



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:13 PM UTC

PDB ID : 4A3C / pdb_00004a3c
Title : RNA Polymerase II initial transcribing complex with a 5nt DNA-RNA hybrid
Authors : Cheung, A.C.M.; Sainsbury, S.; Cramer, P.
Deposited on : 2011-09-30
Resolution : 3.50 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

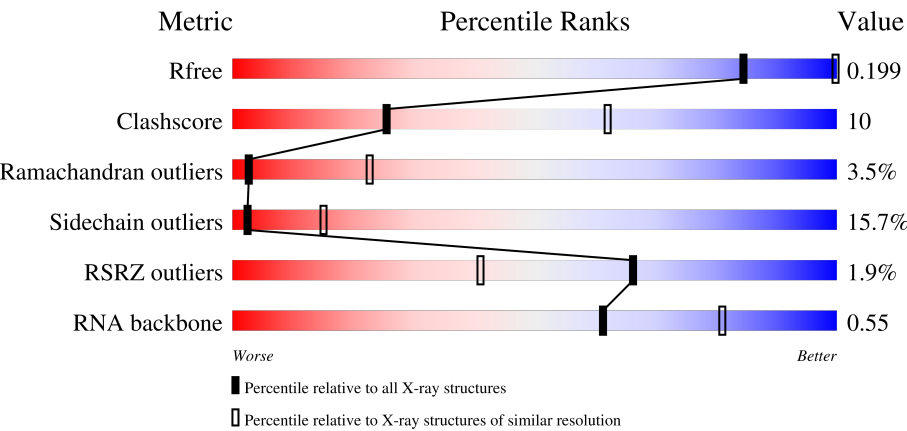
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.



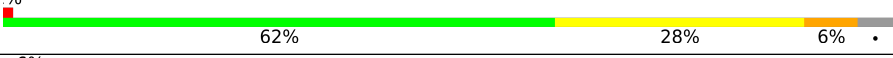
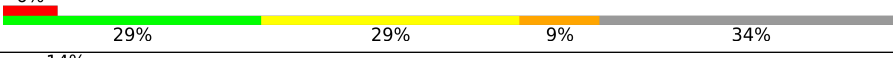
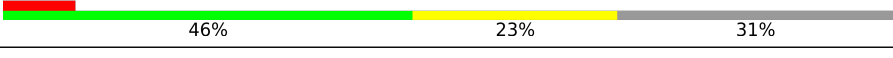
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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	2% 51%23%6%18%
2	B	1224	2% 58%27%5%9%
3	C	318	51%25%7%16%
4	D	221	5% 49%24%7%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	5	
15	T	26	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31858 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	1115	Total	C	N	O	S	0	0	0
			8859	5609	1554	1641	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 NON TEMPLATE DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	10	Total	C	N	O	P	0	0	0
			207	99	39	59	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	4	Total	C	N	O	P	0	0	0
			90	40	20	26	4			

- Molecule 15 is a DNA chain called TEMPLATE DNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
15	T	18	Total	Br	C	N	O	P	0	0	0
			365	1	175	58	113	18			

