2	1.28	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:TYR:CD2	1:E:88:TYR:CZ	2.68	0.81
1:A:127:ASN:HB3	3:A:805:HOH:O	1.80	0.81
1:D:88:TYR:CD2	3:D:689:HOH:O	2.29	0.81
1:K:9:LYS:H	1:K:103:GLN:HE22	1.28	0.81
1:F:66:ALA:HB1	1:F:187:THR:HG22	1.60	0.81
1:H:243:THR:HG21	3:H:634:HOH:O	1.81	0.80
1:F:438:HIS:HE1	1:L:438:HIS:HE1	1.29	0.80
1:L:191:LYS:HG2	1:L:220:VAL:O	1.82	0.79
1:E:9:LYS:H	1:E:103:GLN:HE22	1.29	0.79
1:C:239:LYS:HZ3	1:C:262:HIS:HD2	1.30	0.79
1:L:201:LEU:HD11	1:L:221:PRO:HG3	1.64	0.79
1:F:494:LYS:HG2	1:K:435:LYS:HE3	1.65	0.78
1:B:88:TYR:CD2	1:G:88:TYR:CE2	2.72	0.78
1:I:78:MET:HG2	1:I:82:GLU:HB2	1.63	0.78
1:D:127[A]:ASN:OD1	3:D:757:HOH:O	2.01	0.78
1:J:436:THR:HG21	3:J:671:HOH:O	1.81	0.78
1:F:188:ILE:HD13	1:F:190:LEU:HB2	1.66	0.77
1:B:88:TYR:CE2	1:G:88:TYR:CD2	2.73	0.77
1:G:243:THR:HG21	3:G:646:HOH:O	1.85	0.77
1:E:169:PHE:HB3	1:E:172:VAL:HG13	1.67	0.77
1:L:78:MET:HG2	1:L:82:GLU:HB2	1.66	0.76
1:C:494:LYS:HG3	1:E:435:LYS:HD3	1.67	0.76
1:F:243:THR:HB	1:F:266:GLU:HB2	1.67	0.76
1:H:9:LYS:H	1:H:103:GLN:HE22	1.32	0.76
1:A:438:HIS:HE1	1:E:438:HIS:HE1	1.33	0.76
1:A:88:TYR:CZ	1:D:88:TYR:CD2	2.74	0.75
1:K:433:ASN:HD22	1:K:436:THR:H	1.35	0.75
1:I:173:MET:CE	1:I:243:THR:HG21	2.16	0.75
1:K:59:ILE:HD13	1:K:231:ILE:HG13	1.67	0.75
1:D:258:GLU:OE1	3:D:812:HOH:O	2.06	0.74
1:E:66:ALA:O	1:E:187:THR:HG21	1.86	0.74
1:K:66:ALA:O	1:K:187:THR:HG21	1.87	0.74
1:G:387:VAL:CG1	1:G:394:VAL:HG11	2.17	0.73
1:A:105:GLU:OE1	1:A:199[B]:SER:OG	2.05	0.73
1:B:9:LYS:H	1:B:103:GLN:HE22	1.34	0.73
1:F:374:GLU:HB2	1:F:375:LYS:CD	2.19	0.73
1:G:126:GLU:HG2	3:G:708:HOH:O	1.88	0.73
1:A:9:LYS:H	1:A:103:GLN:HE22	1.37	0.73
1:H:88:TYR:CE2	1:I:88:TYR:CE2	2.77	0.73
1:H:107:LEU:HD13	1:H:333:MET:HG3	1.70	0.72
1:B:22:MET:HG2	1:B:221:PRO:HD2	1.70	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ASP:O	1:D:124:THR:HG23	1.88	0.72
1:G:239:LYS:HZ3	1:G:262:HIS:HD2	1.37	0.72
1:L:26:GLY:HA3	1:L:214:ASN:HD22	1.55	0.72
1:C:88:TYR:CE2	1:E:88:TYR:CD2	2.78	0.72
1:E:66:ALA:HB1	1:E:187:THR:HG23	1.72	0.72
1:G:245:SER:HG	1:G:248:THR:HG1	1.36	0.72
1:K:357:GLN:OE1	1:K:360:LYS:HE2	1.90	0.71
1:C:239:LYS:NZ	1:C:262:HIS:HD2	1.88	0.71
1:A:19:GLU:OE2	3:A:834:HOH:O	2.07	0.71
1:G:188:ILE:HD11	1:G:190:LEU:HB2	1.71	0.71
1:K:438:HIS:HD2	1:L:152:TYR:OH	1.72	0.71
1:D:9:LYS:H	1:D:103:GLN:HE22	1.38	0.70
1:C:66:ALA:O	1:C:187:THR:HG21	1.91	0.70
1:B:438:HIS:HE1	1:H:438:HIS:HE1	1.40	0.70
1:L:324:ALA:O	1:L:327:VAL:HG12	1.91	0.70
1:J:169:PHE:O	1:J:173:MET:HB2	1.91	0.69
1:L:191:LYS:HD3	1:L:192:PRO:O	1.91	0.69
1:B:239:LYS:HZ3	1:B:262:HIS:HD2	1.41	0.69
1:C:88:TYR:CE2	1:E:88:TYR:CE2	2.80	0.69
1:G:78:MET:HG2	1:G:82:GLU:HB2	1.74	0.69
1:B:342:LEU:HD22	1:B:379:VAL:HG13	1.74	0.69
1:I:9:LYS:H	1:I:103:GLN:HE22	1.40	0.68
1:J:308:VAL:HG21	1:J:316:VAL:HG21	1.74	0.68
1:B:433:ASN:HD22	1:B:436:THR:H	1.41	0.68
1:A:120:ASP:O	1:A:124:THR:HG23	1.93	0.68
1:F:9:LYS:H	1:F:103:GLN:HE22	1.42	0.68
1:J:169:PHE:HB3	1:J:172:VAL:HG13	1.76	0.68
1:J:139:ILE:HD12	1:K:141:GLN:HG2	1.76	0.68
1:J:433:ASN:HB3	1:J:436:THR:HG23	1.76	0.68
1:A:264:THR:HB	3:A:730:HOH:O	1.94	0.67
1:G:438:HIS:HE1	1:I:438:HIS:HE1	1.41	0.67
1:L:433:ASN:HB3	1:L:436:THR:HG23	1.75	0.67
1:F:374:GLU:HB2	1:F:375:LYS:HD2	1.76	0.67
1:H:66:ALA:O	1:H:187:THR:HG21	1.95	0.67
1:K:12:VAL:HG11	1:K:103:GLN:HE21	1.58	0.67
1:J:433:ASN:HD22	1:J:436:THR:HG22	1.58	0.67
1:E:124:THR:HG21	1:E:171:LEU:HD13	1.77	0.66
1:L:66:ALA:O	1:L:187:THR:HG21	1.95	0.66
1:B:308:VAL:HG21	1:B:316:VAL:HG21	1.78	0.66
1:A:438:HIS:CE1	1:E:438:HIS:HE1	2.13	0.66
1:D:433:ASN:HD22	1:D:436:THR:H	1.44	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:243:THR:HB	1:L:266:GLU:HB2	1.77	0.66
1:A:88:TYR:CD1	3:A:821:HOH:O	2.48	0.66
1:D:107:LEU:HD13	1:D:333:MET:HG3	1.77	0.66
1:H:88:TYR:CZ	1:I:88:TYR:CD2	2.84	0.66
1:C:438:HIS:HE1	1:D:438:HIS:HE1	1.43	0.65
1:E:387:VAL:CG1	1:E:394:VAL:HG11	2.27	0.65
1:K:266:GLU:OE1	1:K:464:GLY:HA2	1.96	0.65
1:H:66:ALA:HB1	1:H:187:THR:HG23	1.78	0.65
1:E:239:LYS:HZ3	1:E:262:HIS:HD2	1.42	0.65
1:I:239:LYS:HZ3	1:I:262:HIS:HD2	1.45	0.65
1:K:254:ARG:HG2	1:L:254:ARG:HG3	1.78	0.65
1:I:364:THR:HG23	1:I:386:ASP:HB2	1.79	0.65
1:A:239:LYS:NZ	1:A:262:HIS:HD2	1.94	0.64
1:E:277:GLU:O	1:E:312:HIS:HE1	1.80	0.64
1:F:494:LYS:HG2	1:K:435:LYS:CE	2.28	0.64
1:A:88:TYR:CE2	1:D:88:TYR:CE2	2.85	0.64
1:J:356:GLU:O	1:J:360:LYS:HG2	1.98	0.64
1:H:243:THR:HB	1:H:266:GLU:HB2	1.79	0.64
1:A:277:GLU:OE2	1:A:311:LYS:HE3	1.98	0.64
1:B:438:HIS:CE1	1:H:438:HIS:HE1	2.15	0.64
1:F:438:HIS:CE1	1:L:438:HIS:HE1	2.13	0.64
1:B:448:THR:HG23	3:B:632:HOH:O	1.97	0.64
1:I:22:MET:HG3	1:I:221:PRO:HD2	1.80	0.64
1:E:120:ASP:O	1:E:124:THR:HG23	1.98	0.63
1:H:120:ASP:O	1:H:124:THR:HG23	1.98	0.63
1:B:78:MET:HG2	1:B:82:GLU:HB2	1.80	0.63
1:J:259:MET:SD	1:J:261:LYS:HE3	2.38	0.63
1:C:88:TYR:CD2	1:E:88:TYR:CE2	2.86	0.62
1:A:88:TYR:CD2	1:D:88:TYR:CE2	2.87	0.62
1:L:239:LYS:HD2	1:L:482:ASN:O	2.00	0.62
1:E:239:LYS:NZ	1:E:262:HIS:HD2	1.97	0.62
1:B:158:VAL:HG12	1:B:485:GLU:HG2	1.80	0.61
1:A:433:ASN:HD22	1:A:436:THR:H	1.46	0.61
1:G:127:ASN:HB3	3:G:723:HOH:O	2.00	0.61
1:G:264:THR:CG2	1:G:264:THR:CA	2.77	0.61
1:J:387:VAL:HG13	1:J:394:VAL:HG21	1.82	0.61
1:H:436:THR:HG21	3:H:736:HOH:O	2.00	0.61
1:K:438:HIS:CD2	1:L:152:TYR:OH	2.52	0.61
1:F:374:GLU:CB	1:F:375:LYS:HD2	2.29	0.61
1:F:374:GLU:HB2	1:F:375:LYS:HD3	1.82	0.61
