



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:12 AM UTC

PDB ID : 4A93 / pdb_00004a93
Title : RNA Polymerase II elongation complex containing a CPD Lesion
Authors : Walmacq, C.; Cheung, A.C.M.; Kireeva, M.L.; Lubkowska, L.; Ye, C.; Gotte, D.; Strathern, J.N.; Carell, T.; Cramer, P.; Kashlev, M.
Deposited on : 2011-11-23
Resolution : 3.40 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

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)
Xtriage (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

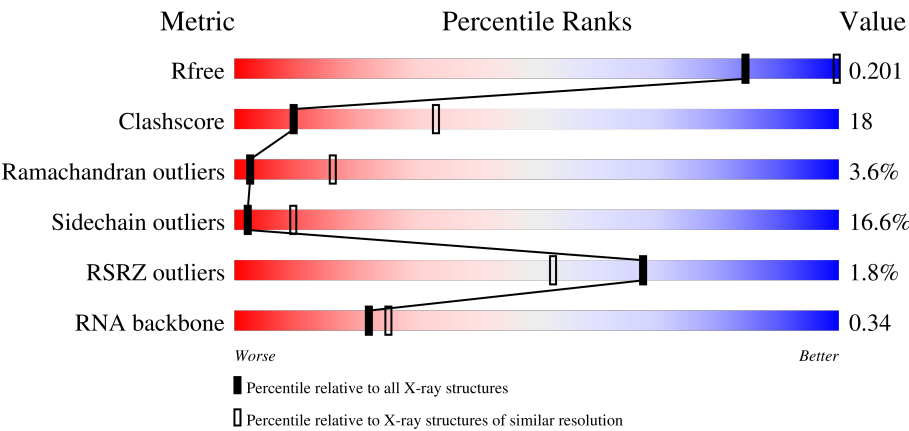
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



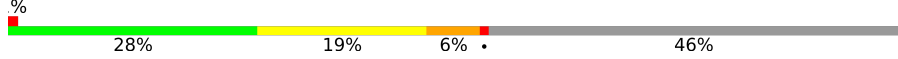
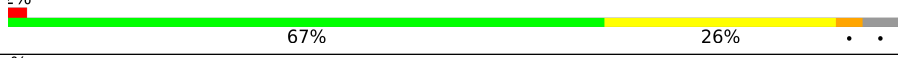
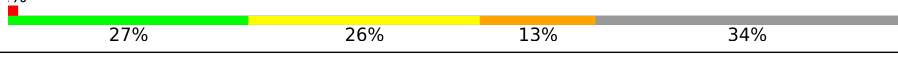
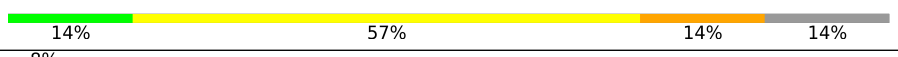
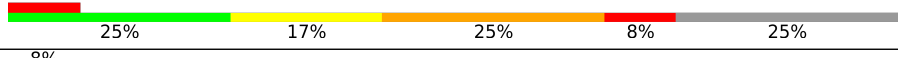
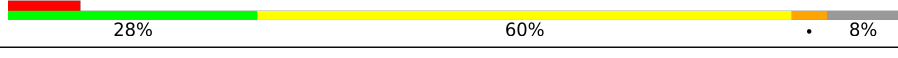
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)
RNA backbone	3983	1157 (3.80-3.00)

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 ≥ 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	1732	0.201 44% 29% 8% 18%
2	B	1224	3% 49% 33% 8% 9%
3	C	318	47% 31% 6% 16%
4	D	221	4% 40% 27% 11% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	14	
14	P	12	
15	T	25	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32105 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1422	Total	C	N	O	S	0	0	0
			11174	7037	1954	2121	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1113	Total	C	N	O	S	0	0	0
			8839	5597	1548	1639	55			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 7 is a protein called RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	1
			920	590	157	171	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is a DNA chain called 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP*GP*CP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	12	Total	C	N	O	P	0	0	0
			247	118	44	73	12			

- Molecule 14 is a RNA chain called 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	9	Total	C	N	O	P	0	0	0
			197	88	41	59	9			

- Molecule 15 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*TTTP*TP*TP*CP*C BRUP*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	23	Total	Br	C	N	O	P	0	0
			485	1	234	81	146	23		

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	2	Total	Zn	0	0
			2	2		
16	B	1	Total	Zn	0	0
			1	1		
16	C	1	Total	Zn	0	0
			1	1		
16	I	2	Total	Zn	0	0
			2	2		
16	J	1	Total	Zn	0	0
			1	1		
16	L	1	Total	Zn	0	0
			1	1		

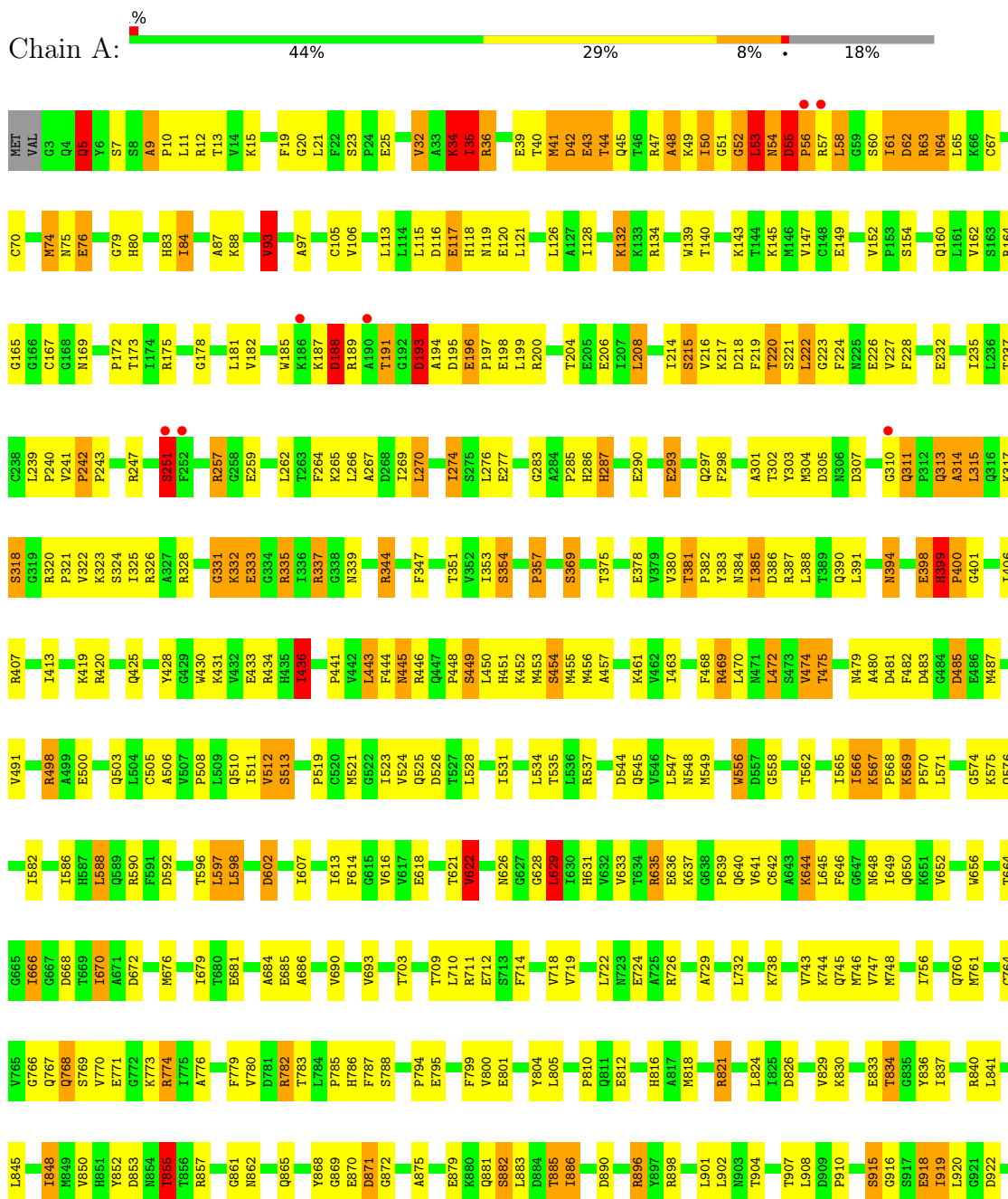
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

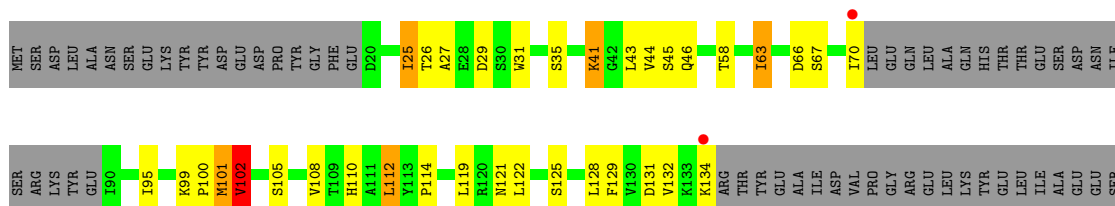
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1







Response	Percentage
Doing a good job	47%
Not doing a good job	31%
Don't know	6%
Refuse to answer	16%



- Molecule 7: RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G: 58% 36% 5% .



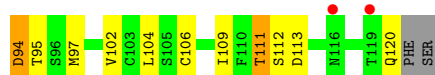
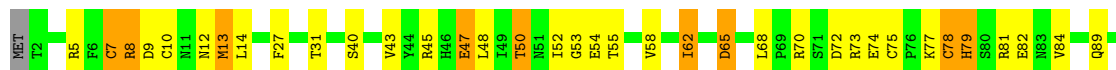
- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H: 3% 38% 41% 12% 9% .



- Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

Chain I: 2% 59% 30% 9% .



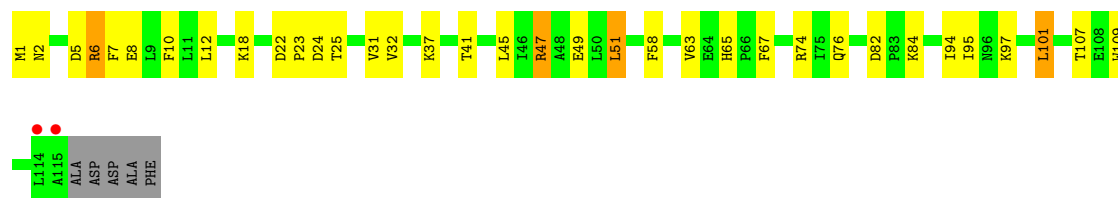
- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J: 47% 34% 10% 7% .

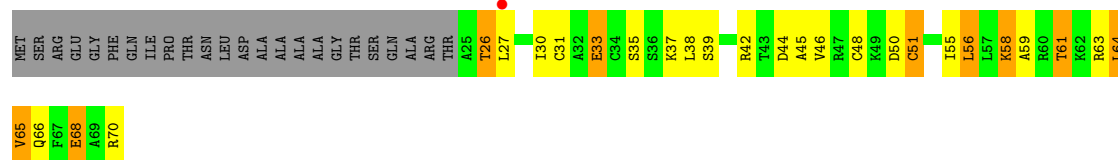
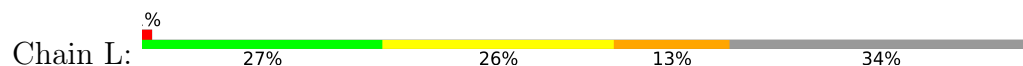


- Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

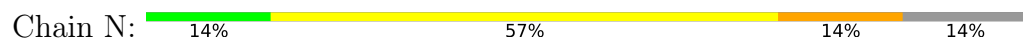
Chain K: 2% 67% 26% . .



- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4



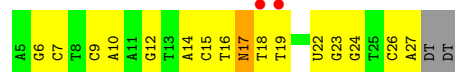
- Molecule 13: 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP*GP*CP*TP)-3'



- Molecule 14: 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP*AP)-3'



- Molecule 15: 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*T*TTP*TP*TP*CP*C B RUP*GP*GP*TP*CP*AP*TP*T)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	221.64Å 391.52Å 281.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.09 – 3.40 54.09 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.09-3.40) 99.9 (54.09-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 3.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.165 , 0.199 0.172 , 0.201	Depositor DCC
R_{free} test set	3298 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	103.5	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 109.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.025 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.029 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32105	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: TT, MG, BRU, 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	0.67	1/11374 (0.0%)	1.10	42/15383 (0.3%)
2	B	0.62	0/9010	1.06	48/12149 (0.4%)
3	C	0.61	0/2133	1.03	8/2891 (0.3%)
4	D	0.79	3/1444 (0.2%)	1.11	7/1935 (0.4%)
5	E	0.51	0/1788	0.99	5/2406 (0.2%)
6	F	0.82	1/691 (0.1%)	1.28	7/933 (0.8%)
7	G	0.64	0/1368	1.08	6/1844 (0.3%)
8	H	0.47	0/1086	0.97	4/1470 (0.3%)
9	I	0.51	0/989	1.03	8/1331 (0.6%)
10	J	0.67	0/541	1.16	3/727 (0.4%)
11	K	0.63	0/938	0.96	0/1267
12	L	0.68	0/365	1.12	1/485 (0.2%)
13	N	0.38	0/276	1.17	4/424 (0.9%)
14	P	0.48	0/221	0.74	1/343 (0.3%)
15	T	0.31	0/475	0.90	0/725
All	All	0.64	5/32699 (0.0%)	1.07	144/44313 (0.3%)

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	A	0	5
4	D	0	1
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	187	THR	CA-CB	13.01	1.75	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	187	THR	CB-CG2	9.31	1.83	1.52
4	D	25	ALA	CA-C	6.19	1.60	1.53
1	A	1051	ALA	CA-CB	-5.88	1.44	1.53
6	F	82	THR	CA-C	-5.29	1.47	1.53

