



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:30 AM UTC

PDB ID : 3CQZ / pdb_00003cqz
Title : Crystal structure of 10 subunit RNA polymerase II in complex with the inhibitor alpha-amanitin
Authors : Kaplan, C.D.; Larsson, K.-M.; Kornberg, R.D.
Deposited on : 2008-04-03
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

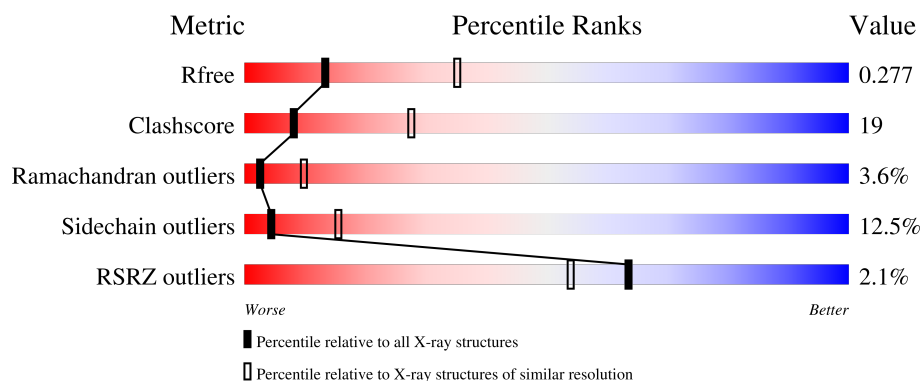
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	1733	2% 48% 23% . . 22%
2	B	1224	2% 55% 25% 5% . 13%
3	C	318	55% 23% 5% 17%
4	E	215	2% 58% 28% 10% . .
5	F	155	38% 13% . . 46%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	H	146	3%32%29%16%.21%
7	I	122	%55%38%7%. .
8	J	70	57%27%9%7%
9	K	120	%56%35%. .6%
10	L	70	29%26%7%39%
11	M	8	50%38%12%

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 27340 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	1349	Total	C	N	O	S	0	0	0
			10616	6710	1838	2009	59			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1061	Total	C	N	O	S	0	0	0
			8419	5340	1465	1563	51			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	265	Total	C	N	O	S	0	0	0
			2087	1313	347	414	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	213	Total	C	N	O	S	0	0	0
			1744	1107	308	318	11			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC2.

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

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	116	Total	C	N	O	S	0	0	0
			932	589	154	185	4			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	121	Total	C	N	O	S	0	0	0
			989	608	181	190	10			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5.

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

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	113	Total	C	N	O	S	0	0	0
			911	585	155	170	1			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	43	Total	C	N	O	S	0	0	0
			342	211	68	59	4			

- Molecule 11 is a protein called ALPHA-AMANITIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	M	8	Total	C	N	O	S	0	0	0
			64	39	10	14	1			

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	1	Total 1	Zn 1	0	0
12	I	2	Total 2	Zn 2	0	0
12	J	1	Total 1	Zn 1	0	0
12	L	1	Total 1	Zn 1	0	0

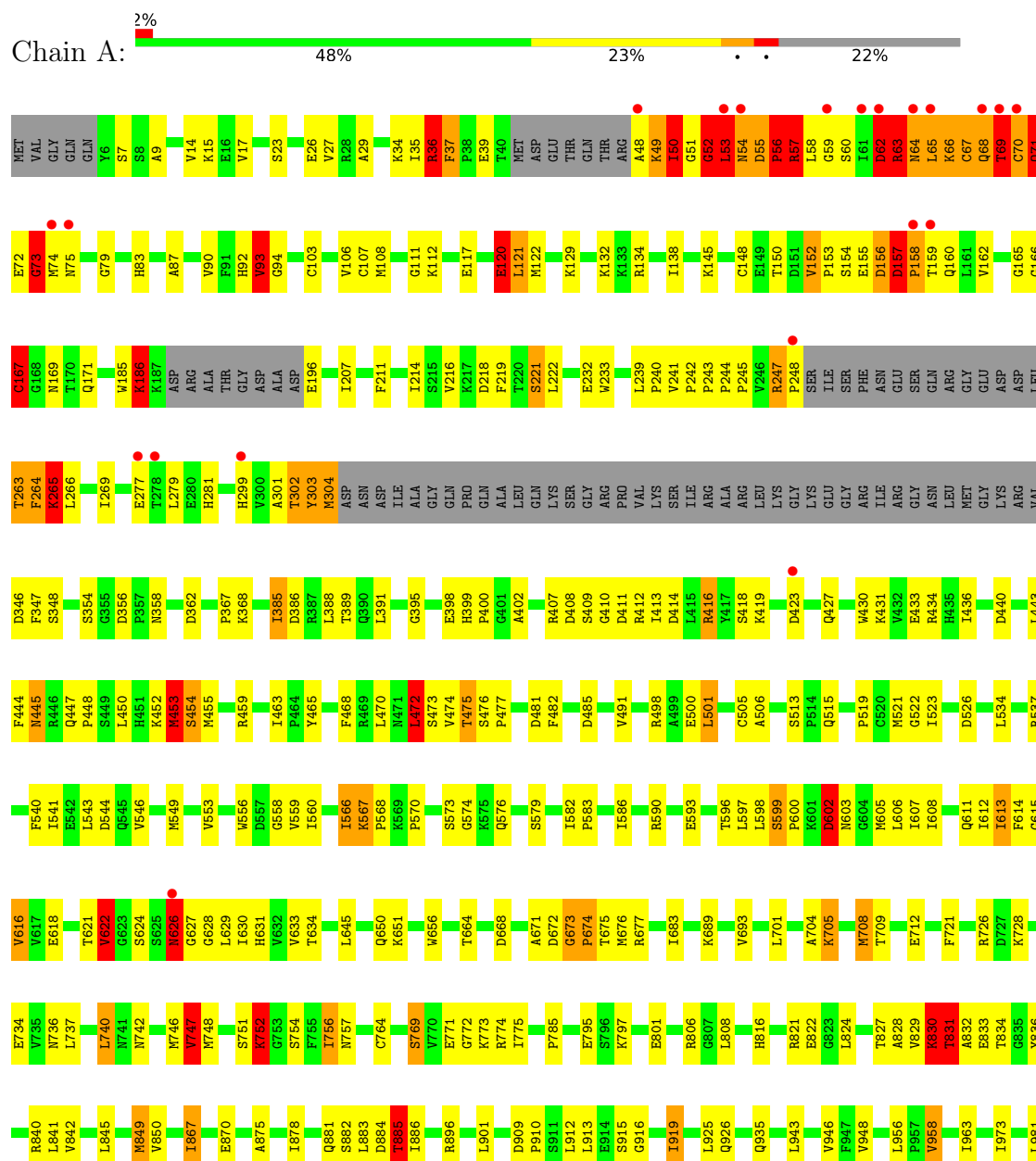
- Molecule 13 is water.

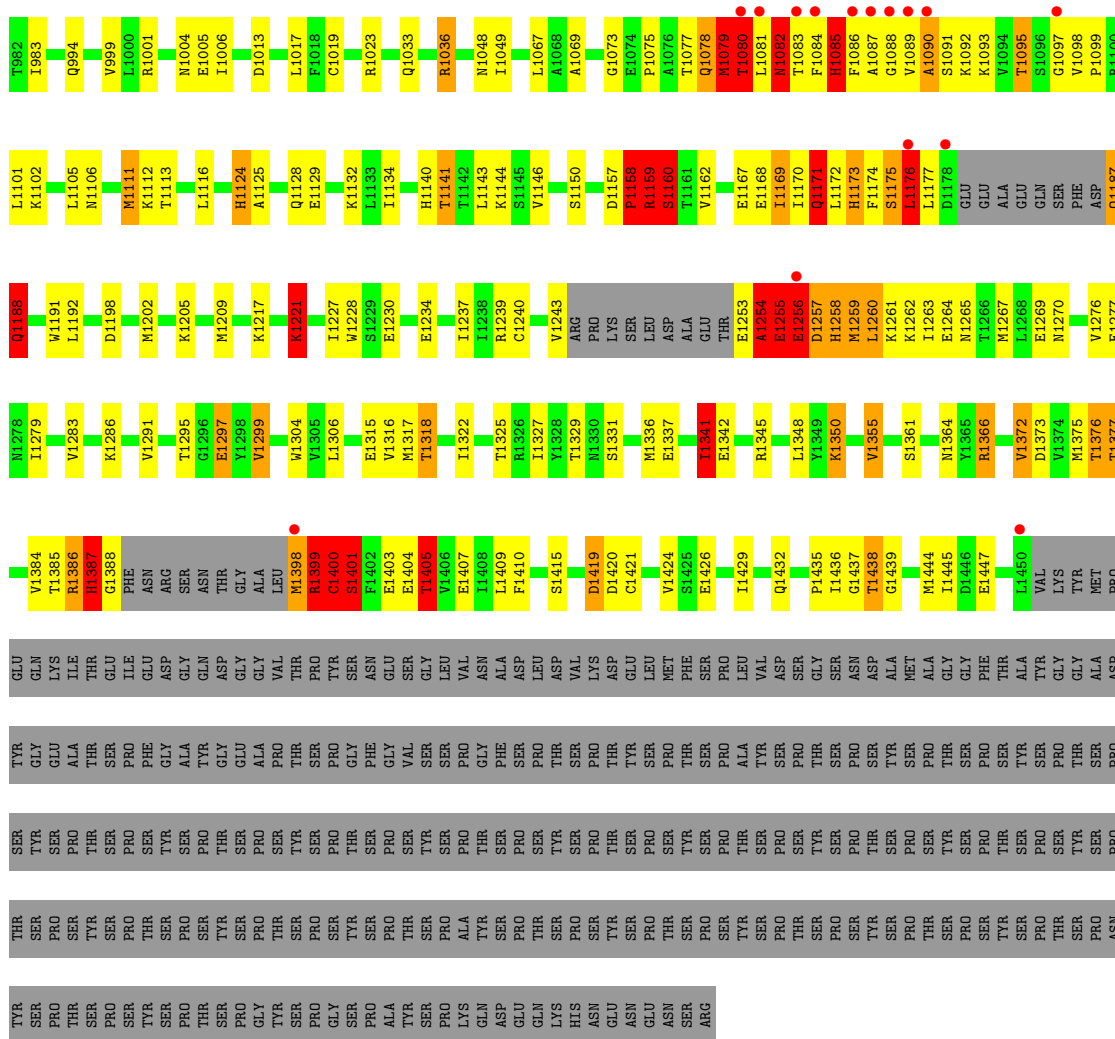
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	11	Total 11	O 11	0	0
13	B	4	Total 4	O 4	0	0
13	E	1	Total 1	O 1	0	0
13	F	1	Total 1	O 1	0	0

3 Residue-property plots

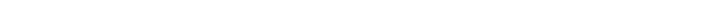
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

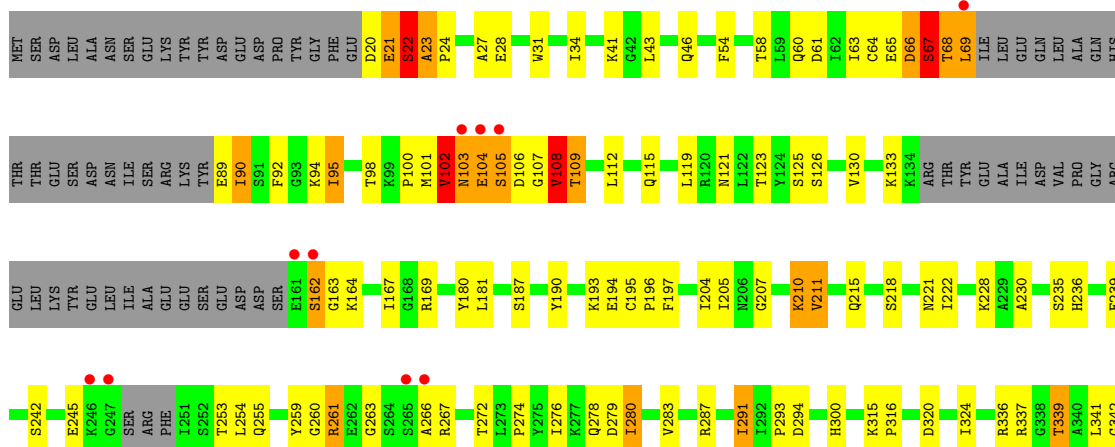
• Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1

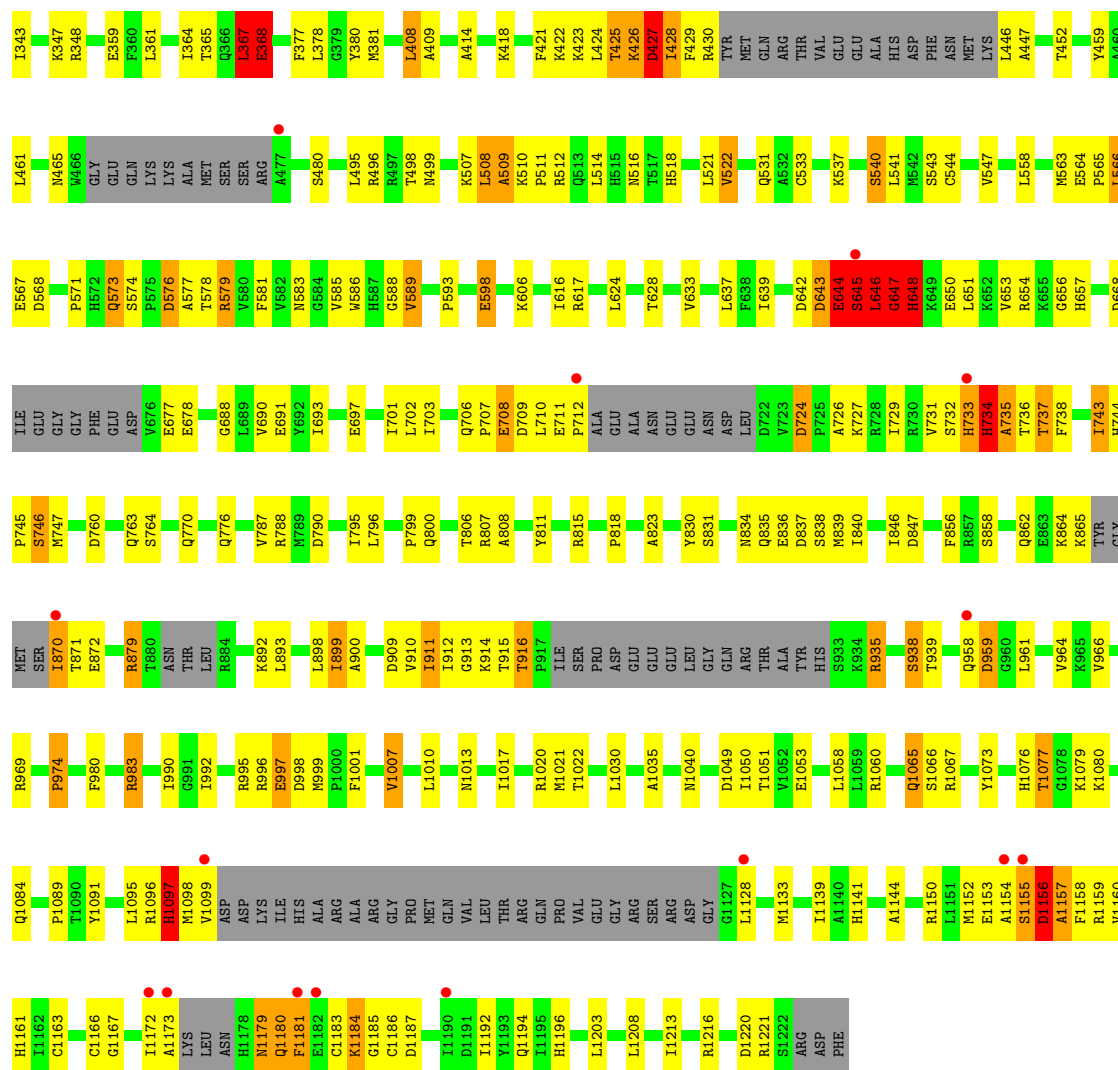




● Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

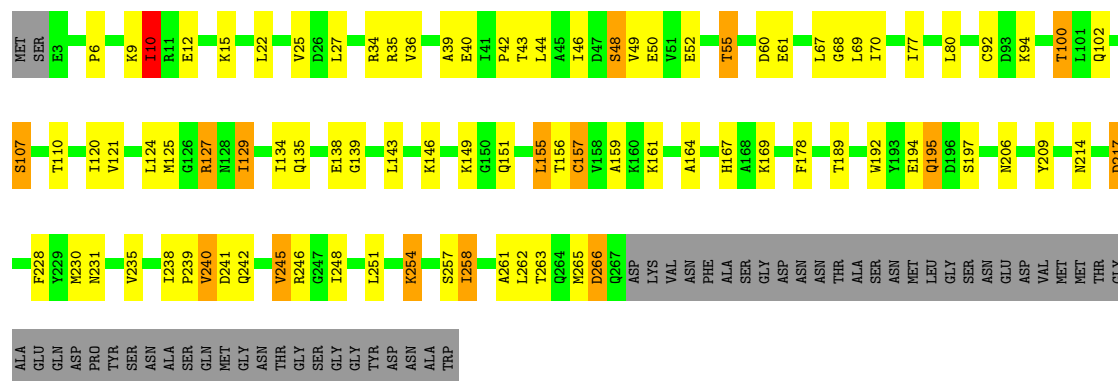
Chain B:  2% 55% 25% 5% 13%





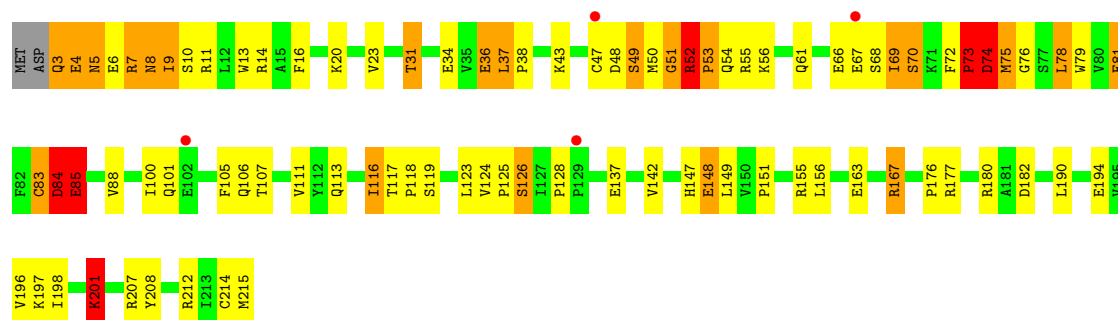
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C: 55% 23% 5% 17%