1:L:387:VAL:CG1	1:L:394:VAL:CG2	2.78	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:370:GLU:HG2	1:G:380:LYS:HD2	1.80	0.61
1:D:239:LYS:HZ3	1:D:262:HIS:HD2	1.49	0.61
1:J:239:LYS:NZ	1:J:262:HIS:HD2	1.98	0.61
1:A:88:TYR:CE1	3:A:821:HOH:O	2.53	0.61
1:F:66:ALA:HB1	1:F:187:THR:CG2	2.30	0.61
1:B:88:TYR:CE2	1:G:88:TYR:CE2	2.88	0.61
1:J:178:MET:HG2	1:J:188:ILE:HD12	1.82	0.61
1:H:277:GLU:O	1:H:312:HIS:HE1	1.84	0.60
1:H:48:LEU:HD11	1:H:107:LEU:HB3	1.83	0.60
1:C:433:ASN:HD22	1:C:436:THR:H	1.49	0.60
1:I:126:GLU:HG3	3:I:690:HOH:O	2.01	0.60
1:G:387:VAL:HG11	1:G:404:VAL:HG11	1.83	0.60
1:H:264:THR:CA	1:H:264:THR:CG2	2.74	0.60
1:B:308:VAL:HG21	1:B:316:VAL:CG2	2.32	0.60
1:H:88:TYR:CD2	1:I:88:TYR:CE2	2.90	0.60
1:I:433:ASN:HD22	1:I:436:THR:H	1.48	0.60
1:F:124:THR:HG21	1:F:171:LEU:HD13	1.83	0.59
1:F:188:ILE:HD12	1:F:188:ILE:C	2.23	0.59
1:J:173:MET:HG3	3:J:646:HOH:O	2.02	0.59
1:J:387:VAL:HG13	1:J:394:VAL:CG2	2.32	0.59
1:D:190:LEU:HD12	1:D:200:LEU:HD21	1.85	0.59
1:H:239:LYS:NZ	1:H:262:HIS:HD2	2.01	0.59
1:I:78:MET:HG2	1:I:82:GLU:CB	2.32	0.59
1:K:105:GLU:OE1	1:K:199:SER:HB3	2.02	0.59
1:F:235:HIS:HA	1:F:259:MET:CE	2.33	0.59
1:F:447:GLY:HA3	1:F:464:GLY:O	2.02	0.59
1:J:9:LYS:H	1:J:103:GLN:HE22	1.48	0.59
1:A:257:ALA:HA	1:C:253:MET:HE3	1.84	0.59
1:D:364:THR:CG2	1:D:386:ASP:OD2	2.51	0.59
1:F:163:GLN:HB2	1:F:190:LEU:HD23	1.85	0.59
1:F:88:TYR:CD2	1:K:88:TYR:CZ	2.91	0.59
1:L:163:GLN:HB2	1:L:190:LEU:HD23	1.84	0.59
1:L:78:MET:HG2	1:L:82:GLU:CB	2.32	0.58
1:J:239:LYS:HZ3	1:J:262:HIS:HD2	1.48	0.58
1:L:277:GLU:O	1:L:312:HIS:HE1	1.87	0.58
1:I:120:ASP:O	1:I:124:THR:HG23	2.03	0.58
1:C:239:LYS:NZ	1:C:262:HIS:CD2	2.71	0.58
1:F:84:ALA:HB2	1:F:135:THR:OG1	2.03	0.58
1:K:260:ILE:HD12	1:L:468:GLN:HB3	1.86	0.58
1:D:67:ARG:O	1:D:71:GLU:HG3	2.03	0.58
1:L:239:LYS:HZ3	1:L:264:THR:HG23	1.68	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:163:GLN:OE1	1:G:188:ILE:CD1	2.51	0.57
1:L:239:LYS:NZ	1:L:264:THR:HG23	2.19	0.57
1:L:447:GLY:HA3	1:L:464:GLY:O	2.05	0.57
1:D:239:LYS:NZ	1:D:262:HIS:HD2	2.02	0.57
1:G:178:MET:HG2	1:G:188:ILE:HD13	1.86	0.57
1:H:433:ASN:HD22	1:H:436:THR:H	1.52	0.57
1:J:492:ASN:ND2	1:J:494:LYS:H	2.02	0.57
1:F:158:VAL:HG12	1:F:485:GLU:HG2	1.87	0.57
1:H:84:ALA:HB2	1:H:135:THR:OG1	2.04	0.57
1:B:120:ASP:O	1:B:124:THR:HG23	2.04	0.57
1:K:19:GLU:OE1	3:K:638:HOH:O	2.17	0.57
1:H:391:MET:HB2	1:H:394:VAL:CG1	2.35	0.56
1:L:387:VAL:CG1	1:L:394:VAL:HG21	2.35	0.56
1:A:239:LYS:HZ1	1:A:264:THR:HG22	1.69	0.56
1:G:239:LYS:NZ	1:G:262:HIS:HD2	2.02	0.56
1:G:112:PRO:HB2	1:G:115:VAL:HG13	1.87	0.56
1:G:88:TYR:CE1	1:G:129:ARG:HG2	2.41	0.56
1:H:350:ARG:NH1	3:H:664:HOH:O	2.29	0.56
1:K:66:ALA:HB1	1:K:187:THR:HG23	1.86	0.56
1:H:371:ARG:HD3	1:H:372:ALA:N	2.20	0.56
1:J:364:THR:HG23	1:J:386:ASP:HB2	1.87	0.56
1:G:357:GLN:HE22	1:G:360:LYS:HE3	1.71	0.56
1:B:124:THR:HG22	1:B:172:VAL:HA	1.87	0.56
1:I:374:GLU:HB2	1:I:375:LYS:HE3	1.88	0.56
1:L:26:GLY:HA3	1:L:214:ASN:ND2	2.20	0.56
1:C:494:LYS:HG3	1:E:435:LYS:CD	2.36	0.55
1:F:194:SER:OG	1:F:223:PHE:CE1	2.54	0.55
1:D:22:MET:CG	1:D:221:PRO:HD2	2.36	0.55
1:J:433:ASN:HD22	1:J:436:THR:CG2	2.18	0.55
1:G:191:LYS:HG2	1:G:220:VAL:O	2.07	0.55
1:I:112:PRO:HB2	1:I:115:VAL:HG13	1.86	0.55
1:G:9:LYS:H	1:G:103:GLN:HE22	1.52	0.55
1:J:78:MET:SD	1:J:83:ARG:HG2	2.47	0.55
1:C:124:THR:HG21	1:C:171:LEU:HD13	1.88	0.55
1:F:235:HIS:HA	1:F:259:MET:HE2	1.87	0.55
1:F:75:TRP:CZ2	1:F:83:ARG:HD2	2.42	0.55
1:G:438:HIS:HE1	1:I:438:HIS:CE1	2.25	0.55
1:L:405:VAL:C	1:L:406:LEU:HD23	2.27	0.55
1:A:484:THR:HG22	3:A:657:HOH:O	2.05	0.55
1:D:235:HIS:HB2	1:D:259:MET:HE3	1.88	0.55
1:C:361:GLU:OE1	3:C:717:HOH:O	2.18	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:LYS:NZ	1:B:262:HIS:HD2	2.03	0.55
1:C:364:THR:HG23	1:C:386:ASP:HB2	1.89	0.55
1:C:78:MET:HG3	1:C:82:GLU:HB2	1.90	0.54
1:E:9:LYS:H	1:E:103:GLN:NE2	2.03	0.54
1:G:387:VAL:CG1	1:G:394:VAL:CG1	2.85	0.54
1:A:260:ILE:HA	1:C:253:MET:HE1	1.88	0.54
1:G:176:TRP:CZ2	1:G:475:LEU:HD11	2.42	0.54
1:C:438:HIS:CE1	1:D:438:HIS:HE1	2.26	0.54
1:K:70:PHE:CZ	1:K:159:GLY:HA2	2.42	0.54
1:G:433:ASN:HD22	1:G:436:THR:H	1.55	0.54
1:H:169:PHE:HB3	1:H:172:VAL:HG22	1.90	0.54
1:J:438:HIS:CE1	1:K:438:HIS:HE1	2.25	0.54
1:F:282:GLU:HA	1:F:282:GLU:OE2	2.07	0.54
1:H:177:LYS:HZ1	1:H:243:THR:HG22	1.72	0.54
1:G:84:ALA:HB2	1:G:135:THR:OG1	2.08	0.54
1:K:26:GLY:HA3	1:K:214:ASN:ND2	2.23	0.54
1:C:48:LEU:HD11	1:C:107:LEU:HB3	1.90	0.54
1:B:492:ASN:C	1:B:492:ASN:HD22	2.11	0.53
1:F:177:LYS:HZ1	1:F:243:THR:HG22	1.73	0.53
1:A:76:ALA:O	1:E:147:LYS:HD3	2.09	0.53
1:K:285:ILE:HG12	1:K:316:VAL:HB	1.89	0.53
1:C:9:LYS:H	1:C:103:GLN:NE2	1.99	0.53
1:K:84:ALA:HB2	1:K:135:THR:OG1	2.08	0.53
1:F:239:LYS:HZ3	1:F:262:HIS:HD2	1.55	0.53
1:L:8:LEU:HA	1:L:103:GLN:HE22	1.73	0.53
1:A:290:GLN:CG	3:A:850:HOH:O	2.57	0.53
1:F:492:ASN:ND2	1:F:494:LYS:H	2.07	0.53
1:L:191:LYS:CG	1:L:220:VAL:O	2.57	0.53
1:C:494:LYS:HE3	1:E:439:GLN:OE1	2.09	0.53
1:F:9:LYS:H	1:F:103:GLN:NE2	2.07	0.53
1:J:448:THR:CG2	3:J:669:HOH:O	2.55	0.53
1:K:364:THR:CG2	1:K:386:ASP:OD2	2.57	0.53
1:E:59:ILE:HD12	1:E:231:ILE:CG1	2.38	0.52
1:I:48:LEU:HD11	1:I:107:LEU:HB3	1.90	0.52
1:F:438:HIS:HD2	1:J:152:TYR:OH	1.92	0.52
1:F:346:LYS:O	1:F:350:ARG:HG3	2.09	0.52
1:D:364:THR:HG23	1:D:386:ASP:OD2	2.09	0.52
1:E:107:LEU:HD13	1:E:333:MET:HG3	1.91	0.52
1:A:239:LYS:HZ1	1:A:264:THR:CG2	2.22	0.52