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	26	THR	N-CA-C	-11.22	99.89	112.57
7	G	62	LEU	CA-C-N	-10.22	107.07	119.84
7	G	62	LEU	C-N-CA	-10.22	107.07	119.84
10	J	5	VAL	N-CA-C	-8.96	98.02	109.58
8	H	92	ASP	N-CA-C	-8.59	102.11	112.59
4	D	187	THR	N-CA-C	-8.50	98.01	110.42
10	J	3	VAL	CB-CA-C	-8.33	101.10	110.68
5	E	52	ARG	CA-C-N	8.16	130.04	119.84
5	E	52	ARG	C-N-CA	8.16	130.04	119.84
1	A	622	VAL	N-CA-C	-7.95	105.27	112.90
1	A	70	CYS	N-CA-C	-7.87	100.37	110.53
2	B	296	GLU	N-CA-C	-7.81	102.39	112.23
2	B	973	ILE	N-CA-C	7.60	116.28	107.77
2	B	732	SER	N-CA-C	7.46	117.86	108.45
4	D	187	THR	CA-CB-CG2	7.45	123.17	110.50
6	F	105	ALA	CA-C-N	7.32	127.76	119.93
6	F	105	ALA	C-N-CA	7.32	127.76	119.93
1	A	1424	VAL	CB-CA-C	-7.29	102.63	111.97
9	I	8	ARG	N-CA-C	-7.25	100.28	110.50
1	A	1301	GLU	CA-C-N	7.09	127.01	119.85
1	A	1301	GLU	C-N-CA	7.09	127.01	119.85
2	B	510	LYS	CA-C-N	7.08	126.90	119.05
2	B	510	LYS	C-N-CA	7.08	126.90	119.05
2	B	1222	ARG	N-CA-C	6.96	118.95	111.36
2	B	361	LEU	CA-C-N	6.89	126.52	119.56
2	B	361	LEU	C-N-CA	6.89	126.52	119.56
1	A	64	ASN	N-CA-C	-6.87	99.72	110.36
1	A	629	LEU	N-CA-C	-6.83	103.83	111.28
1	A	23	SER	N-CA-C	-6.75	101.56	109.93
2	B	1160	VAL	CB-CA-C	-6.71	101.25	110.90
13	N	3	DA	N9-C1'-C2'	6.67	123.51	113.50
10	J	64	ASN	N-CA-C	6.67	124.54	109.81
1	A	55	ASP	CA-C-N	6.63	128.12	119.84
1	A	55	ASP	C-N-CA	6.63	128.12	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	74	ILE	CA-C-N	6.62	126.66	119.90
6	F	74	ILE	C-N-CA	6.62	126.66	119.90
1	A	9	ALA	CA-C-N	6.51	127.97	119.84
1	A	9	ALA	C-N-CA	6.51	127.97	119.84
3	C	18	VAL	CB-CA-C	-6.50	103.46	111.32
8	H	85	GLY	N-CA-C	-6.38	105.07	112.73
1	A	513	SER	CA-C-N	6.30	127.11	120.12
1	A	513	SER	C-N-CA	6.30	127.11	120.12
1	A	1403	GLU	N-CA-C	6.28	124.18	110.80
1	A	34	LYS	N-CA-C	-6.26	98.99	109.07
1	A	886	ILE	N-CA-C	6.23	116.39	110.53
2	B	427	ASP	N-CA-C	-6.21	105.36	113.12
13	N	3	DA	O4'-C1'-C2'	-6.21	97.09	106.40
2	B	276	ILE	N-CA-C	6.18	116.77	107.75
2	B	1166	CYS	N-CA-C	-6.11	101.44	110.48
2	B	1156	ASP	N-CA-C	6.10	123.80	110.80
13	N	3	DA	C1'-O4'-C4'	-6.09	100.57	109.70
2	B	973	ILE	CA-C-N	6.05	127.41	119.84
2	B	973	ILE	C-N-CA	6.05	127.41	119.84
6	F	143	PHE	N-CA-C	6.05	118.05	108.79
4	D	41	GLN	N-CA-C	-6.04	105.08	112.88
2	B	736	THR	N-CA-C	-6.01	105.90	113.72
9	I	75	CYS	CA-C-N	6.01	125.72	119.05
9	I	75	CYS	C-N-CA	6.01	125.72	119.05
2	B	211	VAL	CB-CA-C	-6.00	101.68	110.81
14	P	11	A	O4'-C1'-C2'	-5.99	101.61	107.60
3	C	39	ALA	N-CA-C	5.99	120.65	113.23
7	G	32	GLU	N-CA-C	-5.96	104.47	110.97
2	B	748	ILE	N-CA-C	-5.96	104.97	113.07
1	A	1058	VAL	CB-CA-C	-5.92	102.38	111.08
6	F	82	THR	CB-CA-C	-5.90	100.16	109.42
3	C	90	ASP	CB-CA-C	-5.87	109.79	116.54
1	A	70	CYS	CA-C-N	-5.85	114.46	123.17
1	A	70	CYS	C-N-CA	-5.85	114.46	123.17
1	A	582	ILE	CA-C-N	5.81	125.79	120.21
1	A	582	ILE	C-N-CA	5.81	125.79	120.21
1	A	436	ILE	N-CA-C	-5.77	102.08	109.30
1	A	332	LYS	N-CA-C	-5.75	98.55	110.80
2	B	102	VAL	N-CA-C	5.72	116.24	107.77
8	H	109	LYS	CB-CA-C	-5.70	109.01	115.79
9	I	40	SER	CA-C-N	5.69	125.54	119.28
9	I	40	SER	C-N-CA	5.69	125.54	119.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	150	VAL	CA-C-N	5.64	126.11	120.52
5	E	150	VAL	C-N-CA	5.64	126.11	120.52
2	B	1170	THR	N-CA-C	5.60	122.73	110.80
1	A	242	PRO	CA-C-N	5.60	126.14	120.38
1	A	242	PRO	C-N-CA	5.60	126.14	120.38
2	B	628	THR	N-CA-C	-5.58	107.72	114.75
1	A	5	GLN	N-CA-C	5.57	118.08	110.55
2	B	1177	HIS	N-CA-C	-5.57	106.34	113.02
2	B	230	ALA	N-CA-C	5.54	122.06	109.81
2	B	976	ILE	N-CA-C	5.52	116.18	110.82
2	B	764	SER	CA-C-N	-5.45	113.03	119.84
2	B	764	SER	C-N-CA	-5.45	113.03	119.84
1	A	56	PRO	CA-C-N	5.45	131.95	121.54
1	A	56	PRO	C-N-CA	5.45	131.95	121.54
4	D	31	GLN	N-CA-C	-5.45	105.42	111.36
1	A	331	GLY	N-CA-C	5.43	120.55	112.41
2	B	1211	ASN	N-CA-C	5.42	119.48	112.86
6	F	83	PRO	N-CA-C	-5.42	108.47	114.92
2	B	616	ILE	CB-CA-C	-5.41	102.43	110.33
3	C	226	ASP	N-CA-C	-5.41	101.53	109.81
2	B	825	VAL	N-CA-C	5.39	115.72	108.17
3	C	212	PRO	O-C-N	5.38	123.79	121.31
1	A	724	GLU	N-CA-C	-5.37	105.32	111.07
2	B	229	ALA	N-CA-C	5.36	117.24	110.33
7	G	139	ILE	N-CA-C	5.33	116.06	110.62
2	B	706	GLN	N-CA-C	-5.33	103.22	110.36
2	B	1113	VAL	CB-CA-C	-5.32	105.23	111.94
13	N	7	DC	C5'-C4'-C3'	-5.27	106.99	114.90
3	C	217	ASP	CA-C-N	5.27	125.17	119.85
3	C	217	ASP	C-N-CA	5.27	125.17	119.85
1	A	36	ARG	N-CA-C	-5.27	108.61	114.62
5	E	109	ILE	N-CA-C	5.26	115.09	106.72
2	B	1181	GLU	N-CA-C	5.26	122.00	110.80
2	B	1017	ILE	N-CA-C	5.24	120.20	108.88
1	A	53	LEU	N-CA-CB	5.24	118.37	109.10
4	D	187	THR	N-CA-CB	5.21	117.32	109.34
1	A	1226	VAL	N-CA-C	5.21	115.98	108.48
2	B	851	PHE	N-CA-C	5.20	118.92	112.47
2	B	1101	ASP	N-CA-C	-5.18	107.01	113.38
2	B	1189	ILE	CB-CA-C	-5.17	102.81	111.29
1	A	1407	GLU	N-CA-C	-5.16	105.73	111.36
1	A	222	LEU	N-CA-C	-5.14	103.90	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	510	LYS	N-CA-C	5.14	117.49	108.75
2	B	711	GLU	CA-C-N	-5.14	114.44	119.99
2	B	711	GLU	C-N-CA	-5.14	114.44	119.99
2	B	1109	GLY	CA-C-N	5.12	126.24	119.84
2	B	1109	GLY	C-N-CA	5.12	126.24	119.84
3	C	215	GLU	N-CA-C	5.12	117.60	111.71
2	B	689	LEU	N-CA-C	-5.11	106.45	113.30
4	D	26	THR	CB-CA-C	-5.11	103.14	111.06
2	B	744	HIS	CA-C-N	5.11	126.22	119.84
2	B	744	HIS	C-N-CA	5.11	126.22	119.84
1	A	399	HIS	N-CA-CB	5.10	119.45	110.37
1	A	850	VAL	CB-CA-C	-5.09	104.53	111.15
9	I	65	ASP	CA-C-N	5.09	124.58	119.19
9	I	65	ASP	C-N-CA	5.09	124.58	119.19
1	A	641	VAL	CB-CA-C	-5.09	105.27	112.14
7	G	14	HIS	CA-C-N	5.06	126.16	119.84
7	G	14	HIS	C-N-CA	5.06	126.16	119.84
2	B	610	ASN	CA-C-N	5.05	126.15	119.84
2	B	610	ASN	C-N-CA	5.05	126.15	119.84
8	H	21	ASN	N-CA-C	5.04	117.43	111.33
12	L	33	GLU	N-CA-C	5.04	116.63	111.03
9	I	53	GLY	N-CA-C	-5.04	108.05	114.85
1	A	93	VAL	CB-CA-C	-5.02	105.47	112.04
1	A	357	PRO	N-CA-C	-5.01	108.08	114.35
1	A	251	SER	N-CA-C	5.01	117.31	108.24
2	B	805	THR	N-CA-C	5.00	117.01	109.41

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	311	GLN	Peptide
1	A	34	LYS	Peptide
1	A	399	HIS	Peptide
1	A	55	ASP	Peptide
1	A	63	ARG	Peptide
4	D	25	ALA	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	11174	0	11233	450	0
2	B	8839	0	8876	309	0
3	C	2095	0	2051	76	0
4	D	1434	0	1460	66	0
5	E	1752	0	1776	58	0
6	F	679	0	701	31	0
7	G	1340	0	1357	43	0
8	H	1068	0	1040	54	0
9	I	971	0	927	25	0
10	J	532	0	542	26	0
11	K	920	0	929	29	0
12	L	363	0	386	14	0
13	N	247	0	137	14	0
14	P	197	0	99	27	0
15	T	485	0	273	22	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
All	All	32105	0	31787	1120	0