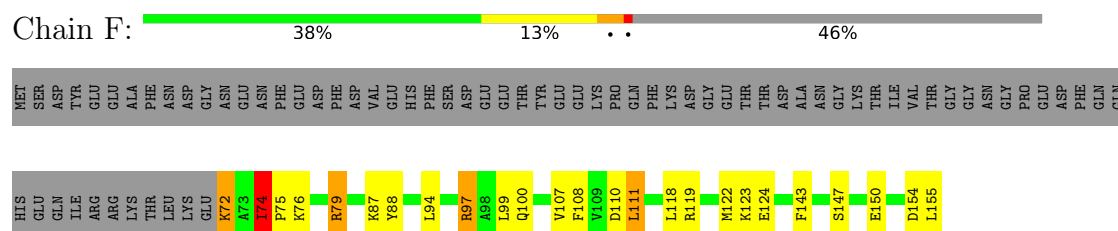


• Molecule 4: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1

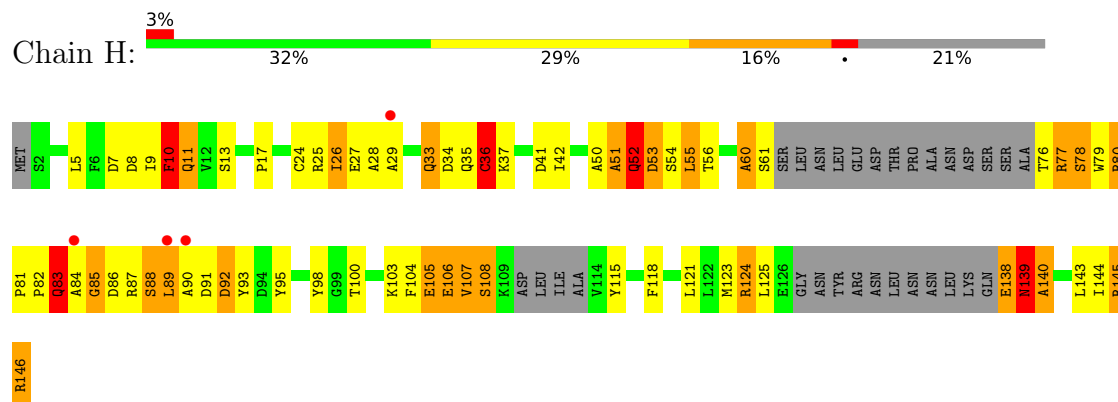
Chain E: 2% 58% 28% 10% ..



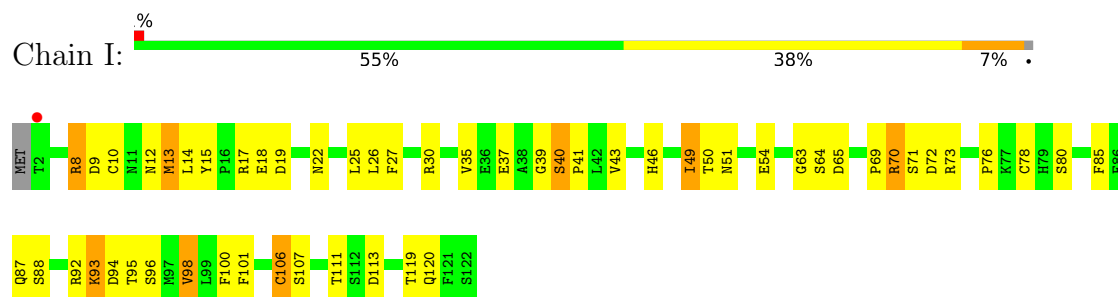
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2



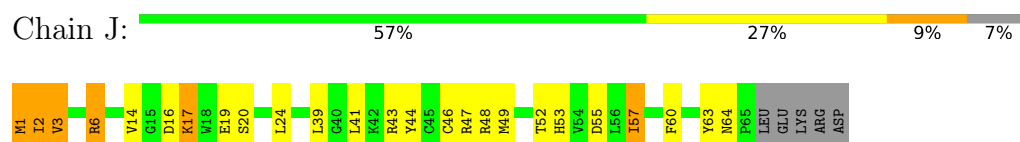
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3



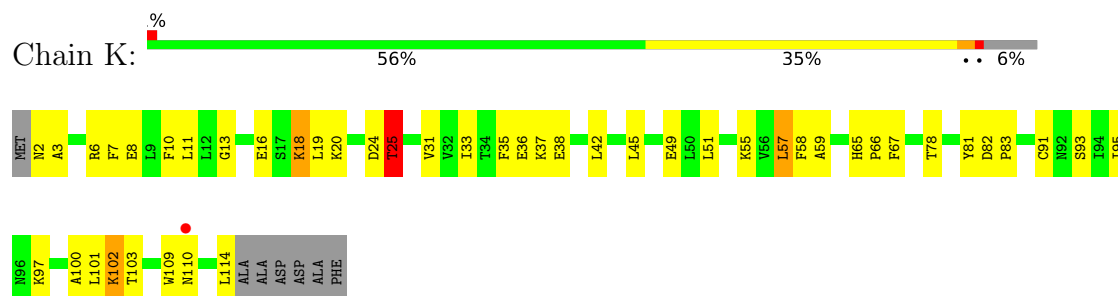
• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



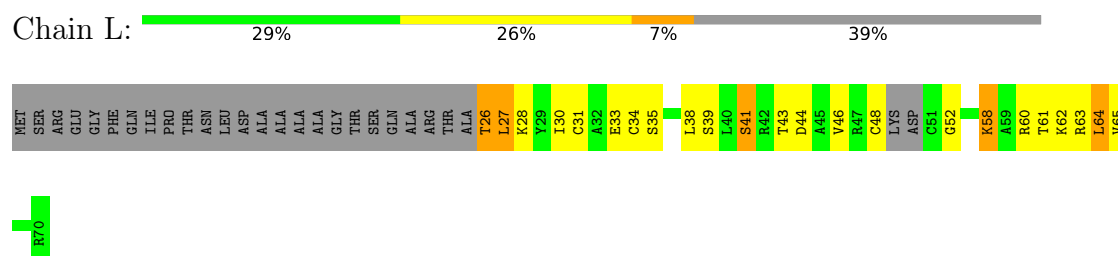
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5



- Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11



- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4



- Molecule 11: ALPHA-AMANITIN



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	122.51Å 222.48Å 374.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.4 (20.00-2.80) 92.7 (20.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.273 0.209 , 0.277	Depositor DCC
R_{free} test set	3507 reflections (2.80%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 25.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27340	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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: HYP, ILX, CSX, TRX, 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	0.91	1/10809 (0.0%)	1.22	80/14624 (0.5%)
2	B	0.90	0/8579	1.16	33/11565 (0.3%)
3	C	0.77	0/2125	1.04	3/2880 (0.1%)
4	E	0.83	1/1780 (0.1%)	1.16	13/2395 (0.5%)
5	F	0.86	0/691	1.17	2/933 (0.2%)
6	H	0.75	0/947	1.25	10/1279 (0.8%)
7	I	0.89	0/1008	1.05	2/1355 (0.1%)
8	J	0.79	0/541	1.17	1/727 (0.1%)
9	K	0.76	0/929	1.01	3/1255 (0.2%)
10	L	0.76	0/343	1.02	0/453
11	M	3.43	2/22 (9.1%)	2.06	0/26
All	All	0.88	4/27774 (0.0%)	1.17	147/37492 (0.4%)

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	16
2	B	0	12
4	E	0	2
8	J	0	1
All	All	0	31

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	4	ILE	C-O	13.26	1.37	1.24
11	M	4	ILE	CA-C	5.94	1.59	1.52
4	E	128	PRO	CA-C	5.74	1.55	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	476	SER	N-CA	-5.00	1.42	1.46

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	ASP	CA-C-N	16.60	140.59	119.84
1	A	157	ASP	C-N-CA	16.60	140.59	119.84
1	A	1257	ASP	N-CA-C	11.91	127.69	108.63
6	H	105	GLU	N-CA-C	11.31	123.15	108.34
4	E	5	ASN	N-CA-C	-9.58	101.52	113.02
2	B	245	GLU	N-CA-C	9.44	121.57	111.28
2	B	733	HIS	N-CA-C	9.17	124.46	112.72
1	A	55	ASP	CA-C-N	8.66	130.66	119.84
1	A	55	ASP	C-N-CA	8.66	130.66	119.84
4	E	74	ASP	N-CA-C	-8.49	92.72	110.80
2	B	1181	PHE	N-CA-C	8.47	123.07	108.76
5	F	74	ILE	CA-C-N	8.27	128.32	119.89
5	F	74	ILE	C-N-CA	8.27	128.32	119.89
1	A	263	THR	CA-C-N	7.88	135.88	121.70
1	A	263	THR	C-N-CA	7.88	135.88	121.70
1	A	1160	SER	N-CA-C	7.84	127.50	110.80
2	B	1179	ASN	N-CA-C	7.79	120.76	111.02
1	A	63	ARG	N-CA-C	-7.70	94.41	110.80
1	A	56	PRO	CA-C-N	7.63	135.44	121.70
1	A	56	PRO	C-N-CA	7.63	135.44	121.70
4	E	83	CYS	N-CA-C	-7.57	98.29	110.32
1	A	1277	GLU	N-CA-C	7.31	119.25	111.28
2	B	871	THR	N-CA-C	7.20	121.23	109.72
1	A	156	ASP	CA-C-N	7.18	134.63	121.70
1	A	156	ASP	C-N-CA	7.18	134.63	121.70
1	A	79	GLY	N-CA-C	-7.04	102.50	111.72
4	E	83	CYS	CA-C-N	6.97	134.25	121.70
4	E	83	CYS	C-N-CA	6.97	134.25	121.70
1	A	1399	ARG	CA-C-N	6.96	134.24	121.70
1	A	1399	ARG	C-N-CA	6.96	134.24	121.70
1	A	1171	GLN	CA-C-N	6.91	134.14	121.70
1	A	1171	GLN	C-N-CA	6.91	134.14	121.70
1	A	1171	GLN	N-CA-C	6.84	119.37	111.02
3	C	40	GLU	CA-C-N	-6.83	117.67	122.59
3	C	40	GLU	C-N-CA	-6.83	117.67	122.59
6	H	140	ALA	N-CA-C	6.83	117.25	108.24
2	B	367	LEU	N-CA-C	6.79	119.97	108.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1187	GLN	CA-C-N	6.73	133.81	121.70
1	A	1187	GLN	C-N-CA	6.73	133.81	121.70
4	E	37	LEU	CA-C-N	6.73	126.76	119.90
4	E	37	LEU	C-N-CA	6.73	126.76	119.90
1	A	1255	GLU	CA-C-N	6.69	133.74	121.70
1	A	1255	GLU	C-N-CA	6.69	133.74	121.70
1	A	472	LEU	N-CA-C	6.68	119.41	111.33
2	B	22	SER	N-CA-C	6.66	124.98	110.80
9	K	3	ALA	CA-C-N	-6.63	113.96	120.52
9	K	3	ALA	C-N-CA	-6.63	113.96	120.52
1	A	303	TYR	CA-C-N	6.55	133.48	121.70
1	A	303	TYR	C-N-CA	6.55	133.48	121.70
4	E	85	GLU	CA-C-N	6.55	128.02	119.84
4	E	85	GLU	C-N-CA	6.55	128.02	119.84
2	B	342	GLY	N-CA-C	6.46	121.57	114.40
1	A	69	THR	CA-C-N	6.41	133.25	121.70
1	A	69	THR	C-N-CA	6.41	133.25	121.70
1	A	169	ASN	N-CA-C	6.40	118.56	110.24
6	H	60	ALA	N-CA-C	6.39	116.43	108.19
2	B	646	LEU	N-CA-C	6.39	124.41	110.80
1	A	265	LYS	N-CA-C	-6.36	103.60	112.45
2	B	644	GLU	CA-C-N	6.36	133.14	121.70
2	B	644	GLU	C-N-CA	6.36	133.14	121.70
3	C	266	ASP	N-CA-C	-6.33	104.26	112.68
8	J	64	ASN	N-CA-C	6.33	121.48	113.25
2	B	280	ILE	CA-C-N	6.32	126.69	119.93
2	B	280	ILE	C-N-CA	6.32	126.69	119.93
1	A	264	PHE	N-CA-C	6.28	128.59	111.00
1	A	1341	ILE	CB-CA-C	-6.26	103.57	112.22
6	H	10	PHE	CA-C-N	6.24	132.93	121.70
6	H	10	PHE	C-N-CA	6.24	132.93	121.70
2	B	648	HIS	N-CA-C	6.23	128.46	111.00
2	B	102	VAL	CB-CA-C	-6.22	100.94	110.95
7	I	71	SER	N-CA-C	6.22	116.48	108.34
2	B	606	LYS	N-CA-C	-6.18	106.05	113.97
4	E	72	PHE	CA-C-N	6.18	127.56	119.84
4	E	72	PHE	C-N-CA	6.18	127.56	119.84
1	A	57	ARG	N-CA-C	6.17	128.28	111.00
1	A	241	VAL	CA-C-N	6.15	126.71	120.38
1	A	241	VAL	C-N-CA	6.15	126.71	120.38
1	A	468	PHE	N-CA-C	-6.09	101.47	110.48
2	B	230	ALA	N-CA-C	6.07	123.23	109.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	602	ASP	N-CA-C	6.07	120.63	113.23
1	A	1112	LYS	N-CA-C	6.07	117.56	111.07
6	H	10	PHE	N-CA-C	-6.00	98.86	109.06
1	A	1085	HIS	N-CA-C	5.97	120.55	109.56
1	A	65	LEU	CA-C-N	5.96	132.43	121.70
1	A	65	LEU	C-N-CA	5.96	132.43	121.70
1	A	1082	ASN	CA-C-N	5.91	132.33	121.70
1	A	1082	ASN	C-N-CA	5.91	132.33	121.70
2	B	647	GLY	CA-C-N	5.90	132.32	121.70
2	B	647	GLY	C-N-CA	5.90	132.32	121.70
2	B	66	ASP	N-CA-C	5.89	117.20	108.60
1	A	9	ALA	N-CA-C	5.82	117.23	109.83
1	A	358	ASN	N-CA-C	5.81	120.06	112.92
6	H	52	GLN	CA-C-N	5.80	132.14	121.70
6	H	52	GLN	C-N-CA	5.80	132.14	121.70
1	A	472	LEU	CA-CB-CG	-5.79	96.05	116.30
1	A	244	PRO	N-CA-C	5.78	117.75	110.70
1	A	628	GLY	N-CA-C	-5.70	96.76	113.30
7	I	64	SER	N-CA-C	-5.70	106.66	113.21
1	A	395	GLY	CA-C-N	5.69	125.54	119.28
1	A	395	GLY	C-N-CA	5.69	125.54	119.28
1	A	67	CYS	CA-C-N	5.67	131.90	121.70
1	A	67	CYS	C-N-CA	5.67	131.90	121.70
2	B	22	SER	CA-C-N	5.65	131.87	121.70
2	B	22	SER	C-N-CA	5.65	131.87	121.70
1	A	303	TYR	CB-CA-C	5.61	120.11	110.86
1	A	1158	PRO	CA-C-N	5.58	132.20	121.54
1	A	1158	PRO	C-N-CA	5.58	132.20	121.54
1	A	73	GLY	N-CA-C	-5.56	97.19	113.30
1	A	1299	VAL	N-CA-C	-5.51	100.54	108.42
2	B	645	SER	CB-CA-C	5.45	120.46	110.10
1	A	1254	ALA	CA-C-N	5.44	131.49	121.70
1	A	1254	ALA	C-N-CA	5.44	131.49	121.70
1	A	1080	THR	N-CA-C	5.43	122.38	110.80
4	E	201	LYS	N-CA-C	-5.41	102.48	110.48
1	A	242	PRO	CA-C-N	5.36	125.90	120.38
1	A	242	PRO	C-N-CA	5.36	125.90	120.38
1	A	1270	ASN	CA-C-N	-5.28	116.28	122.93
1	A	1270	ASN	C-N-CA	-5.28	116.28	122.93
2	B	167	ILE	N-CA-C	5.28	117.96	112.90
1	A	473	SER	N-CA-C	5.27	119.46	113.19
1	A	71	GLN	N-CA-C	5.25	121.98	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	724	ASP	CA-C-N	5.24	125.55	119.47
2	B	724	ASP	C-N-CA	5.24	125.55	119.47
2	B	465	ASN	N-CA-C	5.20	118.15	107.69
2	B	1013	ASN	CA-C-N	5.19	125.24	119.32
2	B	1013	ASN	C-N-CA	5.19	125.24	119.32
1	A	1093	LYS	N-CA-C	5.18	118.18	109.95
6	H	145	ARG	CA-C-N	5.17	131.01	121.70
6	H	145	ARG	C-N-CA	5.17	131.01	121.70
9	K	58	PHE	N-CA-C	5.15	116.76	108.32
1	A	1419	ASP	N-CA-C	5.10	116.50	109.15
1	A	418	SER	N-CA-C	5.10	117.56	109.96
1	A	49	LYS	CA-C-N	5.09	130.87	121.70
1	A	49	LYS	C-N-CA	5.09	130.87	121.70
1	A	1386	ARG	CA-C-N	5.09	130.86	121.70
1	A	1386	ARG	C-N-CA	5.09	130.86	121.70
2	B	368	GLU	N-CA-C	5.07	121.60	110.80
2	B	95	ILE	CB-CA-C	-5.07	103.83	110.98
1	A	52	GLY	CA-C-N	5.06	130.81	121.70
1	A	52	GLY	C-N-CA	5.06	130.81	121.70
1	A	491	VAL	N-CA-C	5.04	113.42	107.77
2	B	67	SER	CA-C-N	5.02	130.74	121.70
2	B	67	SER	C-N-CA	5.02	130.74	121.70
4	E	118	PRO	N-CA-C	-5.02	107.86	114.03
1	A	218	ASP	N-CA-C	5.00	117.38	111.33
1	A	1400	CYS	CA-C-N	5.00	130.71	121.70
1	A	1400	CYS	C-N-CA	5.00	130.71	121.70

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1079	MET	Peptide
1	A	1082	ASN	Peptide
1	A	1085	HIS	Peptide
1	A	1097	GLY	Peptide
1	A	1158	PRO	Peptide
1	A	1159	ARG	Peptide
1	A	1256	GLU	Peptide
1	A	157	ASP	Peptide
1	A	158	PRO	Peptide
1	A	36	ARG	Peptide
1	A	602	ASP	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	62	ASP	Peptide
1	A	624	SER	Peptide
1	A	673	GLY	Peptide
1	A	73	GLY	Peptide
1	A	830	LYS	Peptide
2	B	103	ASN	Peptide
2	B	105	SER	Peptide
2	B	1076	HIS	Peptide
2	B	21	GLU	Peptide
2	B	22	SER	Peptide
2	B	367	LEU	Peptide
2	B	507	LYS	Peptide
2	B	508	LEU	Peptide
2	B	645	SER	Peptide
2	B	647	GLY	Peptide
2	B	732	SER	Peptide
2	B	734	HIS	Peptide
4	E	4	GLU	Peptide
4	E	73	PRO	Peptide
8	J	63	TYR	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	10616	0	10675	475	0
2	B	8419	0	8450	308	0
3	C	2087	0	2047	67	0
4	E	1744	0	1772	88	0
5	F	679	0	701	21	0
6	H	932	0	899	75	0
7	I	989	0	942	35	0
8	J	532	0	542	17	0
9	K	911	0	917	38	0
10	L	342	0	363	17	0
11	M	64	0	51	1	0
12	A	2	0	0	0	0
12	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	C	1	0	0	0	0
12	I	2	0	0	0	0
12	J	1	0	0	0	0
12	L	1	0	0	0	0
13	A	11	0	0	2	0
13	B	4	0	0	1	0
13	E	1	0	0	0	0
13	F	1	0	0	0	0
All	All	27340	0	27359	1058	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 19.

