



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:35 AM UTC

PDB ID : 2DKF / pdb\_00002dkf  
Title : Crystal Structure of TTHA0252 from *Thermus thermophilus* HB8, a RNA Degradation Protein of the Metallo-beta-lactamase Superfamily  
Authors : Ishikawa, I.; Nakagawa, N.; Kuramitsu, S.; Yokoyama, S.; Masui, R.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2006-04-10  
Resolution : 2.80 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

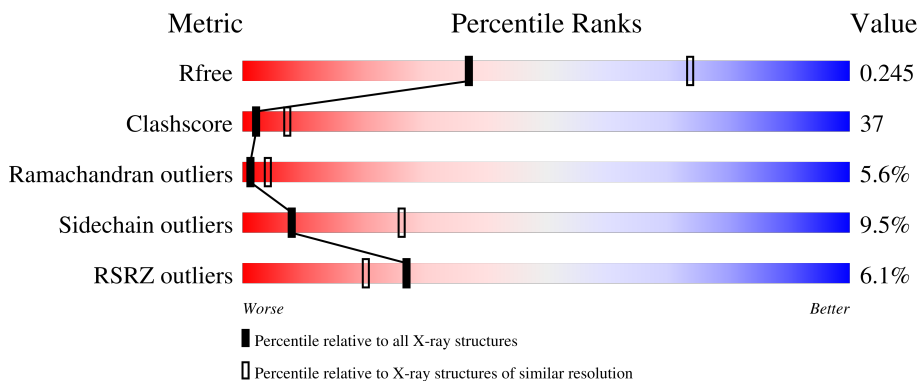
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


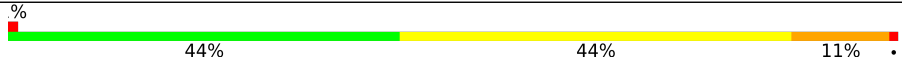
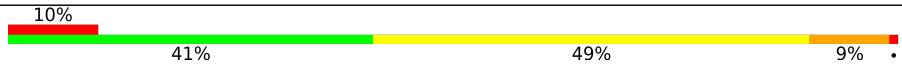
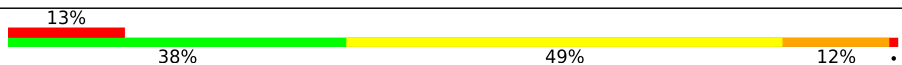
The reported resolution of this entry is 2.80 Å.

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))
$R_{free}$	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	431	
1	B	431	
1	C	431	
1	D	431	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13404 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 metallo-beta-lactamase superfamily protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	431	3326	2127	597	594	1	7	0	0	0
1	B	431	3326	2127	597	594	1	7	0	0	0
1	C	431	3326	2127	597	594	1	7	0	0	0
1	D	431	3326	2127	597	594	1	7	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	GB 55771634
A	32	MSE	MET	modified residue	GB 55771634
A	90	MSE	MET	modified residue	GB 55771634
A	101	MSE	MET	modified residue	GB 55771634
A	253	MSE	MET	modified residue	GB 55771634
A	307	MSE	MET	modified residue	GB 55771634
A	315	MSE	MET	modified residue	GB 55771634
B	1	MSE	MET	modified residue	GB 55771634
B	32	MSE	MET	modified residue	GB 55771634
B	90	MSE	MET	modified residue	GB 55771634
B	101	MSE	MET	modified residue	GB 55771634
B	253	MSE	MET	modified residue	GB 55771634
B	307	MSE	MET	modified residue	GB 55771634
B	315	MSE	MET	modified residue	GB 55771634
C	1	MSE	MET	modified residue	GB 55771634
C	32	MSE	MET	modified residue	GB 55771634
C	90	MSE	MET	modified residue	GB 55771634
C	101	MSE	MET	modified residue	GB 55771634
C	253	MSE	MET	modified residue	GB 55771634
C	307	MSE	MET	modified residue	GB 55771634
C	315	MSE	MET	modified residue	GB 55771634

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MSE	MET	modified residue	GB 55771634
D	32	MSE	MET	modified residue	GB 55771634
D	90	MSE	MET	modified residue	GB 55771634
D	101	MSE	MET	modified residue	GB 55771634
D	253	MSE	MET	modified residue	GB 55771634
D	307	MSE	MET	modified residue	GB 55771634
D	315	MSE	MET	modified residue	GB 55771634

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is water.

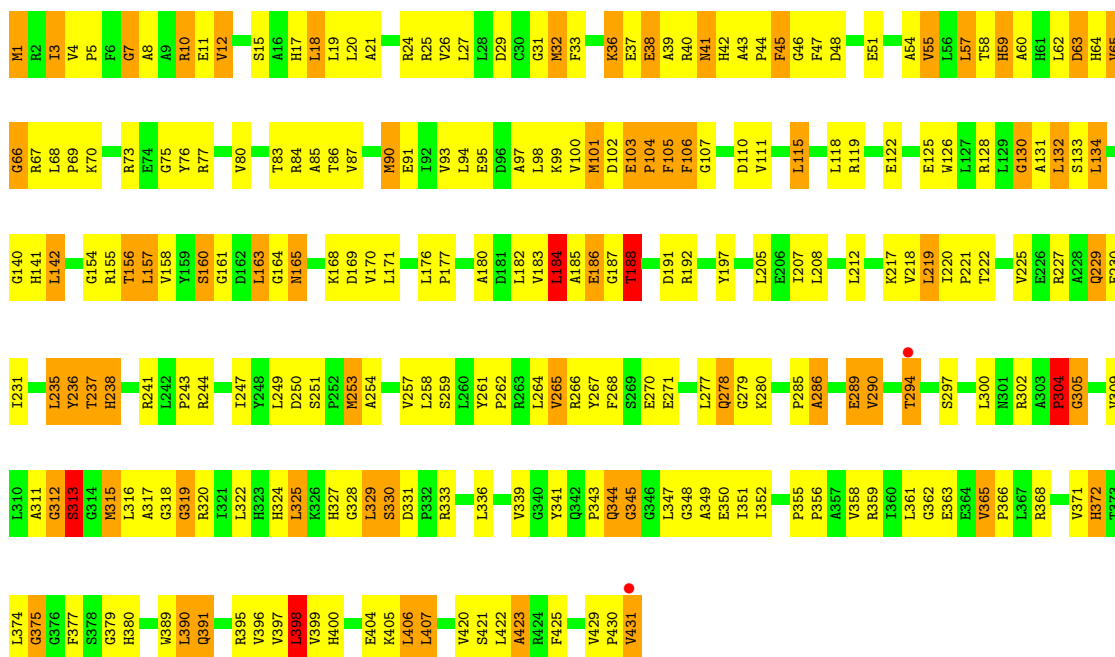
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total 32	O 32	0	0
3	B	28	Total 28	O 28	0	0
3	C	16	Total 16	O 16	0	0
3	D	16	Total 16	O 16	0	0

### 3 Residue-property plots

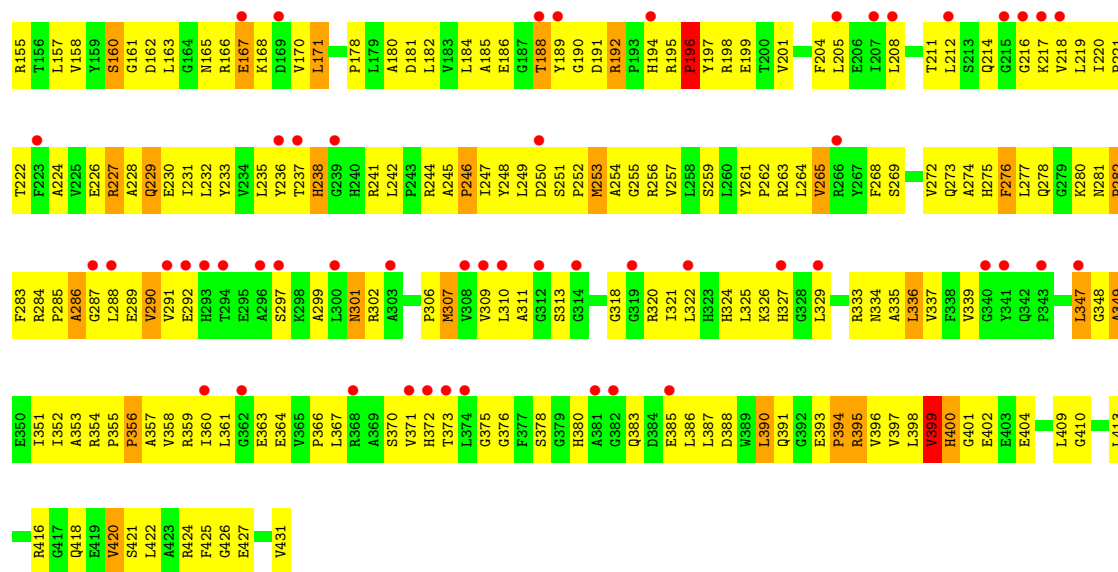
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: metallo-beta-lactamase superfamily protein

Chain A: 







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.22Å 147.10Å 121.23Å 90.00° 109.25° 90.00°	Depositor
Resolution (Å)	19.99 – 2.80 19.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (19.99-2.80) 95.8 (19.99-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	28.81 (at 2.79Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.242 , 0.285 0.246 , 0.245	Depositor DCC
$R_{free}$ test set	2847 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.7	Xtrriage
Anisotropy	0.048	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 55.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13404	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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:  
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	0.79	9/3401 (0.3%)	1.25	39/4603 (0.8%)
1	B	0.78	11/3401 (0.3%)	1.20	41/4603 (0.9%)
1	C	0.62	11/3401 (0.3%)	1.04	23/4603 (0.5%)
1	D	0.59	7/3401 (0.2%)	1.01	18/4603 (0.4%)
All	All	0.70	38/13604 (0.3%)	1.13	121/18412 (0.7%)

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	MSE	SE-CE	-12.04	1.59	1.95
1	A	32	MSE	SE-CE	-10.25	1.64	1.95
1	B	90	MSE	SE-CE	-9.68	1.66	1.95
1	A	253	MSE	SE-CE	-9.16	1.68	1.95
1	B	32	MSE	SE-CE	-8.60	1.69	1.95
1	C	90	MSE	SE-CE	-7.92	1.71	1.95
1	C	32	MSE	SE-CE	-7.72	1.72	1.95
1	D	90	MSE	SE-CE	-7.68	1.72	1.95
1	A	253	MSE	CG-SE	-7.67	1.72	1.95
1	B	101	MSE	SE-CE	-7.43	1.73	1.95
1	B	1	MSE	SE-CE	-7.41	1.73	1.95
1	B	253	MSE	SE-CE	-7.31	1.73	1.95
1	C	253	MSE	SE-CE	-7.21	1.73	1.95
1	D	1	MSE	SE-CE	-7.08	1.74	1.95
1	C	1	MSE	SE-CE	-6.98	1.74	1.95
1	B	307	MSE	SE-CE	-6.93	1.74	1.95
1	B	90	MSE	CG-SE	-6.88	1.74	1.95
1	A	90	MSE	CG-SE	-6.70	1.75	1.95
1	A	101	MSE	SE-CE	-6.54	1.75	1.95
1	C	101	MSE	SE-CE	-6.17	1.76	1.95
1	D	32	MSE	SE-CE	-6.16	1.76	1.95
1	B	315	MSE	SE-CE	-6.14	1.77	1.95

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	253	MSE	SE-CE	-5.90	1.77	1.95
1	D	253	MSE	CG-SE	-5.85	1.77	1.95
1	C	307	MSE	SE-CE	-5.80	1.78	1.95
1	D	307	MSE	SE-CE	-5.71	1.78	1.95
1	C	253	MSE	CG-SE	-5.52	1.78	1.95
1	B	315	MSE	CG-SE	-5.50	1.78	1.95
1	C	315	MSE	CG-SE	-5.42	1.79	1.95
1	C	90	MSE	CG-SE	-5.41	1.79	1.95
1	A	101	MSE	CG-SE	-5.25	1.79	1.95
1	C	315	MSE	SE-CE	-5.25	1.79	1.95
1	A	315	MSE	CG-SE	-5.14	1.80	1.95
1	D	307	MSE	CG-SE	-5.09	1.80	1.95
1	B	253	MSE	CG-SE	-5.07	1.80	1.95
1	B	32	MSE	CG-SE	-5.03	1.80	1.95
1	A	1	MSE	SE-CE	-5.02	1.80	1.95
1	C	32	MSE	CG-SE	-5.01	1.80	1.95