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

All (1120) 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)
4:D:187:THR:CB	4:D:187:THR:CA	1.75	1.60
4:D:187:THR:CB	4:D:187:THR:CG2	1.83	1.55
14:P:11:A:C8	14:P:11:A:H5''	1.77	1.18
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.11	1.14
14:P:11:A:C8	14:P:11:A:C5'	2.30	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.00	1.02
3:C:148:ARG:H	3:C:151:GLN:HG3	1.26	0.99
1:A:53:LEU:HD23	1:A:54:ASN:H	1.30	0.95
3:C:66:ARG:NH2	10:J:3:VAL:O	2.00	0.95
7:G:26:LEU:HD13	7:G:56:ILE:HD11	1.46	0.94
4:D:40:HIS:HB3	7:G:73:LYS:HE3	1.50	0.93
2:B:338:GLY:HA3	2:B:340:ALA:H	1.35	0.90
7:G:1:MET:SD	7:G:2:PHE:N	2.45	0.90
2:B:766:ARG:HE	2:B:1020:ARG:HG2	1.36	0.88
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.56	0.87
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.53	0.87
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.57	0.86
1:A:433:GLU:OE1	2:B:1108:ARG:NH2	2.09	0.85
1:A:855:THR:HG21	1:A:857:ARG:HE	1.42	0.84
15:T:17:TT:H3R	15:T:17:TT:H3'	1.60	0.84
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.13	0.83
1:A:115:LEU:HD21	1:A:145:LYS:HG3	1.59	0.83
2:B:806:THR:HG22	2:B:808:ALA:H	1.41	0.83
10:J:44:TYR:HA	10:J:47:ARG:HG3	1.60	0.83
14:P:11:A:C5'	14:P:11:A:H8	1.89	0.82
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.61	0.82
1:A:53:LEU:CD2	1:A:54:ASN:H	1.93	0.82
7:G:1:MET:HE1	7:G:80:LYS:O	1.80	0.82
2:B:637:LEU:HD13	2:B:693:ILE:HD12	1.61	0.81
2:B:323:VAL:HG23	2:B:324:ILE:HD12	1.64	0.80
2:B:295:GLY:HA2	2:B:298:LEU:HB2	1.63	0.79
14:P:11:A:C8	14:P:11:A:C3'	2.66	0.79
2:B:705:MET:H	2:B:710:LEU:HD12	1.47	0.79
13:N:9:DT:H2'	13:N:10:DG:H8	1.47	0.78
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.64	0.77
4:D:130:LEU:HD13	4:D:142:LYS:HG2	1.66	0.77
14:P:11:A:H8	14:P:11:A:H3'	1.49	0.77
2:B:1037:LEU:O	10:J:47:ARG:NH1	2.17	0.77
6:F:111:LEU:HD12	6:F:111:LEU:H	1.50	0.77
1:A:709:THR:HG22	1:A:711:ARG:H	1.49	0.77
1:A:53:LEU:HD23	1:A:54:ASN:N	2.00	0.76
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.65	0.76
10:J:10:CYS:SG	10:J:43:ARG:NH2	2.57	0.76
13:N:13:DC:N4	15:T:6:DG:O6	2.18	0.76
1:A:834:THR:HG21	1:A:1077:THR:HG23	1.68	0.76
1:A:976:THR:OG1	1:A:977:LYS:N	2.18	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	1.96	0.75
1:A:61:ILE:HG22	1:A:62:ASP:H	1.52	0.75
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.68	0.75
1:A:32:VAL:HG11	1:A:80:HIS:HB3	1.69	0.75
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.68	0.75
14:P:10:A:N6	15:T:19:DT:O4	2.14	0.74
2:B:642:ASP:HA	2:B:649:LYS:HA	1.68	0.74
2:B:843:GLN:HG2	2:B:993:THR:HB	1.69	0.74
4:D:187:THR:CB	4:D:187:THR:HA	2.09	0.74
1:A:332:LYS:H	1:A:337:ARG:HB3	1.52	0.74
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.70	0.74
1:A:810:PRO:HB2	2:B:705:MET:HE2	1.69	0.74
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.70	0.74
1:A:52:GLY:H	1:A:56:PRO:HG3	1.53	0.74
1:A:200:ARG:NH2	1:A:206:GLU:OE2	2.20	0.74
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.68	0.73
4:D:24:ALA:HB3	4:D:26:THR:HG23	1.69	0.73
14:P:11:A:C8	14:P:11:A:H3'	2.24	0.73
1:A:55:ASP:HA	1:A:58:LEU:H	1.54	0.73
2:B:642:ASP:O	2:B:644:GLU:N	2.22	0.73
12:L:68:GLU:HB2	12:L:70:ARG:HD2	1.70	0.72
1:A:54:ASN:HB3	1:A:247:ARG:HH22	1.54	0.72
4:D:187:THR:CA	4:D:187:THR:HB	2.11	0.72
7:G:138:THR:HG22	7:G:139:ILE:H	1.54	0.72
4:D:53:SER:HB3	4:D:152:SER:HB3	1.72	0.72
2:B:792:MET:HE2	2:B:857:ARG:NH2	2.04	0.72
1:A:709:THR:HB	1:A:712:GLU:H	1.54	0.72
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.71	0.72
2:B:1180:PHE:H	2:B:1188:LYS:NZ	1.88	0.72
2:B:322:PHE:O	2:B:325:GLN:NE2	2.23	0.71
10:J:48:ARG:O	10:J:52:THR:HG22	1.90	0.71
1:A:1116:LEU:HD12	1:A:1329:THR:HB	1.71	0.71
2:B:429:PHE:O	2:B:433:GLN:NE2	2.23	0.71
14:P:11:A:C8	14:P:11:A:C4'	2.72	0.71
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.73	0.71
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.70	0.71
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.56	0.71
2:B:315:LYS:HG2	9:I:13:MET:HE1	1.71	0.71
2:B:641:GLU:HB2	2:B:643:ASP:HB2	1.71	0.71
9:I:7:CYS:SG	9:I:10:CYS:HB2	2.30	0.71
12:L:46:VAL:HG13	12:L:56:LEU:HD12	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ARG:NH2	2:B:991:GLY:O	2.24	0.70
2:B:291:ILE:HG22	2:B:297:ILE:HG13	1.74	0.70
2:B:996:ARG:NH2	3:C:174:ALA:O	2.24	0.70
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.74	0.70
2:B:344:LYS:HB3	2:B:347:LYS:HB2	1.74	0.69
13:N:3:DA:H2''	13:N:4:DG:N7	2.07	0.69
1:A:12:ARG:HD2	2:B:1218:THR:HB	1.74	0.69
1:A:88:LYS:HG3	1:A:276:LEU:HD21	1.74	0.69
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.26	0.69
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.74	0.69
13:N:9:DT:H2'	13:N:10:DG:C8	2.26	0.69
14:P:11:A:C8	14:P:11:A:H5'	2.28	0.69
14:P:3:G:O2'	14:P:4:A:OP1	2.11	0.68
7:G:34:VAL:O	7:G:37:SER:HB3	1.93	0.68
13:N:8:DT:O2	15:T:12:DG:N2	2.22	0.68
6:F:73:ALA:HB2	6:F:143:PHE:CZ	2.29	0.68
11:K:24:ASP:OD2	11:K:74:ARG:NH1	2.26	0.68
1:A:1148:ILE:HD12	1:A:1196:GLU:HG2	1.76	0.68
1:A:331:GLY:HA3	1:A:337:ARG:HB2	1.76	0.68
1:A:548:ASN:HD21	11:K:47:ARG:HE	1.43	0.67
1:A:879:GLU:OE2	1:A:962:ARG:NH2	2.27	0.67
1:A:42:ASP:O	1:A:44:THR:N	2.28	0.67
3:C:184:ASN:ND2	3:C:189:THR:O	2.28	0.67
2:B:531:GLN:NE2	15:T:18:DT:O4	2.28	0.67
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.75	0.67
1:A:187:LYS:HE3	1:A:198:GLU:HB2	1.77	0.66
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	1.96	0.66
2:B:890:TYR:OH	2:B:936:ASP:OD2	2.11	0.66
1:A:544:ASP:OD1	1:A:545:GLN:N	2.27	0.66
1:A:744:LYS:HG2	1:A:748:MET:HE2	1.77	0.66
2:B:831:SER:HB2	2:B:833:TYR:HD2	1.60	0.66
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.78	0.66
1:A:265:LYS:HG3	1:A:303:TYR:HB2	1.78	0.66
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.75	0.66
10:J:48:ARG:HE	10:J:49:MET:HE2	1.61	0.66
8:H:62:SER:OG	8:H:63:LEU:N	2.28	0.66
14:P:10:A:C2'	14:P:11:A:OP1	2.44	0.66
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.28	0.66
1:A:890:ASP:OD1	1:A:940:ARG:NH1	2.29	0.66
2:B:641:GLU:HG3	2:B:652:LYS:HE2	1.78	0.66
1:A:34:LYS:HA	1:A:35:ILE:HB	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ASP:HA	1:A:195:ASP:HB2	1.78	0.65
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.30	0.65
7:G:30:LEU:HD22	7:G:72:VAL:HG11	1.78	0.65
4:D:18:VAL:HG22	4:D:19:GLU:HA	1.77	0.65
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.77	0.65
2:B:889:THR:HG22	2:B:891:ASP:H	1.61	0.65
15:T:23:DG:H2'	15:T:24:DG:H8	1.60	0.65
1:A:567:LYS:HA	1:A:568:PRO:C	2.22	0.65
1:A:347:PHE:H	2:B:1107:ALA:HA	1.61	0.65
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.78	0.65
2:B:801:LYS:O	10:J:52:THR:OG1	2.15	0.65
6:F:128:LYS:HG3	6:F:149:GLU:HA	1.79	0.65
9:I:78:CYS:SG	9:I:106:CYS:HB3	2.36	0.65
12:L:61:THR:HB	12:L:63:ARG:HG2	1.79	0.65
8:H:124:ARG:HE	8:H:126:GLU:HG3	1.61	0.64
2:B:328:GLU:OE1	2:B:328:GLU:N	2.26	0.64
4:D:155:ARG:HB3	4:D:219:THR:HG21	1.78	0.64
1:A:369:SER:HB3	11:K:2:ASN:OD1	1.97	0.64
3:C:6:PRO:HB3	3:C:25:VAL:HG13	1.80	0.64
4:D:40:HIS:HB3	7:G:73:LYS:CE	2.25	0.64
3:C:183:TRP:O	3:C:185:LYS:N	2.30	0.64
4:D:158:GLU:CD	4:D:158:GLU:H	2.06	0.64
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.80	0.64
4:D:187:THR:CG2	4:D:187:THR:HB	2.19	0.64
14:P:11:A:H8	14:P:11:A:C3'	2.07	0.64
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.63	0.63
1:A:1387:HIS:CE1	13:N:7:DC:H5'	2.33	0.63
2:B:102:VAL:HG13	2:B:112:LEU:HD22	1.81	0.63
1:A:41:MET:CB	1:A:49:LYS:HA	2.29	0.63
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.47	0.63
1:A:302:THR:HA	1:A:305:ASP:O	1.99	0.63
2:B:298:LEU:HD23	2:B:314:LEU:HD13	1.82	0.62
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.39	0.62
10:J:8:PHE:H	10:J:49:MET:HE3	1.64	0.62
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.80	0.62
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.82	0.62
2:B:822:ASN:O	10:J:48:ARG:NH1	2.32	0.62
2:B:1082:MET:HA	3:C:189:THR:HA	1.81	0.62
5:E:4:GLU:HB3	5:E:7:ARG:NE	2.15	0.62
5:E:145:THR:HG21	5:E:187:TYR:CD2	2.34	0.62
1:A:483:ASP:C	1:A:483:ASP:OD1	2.42	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ASP:N	1:A:481:ASP:OD1	2.30	0.62
2:B:1082:MET:HE3	3:C:190:ASP:HB2	1.82	0.62
2:B:904:ARG:NH1	12:L:66:GLN:O	2.31	0.62
3:C:148:ARG:HD3	3:C:149:LYS:HG2	1.82	0.62
6:F:103:MET:HE1	7:G:66:GLY:H	1.64	0.62
7:G:23:LYS:HE3	7:G:27:LYS:HE3	1.80	0.62
10:J:30:LEU:HD22	10:J:34:THR:HB	1.80	0.62
2:B:839:MET:HE2	2:B:1010:LEU:HD11	1.82	0.62
6:F:109:VAL:HG11	6:F:123:LYS:HG2	1.81	0.62
3:C:148:ARG:HG3	3:C:149:LYS:H	1.65	0.61
4:D:23:ASN:N	4:D:23:ASN:OD1	2.33	0.61
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.65	0.61
2:B:408:LEU:HD21	2:B:545:ILE:HD13	1.82	0.61
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.82	0.61
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.35	0.61
6:F:87:LYS:HA	6:F:155:LEU:HD11	1.82	0.61
7:G:83:LYS:HG3	7:G:149:GLY:HA2	1.82	0.61
2:B:914:LYS:HB3	2:B:937:ALA:HB3	1.80	0.61
1:A:635:ARG:HH11	1:A:635:ARG:HA	1.65	0.61
2:B:806:THR:HB	2:B:809:MET:HG3	1.82	0.61
3:C:147:LEU:HB3	3:C:151:GLN:HB2	1.80	0.61
14:P:6:C:H2'	14:P:7:A:H8	1.65	0.61
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.65	0.61
3:C:148:ARG:N	3:C:151:GLN:HG3	2.07	0.61
9:I:102:VAL:HG22	9:I:109:ILE:HG13	1.82	0.61
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.83	0.61
1:A:1141:THR:HG23	1:A:1205:LYS:HD3	1.82	0.61
1:A:1116:LEU:HD13	1:A:1311:VAL:HG22	1.83	0.61
1:A:1211:GLN:HE22	1:A:1274:ARG:HH12	1.49	0.61
1:A:1350:LYS:O	1:A:1354:ASN:ND2	2.34	0.60
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.35	0.60
4:D:4:SER:OG	4:D:5:THR:N	2.20	0.60
1:A:485:ASP:N	1:A:485:ASP:OD1	2.30	0.60
2:B:169:ARG:N	2:B:454:THR:OG1	2.34	0.60
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.84	0.60
4:D:26:THR:O	4:D:26:THR:OG1	2.18	0.60
14:P:11:A:H8	14:P:11:A:H5'	1.61	0.60
1:A:588:LEU:HD22	1:A:607:ILE:HD12	1.83	0.60
1:A:1172:LEU:C	1:A:1174:PHE:H	2.09	0.60
1:A:335:ARG:NH1	2:B:1206:GLU:OE2	2.33	0.60
1:A:1170:ILE:O	1:A:1174:PHE:HB2	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3:GLU:N	3:C:7:GLN:HE22	2.00	0.60
5:E:215:MET:HE2	5:E:215:MET:HA	1.82	0.60
2:B:651:LEU:H	2:B:651:LEU:HD12	1.65	0.60
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.35	0.60
2:B:475:SER:O	2:B:476:ARG:HB2	2.01	0.60
1:A:49:LYS:HE2	1:A:61:ILE:H	1.66	0.59
1:A:315:LEU:HA	1:A:321:PRO:HA	1.85	0.59
1:A:646:PHE:O	1:A:650:GLN:HG2	2.01	0.59
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.84	0.59
1:A:709:THR:HG23	9:I:94:ASP:HA	1.85	0.59
8:H:4:THR:HA	8:H:60:ALA:HB2	1.84	0.59
1:A:383:TYR:HB3	6:F:115:THR:HG22	1.83	0.59
1:A:1437:GLY:O	1:A:1440:ALA:N	2.35	0.59
3:C:149:LYS:HG3	3:C:150:GLY:H	1.68	0.59
8:H:82:PRO:O	8:H:84:ALA:N	2.36	0.59
2:B:1116:ARG:HG3	2:B:1198:TYR:CD2	2.38	0.59
10:J:14:VAL:HG13	10:J:50:ILE:HD11	1.85	0.59
1:A:974:ASP:C	1:A:976:THR:H	2.11	0.59
2:B:580:VAL:HG22	2:B:624:LEU:HB3	1.85	0.59
1:A:407:ARG:HD3	1:A:413:ILE:HD11	1.83	0.58
2:B:102:VAL:HG11	2:B:122:LEU:HD13	1.86	0.58
2:B:363:HIS:O	2:B:365:THR:N	2.36	0.58
2:B:378:LEU:O	2:B:382:ILE:HG13	2.03	0.58
1:A:448:PRO:HB2	1:A:450:LEU:HD11	1.86	0.58
5:E:23:VAL:HG13	5:E:78:LEU:HD23	1.84	0.58
1:A:567:LYS:HG2	1:A:569:LYS:H	1.67	0.58
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.39	0.58
2:B:428:ILE:HG12	2:B:448:ILE:HG23	1.85	0.58
2:B:936:ASP:OD1	2:B:937:ALA:N	2.36	0.58
4:D:15:LEU:O	4:D:17:LYS:N	2.37	0.58
8:H:127:GLY:HA3	8:H:130:ARG:HH21	1.67	0.58
8:H:38:LEU:HD11	8:H:123:MET:HE2	1.85	0.58
1:A:118:HIS:HB3	1:A:152:VAL:HG11	1.86	0.58
8:H:63:LEU:HB3	8:H:90:ALA:HB2	1.85	0.58
2:B:860:MET:HB2	2:B:965:LYS:HG2	1.86	0.58
1:A:779:PHE:CE2	1:A:785:PRO:HD3	2.39	0.58
1:A:810:PRO:CB	2:B:705:MET:HE2	2.34	0.58
8:H:43:ASN:HD21	8:H:46:LEU:HD23	1.69	0.58
11:K:8:GLU:O	11:K:37:LYS:HD2	2.03	0.57
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.86	0.57
2:B:758:PHE:CE1	2:B:1044:ALA:HA	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:ARG:HD3	3:C:149:LYS:HE2	1.86	0.57
4:D:188:ALA:HB2	4:D:208:GLU:HG3	1.85	0.57
2:B:102:VAL:HG23	2:B:110:HIS:HB3	1.87	0.57
2:B:365:THR:HG23	2:B:367:LEU:HG	1.87	0.57
3:C:100:THR:HG22	3:C:119:VAL:HG13	1.87	0.57
4:D:118:THR:HB	4:D:121:LYS:HG3	1.86	0.57
5:E:78:LEU:HD11	5:E:109:ILE:HG13	1.87	0.57
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.87	0.57
2:B:351:TYR:CZ	2:B:355:ILE:HD11	2.39	0.57
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.40	0.57
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.86	0.56
1:A:1437:GLY:O	1:A:1439:GLY:N	2.38	0.56
2:B:1181:GLU:HB2	2:B:1188:LYS:HE3	1.87	0.56
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.37	0.56
1:A:35:ILE:HG21	1:A:241:VAL:HG21	1.86	0.56
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.40	0.56
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.87	0.56
2:B:732:SER:HB2	2:B:734:HIS:NE2	2.19	0.56
2:B:766:ARG:HA	2:B:766:ARG:HH11	1.70	0.56
2:B:847:ASP:OD2	11:K:6:ARG:NH2	2.38	0.56
14:P:10:A:H2'	14:P:11:A:OP1	2.05	0.56
1:A:629:LEU:O	1:A:633:VAL:HG23	2.05	0.56
1:A:882:SER:O	1:A:1025:ARG:NH2	2.36	0.56
2:B:1043:ASP:OD1	2:B:1045:SER:HB2	2.05	0.56
1:A:41:MET:HG3	1:A:257:ARG:HH21	1.70	0.56
1:A:52:GLY:N	1:A:56:PRO:HG3	2.19	0.56
3:C:178:PHE:CE2	3:C:230:MET:HE2	2.41	0.56
1:A:79:GLY:HA3	1:A:243:PRO:HG2	1.86	0.56
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.87	0.56
1:A:982:THR:H	1:A:985:ASP:HB2	1.70	0.56
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.40	0.56
1:A:226:GLU:HG3	1:A:227:VAL:HG23	1.88	0.56
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.21	0.56
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.40	0.56
2:B:872:GLU:HG2	2:B:916:THR:HG23	1.88	0.56
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.88	0.56
1:A:639:PRO:HG2	1:A:640:GLN:HG2	1.88	0.55
1:A:848:ILE:HG21	1:A:1370:LEU:HD21	1.88	0.55
1:A:852:TYR:O	6:F:81:THR:HG22	2.06	0.55
1:A:35:ILE:HG21	1:A:84:ILE:HG22	1.88	0.55
2:B:577:ALA:HB1	2:B:589:VAL:HB	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.87	0.55
3:C:56:THR:HG21	3:C:145:CYS:SG	2.46	0.55
3:C:114:TYR:HB3	3:C:140:ASN:O	2.07	0.55
4:D:118:THR:O	4:D:120:GLU:N	2.39	0.55
1:A:93:VAL:HG23	1:A:304:MET:HE3	1.88	0.55
1:A:332:LYS:H	1:A:337:ARG:CB	2.20	0.55
2:B:882:THR:HG22	2:B:884:ARG:H	1.71	0.55
8:H:56:THR:OG1	8:H:146:ARG:NH1	2.38	0.55
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.41	0.55
4:D:118:THR:N	4:D:155:ARG:HH12	2.05	0.55
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	2.07	0.55
1:A:508:PRO:O	1:A:511:ILE:HG13	2.06	0.55
4:D:7:THR:CG2	7:G:5:LYS:HZ1	2.19	0.55
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.87	0.55
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.40	0.54
1:A:1130:GLN:O	1:A:1134:ILE:HG13	2.06	0.54
6:F:76:LYS:HA	6:F:79:ARG:CD	2.37	0.54
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.89	0.54
8:H:43:ASN:ND2	8:H:46:LEU:HD23	2.21	0.54
15:T:18:DT:H1'	15:T:19:DT:C5	2.42	0.54
1:A:290:GLU:HA	1:A:293:GLU:HB2	1.88	0.54
1:A:568:PRO:HG2	8:H:46:LEU:HD12	1.88	0.54
1:A:939:ASP:OD2	1:A:1023:ARG:NH1	2.40	0.54
5:E:16:PHE:CE2	5:E:20:LYS:HE2	2.42	0.54
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.89	0.54
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.89	0.54
4:D:8:PHE:HZ	4:D:37:GLN:NE2	2.03	0.54
8:H:106:GLU:HA	8:H:112:ILE:HD12	1.89	0.54
1:A:586:ILE:HD11	1:A:637:LYS:HG2	1.90	0.54
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.90	0.54
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.73	0.54
1:A:1402:PHE:CE2	1:A:1403:GLU:HG3	2.42	0.54
1:A:855:THR:CG2	1:A:857:ARG:HE	2.16	0.54
1:A:636:GLU:OE1	1:A:962:ARG:NH1	2.40	0.54
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.90	0.54
10:J:9:SER:OG	10:J:48:ARG:NH2	2.41	0.54
1:A:34:LYS:HB3	1:A:83:HIS:CE1	2.42	0.54
1:A:41:MET:HB2	1:A:49:LYS:HA	1.90	0.54
1:A:132:LYS:HD2	1:A:1411:GLU:OE1	2.08	0.54
1:A:149:GLU:HB3	1:A:164:ARG:HH21	1.73	0.54
2:B:707:PRO:O	2:B:710:LEU:N	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:LEU:O	1:A:475:THR:HB	2.08	0.54
5:E:176:PRO:O	5:E:212:ARG:HA	2.07	0.54
8:H:82:PRO:C	8:H:84:ALA:H	2.16	0.54
1:A:12:ARG:O	2:B:1194:ILE:HG22	2.08	0.54
1:A:785:PRO:HB2	2:B:703:ILE:HD12	1.88	0.54
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.40	0.54
9:I:77:LYS:O	9:I:79:HIS:N	2.40	0.54
1:A:337:ARG:HD3	2:B:1132:GLU:OE2	2.08	0.53
1:A:761:MET:HA	1:A:804:TYR:HB2	1.90	0.53
1:A:836:TYR:CZ	15:T:16:DT:H2"	2.43	0.53
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.41	0.53
2:B:711:GLU:HB2	2:B:712:PRO:HD3	1.90	0.53
11:K:47:ARG:HB3	11:K:47:ARG:NH1	2.24	0.53
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.90	0.53
2:B:800:GLN:HB3	10:J:52:THR:HG23	1.88	0.53
3:C:244:VAL:O	3:C:248:ILE:HG13	2.08	0.53
1:A:590:ARG:NH1	1:A:592:ASP:OD2	2.41	0.53
15:T:16:DT:H5'	15:T:17:TT:O2P	2.08	0.53
1:A:1116:LEU:H	1:A:1308:THR:HB	1.73	0.53
2:B:766:ARG:NE	2:B:1020:ARG:HG2	2.16	0.53
4:D:13:ARG:HH12	4:D:18:VAL:H	1.57	0.53
10:J:36:LEU:HD11	10:J:51:LEU:HB2	1.91	0.53
1:A:932:GLU:O	1:A:936:LEU:HG	2.09	0.53
5:E:153:HIS:C	5:E:154:ILE:HD12	2.34	0.53
14:P:10:A:C2	14:P:11:A:C2	2.97	0.53
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.23	0.53
2:B:338:GLY:HA3	2:B:340:ALA:N	2.16	0.53
1:A:1333:ILE:HD12	1:A:1333:ILE:H	1.73	0.53
1:A:743:VAL:HA	1:A:746:MET:HE3	1.91	0.53
6:F:72:LYS:O	6:F:72:LYS:HG2	2.09	0.53
7:G:122:ASN:ND2	7:G:125:SER:HB3	2.23	0.53
1:A:119:ASN:OD1	1:A:120:GLU:N	2.42	0.52
2:B:43:LEU:HD13	2:B:492:LEU:HD13	1.91	0.52