- 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		

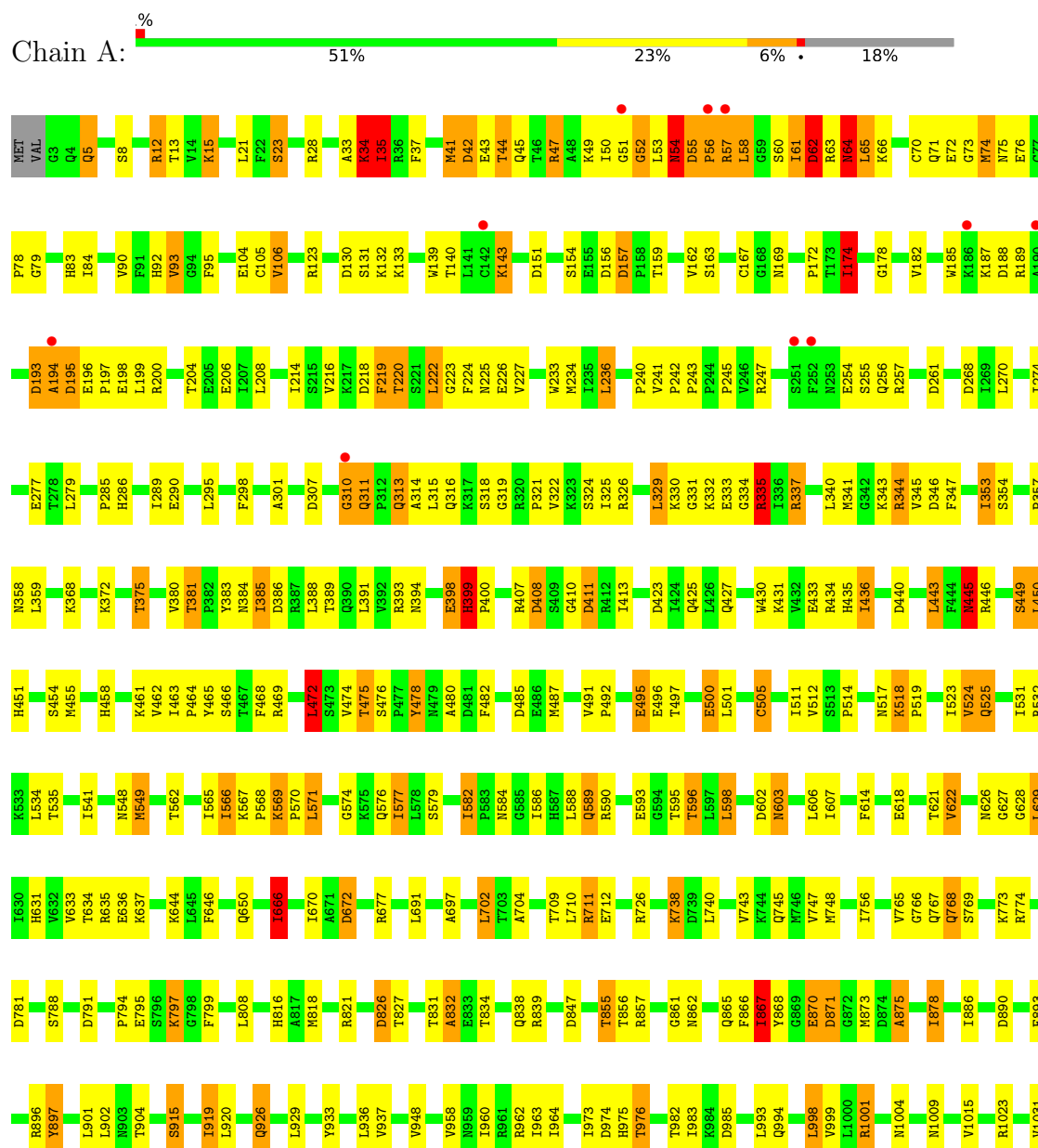
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