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	GLY	N-CA-C	-12.79	92.94	112.51
1	A	63	ASP	N-CA-C	-10.75	97.19	110.41
1	B	349	ALA	N-CA-C	-10.67	99.73	111.36
1	B	375	GLY	N-CA-C	-10.62	95.75	112.85
1	A	237	THR	N-CA-C	-9.97	97.37	110.43
1	A	170	VAL	N-CA-C	9.79	119.79	110.30
1	C	170	VAL	N-CA-C	9.70	119.71	110.30
1	A	254	ALA	N-CA-C	-9.61	100.67	111.82
1	A	105	PHE	N-CA-C	-9.06	98.56	110.53
1	B	40	ARG	N-CA-C	-8.86	101.73	112.54
1	A	365	VAL	N-CA-C	8.74	117.56	107.77
1	C	105	PHE	N-CA-C	-8.66	97.00	110.42
1	B	365	VAL	N-CA-C	8.53	117.45	107.73
1	B	170	VAL	N-CA-C	8.27	118.31	110.53
1	B	60	ALA	N-CA-C	8.22	122.09	112.72
1	D	105	PHE	N-CA-C	-8.19	98.34	110.46
1	A	377	PHE	N-CA-C	-7.91	104.08	112.93
1	B	166	ARG	N-CA-C	7.79	120.67	111.71
1	B	225	VAL	N-CA-C	7.73	122.64	112.98
1	A	169	ASP	N-CA-C	7.66	122.92	113.50
1	A	312	GLY	N-CA-C	7.66	120.32	111.36
1	D	75	GLY	N-CA-C	7.56	123.48	114.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	45	PHE	N-CA-C	-7.56	99.10	110.28
1	C	60	ALA	N-CA-C	7.46	122.23	113.20
1	B	365	VAL	CA-C-N	7.32	127.76	119.93
1	B	365	VAL	C-N-CA	7.32	127.76	119.93
1	A	231	ILE	N-CA-C	-7.31	103.66	110.53
1	A	41	ASN	N-CA-C	-7.13	104.38	113.23
1	B	377	PHE	N-CA-C	-6.99	104.84	113.15
1	A	349	ALA	N-CA-C	-6.95	102.92	111.33
1	B	12	VAL	N-CA-C	6.75	120.56	112.80
1	A	60	ALA	N-CA-C	6.74	120.40	112.72
1	A	227	ARG	N-CA-C	6.71	119.21	111.02
1	B	169	ASP	N-CA-C	6.66	122.90	114.31
1	C	161	GLY	N-CA-C	-6.63	98.66	110.86
1	A	161	GLY	N-CA-C	-6.55	98.69	112.45
1	B	311	ALA	N-CA-C	6.54	119.37	109.23
1	B	147	PHE	N-CA-C	-6.52	100.55	110.14
1	C	377	PHE	N-CA-C	-6.42	104.89	114.64
1	C	184	LEU	N-CA-C	-6.40	98.75	108.67
1	B	105	PHE	N-CA-C	-6.32	102.38	110.53
1	B	4	VAL	N-CA-C	6.25	114.77	107.77
1	C	349	ALA	N-CA-C	-6.25	104.52	111.71
1	B	160	SER	N-CA-C	6.24	118.89	111.71
1	A	184	LEU	N-CA-C	-6.18	97.63	108.20
1	C	237	THR	N-CA-C	-6.17	102.58	110.53
1	B	279	GLY	N-CA-C	6.12	123.48	115.40
1	D	301	ASN	N-CA-C	-6.12	105.82	113.28
1	A	142	LEU	CA-C-N	-6.09	113.25	119.83
1	A	142	LEU	C-N-CA	-6.09	113.25	119.83
1	A	265	VAL	N-CA-C	6.07	117.54	110.62
1	B	239	GLY	N-CA-C	-6.06	108.01	114.67
1	C	176	LEU	N-CA-C	-6.05	102.15	109.83
1	B	429	VAL	CA-C-N	6.02	125.93	119.85
1	B	429	VAL	C-N-CA	6.02	125.93	119.85
1	B	330	SER	N-CA-C	-6.01	105.24	113.30
1	C	169	ASP	N-CA-C	6.01	120.74	113.41
1	A	119	ARG	CA-C-N	5.97	126.28	119.83
1	A	119	ARG	C-N-CA	5.97	126.28	119.83
1	B	292	GLU	N-CA-C	5.93	120.69	112.45
1	A	420	VAL	N-CA-C	5.92	117.00	108.48
1	C	36	LYS	N-CA-C	-5.91	106.20	113.41
1	B	188	THR	N-CA-C	-5.83	102.00	110.64
1	D	160	SER	N-CA-C	5.83	118.38	111.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	THR	N-CA-C	-5.79	101.62	110.30
1	D	41	ASN	N-CA-C	-5.75	106.11	113.01
1	B	290	VAL	N-CA-C	5.72	121.25	109.34
1	A	104	PRO	N-CA-C	5.72	119.44	110.80
1	A	289	GLU	N-CA-C	5.69	120.00	112.72
1	D	148	VAL	N-CA-C	5.68	116.76	108.53
1	A	345	GLY	N-CA-C	-5.66	107.95	114.69
1	B	63	ASP	N-CA-C	-5.64	100.99	109.79
1	B	175	SER	N-CA-C	-5.63	102.14	110.48
1	B	428	GLY	N-CA-C	5.63	117.95	111.36
1	A	398	LEU	N-CA-C	5.62	117.85	109.25
1	B	306	PRO	N-CA-C	-5.59	103.02	111.41
1	A	311	ALA	N-CA-C	5.56	118.29	109.50
1	D	139	ALA	N-CA-C	-5.56	106.62	113.41
1	D	259	SER	N-CA-C	-5.56	106.00	112.89
1	C	180	ALA	N-CA-C	5.54	118.26	109.50
1	C	113	GLU	N-CA-C	-5.54	105.33	111.36
1	D	36	LYS	N-CA-C	-5.53	105.26	111.28
1	A	330	SER	N-CA-C	-5.52	106.31	113.16
1	A	236	TYR	N-CA-C	-5.49	104.93	111.03
1	B	327	HIS	N-CA-C	-5.43	101.69	110.32
1	C	293	HIS	N-CA-C	5.40	117.66	110.53
1	D	161	GLY	N-CA-C	-5.40	101.98	112.02
1	B	265	VAL	N-CA-C	5.39	118.60	111.17
1	C	409	LEU	N-CA-C	-5.37	105.59	111.82
1	D	311	ALA	N-CA-C	5.35	117.55	109.41
1	A	327	HIS	N-CA-C	-5.35	100.97	109.96
1	C	146	ALA	N-CA-C	5.34	116.11	108.74
1	D	349	ALA	N-CA-C	-5.33	105.87	112.38
1	D	276	PHE	N-CA-C	-5.31	105.54	112.23
1	A	294	THR	N-CA-C	5.31	117.98	111.82
1	D	242	LEU	CA-C-N	5.31	126.14	119.98
1	D	242	LEU	C-N-CA	5.31	126.14	119.98
1	B	220	ILE	CA-C-N	-5.30	114.33	119.90
1	B	220	ILE	C-N-CA	-5.30	114.33	119.90
1	C	126	TRP	N-CA-C	5.27	118.14	109.76
1	A	319	GLY	N-CA-C	5.26	125.65	113.18
1	C	78	GLY	CA-C-N	5.25	125.70	120.14
1	C	78	GLY	C-N-CA	5.25	125.70	120.14
1	A	126	TRP	N-CA-C	5.24	118.16	109.46
1	A	7	GLY	N-CA-C	5.24	125.59	113.18
1	B	180	ALA	N-CA-C	5.23	117.76	109.50

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	237	THR	N-CA-C	-5.23	102.79	110.52
1	D	42	HIS	N-CA-C	-5.20	106.62	113.17
1	B	78	GLY	CA-C-N	5.16	125.63	120.52
1	B	78	GLY	C-N-CA	5.16	125.63	120.52
1	A	66	GLY	N-CA-C	5.12	120.36	114.16
1	C	12	VAL	N-CA-C	5.12	116.21	111.81
1	B	58	THR	N-CA-C	-5.11	100.97	109.46
1	B	95	GLU	N-CA-C	-5.10	104.69	112.04
1	C	75	GLY	N-CA-C	5.09	121.77	114.64
1	C	242	LEU	CA-C-N	5.09	125.33	119.83
1	C	242	LEU	C-N-CA	5.09	125.33	119.83
1	B	310	LEU	N-CA-C	-5.08	100.12	108.41
1	D	60	ALA	N-CA-C	5.07	119.18	113.15
1	A	176	LEU	N-CA-C	-5.04	103.13	110.08
1	A	160	SER	N-CA-C	5.00	116.73	111.28

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	3326	0	3351	218	0
1	B	3326	0	3351	235	0
1	C	3326	0	3351	253	0
1	D	3326	0	3351	284	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
3	A	32	0	0	3	0
3	B	28	0	0	0	0
3	C	16	0	0	1	0
3	D	16	0	0	0	0
All	All	13404	0	13404	979	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 37.