2:B:662:MET:HA	2:B:665:GLU:HG3	1.90	0.52
3:C:31:ASN:O	3:C:35:ARG:HG3	2.09	0.52
9:I:82:GLU:HG2	9:I:104:LEU:HD12	1.91	0.52
2:B:979:LYS:NZ	14:P:11:A:OP2	2.41	0.52
2:B:315:LYS:N	2:B:316:PRO:HD2	2.25	0.52
1:A:761:MET:HG3	2:B:1021:MET:HG2	1.91	0.52
4:D:134:THR:HG22	4:D:136:GLY:H	1.75	0.52
1:A:285:PRO:O	1:A:287:HIS:N	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1317:MET:HE2	5:E:142:VAL:HG11	1.92	0.52
2:B:842:ASN:HB3	2:B:845:SER:HB2	1.91	0.52
2:B:986:GLN:HE22	2:B:1022:THR:HG21	1.75	0.52
12:L:48:CYS:HB3	12:L:51:CYS:SG	2.50	0.52
1:A:216:VAL:O	1:A:220:THR:HB	2.09	0.52
1:A:567:LYS:HA	1:A:569:LYS:N	2.25	0.52
1:A:767:GLN:HA	1:A:799:PHE:HA	1.91	0.52
4:D:65:GLU:HA	4:D:68:ARG:HG3	1.92	0.52
1:A:1404:GLU:O	1:A:1408:ILE:HG13	2.10	0.52
1:A:821:ARG:NH1	1:A:821:ARG:HB2	2.24	0.52
2:B:564:GLU:HB2	2:B:589:VAL:HG23	1.91	0.52
5:E:152:LYS:HD2	5:E:199:ILE:HB	1.92	0.52
9:I:50:THR:HG22	9:I:52:ILE:HG12	1.92	0.52
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.91	0.52
3:C:92:CYS:SG	3:C:94:LYS:HB2	2.49	0.52
3:C:196:ASP:HB3	3:C:199:LYS:HB2	1.92	0.52
11:K:23:PRO:HA	11:K:31:VAL:HG23	1.92	0.52
1:A:117:GLU:CD	1:A:117:GLU:H	2.17	0.51
1:A:1293:SER:OG	1:A:1295:THR:HG23	2.10	0.51
2:B:25:ILE:HD12	2:B:653:VAL:HB	1.93	0.51
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.91	0.51
1:A:399:HIS:O	1:A:400:PRO:C	2.53	0.51
2:B:1180:PHE:H	2:B:1188:LYS:HZ1	1.54	0.51
4:D:50:LEU:HD21	7:G:4:ILE:HD12	1.92	0.51
7:G:99:PHE:CE2	7:G:115:MET:HE2	2.46	0.51
7:G:127:PRO:HB2	7:G:139:ILE:HD12	1.93	0.51
1:A:172:PRO:HD3	1:A:185:TRP:NE1	2.24	0.51
2:B:259:TYR:CE1	2:B:270:LYS:HD2	2.44	0.51
4:D:37:GLN:HE22	7:G:5:LYS:NZ	2.09	0.51
4:D:173:HIS:CE1	4:D:201:LYS:HE3	2.46	0.51
5:E:20:LYS:HE3	5:E:34:GLU:HG2	1.92	0.51
4:D:32:GLU:O	7:G:5:LYS:HE2	2.10	0.51
1:A:1268:LEU:HD13	9:I:48:LEU:HD21	1.93	0.51
1:A:1276:VAL:HG11	1:A:1315:GLU:HB3	1.90	0.51
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.46	0.51
2:B:873:THR:O	2:B:914:LYS:HA	2.10	0.51
1:A:871:ASP:CG	1:A:1366:ARG:HH22	2.19	0.51
1:A:907:THR:HG22	1:A:908:LEU:O	2.10	0.51
1:A:1444:MET:HG2	7:G:58:ARG:HB3	1.92	0.51
4:D:159:THR:O	4:D:163:VAL:HG23	2.11	0.51
1:A:40:THR:HG21	1:A:259:GLU:OE2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.92	0.51
2:B:466:TRP:HB2	2:B:479:VAL:HG21	1.91	0.51
5:E:26:ARG:NH2	5:E:133:GLU:OE1	2.44	0.51
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.92	0.51
1:A:1444:MET:HE1	6:F:135:ARG:CB	2.39	0.51
4:D:41:GLN:HB2	4:D:43:GLU:HG2	1.91	0.51
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.46	0.51
1:A:378:GLU:OE2	1:A:387:ARG:NH2	2.43	0.51
2:B:41:LYS:HB3	2:B:45:SER:HB3	1.93	0.51
2:B:597:MET:HG3	2:B:601:ARG:HH12	1.76	0.51
8:H:84:ALA:HA	8:H:87:ARG:HD2	1.93	0.51
10:J:22:LEU:O	10:J:26:GLN:HG3	2.11	0.51
1:A:283:GLY:O	1:A:285:PRO:HD3	2.11	0.50
1:A:998:LEU:HA	1:A:1011:GLN:HE22	1.75	0.50
2:B:900:ALA:HB3	12:L:61:THR:HG23	1.92	0.50
3:C:165:LYS:O	11:K:6:ARG:NH1	2.39	0.50
1:A:483:ASP:OD2	14:P:11:A:O3'	2.30	0.50
1:A:855:THR:HG21	1:A:857:ARG:NE	2.19	0.50
7:G:13:LEU:HD22	7:G:17:PHE:HB2	1.94	0.50
1:A:200:ARG:HH22	1:A:206:GLU:CD	2.16	0.50
1:A:483:ASP:OD1	1:A:485:ASP:OD1	2.30	0.50
2:B:997:GLU:HG2	3:C:39:ALA:HB2	1.92	0.50
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.93	0.50
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.92	0.50
15:T:6:DG:H2''	15:T:7:DC:OP2	2.11	0.50
1:A:188:ASP:O	1:A:193:ASP:HB2	2.11	0.50
1:A:390:GLN:O	1:A:394:ASN:HB2	2.11	0.50
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.92	0.50
1:A:1286:LYS:HD2	1:A:1304:TRP:CZ2	2.45	0.50
2:B:842:ASN:O	2:B:846:ILE:HG13	2.12	0.50
3:C:149:LYS:C	3:C:151:GLN:H	2.18	0.50
1:A:354:SER:O	1:A:469:ARG:HA	2.11	0.50
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.93	0.50
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.92	0.50
11:K:49:GLU:OE2	11:K:97:LYS:NZ	2.33	0.50
7:G:128:PRO:O	7:G:138:THR:HG23	2.11	0.50
1:A:780:VAL:O	1:A:782:ARG:HD3	2.12	0.50
1:A:833:GLU:HG2	13:N:3:DA:H2	1.76	0.50
2:B:779:GLY:HA2	2:B:796:LEU:HB2	1.92	0.50
2:B:1106:ARG:HG3	2:B:1107:ALA:N	2.24	0.50
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:103:LYS:HB3	8:H:115:TYR:CD1	2.47	0.50
14:P:6:C:H2'	14:P:7:A:C8	2.45	0.50
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.94	0.50
1:A:481:ASP:OD2	1:A:483:ASP:OD2	2.30	0.50
1:A:531:ILE:HG21	1:A:622:VAL:HG11	1.94	0.50
1:A:565:ILE:O	1:A:570:PRO:HA	2.12	0.50
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.94	0.50
2:B:287:ARG:NH1	2:B:324:ILE:O	2.41	0.50
2:B:791:THR:O	2:B:792:MET:HB2	2.11	0.50
1:A:537:ARG:HB2	8:H:20:TYR:CE1	2.46	0.50
2:B:882:THR:CG2	2:B:884:ARG:H	2.24	0.50
2:B:897:GLY:O	2:B:898:LEU:HD23	2.12	0.50
1:A:164:ARG:HG3	1:A:165:GLY:H	1.76	0.49
1:A:317:LYS:O	1:A:318:SER:HB3	2.12	0.49
2:B:1152:MET:HB3	2:B:1157:ALA:HB2	1.94	0.49
1:A:62:ASP:O	1:A:64:ASN:N	2.43	0.49
1:A:756:ILE:O	1:A:760:GLN:HG3	2.12	0.49
5:E:26:ARG:HH22	5:E:133:GLU:CD	2.20	0.49
1:A:25:GLU:CD	1:A:25:GLU:H	2.20	0.49
1:A:746:MET:SD	2:B:1015:HIS:HD2	2.35	0.49
1:A:1294:PRO:HG2	1:A:1295:THR:HG22	1.95	0.49
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.94	0.49
1:A:862:ASN:HA	5:E:174:GLN:HB3	1.95	0.49
1:A:1383:SER:HB2	1:A:1385:THR:HG23	1.95	0.49
5:E:198:ILE:HD13	5:E:212:ARG:HG3	1.95	0.49
15:T:23:DG:H2''	15:T:24:DG:C8	2.43	0.49
1:A:481:ASP:O	1:A:485:ASP:OD2	2.30	0.49
2:B:861:ASP:OD1	2:B:862:GLN:N	2.42	0.49
4:D:119:ARG:HB3	4:D:119:ARG:CZ	2.42	0.49
1:A:483:ASP:OD1	14:P:11:A:O3'	2.30	0.49
1:A:535:THR:O	1:A:575:LYS:HE3	2.13	0.49
1:A:1208:THR:OG1	1:A:1211:GLN:HG2	2.12	0.49
1:A:1211:GLN:NE2	1:A:1274:ARG:HH12	2.10	0.49
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.95	0.49
2:B:732:SER:HB2	2:B:734:HIS:CD2	2.48	0.49
2:B:882:THR:C	2:B:884:ARG:H	2.21	0.49
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.95	0.49
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.93	0.49
4:D:186:ASP:O	4:D:187:THR:C	2.55	0.49
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.78	0.49
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:CG	1:A:400:PRO:N	2.78	0.49
1:A:1189:SER:HB2	1:A:1242:VAL:HG23	1.95	0.49
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.94	0.49
2:B:664:THR:HA	2:B:667:GLN:HG3	1.94	0.49
4:D:25:ALA:C	4:D:27:LEU:H	2.21	0.49
2:B:314:LEU:O	2:B:318:VAL:HG23	2.12	0.49
2:B:371:GLU:OE1	2:B:371:GLU:N	2.46	0.49
7:G:106:MET:HG3	7:G:157:ILE:O	2.13	0.49
14:P:10:A:O2'	14:P:11:A:P	2.70	0.49
1:A:105:CYS:SG	1:A:139:TRP:HA	2.53	0.49
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.95	0.49
1:A:670:ILE:HG13	1:A:805:LEU:HD21	1.95	0.49
1:A:853:ASP:OD1	1:A:855:THR:HB	2.12	0.49
1:A:922:ASP:CG	1:A:925:LEU:HD12	2.38	0.49
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.94	0.49
4:D:119:ARG:HB3	4:D:119:ARG:NH1	2.28	0.49
5:E:90:VAL:HA	5:E:93:MET:HB3	1.95	0.49
12:L:61:THR:HB	12:L:63:ARG:H	1.77	0.49
1:A:782:ARG:NH1	1:A:787:PHE:O	2.46	0.49
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.93	0.49
2:B:843:GLN:HG2	2:B:993:THR:CB	2.40	0.49
8:H:15:VAL:HG22	8:H:26:ILE:HD11	1.95	0.49
2:B:344:LYS:O	2:B:348:ARG:HD2	2.12	0.48
14:P:10:A:O2'	14:P:11:A:OP1	2.30	0.48
1:A:297:GLN:NE2	1:A:297:GLN:O	2.45	0.48
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.95	0.48
2:B:552:MET:SD	2:B:552:MET:N	2.87	0.48
6:F:105:ALA:HA	7:G:16:SER:HA	1.94	0.48
1:A:483:ASP:CG	14:P:11:A:O3'	2.55	0.48
1:A:974:ASP:O	1:A:976:THR:N	2.45	0.48
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.95	0.48
2:B:234:ILE:HG21	2:B:237:VAL:HG23	1.95	0.48
2:B:885:MET:HB3	2:B:936:ASP:HB2	1.94	0.48
2:B:952:VAL:HB	12:L:58:LYS:HB2	1.94	0.48
2:B:1116:ARG:HG3	2:B:1198:TYR:CE2	2.49	0.48
3:C:148:ARG:HG3	3:C:149:LYS:N	2.28	0.48
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.48	0.48
1:A:41:MET:HB3	1:A:49:LYS:HA	1.96	0.48
1:A:335:ARG:HD3	2:B:1202:LEU:HD13	1.95	0.48
1:A:1388:GLY:O	1:A:1391:ARG:HG3	2.12	0.48
1:A:836:TYR:OH	1:A:1403:GLU:OE1	2.32	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:990:VAL:O	1:A:994:GLN:HG3	2.12	0.48
2:B:121:ASN:HD21	2:B:860:MET:HE2	1.79	0.48
2:B:705:MET:N	2:B:710:LEU:HD12	2.24	0.48
6:F:94:LEU:HD13	6:F:122:MET:HG2	1.96	0.48
15:T:17:TT:H2R2	15:T:17:TT:H6T	1.64	0.48
1:A:388:LEU:HA	1:A:388:LEU:HD23	1.64	0.48
1:A:512:VAL:HA	1:A:519:PRO:HA	1.96	0.48
3:C:77:ILE:HA	3:C:129:ILE:HD11	1.95	0.48
3:C:125:MET:HB2	3:C:127:ARG:HE	1.78	0.48
4:D:191:ALA:HB2	4:D:211:LEU:HD11	1.95	0.48
5:E:26:ARG:O	5:E:75:MET:HE1	2.14	0.48
1:A:381:THR:HG22	1:A:384:ASN:OD1	2.14	0.48
2:B:351:TYR:CE1	2:B:355:ILE:HD11	2.49	0.48
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.94	0.48
6:F:82:THR:HG22	6:F:83:PRO:HD2	1.95	0.48
1:A:472:LEU:HD13	2:B:835:GLN:NE2	2.29	0.48
1:A:824:LEU:HD21	2:B:765:PRO:HB3	1.95	0.48
2:B:802:PRO:HG3	2:B:814:PHE:HE2	1.79	0.48
2:B:1033:LYS:NZ	2:B:1070:GLU:OE1	2.35	0.48
2:B:1224:PHE:CD1	5:E:171:LYS:HG3	2.49	0.48
5:E:56:LYS:HG3	5:E:84:ASP:OD2	2.14	0.48
7:G:137:ILE:HD13	7:G:143:ILE:HD11	1.96	0.48
8:H:110:ASP:HB3	8:H:128:ASN:OD1	2.13	0.48
1:A:1025:ARG:O	1:A:1035:TYR:HE2	1.97	0.48
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.79	0.48
6:F:90:ARG:HD3	6:F:155:LEU:HD13	1.96	0.48
7:G:83:LYS:H	7:G:83:LYS:HD2	1.78	0.48
1:A:566:ILE:HD12	8:H:96:VAL:HG12	1.96	0.47
1:A:852:TYR:CZ	6:F:136:ARG:HG2	2.49	0.47
15:T:9:DC:H2'	15:T:10:DA:C8	2.49	0.47
1:A:332:LYS:HB2	1:A:337:ARG:CZ	2.43	0.47
3:C:67:LEU:HA	3:C:70:ILE:CD1	2.44	0.47
7:G:92:VAL:O	7:G:139:ILE:HG12	2.14	0.47
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.95	0.47
8:H:89:LEU:HD12	8:H:91:ASP:O	2.13	0.47
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.96	0.47
1:A:353:ILE:HD13	1:A:487:MET:CE	2.45	0.47
1:A:919:ILE:HG13	1:A:925:LEU:HD13	1.96	0.47
2:B:559:SER:HA	2:B:563:MET:HB3	1.96	0.47
6:F:83:PRO:O	6:F:152:ILE:HG13	2.13	0.47
7:G:15:PRO:HD3	7:G:67:SER:HA	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:THR:CG2	1:A:857:ARG:HG3	2.43	0.47
1:A:925:LEU:HD22	1:A:983:ILE:HB	1.96	0.47
2:B:705:MET:HE3	2:B:745:PRO:HB3	1.96	0.47
7:G:49:LEU:HG	7:G:76:ALA:HA	1.96	0.47
8:H:127:GLY:CA	8:H:130:ARG:HH21	2.28	0.47
1:A:882:SER:HB2	1:A:953:ASN:OD1	2.13	0.47
2:B:1150:ARG:HA	2:B:1154:ALA:HB3	1.96	0.47
1:A:1444:MET:HG3	7:G:59:GLY:O	2.15	0.47
2:B:635:ARG:HH12	2:B:742:GLU:CD	2.22	0.47
2:B:1204:PHE:O	2:B:1208:MET:HG3	2.15	0.47
8:H:104:PHE:CE1	8:H:114:VAL:HG12	2.50	0.47
11:K:5:ASP:HB2	11:K:8:GLU:HG3	1.96	0.47
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.50	0.47
1:A:598:LEU:HD22	8:H:25:ARG:NH1	2.29	0.47
1:A:1027:ALA:O	1:A:1031:VAL:HG23	2.15	0.47
2:B:780:VAL:HG21	10:J:56:LEU:CD1	2.45	0.47
5:E:161:LYS:HD2	5:E:195:VAL:HG23	1.97	0.47
13:N:3:DA:H2''	13:N:4:DG:C8	2.49	0.47
1:A:1378:GLN:OE1	1:A:1378:GLN:HA	2.14	0.47
1:A:1445:ILE:HD12	1:A:1445:ILE:O	2.14	0.47
1:A:1450:LEU:HD23	1:A:1450:LEU:O	2.14	0.47
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.47	0.47
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.78	0.47
1:A:216:VAL:HA	1:A:219:PHE:CE2	2.49	0.47
1:A:1343:ALA:HB2	5:E:150:VAL:HG22	1.96	0.47
3:C:145:CYS:SG	3:C:146:LYS:N	2.88	0.47
1:A:870:GLU:HG2	5:E:208:TYR:CD2	2.49	0.47
2:B:100:PRO:HG3	2:B:172:ILE:HG13	1.96	0.47
2:B:635:ARG:NH1	2:B:742:GLU:OE1	2.45	0.47
2:B:1188:LYS:O	2:B:1188:LYS:HE2	2.15	0.47
1:A:41:MET:HE3	1:A:257:ARG:HE	1.79	0.46
1:A:187:LYS:HB3	1:A:188:ASP:H	1.65	0.46
2:B:101:MET:HA	2:B:112:LEU:H	1.80	0.46
12:L:31:CYS:O	12:L:35:SER:HA	2.15	0.46
1:A:242:PRO:HA	1:A:243:PRO:HD3	1.58	0.46
1:A:399:HIS:O	1:A:401:GLY:N	2.48	0.46
1:A:485:ASP:OD1	14:P:11:A:O2'	2.30	0.46
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.97	0.46
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.97	0.46
2:B:1100:ASP:OD2	11:K:1:MET:HB3	2.15	0.46
1:A:227:VAL:HG12	1:A:228:PHE:CD1	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:LEU:HD13	1:A:597:LEU:HA	1.69	0.46
2:B:901:PRO:HD3	12:L:58:LYS:HB3	1.96	0.46
9:I:72:ASP:O	9:I:81:ARG:HG2	2.16	0.46
1:A:916:GLY:O	1:A:919:ILE:HG22	2.16	0.46
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.96	0.46
1:A:270:LEU:HD22	1:A:270:LEU:HA	1.74	0.46
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.98	0.46
3:C:262:LEU:HD23	3:C:262:LEU:HA	1.75	0.46
1:A:896:ARG:HD3	1:A:1030:ARG:HD2	1.98	0.46
1:A:997:LEU:O	1:A:1011:GLN:NE2	2.48	0.46
2:B:519:TRP:CD1	2:B:519:TRP:C	2.93	0.46
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.97	0.46
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.97	0.46
7:G:34:VAL:HG13	7:G:45:ILE:HG21	1.98	0.46
1:A:121:LEU:HD12	1:A:121:LEU:H	1.79	0.46
1:A:239:LEU:HA	1:A:240:PRO:HD2	1.82	0.46
1:A:524:VAL:HG22	1:A:525:GLN:N	2.30	0.46
1:A:714:PHE:O	1:A:718:VAL:HG23	2.16	0.46
1:A:1161:THR:HB	1:A:1170:ILE:HD11	1.97	0.46
1:A:1327:ILE:HD13	1:A:1328:TYR:N	2.30	0.46
2:B:35:SER:HA	2:B:811:TYR:CE1	2.51	0.46
2:B:227:LYS:H	2:B:395:GLN:CD	2.24	0.46
2:B:583:ASN:HD21	2:B:628:THR:CG2	2.28	0.46
5:E:33:GLU:H	5:E:33:GLU:HG3	1.47	0.46
1:A:481:ASP:O	1:A:485:ASP:CG	2.59	0.46
1:A:645:LEU:HD11	1:A:649:ILE:HD11	1.98	0.46
2:B:128:LEU:HD21	2:B:170:LEU:HB2	1.98	0.46
15:T:17:TT:H3'	15:T:17:TT:C3R	2.40	0.46
1:A:41:MET:HG3	1:A:257:ARG:NH2	2.31	0.46
1:A:1438:THR:N	6:F:88:TYR:HB3	2.31	0.46
3:C:69:LEU:HD23	10:J:6:ARG:HB2	1.97	0.46
1:A:35:ILE:HD12	1:A:53:LEU:HA	1.98	0.46
1:A:446:ARG:HB2	1:A:487:MET:SD	2.56	0.46
1:A:830:LYS:O	1:A:834:THR:HB	2.16	0.46
2:B:212:LEU:HD23	2:B:212:LEU:HA	1.66	0.46
2:B:649:LYS:HD3	2:B:736:THR:O	2.16	0.46
2:B:1006:ILE:HG22	2:B:1007:VAL:N	2.30	0.46
7:G:106:MET:HG2	7:G:107:LYS:N	2.30	0.46
9:I:45:ARG:NH2	9:I:47:GLU:OE1	2.48	0.46
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.97	0.45
1:A:826:ASP:HA	1:A:829:VAL:HB	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:979:LYS:HE2	2:B:987:LYS:HB2	1.99	0.45
1:A:106:VAL:HG21	1:A:214:ILE:HG12	1.99	0.45
3:C:128:ASN:O	3:C:129:ILE:HD12	2.15	0.45
4:D:14:ARG:HA	4:D:14:ARG:HD3	1.65	0.45
9:I:111:THR:OG1	9:I:113:ASP:HB2	2.17	0.45
1:A:776:ALA:O	1:A:783:THR:HG22	2.17	0.45
2:B:221:ASN:N	2:B:241:ARG:O	2.34	0.45
3:C:66:ARG:NH2	10:J:2:ILE:HG23	2.32	0.45
5:E:192:ARG:HA	5:E:214:CYS:HB3	1.98	0.45
1:A:19:PHE:O	1:A:1416:ALA:HA	2.15	0.45
1:A:287:HIS:HA	1:A:290:GLU:HG2	1.98	0.45
1:A:1095:THR:HG21	1:A:1112:LYS:HD2	1.99	0.45
1:A:1195:LEU:HA	1:A:1195:LEU:HD23	1.64	0.45
1:A:1224:LEU:HD12	1:A:1241:ARG:O	2.17	0.45
2:B:796:LEU:HD12	2:B:796:LEU:HA	1.70	0.45
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.98	0.45
3:C:33:LEU:HG	3:C:37:MET:HE2	1.99	0.45
3:C:46:ILE:HA	3:C:159:ALA:HA	1.99	0.45
8:H:89:LEU:C	8:H:91:ASP:H	2.25	0.45
1:A:140:THR:HA	1:A:143:LYS:HE2	1.99	0.45
1:A:1120:LEU:HD12	1:A:1120:LEU:HA	1.71	0.45
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.99	0.45
2:B:1156:ASP:OD1	2:B:1198:TYR:N	2.49	0.45
1:A:642:CYS:O	1:A:645:LEU:HB3	2.16	0.45
1:A:685:GLU:HG3	1:A:686:ALA:N	2.31	0.45
2:B:185:THR:HG23	2:B:188:ASP:OD2	2.17	0.45
3:C:15:LYS:O	3:C:240:VAL:HG22	2.16	0.45
5:E:79:TRP:HE1	5:E:81:GLU:HB2	1.82	0.45
1:A:128:ILE:HB	1:A:134:ARG:HB2	1.98	0.45
1:A:218:ASP:O	1:A:222:LEU:HD12	2.17	0.45
2:B:170:LEU:HD12	2:B:171:PRO:HD2	1.98	0.45
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.99	0.45
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.99	0.45
4:D:56:ARG:HB2	4:D:148:LEU:HD22	1.98	0.45
4:D:187:THR:CB	4:D:187:THR:C	2.79	0.45
1:A:547:LEU:HD22	11:K:58:PHE:CD2	2.51	0.45
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.99	0.45
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.17	0.45
2:B:63:ILE:HD12	2:B:63:ILE:HA	1.80	0.45
2:B:558:LEU:HB3	2:B:563:MET:HE2	1.98	0.45
2:B:615:MET:HE3	2:B:615:MET:HB2	1.86	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:871:THR:HG22	2:B:872:GLU:N	2.31	0.45
8:H:46:LEU:HD13	8:H:46:LEU:HA	1.65	0.45
10:J:6:ARG:HG3	10:J:13:VAL:HA	1.97	0.45
1:A:262:LEU:HG	1:A:328:ARG:HH21	1.82	0.45
1:A:262:LEU:HG	1:A:328:ARG:NH2	2.32	0.45
1:A:549:MET:CE	1:A:656:TRP:HD1	2.28	0.45
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.17	0.45
2:B:383:ASN:OD1	2:B:387:LEU:HD22	2.16	0.45
2:B:405:ARG:HB3	2:B:631:GLY:HA3	1.98	0.45
2:B:515:HIS:CE1	2:B:517:THR:HG1	2.34	0.45
2:B:848:ARG:HD2	10:J:8:PHE:O	2.17	0.45
2:B:902:GLY:O	12:L:65:VAL:HG11	2.17	0.45
4:D:52:LEU:O	4:D:53:SER:OG	2.24	0.45
12:L:61:THR:CB	12:L:63:ARG:HG2	2.46	0.45
1:A:419:LYS:HG3	1:A:420:ARG:N	2.31	0.45
1:A:566:ILE:HD11	8:H:98:TYR:HB2	1.99	0.45
1:A:898:ARG:HB2	1:A:933:TYR:CE2	2.52	0.45
1:A:942:PHE:HD2	1:A:943:LEU:HD23	1.80	0.45
2:B:636:PRO:C	2:B:637:LEU:HD12	2.42	0.45
4:D:155:ARG:H	4:D:219:THR:HG21	1.81	0.45
4:D:203:SER:OG	4:D:206:GLU:HB2	2.17	0.45
5:E:67:GLU:O	5:E:70:SER:HB3	2.17	0.45
5:E:94:LYS:O	5:E:98:ILE:HG13	2.17	0.45
8:H:133:ASN:O	8:H:135:LEU:HD12	2.16	0.45
2:B:219:ALA:HB2	2:B:405:ARG:HG2	1.99	0.44
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	2.56	0.44
1:A:9:ALA:HA	1:A:10:PRO:HD2	1.65	0.44
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.99	0.44
1:A:264:PHE:O	1:A:267:ALA:HB3	2.17	0.44
1:A:869:GLY:O	5:E:204:THR:HG21	2.17	0.44
1:A:1438:THR:HB	2:B:1142:GLY:O	2.17	0.44
2:B:189:LEU:O	2:B:192:LEU:N	2.51	0.44
2:B:550:ASP:HA	2:B:551:PRO:HD3	1.84	0.44
12:L:30:ILE:O	12:L:56:LEU:HA	2.17	0.44
1:A:193:ASP:HA	1:A:194:ALA:HA	1.53	0.44
1:A:215:SER:HB3	1:A:218:ASP:OD2	2.17	0.44
1:A:562:THR:O	1:A:576:GLN:NE2	2.51	0.44
1:A:841:LEU:HD23	1:A:841:LEU:HA	1.79	0.44
1:A:1396:ALA:HA	1:A:1399:ARG:NH2	2.32	0.44
1:A:1172:LEU:O	1:A:1174:PHE:N	2.43	0.44
1:A:1402:PHE:O	1:A:1404:GLU:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:ILE:HG23	2:B:296:GLU:HG2	1.99	0.44