All (1058) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1399:ARG:HB3	1:A:1400:CYS:CB	1.60	1.30
4:E:53:PRO:HB2	4:E:54:GLN:CA	1.65	1.25
1:A:1399:ARG:CB	1:A:1400:CYS:HB3	1.68	1.24
4:E:53:PRO:CB	4:E:54:GLN:HA	1.64	1.22
1:A:1398:MET:HA	1:A:1399:ARG:HB2	1.24	1.17
4:E:79:TRP:HE1	4:E:81:GLU:HG3	1.11	1.15
1:A:1386:ARG:HA	1:A:1387:HIS:HB2	1.15	1.14
2:B:645:SER:HB3	2:B:646:LEU:HB2	1.22	1.14
1:A:834:THR:HB	1:A:1077:THR:HG22	1.28	1.13
1:A:57:ARG:HB3	1:A:68:GLN:CG	1.78	1.12
1:A:830:LYS:O	1:A:830:LYS:HG2	1.47	1.12
1:A:67:CYS:HB3	1:A:68:GLN:C	1.73	1.11
1:A:65:LEU:CB	1:A:66:LYS:HB2	1.81	1.10
6:H:52:GLN:H	6:H:53:ASP:HB2	0.98	1.10
1:A:57:ARG:CB	1:A:68:GLN:HG3	1.81	1.10
1:A:65:LEU:HB3	1:A:66:LYS:CB	1.81	1.10
6:H:107:VAL:HG12	6:H:108:SER:H	1.14	1.10
2:B:1179:ASN:HA	2:B:1180:GLN:HB2	1.27	1.10
6:H:138:GLU:HA	6:H:139:ASN:HB2	1.23	1.10
1:A:1187:GLN:HB3	1:A:1188:GLN:HB3	1.34	1.09
2:B:67:SER:HA	2:B:68:THR:HB	1.31	1.08
6:H:52:GLN:N	6:H:53:ASP:HB2	1.66	1.08
2:B:107:GLY:HA2	2:B:108:VAL:HB	1.36	1.07
2:B:276:ILE:HG21	2:B:280:ILE:HD11	1.31	1.07
2:B:68:THR:HG23	2:B:69:LEU:H	0.97	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:643:ASP:HA	2:B:644:GLU:HB2	1.34	1.06
2:B:107:GLY:CA	2:B:108:VAL:HB	1.85	1.06
2:B:1179:ASN:CA	2:B:1180:GLN:HB2	1.86	1.05
1:A:626:ASN:HB3	1:A:627:GLY:HA2	1.35	1.04
2:B:644:GLU:HB3	2:B:645:SER:HB2	1.09	1.04
2:B:1185:GLY:HA2	2:B:1186:CYS:HB2	1.39	1.04
2:B:558:LEU:HB3	2:B:563:MET:HE3	1.38	1.04
6:H:76:THR:HA	6:H:77:ARG:CB	1.88	1.04
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.36	1.01
1:A:56:PRO:HB3	1:A:57:ARG:HG3	1.43	1.00
6:H:76:THR:CA	6:H:77:ARG:HB2	1.91	1.00
2:B:22:SER:N	2:B:23:ALA:HB3	1.76	1.00
1:A:626:ASN:HB3	1:A:627:GLY:CA	1.89	1.00
3:C:69:LEU:O	8:J:6:ARG:NH1	1.95	0.99
4:E:79:TRP:NE1	4:E:81:GLU:HG3	1.78	0.98
2:B:644:GLU:CB	2:B:645:SER:HB2	1.94	0.97
4:E:88:VAL:HB	4:E:116:ILE:HG23	1.47	0.97
1:A:1386:ARG:CA	1:A:1387:HIS:HB2	1.94	0.96
6:H:76:THR:HA	6:H:77:ARG:HB2	0.97	0.96
8:J:1:MET:HG3	8:J:60:PHE:HE2	1.29	0.96
2:B:68:THR:CG2	2:B:69:LEU:H	1.79	0.95
1:A:598:LEU:HD11	6:H:124:ARG:HG2	1.50	0.93
2:B:643:ASP:HA	2:B:644:GLU:CB	1.95	0.93
6:H:11:GLN:H	6:H:54:SER:HA	1.33	0.93
6:H:138:GLU:HA	6:H:139:ASN:CB	1.99	0.93
2:B:278:GLN:NE2	2:B:337:ARG:HE	1.66	0.93
1:A:67:CYS:CB	1:A:68:GLN:C	2.43	0.92
2:B:68:THR:HG23	2:B:69:LEU:N	1.79	0.92
1:A:1254:ALA:HB1	1:A:1255:GLU:C	1.95	0.92
1:A:57:ARG:HB3	1:A:68:GLN:HG3	0.93	0.91
3:C:265:MET:HE1	9:K:19:LEU:HB2	1.52	0.91
1:A:1398:MET:HB2	1:A:1400:CYS:SG	2.10	0.91
1:A:673:GLY:HA2	1:A:674:PRO:C	1.95	0.91
1:A:834:THR:HB	1:A:1077:THR:CG2	2.00	0.91
1:A:566:ILE:O	1:A:567:LYS:HD3	1.70	0.90
1:A:157:ASP:HB3	1:A:160:GLN:H	1.37	0.90
1:A:65:LEU:HB3	1:A:66:LYS:HB2	0.92	0.89
1:A:671:ALA:HB3	1:A:676:MET:HE2	1.55	0.89
2:B:22:SER:H	2:B:23:ALA:HB3	1.38	0.89
6:H:82:PRO:HA	6:H:83:GLN:HB2	1.55	0.89
9:K:65:HIS:HD2	9:K:67:PHE:H	1.20	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1078:GLN:N	1:A:1079:MET:HA	1.88	0.89
1:A:1087:ALA:H	1:A:1088:GLY:HA3	1.36	0.88
1:A:67:CYS:HB3	1:A:69:THR:N	1.88	0.88
2:B:106:ASP:HB3	2:B:107:GLY:HA3	1.53	0.88
1:A:1399:ARG:HG3	1:A:1419:ASP:OD2	1.74	0.88
4:E:7:ARG:HG3	4:E:7:ARG:O	1.74	0.88
4:E:74:ASP:O	4:E:75:MET:HB3	1.73	0.87
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.40	0.87
1:A:1082:ASN:HB3	1:A:1083:THR:HB	1.57	0.87
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.57	0.87
1:A:1386:ARG:HA	1:A:1387:HIS:CB	2.03	0.86
1:A:1084:PHE:CE2	1:A:1087:ALA:HB2	2.10	0.86
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.57	0.86
1:A:673:GLY:HA2	1:A:676:MET:H	1.39	0.86
1:A:1079:MET:HB2	1:A:1080:THR:O	1.76	0.86
2:B:1077:THR:HG22	2:B:1079:LYS:H	1.40	0.85
2:B:21:GLU:HB3	2:B:22:SER:HB2	1.59	0.85
8:J:2:ILE:HG22	8:J:3:VAL:HG23	1.59	0.85
1:A:673:GLY:CA	1:A:676:MET:H	1.90	0.85
2:B:644:GLU:HB3	2:B:645:SER:CB	2.02	0.85
6:H:107:VAL:HG12	6:H:108:SER:N	1.91	0.84
3:C:100:THR:HG21	3:C:102:GLN:HE21	1.41	0.84
1:A:629:LEU:O	1:A:633:VAL:HG23	1.78	0.83
2:B:260:GLY:HA3	2:B:267:ARG:HD2	1.59	0.83
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.59	0.83
5:F:111:LEU:HD12	5:F:111:LEU:H	1.42	0.83
2:B:1185:GLY:CA	2:B:1187:ASP:H	1.92	0.82
8:J:44:TYR:HA	8:J:47:ARG:HG3	1.62	0.82
2:B:1153:GLU:HG3	2:B:1155:SER:H	1.45	0.81
4:E:163:GLU:OE2	4:E:167:ARG:HD2	1.79	0.81
1:A:444:PHE:CE2	1:A:470:LEU:HD21	2.15	0.81
1:A:1086:PHE:N	1:A:1087:ALA:HA	1.95	0.81
6:H:84:ALA:HA	6:H:86:ASP:HB2	1.62	0.81
1:A:1258:HIS:HB2	1:A:1261:LYS:HB2	1.62	0.81
7:I:106:CYS:O	7:I:107:SER:HB2	1.80	0.81
1:A:72:GLU:HB3	1:A:73:GLY:HA2	1.63	0.81
1:A:1078:GLN:H	1:A:1079:MET:HA	1.44	0.81
1:A:50:ILE:HG23	1:A:51:GLY:CA	2.10	0.80
1:A:1158:PRO:HB2	1:A:1159:ARG:HG2	1.63	0.80
2:B:711:GLU:HB2	2:B:712:PRO:HD2	1.63	0.80
6:H:50:ALA:HB3	6:H:53:ASP:OD2	1.80	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:HG23	1:A:51:GLY:HA3	1.63	0.80
1:A:444:PHE:HE2	1:A:470:LEU:HD21	1.46	0.80
3:C:22:LEU:HD12	3:C:230:MET:HE3	1.61	0.80
1:A:156:ASP:HB3	1:A:157:ASP:O	1.81	0.79
4:E:49:SER:HA	4:E:51:GLY:H	1.47	0.79
1:A:48:ALA:HA	1:A:49:LYS:HB2	1.63	0.79
6:H:10:PHE:HB3	6:H:28:ALA:HB1	1.63	0.79
2:B:645:SER:CB	2:B:646:LEU:HB2	2.08	0.79
1:A:50:ILE:HG23	1:A:51:GLY:O	1.82	0.78
2:B:278:GLN:HE21	2:B:337:ARG:HE	1.29	0.78
2:B:103:ASN:HB2	2:B:169:ARG:NH2	1.98	0.78
2:B:1179:ASN:N	2:B:1180:GLN:HB2	1.99	0.78
6:H:26:ILE:HD13	6:H:42:ILE:HD12	1.62	0.78
1:A:829:VAL:O	1:A:830:LYS:HB3	1.83	0.78
1:A:1090:ALA:H	1:A:1092:LYS:HG2	1.49	0.78
2:B:103:ASN:HB2	2:B:169:ARG:HH22	1.47	0.78
1:A:265:LYS:HE2	1:A:299:HIS:HD2	1.46	0.78
2:B:66:ASP:O	2:B:67:SER:HB3	1.84	0.78
1:A:1400:CYS:HA	1:A:1401:SER:HB2	1.66	0.77
5:F:97:ARG:HE	5:F:100:GLN:NE2	1.83	0.77
8:J:48:ARG:CZ	8:J:49:MET:HE1	2.15	0.76
10:L:26:THR:N	10:L:62:LYS:HZ1	1.83	0.76
2:B:106:ASP:HB3	2:B:107:GLY:CA	2.14	0.76
2:B:1022:THR:HA	13:B:2004:HOH:O	1.83	0.76
1:A:1254:ALA:HB1	1:A:1255:GLU:O	1.86	0.76
2:B:1185:GLY:HA3	2:B:1187:ASP:H	1.50	0.76
2:B:67:SER:HA	2:B:68:THR:CB	2.13	0.76
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.16	0.76
2:B:734:HIS:CD2	2:B:734:HIS:H	2.04	0.76
1:A:303:TYR:CD2	1:A:304:MET:HG3	2.21	0.76
1:A:673:GLY:HA2	1:A:676:MET:N	1.99	0.76
1:A:537:ARG:NH2	1:A:602:ASP:HB2	2.00	0.75
7:I:8:ARG:HH11	7:I:8:ARG:HG2	1.52	0.75
6:H:35:GLN:O	6:H:36:CYS:HB3	1.85	0.74
1:A:49:LYS:HB3	1:A:50:ILE:HG22	1.68	0.74
1:A:883:LEU:O	1:A:886:ILE:HG22	1.87	0.74
4:E:7:ARG:O	4:E:8:ASN:HB2	1.86	0.74
4:E:52:ARG:HB3	4:E:53:PRO:CD	2.18	0.73
1:A:1173:HIS:HA	1:A:1174:PHE:HB2	1.69	0.73
2:B:583:ASN:HD21	2:B:628:THR:H	1.35	0.73
2:B:41:LYS:NZ	2:B:544:CYS:SG	2.59	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1179:ASN:HA	2:B:1180:GLN:CB	2.13	0.73
3:C:167:HIS:HD2	3:C:169:LYS:H	1.34	0.73
1:A:453:MET:HE3	1:A:453:MET:H	1.54	0.72
1:A:1079:MET:HG2	1:A:1081:LEU:HB2	1.71	0.72
1:A:1410:PHE:HD2	2:B:1213:ILE:HD11	1.54	0.72
1:A:56:PRO:HB3	1:A:57:ARG:CG	2.18	0.72
1:A:1400:CYS:SG	1:A:1400:CYS:O	2.47	0.72
1:A:673:GLY:HA3	1:A:676:MET:HB2	1.70	0.72
1:A:1265:ASN:HD21	2:B:263:GLY:HA2	1.55	0.72
2:B:893:LEU:HD21	2:B:910:VAL:HG12	1.72	0.72
6:H:107:VAL:O	6:H:108:SER:HB2	1.90	0.72
1:A:445:ASN:CB	1:A:455:MET:HG2	2.19	0.71
2:B:21:GLU:CB	2:B:22:SER:HB2	2.21	0.71
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.89	0.71
4:E:75:MET:CE	4:E:155:ARG:HH22	2.03	0.71
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.72	0.71
1:A:67:CYS:HB3	1:A:68:GLN:CA	2.20	0.71
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.36	0.71
5:F:79:ARG:HH22	5:F:150:GLU:CD	1.99	0.71
2:B:579:ARG:HG2	2:B:586:TRP:CE2	2.26	0.71
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.38	0.70
1:A:1257:ASP:O	1:A:1258:HIS:HB3	1.91	0.70
4:E:49:SER:HA	4:E:51:GLY:N	2.05	0.70
2:B:1051:THR:HG22	2:B:1053:GLU:N	2.06	0.70
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.25	0.70
6:H:10:PHE:O	6:H:55:LEU:N	2.22	0.70
2:B:423:LYS:O	2:B:424:LEU:HB3	1.90	0.70
1:A:50:ILE:HG23	1:A:51:GLY:C	2.16	0.69
1:A:1111:MET:HE1	1:A:1331:SER:HB2	1.72	0.69
6:H:84:ALA:CA	6:H:86:ASP:HB2	2.22	0.69
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.72	0.69
4:E:75:MET:HG2	4:E:76:GLY:H	1.57	0.69
4:E:155:ARG:HD2	4:E:194:GLU:OE2	1.91	0.69
1:A:1084:PHE:HE2	1:A:1087:ALA:HB2	1.54	0.69
1:A:754:SER:H	1:A:757:ASN:HD22	1.40	0.69
7:I:8:ARG:NH1	7:I:9:ASP:OD1	2.26	0.69
1:A:56:PRO:HB3	1:A:57:ARG:HE	1.55	0.69
2:B:514:LEU:HD12	2:B:518:HIS:HD2	1.56	0.69
1:A:1398:MET:CA	1:A:1399:ARG:HB2	2.13	0.69
2:B:205:ILE:HD12	2:B:210:LYS:HG3	1.75	0.69
2:B:509:ALA:C	2:B:511:PRO:HD3	2.18	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.74	0.69
1:A:68:GLN:CB	1:A:69:THR:HA	2.22	0.69
1:A:1116:LEU:HD23	1:A:1329:THR:HB	1.74	0.69
7:I:63:GLY:O	7:I:70:ARG:NH1	2.25	0.69
2:B:294:ASP:H	7:I:12:ASN:ND2	1.92	0.68
1:A:1187:GLN:CB	1:A:1188:GLN:HB3	2.19	0.68
2:B:1173:ALA:HA	2:B:1181:PHE:HB3	1.75	0.68
2:B:558:LEU:CB	2:B:563:MET:HE3	2.20	0.68
1:A:526:ASP:HB2	2:B:835:GLN:OE1	1.93	0.68
2:B:107:GLY:CA	2:B:108:VAL:CB	2.67	0.68
6:H:61:SER:C	6:H:89:LEU:HD11	2.19	0.68
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.75	0.67
2:B:377:PHE:CD2	2:B:381:MET:HE2	2.29	0.67
4:E:74:ASP:O	4:E:75:MET:CB	2.42	0.67
1:A:795:GLU:HG2	2:B:731:VAL:HG11	1.76	0.67
1:A:1079:MET:HB2	1:A:1080:THR:C	2.18	0.67
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.77	0.67
8:J:1:MET:HG3	8:J:60:PHE:CE2	2.22	0.67
2:B:509:ALA:O	2:B:511:PRO:HD3	1.95	0.67
1:A:1401:SER:HB2	1:A:1429:ILE:HD11	1.77	0.67
2:B:734:HIS:CD2	2:B:734:HIS:N	2.62	0.67
3:C:100:THR:CG2	3:C:102:GLN:HE21	2.07	0.67
1:A:67:CYS:CB	1:A:69:THR:N	2.57	0.67
1:A:606:LEU:HD21	1:A:608:ILE:CD1	2.25	0.67
1:A:579:SER:HB3	1:A:611:GLN:OE1	1.94	0.66
4:E:6:GLU:HA	4:E:9:ILE:HG12	1.78	0.66
5:F:119:ARG:HA	5:F:122:MET:HE3	1.76	0.66
4:E:83:CYS:HA	4:E:84:ASP:HB2	1.76	0.66
5:F:97:ARG:HE	5:F:100:GLN:HE21	1.44	0.66
1:A:265:LYS:NZ	1:A:302:THR:HB	2.10	0.66
1:A:534:LEU:O	1:A:574:GLY:HA3	1.95	0.66
10:L:26:THR:HG23	10:L:27:LEU:H	1.60	0.66
1:A:830:LYS:H	1:A:831:THR:C	2.04	0.65
1:A:1078:GLN:N	1:A:1079:MET:CA	2.59	0.65
6:H:11:GLN:H	6:H:54:SER:CA	2.07	0.65
1:A:56:PRO:HB3	1:A:57:ARG:NE	2.11	0.65
1:A:829:VAL:O	1:A:829:VAL:HG12	1.95	0.65
6:H:37:LYS:O	6:H:125:LEU:HD23	1.97	0.65
1:A:606:LEU:HD21	1:A:608:ILE:HD12	1.79	0.65
1:A:1082:ASN:HB3	1:A:1083:THR:CB	2.25	0.65
2:B:1185:GLY:HA2	2:B:1186:CYS:CB	2.14	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:9:LYS:O	3:C:10:ILE:HG13	1.98	0.65
2:B:278:GLN:HE21	2:B:337:ARG:NE	1.94	0.64
1:A:834:THR:CB	1:A:1077:THR:HG22	2.18	0.64
2:B:647:GLY:HA2	2:B:648:HIS:O	1.96	0.64
1:A:166:GLY:CA	1:A:167:CYS:HB3	2.27	0.64
1:A:452:LYS:HG3	2:B:1141:HIS:CE1	2.32	0.64
1:A:606:LEU:HD22	1:A:613:ILE:HB	1.80	0.64
3:C:67:LEU:HD11	3:C:155:LEU:HD11	1.79	0.64
8:J:2:ILE:HG22	8:J:3:VAL:N	2.13	0.64
2:B:107:GLY:HA3	2:B:108:VAL:HB	1.79	0.64
4:E:5:ASN:O	4:E:8:ASN:HB3	1.98	0.63
1:A:771:GLU:HG2	1:A:1086:PHE:CE1	2.32	0.63
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.80	0.63
1:A:1004:ASN:CG	4:E:167:ARG:HD3	2.23	0.63
6:H:138:GLU:CA	6:H:139:ASN:CB	2.75	0.63
3:C:239:PRO:O	3:C:242:GLN:HB2	1.98	0.63
1:A:549:MET:HE1	1:A:656:TRP:CD1	2.29	0.63
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.81	0.63
1:A:540:PHE:C	1:A:541:ILE:HD12	2.24	0.63
2:B:654:ARG:H	2:B:657:HIS:HD2	1.45	0.62
2:B:770:GLN:HA	2:B:770:GLN:OE1	1.99	0.62
6:H:11:GLN:N	6:H:54:SER:HA	2.11	0.62
6:H:82:PRO:HA	6:H:83:GLN:CB	2.28	0.62
1:A:773:LYS:HZ2	1:A:1089:VAL:H	1.46	0.62
4:E:190:LEU:HD23	4:E:214:CYS:HB2	1.79	0.62
9:K:24:ASP:CG	9:K:25:THR:H	2.06	0.62
1:A:56:PRO:CB	1:A:57:ARG:HE	2.12	0.62
1:A:775:ILE:O	1:A:797:LYS:HE3	1.99	0.62
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.34	0.62
1:A:1254:ALA:CB	1:A:1255:GLU:HA	2.29	0.62
1:A:1364:ASN:ND2	1:A:1366:ARG:HH11	1.96	0.62
2:B:522:VAL:HG11	2:B:537:LYS:HD2	1.81	0.62
1:A:69:THR:H	1:A:70:CYS:HB3	1.63	0.62
2:B:899:ILE:N	2:B:899:ILE:HD13	2.15	0.62
2:B:571:PRO:C	2:B:573:GLN:H	2.08	0.62
1:A:23:SER:O	1:A:27:VAL:HG23	2.00	0.62
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.81	0.61
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.63	0.61
6:H:50:ALA:O	6:H:51:ALA:HB2	1.99	0.61
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.81	0.61
2:B:734:HIS:H	2:B:734:HIS:HD2	1.49	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:147:SER:OG	5:F:150:GLU:HB2	2.00	0.61
1:A:452:LYS:C	1:A:454:SER:H	2.08	0.61
1:A:956:LEU:HD21	1:A:1017:LEU:HD23	1.82	0.61
1:A:1404:GLU:O	1:A:1405:THR:C	2.43	0.61
1:A:1364:ASN:HD21	1:A:1366:ARG:NH1	1.99	0.61
2:B:294:ASP:H	7:I:12:ASN:HD22	1.48	0.61
2:B:377:PHE:HD2	2:B:381:MET:HE2	1.64	0.61
1:A:885:THR:CG2	1:A:943:LEU:HD12	2.31	0.61
2:B:260:GLY:CA	2:B:267:ARG:HD2	2.27	0.61
2:B:1185:GLY:CA	2:B:1186:CYS:HB2	2.24	0.61
9:K:57:LEU:HD21	9:K:78:THR:CG2	2.31	0.61
1:A:54:ASN:HB2	1:A:55:ASP:OD1	1.99	0.61
1:A:1254:ALA:HB1	1:A:1255:GLU:CA	2.31	0.61
3:C:77:ILE:HA	3:C:129:ILE:HD11	1.81	0.61
2:B:898:LEU:HB2	10:L:58:LYS:HE3	1.83	0.61
2:B:995:ARG:NH1	2:B:997:GLU:OE2	2.28	0.61
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.66	0.60
1:A:673:GLY:HA2	1:A:675:THR:N	2.16	0.60
1:A:1091:SER:N	1:A:1092:LYS:HA	2.16	0.60
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.83	0.60
1:A:1410:PHE:CD2	2:B:1213:ILE:HD11	2.36	0.60
1:A:53:LEU:N	1:A:53:LEU:HD12	2.15	0.60
1:A:156:ASP:CB	1:A:157:ASP:O	2.49	0.60
1:A:773:LYS:NZ	1:A:1089:VAL:HG22	2.16	0.60
1:A:303:TYR:HD2	1:A:304:MET:HG3	1.66	0.60
1:A:913:LEU:HD11	1:A:981:LEU:O	2.01	0.60
6:H:84:ALA:HA	6:H:86:ASP:N	2.16	0.60
1:A:549:MET:CE	1:A:656:TRP:HD1	2.10	0.60
1:A:1085:HIS:N	1:A:1086:PHE:HB3	2.17	0.60
1:A:1398:MET:HA	1:A:1399:ARG:CB	2.12	0.60
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.83	0.60
1:A:1111:MET:HE1	1:A:1331:SER:CB	2.31	0.60
4:E:53:PRO:HB3	4:E:55:ARG:HH11	1.64	0.60
2:B:67:SER:CA	2:B:68:THR:HB	2.20	0.60
2:B:706:GLN:HB3	2:B:708:GLU:HG2	1.84	0.60
1:A:367:PRO:HB3	9:K:2:ASN:HD21	1.66	0.60
1:A:1191:TRP:HZ3	7:I:43:VAL:HG21	1.67	0.60
6:H:80:ARG:HG2	9:K:57:LEU:HD22	1.83	0.60
9:K:7:PHE:HB2	9:K:11:LEU:HD12	1.83	0.60
1:A:453:MET:H	1:A:453:MET:CE	2.14	0.59
2:B:864:LYS:H	2:B:872:GLU:HB2	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:PHE:HA	2:B:58:THR:HB	1.83	0.59
4:E:84:ASP:H	4:E:113:GLN:HE21	1.49	0.59
1:A:754:SER:OG	1:A:756:ILE:HG22	2.03	0.59
1:A:867:ILE:HD11	1:A:999:VAL:HG11	1.84	0.59
2:B:68:THR:CG2	2:B:90:ILE:O	2.50	0.59
10:L:26:THR:HG23	10:L:27:LEU:N	2.18	0.59
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.50	0.59
1:A:68:GLN:HB2	1:A:69:THR:HA	1.85	0.59
1:A:472:LEU:O	1:A:475:THR:HB	2.03	0.59
1:A:1004:ASN:ND2	4:E:167:ARG:HD3	2.18	0.59
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.18	0.59
1:A:1150:SER:OG	7:I:46:HIS:HB3	2.02	0.59
9:K:65:HIS:CD2	9:K:67:PHE:H	2.11	0.59
2:B:422:LYS:O	2:B:426:LYS:HB2	2.03	0.59
1:A:1315:GLU:O	1:A:1318:THR:HG22	2.02	0.59
4:E:3:GLN:C	4:E:3:GLN:HE21	2.11	0.59
5:F:76:LYS:HA	5:F:79:ARG:HD2	1.83	0.59
1:A:1106:ASN:OD1	1:A:1385:THR:CG2	2.51	0.59
1:A:946:VAL:HG22	4:E:201:LYS:HB2	1.84	0.58
1:A:1098:VAL:H	1:A:1099:PRO:HD2	1.68	0.58
2:B:864:LYS:HG3	2:B:870:ILE:O	2.03	0.58
6:H:138:GLU:CA	6:H:139:ASN:HB2	2.15	0.58
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.84	0.58
1:A:596:THR:HG22	1:A:597:LEU:H	1.68	0.58
4:E:7:ARG:O	4:E:7:ARG:CG	2.49	0.58
1:A:596:THR:HG22	1:A:597:LEU:N	2.19	0.58
2:B:68:THR:CG2	2:B:69:LEU:N	2.50	0.58
2:B:899:ILE:N	2:B:899:ILE:CD1	2.66	0.58
7:I:26:LEU:HD23	7:I:37:GLU:HA	1.85	0.58
1:A:708:MET:HE3	1:A:1091:SER:O	2.03	0.58
1:A:1084:PHE:C	1:A:1086:PHE:HB3	2.28	0.58
2:B:20:ASP:HB3	2:B:23:ALA:HB2	1.85	0.58
2:B:21:GLU:O	2:B:656:GLY:N	2.36	0.58
2:B:98:THR:O	2:B:126:SER:HB3	2.02	0.58
2:B:239:GLU:HG2	2:B:255:GLN:HG2	1.85	0.58
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.39	0.58
2:B:260:GLY:CA	2:B:267:ARG:CD	2.82	0.58
2:B:498:THR:OG1	2:B:537:LYS:HB2	2.03	0.58
2:B:558:LEU:HD13	2:B:563:MET:CE	2.33	0.58
6:H:107:VAL:CG1	6:H:108:SER:N	2.62	0.58
1:A:840:ARG:HB3	1:A:1385:THR:HA	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:ASP:CB	2:B:107:GLY:HA3	2.28	0.58
2:B:514:LEU:HD12	2:B:518:HIS:CD2	2.37	0.58
2:B:996:ARG:HG2	2:B:1007:VAL:HG11	1.84	0.58
7:I:95:THR:HG22	7:I:96:SER:N	2.19	0.58
1:A:112:LYS:HE3	1:A:165:GLY:H	1.69	0.58
1:A:673:GLY:CA	1:A:674:PRO:C	2.71	0.58
1:A:1083:THR:CG2	1:A:1084:PHE:N	2.66	0.58
4:E:36:GLU:O	4:E:38:PRO:HD3	2.04	0.58
1:A:54:ASN:HA	1:A:56:PRO:HD3	1.86	0.57
6:H:103:LYS:HG3	6:H:105:GLU:HB3	1.85	0.57
1:A:53:LEU:HD12	1:A:53:LEU:H	1.70	0.57
1:A:155:GLU:HB2	1:A:156:ASP:CB	2.34	0.57
3:C:238:ILE:HG22	3:C:242:GLN:HB2	1.86	0.57
1:A:626:ASN:CB	1:A:627:GLY:CA	2.66	0.57
1:A:830:LYS:O	1:A:830:LYS:CG	2.34	0.57
3:C:52:GLU:HA	10:L:64:LEU:CD1	2.34	0.57
1:A:265:LYS:HZ1	1:A:302:THR:HB	1.69	0.57
2:B:43:LEU:HD11	2:B:811:TYR:O	2.04	0.57
2:B:339:THR:HG21	2:B:348:ARG:HG2	1.85	0.57
2:B:645:SER:HB3	2:B:646:LEU:CB	2.15	0.57
3:C:241:ASP:HB3	9:K:109:TRP:CZ2	2.40	0.57
1:A:62:ASP:HA	1:A:63:ARG:HG2	1.85	0.57
1:A:1399:ARG:CB	1:A:1400:CYS:CB	2.51	0.57
3:C:15:LYS:HZ1	3:C:135:GLN:HG2	1.69	0.57
4:E:61:GLN:HG3	4:E:105:PHE:CZ	2.40	0.57
7:I:14:LEU:HB3	7:I:27:PHE:HB3	1.85	0.57
7:I:49:ILE:HA	7:I:92:ARG:HH22	1.70	0.57
2:B:856:PHE:CE2	2:B:969:ARG:HG3	2.39	0.57
1:A:122:MET:HE1	1:A:138:ILE:HG23	1.86	0.57
1:A:556:TRP:CH2	1:A:558:GLY:HA2	2.40	0.57
2:B:711:GLU:CB	2:B:712:PRO:HD2	2.34	0.57
3:C:155:LEU:HD21	3:C:157:CYS:SG	2.45	0.57
4:E:79:TRP:HB3	4:E:100:ILE:HD11	1.85	0.57
8:J:2:ILE:HG22	8:J:3:VAL:H	1.69	0.57
10:L:41:SER:C	10:L:43:THR:H	2.12	0.57
3:C:120:ILE:HD13	3:C:124:LEU:HD11	1.86	0.57
4:E:52:ARG:HB3	4:E:53:PRO:HD2	1.85	0.57
6:H:9:ILE:HG12	6:H:56:THR:HG22	1.87	0.57
5:F:97:ARG:HH11	5:F:124:GLU:CD	2.13	0.57
5:F:118:LEU:HG	5:F:122:MET:HE2	1.87	0.57
2:B:1154:ALA:C	2:B:1156:ASP:H	2.13	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:31:THR:O	4:E:34:GLU:HB2	2.05	0.56
6:H:107:VAL:O	6:H:108:SER:CB	2.53	0.56
1:A:56:PRO:CB	1:A:57:ARG:HG3	2.27	0.56
1:A:773:LYS:HZ1	1:A:1089:VAL:HG22	1.69	0.56
2:B:579:ARG:HG2	2:B:586:TRP:CZ2	2.41	0.56
1:A:605:MET:HE1	1:A:612:ILE:HG23	1.87	0.56
1:A:751:SER:O	1:A:752:LYS:HB2	2.04	0.56
2:B:745:PRO:C	2:B:747:MET:H	2.13	0.56
3:C:265:MET:HE1	9:K:19:LEU:CB	2.31	0.56
6:H:8:ASP:CG	6:H:9:ILE:H	2.14	0.56
7:I:85:PHE:HB3	7:I:101:PHE:CD2	2.40	0.56
8:J:48:ARG:NH2	8:J:49:MET:HE1	2.19	0.56
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.88	0.56
7:I:98:VAL:HG21	7:I:113:ASP:HB2	1.86	0.56
1:A:602:ASP:O	1:A:602:ASP:CG	2.48	0.56
1:A:870:GLU:HG2	4:E:208:TYR:CD2	2.41	0.56
3:C:52:GLU:HA	10:L:64:LEU:HD11	1.86	0.56
2:B:651:LEU:HD23	2:B:710:LEU:CD1	2.36	0.56
6:H:145:ARG:HB2	6:H:146:ARG:C	2.30	0.56
1:A:602:ASP:O	1:A:615:GLY:HA2	2.06	0.56
1:A:54:ASN:OD1	1:A:54:ASN:N	2.39	0.56
1:A:450:LEU:HD23	2:B:1133:MET:CE	2.36	0.56
1:A:1401:SER:HA	1:A:1404:GLU:OE2	2.05	0.56
2:B:21:GLU:CA	2:B:22:SER:HB2	2.36	0.56
1:A:68:GLN:HB2	1:A:69:THR:CA	2.36	0.56
1:A:1399:ARG:HB3	1:A:1400:CYS:HB3	0.71	0.56
2:B:1185:GLY:CA	2:B:1187:ASP:N	2.67	0.55
4:E:43:LYS:O	4:E:47:CYS:HB2	2.06	0.55
5:F:72:LYS:O	5:F:72:LYS:HG2	2.06	0.55
1:A:886:ILE:HD12	1:A:943:LEU:HB3	1.89	0.55
1:A:1325:THR:O	4:E:148:GLU:HB2	2.05	0.55
2:B:646:LEU:H	2:B:647:GLY:HA3	1.71	0.55
3:C:100:THR:HG21	3:C:102:GLN:NE2	2.18	0.55
4:E:147:HIS:HD2	4:E:149:LEU:H	1.55	0.55
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.06	0.55
1:A:48:ALA:CA	1:A:49:LYS:HB2	2.35	0.55
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.88	0.55
2:B:421:PHE:O	2:B:425:THR:HB	2.07	0.55
2:B:566:LEU:HD13	2:B:588:GLY:HA2	1.88	0.55
2:B:702:LEU:HD23	2:B:737:THR:HG22	1.88	0.55
2:B:806:THR:HG22	2:B:808:ALA:H	1.70	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1254:ALA:HB1	1:A:1255:GLU:HA	1.89	0.55
1:A:1087:ALA:N	1:A:1088:GLY:HA3	2.08	0.55
1:A:1316:VAL:C	1:A:1318:THR:H	2.14	0.55
2:B:735:ALA:CB	2:B:738:PHE:CE1	2.90	0.55
4:E:6:GLU:HA	4:E:9:ILE:CG1	2.37	0.55
7:I:39:GLY:O	7:I:40:SER:CB	2.54	0.55
1:A:52:GLY:HA3	1:A:53:LEU:C	2.32	0.55
1:A:399:HIS:HE1	1:A:436:ILE:O	1.89	0.55
4:E:75:MET:CG	4:E:76:GLY:H	2.20	0.55
1:A:72:GLU:HB3	1:A:73:GLY:CA	2.36	0.55
2:B:27:ALA:HB2	2:B:708:GLU:OE2	2.07	0.55
2:B:637:LEU:HA	2:B:743:ILE:HD12	1.89	0.55
1:A:1175:SER:HB3	1:A:1177:LEU:HD12	1.89	0.55
3:C:231:ASN:OD1	3:C:231:ASN:C	2.50	0.55
4:E:117:THR:C	4:E:119:SER:H	2.15	0.55
9:K:65:HIS:HD2	9:K:67:PHE:N	1.99	0.55
1:A:64:ASN:HB2	1:A:65:LEU:HG	1.87	0.54
1:A:474:VAL:O	1:A:477:PRO:HD2	2.07	0.54
1:A:709:THR:HG21	7:I:93:LYS:O	2.07	0.54
3:C:206:ASN:HA	3:C:209:TYR:CD1	2.42	0.54
1:A:1342:GLU:OE2	4:E:212:ARG:NH1	2.30	0.54
1:A:67:CYS:SG	1:A:69:THR:HB	2.48	0.54
1:A:1187:GLN:HB3	1:A:1188:GLN:CB	2.22	0.54
2:B:68:THR:HG22	2:B:90:ILE:O	2.07	0.54
1:A:53:LEU:N	1:A:53:LEU:CD1	2.71	0.54
2:B:69:LEU:HB2	2:B:89:GLU:HG2	1.88	0.54
4:E:66:GLU:N	4:E:66:GLU:CD	2.65	0.54
1:A:35:ILE:HG23	1:A:54:ASN:OD1	2.07	0.54
2:B:103:ASN:CB	2:B:169:ARG:HH22	2.17	0.54
3:C:214:ASN:O	3:C:217:ASP:HB2	2.07	0.54
6:H:84:ALA:HA	6:H:85:GLY:C	2.33	0.54
1:A:1254:ALA:C	1:A:1256:GLU:HG2	2.32	0.54
2:B:744:HIS:CD2	2:B:746:SER:H	2.25	0.54
2:B:1067:ARG:NH1	3:C:194:GLU:OE1	2.37	0.54
2:B:1084:GLN:HE22	3:C:192:TRP:H	1.55	0.54
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.90	0.53
4:E:124:VAL:HB	4:E:125:PRO:HD3	1.90	0.53
4:E:198:ILE:CD1	4:E:212:ARG:HG3	2.38	0.53
6:H:35:GLN:O	6:H:36:CYS:CB	2.53	0.53
1:A:672:ASP:CG	1:A:736:ASN:HD21	2.16	0.53
1:A:1098:VAL:O	1:A:1099:PRO:C	2.52	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1400:CYS:HA	1:A:1401:SER:CB	2.36	0.53
2:B:428:ILE:C	2:B:430:ARG:H	2.15	0.53
10:L:30:ILE:HG22	10:L:31:CYS:H	1.72	0.53
1:A:74:MET:O	1:A:75:ASN:HB2	2.09	0.53
1:A:704:ALA:O	1:A:705:LYS:HB2	2.08	0.53
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.49	0.53
6:H:77:ARG:O	6:H:78:SER:HB2	2.08	0.53
7:I:65:ASP:OD1	7:I:65:ASP:C	2.52	0.53
9:K:100:ALA:O	9:K:103:THR:HG22	2.08	0.53
1:A:598:LEU:O	1:A:599:SER:C	2.50	0.53
1:A:1387:HIS:H	1:A:1388:GLY:HA3	1.73	0.53
4:E:147:HIS:CD2	4:E:149:LEU:H	2.26	0.53
6:H:61:SER:O	6:H:89:LEU:HD11	2.08	0.53
1:A:53:LEU:HA	1:A:56:PRO:HD3	1.89	0.53
2:B:581:PHE:HA	2:B:585:VAL:O	2.08	0.53
4:E:75:MET:HE1	4:E:155:ARG:HH22	1.70	0.53
4:E:84:ASP:H	4:E:113:GLN:NE2	2.06	0.53
5:F:154:ASP:O	5:F:155:LEU:HD23	2.08	0.53
1:A:1263:ILE:O	1:A:1267:MET:HG3	2.08	0.53
2:B:1067:ARG:NH1	3:C:194:GLU:CD	2.67	0.53
3:C:107:SER:O	3:C:149:LYS:HB2	2.08	0.53
6:H:11:GLN:HB3	6:H:29:ALA:O	2.09	0.53
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.08	0.53
2:B:1098:MET:HB3	2:B:1099:VAL:HA	1.91	0.53
3:C:254:LYS:HE2	9:K:38:GLU:OE1	2.09	0.53
1:A:134:ARG:HD2	1:A:221:SER:O	2.09	0.52
1:A:1372:VAL:O	1:A:1376:THR:HB	2.09	0.52
9:K:57:LEU:HD21	9:K:78:THR:HG22	1.90	0.52
1:A:50:ILE:CG2	1:A:51:GLY:HA3	2.37	0.52
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.55	0.52
1:A:885:THR:HG22	1:A:943:LEU:HD12	1.91	0.52
6:H:91:ASP:O	6:H:93:TYR:N	2.41	0.52
6:H:41:ASP:HB2	6:H:121:LEU:HB3	1.92	0.52
1:A:751:SER:O	1:A:752:LYS:CB	2.56	0.52
1:A:757:ASN:HA	2:B:1021:MET:HE1	1.92	0.52
1:A:1158:PRO:N	1:A:1159:ARG:HB2	2.25	0.52
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.35	0.52
4:E:83:CYS:SG	4:E:85:GLU:HG3	2.50	0.52
6:H:33:GLN:H	6:H:33:GLN:HE21	1.56	0.52
1:A:1398:MET:O	1:A:1398:MET:HG2	2.09	0.52
7:I:8:ARG:HG2	7:I:8:ARG:NH1	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:ASN:HA	2:B:207:GLY:CA	2.40	0.52
1:A:385:ILE:HG23	1:A:386:ASP:N	2.25	0.51
1:A:412:ARG:NH1	1:A:433:GLU:OE1	2.43	0.51
1:A:1162:VAL:HG11	7:I:41:PRO:HG3	1.91	0.51
2:B:378:LEU:HA	2:B:381:MET:HE3	1.92	0.51
2:B:571:PRO:C	2:B:573:GLN:N	2.67	0.51
1:A:597:LEU:HD21	6:H:103:LYS:HG2	1.90	0.51
2:B:823:ALA:O	2:B:1089:PRO:HA	2.09	0.51
9:K:93:SER:O	9:K:97:LYS:HG3	2.11	0.51
1:A:391:LEU:CD2	1:A:400:PRO:HB2	2.40	0.51
1:A:726:ARG:HD2	11:M:2:TRX:CE3	2.40	0.51
3:C:124:LEU:O	3:C:127:ARG:HD3	2.10	0.51
2:B:254:LEU:CD2	2:B:381:MET:HE1	2.40	0.51
2:B:864:LYS:O	2:B:865:LYS:HB2	2.09	0.51
7:I:78:CYS:SG	7:I:80:SER:HB3	2.50	0.51
8:J:53:HIS:HE1	8:J:55:ASP:OD1	1.94	0.51
1:A:67:CYS:C	1:A:68:GLN:HG2	2.36	0.51
1:A:1191:TRP:CZ3	7:I:43:VAL:HG21	2.45	0.51