All (979) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:GLU:HB3	1:C:40:ARG:HH11	0.97	1.13
1:C:37:GLU:HB3	1:C:40:ARG:NH1	1.76	1.00
1:D:227:ARG:HB2	1:D:227:ARG:HH21	1.25	0.99
1:C:73:ARG:HE	1:C:106:PHE:HA	1.24	0.98
1:C:235:LEU:HD23	1:C:247:ILE:HD13	1.45	0.97
1:C:36:LYS:H	1:C:36:LYS:HD3	1.29	0.97
1:D:59:HIS:CD2	1:D:61:HIS:HB2	2.00	0.96
1:A:36:LYS:H	1:A:36:LYS:HD3	1.31	0.95
1:C:160:SER:HB2	1:C:163:LEU:HD11	1.51	0.93
1:D:90:MSE:HE1	1:D:118:LEU:HD21	1.51	0.92
1:C:61:HIS:O	1:C:65:VAL:HG12	1.70	0.92
1:B:101:MSE:HB3	1:B:104:PRO:HB3	1.51	0.92
1:B:33:PHE:H	1:B:41:ASN:HD21	0.92	0.91
1:D:227:ARG:HH11	1:D:378:SER:HA	1.34	0.91
1:D:360:ILE:HG22	1:D:361:LEU:HD23	1.51	0.91
1:B:348:GLY:O	1:B:352:ILE:HG12	1.72	0.90
1:A:184:LEU:HD23	1:A:397:VAL:HG13	1.55	0.89
1:C:33:PHE:H	1:C:41:ASN:HD21	1.16	0.89
1:C:98:LEU:HD21	1:C:108:PRO:HB3	1.54	0.88
1:C:36:LYS:HD3	1:C:36:LYS:N	1.90	0.86
1:D:33:PHE:H	1:D:41:ASN:HD21	1.18	0.86
1:C:10:ARG:HH12	1:C:424:ARG:HG2	1.38	0.85
1:D:235:LEU:HD23	1:D:247:ILE:HD13	1.57	0.85
1:C:222:THR:HG22	1:C:339:VAL:HG21	1.57	0.85
1:C:37:GLU:CB	1:C:40:ARG:HH11	1.86	0.85
1:B:404:GLU:H	1:B:404:GLU:CD	1.82	0.84
1:B:168:LYS:HG2	1:B:197:TYR:CD2	2.13	0.84
1:A:31:GLY:HA3	1:A:64:HIS:N	1.91	0.84
1:D:420:VAL:HG22	1:D:421:SER:H	1.43	0.83
1:D:155:ARG:HH11	1:D:431:VAL:HG11	1.42	0.83
1:A:155:ARG:HE	1:A:431:VAL:CG2	1.90	0.82
1:C:359:ARG:H	1:C:359:ARG:HD2	1.43	0.82
1:A:48:ASP:OD2	1:A:51:GLU:HG2	1.79	0.82
1:B:141:HIS:HD2	1:B:379:GLY:O	1.62	0.82
1:B:11:GLU:OE1	1:B:37:GLU:HG3	1.80	0.81
1:C:163:LEU:HD21	1:C:389:TRP:CD2	2.15	0.81
1:A:91:GLU:O	1:A:95:GLU:HG2	1.81	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ARG:HE	1:B:431:VAL:HG13	1.45	0.81
1:C:278:GLN:HG3	1:C:280:LYS:HG2	1.64	0.80
1:B:3:ILE:HD11	1:B:17:HIS:HB3	1.62	0.80
1:B:33:PHE:H	1:B:41:ASN:ND2	1.77	0.80
1:C:86:THR:HG22	1:C:90:MSE:HE2	1.65	0.79
1:D:38:GLU:O	1:D:40:ARG:N	2.14	0.79
1:A:348:GLY:O	1:A:352:ILE:HG12	1.82	0.79
1:D:416:ARG:HD2	1:D:418:GLN:OE1	1.81	0.79
1:C:338:PHE:HB2	1:C:373:THR:HA	1.63	0.79
1:B:12:VAL:HG12	1:B:401:GLY:HA2	1.63	0.79
1:C:182:LEU:HD11	1:C:397:VAL:HG12	1.63	0.79
1:C:302:ARG:HH21	1:C:302:ARG:HB2	1.47	0.79
1:B:37:GLU:O	1:B:40:ARG:HG3	1.82	0.78
1:C:328:GLY:C	1:C:330:SER:H	1.89	0.78
1:D:59:HIS:HD2	1:D:61:HIS:HB2	1.48	0.78
1:B:33:PHE:N	1:B:41:ASN:HD21	1.77	0.78
1:D:59:HIS:HB3	1:D:145:SER:CB	2.14	0.78
1:B:63:ASP:O	1:B:65:VAL:N	2.17	0.78
1:A:33:PHE:H	1:A:41:ASN:HD21	1.31	0.77
1:B:61:HIS:O	1:B:65:VAL:HG12	1.84	0.77
1:A:309:VAL:HG11	1:A:324:HIS:ND1	1.99	0.76
1:D:170:VAL:HG21	1:D:230:GLU:HG3	1.66	0.76
1:D:359:ARG:HA	1:D:363:GLU:O	1.85	0.76
1:B:221:PRO:HB3	1:B:321:ILE:HG12	1.66	0.76
1:B:1:MSE:CB	1:B:21:ALA:HB2	2.16	0.76
1:C:132:LEU:HG	1:C:134:LEU:HD11	1.66	0.76
1:A:57:LEU:HG	1:A:65:VAL:HG23	1.68	0.75
1:B:394:PRO:O	1:B:395:ARG:HB2	1.87	0.75
1:D:387:LEU:HB3	1:D:416:ARG:HH12	1.52	0.75
1:B:208:LEU:HD21	1:B:218:VAL:HG11	1.69	0.74
1:A:155:ARG:HE	1:A:431:VAL:HG22	1.50	0.74
1:B:407:LEU:HD13	1:B:422:LEU:HD21	1.70	0.74
1:B:63:ASP:OD1	1:B:63:ASP:N	2.19	0.74
1:B:73:ARG:HE	1:B:106:PHE:HA	1.52	0.74
1:C:409:LEU:O	1:C:413:LEU:HG	1.86	0.74
1:C:123:TYR:HE1	1:C:146:ALA:HB2	1.52	0.74
1:D:220:ILE:HG22	1:D:222:THR:HG23	1.69	0.74
1:B:401:GLY:HA3	1:B:406:LEU:HD11	1.70	0.73
1:C:20:LEU:HD23	1:C:25:ARG:HG2	1.70	0.73
1:A:1:MSE:HG2	1:A:21:ALA:HB1	1.71	0.73
1:C:294:THR:HG22	1:C:320:ARG:HH11	1.52	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:LEU:HD12	1:B:133:SER:H	1.53	0.73
1:C:10:ARG:NH1	1:C:424:ARG:HG2	2.04	0.73
1:D:38:GLU:OE2	1:D:39:ALA:N	2.22	0.73
1:D:227:ARG:NH1	1:D:378:SER:HA	2.04	0.73
1:B:10:ARG:HG2	1:B:10:ARG:HH11	1.53	0.72
1:B:32:MSE:HA	1:B:67:ARG:HG3	1.71	0.72
1:D:27:LEU:HD13	1:D:29:ASP:O	1.88	0.72
1:C:236:TYR:N	1:C:285:PRO:HB3	2.05	0.72
1:A:1:MSE:HB3	1:A:21:ALA:HB2	1.71	0.72
1:D:1:MSE:HG2	1:D:21:ALA:HB1	1.70	0.72
1:D:227:ARG:HB2	1:D:227:ARG:NH2	2.04	0.72
1:D:153:GLU:O	1:D:155:ARG:HG2	1.90	0.72
1:A:103:GLU:O	1:A:103:GLU:HG2	1.89	0.72
1:B:45:PHE:HB3	1:B:47:PHE:CE1	2.25	0.71
1:B:36:LYS:H	1:B:36:LYS:HD3	1.55	0.71
1:C:259:SER:O	1:C:262:PRO:HD2	1.90	0.71
1:D:194:HIS:ND1	1:D:376:GLY:HA2	2.05	0.71
1:A:404:GLU:CD	1:A:404:GLU:H	1.97	0.71
1:A:63:ASP:O	1:A:64:HIS:HB2	1.90	0.71
1:D:214:GLN:NE2	1:D:333:ARG:HA	2.05	0.71
1:C:309:VAL:HG11	1:C:324:HIS:ND1	2.06	0.70
1:D:59:HIS:HB3	1:D:145:SER:HB2	1.73	0.70
1:B:220:ILE:HG22	1:B:222:THR:HG23	1.72	0.70
1:A:313:SER:HB2	1:A:319:GLY:H	1.56	0.70
1:D:309:VAL:HG11	1:D:324:HIS:ND1	2.05	0.70
1:A:208:LEU:HD23	1:A:218:VAL:HG21	1.74	0.70
1:B:155:ARG:HH11	1:B:431:VAL:HG11	1.55	0.70
1:C:10:ARG:HG2	1:C:10:ARG:HH11	1.56	0.70
1:A:155:ARG:HH11	1:A:431:VAL:HG21	1.57	0.69
1:C:49:PRO:HB3	1:C:71:LEU:HD12	1.74	0.69
1:B:63:ASP:C	1:B:65:VAL:H	2.01	0.69
1:D:37:GLU:O	1:D:38:GLU:O	2.11	0.69
1:D:191:ASP:OD2	1:D:192:ARG:HG3	1.93	0.69
1:D:420:VAL:HG22	1:D:421:SER:N	2.05	0.69
1:A:134:LEU:N	1:A:134:LEU:HD12	2.07	0.69
1:C:20:LEU:CD2	1:C:25:ARG:HG2	2.22	0.69
1:A:3:ILE:HD11	1:A:17:HIS:HB3	1.73	0.69
1:D:198:ARG:HG2	1:D:199:GLU:H	1.58	0.69
1:B:240:HIS:CE1	1:B:241:ARG:HH11	2.10	0.69
1:D:227:ARG:HH21	1:D:227:ARG:CB	2.05	0.69
1:D:291:VAL:HG11	1:D:297:SER:HB2	1.73	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MSE:HG2	1:D:21:ALA:CB	2.23	0.68
1:B:38:GLU:O	1:B:39:ALA:HB3	1.93	0.68
1:B:68:LEU:N	1:B:69:PRO:HD2	2.09	0.68
1:B:182:LEU:HD11	1:B:397:VAL:HG12	1.76	0.68
1:C:262:PRO:O	1:C:265:VAL:HG12	1.93	0.68
1:C:1:MSE:HG2	1:C:21:ALA:HB1	1.76	0.68
1:C:10:ARG:HH22	1:C:424:ARG:HG2	1.58	0.68
1:B:141:HIS:CD2	1:B:379:GLY:O	2.47	0.67
1:D:8:ALA:O	1:D:399:VAL:HG22	1.93	0.67
1:C:155:ARG:HB3	1:C:431:VAL:HG13	1.76	0.67
1:D:49:PRO:HB3	1:D:71:LEU:HD12	1.76	0.67
1:B:36:LYS:HD3	1:B:36:LYS:N	2.09	0.67
1:B:250:ASP:OD1	1:B:324:HIS:HE1	1.77	0.67
1:D:348:GLY:O	1:D:352:ILE:HG12	1.94	0.67
1:D:36:LYS:H	1:D:36:LYS:HD3	1.58	0.67
1:B:208:LEU:CD2	1:B:218:VAL:HG11	2.24	0.67
1:C:85:ALA:HB2	1:C:267:TYR:CD2	2.29	0.67
1:C:325:LEU:HG	1:C:329:LEU:HD22	1.77	0.67
1:C:160:SER:HB2	1:C:163:LEU:CD1	2.24	0.67
1:D:214:GLN:HE21	1:D:333:ARG:HA	1.60	0.67
1:D:32:MSE:HA	1:D:67:ARG:HG3	1.75	0.66
1:D:284:ARG:HA	1:D:288:LEU:HD22	1.77	0.66
1:D:313:SER:OG	1:D:318:GLY:HA3	1.95	0.66
1:B:97:ALA:O	1:B:101:MSE:HB2	1.95	0.66
1:B:155:ARG:HE	1:B:431:VAL:CG1	2.08	0.66
1:C:97:ALA:O	1:C:101:MSE:HB2	1.95	0.66
1:D:90:MSE:HE1	1:D:118:LEU:CD2	2.26	0.66
1:A:87:VAL:HG13	1:A:118:LEU:HD13	1.78	0.66
1:C:32:MSE:HA	1:C:67:ARG:HG3	1.78	0.66
1:D:196:PRO:HB2	1:D:199:GLU:OE2	1.96	0.66
1:A:330:SER:HA	1:A:366:PRO:O	1.96	0.65
1:A:191:ASP:OD2	1:A:192:ARG:HG2	1.96	0.65
1:C:153:GLU:O	1:C:155:ARG:HG2	1.95	0.65
1:D:198:ARG:HD2	1:D:198:ARG:N	2.11	0.65
1:A:155:ARG:NH1	1:A:431:VAL:HG21	2.11	0.65
1:D:182:LEU:HD11	1:D:397:VAL:HG12	1.79	0.65
1:B:225:VAL:O	1:B:225:VAL:CG1	2.44	0.65
1:B:398:LEU:CD2	1:B:420:VAL:HG23	2.27	0.65
1:C:313:SER:HB2	1:C:318:GLY:HA3	1.78	0.65
1:A:45:PHE:O	1:A:47:PHE:N	2.29	0.65
1:A:266:ARG:NH2	1:C:273:GLN:HE22	1.94	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MSE:HB2	1:B:21:ALA:HB2	1.77	0.64
1:B:32:MSE:HE2	1:B:105:PHE:HZ	1.61	0.64
1:D:54:ALA:HA	1:D:76:TYR:OH	1.97	0.64
1:D:335:ALA:O	1:D:337:VAL:HG23	1.97	0.64
1:D:402:GLU:HB3	1:D:404:GLU:OE2	1.96	0.64
1:B:87:VAL:HA	1:B:90:MSE:HE3	1.80	0.64
1:D:322:LEU:HB3	1:D:361:LEU:HD21	1.78	0.64
1:D:394:PRO:O	1:D:395:ARG:HB2	1.98	0.64
1:A:86:THR:HG22	1:A:90:MSE:HE3	1.80	0.64
1:D:12:VAL:HB	1:D:401:GLY:N	2.11	0.64
1:B:187:GLY:O	1:B:188:THR:C	2.40	0.64
1:C:177:PRO:HD3	1:C:389:TRP:NE1	2.12	0.64
1:C:415:LEU:C	1:C:417:GLY:H	2.05	0.64
1:B:130:GLY:O	1:B:131:ALA:HB3	1.98	0.63
1:C:3:ILE:HD12	1:C:17:HIS:HB3	1.80	0.63
1:A:302:ARG:HD3	1:A:302:ARG:N	2.13	0.63
1:B:328:GLY:O	1:B:329:LEU:CB	2.46	0.63
1:D:226:GLU:O	1:D:229:GLN:HG2	1.98	0.63
1:A:163:LEU:HD21	1:A:389:TRP:CE2	2.32	0.63
1:A:220:ILE:HG22	1:A:222:THR:HG23	1.79	0.63
1:B:1:MSE:HB3	1:B:21:ALA:HB2	1.80	0.63
1:C:375:GLY:O	1:C:377:PHE:N	2.32	0.63
1:D:289:GLU:O	1:D:290:VAL:HB	1.98	0.63
1:B:309:VAL:C	1:B:310:LEU:HD12	2.24	0.63
1:A:220:ILE:HG22	1:A:222:THR:CG2	2.28	0.63
1:C:348:GLY:O	1:C:352:ILE:HG12	1.98	0.63
1:B:191:ASP:OD2	1:B:192:ARG:HG2	1.98	0.63
1:B:395:ARG:HH22	1:B:431:VAL:HB	1.64	0.63
1:D:221:PRO:HD2	1:D:337:VAL:O	1.97	0.63
1:B:45:PHE:C	1:B:47:PHE:H	2.06	0.62
1:A:155:ARG:HE	1:A:431:VAL:HG21	1.64	0.62
1:C:73:ARG:NE	1:C:106:PHE:HA	2.05	0.62
1:A:12:VAL:HG23	1:A:400:HIS:CE1	2.33	0.62
1:C:96:ASP:O	1:C:100:VAL:HG22	2.00	0.62
1:C:233:TYR:CD1	1:C:282:PRO:HB2	2.35	0.62
1:C:202:ARG:O	1:C:206:GLU:HG3	1.99	0.62
1:C:211:THR:HG21	1:C:218:VAL:HG22	1.82	0.62
1:B:189:TYR:HE2	1:B:341:TYR:CD1	2.17	0.62
1:A:83:THR:O	1:A:87:VAL:HG23	1.99	0.62
1:D:217:LYS:HB2	1:D:334:ASN:OD1	2.00	0.62
1:D:195:ARG:HB3	1:D:375:GLY:O	2.00	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLU:O	1:A:40:ARG:N	2.30	0.62
1:D:32:MSE:HE1	1:D:101:MSE:HE2	1.82	0.62
1:A:398:LEU:HB3	1:A:406:LEU:HG	1.82	0.61
1:D:155:ARG:HE	1:D:431:VAL:HG13	1.65	0.61
1:A:177:PRO:HD3	1:A:389:TRP:CE2	2.34	0.61
1:C:247:ILE:O	1:C:288:LEU:HA	2.00	0.61
1:C:424:ARG:HD3	1:C:427:GLU:OE1	1.99	0.61
1:D:12:VAL:HB	1:D:401:GLY:H	1.66	0.61
1:A:98:LEU:HD13	1:A:106:PHE:CE2	2.36	0.61
1:D:97:ALA:O	1:D:101:MSE:HB2	2.01	0.61
1:B:238:HIS:HA	1:B:240:HIS:CE1	2.34	0.61
1:A:107:GLY:N	1:A:110:ASP:OD2	2.30	0.61
1:A:8:ALA:O	1:A:399:VAL:HG23	2.00	0.61
1:B:225:VAL:O	1:B:225:VAL:HG12	2.01	0.61
1:C:61:HIS:NE2	1:C:225:VAL:HG11	2.15	0.61
1:B:48:ASP:OD2	1:B:51:GLU:HG2	2.00	0.61
1:D:250:ASP:HA	1:D:291:VAL:HB	1.82	0.61
1:B:70:LYS:HE3	1:B:74:GLU:OE1	2.01	0.60
1:C:221:PRO:HD2	1:C:337:VAL:O	2.01	0.60
1:C:358:VAL:HG12	1:C:359:ARG:N	2.15	0.60
1:C:397:VAL:HA	1:C:421:SER:O	1.99	0.60
1:D:224:ALA:CB	1:D:254:ALA:HB2	2.31	0.60
1:C:8:ALA:HB1	1:C:400:HIS:HA	1.84	0.60
1:A:328:GLY:O	1:A:329:LEU:CB	2.49	0.60
1:B:265:VAL:HA	1:B:268:PHE:CD2	2.37	0.60
1:C:164:GLY:HA2	1:C:379:GLY:O	2.01	0.60
1:D:184:LEU:HD23	1:D:397:VAL:HG13	1.83	0.60
1:D:347:LEU:HG	1:D:348:GLY:H	1.67	0.60
1:C:298:LYS:HA	1:C:301:ASN:ND2	2.17	0.60
1:D:347:LEU:HG	1:D:348:GLY:N	2.16	0.60
1:A:253:MSE:O	1:A:257:VAL:HG23	2.02	0.60
1:C:302:ARG:HD3	1:C:302:ARG:N	2.16	0.60
1:B:37:GLU:OE2	1:B:40:ARG:HD2	2.02	0.60
1:B:354:ARG:HG3	1:B:354:ARG:O	2.02	0.60
1:D:190:GLY:O	1:D:409:LEU:HB2	2.01	0.60
1:D:197:TYR:O	1:D:201:VAL:HG23	2.02	0.60
1:A:163:LEU:HD21	1:A:389:TRP:CD2	2.37	0.59
1:C:313:SER:HB3	1:C:321:ILE:HG21	1.83	0.59
1:D:166:ARG:HG2	1:D:385:GLU:OE2	2.02	0.59
1:D:424:ARG:HD3	1:D:427:GLU:OE2	2.01	0.59
1:A:317:ALA:HA	1:A:322:LEU:HD11	1.85	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:PRO:HD3	1:B:389:TRP:CE2	2.36	0.59
1:C:85:ALA:HB3	1:C:144:GLY:HA3	1.85	0.59
1:D:163:LEU:N	1:D:163:LEU:HD12	2.16	0.59
1:D:236:TYR:CA	1:D:285:PRO:HB3	2.31	0.59
1:B:31:GLY:HA3	1:B:64:HIS:N	2.18	0.59
1:C:328:GLY:O	1:C:329:LEU:HB3	2.01	0.59
1:D:387:LEU:HB3	1:D:416:ARG:NH1	2.16	0.59
1:B:224:ALA:HB3	1:B:253:MSE:HE2	1.85	0.59
1:C:2:ARG:NH1	3:C:446:HOH:O	2.32	0.59
1:A:45:PHE:C	1:A:47:PHE:H	2.10	0.59
1:A:155:ARG:NE	1:A:431:VAL:HG21	2.18	0.59
1:C:359:ARG:HA	1:C:364:GLU:HA	1.83	0.59
1:D:237:THR:O	1:D:238:HIS:HB2	2.02	0.59
1:D:238:HIS:HA	1:D:241:ARG:NH1	2.18	0.59
1:C:219:LEU:HD11	1:C:324:HIS:HB3	1.84	0.59
1:B:37:GLU:O	1:B:38:GLU:O	2.21	0.59
1:B:338:PHE:CD1	1:B:342:GLN:NE2	2.71	0.59
1:D:235:LEU:CD2	1:D:247:ILE:HD13	2.32	0.59
1:B:202:ARG:O	1:B:206:GLU:HG3	2.01	0.59
1:C:235:LEU:CD2	1:C:247:ILE:HD13	2.28	0.59
1:C:236:TYR:CA	1:C:285:PRO:HB3	2.33	0.59
1:A:111:VAL:O	1:A:115:LEU:HB2	2.03	0.59
1:A:374:LEU:C	1:A:375:GLY:O	2.37	0.59
1:C:36:LYS:H	1:C:36:LYS:CD	2.03	0.58
1:D:10:ARG:HH22	1:D:424:ARG:NH2	2.00	0.58
1:C:10:ARG:NH2	1:C:424:ARG:HG2	2.18	0.58
1:C:355:PRO:HB2	1:C:356:PRO:HD2	1.85	0.58
1:D:208:LEU:HD23	1:D:218:VAL:HG21	1.83	0.58
1:D:388:ASP:O	1:D:391:GLN:HB3	2.03	0.58
1:A:58:THR:O	1:A:59:HIS:O	2.20	0.58
1:A:222:THR:HG22	1:A:339:VAL:CG2	2.32	0.58
1:B:251:SER:HB3	1:B:254:ALA:HB3	1.85	0.58
1:C:155:ARG:HE	1:C:431:VAL:CG1	2.15	0.58
1:C:357:ALA:HB2	1:C:366:PRO:HA	1.86	0.58
1:A:141:HIS:HD2	1:A:379:GLY:O	1.86	0.58
1:D:98:LEU:HD21	1:D:108:PRO:HB3	1.85	0.58
1:A:165:ASN:C	1:A:165:ASN:HD22	2.10	0.58
1:C:209:GLU:C	1:C:211:THR:H	2.12	0.58
1:D:394:PRO:O	1:D:395:ARG:CB	2.51	0.58
1:A:289:GLU:O	1:A:290:VAL:HB	2.04	0.58
1:A:328:GLY:O	1:A:329:LEU:HB2	2.02	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:VAL:HA	1:B:268:PHE:HD2	1.66	0.58
1:D:246:PRO:HB2	1:D:248:TYR:CE1	2.37	0.58
1:A:186:GLU:OE2	1:A:188:THR:OG1	2.21	0.58
1:A:359:ARG:NH2	1:A:362:GLY:HA2	2.19	0.58
1:B:91:GLU:O	1:B:95:GLU:HG2	2.04	0.57
1:D:90:MSE:C	1:D:92:ILE:H	2.11	0.57
1:B:316:LEU:O	1:B:317:ALA:C	2.47	0.57
1:B:317:ALA:HA	1:B:322:LEU:HD11	1.86	0.57
1:A:86:THR:O	1:A:90:MSE:HB2	2.05	0.57
1:C:251:SER:HB3	1:C:254:ALA:HB3	1.86	0.57
1:B:10:ARG:CD	1:B:403:GLU:HG3	2.33	0.57
1:A:86:THR:HG22	1:A:90:MSE:CE	2.34	0.57
1:A:250:ASP:OD2	1:A:320:ARG:NH2	2.37	0.57
1:C:87:VAL:HA	1:C:90:MSE:HE3	1.87	0.57
1:D:275:HIS:HA	1:D:278:GLN:HG2	1.86	0.57
1:C:296:ALA:HA	1:C:299:ALA:HB3	1.87	0.57
1:D:274:ALA:O	1:D:277:LEU:HB3	2.05	0.57
1:A:157:LEU:HG	1:A:158:VAL:N	2.15	0.57
1:D:395:ARG:HH22	1:D:431:VAL:HB	1.69	0.57
1:C:61:HIS:CD2	1:C:225:VAL:HG11	2.39	0.57
1:C:387:LEU:HD22	1:C:416:ARG:NH1	2.19	0.57
1:A:85:ALA:HB2	1:A:267:TYR:CD2	2.39	0.57
1:B:32:MSE:HE2	1:B:105:PHE:CZ	2.39	0.57
1:B:238:HIS:O	1:B:241:ARG:HG2	2.05	0.57
1:A:186:GLU:OE1	1:A:380:HIS:HD2	1.88	0.56
1:B:101:MSE:HE1	1:B:106:PHE:CE1	2.40	0.56
1:D:33:PHE:H	1:D:41:ASN:ND2	1.96	0.56
1:D:198:ARG:HG2	1:D:199:GLU:N	2.19	0.56
1:B:404:GLU:OE2	1:B:404:GLU:N	2.31	0.56
1:C:360:ILE:O	1:C:361:LEU:HB2	2.05	0.56
1:D:347:LEU:O	1:D:349:ALA:N	2.38	0.56
1:C:57:LEU:HD22	1:C:80:VAL:HG12	1.88	0.56
1:C:7:GLY:HA3	1:C:14:GLY:O	2.06	0.56
1:C:233:TYR:CE1	1:C:282:PRO:HB2	2.40	0.56
1:C:296:ALA:HA	1:C:299:ALA:CB	2.36	0.56
1:B:103:GLU:N	1:B:104:PRO:HD3	2.21	0.56
1:C:68:LEU:N	1:C:69:PRO:HD2	2.19	0.56
1:C:204:PHE:HB2	1:C:374:LEU:HD13	1.88	0.56
1:B:61:HIS:O	1:B:63:ASP:O	2.23	0.56
1:C:10:ARG:HH22	1:C:424:ARG:HH21	1.54	0.56
1:D:12:VAL:HG23	1:D:400:HIS:ND1	2.21	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:GLU:C	1:A:38:GLU:O	2.49	0.55
1:A:333:ARG:HG2	1:A:333:ARG:HH21	1.71	0.55
1:B:224:ALA:CB	1:B:253:MSE:HE2	2.36	0.55
1:C:10:ARG:NH2	1:C:424:ARG:HH21	2.04	0.55
1:C:148:VAL:HG12	1:C:149:VAL:N	2.21	0.55
1:C:339:VAL:HG23	1:C:340:GLY:H	1.70	0.55
1:D:12:VAL:HG22	1:D:12:VAL:O	2.06	0.55
1:D:236:TYR:HA	1:D:285:PRO:HB3	1.88	0.55
1:B:1:MSE:HB3	1:B:21:ALA:CB	2.37	0.55
1:B:187:GLY:O	1:B:190:GLY:N	2.39	0.55
1:C:1:MSE:O	1:C:431:VAL:N	2.37	0.55
1:A:222:THR:HG22	1:A:339:VAL:HG21	1.87	0.55
1:B:38:GLU:O	1:B:39:ALA:CB	2.54	0.55
1:B:401:GLY:CA	1:B:406:LEU:HD11	2.37	0.55
1:D:347:LEU:CG	1:D:348:GLY:H	2.19	0.55
1:A:97:ALA:HA	1:A:100:VAL:HG22	1.88	0.55
1:C:85:ALA:HB2	1:C:267:TYR:CE2	2.41	0.55
1:B:327:HIS:O	1:B:328:GLY:O	2.25	0.55
1:B:395:ARG:HA	1:B:419:GLU:O	2.07	0.55
1:D:248:TYR:O	1:D:310:LEU:HD12	2.07	0.55
1:B:1:MSE:O	1:B:431:VAL:N	2.40	0.55
1:C:302:ARG:HD3	1:C:302:ARG:H	1.72	0.55
1:C:328:GLY:C	1:C:330:SER:N	2.59	0.55
1:B:220:ILE:HG22	1:B:222:THR:CG2	2.37	0.55
1:B:304:PRO:O	1:B:305:GLY:O	2.25	0.55
1:C:38:GLU:C	1:C:40:ARG:H	2.14	0.55
1:C:177:PRO:HD3	1:C:389:TRP:CE2	2.42	0.55
1:D:55:VAL:CG2	1:D:80:VAL:HG13	2.36	0.55
1:A:57:LEU:HD22	1:A:80:VAL:CG1	2.37	0.55
1:C:415:LEU:C	1:C:417:GLY:N	2.66	0.54
1:D:354:ARG:HG3	1:D:354:ARG:O	2.07	0.54
1:B:225:VAL:O	1:B:226:GLU:HB2	2.07	0.54
1:A:3:ILE:HD13	1:A:4:VAL:N	2.22	0.54
1:A:65:VAL:HG13	1:A:65:VAL:O	2.07	0.54
1:A:259:SER:O	1:A:262:PRO:HD2	2.08	0.54
1:B:88:LEU:HD12	1:B:264:LEU:HD11	1.90	0.54
1:D:49:PRO:CB	1:D:71:LEU:HD12	2.38	0.54
1:D:204:PHE:CE1	1:D:208:LEU:HD11	2.42	0.54
1:C:195:ARG:HH21	1:C:195:ARG:HG3	1.72	0.54
1:C:237:THR:HG22	1:C:238:HIS:ND1	2.23	0.54
1:D:353:ALA:HB3	1:D:355:PRO:HD3	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MSE:HG2	1:A:21:ALA:CB	2.38	0.54
1:C:360:ILE:HG22	1:C:361:LEU:CD2	2.38	0.54
1:D:12:VAL:HB	1:D:401:GLY:CA	2.38	0.54
1:D:38:GLU:C	1:D:40:ARG:H	2.11	0.54
1:A:1:MSE:CB	1:A:21:ALA:HB2	2.37	0.54
1:B:189:TYR:CE2	1:B:341:TYR:CD1	2.95	0.54
1:C:332:PRO:HD3	1:C:368:ARG:HB3	1.90	0.54
1:A:11:GLU:OE1	1:A:40:ARG:NH1	2.41	0.54
1:D:237:THR:HG22	1:D:238:HIS:ND1	2.23	0.54
1:D:257:VAL:HG12	1:D:261:TYR:CD2	2.42	0.54
1:C:128:ARG:NH2	1:C:128:ARG:HG3	2.23	0.53
1:D:244:ARG:HG3	1:D:244:ARG:HH11	1.74	0.53
1:A:3:ILE:CD1	1:A:17:HIS:HB3	2.36	0.53
1:B:399:VAL:HG22	1:B:400:HIS:H	1.71	0.53
1:C:94:LEU:HD13	1:C:111:VAL:HG13	1.89	0.53
1:A:54:ALA:HA	1:A:76:TYR:OH	2.08	0.53
1:C:32:MSE:HE2	1:C:105:PHE:HZ	1.74	0.53
1:D:396:VAL:HG12	1:D:398:LEU:HD22	1.90	0.53
1:C:36:LYS:N	1:C:36:LYS:CD	2.66	0.53
1:C:360:ILE:HG22	1:C:361:LEU:HD23	1.88	0.53
1:D:248:TYR:CE1	1:D:307:MSE:HE2	2.43	0.53
1:D:249:LEU:HB3	1:D:290:VAL:HA	1.89	0.53
1:D:251:SER:HB3	1:D:254:ALA:HB3	1.90	0.53
1:A:399:VAL:HG22	1:A:400:HIS:N	2.22	0.53
1:C:10:ARG:HH11	1:C:10:ARG:CG	2.22	0.53
1:A:191:ASP:CG	1:A:405:LYS:HD3	2.33	0.53
1:B:5:PRO:HA	1:B:17:HIS:HD2	1.73	0.53
1:C:302:ARG:HH21	1:C:302:ARG:CB	2.19	0.53
1:D:130:GLY:C	1:D:132:LEU:H	2.16	0.53
1:D:182:LEU:HD11	1:D:397:VAL:CG1	2.39	0.53
1:D:278:GLN:O	1:D:280:LYS:HG2	2.09	0.53
1:D:309:VAL:HG11	1:D:324:HIS:CE1	2.44	0.53
1:A:156:THR:HG22	1:A:180:ALA:CB	2.39	0.53
1:A:229:GLN:HG3	1:A:261:TYR:CZ	2.44	0.53
1:B:28:LEU:O	1:B:29:ASP:HB2	2.09	0.53
1:B:398:LEU:HD22	1:B:398:LEU:H	1.74	0.53
1:C:204:PHE:O	1:C:208:LEU:HG	2.09	0.53
1:D:420:VAL:CG2	1:D:421:SER:H	2.17	0.53
1:C:243:PRO:O	1:C:244:ARG:C	2.52	0.53
1:C:45:PHE:HB3	1:C:47:PHE:CE1	2.43	0.53
1:A:207:ILE:HG12	1:A:372:HIS:CE1	2.44	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:LEU:HD12	1:C:163:LEU:N	2.24	0.52
1:D:65:VAL:HG21	1:D:90:MSE:SE	2.58	0.52
1:D:142:LEU:HD12	1:D:226:GLU:HG3	1.91	0.52
1:B:45:PHE:O	1:B:47:PHE:N	2.43	0.52
1:B:250:ASP:OD1	1:B:324:HIS:CE1	2.61	0.52
1:A:36:LYS:H	1:A:36:LYS:CD	2.08	0.52
1:B:310:LEU:HD12	1:B:310:LEU:N	2.24	0.52
1:D:195:ARG:O	1:D:196:PRO:C	2.53	0.52
1:B:105:PHE:O	1:B:106:PHE:O	2.27	0.52
1:D:165:ASN:HB2	1:D:380:HIS:O	2.09	0.52
1:D:269:SER:O	1:D:273:GLN:HG3	2.10	0.52
1:A:315:MSE:HG2	1:A:343:PRO:HD3	1.91	0.52
1:C:375:GLY:O	1:C:376:GLY:C	2.53	0.52
1:A:31:GLY:HA3	1:A:64:HIS:H	1.70	0.52
1:A:422:LEU:O	1:A:423:ALA:C	2.52	0.52
1:B:350:GLU:O	1:B:353:ALA:HB3	2.10	0.52
1:D:87:VAL:HG13	1:D:118:LEU:HD13	1.91	0.52
1:D:324:HIS:O	1:D:325:LEU:HD12	2.10	0.52
1:B:37:GLU:HB3	1:B:40:ARG:HD3	1.91	0.52
1:B:140:GLY:O	1:B:164:GLY:HA3	2.10	0.52
1:B:410:GLY:CA	1:B:420:VAL:HG21	2.40	0.52
1:D:129:LEU:O	1:D:130:GLY:O	2.27	0.52
1:D:216:GLY:HA3	1:D:333:ARG:O	2.09	0.52
1:D:233:TYR:HD1	1:D:282:PRO:O	1.92	0.52
1:D:347:LEU:CG	1:D:348:GLY:N	2.72	0.52
1:C:424:ARG:HG2	1:C:424:ARG:HH21	1.76	0.51
1:D:162:ASP:HA	1:D:186:GLU:OE1	2.10	0.51
1:B:5:PRO:HG2	1:B:423:ALA:HB1	1.92	0.51
1:D:9:ALA:C	1:D:11:GLU:H	2.17	0.51
1:A:128:ARG:NH2	1:A:128:ARG:HG3	2.24	0.51
1:A:266:ARG:NH2	1:C:273:GLN:NE2	2.56	0.51
1:B:80:VAL:HB	1:B:118:LEU:HD23	1.92	0.51
1:B:325:LEU:HG	1:B:329:LEU:HD22	1.92	0.51
1:C:87:VAL:HG13	1:C:118:LEU:HD13	1.92	0.51
1:C:249:LEU:HB3	1:C:290:VAL:HA	1.92	0.51
1:D:163:LEU:N	1:D:163:LEU:CD1	2.73	0.51
1:D:410:GLY:HA2	1:D:420:VAL:HG21	1.93	0.51
1:B:63:ASP:C	1:B:65:VAL:N	2.62	0.51
1:C:209:GLU:OE1	1:C:209:GLU:HA	2.10	0.51
1:D:233:TYR:CE1	1:D:282:PRO:HB2	2.45	0.51
1:D:253:MSE:HA	1:D:256:ARG:CZ	2.41	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:ILE:O	1:D:325:LEU:HD13	2.10	0.51
1:A:430:PRO:O	1:A:431:VAL:HB	2.10	0.51
1:B:36:LYS:N	1:B:36:LYS:CD	2.71	0.51
1:C:223:PHE:HE2	1:C:315:MSE:HE2	1.76	0.51
1:A:130:GLY:O	1:A:131:ALA:HB3	2.09	0.51
1:D:181:ASP:O	1:D:395:ARG:HB2	2.11	0.51
1:B:31:GLY:HA3	1:B:64:HIS:H	1.76	0.51
1:C:375:GLY:O	1:C:377:PHE:HB2	2.11	0.51
1:A:73:ARG:HB2	1:A:110:ASP:OD1	2.09	0.51
1:A:266:ARG:HH21	1:C:273:GLN:HE22	1.57	0.51
1:B:126:TRP:CE3	1:D:178:PRO:HB3	2.45	0.51
1:B:251:SER:HB3	1:B:254:ALA:CB	2.40	0.50
1:A:155:ARG:CZ	1:A:431:VAL:HG21	2.40	0.50
1:A:219:LEU:HD13	1:A:219:LEU:N	2.26	0.50
1:B:327:HIS:C	1:B:328:GLY:O	2.54	0.50
1:C:177:PRO:HD3	1:C:389:TRP:CD1	2.47	0.50
1:D:188:THR:C	1:D:190:GLY:N	2.68	0.50
1:D:284:ARG:NH2	1:D:288:LEU:HD23	2.26	0.50
1:D:301:ASN:HB3	1:D:327:HIS:HB3	1.93	0.50
1:A:358:VAL:HG12	1:A:359:ARG:N	2.26	0.50
1:C:155:ARG:HE	1:C:431:VAL:HG11	1.75	0.50
1:C:204:PHE:CE1	1:C:208:LEU:HD11	2.46	0.50
1:D:10:ARG:HE	1:D:422:LEU:HB3	1.76	0.50
1:B:22:GLY:O	1:B:130:GLY:O	2.30	0.50
1:D:92:ILE:O	1:D:95:GLU:N	2.45	0.50
1:A:84:ARG:NH2	1:A:122:GLU:HG2	2.27	0.50
1:B:62:LEU:O	1:B:66:GLY:N	2.44	0.50
1:B:404:GLU:CD	1:B:404:GLU:N	2.62	0.50
1:C:281:ASN:O	1:C:283:PHE:N	2.44	0.50
1:C:411:LYS:O	1:C:414:ALA:HB3	2.12	0.50
1:D:244:ARG:HG3	1:D:244:ARG:NH1	2.26	0.50
1:D:425:PHE:C	1:D:427:GLU:H	2.20	0.50
1:D:90:MSE:C	1:D:92:ILE:N	2.69	0.50
1:D:112:GLU:HG3	1:D:113:GLU:N	2.26	0.50
1:C:354:ARG:NH1	1:C:371:VAL:HG23	2.27	0.50
1:D:130:GLY:O	1:D:132:LEU:N	2.45	0.50
1:C:207:ILE:HD13	1:C:372:HIS:CG	2.46	0.50
1:B:9:ALA:O	1:B:11:GLU:HG2	2.12	0.50
1:C:62:LEU:HD22	1:C:93:VAL:HG13	1.94	0.50
1:C:258:LEU:HD21	1:C:283:PHE:HB3	1.93	0.50
1:C:357:ALA:CB	1:C:366:PRO:HA	2.41	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:VAL:HG23	1:C:340:GLY:N	2.26	0.49
1:A:236:TYR:C	1:A:237:THR:O	2.46	0.49
1:C:105:PHE:O	1:C:106:PHE:O	2.30	0.49