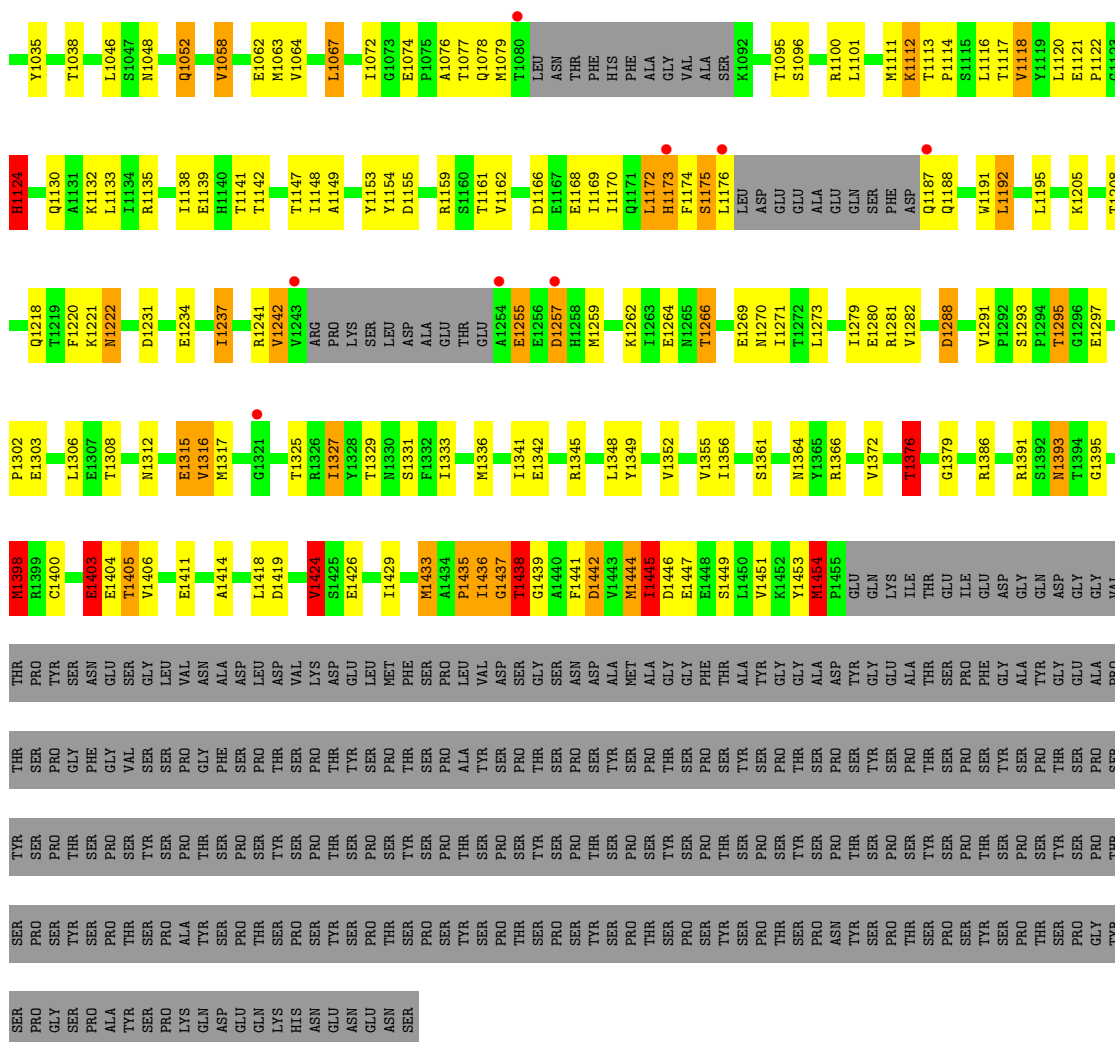
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

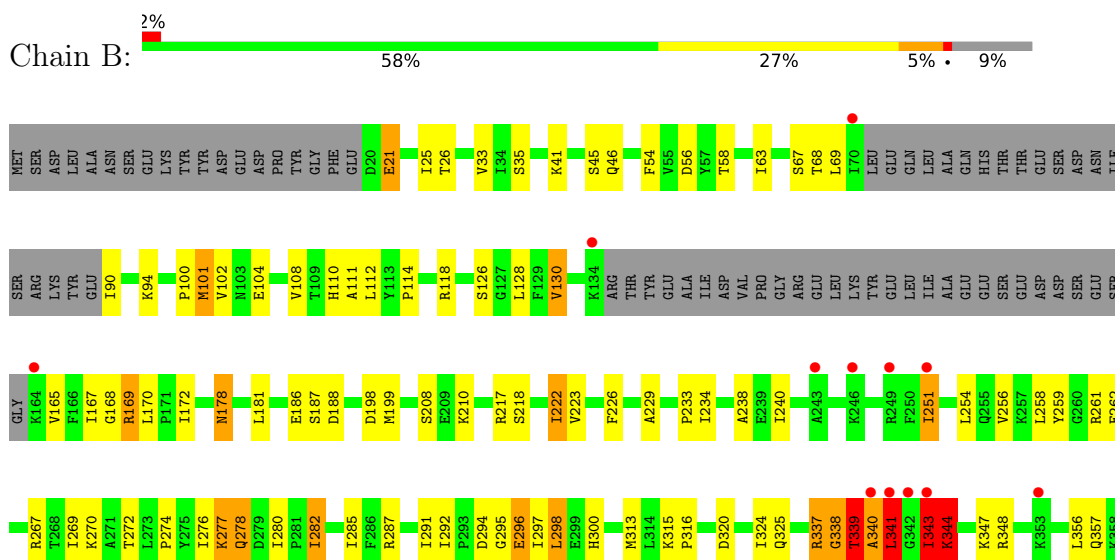
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