1:A:78:MET:HG2	1:A:82:GLU:HB2	1.92	0.52
1:E:387:VAL:HG13	1:E:394:VAL:CG1	2.40	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:433:ASN:HD22	1:F:436:THR:H	1.57	0.52
1:G:253:MET:HG3	1:G:265:LEU:HD11	1.90	0.52
1:I:107:LEU:HD13	1:I:333:MET:HG3	1.92	0.52
1:K:59:ILE:HD12	1:K:230:ALA:HB3	1.92	0.52
1:A:88:TYR:CE2	1:D:88:TYR:CD2	2.97	0.52
1:C:415:ILE:HD13	1:C:443:LYS:HD2	1.91	0.52
1:I:163:GLN:HB2	1:I:190:LEU:HD23	1.92	0.52
1:I:190:LEU:HD12	1:I:200:LEU:HD21	1.92	0.52
1:K:364:THR:HG21	1:K:386:ASP:OD2	2.09	0.52
1:G:124:THR:HG21	1:G:171:LEU:HD13	1.91	0.52
1:B:387:VAL:HG13	1:B:394:VAL:HG11	1.91	0.52
1:E:188:ILE:CD1	1:E:190:LEU:HB2	2.39	0.52
1:A:492:ASN:C	1:A:492:ASN:HD22	2.13	0.52
1:B:48:LEU:HD11	1:B:107:LEU:HB3	1.92	0.52
1:C:84:ALA:HB2	1:C:135:THR:OG1	2.09	0.52
1:D:190:LEU:HD12	1:D:200:LEU:CD2	2.39	0.52
1:E:387:VAL:CG1	1:E:394:VAL:CG1	2.88	0.51
1:I:166:PRO:HD3	1:I:243:THR:HB	1.91	0.51
1:L:251:TYR:O	1:L:255:GLN:HG2	2.10	0.51
1:I:105:GLU:HA	1:I:105:GLU:OE1	2.10	0.51
1:K:188:ILE:CD1	1:K:190:LEU:HB2	2.41	0.51
1:E:492:ASN:ND2	1:E:494:LYS:H	2.09	0.51
1:J:438:HIS:HE1	1:K:438:HIS:HE1	1.58	0.51
1:K:12:VAL:HG11	1:K:103:GLN:NE2	2.24	0.51
1:F:492:ASN:C	1:F:492:ASN:HD22	2.14	0.51
1:G:357:GLN:HE22	1:G:360:LYS:CE	2.23	0.51
1:J:329:LEU:HD12	1:J:339:MET:HB3	1.91	0.51
1:J:107:LEU:HD13	1:J:333:MET:HG3	1.92	0.51
1:F:88:TYR:CE2	1:K:88:TYR:CE2	2.99	0.51
1:F:438:HIS:HE1	1:L:438:HIS:CE1	2.19	0.51
1:H:387:VAL:CG1	1:H:394:VAL:HG11	2.40	0.51
1:A:277:GLU:OE2	1:A:311:LYS:CE	2.57	0.51
1:E:387:VAL:HG13	1:E:394:VAL:HG11	1.92	0.51
1:I:243:THR:HG23	1:I:266:GLU:HB3	1.92	0.51
1:K:492:ASN:ND2	1:K:494:LYS:H	2.09	0.51
1:B:342:LEU:HD22	1:B:379:VAL:CG1	2.39	0.51
1:D:163:GLN:HB2	1:D:190:LEU:HD23	1.92	0.51
1:D:364:THR:HG23	1:D:386:ASP:HB2	1.93	0.51
1:G:438:HIS:CE1	1:I:438:HIS:HE1	2.24	0.51
1:K:372:ALA:HB2	1:K:380:LYS:HG3	1.93	0.51
1:L:239:LYS:NZ	1:L:262:HIS:HD2	2.08	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:GLU:O	1:B:103:GLN:HG3	2.10	0.51
1:H:387:VAL:CG1	1:H:394:VAL:CG1	2.89	0.51
1:K:254:ARG:HG2	1:L:254:ARG:CG	2.40	0.51
1:L:327:VAL:HG13	1:L:327:VAL:O	2.10	0.51
1:B:22:MET:CG	1:B:221:PRO:HD2	2.41	0.51
1:E:364:THR:CG2	1:E:386:ASP:OD2	2.59	0.51
1:F:188:ILE:CD1	1:F:190:LEU:HB2	2.38	0.51
1:H:388:THR:O	1:H:394:VAL:HG11	2.11	0.51
1:I:84:ALA:HB2	1:I:135:THR:OG1	2.11	0.51
1:I:239:LYS:NZ	1:I:262:HIS:HD2	2.08	0.51
1:B:78:MET:SD	1:B:83:ARG:HG2	2.51	0.50
1:L:66:ALA:HB1	1:L:187:THR:HG23	1.93	0.50
1:L:9:LYS:H	1:L:103:GLN:HE22	1.57	0.50
1:G:152:TYR:OH	1:H:438:HIS:HD2	1.94	0.50
1:L:235:HIS:HA	1:L:259:MET:SD	2.51	0.50
1:D:253:MET:HG3	1:D:265:LEU:HD11	1.93	0.50
1:E:59:ILE:CD1	1:E:220:VAL:HG21	2.42	0.50
1:J:149:TYR:CD1	1:J:492:ASN:HA	2.46	0.50
1:K:26:GLY:HA3	1:K:214:ASN:HD22	1.77	0.50
1:K:67:ARG:O	1:K:71:GLU:HG2	2.10	0.50
1:B:484:THR:HG21	3:B:635:HOH:O	2.11	0.50
1:C:492:ASN:HD22	1:C:492:ASN:C	2.15	0.50
1:D:18:GLU:HG3	3:D:711:HOH:O	2.12	0.50
1:F:312:HIS:O	1:F:316:VAL:HG13	2.11	0.50
1:I:415:ILE:HD13	1:I:443:LYS:HD2	1.93	0.50
1:K:21:LYS:HE2	1:K:29:VAL:HA	1.92	0.50
1:I:374:GLU:HB2	1:I:375:LYS:CE	2.41	0.50
1:A:112:PRO:HB2	1:A:115:VAL:HG13	1.94	0.50
1:A:178:MET:HG2	1:A:188:ILE:HD13	1.94	0.50
1:F:112:PRO:HB2	1:F:115:VAL:HG13	1.94	0.50
1:B:148:ASP:HB3	1:B:494:LYS:HG3	1.93	0.50
1:E:253:MET:HE2	1:E:265:LEU:HD11	1.92	0.50
1:K:120:ASP:O	1:K:124:THR:HG23	2.11	0.50
1:L:254:ARG:O	1:L:257:ALA:HB3	2.12	0.50
1:C:239:LYS:HZ3	1:C:262:HIS:CD2	2.19	0.50
1:G:163:GLN:OE1	1:G:188:ILE:HD12	2.12	0.50
1:H:120:ASP:O	1:H:124:THR:CG2	2.60	0.50
1:G:169:PHE:HB3	1:G:172:VAL:HG13	1.94	0.50
1:K:178:MET:HG2	1:K:188:ILE:HD13	1.93	0.50
1:E:201:LEU:HD11	1:E:221:PRO:HG3	1.93	0.49
1:J:9:LYS:HB2	1:J:12:VAL:HG13	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:492:ASN:C	1:L:492:ASN:HD22	2.15	0.49
1:B:438:HIS:HD2	1:I:152:TYR:OH	1.95	0.49
1:G:153:THR:HA	1:G:487:LYS:O	2.12	0.49
1:K:239:LYS:HZ3	1:K:262:HIS:HD2	1.58	0.49
1:G:78:MET:SD	1:G:83:ARG:HG2	2.52	0.49
1:H:264:THR:HA	1:H:264:THR:CG2	2.41	0.49
1:H:364:THR:CG2	1:H:386:ASP:OD2	2.60	0.49
1:L:105:GLU:OE1	1:L:199:SER:OG	2.21	0.49
1:B:84:ALA:HB2	1:B:135:THR:OG1	2.13	0.49
1:H:124:THR:HG21	1:H:171:LEU:HD13	1.94	0.49
1:J:190:LEU:HD12	1:J:200:LEU:CD2	2.42	0.49
1:K:433:ASN:HD21	1:K:435:LYS:HB2	1.78	0.49
1:K:85:HIS:CE1	1:K:89:LYS:HE2	2.47	0.49
1:K:391:MET:HB2	1:K:394:VAL:HG13	1.94	0.49
1:K:98:ARG:CZ	1:K:117:LEU:HD11	2.43	0.49
1:L:327:VAL:HG11	1:L:381:PRO:CG	2.36	0.49
1:C:447:GLY:HA3	1:C:464:GLY:O	2.12	0.49
1:J:161:VAL:O	1:J:161:VAL:HG13	2.12	0.49
1:K:327:VAL:HG22	1:K:329:LEU:CD2	2.43	0.49
1:C:372:ALA:HB2	1:C:380:LYS:HG3	1.95	0.49
1:G:391:MET:HB2	1:G:394:VAL:HG13	1.95	0.49
1:F:317:VAL:HG22	1:F:405:VAL:HG11	1.95	0.49
1:L:464:GLY:HA3	1:L:473:ARG:HD3	1.94	0.49
1:B:9:LYS:H	1:B:103:GLN:NE2	2.06	0.49
1:G:177:LYS:HZ1	1:G:243:THR:CG2	2.25	0.49
1:L:387:VAL:HG11	1:L:394:VAL:CG2	2.42	0.49
1:I:163:GLN:CB	1:I:190:LEU:HD23	2.42	0.48
1:A:35:LYS:HG3	3:A:696:HOH:O	2.13	0.48
1:E:59:ILE:HD12	1:E:231:ILE:HG12	1.95	0.48
1:G:277:GLU:O	1:G:312:HIS:HE1	1.95	0.48
1:G:471:ILE:HG13	1:H:260:ILE:HG22	1.95	0.48
1:H:92:ASP:O	1:H:96:GLU:HG3	2.13	0.48
1:I:156:GLU:O	1:I:484:THR:HA	2.13	0.48
1:J:161:VAL:HG12	1:J:187:THR:O	2.12	0.48
1:K:161:VAL:HG21	1:K:483:TYR:CE1	2.48	0.48
1:L:493:ILE:O	1:L:494:LYS:HB2	2.13	0.48
1:B:178:MET:HG2	1:B:188:ILE:HD13	1.94	0.48
1:G:107:LEU:HD13	1:G:333:MET:HG3	1.94	0.48