1:C:123:TYR:CE1	1:C:146:ALA:HB2	2.39	0.49
1:C:186:GLU:HA	1:C:399:VAL:O	2.13	0.49
1:C:309:VAL:C	1:C:310:LEU:HD12	2.38	0.49
1:D:233:TYR:HE1	1:D:282:PRO:HB2	1.76	0.49
1:D:287:GLY:O	1:D:288:LEU:C	2.55	0.49
1:A:205:LEU:HD11	1:A:238:HIS:CD2	2.47	0.49
1:A:244:ARG:HB3	1:B:295:GLU:OE1	2.12	0.49
1:B:132:LEU:HD12	1:B:133:SER:N	2.24	0.49
1:C:1:MSE:HG2	1:C:21:ALA:CB	2.40	0.49
1:C:396:VAL:HG12	1:C:398:LEU:HD22	1.93	0.49
1:D:32:MSE:HE1	1:D:101:MSE:CE	2.42	0.49
1:D:352:ILE:HG22	1:D:352:ILE:O	2.10	0.49
1:D:421:SER:C	1:D:422:LEU:HD12	2.37	0.49
1:C:10:ARG:HH12	1:C:424:ARG:CG	2.18	0.49
1:C:27:LEU:HD13	1:C:29:ASP:O	2.12	0.49
1:C:55:VAL:HG22	1:C:80:VAL:HG13	1.95	0.49
1:C:195:ARG:O	1:C:196:PRO:C	2.55	0.49
1:C:237:THR:HG22	1:C:238:HIS:N	2.28	0.49
1:D:237:THR:O	1:D:238:HIS:CB	2.60	0.49
1:B:237:THR:C	1:B:239:GLY:H	2.19	0.49
1:B:250:ASP:OD2	1:B:320:ARG:NH2	2.42	0.49
1:A:277:LEU:C	1:A:279:GLY:H	2.20	0.49
1:A:290:VAL:HG12	1:A:290:VAL:O	2.13	0.49
1:B:12:VAL:HG12	1:B:401:GLY:CA	2.38	0.49
1:B:324:HIS:O	1:B:327:HIS:O	2.31	0.49
1:C:193:PRO:HD3	1:C:383:GLN:HE21	1.78	0.49
1:C:246:PRO:HB2	1:C:248:TYR:CZ	2.47	0.49
1:D:77:ARG:NE	1:D:113:GLU:OE1	2.44	0.49
1:D:188:THR:O	1:D:189:TYR:C	2.54	0.49
1:D:269:SER:OG	1:D:272:VAL:HG23	2.13	0.49
1:A:8:ALA:HB3	1:A:399:VAL:HG22	1.95	0.49
1:A:105:PHE:O	1:A:106:PHE:O	2.30	0.49
1:B:105:PHE:CD1	1:B:106:PHE:HD1	2.31	0.49
1:A:63:ASP:O	1:A:64:HIS:CB	2.57	0.49
1:C:359:ARG:HH21	1:C:359:ARG:HG3	1.78	0.49
1:D:59:HIS:NE2	1:D:61:HIS:HB2	2.26	0.49
1:D:228:ALA:O	1:D:232:LEU:HG	2.13	0.49
1:D:337:VAL:HG13	1:D:372:HIS:O	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:GLU:O	1:A:38:GLU:O	2.31	0.49
1:B:19:LEU:CD2	1:B:132:LEU:HD21	2.42	0.49
1:C:37:GLU:O	1:C:38:GLU:O	2.31	0.49
1:C:94:LEU:HD12	1:C:115:LEU:HD11	1.94	0.49
1:C:163:LEU:HD21	1:C:389:TRP:CE2	2.48	0.49
1:C:246:PRO:HB2	1:C:248:TYR:CE1	2.48	0.49
1:B:22:GLY:CA	1:B:131:ALA:HB3	2.43	0.49
1:B:103:GLU:N	1:B:104:PRO:CD	2.76	0.49
1:B:209:GLU:O	1:B:213:SER:HB2	2.13	0.49
1:D:198:ARG:HD2	1:D:198:ARG:H	1.78	0.49
1:A:8:ALA:O	1:A:399:VAL:CG2	2.61	0.48
1:A:10:ARG:NH1	1:A:10:ARG:HG2	2.28	0.48
1:A:396:VAL:HG12	1:A:398:LEU:HD13	1.94	0.48
1:A:398:LEU:HD23	1:A:406:LEU:O	2.12	0.48
1:B:188:THR:HG22	1:B:189:TYR:CD1	2.48	0.48
1:C:366:PRO:HB3	1:C:368:ARG:HH12	1.78	0.48
1:D:3:ILE:CD1	1:D:17:HIS:HB3	2.43	0.48
1:B:422:LEU:HD12	1:B:422:LEU:N	2.28	0.48
1:D:351:ILE:C	1:D:353:ALA:H	2.21	0.48
1:C:111:VAL:O	1:C:115:LEU:HD13	2.13	0.48
1:C:27:LEU:O	1:C:55:VAL:HA	2.13	0.48
1:C:38:GLU:O	1:C:40:ARG:N	2.41	0.48
1:C:348:GLY:H	1:C:351:ILE:HG13	1.78	0.48
1:B:230:GLU:O	1:B:234:VAL:HG23	2.14	0.48
1:C:84:ARG:HD2	1:C:122:GLU:OE2	2.12	0.48
1:C:137:GLY:O	1:C:146:ALA:HB1	2.13	0.48
1:A:102:ASP:O	1:A:103:GLU:C	2.57	0.48
1:A:165:ASN:C	1:A:165:ASN:ND2	2.71	0.48
1:B:394:PRO:O	1:B:395:ARG:CB	2.57	0.48
1:C:212:LEU:C	1:C:214:GLN:H	2.20	0.48
1:D:7:GLY:O	1:D:9:ALA:N	2.45	0.48
1:C:10:ARG:HH22	1:C:424:ARG:CG	2.26	0.48
1:A:250:ASP:OD1	1:A:297:SER:OG	2.29	0.48
1:D:233:TYR:C	1:D:235:LEU:H	2.21	0.48
1:D:363:GLU:HG3	1:D:364:GLU:N	2.29	0.48
1:A:68:LEU:N	1:A:69:PRO:HD2	2.28	0.48
1:A:103:GLU:N	1:A:104:PRO:CD	2.77	0.48
1:A:155:ARG:NE	1:A:431:VAL:CG2	2.66	0.48
1:A:237:THR:HG22	1:A:238:HIS:ND1	2.29	0.48
1:D:219:LEU:N	1:D:219:LEU:HD22	2.28	0.48
1:D:245:ALA:O	1:D:246:PRO:C	2.57	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:TYR:CE2	1:D:289:GLU:HG2	2.48	0.48
1:D:263:ARG:C	1:D:265:VAL:H	2.22	0.48
1:D:422:LEU:HD12	1:D:422:LEU:N	2.28	0.48
1:A:75:GLY:O	1:A:77:ARG:HG2	2.13	0.47
1:C:10:ARG:NH1	1:C:423:ALA:O	2.47	0.47
1:C:61:HIS:HE2	1:C:225:VAL:HG11	1.78	0.47
1:D:160:SER:HB2	1:D:163:LEU:HD11	1.95	0.47
1:D:409:LEU:O	1:D:413:LEU:HG	2.14	0.47
1:A:421:SER:C	1:A:422:LEU:HD12	2.39	0.47
1:C:237:THR:HG22	1:C:238:HIS:H	1.79	0.47
1:D:1:MSE:HE1	1:D:157:LEU:CB	2.44	0.47
1:B:32:MSE:HE1	1:B:101:MSE:HE2	1.95	0.47
1:B:358:VAL:CG1	1:B:359:ARG:N	2.76	0.47
1:C:8:ALA:O	1:C:399:VAL:CG2	2.62	0.47
1:D:19:LEU:HD13	1:D:157:LEU:CD2	2.44	0.47
1:B:142:LEU:O	1:B:143:PRO:C	2.53	0.47
1:C:8:ALA:O	1:C:399:VAL:HG22	2.15	0.47
1:D:148:VAL:O	1:D:158:VAL:HA	2.14	0.47
1:D:212:LEU:HD22	1:D:306:PRO:HB2	1.97	0.47
1:D:222:THR:HG22	1:D:339:VAL:HG21	1.95	0.47
1:A:97:ALA:O	1:A:101:MSE:HB2	2.13	0.47
1:A:122:GLU:O	1:A:125:GLU:HB2	2.13	0.47
1:A:344:GLN:OE1	1:A:345:GLY:N	2.48	0.47
1:B:68:LEU:N	1:B:69:PRO:CD	2.76	0.47
1:C:10:ARG:CZ	1:C:424:ARG:HG2	2.43	0.47
1:C:219:LEU:HD22	1:C:219:LEU:N	2.29	0.47
1:C:341:TYR:HD1	1:C:341:TYR:H	1.61	0.47
1:A:67:ARG:C	1:A:69:PRO:HD2	2.39	0.47
1:B:9:ALA:C	1:B:11:GLU:H	2.23	0.47
1:D:265:VAL:HA	1:D:268:PHE:HD2	1.78	0.47
1:D:278:GLN:HG3	1:D:280:LYS:HG2	1.95	0.47
1:A:168:LYS:NZ	1:A:230:GLU:OE1	2.44	0.47
1:B:24:ARG:HG3	1:B:24:ARG:HH11	1.80	0.47
1:B:86:THR:HG22	1:B:90:MSE:HE2	1.96	0.47
1:B:166:ARG:HG2	1:B:385:GLU:OE2	2.14	0.47
1:C:258:LEU:HD11	1:C:283:PHE:O	2.14	0.47
1:C:358:VAL:CG1	1:C:359:ARG:N	2.77	0.47
1:B:101:MSE:CB	1:B:104:PRO:HB3	2.36	0.47
1:B:233:TYR:OH	1:B:271:GLU:OE1	2.29	0.47
1:B:36:LYS:H	1:B:36:LYS:CD	2.19	0.47
1:C:224:ALA:HB3	1:C:253:MSE:HE2	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:HIS:HD2	1:D:61:HIS:H	1.62	0.47
1:D:59:HIS:HB3	1:D:145:SER:HB3	1.96	0.47
1:A:45:PHE:C	1:A:47:PHE:N	2.72	0.47
1:B:208:LEU:CD2	1:B:218:VAL:HG21	2.45	0.47
1:B:328:GLY:O	1:B:329:LEU:HB2	2.14	0.47
1:D:399:VAL:O	1:D:400:HIS:O	2.33	0.47
1:A:425:PHE:C	1:A:425:PHE:CD2	2.92	0.46
1:B:48:ASP:C	1:B:50:LYS:H	2.23	0.46
1:B:188:THR:HG22	1:B:189:TYR:CE1	2.50	0.46
1:B:317:ALA:H	1:B:322:LEU:HD21	1.80	0.46
1:A:62:LEU:HD13	1:A:93:VAL:HG12	1.96	0.46
1:A:366:PRO:HB3	1:A:368:ARG:HH12	1.81	0.46
1:A:397:VAL:HG13	1:A:397:VAL:O	2.15	0.46
1:B:400:HIS:O	1:B:400:HIS:ND1	2.48	0.46
1:C:313:SER:HB3	1:C:321:ILE:CG2	2.45	0.46
1:D:1:MSE:HE1	1:D:157:LEU:HB2	1.97	0.46
1:D:166:ARG:C	1:D:168:LYS:H	2.23	0.46
1:D:248:TYR:CD2	1:D:289:GLU:HG2	2.50	0.46
1:D:336:LEU:C	1:D:336:LEU:HD23	2.40	0.46
1:C:222:THR:HG22	1:C:339:VAL:CG2	2.36	0.46
1:B:21:ALA:HB3	1:B:132:LEU:HD22	1.97	0.46
1:C:84:ARG:HB2	1:C:267:TYR:OH	2.15	0.46
1:C:359:ARG:HG3	1:C:359:ARG:NH2	2.31	0.46
1:D:57:LEU:HD23	1:D:90:MSE:SE	2.64	0.46
1:B:182:LEU:HD11	1:B:397:VAL:CG1	2.44	0.46
1:B:235:LEU:HD12	1:B:242:LEU:HD11	1.96	0.46
1:C:57:LEU:HD22	1:C:80:VAL:CG1	2.46	0.46
1:C:233:TYR:HA	1:C:282:PRO:O	2.15	0.46
1:D:357:ALA:HA	1:D:366:PRO:HA	1.96	0.46
1:B:96:ASP:O	1:B:100:VAL:HG22	2.16	0.46
1:B:110:ASP:O	1:B:113:GLU:N	2.48	0.46
1:B:329:LEU:HA	1:B:369:ALA:CB	2.46	0.46
1:C:132:LEU:HG	1:C:134:LEU:CD1	2.40	0.46
1:D:92:ILE:O	1:D:93:VAL:C	2.57	0.46
1:A:62:LEU:C	1:A:63:ASP:O	2.55	0.46
1:A:331:ASP:OD2	1:A:331:ASP:C	2.59	0.46
1:A:333:ARG:HG2	1:A:333:ARG:NH2	2.31	0.46
1:B:353:ALA:O	1:B:354:ARG:HB3	2.16	0.46
1:A:5:PRO:HG2	1:A:423:ALA:HB1	1.97	0.46
1:D:347:LEU:CD1	1:D:348:GLY:H	2.28	0.46
1:D:355:PRO:HB2	1:D:356:PRO:HD2	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:GLU:O	1:B:38:GLU:C	2.58	0.46
1:B:84:ARG:HE	1:B:266:ARG:HH12	1.63	0.46
1:B:388:ASP:O	1:B:391:GLN:HB3	2.16	0.46
1:B:425:PHE:C	1:B:427:GLU:H	2.23	0.46
1:C:258:LEU:HD21	1:C:283:PHE:CB	2.46	0.46
1:D:354:ARG:N	1:D:355:PRO:CD	2.79	0.46
1:D:360:ILE:O	1:D:363:GLU:HB3	2.16	0.46
1:B:295:GLU:OE2	1:B:295:GLU:HA	2.14	0.46
1:D:281:ASN:C	1:D:283:PHE:H	2.23	0.46
1:A:26:VAL:HA	1:A:54:ALA:O	2.16	0.45
1:A:29:ASP:HA	1:A:57:LEU:HD12	1.98	0.45
1:A:65:VAL:HG21	1:A:90:MSE:HE2	1.96	0.45
1:A:177:PRO:HD3	1:A:389:TRP:NE1	2.31	0.45
1:D:33:PHE:CD2	1:D:40:ARG:HB2	2.51	0.45
1:D:285:PRO:O	1:D:286:ALA:C	2.59	0.45
1:D:336:LEU:O	1:D:371:VAL:HA	2.16	0.45
1:B:68:LEU:O	1:B:71:LEU:HB3	2.16	0.45
1:C:141:HIS:O	1:C:141:HIS:CG	2.69	0.45
1:D:198:ARG:N	1:D:198:ARG:CD	2.78	0.45
1:A:55:VAL:HG22	1:A:80:VAL:HG13	1.98	0.45
1:A:285:PRO:O	1:A:286:ALA:C	2.59	0.45
1:A:75:GLY:O	1:A:76:TYR:C	2.58	0.45
1:B:59:HIS:CE1	1:B:64:HIS:CD2	3.05	0.45
1:A:160:SER:OG	1:A:185:ALA:HA	2.16	0.45
1:A:235:LEU:HD23	1:A:247:ILE:HD13	1.98	0.45
1:B:365:VAL:HA	1:B:366:PRO:HD3	1.71	0.45
1:B:422:LEU:N	1:B:422:LEU:CD1	2.79	0.45
1:B:425:PHE:O	1:B:427:GLU:N	2.50	0.45
1:C:128:ARG:HG3	1:C:128:ARG:HH21	1.81	0.45
1:C:357:ALA:O	1:C:358:VAL:HG23	2.17	0.45
1:D:55:VAL:HG22	1:D:80:VAL:HG13	1.99	0.45
1:D:68:LEU:HB3	1:D:69:PRO:CD	2.47	0.45
1:A:128:ARG:HG3	1:A:128:ARG:HH21	1.82	0.45
1:B:162:ASP:OD1	1:B:380:HIS:NE2	2.47	0.45
1:C:48:ASP:O	1:C:51:GLU:HB2	2.16	0.45
1:C:210:LYS:O	1:C:210:LYS:HG2	2.16	0.45
1:C:333:ARG:HG2	1:C:333:ARG:HH11	1.81	0.45
1:D:142:LEU:HG	1:D:143:PRO:HD2	1.98	0.45
1:A:309:VAL:HG11	1:A:324:HIS:CE1	2.49	0.45
1:B:10:ARG:HD2	1:B:403:GLU:HG3	1.97	0.45
1:C:101:MSE:SE	1:C:104:PRO:HB3	2.66	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:TYR:C	1:D:235:LEU:N	2.74	0.45
1:D:238:HIS:HA	1:D:241:ARG:HH12	1.81	0.45
1:D:253:MSE:HB2	1:D:256:ARG:NH1	2.32	0.45
1:B:31:GLY:CA	1:B:64:HIS:N	2.79	0.45
1:B:39:ALA:C	1:B:41:ASN:N	2.74	0.45
1:B:95:GLU:O	1:B:98:LEU:HB3	2.17	0.45
1:B:113:GLU:O	1:B:117:HIS:HD2	1.99	0.45
1:B:200:THR:HG22	1:B:377:PHE:CE1	2.51	0.45
1:C:105:PHE:CD1	1:C:106:PHE:HD1	2.34	0.45
1:D:43:ALA:HB1	1:D:44:PRO:HD2	1.99	0.45
1:D:198:ARG:O	1:D:201:VAL:N	2.49	0.45
1:D:302:ARG:HD3	1:D:302:ARG:N	2.31	0.45
1:D:425:PHE:O	1:D:427:GLU:N	2.49	0.45
1:A:341:TYR:CZ	1:A:375:GLY:HA3	2.52	0.45
1:A:347:LEU:HA	1:A:350:GLU:HB3	1.99	0.45
1:B:237:THR:C	1:B:239:GLY:N	2.74	0.45
1:C:10:ARG:NH1	1:C:10:ARG:CG	2.80	0.45
1:C:106:PHE:CD2	1:C:106:PHE:C	2.95	0.45
1:C:107:GLY:O	1:C:110:ASP:HB2	2.17	0.45
1:C:219:LEU:HD13	1:C:309:VAL:HB	1.99	0.45
1:A:99:LYS:HG2	1:A:100:VAL:N	2.32	0.45
1:A:422:LEU:O	1:A:423:ALA:O	2.35	0.45
1:B:236:TYR:C	1:B:236:TYR:CD2	2.95	0.45
1:B:410:GLY:HA3	1:B:420:VAL:HG21	1.99	0.45
1:C:212:LEU:C	1:C:214:GLN:N	2.76	0.45
1:D:253:MSE:C	1:D:255:GLY:N	2.73	0.45
1:A:45:PHE:HB3	1:A:47:PHE:CE1	2.52	0.44
1:A:94:LEU:O	1:A:95:GLU:C	2.59	0.44
1:D:404:GLU:H	1:D:404:GLU:CD	2.26	0.44
1:C:163:LEU:HD21	1:C:389:TRP:CE3	2.51	0.44
1:A:168:LYS:HA	1:A:197:TYR:CD1	2.52	0.44
1:A:372:HIS:CD2	1:A:372:HIS:N	2.84	0.44
1:A:407:LEU:HD13	1:A:422:LEU:HD21	1.99	0.44
1:B:72:PHE:O	1:B:73:ARG:C	2.61	0.44
1:D:252:PRO:HB2	1:D:256:ARG:HH22	1.82	0.44
1:B:410:GLY:HA2	1:B:420:VAL:HG21	1.99	0.44
1:D:45:PHE:C	1:D:47:PHE:H	2.25	0.44
1:A:244:ARG:NH2	3:A:447:HOH:O	2.33	0.44
1:A:359:ARG:HH21	1:A:362:GLY:HA2	1.82	0.44
1:B:10:ARG:HG2	1:B:10:ARG:NH1	2.27	0.44
1:B:19:LEU:HD21	1:B:132:LEU:HD21	1.98	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:MSE:HE1	1:B:106:PHE:HE1	1.82	0.44
1:B:205:LEU:HD11	1:B:238:HIS:CD2	2.53	0.44
1:C:3:ILE:CD1	1:C:17:HIS:HB3	2.47	0.44
1:D:188:THR:O	1:D:190:GLY:N	2.50	0.44
1:D:272:VAL:HG12	1:D:272:VAL:O	2.18	0.44
1:A:8:ALA:HB1	1:A:400:HIS:HA	1.98	0.44
1:A:41:ASN:O	1:A:70:LYS:NZ	2.47	0.44
1:C:313:SER:CB	1:C:318:GLY:HA3	2.45	0.44
1:B:84:ARG:HE	1:B:266:ARG:NH1	2.15	0.44
1:B:287:GLY:O	1:B:288:LEU:C	2.61	0.44
1:C:152:GLY:O	1:C:153:GLU:HB2	2.18	0.44
1:C:155:ARG:HE	1:C:431:VAL:HG13	1.82	0.44
1:C:275:HIS:O	1:C:278:GLN:HG2	2.18	0.44
1:D:205:LEU:HD11	1:D:238:HIS:CD2	2.53	0.44
1:A:98:LEU:HD22	1:A:111:VAL:HG21	1.98	0.44
1:A:302:ARG:HD3	1:A:302:ARG:H	1.82	0.44
1:B:179:LEU:CD2	1:D:131:ALA:HA	2.48	0.44
1:C:343:PRO:O	1:C:349:ALA:HB2	2.18	0.44
1:C:359:ARG:O	1:C:359:ARG:HG2	2.17	0.44
1:A:244:ARG:NH1	3:A:447:HOH:O	2.30	0.43
1:A:355:PRO:O	1:A:356:PRO:C	2.61	0.43
1:C:32:MSE:CA	1:C:67:ARG:HG3	2.46	0.43
1:C:357:ALA:O	1:C:358:VAL:CG2	2.66	0.43
1:D:227:ARG:O	1:D:231:ILE:HG12	2.18	0.43
1:A:212:LEU:HB2	1:A:243:PRO:CG	2.48	0.43
1:C:182:LEU:HD12	1:C:183:VAL:H	1.83	0.43
1:C:415:LEU:O	1:C:417:GLY:N	2.51	0.43
1:D:11:GLU:O	1:D:401:GLY:N	2.51	0.43
1:D:38:GLU:OE2	1:D:38:GLU:C	2.61	0.43
1:C:332:PRO:HA	1:C:368:ARG:O	2.18	0.43
1:D:383:GLN:O	1:D:387:LEU:HG	2.17	0.43
1:A:95:GLU:OE1	1:A:95:GLU:HA	2.18	0.43
1:A:208:LEU:HD21	1:A:218:VAL:HG11	2.00	0.43
1:B:315:MSE:O	1:B:316:LEU:O	2.36	0.43
1:B:328:GLY:O	1:B:329:LEU:HB3	2.19	0.43
1:A:182:LEU:HG	1:A:183:VAL:N	2.32	0.43
1:A:325:LEU:HD12	1:A:325:LEU:HA	1.77	0.43
1:A:429:VAL:HG13	1:A:430:PRO:HD2	2.00	0.43
1:A:429:VAL:HG12	1:A:430:PRO:N	2.32	0.43
1:C:183:VAL:HG12	1:C:185:ALA:HB2	2.00	0.43
1:C:233:TYR:HD1	1:C:282:PRO:HB2	1.82	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:ILE:HG23	1:C:322:LEU:N	2.33	0.43
1:D:17:HIS:ND1	1:D:17:HIS:N	2.65	0.43
1:A:18:LEU:HD12	1:A:19:LEU:N	2.33	0.43
1:A:36:LYS:HD3	1:A:36:LYS:N	2.15	0.43
1:A:100:VAL:HG23	1:A:101:MSE:N	2.33	0.43
1:A:134:LEU:N	1:A:134:LEU:CD1	2.80	0.43
1:C:298:LYS:HA	1:C:301:ASN:HD21	1.84	0.43
1:D:19:LEU:HD13	1:D:157:LEU:HD23	2.00	0.43
1:D:186:GLU:OE2	1:D:380:HIS:HD2	2.02	0.43
1:D:397:VAL:HG13	1:D:397:VAL:O	2.18	0.43
1:A:131:ALA:HA	1:C:179:LEU:HD22	2.01	0.43
1:B:129:LEU:O	1:B:130:GLY:O	2.37	0.43
1:C:234:VAL:O	1:C:237:THR:O	2.37	0.43
1:D:83:THR:O	1:D:87:VAL:HG23	2.19	0.43
1:A:33:PHE:H	1:A:41:ASN:ND2	2.09	0.43
1:A:186:GLU:HA	1:A:399:VAL:O	2.19	0.43
1:C:404:GLU:O	1:C:407:LEU:N	2.51	0.43
1:D:26:VAL:HA	1:D:54:ALA:O	2.19	0.43
1:D:262:PRO:HA	1:D:276:PHE:CZ	2.54	0.43
1:A:187:GLY:HA3	1:A:406:LEU:HD12	2.01	0.43
1:A:265:VAL:HA	1:A:268:PHE:HD2	1.83	0.43
1:B:110:ASP:O	1:B:113:GLU:HB3	2.19	0.43
1:B:253:MSE:O	1:B:254:ALA:C	2.58	0.43
1:B:376:GLY:C	1:B:378:SER:H	2.27	0.43
1:D:170:VAL:HB	1:D:171:LEU:HD22	2.01	0.43
1:D:219:LEU:HD12	1:D:324:HIS:HB3	1.99	0.43
1:B:37:GLU:HB3	1:B:40:ARG:CD	2.49	0.43
1:B:105:PHE:CD2	1:B:105:PHE:N	2.86	0.43
1:C:209:GLU:C	1:C:211:THR:N	2.76	0.43
1:D:358:VAL:HG12	1:D:359:ARG:N	2.34	0.43
1:A:305:GLY:HA3	1:B:302:ARG:HH22	1.83	0.42
1:B:398:LEU:HD21	1:B:420:VAL:HG23	1.99	0.42
1:D:157:LEU:HD12	1:D:158:VAL:H	1.84	0.42
1:D:281:ASN:O	1:D:283:PHE:N	2.52	0.42
1:D:335:ALA:HA	1:D:370:SER:O	2.19	0.42
1:B:130:GLY:O	1:B:131:ALA:CB	2.63	0.42
1:B:310:LEU:N	1:B:310:LEU:CD1	2.82	0.42
1:C:62:LEU:C	1:C:64:HIS:H	2.27	0.42
1:D:129:LEU:O	1:D:130:GLY:C	2.63	0.42
1:D:290:VAL:O	1:D:292:GLU:OE2	2.37	0.42
1:D:325:LEU:HD21	1:D:336:LEU:HD11	2.00	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ALA:O	1:A:42:HIS:HB2	2.19	0.42
1:A:217:LYS:NZ	1:A:300:LEU:O	2.52	0.42
1:A:371:VAL:C	1:A:372:HIS:CD2	2.97	0.42
1:B:189:TYR:CE2	1:B:341:TYR:CE1	3.07	0.42
1:C:223:PHE:CE2	1:C:315:MSE:HE2	2.53	0.42
1:C:224:ALA:HB3	1:C:253:MSE:CE	2.49	0.42
1:D:9:ALA:C	1:D:11:GLU:N	2.78	0.42
1:D:109:GLU:H	1:D:109:GLU:CD	2.26	0.42
1:D:326:LYS:HD2	1:D:361:LEU:HB2	2.00	0.42
1:A:24:ARG:NH1	3:A:436:HOH:O	2.52	0.42
1:B:10:ARG:HH11	1:B:10:ARG:CG	2.24	0.42
1:B:270:GLU:O	1:B:271:GLU:C	2.61	0.42
1:C:37:GLU:C	1:C:38:GLU:O	2.63	0.42
1:C:294:THR:CG2	1:C:320:ARG:HH11	2.25	0.42
1:D:226:GLU:HG2	1:D:261:TYR:OH	2.20	0.42
1:A:39:ALA:C	1:A:41:ASN:H	2.27	0.42
1:A:133:SER:C	1:A:134:LEU:HD12	2.45	0.42
1:B:212:LEU:O	1:B:214:GLN:N	2.53	0.42
1:C:32:MSE:HB2	1:C:41:ASN:OD1	2.19	0.42
1:C:101:MSE:SE	1:C:104:PRO:CB	3.18	0.42
1:C:294:THR:O	1:C:297:SER:HB3	2.20	0.42
1:D:72:PHE:CE1	1:D:114:ALA:HA	2.55	0.42
1:D:383:GLN:HA	1:D:386:LEU:HD12	2.01	0.42
1:D:388:ASP:O	1:D:391:GLN:CB	2.67	0.42
1:A:358:VAL:O	1:A:365:VAL:HG12	2.19	0.42
1:C:253:MSE:C	1:C:255:GLY:N	2.77	0.42
1:D:105:PHE:CD2	1:D:105:PHE:N	2.81	0.42
1:D:130:GLY:C	1:D:132:LEU:N	2.77	0.42
1:A:131:ALA:HA	1:C:179:LEU:CD2	2.50	0.42
1:A:404:GLU:OE2	1:A:404:GLU:N	2.44	0.42
1:B:155:ARG:NH1	1:B:431:VAL:HG11	2.28	0.42
1:C:229:GLN:HE21	1:C:229:GLN:HB3	1.59	0.42
1:C:387:LEU:HD11	1:C:412:LEU:HD13	2.01	0.42
1:D:165:ASN:HA	1:D:385:GLU:OE1	2.19	0.42
1:D:325:LEU:HD11	1:D:336:LEU:HD12	2.02	0.42
1:A:20:LEU:CD2	1:A:25:ARG:HE	2.33	0.42
1:A:304:PRO:O	1:A:305:GLY:O	2.38	0.42
1:C:6:PHE:HB2	1:C:16:ALA:O	2.19	0.42
1:C:357:ALA:C	1:C:358:VAL:HG23	2.45	0.42
1:D:257:VAL:HG12	1:D:261:TYR:CE2	2.54	0.42
1:D:324:HIS:C	1:D:325:LEU:HD12	2.45	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:LEU:HD12	1:D:348:GLY:H	1.84	0.42
1:A:10:ARG:CG	1:A:10:ARG:HH11	2.33	0.42
1:A:85:ALA:HB2	1:A:267:TYR:CE2	2.54	0.42
1:B:139:ALA:HB2	1:B:146:ALA:C	2.45	0.42
1:C:11:GLU:C	1:C:401:GLY:H	2.26	0.42
1:D:373:THR:O	1:D:373:THR:HG22	2.20	0.42
1:A:250:ASP:OD1	1:A:324:HIS:CE1	2.73	0.42
1:B:62:LEU:O	1:B:66:GLY:HA3	2.20	0.42
1:B:315:MSE:SE	1:B:343:PRO:HD3	2.70	0.42
1:C:163:LEU:CD1	1:C:163:LEU:N	2.82	0.42
1:D:157:LEU:HD12	1:D:158:VAL:N	2.34	0.42
1:D:198:ARG:CG	1:D:199:GLU:H	2.29	0.42
1:D:299:ALA:HA	1:D:302:ARG:HH21	1.85	0.42
1:B:225:VAL:HG23	1:B:253:MSE:HE1	2.02	0.41
1:B:398:LEU:CD1	1:B:409:LEU:HD23	2.50	0.41
1:C:21:ALA:O	1:C:24:ARG:N	2.46	0.41
1:C:49:PRO:HB3	1:C:71:LEU:CD1	2.48	0.41
1:D:114:ALA:O	1:D:115:LEU:C	2.63	0.41
1:B:48:ASP:O	1:B:50:LYS:N	2.52	0.41
1:D:160:SER:HB3	1:D:185:ALA:HA	2.02	0.41
1:A:32:MSE:HE3	1:A:62:LEU:HG	2.02	0.41
1:A:55:VAL:HG13	1:A:80:VAL:HG22	2.02	0.41
1:A:229:GLN:CD	1:A:229:GLN:H	2.27	0.41
1:A:348:GLY:O	1:A:351:ILE:N	2.52	0.41
1:B:297:SER:OG	1:B:320:ARG:HD3	2.21	0.41
1:D:167:GLU:O	1:D:197:TYR:CG	2.73	0.41
1:A:57:LEU:HG	1:A:65:VAL:CG2	2.43	0.41
1:A:221:PRO:C	1:A:222:THR:HG23	2.46	0.41
1:A:279:GLY:C	1:A:280:LYS:HG2	2.45	0.41
1:B:185:ALA:O	1:B:399:VAL:HG12	2.21	0.41
1:B:196:PRO:HG2	1:B:199:GLU:OE2	2.21	0.41
1:D:181:ASP:OD1	1:D:181:ASP:N	2.52	0.41
1:D:247:ILE:HD12	1:D:286:ALA:HB3	2.02	0.41
1:D:399:VAL:HG13	1:D:400:HIS:N	2.34	0.41
1:A:37:GLU:OE2	1:A:37:GLU:HA	2.19	0.41
1:A:163:LEU:HA	1:A:163:LEU:HD12	1.57	0.41
1:B:113:GLU:OE2	1:B:113:GLU:HA	2.21	0.41
1:B:188:THR:OG1	1:B:400:HIS:CE1	2.73	0.41
1:C:68:LEU:O	1:C:71:LEU:HB3	2.21	0.41
1:C:281:ASN:C	1:C:283:PHE:H	2.27	0.41
1:D:90:MSE:O	1:D:92:ILE:N	2.54	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:VAL:HA	1:A:5:PRO:HD3	1.92	0.41
1:A:26:VAL:O	1:A:26:VAL:HG23	2.19	0.41
1:A:97:ALA:O	1:A:101:MSE:CB	2.68	0.41
1:B:17:HIS:O	1:B:27:LEU:HD23	2.21	0.41
1:B:91:GLU:HG3	1:B:92:ILE:N	2.35	0.41
1:C:188:THR:HG22	1:C:189:TYR:CD1	2.56	0.41
1:D:3:ILE:HD13	1:D:4:VAL:H	1.86	0.41
1:D:36:LYS:HG2	1:D:37:GLU:N	2.36	0.41
1:D:318:GLY:H	1:D:322:LEU:HD11	1.85	0.41
1:A:115:LEU:HD12	1:A:115:LEU:HA	1.88	0.41
1:A:130:GLY:C	1:A:132:LEU:H	2.28	0.41
1:A:329:LEU:HD11	1:A:336:LEU:HD12	2.02	0.41
1:A:358:VAL:CG1	1:A:359:ARG:N	2.83	0.41
1:B:9:ALA:C	1:B:11:GLU:N	2.78	0.41
1:B:208:LEU:HD23	1:B:218:VAL:HG21	2.03	0.41
1:B:332:PRO:HA	1:B:369:ALA:HA	2.03	0.41
1:C:235:LEU:HD23	1:C:247:ILE:HG21	2.02	0.41
1:C:258:LEU:HD21	1:C:283:PHE:O	2.21	0.41
1:D:17:HIS:N	1:D:17:HIS:HD1	2.19	0.41
1:D:90:MSE:CE	1:D:118:LEU:HD11	2.51	0.41
1:D:196:PRO:HB3	1:D:198:ARG:HD3	2.02	0.41
1:D:227:ARG:HA	1:D:227:ARG:HD3	1.96	0.41
1:A:155:ARG:HH11	1:A:431:VAL:HG11	1.85	0.41
1:B:57:LEU:HD22	1:B:80:VAL:CG1	2.51	0.41
1:B:58:THR:O	1:B:59:HIS:O	2.39	0.41
1:B:126:TRP:CD2	1:D:178:PRO:HB3	2.56	0.41
1:B:195:ARG:O	1:B:196:PRO:C	2.64	0.41
1:C:321:ILE:HG23	1:C:322:LEU:HG	2.02	0.41
1:D:58:THR:HB	1:D:146:ALA:O	2.20	0.41
1:D:158:VAL:HG23	1:D:180:ALA:HB2	2.02	0.41
1:D:168:LYS:HZ2	1:D:230:GLU:CD	2.29	0.41
1:D:221:PRO:O	1:D:339:VAL:HG22	2.20	0.41
1:A:103:GLU:N	1:A:104:PRO:HD3	2.35	0.41
1:B:57:LEU:HD12	1:B:57:LEU:HA	1.92	0.41
1:B:178:PRO:HB3	1:D:126:TRP:CD2	2.56	0.41
1:B:431:VAL:O	1:B:431:VAL:HG12	2.20	0.41
1:C:105:PHE:O	1:C:106:PHE:CD1	2.74	0.41
1:C:150:ALA:HB3	1:C:157:LEU:HB3	2.03	0.41
1:D:219:LEU:CD1	1:D:324:HIS:HB3	2.51	0.41
1:D:390:LEU:O	1:D:418:GLN:NE2	2.53	0.41
1:A:19:LEU:HB3	1:A:26:VAL:HG22	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:PRO:HA	1:B:17:HIS:CD2	2.54	0.41
1:B:155:ARG:HD2	1:B:155:ARG:HA	1.82	0.41
1:A:59:HIS:HE1	1:A:64:HIS:CE1	2.38	0.40
1:A:270:GLU:O	1:A:271:GLU:C	2.64	0.40
1:B:54:ALA:HA	1:B:76:TYR:OH	2.21	0.40
1:B:325:LEU:HA	1:B:325:LEU:HD12	1.84	0.40
1:C:386:LEU:O	1:C:390:LEU:HD23	2.21	0.40
1:D:113:GLU:HA	1:D:113:GLU:OE2	2.21	0.40
1:D:119:ARG:HA	1:D:120:PRO:HD3	1.85	0.40
1:D:211:THR:HG21	1:D:218:VAL:HG22	2.03	0.40
1:A:62:LEU:O	1:A:66:GLY:N	2.53	0.40
1:A:312:GLY:O	1:A:313:SER:HB2	2.21	0.40
1:B:72:PHE:CD2	1:B:113:GLU:HG3	2.56	0.40
1:C:375:GLY:C	1:C:377:PHE:N	2.77	0.40
1:D:8:ALA:H	1:D:15:SER:HA	1.86	0.40
1:D:68:LEU:O	1:D:71:LEU:HB3	2.21	0.40
1:D:109:GLU:HA	1:D:112:GLU:HG2	2.02	0.40
1:D:231:ILE:C	1:D:233:TYR:H	2.29	0.40
1:A:390:LEU:O	1:A:391:GLN:C	2.65	0.40
1:C:141:HIS:HB2	1:C:164:GLY:N	2.36	0.40
1:C:163:LEU:CD2	1:C:389:TRP:CD2	2.98	0.40
1:C:387:LEU:O	1:C:416:ARG:NH2	2.55	0.40
1:C:390:LEU:O	1:C:393:GLU:HB2	2.20	0.40
1:D:10:ARG:HH22	1:D:424:ARG:HH21	1.66	0.40
1:D:184:LEU:HA	1:D:397:VAL:HG13	2.02	0.40
1:A:18:LEU:HD12	1:A:19:LEU:H	1.86	0.40
1:A:140:GLY:O	1:A:164:GLY:HA3	2.20	0.40
1:A:249:LEU:O	1:A:290:VAL:HA	2.21	0.40
1:B:3:ILE:HG23	1:B:3:ILE:O	2.21	0.40
1:B:251:SER:O	1:B:252:PRO:C	2.63	0.40
1:B:427:GLU:HA	1:B:427:GLU:OE1	2.21	0.40
1:C:191:ASP:OD2	1:C:192:ARG:N	2.53	0.40
1:C:333:ARG:HG2	1:C:333:ARG:NH1	2.36	0.40
1:C:424:ARG:O	1:C:425:PHE:C	2.63	0.40
1:A:105:PHE:HD2	1:A:105:PHE:H	1.66	0.40
1:B:3:ILE:HD11	1:B:17:HIS:CB	2.43	0.40
1:C:38:GLU:O	1:C:39:ALA:HB3	2.21	0.40
1:D:194:HIS:CG	1:D:376:GLY:HA2	2.56	0.40
1:D:351:ILE:HG23	1:D:367:LEU:HD22	2.04	0.40
1:D:393:GLU:O	1:D:418:GLN:HG2	2.21	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	429/431 (100%)	361 (84%)	45 (10%)	23 (5%)	<b>1</b> <b>4</b>
1	B	429/431 (100%)	364 (85%)	45 (10%)	20 (5%)	<b>2</b> <b>6</b>
1	C	429/431 (100%)	340 (79%)	64 (15%)	25 (6%)	<b>1</b> <b>4</b>
1	D	429/431 (100%)	333 (78%)	68 (16%)	28 (6%)	<b>1</b> <b>3</b>
All	All	1716/1724 (100%)	1398 (82%)	222 (13%)	96 (6%)	<b>1</b> <b>4</b>