2:B:753:ALA:HA	2:B:756:ILE:HD12	1.98	0.44
2:B:914:LYS:HE2	2:B:937:ALA:HB1	1.99	0.44
8:H:16:ASP:HA	8:H:17:PRO:HD3	1.83	0.44
11:K:37:LYS:HA	11:K:37:LYS:HD3	1.87	0.44
1:A:337:ARG:HH22	15:T:17:TT:P	2.41	0.44
1:A:898:ARG:HD3	1:A:933:TYR:CD2	2.52	0.44
4:D:7:THR:HB	4:D:8:PHE:H	1.19	0.44
8:H:95:TYR:CE1	8:H:97:MET:HG3	2.52	0.44
15:T:26:DC:N3	15:T:27:DA:N6	2.66	0.44
1:A:251:SER:HA	1:A:257:ARG:O	2.17	0.44
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	2.00	0.44
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.53	0.44
2:B:613:VAL:HG22	2:B:627:PHE:O	2.18	0.44
3:C:148:ARG:H	3:C:151:GLN:CG	2.13	0.44
4:D:206:GLU:O	4:D:209:ARG:HB2	2.17	0.44
6:F:72:LYS:N	6:F:72:LYS:HE2	2.33	0.44
11:K:65:HIS:CE1	11:K:67:PHE:CG	3.05	0.44
1:A:270:LEU:O	1:A:274:ILE:HG13	2.17	0.44
1:A:779:PHE:CZ	1:A:785:PRO:HD3	2.53	0.44
1:A:853:ASP:CG	1:A:855:THR:HB	2.42	0.44
2:B:879:ARG:NE	2:B:883:LEU:HG	2.33	0.44
4:D:167:LEU:O	4:D:169:SER:N	2.51	0.44
4:D:176:GLU:OE2	4:D:197:SER:HB2	2.18	0.44
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.83	0.44
6:F:83:PRO:HG2	6:F:84:TYR:CD1	2.53	0.44
8:H:12:VAL:HG23	8:H:53:ASP:O	2.18	0.44
1:A:222:LEU:O	1:A:224:PHE:N	2.51	0.44
1:A:644:LYS:HA	1:A:644:LYS:HD2	1.73	0.44
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	2.00	0.44
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.58	0.44
1:A:1032:LEU:O	1:A:1036:ARG:HD3	2.18	0.44
1:A:1170:ILE:H	1:A:1170:ILE:HG13	1.64	0.44
2:B:351:TYR:O	2:B:354:ASP:HB2	2.18	0.44
2:B:1032:SER:HB3	2:B:1089:PRO:HB2	2.00	0.44
8:H:4:THR:HA	8:H:60:ALA:CB	2.48	0.44
11:K:32:VAL:HG22	11:K:74:ARG:HG3	2.00	0.44
15:T:18:DT:C6	15:T:19:DT:H73	2.53	0.44
1:A:265:LYS:HD3	1:A:265:LYS:HA	1.84	0.44
1:A:353:ILE:HD13	1:A:487:MET:HE3	2.00	0.44
1:A:380:VAL:HG12	1:A:428:TYR:HA	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:ASN:OD1	1:A:1012:ARG:NH1	2.50	0.44
2:B:871:THR:HG22	2:B:872:GLU:O	2.18	0.44
8:H:101:ALA:HB2	8:H:116:TYR:CE1	2.52	0.44
9:I:77:LYS:C	9:I:79:HIS:H	2.25	0.44
1:A:394:ASN:OD1	1:A:398:GLU:HG2	2.18	0.43
1:A:1199:ARG:NH2	1:A:1231:ASP:O	2.46	0.43
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.53	0.43
2:B:225:VAL:HG11	2:B:385:LEU:HA	2.00	0.43
2:B:246:LYS:HG2	2:B:418:LYS:HZ1	1.82	0.43
2:B:1197:PRO:O	2:B:1200:ALA:N	2.47	0.43
11:K:51:LEU:HD12	11:K:51:LEU:HA	1.68	0.43
1:A:285:PRO:C	1:A:287:HIS:H	2.26	0.43
2:B:294:ASP:HB2	9:I:12:ASN:HA	2.00	0.43
2:B:819:ALA:HB1	2:B:1093:GLN:HE21	1.83	0.43
3:C:201:TRP:HA	3:C:202:PRO:HD3	1.71	0.43
7:G:131:GLN:HG2	7:G:136:VAL:HG23	2.00	0.43
1:A:857:ARG:HD3	1:A:861:GLY:O	2.18	0.43
1:A:1202:MET:O	1:A:1207:LEU:N	2.47	0.43
2:B:1138:MET:HE2	2:B:1146:PHE:CD2	2.53	0.43
4:D:158:GLU:OE1	4:D:158:GLU:N	2.51	0.43
8:H:142:LEU:C	8:H:143:LEU:HD12	2.43	0.43
9:I:62:ILE:HA	9:I:62:ILE:HD12	1.78	0.43
1:A:709:THR:HG22	1:A:710:LEU:N	2.34	0.43
1:A:818:MET:HE3	2:B:514:LEU:O	2.17	0.43
1:A:872:GLY:O	1:A:1058:VAL:HG22	2.18	0.43
1:A:1430:LEU:HB3	1:A:1432:GLN:HG3	1.99	0.43
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.99	0.43
3:C:124:LEU:O	3:C:127:ARG:HG2	2.18	0.43
4:D:51:ASN:OD1	4:D:54:GLU:HB2	2.18	0.43
4:D:217:LEU:O	4:D:219:THR:N	2.52	0.43
8:H:10:PHE:HB3	8:H:28:ALA:HB1	1.99	0.43
9:I:74:GLU:HB3	9:I:81:ARG:HG3	1.99	0.43
15:T:18:DT:C2	15:T:19:DT:O4	2.71	0.43
1:A:313:GLN:O	1:A:314:ALA:C	2.62	0.43
1:A:745:GLN:HA	1:A:748:MET:HE3	2.00	0.43
1:A:868:TYR:CD2	1:A:1058:VAL:HG11	2.53	0.43
1:A:879:GLU:CD	1:A:962:ARG:HH21	2.25	0.43
1:A:949:ASP:OD2	1:A:951:GLU:HB2	2.18	0.43
1:A:1095:THR:HG21	1:A:1112:LYS:HB3	2.00	0.43
2:B:101:MET:HB2	2:B:101:MET:HE3	1.71	0.43
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:44:ALA:O	5:E:45:LYS:HB2	2.19	0.43
1:A:7:SER:HB3	2:B:1193:GLN:OE1	2.18	0.43
2:B:1031:LEU:HB2	2:B:1055:ILE:HD13	2.00	0.43
4:D:144:THR:HG21	7:G:46:LEU:HD13	2.00	0.43
6:F:97:ARG:HD2	6:F:97:ARG:HA	1.66	0.43
8:H:26:ILE:HD12	8:H:26:ILE:HA	1.74	0.43
14:P:11:A:H5 ⁺	14:P:11:A:N9	2.23	0.43
1:A:963:ILE:HD13	1:A:1048:ASN:HB3	2.00	0.43
4:D:46:GLU:HG2	4:D:47:LEU:H	1.84	0.43
5:E:13:TRP:CZ3	5:E:39:LEU:HB2	2.54	0.43
6:F:101:ILE:HD13	6:F:120:ILE:CG2	2.49	0.43
1:A:208:LEU:HD23	1:A:235:ILE:HD12	2.01	0.43
1:A:456:MET:HE1	1:A:474:VAL:CG2	2.48	0.43
1:A:614:PHE:CD1	1:A:614:PHE:C	2.97	0.43
1:A:1436:ILE:O	1:A:1437:GLY:C	2.61	0.43
2:B:185:THR:O	2:B:188:ASP:HB2	2.19	0.43
2:B:199:MET:HE2	2:B:492:LEU:CD2	2.49	0.43
2:B:455:SER:HA	2:B:458:LYS:HB2	1.99	0.43
2:B:649:LYS:HE2	2:B:738:PHE:O	2.19	0.43
2:B:666:TYR:C	2:B:668:ASP:H	2.26	0.43
3:C:177:GLU:O	3:C:230:MET:HA	2.19	0.43
7:G:154:VAL:HG23	7:G:155:SER:H	1.83	0.43
1:A:407:ARG:CD	1:A:413:ILE:HD11	2.48	0.43
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.54	0.43
4:D:121:LYS:HB3	4:D:121:LYS:HE2	1.83	0.43
7:G:126:ASN:HA	7:G:127:PRO:HA	1.81	0.43
8:H:63:LEU:CB	8:H:90:ALA:HB2	2.48	0.43
11:K:7:PHE:HA	11:K:10:PHE:CE1	2.54	0.43
1:A:344:ARG:HB3	2:B:1118:PRO:HB2	2.00	0.43
2:B:1058:LEU:O	2:B:1061:GLU:HB2	2.19	0.43
2:B:1110:PRO:O	2:B:1119:VAL:HG13	2.19	0.43
7:G:1:MET:CG	7:G:2:PHE:N	2.82	0.43
1:A:915:SER:HA	1:A:918:GLU:OE2	2.18	0.42
1:A:1364:ASN:OD1	1:A:1366:ARG:HG2	2.18	0.42
2:B:401:PHE:HD2	2:B:521:LEU:HD12	1.84	0.42
2:B:498:THR:O	2:B:536:VAL:HA	2.18	0.42
2:B:773:MET:HE1	2:B:985:GLY:HA2	2.01	0.42
2:B:882:THR:HG22	2:B:884:ARG:N	2.34	0.42
2:B:1176:ASN:H	2:B:1178:ASN:H	1.67	0.42
7:G:111:THR:HG22	7:G:113:HIS:H	1.84	0.42
8:H:40:LEU:HD13	8:H:123:MET:HE3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:13:MET:HE3	9:I:13:MET:HB2	1.77	0.42
10:J:21:TYR:O	10:J:25:LEU:HG	2.19	0.42
1:A:49:LYS:HZ3	1:A:60:SER:HA	1.83	0.42
1:A:436:ILE:HA	1:A:436:ILE:HD12	1.67	0.42
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.44	0.42
1:A:800:VAL:HG13	1:A:812:GLU:OE1	2.19	0.42
1:A:1173:HIS:HB3	1:A:1227:ILE:HG23	2.00	0.42
1:A:1215:ARG:HD3	1:A:1218:GLN:NE2	2.35	0.42
2:B:112:LEU:O	2:B:180:TYR:HE2	2.02	0.42
2:B:408:LEU:HA	2:B:408:LEU:HD13	1.79	0.42
2:B:551:PRO:HG3	2:B:628:THR:HG21	2.01	0.42
5:E:163:GLU:OE2	5:E:167:ARG:NE	2.51	0.42
8:H:92:ASP:H	8:H:93:TYR:HD1	1.67	0.42
1:A:20:GLY:O	1:A:21:LEU:HD23	2.19	0.42
1:A:49:LYS:CE	1:A:61:ILE:H	2.32	0.42
1:A:335:ARG:O	1:A:339:ASN:HB2	2.19	0.42
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.18	0.42
1:A:1189:SER:O	1:A:1241:ARG:HD3	2.19	0.42
2:B:125:SER:O	2:B:169:ARG:NH1	2.52	0.42
3:C:57:VAL:H	3:C:57:VAL:HG13	1.55	0.42
3:C:163:ILE:HD12	3:C:165:LYS:HB2	2.00	0.42
4:D:9:GLN:C	4:D:11:ARG:H	2.28	0.42
4:D:135:GLY:O	4:D:137:ASN:N	2.45	0.42
7:G:132:SER:HB3	7:G:135:ASP:H	1.83	0.42
1:A:331:GLY:O	1:A:332:LYS:HB3	2.19	0.42
1:A:382:PRO:N	1:A:428:TYR:HE1	2.17	0.42
1:A:743:VAL:O	1:A:747:VAL:HG23	2.20	0.42
1:A:786:HIS:HE1	2:B:519:TRP:CE2	2.37	0.42
1:A:818:MET:HE2	1:A:818:MET:HB3	1.95	0.42
1:A:883:LEU:O	1:A:886:ILE:HG22	2.19	0.42
2:B:854:LEU:HD23	2:B:854:LEU:HA	1.73	0.42
3:C:164:ALA:HA	3:C:167:HIS:O	2.19	0.42
4:D:46:GLU:HG2	4:D:47:LEU:N	2.34	0.42
4:D:187:THR:O	4:D:190:GLU:HB3	2.18	0.42
1:A:219:PHE:HA	1:A:222:LEU:CD1	2.49	0.42
1:A:406:ILE:HB	1:A:431:LYS:HB2	2.02	0.42
1:A:602:ASP:HB3	1:A:616:VAL:HG23	2.02	0.42
1:A:1147:THR:HG22	9:I:48:LEU:HD13	2.00	0.42
4:D:63:LEU:O	4:D:133:THR:HG21	2.20	0.42
5:E:211:TYR:CD1	5:E:211:TYR:N	2.87	0.42
1:A:126:LEU:HD23	1:A:126:LEU:HA	1.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1100:ARG:O	1:A:1104:ILE:HG13	2.19	0.42
1:A:1223:ASP:HA	1:A:1243:VAL:HB	2.02	0.42
2:B:879:ARG:HB3	2:B:880:THR:H	1.56	0.42
2:B:969:ARG:HH11	3:C:61:GLU:CD	2.27	0.42
3:C:66:ARG:O	3:C:70:ILE:HD12	2.19	0.42
3:C:92:CYS:O	3:C:96:SER:OG	2.35	0.42
5:E:52:ARG:HA	5:E:53:PRO:HD2	1.66	0.42
8:H:109:LYS:HB3	8:H:110:ASP:H	1.53	0.42
1:A:219:PHE:HA	1:A:222:LEU:HD12	2.00	0.42
1:A:648:ASN:O	1:A:652:VAL:HG23	2.20	0.42
1:A:1387:HIS:CE1	13:N:6:DA:H2"	2.55	0.42
2:B:582:VAL:HG22	2:B:626:ILE:HB	2.01	0.42
2:B:1167:GLY:H	2:B:1215:ARG:HD3	1.85	0.42
5:E:195:VAL:HG22	5:E:213:ILE:HG13	2.00	0.42
1:A:380:VAL:HG13	1:A:385:ILE:HG12	2.01	0.42
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.55	0.42
1:A:664:THR:HG22	2:B:1014:PRO:HB3	2.02	0.42
1:A:710:LEU:HD12	1:A:710:LEU:HA	1.83	0.42
1:A:1004:ASN:CG	5:E:167:ARG:HD2	2.43	0.42
2:B:744:HIS:CE1	2:B:746:SER:HG	2.38	0.42
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.54	0.42
4:D:13:ARG:NH1	4:D:18:VAL:H	2.18	0.42
7:G:46:LEU:HD23	7:G:46:LEU:HA	1.88	0.42
8:H:47:PHE:HB3	8:H:95:TYR:CD2	2.55	0.42
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.82	0.42
1:A:74:MET:O	1:A:76:GLU:N	2.52	0.42
1:A:196:GLU:HA	1:A:197:PRO:HD3	1.90	0.42
1:A:444:PHE:HE2	1:A:470:LEU:HD23	1.83	0.42
1:A:1318:THR:HG22	5:E:142:VAL:HG23	2.00	0.42
1:A:1377:THR:HG22	5:E:176:PRO:HB3	2.02	0.42
1:A:1412:ALA:HA	1:A:1417:GLU:HG3	2.02	0.42
2:B:422:LYS:HA	2:B:425:THR:HB	2.02	0.42
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.20	0.42
2:B:956:THR:HA	2:B:961:LEU:O	2.19	0.42
3:C:31:ASN:O	3:C:34:ARG:HB3	2.19	0.42
3:C:41:ILE:HB	3:C:172:PRO:HG3	2.02	0.42
4:D:24:ALA:HB3	4:D:26:THR:CG2	2.44	0.42
5:E:65:THR:O	5:E:69:ILE:HG13	2.20	0.42
2:B:412:LEU:HD13	2:B:412:LEU:HA	1.84	0.42
2:B:821:GLN:OE1	2:B:850:LEU:HD12	2.20	0.42
5:E:135:PHE:CD2	5:E:140:LEU:HD21	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:82:ASP:OD2	11:K:84:LYS:HB2	2.20	0.42
14:P:6:C:C2	14:P:7:A:C8	3.08	0.42
1:A:681:GLU:HA	1:A:684:ALA:HB3	2.01	0.41
1:A:848:ILE:HA	1:A:857:ARG:O	2.20	0.41
2:B:426:LYS:O	2:B:430:ARG:HD2	2.19	0.41
2:B:853:SER:HB3	2:B:1094:ARG:HH11	1.85	0.41
3:C:62:PHE:O	3:C:66:ARG:HG3	2.20	0.41
5:E:4:GLU:HB3	5:E:7:ARG:CZ	2.50	0.41
8:H:15:VAL:HA	8:H:26:ILE:HD12	2.01	0.41
8:H:82:PRO:HB2	8:H:83:GLN:H	1.61	0.41
13:N:6:DA:C2	13:N:7:DC:C2	3.08	0.41
1:A:116:ASP:OD1	1:A:116:ASP:N	2.53	0.41
1:A:452:LYS:HG2	2:B:1141:HIS:CE1	2.55	0.41
1:A:928:LEU:HD23	1:A:928:LEU:HA	1.86	0.41
1:A:986:ILE:HG21	1:A:1028:THR:HA	2.01	0.41
2:B:336:ARG:HG3	2:B:348:ARG:NH2	2.35	0.41
2:B:1081:LEU:HD23	2:B:1081:LEU:HA	1.86	0.41
5:E:35:VAL:O	5:E:37:LEU:N	2.51	0.41
1:A:770:VAL:HG12	1:A:771:GLU:HG3	2.02	0.41
2:B:26:THR:OG1	2:B:27:ALA:N	2.54	0.41
2:B:276:ILE:HA	2:B:338:GLY:O	2.20	0.41
2:B:554:ILE:O	2:B:558:LEU:N	2.47	0.41
2:B:1065:GLN:HG2	3:C:201:TRP:CZ3	2.55	0.41
2:B:1224:PHE:HD1	5:E:171:LYS:HG3	1.86	0.41
4:D:54:GLU:O	4:D:58:VAL:HG23	2.19	0.41
1:A:11:LEU:HD13	2:B:1193:GLN:HG3	2.03	0.41
1:A:239:LEU:HD12	1:A:239:LEU:HA	1.81	0.41
1:A:335:ARG:HA	1:A:339:ASN:HB2	2.02	0.41
1:A:534:LEU:O	1:A:574:GLY:HA3	2.20	0.41
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.35	0.41
1:A:1258:HIS:HB3	1:A:1262:LYS:HZ1	1.85	0.41
2:B:461:LEU:HD12	2:B:461:LEU:H	1.86	0.41
2:B:770:GLN:HG2	2:B:983:ARG:O	2.20	0.41
2:B:916:THR:HA	2:B:917:PRO:HD3	1.90	0.41
3:C:149:LYS:C	3:C:151:GLN:N	2.78	0.41
3:C:251:LEU:O	3:C:255:VAL:HG23	2.20	0.41
13:N:4:DG:N2	13:N:5:DT:C2	2.88	0.41
15:T:26:DC:C4	15:T:27:DA:N6	2.89	0.41
1:A:43:GLU:OE2	1:A:48:ALA:HB3	2.21	0.41
1:A:49:LYS:NZ	1:A:60:SER:HA	2.35	0.41
1:A:181:LEU:HA	1:A:181:LEU:HD23	1.80	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:PRO:HB2	3:C:221:TYR:CE2	2.56	0.41
2:B:99:LYS:HB3	2:B:180:TYR:CE1	2.56	0.41
2:B:453:ILE:HD12	2:B:453:ILE:H	1.86	0.41
8:H:118:PHE:HB2	8:H:121:LEU:HB2	2.03	0.41
9:I:50:THR:CG2	9:I:52:ILE:HG12	2.49	0.41
9:I:73:ARG:HH12	9:I:112:SER:CB	2.34	0.41
9:I:97:MET:HE3	9:I:97:MET:HB2	1.87	0.41
11:K:10:PHE:HA	11:K:37:LYS:HB3	2.01	0.41
1:A:679:ILE:HG23	1:A:729:ALA:HB1	2.03	0.41
1:A:993:LEU:O	1:A:993:LEU:HD12	2.20	0.41
2:B:66:ASP:CG	2:B:67:SER:H	2.28	0.41
2:B:254:LEU:HD22	2:B:361:LEU:HD13	2.02	0.41
2:B:344:LYS:HZ3	2:B:346:GLU:H	1.68	0.41
2:B:879:ARG:HD2	2:B:879:ARG:HA	1.58	0.41
3:C:47:ASP:HA	3:C:169:LYS:NZ	2.36	0.41
4:D:144:THR:CG2	4:D:148:LEU:HD12	2.50	0.41
9:I:14:LEU:HB3	9:I:27:PHE:HB3	2.01	0.41
1:A:41:MET:HA	1:A:50:ILE:H	1.86	0.41
1:A:1064:VAL:HG12	1:A:1064:VAL:O	2.21	0.41
1:A:1366:ARG:HG2	1:A:1366:ARG:H	1.41	0.41
2:B:530:GLY:H	2:B:533:CYS:HB2	1.86	0.41
2:B:680:THR:O	2:B:683:SER:HB2	2.20	0.41
2:B:710:LEU:HA	2:B:733:HIS:HB3	2.03	0.41
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.21	0.41
5:E:29:PHE:N	5:E:63:ASN:O	2.41	0.41
6:F:74:ILE:HA	6:F:75:PRO:HD2	1.70	0.41
8:H:13:SER:N	8:H:27:GLU:O	2.38	0.41
12:L:61:THR:HG21	12:L:63:ARG:NE	2.35	0.41
1:A:54:ASN:HB3	1:A:247:ARG:NH2	2.30	0.41
1:A:262:LEU:HD11	1:A:325:ILE:HG12	2.03	0.41
1:A:503:GLN:OE1	6:F:90:ARG:NH2	2.50	0.41
1:A:626:ASN:O	1:A:631:HIS:CD2	2.74	0.41
1:A:1261:LYS:HE3	1:A:1261:LYS:HB2	1.60	0.41
2:B:95:ILE:HD11	2:B:128:LEU:HD12	2.03	0.41
2:B:221:ASN:OD1	2:B:242:SER:HA	2.21	0.41
2:B:305:VAL:O	2:B:305:VAL:HG12	2.21	0.41
2:B:368:GLU:O	2:B:370:PHE:N	2.50	0.41
2:B:469:GLN:HG2	2:B:470:LYS:HE2	2.03	0.41
2:B:485:ARG:CZ	2:B:782:LEU:HD11	2.51	0.41
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.56	0.41
2:B:848:ARG:HH22	2:B:996:ARG:HH11	1.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.85	0.41
7:G:138:THR:HG22	7:G:139:ILE:N	2.30	0.41
11:K:63:VAL:HG23	11:K:63:VAL:O	2.21	0.41
11:K:65:HIS:HE1	11:K:67:PHE:CD1	2.38	0.41
1:A:88:LYS:HD2	1:A:293:GLU:CD	2.46	0.41
1:A:266:LEU:HD21	1:A:303:TYR:CZ	2.56	0.41
1:A:391:LEU:HA	1:A:394:ASN:HB2	2.03	0.41
1:A:451:HIS:HB2	1:A:454:SER:HB2	2.02	0.41
1:A:1123:GLY:O	1:A:1125:ALA:N	2.54	0.41
1:A:1387:HIS:HE1	13:N:6:DA:H2'	1.86	0.41
2:B:283:VAL:HG21	2:B:317:CYS:O	2.21	0.41
2:B:367:LEU:HB2	2:B:368:GLU:H	1.66	0.41
2:B:775:LYS:HE3	2:B:775:LYS:HB2	1.94	0.41
3:C:18:VAL:CG2	3:C:240:VAL:HB	2.51	0.41
3:C:50:GLU:HG3	3:C:156:THR:HB	2.03	0.41
5:E:118:PRO:HA	5:E:121:MET:HB2	2.02	0.41
6:F:118:LEU:HD12	6:F:118:LEU:HA	1.85	0.41
8:H:93:TYR:CD1	8:H:143:LEU:HD23	2.56	0.41
11:K:84:LYS:HB3	11:K:84:LYS:HE3	1.89	0.41
13:N:10:DG:H2'	13:N:11:DA:C8	2.56	0.41
1:A:265:LYS:O	1:A:269:ILE:HG13	2.21	0.41
1:A:347:PHE:CD1	2:B:1107:ALA:HB1	2.56	0.41
1:A:821:ARG:HB2	1:A:821:ARG:HH11	1.86	0.41
1:A:1116:LEU:HG	1:A:1327:ILE:HD11	2.03	0.41
2:B:129:PHE:HA	2:B:165:VAL:O	2.21	0.41
8:H:77:ARG:HH11	8:H:77:ARG:HB2	1.85	0.41
8:H:104:PHE:CD1	8:H:114:VAL:HG12	2.56	0.41
15:T:7:DC:H6	15:T:7:DC:H2'	1.70	0.41
1:A:42:ASP:OD2	1:A:45:GLN:HA	2.21	0.40
1:A:353:ILE:HG13	1:A:482:PHE:HD1	1.86	0.40
1:A:498:ARG:HH11	1:A:498:ARG:HD3	1.74	0.40
1:A:525:GLN:HG3	2:B:836:GLU:HG2	2.03	0.40
1:A:1000:LEU:HD12	1:A:1011:GLN:HA	2.04	0.40
2:B:211:VAL:HG23	2:B:481:GLN:O	2.21	0.40
3:C:259:LEU:HD12	3:C:259:LEU:HA	1.92	0.40
8:H:83:GLN:O	8:H:86:ASP:N	2.45	0.40
9:I:70:ARG:HA	9:I:70:ARG:HD3	1.91	0.40
1:A:767:GLN:NE2	1:A:774:ARG:HD2	2.36	0.40
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	2.02	0.40
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.52	0.40
2:B:128:LEU:HD21	2:B:170:LEU:CB	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:365:THR:HG21	2:B:370:PHE:CD1	2.56	0.40
3:C:5:GLY:HA3	3:C:6:PRO:HD2	1.95	0.40
3:C:116:LYS:HD3	3:C:140:ASN:HA	2.03	0.40
4:D:39:ASN:O	4:D:42:GLY:N	2.44	0.40
4:D:41:GLN:OE1	4:D:41:GLN:N	2.54	0.40
4:D:138:ASN:ND2	7:G:35:GLU:HG2	2.35	0.40
5:E:69:ILE:HG13	5:E:69:ILE:H	1.70	0.40
5:E:118:PRO:O	5:E:122:LYS:HG2	2.21	0.40
5:E:156:LEU:HA	5:E:160:GLU:OE1	2.22	0.40
5:E:181:ALA:HA	5:E:186:LEU:HD21	2.03	0.40
10:J:8:PHE:N	10:J:49:MET:HE3	2.33	0.40
11:K:5:ASP:HB3	11:K:7:PHE:CE2	2.56	0.40
11:K:47:ARG:HD2	11:K:51:LEU:HD22	2.02	0.40
1:A:483:ASP:CG	14:P:11:A:HO3'	2.26	0.40
1:A:804:TYR:OH	2:B:763:GLN:HA	2.21	0.40
2:B:31:TRP:CZ2	2:B:807:ARG:HB2	2.56	0.40
4:D:126:ILE:HG21	4:D:145:MET:HB3	2.03	0.40
6:F:136:ARG:O	6:F:143:PHE:HB2	2.21	0.40
11:K:101:LEU:HD23	11:K:101:LEU:HA	1.81	0.40
15:T:14:DA:H1'	15:T:15:DC:H5'	2.01	0.40
1:A:567:LYS:HG2	1:A:569:LYS:N	2.35	0.40
1:A:1424:VAL:HG13	1:A:1436:ILE:HG12	2.03	0.40
2:B:295:GLY:N	2:B:298:LEU:HD12	2.37	0.40
2:B:491:THR:O	2:B:495:LEU:HD12	2.22	0.40
2:B:571:PRO:C	2:B:573:GLN:N	2.79	0.40
2:B:610:ASN:OD1	2:B:610:ASN:C	2.64	0.40
2:B:722:ASP:OD2	2:B:723:VAL:HG23	2.21	0.40
6:F:116:ASP:HA	6:F:117:PRO:HD2	1.91	0.40
8:H:58:THR:HB	8:H:143:LEU:HB2	2.04	0.40
8:H:135:LEU:HB2	8:H:137:GLN:HG3	2.03	0.40
10:J:6:ARG:HA	10:J:12:LYS:O	2.21	0.40
15:T:14:DA:C2	15:T:15:DC:C2	3.10	0.40
1:A:15:LYS:HA	1:A:15:LYS:HD3	1.89	0.40
1:A:134:ARG:NH1	1:A:221:SER:HA	2.36	0.40
1:A:351:THR:HG22	1:A:468:PHE:CD2	2.57	0.40
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.72	0.40
1:A:722:LEU:HD11	1:A:794:PRO:HB3	2.04	0.40
1:A:852:TYR:CE1	1:A:1060:PRO:HB2	2.55	0.40
1:A:868:TYR:CZ	1:A:1064:VAL:HG11	2.54	0.40
1:A:984:LYS:HB3	1:A:988:LEU:HD12	2.04	0.40
2:B:377:PHE:CD2	2:B:381:MET:HE2	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:765:PRO:O	2:B:769:TYR:HD1	2.05	0.40
2:B:1098:MET:HB2	2:B:1098:MET:HE3	1.88	0.40
2:B:1167:GLY:H	2:B:1215:ARG:HG2	1.87	0.40
3:C:3:GLU:O	3:C:4:GLU:HG3	2.22	0.40
3:C:22:LEU:O	3:C:227:THR:HA	2.20	0.40
5:E:35:VAL:C	5:E:37:LEU:H	2.29	0.40
10:J:48:ARG:HE	10:J:49:MET:CE	2.31	0.40
13:N:10:DG:H2'	13:N:11:DA:H8	1.86	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	1414/1732 (82%)	1209 (86%)	145 (10%)	60 (4%)	2	14
2	B	1096/1224 (90%)	945 (86%)	120 (11%)	31 (3%)	4	19
3	C	264/318 (83%)	237 (90%)	23 (9%)	4 (2%)	8	30
4	D	174/221 (79%)	146 (84%)	15 (9%)	13 (8%)	1	5
5	E	212/215 (99%)	193 (91%)	14 (7%)	5 (2%)	4	22
6	F	82/155 (53%)	74 (90%)	7 (8%)	1 (1%)	10	35
7	G	169/171 (99%)	153 (90%)	13 (8%)	3 (2%)	6	26
8	H	129/146 (88%)	102 (79%)	19 (15%)	8 (6%)	1	7
9	I	117/122 (96%)	100 (86%)	12 (10%)	5 (4%)	2	13
10	J	63/70 (90%)	56 (89%)	4 (6%)	3 (5%)	2	11
11	K	113/120 (94%)	104 (92%)	9 (8%)	0	100	100
12	L	44/70 (63%)	31 (70%)	6 (14%)	7 (16%)	0	0
All	All	3877/4564 (85%)	3350 (86%)	387 (10%)	140 (4%)	2	16