1:I:191:LYS:HG2	1:I:220:VAL:O	2.13	0.48
1:F:35:LYS:HB2	3:F:701:HOH:O	2.12	0.48
1:B:372:ALA:HB2	1:B:380:LYS:HG3	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:78:MET:HG2	1:G:82:GLU:CB	2.42	0.48
1:H:387:VAL:HG12	1:H:394:VAL:HG11	1.96	0.48
1:J:190:LEU:HD12	1:J:200:LEU:HD21	1.95	0.48
1:K:433:ASN:ND2	1:K:436:THR:HG23	2.28	0.48
1:L:173:MET:HE2	1:L:173:MET:HA	1.95	0.48
1:L:259:MET:HE2	1:L:261:LYS:HE2	1.95	0.48
1:D:492:ASN:C	1:D:492:ASN:HD22	2.16	0.48
1:E:350:ARG:HD3	3:E:657:HOH:O	2.13	0.48
1:H:59:ILE:HG13	1:H:230:ALA:HB3	1.95	0.48
1:K:357:GLN:O	1:K:361:GLU:HB2	2.14	0.48
1:L:290:GLN:HB3	3:L:613:HOH:O	2.13	0.48
1:B:190:LEU:CD1	1:B:200:LEU:CD2	2.92	0.48
1:D:22:MET:HG2	1:D:221:PRO:HD2	1.96	0.48
1:E:492:ASN:HD22	1:E:492:ASN:C	2.17	0.48
1:F:296:HIS:N	1:F:296:HIS:CD2	2.81	0.48
1:H:9:LYS:H	1:H:103:GLN:NE2	2.08	0.48
1:J:165:ILE:HG22	1:J:177:LYS:HE2	1.96	0.48
1:A:21:LYS:NZ	3:A:834:HOH:O	2.22	0.48
1:C:165:ILE:HB	1:C:166:PRO:HD2	1.96	0.48
1:D:22:MET:HG3	1:D:221:PRO:HD2	1.95	0.48
1:G:177:LYS:NZ	1:G:243:THR:CG2	2.77	0.48
1:B:391:MET:HB2	1:B:394:VAL:HG13	1.94	0.48
1:B:438:HIS:HE1	1:H:438:HIS:CE1	2.26	0.48
1:C:107:LEU:HD13	1:C:333:MET:HG3	1.95	0.48
1:H:177:LYS:HZ1	1:H:243:THR:CG2	2.25	0.48
1:H:328:LYS:HE3	1:H:336:GLU:HB3	1.96	0.48
1:K:112:PRO:HB2	1:K:115:VAL:HG13	1.94	0.47
1:K:246:THR:HG22	1:K:250:LYS:HE3	1.96	0.47
1:K:325:ASN:HD21	1:K:367:ALA:HB1	1.78	0.47
1:L:194:SER:HB3	1:L:222:GLY:O	2.14	0.47
1:C:78:MET:HG3	1:C:82:GLU:CB	2.43	0.47
1:C:88:TYR:CZ	1:C:129:ARG:HG2	2.49	0.47
1:D:103:GLN:O	1:D:107:LEU:HD22	2.14	0.47
1:K:75:TRP:CH2	1:K:83:ARG:HG3	2.49	0.47
1:F:142:THR:OG1	1:L:140:GLY:HA3	2.15	0.47
1:A:78:MET:SD	1:A:83:ARG:HG2	2.54	0.47
1:D:78:MET:HG2	1:D:82:GLU:CB	2.45	0.47
1:I:451:ILE:O	1:I:452:ASN:HB2	2.14	0.47
1:K:351:VAL:CG2	1:K:379:VAL:HG21	2.45	0.47
1:F:280:ASP:HB2	1:F:432:GLN:OE1	2.15	0.47
1:H:239:LYS:HZ3	1:H:262:HIS:CD2	2.19	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:277:GLU:O	1:I:312:HIS:HE1	1.96	0.47
1:E:59:ILE:HD11	1:E:220:VAL:HG21	1.95	0.47
1:F:99:GLU:O	1:F:103:GLN:HG3	2.14	0.47
1:G:177:LYS:HZ1	1:G:243:THR:HG22	1.78	0.47
1:I:9:LYS:H	1:I:103:GLN:NE2	2.09	0.47
1:C:9:LYS:N	1:C:103:GLN:HE22	2.02	0.47
1:F:438:HIS:CE1	1:L:438:HIS:CE1	3.00	0.47
1:G:188:ILE:CD1	1:G:190:LEU:HB2	2.43	0.47
1:G:357:GLN:NE2	1:G:360:LYS:HE3	2.29	0.47
1:H:135:THR:HG22	1:H:183:ALA:HA	1.95	0.47
1:I:135:THR:HG22	1:I:183:ALA:HA	1.96	0.47
1:B:492:ASN:HD21	1:B:494:LYS:HB2	1.79	0.47
1:D:364:THR:HG21	1:D:386:ASP:OD2	2.14	0.47
1:L:163:GLN:CB	1:L:190:LEU:HD23	2.43	0.47
1:L:78:MET:SD	1:L:83:ARG:HG2	2.54	0.47
1:F:88:TYR:CE2	1:K:88:TYR:CD2	3.03	0.47
1:B:78:MET:HG2	1:B:82:GLU:CB	2.45	0.47
1:C:438:HIS:HE1	1:D:438:HIS:CE1	2.27	0.47
1:F:147:LYS:HD2	1:L:76:ALA:O	2.14	0.47
1:G:387:VAL:HG11	1:G:394:VAL:CG1	2.45	0.47
1:I:296:HIS:CD2	1:I:296:HIS:N	2.83	0.47
1:J:448:THR:HG23	3:J:669:HOH:O	2.15	0.47
1:J:173:MET:CE	1:J:173:MET:HA	2.45	0.47
1:E:391:MET:HB2	1:E:394:VAL:HG13	1.97	0.47
1:K:172:VAL:HG13	3:K:641:HOH:O	2.15	0.47
1:K:43:ALA:HB2	3:K:642:HOH:O	2.14	0.47
1:A:8:LEU:HB3	1:A:13:GLU:OE2	2.15	0.46
1:F:493:ILE:HA	1:K:435:LYS:HG3	1.96	0.46
1:I:364:THR:HG21	1:I:386:ASP:OD2	2.15	0.46
1:L:134:TRP:O	1:L:138:ILE:HG13	2.15	0.46
1:A:290:GLN:HG3	3:A:850:HOH:O	2.13	0.46
1:H:163:GLN:OE1	1:H:188:ILE:HD13	2.14	0.46
1:H:88:TYR:CD2	1:I:88:TYR:CZ	3.04	0.46
1:J:347:GLN:O	1:J:351:VAL:HG13	2.14	0.46
1:L:228:GLY:O	1:L:232:VAL:HG12	2.15	0.46
1:A:439:GLN:HE22	1:D:494:LYS:HE3	1.80	0.46
1:E:9:LYS:CE	1:E:99:GLU:OE2	2.62	0.46
1:A:277:GLU:O	1:A:312:HIS:HE1	1.99	0.46
1:C:75:TRP:CH2	1:C:83:ARG:HG3	2.51	0.46
1:G:19:GLU:OE1	3:G:743:HOH:O	2.21	0.46
1:A:239:LYS:HZ3	1:A:262:HIS:HD2	1.61	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:LYS:HE2	1:C:482:ASN:O	2.16	0.46
1:D:9:LYS:H	1:D:103:GLN:NE2	2.09	0.46
1:H:67:ARG:O	1:H:71:GLU:HG3	2.15	0.46
1:I:124:THR:HG21	1:I:171:LEU:HB3	1.98	0.46
1:L:153:THR:HA	1:L:487:LYS:O	2.15	0.46
1:B:207:PHE:CD2	1:B:217:VAL:HG11	2.50	0.46
1:H:296:HIS:N	1:H:296:HIS:CD2	2.84	0.46
1:J:492:ASN:C	1:J:492:ASN:HD22	2.19	0.46
1:C:126:GLU:HG3	3:C:731:HOH:O	2.15	0.46
1:K:242:PHE:CZ	1:K:248:THR:HB	2.50	0.46
1:L:9:LYS:NZ	1:L:99:GLU:OE2	2.47	0.46
1:C:434:ILE:HB	1:D:434:ILE:HA	1.98	0.46
1:I:272:PRO:HG3	1:I:418:ALA:HB1	1.98	0.46
1:J:48:LEU:HD11	1:J:107:LEU:HB3	1.98	0.46
1:J:296:HIS:CD2	1:J:296:HIS:N	2.84	0.46
1:H:124:THR:HG22	1:H:172:VAL:HG12	1.97	0.45
1:H:149:TYR:CD1	1:H:492:ASN:HA	2.51	0.45
1:A:124:THR:HG22	1:A:172:VAL:HA	1.98	0.45
1:A:308:VAL:HG11	1:A:316:VAL:HG13	1.97	0.45
1:E:188:ILE:HG12	1:E:217:VAL:HG22	1.98	0.45
1:F:75:TRP:CH2	1:F:83:ARG:HD2	2.51	0.45
1:H:75:TRP:CZ3	1:H:83:ARG:HG2	2.51	0.45
1:J:59:ILE:HD12	1:J:220:VAL:HG21	1.99	0.45
1:K:9:LYS:H	1:K:103:GLN:NE2	2.04	0.45
1:B:296:HIS:ND1	1:B:341:PRO:O	2.47	0.45
1:H:88:TYR:CG	1:I:88:TYR:CZ	3.05	0.45
1:K:289:PHE:CG	1:K:323:MET:HE2	2.51	0.45
1:H:364:THR:HG23	1:H:386:ASP:OD2	2.16	0.45
1:B:152:TYR:OH	1:I:438:HIS:HD2	1.99	0.45
1:K:188:ILE:HD12	1:K:190:LEU:HB2	1.98	0.45
1:L:342:LEU:CD2	1:L:351:VAL:HG21	2.46	0.45
1:F:44:THR:O	1:F:45:GLU:HB2	2.17	0.45
1:K:158:VAL:HG23	1:K:483:TYR:O	2.16	0.45
1:H:433:ASN:ND2	1:H:436:THR:HG23	2.31	0.45
1:J:166:PRO:HD2	1:J:173:MET:HG2	1.98	0.45
1:J:433:ASN:ND2	1:J:436:THR:HG22	2.28	0.45
1:L:254:ARG:NH1	1:L:255:GLN:OE1	2.49	0.45
1:C:492:ASN:ND2	1:C:494:LYS:H	2.14	0.45