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	GLU
1	A	59	HIS
1	A	106	PHE
1	A	286	ALA
1	A	304	PRO
1	A	423	ALA
1	B	38	GLU
1	B	59	HIS
1	B	106	PHE
1	B	213	SER
1	B	290	VAL
1	B	304	PRO
1	B	305	GLY
1	B	316	LEU
1	C	38	GLU
1	C	106	PHE
1	C	286	ALA
1	C	366	PRO
1	D	38	GLU
1	D	39	ALA
1	D	59	HIS
1	D	106	PHE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	130	GLY
1	D	286	ALA
1	D	395	ARG
1	A	46	GLY
1	A	130	GLY
1	A	305	GLY
1	A	313	SER
1	A	329	LEU
1	A	395	ARG
1	B	130	GLY
1	B	226	GLU
1	B	286	ALA
1	B	329	LEU
1	B	426	GLY
1	C	130	GLY
1	C	196	PRO
1	C	280	LYS
1	C	282	PRO
1	C	312	GLY
1	C	376	GLY
1	D	8	ALA
1	D	329	LEU
1	D	347	LEU
1	D	400	HIS
1	D	420	VAL
1	A	7	GLY
1	A	44	PRO
1	C	30	CYS
1	C	225	VAL
1	C	292	GLU
1	C	295	GLU
1	C	304	PRO
1	C	395	ARG
1	D	93	VAL
1	D	131	ALA
1	D	196	PRO
1	D	282	PRO
1	D	356	PRO
1	D	426	GLY
1	A	391	GLN
1	B	46	GLY
1	B	317	ALA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	328	GLY
1	B	399	VAL
1	C	285	PRO
1	C	313	SER
1	C	416	ARG
1	D	167	GLU
1	D	238	HIS
1	A	154	GLY
1	A	225	VAL
1	A	238	HIS
1	A	278	GLN
1	B	49	PRO
1	B	318	GLY
1	C	347	LEU
1	D	12	VAL
1	D	290	VAL
1	D	320	ARG
1	A	290	VAL
1	A	316	LEU
1	B	64	HIS
1	C	45	PHE
1	C	290	VAL
1	D	399	VAL
1	A	43	ALA
1	C	65	VAL
1	D	246	PRO
1	D	394	PRO
1	C	331	ASP
1	C	93	VAL
1	D	143	PRO
1	A	318	GLY
1	D	265	VAL