1:A:1083:THR:HG23	1:A:1084:PHE:H	1.76	0.51
2:B:735:ALA:O	2:B:737:THR:N	2.44	0.51
1:A:1254:ALA:CB	1:A:1255:GLU:CA	2.89	0.51
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.93	0.51
2:B:724:ASP:HB3	2:B:727:LYS:HD2	1.92	0.51
6:H:87:ARG:O	6:H:88:SER:HB3	2.10	0.51
9:K:55:LYS:HB3	9:K:81:TYR:CD1	2.45	0.51
2:B:508:LEU:HD13	2:B:508:LEU:O	2.11	0.51
1:A:633:VAL:HG21	1:A:645:LEU:HD22	1.93	0.51
3:C:80:LEU:HD12	3:C:127:ARG:NH2	2.26	0.51
6:H:139:ASN:C	6:H:139:ASN:HD22	2.18	0.51
2:B:744:HIS:HD2	2:B:746:SER:H	1.57	0.51
4:E:52:ARG:CB	4:E:53:PRO:CD	2.88	0.51
1:A:541:ILE:HD12	1:A:541:ILE:N	2.25	0.50
2:B:583:ASN:ND2	2:B:628:THR:H	2.06	0.50
3:C:42:PRO:HB3	3:C:161:LYS:HE3	1.94	0.50
5:F:143:PHE:C	5:F:143:PHE:CD1	2.89	0.50
2:B:708:GLU:O	2:B:711:GLU:HG2	2.11	0.50
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.93	0.50
2:B:913:GLY:HA2	2:B:938:SER:HB3	1.92	0.50
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.11	0.50
2:B:651:LEU:HD11	2:B:707:PRO:HB3	1.93	0.50
2:B:862:GLN:NE2	2:B:961:LEU:HD13	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:509:ALA:O	2:B:511:PRO:CD	2.58	0.50
1:A:132:LYS:HE2	1:A:1415:SER:OG	2.12	0.50
2:B:836:GLU:O	2:B:837:ASP:HB2	2.12	0.50
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.76	0.50
1:A:67:CYS:HB2	1:A:68:GLN:C	2.34	0.50
1:A:414:ASP:OD2	1:A:416:ARG:NH2	2.35	0.50
1:A:472:LEU:HD13	2:B:835:GLN:NE2	2.27	0.50
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.94	0.50
1:A:1258:HIS:HD2	1:A:1262:LYS:HE3	1.77	0.50
4:E:123:LEU:O	4:E:126:SER:HB3	2.12	0.50
2:B:22:SER:N	2:B:23:ALA:CB	2.64	0.50
2:B:1067:ARG:HG3	2:B:1067:ARG:HH11	1.77	0.50
4:E:73:PRO:O	4:E:74:ASP:HB2	2.11	0.50
10:L:30:ILE:HG22	10:L:31:CYS:N	2.27	0.50
1:A:884:ASP:O	1:A:886:ILE:N	2.45	0.50
1:A:1129:GLU:HA	1:A:1132:LYS:HD2	1.93	0.50
1:A:54:ASN:CB	1:A:55:ASP:OD1	2.59	0.49
2:B:68:THR:HG21	2:B:90:ILE:O	2.12	0.49
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.94	0.49
5:F:99:LEU:HD12	5:F:99:LEU:O	2.11	0.49
1:A:57:ARG:CA	1:A:68:GLN:HG3	2.39	0.49
4:E:79:TRP:HE1	4:E:81:GLU:CG	2.02	0.49
1:A:537:ARG:CZ	1:A:602:ASP:HB2	2.42	0.49
1:A:567:LYS:HD2	1:A:568:PRO:C	2.38	0.49
1:A:1168:GLU:O	1:A:1171:GLN:HB2	2.12	0.49
2:B:1035:ALA:HB1	2:B:1040:ASN:O	2.11	0.49
4:E:61:GLN:HG3	4:E:105:PHE:HZ	1.78	0.49
1:A:830:LYS:N	1:A:831:THR:C	2.70	0.49
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.95	0.49
2:B:654:ARG:N	2:B:657:HIS:HD2	2.10	0.49
4:E:66:GLU:CD	4:E:66:GLU:H	2.20	0.49
1:A:1073:GLY:O	1:A:1077:THR:HG23	2.12	0.49
2:B:294:ASP:CG	7:I:12:ASN:HD22	2.20	0.49
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.78	0.49
2:B:727:LYS:HE2	2:B:1049:ASP:OD2	2.11	0.49
1:A:1341:ILE:O	1:A:1345:ARG:N	2.37	0.49
4:E:16:PHE:CE2	4:E:20:LYS:NZ	2.79	0.49
6:H:106:GLU:O	6:H:107:VAL:HB	2.12	0.49
1:A:117:GLU:CD	1:A:117:GLU:H	2.21	0.49
1:A:1141:THR:HG21	1:A:1205:LYS:HD3	1.94	0.49
1:A:1295:THR:OG1	1:A:1297:GLU:OE1	2.22	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:GLU:O	2:B:656:GLY:HA3	2.13	0.49
7:I:15:TYR:CD1	7:I:30:ARG:HG3	2.47	0.49
1:A:606:LEU:C	1:A:606:LEU:HD23	2.38	0.49
1:A:994:GLN:NE2	1:A:1023:ARG:HE	2.09	0.49
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	2.28	0.49
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.94	0.49
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.10	0.49
2:B:508:LEU:N	2:B:509:ALA:CB	2.76	0.48
2:B:899:ILE:CD1	2:B:899:ILE:H	2.26	0.48
2:B:1077:THR:CG2	2:B:1079:LYS:H	2.20	0.48
2:B:914:LYS:H	2:B:938:SER:HB3	1.78	0.48
2:B:205:ILE:HD11	2:B:461:LEU:HD23	1.94	0.48
3:C:46:ILE:HA	3:C:159:ALA:HA	1.95	0.48
4:E:23:VAL:HG22	4:E:78:LEU:HD21	1.95	0.48
4:E:79:TRP:HB3	4:E:100:ILE:CD1	2.43	0.48
4:E:176:PRO:O	4:E:212:ARG:HA	2.13	0.48
1:A:166:GLY:HA3	1:A:167:CYS:HB3	1.94	0.48
1:A:740:LEU:C	1:A:740:LEU:CD2	2.86	0.48
1:A:1036:ARG:HH11	1:A:1036:ARG:HG2	1.77	0.48
1:A:1316:VAL:C	1:A:1318:THR:N	2.70	0.48
1:A:68:GLN:HB2	1:A:69:THR:OG1	2.14	0.48
1:A:166:GLY:CA	1:A:167:CYS:CB	2.90	0.48
1:A:598:LEU:HG	6:H:115:TYR:HE2	1.78	0.48
1:A:1106:ASN:OD1	1:A:1385:THR:HG21	2.13	0.48
1:A:1364:ASN:ND2	1:A:1366:ARG:H	2.11	0.48
2:B:795:ILE:HG22	2:B:796:LEU:O	2.13	0.48
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.48	0.48
4:E:50:MET:O	4:E:50:MET:HG2	2.14	0.48
7:I:19:ASP:OD1	7:I:22:ASN:HB2	2.13	0.48
1:A:772:GLY:HA3	1:A:1086:PHE:H	1.79	0.48
1:A:1075:PRO:HA	1:A:1078:GLN:HB3	1.95	0.48
2:B:830:TYR:O	2:B:831:SER:CB	2.61	0.48
2:B:959:ASP:OD2	2:B:959:ASP:N	2.46	0.48
1:A:152:VAL:HG13	1:A:153:PRO:CD	2.40	0.48
1:A:157:ASP:HB3	1:A:160:GLN:N	2.18	0.48
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.28	0.48
6:H:17:PRO:HA	6:H:24:CYS:SG	2.54	0.48
10:L:33:GLU:C	10:L:35:SER:H	2.22	0.48
1:A:541:ILE:CG2	1:A:546:VAL:HG23	2.43	0.48
1:A:598:LEU:HG	6:H:115:TYR:CE2	2.49	0.48
1:A:1084:PHE:CG	1:A:1085:HIS:N	2.81	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1399:ARG:HB3	1:A:1400:CYS:SG	2.53	0.48
2:B:108:VAL:HG13	2:B:108:VAL:O	2.13	0.48
10:L:48:CYS:HB3	10:L:52:GLY:H	1.79	0.48
1:A:92:HIS:C	1:A:92:HIS:CD2	2.91	0.48
1:A:155:GLU:HB2	1:A:156:ASP:CG	2.38	0.48
2:B:1183:CYS:O	2:B:1184:LYS:HG2	2.14	0.48
4:E:55:ARG:HD3	4:E:84:ASP:HA	1.96	0.48
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.53	0.47
1:A:185:TRP:O	1:A:186:LYS:HB2	2.13	0.47
1:A:919:ILE:HD11	1:A:925:LEU:HD12	1.96	0.47
1:A:1158:PRO:HB2	1:A:1159:ARG:CG	2.40	0.47
2:B:514:LEU:CD1	2:B:518:HIS:HD2	2.27	0.47
6:H:13:SER:N	6:H:27:GLU:O	2.41	0.47
1:A:1083:THR:CG2	1:A:1084:PHE:H	2.27	0.47
2:B:427:ASP:O	2:B:430:ARG:HB3	2.14	0.47
2:B:864:LYS:CG	2:B:865:LYS:H	2.26	0.47
1:A:93:VAL:HG21	1:A:304:MET:HB3	1.96	0.47
1:A:120:GLU:HB2	1:A:121:LEU:HG	1.96	0.47
2:B:64:CYS:C	2:B:66:ASP:H	2.22	0.47
1:A:477:PRO:HG3	1:A:521:MET:HG2	1.95	0.47
1:A:885:THR:HG21	1:A:943:LEU:HD12	1.96	0.47
2:B:992:ILE:HD11	9:K:66:PRO:HB2	1.95	0.47
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.95	0.47
7:I:17:ARG:O	7:I:25:LEU:HD12	2.14	0.47
7:I:51:ASN:O	7:I:54:GLU:HB2	2.14	0.47
1:A:15:LYS:HB2	2:B:1220:ASP:O	2.14	0.47
2:B:651:LEU:CD2	2:B:710:LEU:CD1	2.92	0.47
4:E:117:THR:C	4:E:119:SER:N	2.72	0.47
5:F:97:ARG:NH1	5:F:124:GLU:OE2	2.48	0.47
5:F:107:VAL:HG12	5:F:108:PHE:N	2.30	0.47
9:K:13:GLY:HA2	9:K:16:GLU:HB2	1.95	0.47
1:A:664:THR:OG1	1:A:746:MET:HE2	2.15	0.47
1:A:841:LEU:O	1:A:842:VAL:C	2.57	0.47
1:A:1124:HIS:O	1:A:1125:ALA:HB3	2.14	0.47
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.96	0.47
7:I:69:PRO:HB2	7:I:85:PHE:CZ	2.50	0.47
2:B:260:GLY:HA3	2:B:267:ARG:CD	2.34	0.47
2:B:1020:ARG:O	2:B:1021:MET:HB2	2.14	0.47
2:B:1067:ARG:HH12	3:C:194:GLU:CD	2.23	0.47
1:A:560:ILE:HB	6:H:79:TRP:HB3	1.97	0.47
1:A:567:LYS:NZ	1:A:570:PRO:HD3	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:ARG:HD2	13:A:2005:HOH:O	2.15	0.47
2:B:190:TYR:CZ	2:B:196:PRO:HG2	2.50	0.47
2:B:1065:GLN:OE1	2:B:1067:ARG:HB2	2.15	0.47
2:B:1185:GLY:HA2	2:B:1187:ASP:H	1.73	0.47
4:E:13:TRP:NE1	4:E:37:LEU:O	2.43	0.47
4:E:177:ARG:HD3	4:E:215:MET:SD	2.54	0.47
3:C:240:VAL:C	3:C:242:GLN:N	2.71	0.47
1:A:65:LEU:CA	1:A:66:LYS:HB2	2.43	0.46
1:A:674:PRO:O	1:A:675:THR:C	2.57	0.46
4:E:55:ARG:HD3	4:E:84:ASP:N	2.30	0.46
4:E:177:ARG:HB3	4:E:215:MET:HG2	1.96	0.46
1:A:1090:ALA:H	1:A:1092:LYS:CG	2.25	0.46
2:B:21:GLU:O	2:B:656:GLY:CA	2.63	0.46
3:C:60:ASP:OD2	10:L:60:ARG:NH2	2.48	0.46
3:C:195:GLN:HE21	3:C:195:GLN:HB2	1.60	0.46
10:L:28:LYS:HD2	10:L:39:SER:OG	2.15	0.46
1:A:673:GLY:CA	1:A:676:MET:N	2.66	0.46
1:A:709:THR:HB	1:A:712:GLU:H	1.79	0.46
2:B:92:PHE:HB3	2:B:130:VAL:HG11	1.97	0.46
6:H:25:ARG:HG3	6:H:41:ASP:OD2	2.15	0.46
1:A:427:GLN:HB2	1:A:430:TRP:NE1	2.30	0.46
1:A:650:GLN:O	1:A:651:LYS:C	2.59	0.46
2:B:60:GLN:HA	2:B:95:ILE:CD1	2.45	0.46
2:B:650:GLU:HB3	2:B:654:ARG:HH21	1.81	0.46
2:B:864:LYS:HG2	2:B:865:LYS:H	1.79	0.46
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.48	0.46
1:A:673:GLY:HA3	1:A:676:MET:H	1.78	0.46
1:A:1258:HIS:H	1:A:1260:LEU:HB3	1.80	0.46
1:A:1258:HIS:HA	1:A:1260:LEU:N	2.30	0.46
1:A:1421:CYS:HA	1:A:1426:GLU:HG3	1.98	0.46
2:B:291:ILE:HD13	2:B:300:HIS:CE1	2.50	0.46
2:B:799:PRO:HB2	2:B:818:PRO:HG2	1.98	0.46
2:B:1156:ASP:O	2:B:1157:ALA:C	2.57	0.46
4:E:180:ARG:HE	4:E:180:ARG:HB2	1.62	0.46
1:A:301:ALA:C	1:A:303:TYR:H	2.24	0.46
1:A:452:LYS:C	1:A:454:SER:N	2.73	0.46
2:B:763:GLN:HB2	2:B:1021:MET:HB2	1.97	0.46
2:B:911:ILE:HD13	2:B:911:ILE:HA	1.84	0.46
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	2.51	0.46
6:H:50:ALA:HB3	6:H:53:ASP:CG	2.41	0.46
7:I:63:GLY:C	7:I:65:ASP:H	2.23	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASP:HB2	1:A:160:GLN:HG3	1.97	0.46
2:B:162:SER:HA	2:B:163:GLY:HA2	1.70	0.46
4:E:69:ILE:H	4:E:69:ILE:HG12	1.65	0.46
1:A:63:ARG:NH1	1:A:75:ASN:HD22	2.14	0.46
1:A:626:ASN:CB	1:A:627:GLY:HA2	2.25	0.46
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.98	0.46
1:A:870:GLU:HG2	4:E:208:TYR:CG	2.51	0.46
1:A:915:SER:O	1:A:919:ILE:HB	2.15	0.46
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.30	0.46
9:K:7:PHE:CD1	9:K:7:PHE:C	2.93	0.46
1:A:7:SER:OG	2:B:1161:HIS:HE1	1.99	0.46
1:A:673:GLY:HA3	1:A:676:MET:CB	2.43	0.46
1:A:1258:HIS:CD2	1:A:1262:LYS:HE3	2.51	0.46
1:A:1336:MET:HE2	1:A:1337:GLU:HG3	1.97	0.46
2:B:879:ARG:HE	2:B:879:ARG:HB3	1.65	0.46
8:J:17:LYS:HG2	8:J:39:LEU:HD13	1.97	0.46
1:A:63:ARG:HD3	1:A:74:MET:CB	2.47	0.45
2:B:336:ARG:HG2	2:B:348:ARG:HD3	1.97	0.45
7:I:69:PRO:HG2	7:I:85:PHE:O	2.16	0.45
9:K:8:GLU:O	9:K:37:LYS:HD2	2.15	0.45
1:A:881:GLN:NE2	1:A:958:VAL:O	2.48	0.45
1:A:884:ASP:C	1:A:886:ILE:H	2.24	0.45
1:A:1095:THR:HG22	1:A:1113:THR:OG1	2.17	0.45
2:B:28:GLU:OE2	2:B:807:ARG:NH2	2.49	0.45
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.98	0.45
2:B:899:ILE:HD12	2:B:911:ILE:O	2.17	0.45
2:B:565:PRO:O	2:B:568:ASP:HB2	2.16	0.45
2:B:745:PRO:C	2:B:747:MET:N	2.74	0.45
3:C:48:SER:O	3:C:157:CYS:HA	2.16	0.45
6:H:50:ALA:O	6:H:51:ALA:CB	2.63	0.45
1:A:829:VAL:O	1:A:830:LYS:CB	2.62	0.45
5:F:97:ARG:NH1	5:F:124:GLU:CD	2.75	0.45
1:A:1160:SER:H	1:A:1170:ILE:HG21	1.82	0.45
2:B:564:GLU:HB2	2:B:589:VAL:HG12	1.99	0.45
9:K:57:LEU:HD21	9:K:78:THR:HG23	1.99	0.45
1:A:92:HIS:HD2	1:A:94:GLY:H	1.65	0.45
1:A:1327:ILE:O	4:E:147:HIS:HE1	1.99	0.45
2:B:459:TYR:C	2:B:459:TYR:CD2	2.95	0.45
2:B:980:PHE:CE2	2:B:990:ILE:HD11	2.52	0.45
1:A:824:LEU:HD23	1:A:824:LEU:HA	1.82	0.45
2:B:566:LEU:HD11	2:B:586:TRP:CE2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LEU:N	1:A:59:GLY:CA	2.80	0.45
1:A:87:ALA:HB2	1:A:277:GLU:HG3	1.98	0.45
1:A:408:ASP:O	1:A:410:GLY:N	2.50	0.45
2:B:34:ILE:HD11	2:B:743:ILE:HG22	1.98	0.45
2:B:235:SER:HB2	2:B:236:HIS:CD2	2.52	0.45
2:B:577:ALA:HB1	2:B:589:VAL:HG22	1.99	0.45
2:B:892:LYS:HE3	2:B:909:ASP:OD2	2.17	0.45
2:B:1067:ARG:HH11	2:B:1067:ARG:CG	2.30	0.45
4:E:75:MET:HE1	4:E:155:ARG:NH2	2.32	0.45
8:J:48:ARG:CZ	8:J:49:MET:CE	2.93	0.45
9:K:24:ASP:CG	9:K:25:THR:N	2.74	0.45
1:A:63:ARG:HD3	1:A:74:MET:HB3	1.98	0.44
1:A:1318:THR:HG21	4:E:11:ARG:HH12	1.83	0.44
1:A:69:THR:H	1:A:70:CYS:CB	2.30	0.44
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.99	0.44
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.99	0.44
2:B:800:GLN:HB3	8:J:52:THR:OG1	2.17	0.44
1:A:346:ASP:O	1:A:347:PHE:HB2	2.18	0.44
1:A:1083:THR:HG22	1:A:1084:PHE:N	2.31	0.44
2:B:315:LYS:N	2:B:316:PRO:HD2	2.32	0.44
2:B:1030:LEU:HD12	2:B:1030:LEU:HA	1.87	0.44
3:C:68:GLY:O	3:C:169:LYS:HB2	2.17	0.44
4:E:55:ARG:O	4:E:56:LYS:C	2.61	0.44
6:H:42:ILE:HG23	6:H:95:TYR:CZ	2.52	0.44
1:A:522:GLY:HA2	1:A:630:ILE:HD13	2.00	0.44
2:B:31:TRP:CH2	2:B:807:ARG:HB2	2.53	0.44
1:A:92:HIS:CD2	1:A:94:GLY:H	2.35	0.44
1:A:427:GLN:HB2	1:A:430:TRP:CD1	2.53	0.44
1:A:1286:LYS:HE3	1:A:1304:TRP:CE2	2.52	0.44
2:B:205:ILE:CD1	2:B:210:LYS:HG3	2.45	0.44
2:B:735:ALA:HB3	2:B:738:PHE:CE1	2.53	0.44
2:B:872:GLU:CD	2:B:914:LYS:HE2	2.42	0.44
2:B:1153:GLU:HG2	2:B:1155:SER:HB2	1.98	0.44
1:A:668:ASP:CG	1:A:742:ASN:HD22	2.26	0.44
1:A:1157:ASP:C	1:A:1159:ARG:HB2	2.43	0.44
2:B:422:LYS:HA	2:B:425:THR:HG22	2.00	0.44
1:A:912:LEU:HD22	1:A:1033:GLN:HA	1.99	0.44
2:B:426:LYS:HB3	2:B:427:ASP:H	1.63	0.44
4:E:5:ASN:O	4:E:9:ILE:HG12	2.17	0.44
4:E:7:ARG:O	4:E:8:ASN:CB	2.60	0.44
5:F:72:LYS:HD3	5:F:72:LYS:N	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:10:PHE:N	6:H:10:PHE:CD1	2.86	0.44
6:H:105:GLU:HB2	6:H:106:GLU:H	1.66	0.44
1:A:103:CYS:HA	1:A:106:VAL:HG12	2.00	0.44
1:A:265:LYS:HE2	1:A:299:HIS:CD2	2.38	0.44
1:A:821:ARG:O	1:A:822:GLU:C	2.60	0.44
2:B:644:GLU:CB	2:B:645:SER:CB	2.79	0.44
3:C:9:LYS:HB3	3:C:10:ILE:H	1.56	0.44
6:H:11:GLN:H	6:H:54:SER:CB	2.31	0.44
1:A:155:GLU:HB2	1:A:156:ASP:HB2	2.00	0.44
1:A:391:LEU:HD21	1:A:400:PRO:HB2	2.00	0.44
1:A:402:ALA:HA	1:A:434:ARG:HA	1.99	0.44
1:A:579:SER:HA	1:A:582:ILE:HD12	2.00	0.44
1:A:599:SER:O	1:A:600:PRO:C	2.59	0.44
1:A:884:ASP:C	1:A:886:ILE:N	2.76	0.44
1:A:1169:ILE:O	1:A:1172:LEU:O	2.36	0.44
2:B:446:LEU:HA	2:B:447:ALA:HA	1.64	0.44
2:B:496:ARG:HH11	2:B:496:ARG:HG2	1.81	0.44
2:B:847:ASP:CG	9:K:6:ARG:HH12	2.26	0.44
2:B:1001:PHE:CE1	3:C:178:PHE:HB3	2.53	0.44
1:A:605:MET:HE2	1:A:607:ILE:HD11	2.00	0.43
1:A:689:LYS:O	1:A:693:VAL:HG23	2.18	0.43
1:A:829:VAL:O	1:A:829:VAL:CG1	2.64	0.43
1:A:1134:ILE:HG22	1:A:1306:LEU:CD1	2.48	0.43
6:H:60:ALA:O	6:H:140:ALA:HB1	2.17	0.43
10:L:41:SER:C	10:L:43:THR:N	2.76	0.43
1:A:1175:SER:HA	1:A:1176:LEU:C	2.43	0.43
1:A:1350:LYS:HE3	1:A:1350:LYS:HB3	1.51	0.43
1:A:1424:VAL:HG21	2:B:1139:ILE:HD11	2.00	0.43
2:B:341:LEU:O	2:B:341:LEU:HD12	2.18	0.43
2:B:1067:ARG:NH1	3:C:194:GLU:OE2	2.51	0.43
5:F:74:ILE:HA	5:F:75:PRO:HD3	1.71	0.43
1:A:14:VAL:N	1:A:1432:GLN:HE22	2.17	0.43
1:A:1217:LYS:O	1:A:1221:LYS:HA	2.18	0.43
2:B:770:GLN:HG2	2:B:983:ARG:O	2.18	0.43
2:B:865:LYS:NZ	2:B:961:LEU:HD11	2.33	0.43
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.99	0.43
9:K:10:PHE:CD1	9:K:11:LEU:HG	2.53	0.43
1:A:362:ASP:OD1	1:A:459:ARG:HD3	2.18	0.43
1:A:515:GLN:HE22	1:A:1075:PRO:HD3	1.83	0.43
1:A:909:ASP:HA	1:A:910:PRO:HD2	1.82	0.43
1:A:1342:GLU:HG2	4:E:151:PRO:HG2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:760:ASP:OD1	2:B:760:ASP:N	2.51	0.43
3:C:155:LEU:HD23	3:C:155:LEU:C	2.43	0.43
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.47	0.43
3:C:248:ILE:HD13	9:K:102:LYS:HA	1.99	0.43
4:E:4:GLU:HA	4:E:6:GLU:H	1.82	0.43
6:H:83:GLN:NE2	6:H:83:GLN:HA	2.33	0.43
1:A:785:PRO:HG2	2:B:703:ILE:HD12	2.00	0.43
2:B:211:VAL:HG13	2:B:495:LEU:HD23	1.99	0.43
2:B:316:PRO:O	2:B:320:ASP:HB2	2.18	0.43
3:C:22:LEU:HD21	9:K:101:LEU:HD13	1.99	0.43
3:C:258:ILE:HG12	9:K:35:PHE:HE2	1.84	0.43
1:A:368:LYS:HE3	1:A:368:LYS:HB2	1.83	0.43
1:A:505:CYS:O	1:A:506:ALA:C	2.60	0.43
1:A:832:ALA:C	1:A:834:THR:H	2.26	0.43
1:A:1157:ASP:O	1:A:1159:ARG:N	2.51	0.43
2:B:846:ILE:HG12	2:B:974:PRO:HB2	2.01	0.43
3:C:134:ILE:HG21	3:C:139:GLY:HA2	2.01	0.43
4:E:75:MET:CE	4:E:155:ARG:NH2	2.79	0.43
9:K:20:LYS:O	9:K:33:ILE:HA	2.18	0.43
1:A:56:PRO:HB3	1:A:57:ARG:CD	2.48	0.43
1:A:522:GLY:HA2	1:A:630:ILE:CD1	2.49	0.43
1:A:1403:GLU:OE2	1:A:1403:GLU:HA	2.19	0.43
2:B:639:ILE:HD12	2:B:688:GLY:O	2.18	0.43
2:B:916:THR:HB	2:B:935:ARG:HG3	2.00	0.43
1:A:633:VAL:O	1:A:634:THR:C	2.61	0.43
2:B:211:VAL:O	2:B:480:SER:HA	2.18	0.43
2:B:1157:ALA:HB1	2:B:1196:HIS:HB3	1.99	0.43
6:H:10:PHE:HA	6:H:29:ALA:O	2.17	0.43
10:L:61:THR:HB	10:L:63:ARG:H	1.83	0.43
1:A:34:LYS:HA	1:A:83:HIS:CE1	2.54	0.43
1:A:36:ARG:O	1:A:37:PHE:CD1	2.72	0.43
1:A:62:ASP:HA	1:A:63:ARG:CG	2.49	0.43
1:A:831:THR:HA	1:A:832:ALA:HA	1.78	0.43
1:A:834:THR:C	1:A:836:TYR:N	2.77	0.43
1:A:849:MET:HG3	1:A:850:VAL:N	2.34	0.43
1:A:919:ILE:HD12	1:A:919:ILE:HA	1.73	0.43
1:A:1348:LEU:HD21	1:A:1375:MET:SD	2.59	0.43
4:E:55:ARG:HD3	4:E:84:ASP:H	1.84	0.43
1:A:583:PRO:O	1:A:586:ILE:HG12	2.19	0.43
1:A:963:ILE:HD12	1:A:1049:ILE:HG13	1.99	0.43
1:A:1078:GLN:O	1:A:1078:GLN:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:HG23	1:A:111:GLY:O	2.19	0.42
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.54	0.42
2:B:228:LYS:O	2:B:261:ARG:NH1	2.51	0.42
2:B:1203:LEU:HD23	2:B:1203:LEU:HA	1.88	0.42
1:A:17:VAL:HA	2:B:1216:ARG:O	2.19	0.42
1:A:901:LEU:N	1:A:926:GLN:OE1	2.51	0.42
1:A:1209:MET:HB3	1:A:1228:TRP:CD1	2.54	0.42
1:A:1317:MET:O	1:A:1322:ILE:HD11	2.19	0.42
2:B:181:LEU:HD13	2:B:194:GLU:HG2	2.02	0.42
1:A:356:ASP:OD2	9:K:65:HIS:HE1	2.03	0.42
1:A:447:GLN:HA	1:A:448:PRO:C	2.43	0.42
1:A:602:ASP:O	1:A:616:VAL:HG23	2.18	0.42
1:A:747:VAL:HG12	1:A:748:MET:N	2.33	0.42
2:B:651:LEU:HD23	2:B:710:LEU:HD11	2.01	0.42
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.84	0.42
7:I:72:ASP:O	7:I:73:ARG:C	2.62	0.42
1:A:26:GLU:HA	1:A:29:ALA:HB3	2.01	0.42
1:A:70:CYS:H	2:B:1172:ILE:HG23	1.84	0.42
1:A:416:ARG:HE	1:A:416:ARG:HB2	1.45	0.42
1:A:1341:ILE:HG13	4:E:182:ASP:OD2	2.19	0.42
2:B:1163:CYS:O	2:B:1167:GLY:HA2	2.19	0.42
6:H:145:ARG:HB2	6:H:146:ARG:O	2.18	0.42
1:A:1067:LEU:HD12	1:A:1067:LEU:HA	1.80	0.42
1:A:1399:ARG:CB	1:A:1400:CYS:SG	3.06	0.42
2:B:276:ILE:CG2	2:B:280:ILE:HD11	2.23	0.42
2:B:408:LEU:O	2:B:409:ALA:C	2.60	0.42
2:B:872:GLU:OE1	2:B:914:LYS:HE2	2.19	0.42
9:K:91:CYS:O	9:K:95:ILE:HG12	2.19	0.42
1:A:239:LEU:HD23	1:A:240:PRO:HD2	2.02	0.42
1:A:701:LEU:HD23	1:A:701:LEU:HA	1.88	0.42
1:A:806:ARG:NH1	2:B:729:ILE:HD11	2.34	0.42
1:A:830:LYS:CA	1:A:831:THR:C	2.93	0.42
1:A:1128:GLN:O	1:A:1128:GLN:HG2	2.19	0.42
4:E:156:LEU:HD21	4:E:197:LYS:HB2	2.00	0.42
1:A:63:ARG:HH12	1:A:75:ASN:HD22	1.67	0.42
1:A:445:ASN:HB3	1:A:455:MET:HE3	2.01	0.42
1:A:559:VAL:HG13	6:H:78:SER:HA	2.02	0.42
2:B:377:PHE:O	2:B:380:TYR:HB3	2.19	0.42
2:B:414:ALA:O	2:B:418:LYS:HB2	2.19	0.42
2:B:508:LEU:N	2:B:509:ALA:HB2	2.34	0.42
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:VAL:C	1:A:477:PRO:HD2	2.45	0.42
1:A:1253:GLU:O	1:A:1254:ALA:HB3	2.20	0.42
2:B:123:THR:HA	2:B:204:ILE:O	2.20	0.42
2:B:1058:LEU:HD23	2:B:1058:LEU:HA	1.92	0.42
4:E:124:VAL:O	4:E:126:SER:N	2.53	0.42
8:J:2:ILE:HD11	8:J:57:ILE:HD13	2.01	0.42
9:K:51:LEU:HD13	9:K:59:ALA:HB3	2.01	0.42
9:K:82:ASP:HA	9:K:83:PRO:HD2	1.85	0.42
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.68	0.42
1:A:247:ARG:N	1:A:248:PRO:HD3	2.35	0.42
1:A:613:ILE:HG22	1:A:614:PHE:CD2	2.55	0.42
1:A:1438:THR:HA	5:F:88:TYR:HB3	2.00	0.42
2:B:221:ASN:OD1	2:B:242:SER:HA	2.20	0.42
4:E:198:ILE:HD11	4:E:212:ARG:HG3	2.02	0.42
6:H:52:GLN:O	6:H:52:GLN:HG3	2.20	0.42
7:I:98:VAL:HG21	7:I:113:ASP:CB	2.50	0.42
1:A:166:GLY:HA2	1:A:167:CYS:CB	2.49	0.42
1:A:1175:SER:HA	1:A:1176:LEU:O	2.19	0.42
1:A:1436:ILE:C	1:A:1436:ILE:HD12	2.45	0.42
2:B:1067:ARG:HA	2:B:1067:ARG:HD3	1.47	0.42
3:C:245:VAL:HA	3:C:248:ILE:HD12	2.02	0.42
4:E:111:VAL:HG12	4:E:137:GLU:HG3	2.02	0.42
5:F:94:LEU:HD23	5:F:94:LEU:HA	1.89	0.42
5:F:143:PHE:CD1	5:F:143:PHE:O	2.73	0.42
9:K:18:LYS:CE	9:K:36:GLU:O	2.67	0.42
1:A:56:PRO:CG	1:A:57:ARG:HE	2.32	0.41
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.55	0.41
1:A:840:ARG:HA	1:A:840:ARG:HD3	1.73	0.41
1:A:1088:GLY:HA2	1:A:1089:VAL:HA	1.86	0.41
1:A:1255:GLU:N	1:A:1256:GLU:HB3	2.35	0.41
2:B:521:LEU:HD22	2:B:633:VAL:HG12	2.02	0.41
2:B:735:ALA:HB1	2:B:738:PHE:CE1	2.53	0.41
2:B:776:GLN:O	2:B:1095:LEU:HA	2.19	0.41
3:C:262:LEU:HD23	3:C:265:MET:HE3	2.01	0.41
9:K:42:LEU:HD23	9:K:42:LEU:HA	1.86	0.41
1:A:49:LYS:HA	1:A:50:ILE:HB	2.02	0.41
1:A:70:CYS:SG	1:A:71:GLN:N	2.93	0.41
1:A:1013:ASP:HB3	4:E:207:ARG:O	2.20	0.41
1:A:1124:HIS:ND1	1:A:1124:HIS:N	2.67	0.41
2:B:22:SER:CA	2:B:23:ALA:HB3	2.49	0.41
2:B:115:GLN:HE21	2:B:119:LEU:HG	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:858:SER:HA	2:B:966:VAL:O	2.21	0.41
2:B:1184:LYS:HA	2:B:1185:GLY:HA3	1.60	0.41
3:C:261:ALA:O	3:C:265:MET:HG2	2.20	0.41
6:H:98:TYR:O	6:H:118:PHE:HD2	2.03	0.41
1:A:440:ASP:OD1	1:A:498:ARG:NH1	2.53	0.41
6:H:52:GLN:N	6:H:53:ASP:CB	2.58	0.41
8:J:43:ARG:HH11	8:J:43:ARG:HD3	1.71	0.41
1:A:443:LEU:HD13	1:A:501:LEU:HD13	2.01	0.41
1:A:481:ASP:O	1:A:485:ASP:HB2	2.20	0.41
1:A:566:ILE:HD11	6:H:98:TYR:HB2	2.03	0.41
1:A:867:ILE:HD11	1:A:999:VAL:CG1	2.50	0.41
2:B:598:GLU:OE2	2:B:598:GLU:HA	2.08	0.41
3:C:240:VAL:O	3:C:241:ASP:C	2.63	0.41
3:C:265:MET:CE	9:K:19:LEU:HD12	2.50	0.41
4:E:52:ARG:HG3	4:E:53:PRO:HD3	2.02	0.41
7:I:13:MET:CE	7:I:15:TYR:CE2	3.03	0.41
1:A:108:MET:HG2	1:A:171:GLN:HE22	1.86	0.41
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.84	0.41
1:A:573:SER:HB3	1:A:576:GLN:H	1.84	0.41
1:A:828:ALA:O	1:A:831:THR:O	2.38	0.41
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.20	0.41
1:A:1256:GLU:HG3	1:A:1256:GLU:O	2.20	0.41
2:B:576:ASP:OD1	2:B:576:ASP:N	2.53	0.41
6:H:118:PHE:O	6:H:121:LEU:HD12	2.19	0.41
10:L:38:LEU:HD23	10:L:39:SER:N	2.36	0.41
1:A:1102:LYS:HE3	1:A:1102:LYS:HB2	1.76	0.41
2:B:361:LEU:HB3	2:B:364:ILE:HD12	2.02	0.41
2:B:428:ILE:C	2:B:430:ARG:N	2.77	0.41
2:B:498:THR:HG1	2:B:537:LYS:HB2	1.85	0.41
2:B:512:ARG:HG2	2:B:533:CYS:O	2.20	0.41
2:B:1159:ARG:HD3	2:B:1194:GLN:HG3	2.02	0.41
7:I:50:THR:H	7:I:92:ARG:NH2	2.19	0.41
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.53	0.41
1:A:994:GLN:HG2	1:A:1019:CYS:SG	2.60	0.41
1:A:1403:GLU:HB3	1:A:1405:THR:H	1.85	0.41
2:B:23:ALA:HA	2:B:24:PRO:HD2	1.86	0.41
4:E:6:GLU:HG3	4:E:9:ILE:HG13	2.02	0.41
6:H:52:GLN:HE21	6:H:52:GLN:HB2	1.61	0.41
1:A:53:LEU:HA	1:A:54:ASN:HA	1.87	0.41
1:A:216:VAL:HA	1:A:219:PHE:CE2	2.54	0.41
1:A:769:SER:HB2	13:A:2006:HOH:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1259:MET:O	1:A:1260:LEU:HB2	2.20	0.41
1:A:1316:VAL:O	1:A:1318:THR:N	2.54	0.41
3:C:92:CYS:SG	3:C:94:LYS:HB2	2.61	0.41
4:E:67:GLU:HA	4:E:70:SER:HB2	2.02	0.41
7:I:88:SER:HB2	7:I:100:PHE:HE1	1.85	0.41
8:J:41:LEU:HD22	8:J:46:CYS:HB3	2.03	0.41
1:A:35:ILE:O	1:A:36:ARG:HB2	2.19	0.41
1:A:943:LEU:HD23	1:A:943:LEU:HA	1.93	0.41
1:A:1101:LEU:O	1:A:1105:LEU:HG	2.21	0.41
1:A:1106:ASN:OD1	1:A:1385:THR:HG23	2.20	0.41
1:A:1342:GLU:CG	4:E:151:PRO:HG2	2.51	0.41
2:B:516:ASN:H	2:B:516:ASN:HD22	1.69	0.41
2:B:646:LEU:HD12	2:B:646:LEU:O	2.21	0.41
2:B:745:PRO:O	2:B:747:MET:N	2.54	0.41
2:B:1158:PHE:CE2	2:B:1160:VAL:HG22	2.56	0.41
9:K:24:ASP:OD1	9:K:25:THR:N	2.29	0.41
1:A:519:PRO:HD3	1:A:631:HIS:ND1	2.35	0.41
2:B:259:TYR:OH	2:B:279:ASP:OD2	2.34	0.41
6:H:33:GLN:HE21	6:H:33:GLN:N	2.18	0.41
3:C:55:THR:HG22	3:C:151:GLN:HA	2.02	0.40
3:C:238:ILE:CG2	3:C:242:GLN:CB	2.99	0.40
6:H:85:GLY:HA3	6:H:86:ASP:HA	1.80	0.40
1:A:54:ASN:HA	1:A:56:PRO:CD	2.50	0.40
1:A:58:LEU:H	1:A:59:GLY:CA	2.34	0.40
1:A:348:SER:OG	2:B:1128:LEU:HD23	2.21	0.40
1:A:423:ASP:O	1:A:423:ASP:CG	2.64	0.40
2:B:115:GLN:HG2	2:B:193:LYS:HB2	2.03	0.40
3:C:49:VAL:HG13	3:C:155:LEU:HG	2.02	0.40
6:H:81:PRO:O	6:H:83:GLN:HG2	2.22	0.40
1:A:746:MET:HB3	1:A:752:LYS:O	2.21	0.40
1:A:1341:ILE:HD12	1:A:1342:GLU:H	1.86	0.40
1:A:1373:ASP:O	1:A:1377:THR:HB	2.21	0.40
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.56	0.40
2:B:287:ARG:NH1	2:B:324:ILE:O	2.54	0.40
3:C:6:PRO:HB2	9:K:101:LEU:HB2	2.04	0.40
4:E:53:PRO:HB3	4:E:55:ARG:NH1	2.34	0.40
1:A:232:GLU:HG2	1:A:233:TRP:CD1	2.56	0.40
1:A:771:GLU:HA	1:A:1086:PHE:CZ	2.56	0.40
2:B:496:ARG:NH2	2:B:540:SER:O	2.55	0.40
6:H:56:THR:N	6:H:145:ARG:O	2.55	0.40
7:I:39:GLY:O	7:I:40:SER:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:CG2	1:A:51:GLY:O	2.62	0.40
1:A:211:PHE:HA	1:A:214:ILE:HD12	2.02	0.40
1:A:596:THR:C	1:A:598:LEU:H	2.29	0.40
1:A:1409:LEU:HD13	2:B:1208:LEU:HD21	2.04	0.40
2:B:293:PRO:O	2:B:294:ASP:C	2.64	0.40
2:B:701:ILE:HD11	2:B:703:ILE:HD11	2.02	0.40
2:B:1220:ASP:OD2	2:B:1220:ASP:C	2.63	0.40
8:J:16:ASP:OD1	8:J:17:LYS:HE3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1333/1733 (77%)	1168 (88%)	110 (8%)	55 (4%)	2	8
2	B	1035/1224 (85%)	920 (89%)	79 (8%)	36 (4%)	3	10
3	C	263/318 (83%)	243 (92%)	19 (7%)	1 (0%)	30	60
4	E	211/215 (98%)	189 (90%)	12 (6%)	10 (5%)	2	6
5	F	82/155 (53%)	78 (95%)	4 (5%)	0	100	100
6	H	108/146 (74%)	76 (70%)	17 (16%)	15 (14%)	0	0
7	I	119/122 (98%)	106 (89%)	11 (9%)	2 (2%)	7	25
8	J	63/70 (90%)	62 (98%)	1 (2%)	0	100	100
9	K	111/120 (92%)	99 (89%)	10 (9%)	2 (2%)	6	23
10	L	39/70 (56%)	29 (74%)	9 (23%)	1 (3%)	4	15
11	M	4/8 (50%)	3 (75%)	1 (25%)	0	100	100
All	All	3368/4181 (81%)	2973 (88%)	273 (8%)	122 (4%)	2	10