1:G:188:ILE:HD11	1:G:190:LEU:HD12	1.98	0.45
1:H:85:HIS:HD2	1:I:88:TYR:OH	1.99	0.45
1:B:139:ILE:HD12	1:H:141:GLN:HG2	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:ASN:OD1	1:C:459:ALA:HB2	2.16	0.45
1:D:120:ASP:O	1:D:124:THR:CG2	2.61	0.45
1:J:433:ASN:HD21	1:J:435:LYS:HB2	1.82	0.45
1:K:188:ILE:HG12	1:K:217:VAL:HG22	1.99	0.45
1:A:239:LYS:HZ1	1:A:262:HIS:HD2	1.62	0.45
1:A:38:GLU:OE2	1:G:35:LYS:NZ	2.50	0.45
1:F:138:ILE:HG12	1:F:480:LEU:HD13	1.99	0.45
1:J:387:VAL:CG1	1:J:394:VAL:CG2	2.95	0.45
1:L:158:VAL:HG22	1:L:483:TYR:O	2.16	0.45
1:C:67:ARG:O	1:C:71:GLU:HG3	2.17	0.45
1:E:190:LEU:HD12	1:E:200:LEU:CD2	2.47	0.45
1:F:66:ALA:HA	1:F:187:THR:HG21	1.98	0.45
1:G:245:SER:OG	1:G:248:THR:OG1	2.08	0.45
1:G:264:THR:CG2	1:G:264:THR:OG1	2.54	0.45
1:B:239:LYS:HE2	1:B:482:ASN:O	2.18	0.44
1:D:161:VAL:HG22	1:D:188:ILE:HD13	1.98	0.44
1:H:201:LEU:HD11	1:H:221:PRO:HG3	1.99	0.44
1:I:447:GLY:HA3	1:I:464:GLY:O	2.17	0.44
1:E:364:THR:HG23	1:E:386:ASP:HB2	1.99	0.44
1:F:260:ILE:HA	1:J:253:MET:HE1	1.99	0.44
1:H:245:SER:OG	1:H:248:THR:HG23	2.17	0.44
1:H:78:MET:HG2	1:H:82:GLU:HB2	2.00	0.44
1:J:387:VAL:CG1	1:J:394:VAL:HG21	2.46	0.44
1:I:296:HIS:CD2	1:I:339:MET:HG3	2.52	0.44
1:I:464:GLY:HA3	1:I:473:ARG:HD3	1.98	0.44
1:A:239:LYS:HE2	1:A:482:ASN:O	2.18	0.44
1:D:78:MET:HG2	1:D:82:GLU:HB2	2.00	0.44
1:I:158:VAL:HG23	1:I:483:TYR:C	2.37	0.44
1:L:191:LYS:HA	1:L:192:PRO:HD2	1.88	0.44
1:A:152:TYR:OH	1:C:438:HIS:HD2	2.01	0.44
1:F:8:LEU:HA	1:F:103:GLN:HE22	1.81	0.44
1:G:177:LYS:NZ	1:G:474:GLU:OE2	2.49	0.44
1:K:217:VAL:HG13	1:K:219:PHE:CZ	2.53	0.44
1:L:190:LEU:HD22	1:L:191:LYS:N	2.33	0.44
1:L:484:THR:HG22	3:L:659:HOH:O	2.17	0.44
1:A:201:LEU:HD11	1:A:221:PRO:HG3	2.00	0.44
1:F:66:ALA:CA	1:F:187:THR:HG21	2.47	0.44
1:L:296:HIS:N	1:L:296:HIS:CD2	2.86	0.44
1:L:364:THR:CG2	1:L:386:ASP:OD2	2.65	0.44
1:A:438:HIS:HD2	1:C:152:TYR:OH	2.01	0.44
1:H:78:MET:SD	1:H:83:ARG:HG3	2.57	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:48:LEU:HD13	1:J:198:LEU:CD1	2.48	0.44
1:L:158:VAL:HG13	1:L:485:GLU:HG2	1.99	0.44
1:F:78:MET:HG2	1:F:82:GLU:HB3	2.00	0.44
1:F:88:TYR:CZ	1:K:88:TYR:CG	3.06	0.44
1:G:74:PRO:O	1:G:78:MET:HB2	2.18	0.44
1:H:292:ILE:HG12	1:H:403:VAL:HB	2.00	0.44
1:J:328:LYS:HE3	1:J:336:GLU:HB3	1.99	0.44
1:C:190:LEU:HD12	1:C:200:LEU:CD2	2.48	0.43
1:J:239:LYS:HE2	1:J:482:ASN:O	2.18	0.43
1:K:67:ARG:O	1:K:71:GLU:CG	2.66	0.43
1:L:351:VAL:CG2	1:L:379:VAL:HG21	2.47	0.43
1:I:190:LEU:HD12	1:I:200:LEU:CD2	2.48	0.43
1:J:251:TYR:O	1:J:255:GLN:HG2	2.17	0.43
1:K:277:GLU:OE2	1:K:311:LYS:NZ	2.36	0.43
1:G:264:THR:CG2	1:G:264:THR:HA	2.47	0.43
1:H:88:TYR:CE2	1:I:88:TYR:CD2	3.05	0.43
1:K:326:ASN:HD22	1:K:326:ASN:HA	1.60	0.43
1:K:364:THR:HG23	1:K:386:ASP:HB2	2.00	0.43
1:A:134:TRP:O	1:A:138:ILE:HG13	2.19	0.43
1:B:447:GLY:HA3	1:B:464:GLY:O	2.18	0.43
1:A:239:LYS:HZ1	1:A:262:HIS:CD2	2.35	0.43
1:B:190:LEU:CD1	1:B:200:LEU:HD22	2.49	0.43
1:F:296:HIS:CD2	1:F:339:MET:HG3	2.54	0.43
1:K:492:ASN:C	1:K:492:ASN:HD22	2.21	0.43
1:L:405:VAL:O	1:L:406:LEU:HD23	2.19	0.43
1:A:123:ALA:O	1:A:127:ASN:CG	2.56	0.43
1:C:224:GLY:N	1:C:225:PRO:CD	2.82	0.43
1:F:66:ALA:CB	1:F:187:THR:HG22	2.42	0.43
1:I:191:LYS:CD	1:I:192:PRO:O	2.67	0.43
1:L:48:LEU:HD13	1:L:198:LEU:HD12	2.00	0.43
1:A:21:LYS:NZ	1:A:30:SER:OG	2.48	0.43
1:C:308:VAL:O	1:C:407:PRO:HA	2.19	0.43
1:H:239:LYS:HE2	1:H:482:ASN:O	2.19	0.43
1:I:173:MET:HE1	1:I:243:THR:CG2	2.34	0.43
1:J:165:ILE:CG2	1:J:177:LYS:HG3	2.49	0.43
1:J:371:ARG:HD3	1:J:372:ALA:N	2.34	0.43
1:K:83:ARG:HD3	1:K:182:LEU:O	2.18	0.43
1:K:239:LYS:NZ	1:K:262:HIS:HD2	2.15	0.43
1:F:78:MET:HG2	1:F:82:GLU:CB	2.49	0.43
1:L:84:ALA:HB2	1:L:135:THR:OG1	2.18	0.43
1:A:492:ASN:ND2	1:A:494:LYS:H	2.16	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:THR:HG22	1:D:172:VAL:HA	2.01	0.43
1:J:138:ILE:O	1:J:138:ILE:HG22	2.19	0.43
1:F:48:LEU:HD11	1:F:107:LEU:HB3	2.01	0.43
1:H:253:MET:HE2	1:H:265:LEU:HD11	1.99	0.43
1:H:433:ASN:HD22	1:H:436:THR:HG23	1.84	0.43
1:L:48:LEU:HD11	1:L:107:LEU:HB3	2.01	0.43
1:A:135:THR:HG22	1:A:183:ALA:HA	2.01	0.42
1:B:190:LEU:CD1	1:B:200:LEU:HD21	2.49	0.42
1:E:78:MET:CG	1:E:82:GLU:HB2	2.49	0.42
1:C:88:TYR:CD2	1:E:88:TYR:CE1	3.05	0.42
1:E:364:THR:HG21	1:E:386:ASP:OD2	2.19	0.42
1:A:432:GLN:NE2	1:E:433:ASN:HD21	2.17	0.42
1:F:451:ILE:O	1:F:452:ASN:HB2	2.19	0.42
1:G:190:LEU:C	1:G:190:LEU:HD23	2.39	0.42
1:B:253:MET:HE2	1:B:265:LEU:HD11	2.02	0.42
1:A:471:ILE:HG13	1:C:260:ILE:HG22	2.00	0.42
1:I:296:HIS:O	1:I:401:PRO:HD3	2.18	0.42
1:I:78:MET:CG	1:I:82:GLU:CB	2.97	0.42
1:D:169:PHE:O	1:D:173:MET:HG2	2.19	0.42
1:G:448:THR:HA	1:H:488:SER:O	2.20	0.42
1:I:364:THR:CG2	1:I:386:ASP:OD2	2.66	0.42
1:L:292:ILE:O	1:L:297:GLY:HA2	2.20	0.42
1:F:239:LYS:NZ	1:F:262:HIS:HD2	2.15	0.42
1:G:124:THR:HG22	1:G:172:VAL:HB	2.01	0.42
1:G:163:GLN:OE1	1:G:188:ILE:HD13	2.20	0.42
1:G:387:VAL:CG1	1:G:388:THR:N	2.83	0.42
1:H:177:LYS:NZ	1:H:243:THR:CG2	2.83	0.42
1:J:78:MET:HG3	1:J:83:ARG:HG3	2.01	0.42
1:K:124:THR:HG21	1:K:171:LEU:HD13	2.01	0.42
1:A:239:LYS:NZ	1:A:264:THR:CG2	2.81	0.42
1:C:135:THR:OG1	1:C:136:THR:N	2.53	0.42
1:L:199:SER:HB2	3:L:623:HOH:O	2.19	0.42
1:D:447:GLY:HA3	1:D:464:GLY:O	2.20	0.42
1:K:60:ASP:OD1	1:K:60:ASP:N	2.51	0.42
1:A:239:LYS:NZ	1:A:264:THR:HG23	2.35	0.42
1:A:253:MET:HE2	1:A:265:LEU:HD11	2.02	0.42
1:B:107:LEU:HD13	1:B:333:MET:HG3	2.01	0.42