### 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	342/335 (102%)	297 (87%)	45 (13%)	4	14
1	B	342/335 (102%)	306 (90%)	36 (10%)	6	22
1	C	342/335 (102%)	319 (93%)	23 (7%)	15	42
1	D	342/335 (102%)	316 (92%)	26 (8%)	12	36
All	All	1368/1340 (102%)	1238 (90%)	130 (10%)	8	26

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	10	ARG
1	A	12	VAL
1	A	15	SER
1	A	18	LEU
1	A	27	LEU
1	A	36	LYS
1	A	45	PHE
1	A	55	VAL
1	A	57	LEU
1	A	65	VAL
1	A	103	GLU
1	A	115	LEU
1	A	132	LEU
1	A	134	LEU
1	A	142	LEU
1	A	156	THR
1	A	157	LEU
1	A	163	LEU
1	A	165	ASN
1	A	171	LEU
1	A	184	LEU
1	A	186	GLU
1	A	188	THR
1	A	219	LEU
1	A	229	GLN
1	A	235	LEU
1	A	241	ARG
1	A	251	SER
1	A	258	LEU
1	A	264	LEU
1	A	278	GLN
1	A	294	THR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	304	PRO
1	A	313	SER
1	A	325	LEU
1	A	344	GLN
1	A	361	LEU
1	A	363	GLU
1	A	372	HIS
1	A	390	LEU
1	A	398	LEU
1	A	406	LEU
1	A	407	LEU
1	A	431	VAL
1	B	3	ILE
1	B	12	VAL
1	B	26	VAL
1	B	27	LEU
1	B	28	LEU
1	B	36	LYS
1	B	38	GLU
1	B	55	VAL
1	B	57	LEU
1	B	62	LEU
1	B	63	ASP
1	B	86	THR
1	B	104	PRO
1	B	105	PHE
1	B	127	LEU
1	B	163	LEU
1	B	165	ASN
1	B	175	SER
1	B	184	LEU
1	B	219	LEU
1	B	227	ARG
1	B	229	GLN
1	B	235	LEU
1	B	258	LEU
1	B	264	LEU
1	B	265	VAL
1	B	294	THR
1	B	325	LEU
1	B	336	LEU
1	B	358	VAL