All (140) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	48	ALA
1	A	57	ARG
1	A	58	LEU
1	A	74	MET
1	A	76	GLU
1	A	169	ASN
1	A	193	ASP
1	A	257	ARG
1	A	286	HIS
1	A	311	GLN
1	A	399	HIS
1	A	556	TRP
1	A	885	THR
1	A	1403	GLU
1	A	1438	THR
2	B	340	ALA
2	B	343	ILE
2	B	367	LEU
2	B	476	ARG
2	B	643	ASP
2	B	707	PRO
2	B	731	VAL
2	B	879	ARG
2	B	881	ASN
2	B	959	ASP
2	B	1046	PRO
2	B	1170	THR
4	D	13	ARG
4	D	15	LEU
4	D	16	LYS
4	D	18	VAL
4	D	53	SER
4	D	119	ARG
4	D	169	SER
4	D	198	LEU
7	G	154	VAL
8	H	83	GLN
9	I	95	THR
10	J	2	ILE
10	J	6	ARG
12	L	39	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	97	ALA
1	A	167	CYS
1	A	178	GLY
1	A	223	GLY
1	A	310	GLY
1	A	314	ALA
1	A	318	SER
1	A	628	GLY
1	A	774	ARG
1	A	855	THR
1	A	1123	GLY
1	A	1124	HIS
1	A	1173	HIS
1	A	1175	SER
1	A	1232	ASN
1	A	1233	ASP
1	A	1405	THR
2	B	108	VAL
2	B	867	GLY
2	B	937	ALA
2	B	1155	SER
2	B	1176	ASN
2	B	1181	GLU
3	C	136	ASP
3	C	184	ASN
4	D	218	GLU
5	E	36	GLU
5	E	45	LYS
8	H	81	PRO
8	H	82	PRO
9	I	9	ASP
9	I	78	CYS
9	I	79	HIS
12	L	56	LEU
1	A	51	GLY
1	A	63	ARG
1	A	75	ASN
1	A	189	ARG
1	A	333	GLU
1	A	400	PRO
1	A	449	SER
1	A	958	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	975	HIS
2	B	249	ARG
2	B	363	HIS
2	B	711	GLU
2	B	772	ALA
2	B	883	LEU
2	B	943	SER
2	B	1108	ARG
2	B	1156	ASP
4	D	40	HIS
4	D	138	ASN
4	D	168	LYS
5	E	113	GLN
8	H	128	ASN
12	L	45	ALA
12	L	64	LEU
1	A	44	THR
1	A	65	LEU
1	A	196	GLU
1	A	569	LYS
1	A	1255	GLU
2	B	667	GLN
2	B	708	GLU
2	B	713	ALA
3	C	4	GLU
3	C	214	ASN
4	D	10	THR
5	E	43	LYS
8	H	17	PRO
8	H	60	ALA
8	H	77	ARG
8	H	132	LEU
9	I	47	GLU
12	L	26	THR
12	L	59	ALA
1	A	188	ASP
1	A	191	THR
1	A	510	GLN
1	A	1127	ASP
5	E	140	LEU
6	F	73	ALA
7	G	57	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	64	ASN
12	L	42	ARG
1	A	42	ASP
1	A	54	ASN
1	A	453	MET
1	A	567	LYS
1	A	1448	GLU
7	G	63	PRO
1	A	35	ILE
1	A	1242	VAL
2	B	263	GLY
1	A	52	GLY
1	A	61	ILE
2	B	369	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	1240/1519 (82%)	1032 (83%)	208 (17%)	2	9
2	B	964/1061 (91%)	789 (82%)	175 (18%)	2	7
3	C	234/274 (85%)	196 (84%)	38 (16%)	2	10
4	D	160/200 (80%)	132 (82%)	28 (18%)	2	8
5	E	196/197 (100%)	172 (88%)	24 (12%)	5	19
6	F	74/137 (54%)	64 (86%)	10 (14%)	4	15
7	G	152/152 (100%)	131 (86%)	21 (14%)	3	14
8	H	117/128 (91%)	98 (84%)	19 (16%)	2	10
9	I	113/116 (97%)	97 (86%)	16 (14%)	3	13
10	J	60/65 (92%)	52 (87%)	8 (13%)	4	15
11	K	99/102 (97%)	88 (89%)	11 (11%)	6	21
12	L	40/57 (70%)	26 (65%)	14 (35%)	0	0
All	All	3449/4008 (86%)	2877 (83%)	572 (17%)	2	10