All (122) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	56	PRO
1	A	63	ARG
1	A	70	CYS
1	A	157	ASP
1	A	167	CYS
1	A	186	LYS
1	A	603	ASN
1	A	674	PRO
1	A	752	LYS
1	A	830	LYS
1	A	885	THR
1	A	1160	SER
1	A	1175	SER
1	A	1188	GLN
1	A	1221	LYS
1	A	1256	GLU
1	A	1260	LEU
1	A	1387	HIS
1	A	1399	ARG
1	A	1400	CYS
1	A	1401	SER
2	B	68	THR
2	B	104	GLU
2	B	105	SER
2	B	108	VAL
2	B	427	ASP
2	B	645	SER
2	B	648	HIS
2	B	1155	SER
2	B	1156	ASP
2	B	1180	GLN
3	C	10	ILE
4	E	49	SER
4	E	52	ARG
4	E	74	ASP
4	E	148	GLU
6	H	36	CYS
6	H	51	ALA
6	H	77	ARG
6	H	78	SER
6	H	85	GLY
6	H	92	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	H	106	GLU
6	H	107	VAL
6	H	108	SER
6	H	139	ASN
7	I	40	SER
1	A	52	GLY
1	A	53	LEU
1	A	62	ASP
1	A	120	GLU
1	A	279	LEU
1	A	409	SER
1	A	419	LYS
1	A	626	ASN
1	A	831	THR
1	A	1080	THR
1	A	1176	LEU
1	A	1405	THR
2	B	22	SER
2	B	67	SER
2	B	266	ALA
2	B	368	GLU
2	B	426	LYS
2	B	429	PHE
2	B	735	ALA
2	B	736	THR
2	B	1097	HIS
2	B	1157	ALA
4	E	8	ASN
4	E	53	PRO
4	E	84	ASP
6	H	83	GLN
6	H	90	ALA
1	A	36	ARG
1	A	66	LYS
1	A	71	GLN
1	A	158	PRO
1	A	465	TYR
1	A	705	LYS
1	A	747	VAL
1	A	764	CYS
1	A	833	GLU
1	A	1158	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1159	ARG
2	B	644	GLU
2	B	1066	SER
2	B	1184	LYS
6	H	52	GLN
6	H	88	SER
1	A	154	SER
1	A	599	SER
2	B	109	THR
2	B	509	ALA
2	B	510	LYS
2	B	746	SER
4	E	75	MET
9	K	25	THR
10	L	64	LEU
1	A	453	MET
1	A	958	VAL
1	A	1090	ALA
1	A	1254	ALA
2	B	1152	MET
6	H	11	GLN
9	K	45	LEU
1	A	221	SER
2	B	23	ALA
2	B	261	ARG
2	B	574	SER
2	B	646	LEU
2	B	1166	CYS
4	E	73	PRO
1	A	93	VAL
4	E	51	GLY
7	I	76	PRO
1	A	622	VAL
2	B	647	GLY
2	B	974	PRO
2	B	1017	ILE
1	A	1437	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	1182/1520 (78%)	1033 (87%)	149 (13%)	4	15
2	B	919/1061 (87%)	823 (90%)	96 (10%)	7	22
3	C	233/274 (85%)	200 (86%)	33 (14%)	3	12
4	E	195/197 (99%)	169 (87%)	26 (13%)	4	14
5	F	74/137 (54%)	66 (89%)	8 (11%)	6	21
6	H	102/128 (80%)	79 (78%)	23 (22%)	1	3
7	I	115/116 (99%)	100 (87%)	15 (13%)	4	14
8	J	60/65 (92%)	50 (83%)	10 (17%)	2	8
9	K	98/102 (96%)	90 (92%)	8 (8%)	10	33
10	L	38/57 (67%)	30 (79%)	8 (21%)	1	4
11	M	2/2 (100%)	2 (100%)	0	100	100
All	All	3018/3659 (82%)	2642 (88%)	376 (12%)	4	15