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	361	LEU
1	B	365	VAL
1	B	390	LEU
1	B	391	GLN
1	B	407	LEU
1	B	427	GLU
1	C	3	ILE
1	C	26	VAL
1	C	27	LEU
1	C	28	LEU
1	C	36	LYS
1	C	55	VAL
1	C	57	LEU
1	C	62	LEU
1	C	112	GLU
1	C	184	LEU
1	C	186	GLU
1	C	196	PRO
1	C	229	GLN
1	C	258	LEU
1	C	264	LEU
1	C	265	VAL
1	C	293	HIS
1	C	302	ARG
1	C	336	LEU
1	C	377	PHE
1	C	390	LEU
1	C	397	VAL
1	C	402	GLU
1	D	3	ILE
1	D	13	THR
1	D	26	VAL
1	D	27	LEU
1	D	28	LEU
1	D	32	MSE
1	D	36	LYS
1	D	38	GLU
1	D	55	VAL
1	D	57	LEU
1	D	61	HIS
1	D	96	ASP
1	D	106	PHE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	112	GLU
1	D	115	LEU
1	D	129	LEU
1	D	171	LEU
1	D	188	THR
1	D	192	ARG
1	D	196	PRO
1	D	227	ARG
1	D	229	GLN
1	D	264	LEU
1	D	336	LEU
1	D	390	LEU
1	D	399	VAL