All (572) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	13	THR
1	A	32	VAL
1	A	35	ILE
1	A	36	ARG
1	A	39	GLU
1	A	41	MET
1	A	47	ARG
1	A	50	ILE
1	A	53	LEU
1	A	62	ASP
1	A	67	CYS
1	A	84	ILE
1	A	93	VAL
1	A	113	LEU
1	A	117	GLU
1	A	132	LYS
1	A	147	VAL
1	A	160	GLN
1	A	173	THR
1	A	175	ARG
1	A	182	VAL
1	A	188	ASP
1	A	191	THR
1	A	193	ASP
1	A	199	LEU
1	A	204	THR
1	A	208	LEU
1	A	215	SER
1	A	217	LYS
1	A	220	THR
1	A	232	GLU
1	A	237	THR
1	A	251	SER
1	A	270	LEU
1	A	274	ILE
1	A	277	GLU
1	A	287	HIS
1	A	293	GLU
1	A	307	ASP
1	A	313	GLN
1	A	315	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	320	ARG
1	A	322	VAL
1	A	323	LYS
1	A	324	SER
1	A	333	GLU
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	354	SER
1	A	369	SER
1	A	375	THR
1	A	381	THR
1	A	385	ILE
1	A	386	ASP
1	A	394	ASN
1	A	398	GLU
1	A	425	GLN
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	449	SER
1	A	454	SER
1	A	461	LYS
1	A	463	ILE
1	A	469	ARG
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	479	ASN
1	A	485	ASP
1	A	498	ARG
1	A	500	GLU
1	A	505	CYS
1	A	512	VAL
1	A	513	SER
1	A	521	MET
1	A	528	LEU
1	A	566	ILE
1	A	571	LEU
1	A	588	LEU
1	A	596	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	597	LEU
1	A	598	LEU
1	A	602	ASP
1	A	613	ILE
1	A	618	GLU
1	A	622	VAL
1	A	629	LEU
1	A	635	ARG
1	A	644	LYS
1	A	666	ILE
1	A	670	ILE
1	A	672	ASP
1	A	676	MET
1	A	690	VAL
1	A	693	VAL
1	A	703	THR
1	A	719	VAL
1	A	732	LEU
1	A	738	LYS
1	A	764	CYS
1	A	768	GLN
1	A	769	SER
1	A	773	LYS
1	A	782	ARG
1	A	788	SER
1	A	795	GLU
1	A	801	GLU
1	A	821	ARG
1	A	834	THR
1	A	837	ILE
1	A	848	ILE
1	A	855	THR
1	A	865	GLN
1	A	871	ASP
1	A	881	GLN
1	A	882	SER
1	A	885	THR
1	A	896	ARG
1	A	904	THR
1	A	915	SER
1	A	918	GLU
1	A	919	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	920	LEU
1	A	926	GLN
1	A	927	VAL
1	A	932	GLU
1	A	934	LYS
1	A	941	LYS
1	A	943	LEU
1	A	948	VAL
1	A	963	ILE
1	A	964	ILE
1	A	969	GLN
1	A	973	ILE
1	A	976	THR
1	A	982	THR
1	A	986	ILE
1	A	993	LEU
1	A	1001	ARG
1	A	1006	ILE
1	A	1046	LEU
1	A	1058	VAL
1	A	1062	GLU
1	A	1064	VAL
1	A	1067	LEU
1	A	1078	GLN
1	A	1112	LYS
1	A	1113	THR
1	A	1116	LEU
1	A	1120	LEU
1	A	1124	HIS
1	A	1133	LEU
1	A	1135	ARG
1	A	1147	THR
1	A	1165	GLU
1	A	1170	ILE
1	A	1172	LEU
1	A	1173	HIS
1	A	1174	PHE
1	A	1176	LEU
1	A	1199	ARG
1	A	1205	LYS
1	A	1215	ARG
1	A	1222	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1223	ASP
1	A	1226	VAL
1	A	1234	GLU
1	A	1237	ILE
1	A	1242	VAL
1	A	1260	LEU
1	A	1261	LYS
1	A	1264	GLU
1	A	1270	ASN
1	A	1271	ILE
1	A	1273	LEU
1	A	1280	GLU
1	A	1291	VAL
1	A	1293	SER
1	A	1295	THR
1	A	1297	GLU
1	A	1301	GLU
1	A	1315	GLU
1	A	1327	ILE
1	A	1336	MET
1	A	1341	ILE
1	A	1356	ILE
1	A	1366	ARG
1	A	1372	VAL
1	A	1376	THR
1	A	1387	HIS
1	A	1391	ARG
1	A	1394	THR
1	A	1400	CYS
1	A	1403	GLU
1	A	1420	ASP
1	A	1426	GLU
1	A	1436	ILE
1	A	1438	THR
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1451	VAL
1	A	1453	TYR
1	A	1454	MET
2	B	25	ILE
2	B	41	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	44	VAL
2	B	46	GLN
2	B	58	THR
2	B	63	ILE
2	B	70	ILE
2	B	101	MET
2	B	102	VAL
2	B	105	SER
2	B	112	LEU
2	B	119	LEU
2	B	131	ASP
2	B	132	VAL
2	B	134	LYS
2	B	165	VAL
2	B	169	ARG
2	B	183	GLU
2	B	185	THR
2	B	211	VAL
2	B	217	ARG
2	B	218	SER
2	B	222	ILE
2	B	225	VAL
2	B	228	LYS
2	B	248	SER
2	B	251	ILE
2	B	261	ARG
2	B	265	SER
2	B	267	ARG
2	B	272	THR
2	B	278	GLN
2	B	283	VAL
2	B	313	MET
2	B	325	GLN
2	B	334	ILE
2	B	337	ARG
2	B	343	ILE
2	B	344	LYS
2	B	346	GLU
2	B	347	LYS
2	B	348	ARG
2	B	355	ILE
2	B	357	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	361	LEU
2	B	365	THR
2	B	367	LEU
2	B	387	LEU
2	B	393	LYS
2	B	394	ASP
2	B	401	PHE
2	B	408	LEU
2	B	412	LEU
2	B	416	LEU
2	B	419	THR
2	B	423	LYS
2	B	425	THR
2	B	429	PHE
2	B	430	ARG
2	B	434	ARG
2	B	446	LEU
2	B	448	ILE
2	B	453	ILE
2	B	455	SER
2	B	470	LYS
2	B	475	SER
2	B	476	ARG
2	B	480	SER
2	B	482	VAL
2	B	485	ARG
2	B	487	THR
2	B	490	SER
2	B	498	THR
2	B	502	ILE
2	B	529	GLU
2	B	547	VAL
2	B	552	MET
2	B	559	SER
2	B	563	MET
2	B	570	VAL
2	B	574	SER
2	B	580	VAL
2	B	582	VAL
2	B	598	GLU
2	B	603	LEU
2	B	612	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	613	VAL
2	B	615	MET
2	B	616	ILE
2	B	620	ARG
2	B	628	THR
2	B	641	GLU
2	B	642	ASP
2	B	648	HIS
2	B	653	VAL
2	B	658	ILE
2	B	678	GLU
2	B	690	VAL
2	B	706	GLN
2	B	708	GLU
2	B	730	ARG
2	B	734	HIS
2	B	737	THR
2	B	746	SER
2	B	754	SER
2	B	764	SER
2	B	766	ARG
2	B	773	MET
2	B	775	LYS
2	B	786	ASN
2	B	787	VAL
2	B	790	ASP
2	B	825	VAL
2	B	831	SER
2	B	835	GLN
2	B	837	ASP
2	B	843	GLN
2	B	844	SER
2	B	857	ARG
2	B	858	SER
2	B	862	GLN
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	884	ARG
2	B	887	HIS
2	B	889	THR
2	B	904	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	911	ILE
2	B	915	THR
2	B	916	THR
2	B	944	THR
2	B	945	GLU
2	B	953	LEU
2	B	956	THR
2	B	959	ASP
2	B	964	VAL
2	B	970	THR
2	B	976	ILE
2	B	983	ARG
2	B	986	GLN
2	B	987	LYS
2	B	997	GLU
2	B	999	MET
2	B	1002	THR
2	B	1007	VAL
2	B	1045	SER
2	B	1048	THR
2	B	1050	ILE
2	B	1051	THR
2	B	1052	VAL
2	B	1060	ARG
2	B	1065	GLN
2	B	1072	MET
2	B	1102	LYS
2	B	1106	ARG
2	B	1112	GLN
2	B	1147	LEU
2	B	1150	ARG
2	B	1151	LEU
2	B	1159	ARG
2	B	1160	VAL
2	B	1168	LEU
2	B	1169	MET
2	B	1170	THR
2	B	1172	ILE
2	B	1175	LEU
2	B	1182	CYS
2	B	1183	LYS
2	B	1188	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1191	ILE
2	B	1196	ILE
2	B	1202	LEU
2	B	1220	ARG
2	B	1221	SER
3	C	7	GLN
3	C	9	LYS
3	C	16	ASP
3	C	22	LEU
3	C	23	SER
3	C	25	VAL
3	C	27	LEU
3	C	50	GLU
3	C	55	THR
3	C	56	THR
3	C	57	VAL
3	C	81	GLU
3	C	89	GLU
3	C	100	THR
3	C	108	GLU
3	C	111	THR
3	C	119	VAL
3	C	121	VAL
3	C	124	LEU
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	134	ILE
3	C	137	LYS
3	C	148	ARG
3	C	158	VAL
3	C	195	GLN
3	C	200	GLU
3	C	204	SER
3	C	215	GLU
3	C	224	GLN
3	C	235	VAL
3	C	238	ILE
3	C	240	VAL
3	C	259	LEU
3	C	263	THR
3	C	265	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	268	ASP
4	D	5	THR
4	D	7	THR
4	D	9	GLN
4	D	18	VAL
4	D	23	ASN
4	D	26	THR
4	D	34	GLN
4	D	52	LEU
4	D	63	LEU
4	D	67	ARG
4	D	73	SER
4	D	118	THR
4	D	121	LYS
4	D	126	ILE
4	D	139	LYS
4	D	141	LEU
4	D	144	THR
4	D	146	GLN
4	D	148	LEU
4	D	158	GLU
4	D	159	THR
4	D	186	ASP
4	D	187	THR
4	D	197	SER
4	D	202	ILE
4	D	213	GLU
4	D	217	LEU
4	D	219	THR
5	E	2	ASP
5	E	5	ASN
5	E	6	GLU
5	E	10	SER
5	E	18	THR
5	E	31	THR
5	E	33	GLU
5	E	45	LYS
5	E	49	SER
5	E	52	ARG
5	E	65	THR
5	E	84	ASP
5	E	85	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	90	VAL
5	E	95	THR
5	E	114	ASN
5	E	131	THR
5	E	144	ILE
5	E	173	SER
5	E	174	GLN
5	E	184	VAL
5	E	191	LYS
5	E	200	ARG
5	E	203	GLU
6	F	72	LYS
6	F	82	THR
6	F	93	ILE
6	F	109	VAL
6	F	111	LEU
6	F	115	THR
6	F	128	LYS
6	F	134	ILE
6	F	148	VAL
6	F	153	VAL
7	G	2	PHE
7	G	13	LEU
7	G	22	MET
7	G	34	VAL
7	G	64	THR
7	G	75	ARG
7	G	83	LYS
7	G	92	VAL
7	G	93	SER
7	G	95	SER
7	G	114	LEU
7	G	118	ASP
7	G	134	GLU
7	G	136	VAL
7	G	143	ILE
7	G	145	VAL
7	G	151	ILE
7	G	152	SER
7	G	154	VAL
7	G	155	SER
7	G	162	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	12	VAL
8	H	14	GLU
8	H	26	ILE
8	H	32	THR
8	H	42	ILE
8	H	46	LEU
8	H	76	THR
8	H	77	ARG
8	H	86	ASP
8	H	89	LEU
8	H	91	ASP
8	H	100	THR
8	H	103	LYS
8	H	106	GLU
8	H	107	VAL
8	H	108	SER
8	H	114	VAL
8	H	130	ARG
8	H	138	GLU
9	I	5	ARG
9	I	7	CYS
9	I	8	ARG
9	I	13	MET
9	I	31	THR
9	I	43	VAL
9	I	50	THR
9	I	54	GLU
9	I	55	THR
9	I	58	VAL
9	I	62	ILE
9	I	84	VAL
9	I	89	GLN
9	I	94	ASP
9	I	111	THR
9	I	120	GLN
10	J	3	VAL
10	J	7	CYS
10	J	13	VAL
10	J	14	VAL
10	J	22	LEU
10	J	23	ASN
10	J	34	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	42	LYS
11	K	6	ARG
11	K	12	LEU
11	K	18	LYS
11	K	22	ASP
11	K	25	THR
11	K	41	THR
11	K	47	ARG
11	K	51	LEU
11	K	95	ILE
11	K	101	LEU
11	K	107	THR
12	L	26	THR
12	L	27	LEU
12	L	33	GLU
12	L	37	LYS
12	L	38	LEU
12	L	44	ASP
12	L	50	ASP
12	L	51	CYS
12	L	55	ILE
12	L	58	LYS
12	L	61	THR
12	L	64	LEU
12	L	65	VAL
12	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	GLN
1	A	390	GLN
1	A	445	ASN
1	A	548	ASN
1	A	611	GLN
1	A	698	GLN
1	A	742	ASN
1	A	760	GLN
1	A	767	GLN
1	A	768	GLN
1	A	1265	ASN
1	A	1387	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	121	ASN
2	B	224	GLN
2	B	395	GLN
2	B	481	GLN
2	B	770	GLN
2	B	986	GLN
2	B	1084	GLN
2	B	1093	GLN
2	B	1117	GLN
3	C	7	GLN
3	C	102	GLN
3	C	131	HIS
3	C	135	GLN
3	C	140	ASN
3	C	151	GLN
4	D	9	GLN
4	D	37	GLN
5	E	115	ASN
7	G	122	ASN
8	H	11	GLN
8	H	52	GLN
8	H	83	GLN
8	H	131	ASN
9	I	79	HIS
10	J	64	ASN
11	K	96	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	9/12 (75%)	2 (22%)	2 (22%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	4	A
14	P	11	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	P	3	G
14	P	10	A