All (376) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	37	PHE
1	A	39	GLU
1	A	50	ILE
1	A	53	LEU
1	A	54	ASN
1	A	56	PRO
1	A	57	ARG
1	A	60	SER
1	A	63	ARG
1	A	64	ASN
1	A	68	GLN
1	A	69	THR
1	A	71	GLN
1	A	90	VAL
1	A	93	VAL
1	A	120	GLU
1	A	121	LEU
1	A	129	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	145	LYS
1	A	150	THR
1	A	152	VAL
1	A	159	THR
1	A	162	VAL
1	A	167	CYS
1	A	186	LYS
1	A	196	GLU
1	A	207	ILE
1	A	222	LEU
1	A	247	ARG
1	A	263	THR
1	A	264	PHE
1	A	265	LYS
1	A	266	LEU
1	A	281	HIS
1	A	302	THR
1	A	304	MET
1	A	354	SER
1	A	385	ILE
1	A	389	THR
1	A	398	GLU
1	A	411	ASP
1	A	416	ARG
1	A	431	LYS
1	A	445	ASN
1	A	453	MET
1	A	454	SER
1	A	463	ILE
1	A	472	LEU
1	A	475	THR
1	A	501	LEU
1	A	513	SER
1	A	543	LEU
1	A	544	ASP
1	A	553	VAL
1	A	566	ILE
1	A	567	LYS
1	A	593	GLU
1	A	613	ILE
1	A	616	VAL
1	A	618	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	622	VAL
1	A	626	ASN
1	A	677	ARG
1	A	708	MET
1	A	728	LYS
1	A	734	GLU
1	A	737	LEU
1	A	740	LEU
1	A	747	VAL
1	A	752	LYS
1	A	756	ILE
1	A	769	SER
1	A	808	LEU
1	A	827	THR
1	A	830	LYS
1	A	831	THR
1	A	849	MET
1	A	867	ILE
1	A	878	ILE
1	A	882	SER
1	A	885	THR
1	A	896	ARG
1	A	919	ILE
1	A	935	GLN
1	A	948	VAL
1	A	973	ILE
1	A	983	ILE
1	A	1001	ARG
1	A	1005	GLU
1	A	1006	ILE
1	A	1036	ARG
1	A	1048	ASN
1	A	1078	GLN
1	A	1079	MET
1	A	1095	THR
1	A	1111	MET
1	A	1124	HIS
1	A	1141	THR
1	A	1143	LEU
1	A	1144	LYS
1	A	1146	VAL
1	A	1159	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1160	SER
1	A	1167	GLU
1	A	1169	ILE
1	A	1171	GLN
1	A	1173	HIS
1	A	1176	LEU
1	A	1188	GLN
1	A	1221	LYS
1	A	1227	ILE
1	A	1230	GLU
1	A	1234	GLU
1	A	1237	ILE
1	A	1240	CYS
1	A	1243	VAL
1	A	1255	GLU
1	A	1258	HIS
1	A	1259	MET
1	A	1264	GLU
1	A	1269	GLU
1	A	1279	ILE
1	A	1283	VAL
1	A	1291	VAL
1	A	1297	GLU
1	A	1299	VAL
1	A	1318	THR
1	A	1341	ILE
1	A	1350	LYS
1	A	1355	VAL
1	A	1361	SER
1	A	1366	ARG
1	A	1372	VAL
1	A	1376	THR
1	A	1377	THR
1	A	1384	VAL
1	A	1387	HIS
1	A	1398	MET
1	A	1399	ARG
1	A	1400	CYS
1	A	1401	SER
1	A	1405	THR
1	A	1407	GLU
1	A	1420	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1438	THR
1	A	1444	MET
1	A	1445	ILE
1	A	1447	GLU
2	B	22	SER
2	B	46	GLN
2	B	61	ASP
2	B	63	ILE
2	B	65	GLU
2	B	69	LEU
2	B	90	ILE
2	B	94	LYS
2	B	101	MET
2	B	102	VAL
2	B	104	GLU
2	B	108	VAL
2	B	109	THR
2	B	125	SER
2	B	133	LYS
2	B	162	SER
2	B	164	LYS
2	B	187	SER
2	B	210	LYS
2	B	211	VAL
2	B	218	SER
2	B	222	ILE
2	B	253	THR
2	B	272	THR
2	B	283	VAL
2	B	291	ILE
2	B	339	THR
2	B	343	ILE
2	B	347	LYS
2	B	365	THR
2	B	367	LEU
2	B	368	GLU
2	B	408	LEU
2	B	425	THR
2	B	427	ASP
2	B	428	ILE
2	B	452	THR
2	B	522	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	531	GLN
2	B	540	SER
2	B	541	LEU
2	B	543	SER
2	B	547	VAL
2	B	566	LEU
2	B	567	GLU
2	B	573	GLN
2	B	576	ASP
2	B	578	THR
2	B	579	ARG
2	B	589	VAL
2	B	598	GLU
2	B	624	LEU
2	B	642	ASP
2	B	643	ASP
2	B	646	LEU
2	B	648	HIS
2	B	653	VAL
2	B	668	ASP
2	B	677	GLU
2	B	678	GLU
2	B	690	VAL
2	B	693	ILE
2	B	708	GLU
2	B	709	ASP
2	B	733	HIS
2	B	734	HIS
2	B	737	THR
2	B	743	ILE
2	B	787	VAL
2	B	815	ARG
2	B	838	SER
2	B	870	ILE
2	B	879	ARG
2	B	899	ILE
2	B	911	ILE
2	B	915	THR
2	B	916	THR
2	B	935	ARG
2	B	938	SER
2	B	939	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	958	GLN
2	B	959	ASP
2	B	964	VAL
2	B	983	ARG
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1050	ILE
2	B	1060	ARG
2	B	1065	GLN
2	B	1077	THR
2	B	1097	HIS
2	B	1150	ARG
2	B	1156	ASP
2	B	1192	ILE
2	B	1221	ARG
3	C	10	ILE
3	C	12	GLU
3	C	25	VAL
3	C	34	ARG
3	C	36	VAL
3	C	43	THR
3	C	48	SER
3	C	50	GLU
3	C	55	THR
3	C	100	THR
3	C	107	SER
3	C	110	THR
3	C	121	VAL
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	138	GLU
3	C	155	LEU
3	C	156	THR
3	C	157	CYS
3	C	189	THR
3	C	195	GLN
3	C	197	SER
3	C	217	ASP
3	C	235	VAL
3	C	240	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	245	VAL
3	C	251	LEU
3	C	254	LYS
3	C	257	SER
3	C	258	ILE
3	C	263	THR
3	C	266	ASP
4	E	3	GLN
4	E	7	ARG
4	E	9	ILE
4	E	10	SER
4	E	14	ARG
4	E	31	THR
4	E	36	GLU
4	E	48	ASP
4	E	52	ARG
4	E	68	SER
4	E	69	ILE
4	E	70	SER
4	E	74	ASP
4	E	78	LEU
4	E	81	GLU
4	E	84	ASP
4	E	85	GLU
4	E	101	GLN
4	E	106	GLN
4	E	107	THR
4	E	116	ILE
4	E	126	SER
4	E	142	VAL
4	E	167	ARG
4	E	196	VAL
4	E	201	LYS
5	F	72	LYS
5	F	74	ILE
5	F	79	ARG
5	F	87	LYS
5	F	97	ARG
5	F	110	ASP
5	F	111	LEU
5	F	123	LYS
6	H	5	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	H	7	ASP
6	H	10	PHE
6	H	26	ILE
6	H	33	GLN
6	H	34	ASP
6	H	36	CYS
6	H	52	GLN
6	H	53	ASP
6	H	55	LEU
6	H	80	ARG
6	H	83	GLN
6	H	89	LEU
6	H	92	ASP
6	H	100	THR
6	H	104	PHE
6	H	123	MET
6	H	124	ARG
6	H	138	GLU
6	H	139	ASN
6	H	143	LEU
6	H	144	ILE
6	H	146	ARG
7	I	8	ARG
7	I	10	CYS
7	I	13	MET
7	I	18	GLU
7	I	35	VAL
7	I	49	ILE
7	I	70	ARG
7	I	87	GLN
7	I	93	LYS
7	I	94	ASP
7	I	98	VAL
7	I	106	CYS
7	I	111	THR
7	I	119	THR
7	I	120	GLN
8	J	1	MET
8	J	2	ILE
8	J	3	VAL
8	J	6	ARG
8	J	14	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	J	17	LYS
8	J	19	GLU
8	J	20	SER
8	J	24	LEU
8	J	57	ILE
9	K	18	LYS
9	K	25	THR
9	K	31	VAL
9	K	49	GLU
9	K	57	LEU
9	K	102	LYS
9	K	110	ASN
9	K	114	LEU
10	L	26	THR
10	L	27	LEU
10	L	34	CYS
10	L	41	SER
10	L	44	ASP
10	L	46	VAL
10	L	58	LYS
10	L	65	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	92	HIS
1	A	299	HIS
1	A	394	ASN
1	A	397	ASN
1	A	399	HIS
1	A	479	ASN
1	A	515	GLN
1	A	517	ASN
1	A	626	ASN
1	A	659	HIS
1	A	736	ASN
1	A	742	ASN
1	A	757	ASN
1	A	767	GLN
1	A	854	ASN
1	A	994	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1048	ASN
1	A	1070	GLN
1	A	1128	GLN
1	A	1171	GLN
1	A	1173	HIS
1	A	1258	HIS
1	A	1265	ASN
1	A	1364	ASN
1	A	1432	GLN
2	B	115	GLN
2	B	121	ASN
2	B	215	GLN
2	B	236	HIS
2	B	278	GLN
2	B	366	GLN
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	572	HIS
2	B	583	ASN
2	B	648	HIS
2	B	657	HIS
2	B	667	GLN
2	B	706	GLN
2	B	734	HIS
2	B	744	HIS
2	B	862	GLN
2	B	951	GLN
2	B	1025	HIS
2	B	1076	HIS
2	B	1084	GLN
2	B	1141	HIS
2	B	1161	HIS
2	B	1179	ASN
2	B	1180	GLN
3	C	17	ASN
3	C	24	ASN
3	C	65	HIS
3	C	102	GLN
3	C	112	ASN
3	C	131	HIS
3	C	135	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	167	HIS
3	C	195	GLN
3	C	203	GLN
3	C	242	GLN
3	C	252	GLN
3	C	267	GLN
4	E	3	GLN
4	E	5	ASN
4	E	32	GLN
4	E	63	ASN
4	E	113	GLN
4	E	147	HIS
5	F	100	GLN
6	H	33	GLN
6	H	52	GLN
6	H	83	GLN
7	I	12	ASN
7	I	46	HIS
7	I	51	ASN
8	J	53	HIS
9	K	2	ASN
9	K	65	HIS
9	K	76	GLN
9	K	89	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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
11	TRX	M	2	11	15,16,17	4.35	7 (46%)	17,22,24	2.24	5 (29%)
11	CSX	M	6	11	3,6,7	2.84	2 (66%)	1,6,8	0.85	0
11	HYP	M	8	11	7,8,9	0.70	0	5,10,12	1.15	0
11	ILX	M	1	11	8,9,10	0.95	0	8,11,13	1.65	2 (25%)