1:E:364:THR:HG23	1:E:386:ASP:OD2	2.19	0.42
1:H:464:GLY:HA3	1:H:473:ARG:HD3	2.02	0.42
1:D:163:GLN:CB	1:D:190:LEU:HD23	2.50	0.42
1:G:348:GLN:HB2	1:G:377:TYR:HB3	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:387:VAL:HG13	1:K:394:VAL:HG11	2.02	0.42
1:K:447:GLY:HA3	1:K:464:GLY:O	2.20	0.42
1:L:433:ASN:HD22	1:L:436:THR:H	1.68	0.42
1:B:59:ILE:HD12	1:B:220:VAL:HG21	2.01	0.41
1:E:9:LYS:HE3	1:E:99:GLU:OE2	2.20	0.41
1:F:66:ALA:CB	1:F:187:THR:CG2	2.97	0.41
1:F:66:ALA:O	1:F:187:THR:HG21	2.20	0.41
1:F:167:TRP:CD2	1:F:343:VAL:HG11	2.54	0.41
1:G:281:LEU:HA	1:G:281:LEU:HD12	1.89	0.41
1:I:99:GLU:O	1:I:103:GLN:HG3	2.19	0.41
1:K:59:ILE:CD1	1:K:227:ALA:O	2.68	0.41
1:K:433:ASN:HD22	1:K:436:THR:HG23	1.85	0.41
1:L:364:THR:HG23	1:L:386:ASP:HB2	2.02	0.41
1:B:9:LYS:HB2	1:B:12:VAL:HG13	2.00	0.41
1:D:235:HIS:HA	1:D:259:MET:HE2	2.03	0.41
1:D:235:HIS:HA	1:D:259:MET:CE	2.49	0.41
1:D:438:HIS:HD2	1:E:152:TYR:OH	2.03	0.41
1:G:191:LYS:HD3	1:G:192:PRO:O	2.21	0.41
1:G:311:LYS:HD2	1:G:312:HIS:NE2	2.34	0.41
1:H:259:MET:O	1:H:260:ILE:C	2.57	0.41
1:L:167:TRP:CZ3	1:L:343:VAL:HB	2.54	0.41
1:C:235:HIS:HB3	3:C:775:HOH:O	2.21	0.41
1:F:299:ASN:HB3	1:F:302:ALA:HB2	2.01	0.41
1:J:17:ASN:OD1	1:J:17:ASN:O	2.38	0.41
1:L:364:THR:HG23	1:L:386:ASP:OD2	2.20	0.41
1:B:438:HIS:CE1	1:H:438:HIS:CE1	3.03	0.41
1:C:391:MET:HB2	1:C:394:VAL:HG13	2.02	0.41
1:A:88:TYR:CE1	1:D:88:TYR:CG	3.08	0.41
1:J:433:ASN:HB3	1:J:436:THR:CG2	2.48	0.41
1:J:8:LEU:HA	1:J:103:GLN:HE22	1.86	0.41
1:A:324:ALA:O	1:A:327:VAL:HG13	2.20	0.41
1:D:92:ASP:O	1:D:96:GLU:HG3	2.21	0.41
1:E:253:MET:HE2	1:E:253:MET:HB2	1.82	0.41
1:F:188:ILE:CD1	1:F:190:LEU:CB	2.98	0.41
1:G:296:HIS:CD2	1:G:296:HIS:N	2.87	0.41
1:J:372:ALA:HB2	1:J:380:LYS:HG3	2.03	0.41
1:J:404:VAL:CG1	1:J:406:LEU:HD11	2.51	0.41
1:K:190:LEU:HD12	1:K:200:LEU:HD21	2.03	0.41
1:L:161:VAL:O	1:L:161:VAL:HG13	2.20	0.41
1:B:277:GLU:O	1:B:312:HIS:HE1	2.03	0.41
1:B:342:LEU:HB2	1:B:377:TYR:O	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:TYR:OH	1:E:438:HIS:HD2	2.03	0.41
1:B:254:ARG:HG3	1:I:254:ARG:HG3	2.01	0.41
1:B:260:ILE:N	1:B:260:ILE:HD12	2.35	0.41
1:D:107:LEU:HD13	1:D:333:MET:CG	2.46	0.41
1:A:88:TYR:CE1	1:D:88:TYR:CD2	3.08	0.41
1:F:163:GLN:CD	1:F:177:LYS:HB3	2.40	0.41
1:F:235:HIS:HA	1:F:259:MET:HE3	2.03	0.41
1:J:308:VAL:HG21	1:J:316:VAL:CG2	2.46	0.41
1:H:112:PRO:HB2	1:H:115:VAL:HG13	2.02	0.41
1:I:124:THR:HG22	1:I:172:VAL:HA	2.02	0.41
1:J:434:ILE:HA	1:K:434:ILE:HB	2.01	0.41
1:G:260:ILE:HA	1:H:253:MET:HE1	2.02	0.41
1:H:329:LEU:HD12	1:H:339:MET:HB3	2.02	0.41
1:I:357:GLN:O	1:I:357:GLN:HG3	2.21	0.41
1:B:492:ASN:ND2	1:B:494:LYS:H	2.19	0.41
1:F:308:VAL:HG11	1:F:316:VAL:HG13	2.02	0.41
1:G:239:LYS:HZ3	1:G:262:HIS:CD2	2.27	0.41
1:D:107:LEU:CD1	1:D:333:MET:HG3	2.47	0.40
1:F:59:ILE:N	1:F:59:ILE:HD13	2.36	0.40
1:B:88:TYR:CZ	1:G:88:TYR:CD2	3.09	0.40
1:J:177:LYS:NZ	1:J:474:GLU:OE2	2.45	0.40
1:L:135:THR:OG1	1:L:136:THR:N	2.54	0.40
1:H:264:THR:OG1	1:H:264:THR:CG2	2.56	0.40
1:I:275:ILE:HG12	1:I:284:ALA:HB1	2.03	0.40
1:L:22:MET:HE3	1:L:24:ILE:CD1	2.51	0.40
1:L:161:VAL:HG21	1:L:483:TYR:HE1	1.86	0.40
1:E:357:GLN:HE22	1:E:360:LYS:NZ	2.18	0.40
1:F:277:GLU:O	1:F:312:HIS:HE1	2.04	0.40
1:G:492:ASN:ND2	1:G:494:LYS:H	2.19	0.40
1:I:371:ARG:NH1	1:I:372:ALA:O	2.50	0.40
1:J:433:ASN:HD22	1:J:436:THR:H	1.68	0.40
1:K:134:TRP:CG	1:K:480:LEU:HD11	2.56	0.40
1:K:296:HIS:N	1:K:296:HIS:CD2	2.89	0.40
1:L:407:PRO:O	1:L:417:ARG:NH1	2.47	0.40
1:L:426:ALA:HA	1:L:448:THR:O	2.22	0.40
1:A:107:LEU:HD13	1:A:333:MET:HG3	2.03	0.40
1:F:177:LYS:NZ	1:F:243:THR:CG2	2.84	0.40
1:G:438:HIS:CE1	1:I:438:HIS:CE1	3.06	0.40
1:I:345:LYS:HE3	1:I:349:GLU:OE2	2.22	0.40
1:I:492:ASN:ND2	1:I:494:LYS:H	2.19	0.40
1:B:484:THR:HG22	3:B:634:HOH:O	2.21	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:ILE:HD12	1:E:468:GLN:HB3	2.03	0.40
1:E:124:THR:HG22	1:E:172:VAL:HA	2.02	0.40
1:J:364:THR:O	1:J:384:PHE:HA	2.22	0.40
1:K:17:ASN:O	1:K:18:GLU:OE2	2.40	0.40
1:K:484:THR:HG22	1:K:485:GLU:N	2.37	0.40
1:L:124:THR:HG21	1:L:171:LEU:HD13	2.04	0.40
1:L:342:LEU:HD12	1:L:342:LEU:HA	1.85	0.40
1:L:321:VAL:HG13	1:L:367:ALA:HB2	2.03	0.40
1:L:67:ARG:O	1:L:71:GLU:HG2	2.21	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	490/494 (99%)	478 (98%)	12 (2%)	0	100	100
1	B	490/494 (99%)	471 (96%)	19 (4%)	0	100	100
1	C	490/494 (99%)	476 (97%)	13 (3%)	1 (0%)	47	38
1	D	490/494 (99%)	476 (97%)	14 (3%)	0	100	100
1	E	488/494 (99%)	474 (97%)	14 (3%)	0	100	100
1	F	491/494 (99%)	475 (97%)	16 (3%)	0	100	100
1	G	488/494 (99%)	473 (97%)	15 (3%)	0	100	100
1	H	489/494 (99%)	473 (97%)	16 (3%)	0	100	100
1	I	489/494 (99%)	471 (96%)	18 (4%)	0	100	100
1	J	489/494 (99%)	471 (96%)	17 (4%)	1 (0%)	47	38
1	K	487/494 (99%)	470 (96%)	17 (4%)	0	100	100
1	L	486/494 (98%)	466 (96%)	18 (4%)	2 (0%)	34	24
All	All	5867/5928 (99%)	5674 (97%)	189 (3%)	4 (0%)	51	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	78	MET
1	C	373	LEU
1	L	424	GLY
1	J	424	GLY

### 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	399/401 (100%)	375 (94%)	24 (6%)	19	9
1	B	399/401 (100%)	369 (92%)	30 (8%)	13	5
1	C	399/401 (100%)	376 (94%)	23 (6%)	20	10
1	D	399/401 (100%)	374 (94%)	25 (6%)	18	8
1	E	397/401 (99%)	373 (94%)	24 (6%)	19	9
1	F	400/401 (100%)	372 (93%)	28 (7%)	15	7
1	G	397/401 (99%)	367 (92%)	30 (8%)	13	5
1	H	398/401 (99%)	364 (92%)	34 (8%)	10	4