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

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	41	ASN
1	A	117	HIS
1	A	141	HIS
1	A	165	ASN
1	A	229	GLN
1	A	324	HIS
1	A	380	HIS
1	A	391	GLN
1	B	41	ASN
1	B	117	HIS
1	B	141	HIS
1	B	165	ASN
1	B	214	GLN
1	B	229	GLN
1	B	278	GLN
1	B	323	HIS
1	B	324	HIS
1	B	383	GLN
1	C	34	GLN
1	C	41	ASN
1	C	117	HIS
1	C	165	ASN
1	C	229	GLN
1	C	273	GLN
1	C	380	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	383	GLN
1	D	41	ASN
1	D	141	HIS
1	D	165	ASN
1	D	194	HIS
1	D	214	GLN
1	D	229	GLN
1	D	240	HIS
1	D	278	GLN
1	D	372	HIS
1	D	380	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 oligosaccharides in this entry.

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

Of 8 ligands modelled in this entry, 8 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 [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	424/431 (98%)	-0.11	2 (0%) 87 82	21, 44, 66, 81	0
1	B	424/431 (98%)	0.04	5 (1%) 76 68	22, 45, 77, 93	0
1	C	424/431 (98%)	0.68	43 (10%) 12 9	33, 78, 134, 141	0
1	D	424/431 (98%)	0.85	54 (12%) 8 6	36, 90, 146, 160	0
All	All	1696/1724 (98%)	0.37	104 (6%) 27 20	21, 56, 136, 160	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	311	ALA	6.1
1	D	216	GLY	4.6
1	D	303	ALA	4.3
1	D	188	THR	3.9
1	D	371	VAL	3.7
1	D	169	ASP	3.7
1	D	250	ASP	3.6
1	A	431	VAL	3.5
1	C	312	GLY	3.4
1	D	308	VAL	3.4
1	C	376	GLY	3.4
1	B	37	GLU	3.3
1	D	205	LEU	3.3
1	D	167	GLU	3.2
1	C	212	LEU	3.1
1	D	236	TYR	3.0
1	D	218	VAL	2.9
1	C	185	ALA	2.9
1	C	290	VAL	2.9
1	D	189	TYR	2.9
1	D	207	ILE	2.8

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	291	VAL	2.8
1	D	309	VAL	2.8
1	C	250	ASP	2.8
1	D	327	HIS	2.8
1	C	188	THR	2.8
1	B	431	VAL	2.7
1	D	288	LEU	2.7
1	D	194	HIS	2.7
1	D	314	GLY	2.7
1	C	385	GLU	2.7
1	C	325	LEU	2.7
1	C	308	VAL	2.7
1	D	223	PHE	2.6
1	C	362	GLY	2.6
1	D	312	GLY	2.6
1	C	377	PHE	2.6
1	C	324	HIS	2.6
1	D	300	LEU	2.6
1	D	215	GLY	2.5
1	D	296	ALA	2.5
1	C	333	ARG	2.5
1	D	293	HIS	2.5
1	D	292	GLU	2.5
1	C	343	PRO	2.5
1	C	236	TYR	2.5
1	C	326	LYS	2.5
1	D	341	TYR	2.4
1	D	343	PRO	2.4
1	D	291	VAL	2.4
1	D	266	ARG	2.4
1	D	294	THR	2.4
1	D	287	GLY	2.4
1	D	368	ARG	2.4
1	C	378	SER	2.4
1	C	369	ALA	2.4
1	C	327	HIS	2.4
1	D	362	GLY	2.4
1	C	380	HIS	2.4
1	D	373	THR	2.3
1	C	321	ILE	2.3
1	C	355	PRO	2.3
1	C	338	PHE	2.3

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	385	GLU	2.3
1	C	374	LEU	2.3
1	C	246	PRO	2.3
1	C	252	PRO	2.3
1	C	303	ALA	2.2
1	C	351	ILE	2.2
1	D	237	THR	2.2
1	C	7	GLY	2.2
1	C	379	GLY	2.2
1	C	367	LEU	2.2
1	D	322	LEU	2.2
1	C	220	ILE	2.2
1	D	7	GLY	2.2
1	D	208	LEU	2.2
1	D	239	GLY	2.2
1	D	310	LEU	2.2
1	B	376	GLY	2.2
1	C	322	LEU	2.2
1	D	212	LEU	2.2
1	C	225	VAL	2.1
1	D	217	LYS	2.1
1	C	346	GLY	2.1
1	D	329	LEU	2.1
1	B	103	GLU	2.1
1	C	365	VAL	2.1
1	D	319	GLY	2.1
1	D	347	LEU	2.1
1	D	360	ILE	2.1
1	D	372	HIS	2.1
1	D	340	GLY	2.1
1	D	374	LEU	2.1
1	C	341	TYR	2.1
1	A	294	THR	2.1
1	C	347	LEU	2.0
1	B	45	PHE	2.0
1	D	382	GLY	2.0
1	C	297	SER	2.0
1	D	297	SER	2.0
1	D	381	ALA	2.0
1	C	363	GLU	2.0
1	D	103	GLU	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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	A	433	1/1	0.83	0.13	37,37,37,37	1
2	ZN	B	433	1/1	0.85	0.16	42,42,42,42	1
2	ZN	B	432	1/1	0.87	0.19	28,28,28,28	1
2	ZN	D	432	1/1	0.89	0.20	59,59,59,59	1
2	ZN	D	433	1/1	0.90	0.19	73,73,73,73	1
2	ZN	C	432	1/1	0.94	0.14	48,48,48,48	1
2	ZN	C	433	1/1	0.95	0.12	44,44,44,44	1
2	ZN	A	432	1/1	0.97	0.10	19,19,19,19	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.