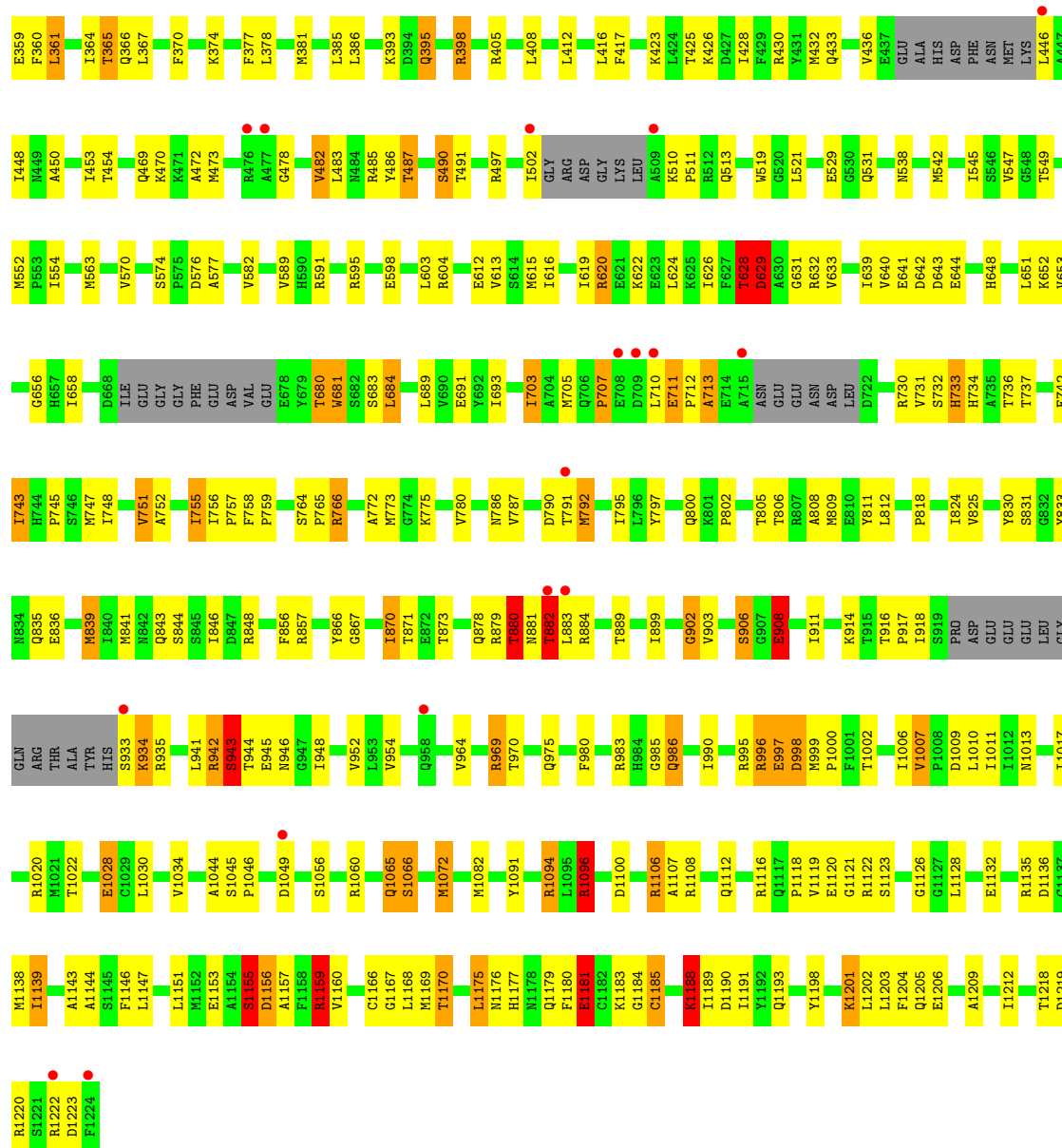
• Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1