1	I	398/401 (99%)	370 (93%)	28 (7%)	15	7
1	J	398/401 (99%)	360 (90%)	38 (10%)	8	3
1	K	396/401 (99%)	361 (91%)	35 (9%)	10	4
1	L	395/401 (98%)	355 (90%)	40 (10%)	7	2
All	All	4775/4812 (99%)	4416 (92%)	359 (8%)	13	5

All (359) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	18	GLU
1	A	59	ILE
1	A	71	GLU
1	A	104	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	105	GLU
1	A	107	LEU
1	A	120	ASP
1	A	121	ILE
1	A	124	THR
1	A	158	VAL
1	A	166	PRO
1	A	171	LEU
1	A	264	THR
1	A	296	HIS
1	A	316	VAL
1	A	329	LEU
1	A	342	LEU
1	A	353	ASN
1	A	375	LYS
1	A	387	VAL
1	A	399	PHE
1	A	484	THR
1	A	492	ASN
1	B	12	VAL
1	B	48	LEU
1	B	71	GLU
1	B	104	LEU
1	B	105	GLU
1	B	107	LEU
1	B	111	LYS
1	B	115	VAL
1	B	120	ASP
1	B	121	ILE
1	B	124	THR
1	B	147	LYS
1	B	158	VAL
1	B	166	PRO
1	B	171	LEU
1	B	190	LEU
1	B	217	VAL
1	B	290	GLN
1	B	306	VAL
1	B	311	LYS
1	B	335	LYS
1	B	342	LEU
1	B	387	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	390	ASP
1	B	394	VAL
1	B	399	PHE
1	B	448	THR
1	B	453	ASP
1	B	484	THR
1	B	492	ASN
1	C	4	THR
1	C	8	LEU
1	C	27	GLU
1	C	48	LEU
1	C	77	GLU
1	C	88	TYR
1	C	107	LEU
1	C	120	ASP
1	C	121	ILE
1	C	158	VAL
1	C	171	LEU
1	C	187	THR
1	C	247	VAL
1	C	311	LYS
1	C	316	VAL
1	C	322	LYS
1	C	360	LYS
1	C	364	THR
1	C	371	ARG
1	C	374	GLU
1	C	375	LYS
1	C	399	PHE
1	C	492	ASN
1	D	7	GLU
1	D	8	LEU
1	D	88	TYR
1	D	105	GLU
1	D	107	LEU
1	D	109	ASN
1	D	120	ASP
1	D	121	ILE
1	D	124	THR
1	D	147	LYS
1	D	158	VAL
1	D	171	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	217	VAL
1	D	282	GLU
1	D	290	GLN
1	D	311	LYS
1	D	364	THR
1	D	365	VAL
1	D	371	ARG
1	D	375	LYS
1	D	385	THR
1	D	387	VAL
1	D	399	PHE
1	D	484	THR
1	D	492	ASN
1	E	7	GLU
1	E	13	GLU
1	E	104	LEU
1	E	105	GLU
1	E	107	LEU
1	E	109	ASN
1	E	120	ASP
1	E	124	THR
1	E	171	LEU
1	E	172	VAL
1	E	187	THR
1	E	188	ILE
1	E	194	SER
1	E	217	VAL
1	E	253	MET
1	E	296	HIS
1	E	310	ARG
1	E	329	LEU
1	E	364	THR
1	E	371	ARG
1	E	375	LYS
1	E	399	PHE
1	E	453	ASP
1	E	492	ASN
1	F	13	GLU
1	F	17	ASN
1	F	18	GLU
1	F	35	LYS
1	F	48	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	F	60	ASP
1	F	77	GLU
1	F	104	LEU
1	F	105	GLU
1	F	107	LEU
1	F	115	VAL
1	F	120	ASP
1	F	171	LEU
1	F	188	ILE
1	F	217	VAL
1	F	225	PRO
1	F	243	THR
1	F	246	THR
1	F	328	LYS
1	F	329	LEU
1	F	371	ARG
1	F	375	LYS
1	F	399	PHE
1	F	412	GLU
1	F	453	ASP
1	F	457	GLU
1	F	484	THR
1	F	492	ASN
1	G	7	GLU
1	G	8	LEU
1	G	9	LYS
1	G	27	GLU
1	G	71	GLU
1	G	105	GLU
1	G	107	LEU
1	G	109	ASN
1	G	124	THR
1	G	171	LEU
1	G	172	VAL
1	G	188	ILE
1	G	191	LYS
1	G	194	SER
1	G	217	VAL
1	G	243	THR
1	G	246	THR
1	G	264	THR
1	G	290	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	322	LYS
1	G	327	VAL
1	G	329	LEU
1	G	342	LEU
1	G	364	THR
1	G	375	LYS
1	G	394	VAL
1	G	399	PHE
1	G	406	LEU
1	G	453	ASP
1	G	492	ASN
1	H	8	LEU
1	H	13	GLU
1	H	27	GLU
1	H	48	LEU
1	H	71	GLU
1	H	104	LEU
1	H	105	GLU
1	H	107	LEU
1	H	120	ASP
1	H	121	ILE
1	H	124	THR
1	H	158	VAL
1	H	171	LEU
1	H	172	VAL
1	H	187	THR
1	H	188	ILE
1	H	217	VAL
1	H	243	THR
1	H	248	THR
1	H	264	THR
1	H	282	GLU
1	H	296	HIS
1	H	329	LEU
1	H	342	LEU
1	H	364	THR
1	H	371	ARG
1	H	375	LYS
1	H	385	THR
1	H	394	VAL
1	H	399	PHE
1	H	412	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	453	ASP
1	H	484	THR
1	H	492	ASN
1	I	4	THR
1	I	8	LEU
1	I	18	GLU
1	I	48	LEU
1	I	50	VAL
1	I	60	ASP
1	I	104	LEU
1	I	107	LEU
1	I	120	ASP
1	I	121	ILE
1	I	124	THR
1	I	147	LYS
1	I	171	LEU
1	I	191	LYS
1	I	246	THR
1	I	252	ILE
1	I	266	GLU
1	I	311	LYS
1	I	316	VAL
1	I	322	LYS
1	I	342	LEU
1	I	357	GLN
1	I	364	THR
1	I	371	ARG
1	I	375	LYS
1	I	399	PHE
1	I	484	THR
1	I	492	ASN
1	J	9	LYS
1	J	12	VAL
1	J	13	GLU
1	J	18	GLU
1	J	19	GLU
1	J	27	GLU
1	J	48	LEU
1	J	59	ILE
1	J	71	GLU
1	J	104	LEU
1	J	105	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	J	107	LEU
1	J	109	ASN
1	J	115	VAL
1	J	120	ASP
1	J	121	ILE
1	J	171	LEU
1	J	172	VAL
1	J	173	MET
1	J	245	SER
1	J	259	MET
1	J	316	VAL
1	J	327	VAL
1	J	329	LEU
1	J	342	LEU
1	J	360	LYS
1	J	364	THR
1	J	365	VAL
1	J	371	ARG
1	J	387	VAL
1	J	399	PHE
1	J	405	VAL
1	J	435	LYS
1	J	436	THR
1	J	448	THR
1	J	453	ASP
1	J	484	THR
1	J	492	ASN
1	K	8	LEU
1	K	12	VAL
1	K	18	GLU
1	K	27	GLU
1	K	48	LEU
1	K	71	GLU
1	K	77	GLU
1	K	104	LEU
1	K	107	LEU
1	K	115	VAL
1	K	124	THR
1	K	158	VAL
1	K	161	VAL
1	K	171	LEU
1	K	187	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	K	188	ILE
1	K	190	LEU
1	K	194	SER
1	K	217	VAL
1	K	220	VAL
1	K	232	VAL
1	K	246	THR
1	K	316	VAL
1	K	329	LEU
1	K	335	LYS
1	K	342	LEU
1	K	343	VAL
1	K	364	THR
1	K	375	LYS
1	K	380	LYS
1	K	394	VAL
1	K	399	PHE
1	K	429	VAL
1	K	435	LYS
1	K	492	ASN
1	L	8	LEU
1	L	9	LYS
1	L	13	GLU
1	L	22	MET
1	L	48	LEU
1	L	104	LEU
1	L	105	GLU
1	L	107	LEU
1	L	115	VAL
1	L	120	ASP
1	L	124	THR
1	L	126	GLU
1	L	158	VAL
1	L	171	LEU
1	L	187	THR
1	L	191	LYS
1	L	217	VAL
1	L	218	ASN
1	L	232	VAL
1	L	239	LYS
1	L	243	THR
1	L	246	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	L	248	THR
1	L	290	GLN
1	L	316	VAL
1	L	342	LEU
1	L	353	ASN
1	L	364	THR
1	L	375	LYS
1	L	381	PRO
1	L	385	THR
1	L	405	VAL
1	L	412	GLU
1	L	429	VAL
1	L	431	THR
1	L	434	ILE
1	L	436	THR
1	L	448	THR
1	L	484	THR
1	L	492	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (155) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	114	GLN
1	A	214	ASN
1	A	262	HIS
1	A	312	HIS
1	A	325	ASN
1	A	326	ASN
1	A	353	ASN
1	A	432	GLN
1	A	433	ASN
1	A	438	HIS
1	A	442	ASN
1	A	492	ASN
1	B	85	HIS