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
11	TRX	M	2	11	-	3/5/6/8	0/2/2/2
11	CSX	M	6	11	-	0/2/5/7	-
11	HYP	M	8	11	-	0/0/11/13	0/1/1/1
11	ILX	M	1	11	-	4/11/12/14	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	2	TRX	CZ2-CH2	11.87	1.56	1.39
11	M	2	TRX	CZ2-CE2	9.74	1.54	1.39
11	M	6	CSX	O-C	4.28	1.36	1.20
11	M	2	TRX	CB-CG	3.66	1.57	1.50
11	M	2	TRX	CD1-CG	3.03	1.41	1.36
11	M	2	TRX	CE2-NE1	-2.96	1.33	1.37
11	M	2	TRX	CD1-NE1	-2.42	1.33	1.37
11	M	6	CSX	CB-CA	2.34	1.59	1.53
11	M	2	TRX	CD2-CG	-2.15	1.40	1.44

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	2	TRX	CE2-CZ2-CH2	-5.56	109.12	117.87
11	M	2	TRX	CZ2-CE2-NE1	-4.20	125.14	131.62
11	M	2	TRX	CZ2-CE2-CD2	3.55	125.35	122.52
11	M	1	ILX	O-C-CA	-2.91	117.30	124.77
11	M	1	ILX	CG2-CB-CG1	2.68	115.36	111.09
11	M	2	TRX	CE3-CZ3-CH2	2.41	122.43	119.88
11	M	2	TRX	CD2-CE2-NE1	2.38	109.50	107.52