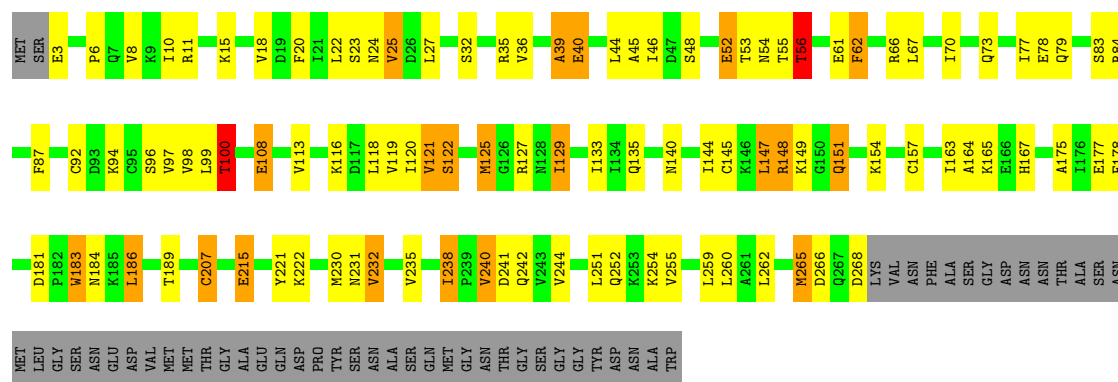
• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2



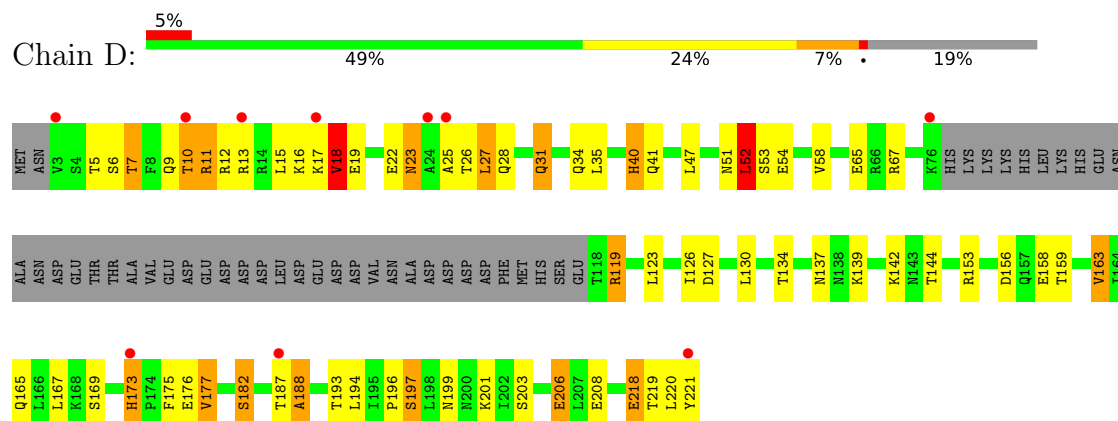


• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

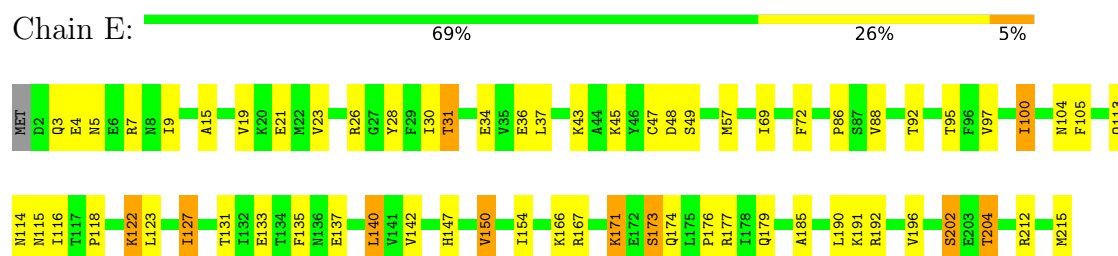
Chain C:



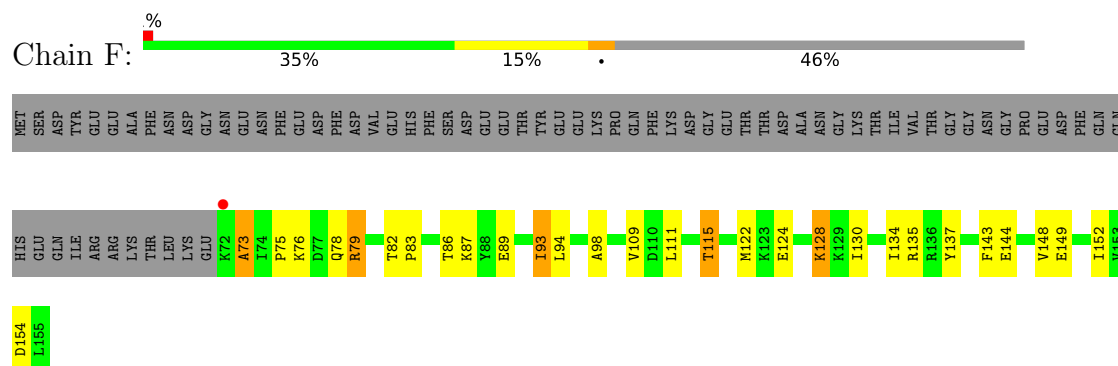
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4