1	B	103	GLN
1	B	214	ASN
1	B	262	HIS
1	B	312	HIS
1	B	325	ASN
1	B	353	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	357	GLN
1	B	432	GLN
1	B	433	ASN
1	B	438	HIS
1	B	442	ASN
1	B	482	ASN
1	B	492	ASN
1	C	103	GLN
1	C	214	ASN
1	C	262	HIS
1	C	312	HIS
1	C	325	ASN
1	C	326	ASN
1	C	432	GLN
1	C	433	ASN
1	C	438	HIS
1	C	442	ASN
1	C	482	ASN
1	C	492	ASN
1	D	103	GLN
1	D	214	ASN
1	D	262	HIS
1	D	312	HIS
1	D	325	ASN
1	D	326	ASN
1	D	357	GLN
1	D	432	GLN
1	D	433	ASN
1	D	438	HIS
1	D	442	ASN
1	D	482	ASN
1	D	492	ASN
1	E	103	GLN
1	E	214	ASN
1	E	262	HIS
1	E	312	HIS
1	E	325	ASN
1	E	326	ASN
1	E	348	GLN
1	E	357	GLN
1	E	432	GLN
1	E	438	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	442	ASN
1	E	482	ASN
1	E	492	ASN
1	F	103	GLN
1	F	214	ASN
1	F	262	HIS
1	F	312	HIS
1	F	325	ASN
1	F	353	ASN
1	F	357	GLN
1	F	433	ASN
1	F	438	HIS
1	F	442	ASN
1	F	492	ASN
1	G	85	HIS
1	G	103	GLN
1	G	214	ASN
1	G	262	HIS
1	G	312	HIS
1	G	325	ASN
1	G	326	ASN
1	G	357	GLN
1	G	432	GLN
1	G	433	ASN
1	G	438	HIS
1	G	442	ASN
1	G	482	ASN
1	G	492	ASN
1	H	85	HIS
1	H	103	GLN
1	H	214	ASN
1	H	262	HIS
1	H	312	HIS
1	H	325	ASN
1	H	326	ASN
1	H	357	GLN
1	H	432	GLN
1	H	433	ASN
1	H	438	HIS
1	H	442	ASN
1	H	482	ASN
1	H	492	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	I	103	GLN
1	I	214	ASN
1	I	262	HIS
1	I	312	HIS
1	I	325	ASN
1	I	326	ASN
1	I	432	GLN
1	I	433	ASN
1	I	438	HIS
1	I	442	ASN
1	I	482	ASN
1	I	492	ASN
1	J	103	GLN
1	J	214	ASN
1	J	262	HIS
1	J	290	GLN
1	J	312	HIS
1	J	325	ASN
1	J	326	ASN
1	J	432	GLN
1	J	433	ASN
1	J	438	HIS
1	J	442	ASN
1	J	482	ASN
1	J	492	ASN
1	K	103	GLN
1	K	214	ASN
1	K	262	HIS
1	K	290	GLN
1	K	298	GLN
1	K	312	HIS
1	K	325	ASN
1	K	326	ASN
1	K	433	ASN
1	K	438	HIS
1	K	442	ASN
1	K	482	ASN
1	K	492	ASN
1	L	103	GLN
1	L	114	GLN
1	L	214	ASN
1	L	262	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	L	312	HIS
1	L	325	ASN
1	L	326	ASN
1	L	432	GLN
1	L	433	ASN
1	L	438	HIS
1	L	442	ASN
1	L	482	ASN
1	L	492	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

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	491/494 (99%)	-0.14	1 (0%) 95 95	5, 10, 21, 35	0
1	B	491/494 (99%)	0.02	4 (0%) 86 87	10, 17, 30, 45	0
1	C	491/494 (99%)	-0.12	1 (0%) 95 95	5, 12, 25, 43	0
1	D	489/494 (98%)	-0.07	2 (0%) 92 93	5, 12, 25, 37	0
1	E	490/494 (99%)	-0.12	1 (0%) 95 95	5, 11, 23, 43	0
1	F	491/494 (99%)	0.07	2 (0%) 92 93	9, 17, 31, 43	0
1	G	490/494 (99%)	0.02	5 (1%) 82 84	10, 16, 29, 52	0
1	H	490/494 (99%)	0.03	3 (0%) 89 90	10, 16, 29, 58	0
1	I	491/494 (99%)	0.02	5 (1%) 82 84	11, 18, 30, 46	0
1	J	491/494 (99%)	0.15	7 (1%) 75 77	10, 21, 34, 53	0
1	K	489/494 (98%)	0.46	22 (4%) 33 36	13, 21, 34, 50	0
1	L	488/494 (98%)	0.56	26 (5%) 26 29	13, 22, 35, 57	0
All	All	5882/5928 (99%)	0.07	79 (1%) 77 79	5, 17, 30, 58	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	43	ALA	5.5
1	H	5	ASN	4.6
1	J	33	GLY	4.3
1	E	5	ASN	3.9
1	K	390	ASP	3.4
1	L	387	VAL	3.3
1	L	351	VAL	3.2
1	K	318	ASP	3.1
1	L	381	PRO	3.0
1	L	374	GLU	3.0
1	K	336	GLU	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	L	373	LEU	3.0
1	L	358	GLY	2.9
1	J	32	ILE	2.9
1	K	281	LEU	2.9
1	L	335	LYS	2.8
1	J	4	THR	2.8
1	H	17	ASN	2.8
1	C	88	TYR	2.7
1	L	46	ASP	2.7
1	G	5	ASN	2.7
1	K	235	HIS	2.6
1	K	374	GLU	2.6
1	K	317	VAL	2.5
1	G	235	HIS	2.5
1	K	276	LEU	2.5
1	B	247	VAL	2.5
1	I	73	GLY	2.5
1	L	73	GLY	2.5
1	B	4	THR	2.5
1	F	247	VAL	2.4
1	K	282	GLU	2.4
1	L	17	ASN	2.4
1	L	44	THR	2.4
1	L	235	HIS	2.4
1	J	335	LYS	2.4
1	K	360	LYS	2.4
1	L	282	GLU	2.4
1	L	383	VAL	2.4
1	K	376	GLY	2.3
1	L	62	ALA	2.3
1	F	335	LYS	2.3
1	L	7	GLU	2.3
1	D	88	TYR	2.3
1	K	408	PHE	2.3
1	K	363	ALA	2.3
1	L	48	LEU	2.3
1	L	23	PHE	2.3
1	A	247	VAL	2.3
1	K	247	VAL	2.3
1	I	88	TYR	2.2
1	K	32	ILE	2.2
1	L	336	GLU	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	L	72	SER	2.1
1	G	335	LYS	2.1
1	K	313	TYR	2.1
1	G	247	VAL	2.1
1	K	314	GLU	2.1
1	L	316	VAL	2.1
1	G	6	ILE	2.1
1	K	69	ALA	2.1
1	K	412	GLU	2.1
1	B	335	LYS	2.1
1	L	384	PHE	2.1
1	D	374	GLU	2.1
1	I	363	ALA	2.1
1	J	5	ASN	2.1
1	K	369	GLY	2.1
1	I	4	THR	2.1
1	I	247	VAL	2.1
1	J	357	GLN	2.1
1	J	390	ASP	2.1
1	B	235	HIS	2.1
1	H	336	GLU	2.0
1	L	68	SER	2.0
1	L	35	LYS	2.0
1	K	320	LEU	2.0
1	K	12	VAL	2.0
1	L	75	TRP	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](#)

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( $\text{\AA}^2$ )	Q<0.9
2	NA	F	501	1/1	0.93	0.10	16,16,16,16	0
2	NA	J	502	1/1	0.94	0.10	21,21,21,21	0
2	NA	K	502	1/1	0.94	0.14	23,23,23,23	0
2	NA	L	501	1/1	0.94	0.21	21,21,21,21	0
2	NA	B	501	1/1	0.94	0.09	17,17,17,17	0
2	NA	K	501	1/1	0.95	0.17	20,20,20,20	0
2	NA	B	502	1/1	0.96	0.07	14,14,14,14	0
2	NA	H	501	1/1	0.97	0.07	15,15,15,15	0
2	NA	J	501	1/1	0.97	0.26	20,20,20,20	0
2	NA	I	501	1/1	0.98	0.10	19,19,19,19	0
2	NA	F	502	1/1	0.98	0.06	13,13,13,13	0
2	NA	L	502	1/1	0.98	0.07	23,23,23,23	0
2	NA	H	502	1/1	0.98	0.06	16,16,16,16	0
2	NA	C	501	1/1	0.98	0.09	12,12,12,12	0
2	NA	D	502	1/1	0.98	0.07	12,12,12,12	0
2	NA	I	502	1/1	0.98	0.09	15,15,15,15	0
2	NA	E	501	1/1	0.99	0.13	10,10,10,10	0
2	NA	A	502	1/1	0.99	0.06	10,10,10,10	0
2	NA	G	501	1/1	0.99	0.09	14,14,14,14	0
2	NA	C	502	1/1	0.99	0.08	9,9,9,9	0
2	NA	A	501	1/1	0.99	0.10	10,10,10,10	0
2	NA	G	502	1/1	0.99	0.05	15,15,15,15	0
2	NA	D	501	1/1	0.99	0.11	11,11,11,11	0
2	NA	E	502	1/1	1.00	0.06	12,12,12,12	0

## 6.5 Other polymers

There are no such residues in this entry.