5.4 Non-standard residues in protein, DNA, RNA chains

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BRU	T	22	14,15	18,21,22	1.49	4 (22%)	25,30,33	2.51	9 (36%)
15	TT	T	17	15	40,43,44	1.28	5 (12%)	58,69,72	2.08	14 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BRU	T	22	14,15	-	2/7/21/22	0/2/2/2
15	TT	T	17	15	-	9/18/105/106	0/5/6/6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	17	TT	C2-N3	-3.28	1.32	1.38
15	T	17	TT	C2-N1	3.04	1.42	1.36
15	T	17	TT	C1R-N1T	3.02	1.49	1.45
15	T	17	TT	C4-N3	-2.94	1.32	1.37
15	T	22	BRU	C4-N3	-2.86	1.33	1.38
15	T	22	BRU	C6-N1	-2.57	1.33	1.38
15	T	22	BRU	C2-N3	-2.52	1.33	1.38
15	T	22	BRU	C2-N1	2.36	1.42	1.38
15	T	17	TT	C2T-N3T	-2.03	1.34	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	17	TT	O4R-C1R-N1T	8.05	118.19	108.65
15	T	17	TT	C4-N3-C2	-6.42	116.98	126.67
15	T	22	BRU	C5-C4-N3	5.74	119.95	113.34
15	T	22	BRU	C4-N3-C2	-5.31	120.37	127.34
15	T	22	BRU	O4-C4-C5	-5.12	119.27	125.80
15	T	22	BRU	N3-C2-N1	4.39	120.61	114.89
15	T	22	BRU	C2'-C1'-N1	-4.16	103.41	113.81
15	T	17	TT	C2'-C1'-N1	-3.84	110.39	115.59
15	T	17	TT	O4T-C4T-C5T	-3.28	119.66	122.71
15	T	17	TT	O4-C4-C5	-3.09	119.83	122.71
15	T	17	TT	C4T-N3T-C2T	-3.00	122.15	126.67
15	T	17	TT	C2R-C1R-N1T	-2.91	111.66	115.59
15	T	17	TT	N3T-C2T-N1T	2.73	119.64	116.78
15	T	17	TT	O2-C2-N1	-2.58	119.58	123.44
15	T	17	TT	O4R-C4R-C5R	2.56	117.52	109.33
15	T	17	TT	O5R-C5R-C4R	2.40	114.84	109.24
15	T	17	TT	C5'-C4'-C3'	-2.37	108.95	114.57
15	T	22	BRU	C6-C5-C4	-2.20	118.44	120.67
15	T	17	TT	O2T-C2T-N1T	-2.17	120.18	123.44
15	T	22	BRU	C1'-N1-C6	-2.12	117.17	120.74
15	T	22	BRU	BR-C5-C4	2.12	120.47	118.02
15	T	17	TT	C3'-C2'-C1'	2.08	106.85	102.89
15	T	22	BRU	O2-C2-N3	-2.01	117.78	121.49

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	22	BRU	C3'-C4'-C5'-O5'
15	T	22	BRU	O4'-C4'-C5'-O5'
15	T	17	TT	C2R-C1R-N1T-C6T
15	T	17	TT	O3'-C7-O5R-C5R
15	T	17	TT	C3'-C4'-C5'-O5'
15	T	17	TT	O4'-C4'-C5'-O5'
15	T	17	TT	O4R-C1R-N1T-C6T
15	T	17	TT	C2R-C1R-N1T-C2T
15	T	17	TT	O4R-C1R-N1T-C2T
15	T	17	TT	C4'-C5'-O5'-P
15	T	17	TT	C4'-C3'-O3'-C7

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	T	17	TT	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	1422/1732 (82%)	-0.46	15 (1%) 78 65	56, 101, 162, 298	0
2	B	1113/1224 (90%)	-0.18	34 (3%) 51 38	53, 113, 185, 237	0
3	C	266/318 (83%)	-0.65	0 100 100	72, 102, 141, 189	0
4	D	178/221 (80%)	-0.25	8 (4%) 38 28	80, 116, 180, 211	0
5	E	214/215 (99%)	-0.40	1 (0%) 87 78	77, 137, 188, 195	0
6	F	84/155 (54%)	-0.78	1 (1%) 76 63	59, 80, 109, 134	0
7	G	171/171 (100%)	-0.45	0 100 100	63, 100, 139, 166	0
8	H	133/146 (91%)	-0.00	5 (3%) 44 31	106, 151, 194, 218	0
9	I	119/122 (97%)	-0.16	2 (1%) 69 54	107, 141, 182, 219	0
10	J	65/70 (92%)	-0.54	1 (1%) 72 57	77, 106, 146, 157	0
11	K	115/120 (95%)	-0.64	2 (1%) 69 54	66, 101, 137, 163	0
12	L	46/70 (65%)	0.23	1 (2%) 62 47	91, 154, 198, 202	0
13	N	12/14 (85%)	0.32	0 100 100	164, 177, 260, 301	0
14	P	9/12 (75%)	-0.01	1 (11%) 10 11	132, 150, 197, 204	0
15	T	21/25 (84%)	0.30	2 (9%) 14 13	125, 177, 286, 307	0
All	All	3968/4615 (85%)	-0.35	73 (1%) 67 53	53, 110, 179, 307	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	502	ILE	6.5
1	A	1080	THR	6.3
2	B	1224	PHE	6.0
8	H	63	LEU	5.5
2	B	883	LEU	5.2
10	J	65	PRO	4.8
2	B	882	THR	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	K	114	LEU	4.6
2	B	709	ASP	4.5
2	B	933	SER	4.5
2	B	708	GLU	4.1
2	B	1222	ARG	4.1
12	L	27	LEU	4.0
2	B	341	LEU	4.0
2	B	918	ILE	3.9
2	B	134	LYS	3.9
1	A	1243	VAL	3.8
2	B	446	LEU	3.8
1	A	1254	ALA	3.8
6	F	72	LYS	3.6
1	A	252	PHE	3.6
2	B	262	GLU	3.5
1	A	1455	PRO	3.4
2	B	70	ILE	3.4
15	T	18	DT	3.3
2	B	880	THR	3.2
2	B	881	ASN	3.1
4	D	25	ALA	3.0
1	A	251	SER	3.0
2	B	343	ILE	3.0
2	B	509	ALA	2.8
4	D	20	GLU	2.8
8	H	2	SER	2.7
1	A	1176	LEU	2.7
4	D	3	VAL	2.7
11	K	115	ALA	2.7
2	B	769	TYR	2.7
1	A	310	GLY	2.6
2	B	715	ALA	2.6
1	A	1187	GLN	2.6
1	A	190	ALA	2.6
8	H	135	LEU	2.6
1	A	1381	LEU	2.5
2	B	164	LYS	2.5
2	B	884	ARG	2.5
2	B	252	SER	2.5
2	B	473	MET	2.5
15	T	19	DT	2.4
4	D	187	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	I	116	ASN	2.3
4	D	18	VAL	2.3
2	B	249	ARG	2.3
1	A	56	PRO	2.3
2	B	860	MET	2.3
1	A	186	LYS	2.3
2	B	879	ARG	2.2
2	B	870	ILE	2.2
4	D	13	ARG	2.2
9	I	119	THR	2.2
4	D	221	TYR	2.1
2	B	469	GLN	2.1
2	B	468	GLU	2.1
1	A	1092	LYS	2.1
2	B	251	ILE	2.1
2	B	340	ALA	2.1
8	H	132	LEU	2.1
2	B	987	LYS	2.1
14	P	11	A	2.1
4	D	155	ARG	2.0
2	B	936	ASP	2.0
8	H	76	THR	2.0
1	A	57	ARG	2.0
5	E	57	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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 ²)	Q<0.9
15	TT	T	17	38/39	0.89	0.18	112,230,240,242	0
15	BRU	T	22	20/21	0.90	0.11	161,193,214,215	0

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, 95th 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
17	MG	A	2458	1/1	0.94	0.14	124,124,124,124	0
16	ZN	L	1071	1/1	0.99	0.03	187,187,187,187	0
16	ZN	I	1122	1/1	0.99	0.03	196,196,196,196	0
16	ZN	C	1269	1/1	1.00	0.02	75,75,75,75	0
16	ZN	I	1121	1/1	1.00	0.03	120,120,120,120	0
16	ZN	A	2456	1/1	1.00	0.02	127,127,127,127	0
16	ZN	J	1066	1/1	1.00	0.03	90,90,90,90	0
16	ZN	A	2457	1/1	1.00	0.01	70,70,70,70	0
16	ZN	B	2225	1/1	1.00	0.01	75,75,75,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.