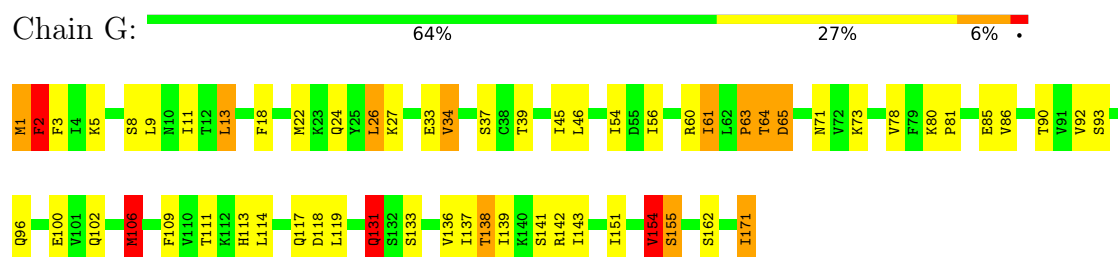
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1



• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

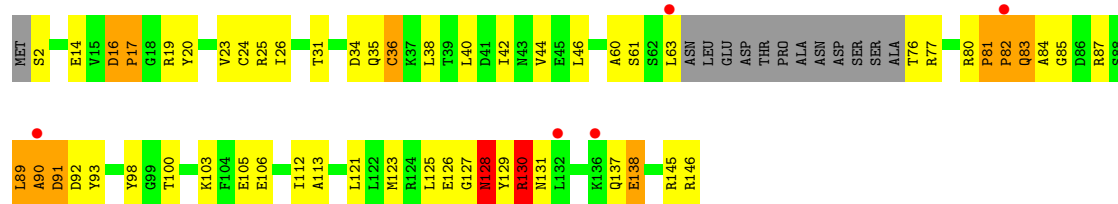


• Molecule 7: RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

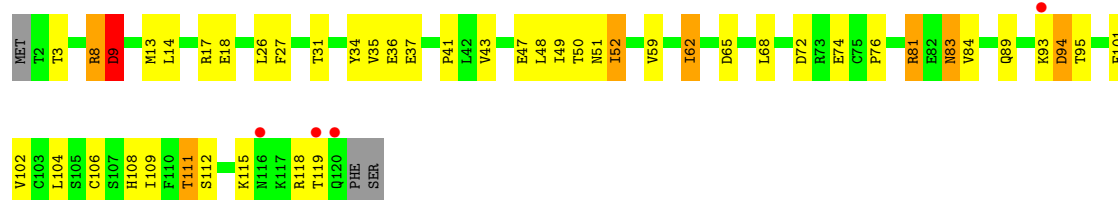


• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3





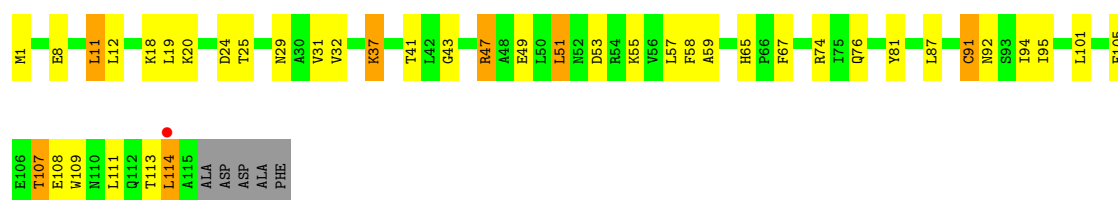
● Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