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	M	1	ILX	CG2-CB-CG1-CD1
11	M	1	ILX	OD1-CD1-CG1-OG1
11	M	2	TRX	CA-CB-CG-CD2
11	M	1	ILX	C-CA-CB-CG2
11	M	2	TRX	CA-CB-CG-CD1
11	M	1	ILX	OD1-CD1-CG1-CB
11	M	2	TRX	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	M	2	TRX	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	1349/1733 (77%)	-0.06	36 (2%) 56 46	2, 30, 63, 104	0
2	B	1061/1224 (86%)	-0.15	25 (2%) 59 49	6, 29, 63, 77	0
3	C	265/318 (83%)	-0.10	0 100 100	16, 26, 43, 59	0
4	E	213/215 (99%)	-0.04	4 (1%) 66 57	13, 35, 60, 70	0
5	F	84/155 (54%)	-0.38	0 100 100	10, 23, 41, 49	0
6	H	116/146 (79%)	0.62	4 (3%) 48 39	35, 48, 71, 72	0
7	I	121/122 (99%)	-0.28	1 (0%) 82 75	6, 24, 52, 65	0
8	J	65/70 (92%)	-0.29	0 100 100	17, 26, 45, 46	0
9	K	113/120 (94%)	0.01	1 (0%) 81 74	17, 32, 54, 57	0
10	L	43/70 (61%)	0.44	0 100 100	34, 57, 72, 76	0
11	M	4/8 (50%)	0.36	0 100 100	44, 45, 48, 48	0
All	All	3434/4181 (82%)	-0.08	71 (2%) 63 54	2, 30, 62, 104	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1090	ALA	5.2
1	A	54	ASN	5.0
1	A	69	THR	4.7
1	A	62	ASP	4.7
1	A	1083	THR	4.4
1	A	1087	ALA	4.3
2	B	247	GLY	4.3
1	A	48	ALA	3.8
2	B	1172	ILE	3.8
6	H	89	LEU	3.8
1	A	1088	GLY	3.8
2	B	870	ILE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	3.6
1	A	1084	PHE	3.4
1	A	70	CYS	3.4
2	B	1155	SER	3.4
2	B	266	ALA	3.2
2	B	265	SER	3.1
1	A	158	PRO	3.0
1	A	1081	LEU	3.0
2	B	105	SER	3.0
1	A	53	LEU	3.0
2	B	1190	ILE	2.9
2	B	1173	ALA	2.9
1	A	299	HIS	2.9
1	A	75	ASN	2.9
1	A	1398	MET	2.8
4	E	47	CYS	2.8
2	B	104	GLU	2.8
2	B	1154	ALA	2.8
6	H	90	ALA	2.7
1	A	1080	THR	2.7
1	A	64	ASN	2.7
2	B	477	ALA	2.7
1	A	1089	VAL	2.6
2	B	246	LYS	2.6
1	A	65	LEU	2.6
9	K	110	ASN	2.6
1	A	61	ILE	2.6
1	A	1086	PHE	2.5
1	A	278	THR	2.5
2	B	162	SER	2.5
2	B	1181	PHE	2.5
1	A	68	GLN	2.4
1	A	1178	ASP	2.4
2	B	1099	VAL	2.4
2	B	103	ASN	2.3
1	A	1450	LEU	2.3
1	A	248	PRO	2.3
1	A	626	ASN	2.3
4	E	102	GLU	2.3
2	B	1128	LEU	2.3
2	B	712	PRO	2.3
1	A	74	MET	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	H	29	ALA	2.2
2	B	733	HIS	2.2
2	B	69	LEU	2.2
2	B	958	GLN	2.2
1	A	277	GLU	2.2
1	A	423	ASP	2.2
4	E	129	PRO	2.1
2	B	161	GLU	2.1
2	B	645	SER	2.1
1	A	59	GLY	2.1
7	I	2	THR	2.1
1	A	1097	GLY	2.1
6	H	84	ALA	2.1
4	E	67	GLU	2.1
1	A	1256	GLU	2.0
2	B	1182	GLU	2.0
1	A	159	THR	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
11	ILX	M	1	10/11	0.91	0.10	37,40,44,44	0
11	CSX	M	6	7/8	0.91	0.09	48,50,52,54	0
11	TRX	M	2	15/16	0.93	0.10	44,50,51,51	0
11	HYP	M	8	8/9	0.95	0.08	42,47,48,48	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
12	ZN	L	3005	1/1	0.95	0.05	73,73,73,73	0
12	ZN	A	3008	1/1	0.96	0.06	77,77,77,77	0
12	ZN	C	3002	1/1	0.97	0.04	39,39,39,39	0
12	ZN	I	3004	1/1	0.98	0.03	46,46,46,46	0
12	ZN	A	3006	1/1	0.98	0.02	46,46,46,46	0
12	ZN	B	3007	1/1	0.99	0.03	60,60,60,60	0
12	ZN	J	3001	1/1	0.99	0.02	34,34,34,34	0
12	ZN	I	3003	1/1	0.99	0.02	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.