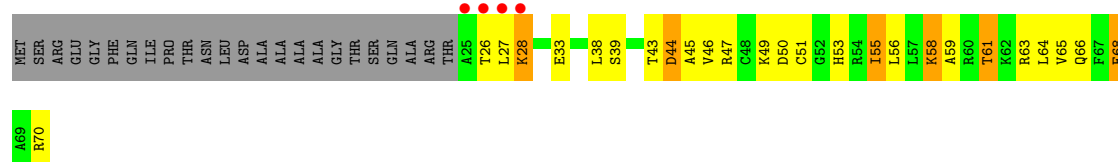
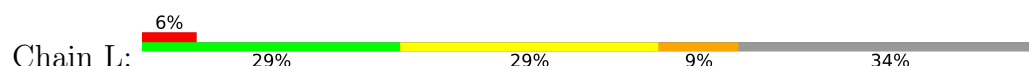
● Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



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

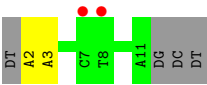


● Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

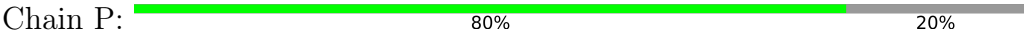


● Molecule 13: NON TEMPLATE DNA





● Molecule 14: TRANSCRIPT RNA, 5'-R(*CP*AP*GP*GP*AP)-3'



● Molecule 15: TEMPLATE DNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	221.41Å 393.12Å 282.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 3.50 49.85 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.85-3.50) 99.9 (49.85-3.50)	Depositor EDS
R_{merge}	0.89	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.158 , 0.184 0.179 , 0.199	Depositor DCC
R_{free} test set	3047 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	97.9	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 103.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.029 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.035 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31858	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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: MG, ZN, BRU

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	0.92	9/11374 (0.1%)	1.56	144/15383 (0.9%)
2	B	0.87	3/9029 (0.0%)	1.48	99/12171 (0.8%)
3	C	0.82	0/2133	1.47	28/2891 (1.0%)
4	D	0.91	2/1444 (0.1%)	1.66	24/1935 (1.2%)
5	E	0.84	0/1788	1.44	12/2406 (0.5%)
6	F	0.99	1/691 (0.1%)	1.45	5/933 (0.5%)
7	G	0.90	1/1368 (0.1%)	1.42	12/1844 (0.7%)
8	H	0.91	0/1086	1.47	19/1470 (1.3%)
9	I	0.80	0/989	1.37	9/1331 (0.7%)
10	J	0.92	1/541 (0.2%)	1.57	4/727 (0.6%)
11	K	0.80	0/938	1.40	7/1267 (0.6%)
12	L	0.90	0/365	1.48	4/485 (0.8%)
13	N	0.50	0/232	0.66	0/356
14	P	0.73	0/101	0.66	0/156
15	T	0.55	0/383	0.64	0/586
All	All	0.88	17/32462 (0.1%)	1.49	367/43941 (0.8%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	25	ALA	CA-C	9.73	1.64	1.53
1	A	867	ILE	CG1-CD1	7.87	1.82	1.51
7	G	1	MET	C-N	7.26	1.43	1.33
1	A	1398	MET	SD-CE	7.12	1.97	1.79
1	A	57	ARG	CA-C	6.34	1.61	1.52
1	A	54	ASN	CA-C	6.27	1.61	1.52
1	A	57	ARG	C-N	5.66	1.41	1.33
10	J	49	MET	SD-CE	-5.47	1.65	1.79
1	A	1454	MET	CA-C	5.44	1.59	1.52
2	B	881	ASN	C-N	5.34	1.40	1.33
1	A	56	PRO	C-N	5.31	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	128	LYS	CA-C	5.27	1.59	1.52
4	D	18	VAL	CA-C	5.25	1.59	1.52
1	A	549	MET	SD-CE	-5.18	1.66	1.79
1	A	52	GLY	C-N	5.15	1.41	1.33
2	B	830	TYR	CA-C	5.14	1.55	1.52
2	B	990	ILE	CA-C	5.11	1.59	1.52

All (367) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	26	THR	N-CA-C	-12.41	95.42	112.30
4	D	31	GLN	N-CA-C	-9.33	101.07	111.14
4	D	25	ALA	CA-C-N	9.32	137.71	122.14
4	D	25	ALA	C-N-CA	9.32	137.71	122.14
8	H	92	ASP	N-CA-C	-8.84	101.47	112.88
3	C	39	ALA	N-CA-C	8.79	124.67	112.45
10	J	5	VAL	N-CA-C	-8.74	98.30	109.58
8	H	129	TYR	N-CA-C	8.64	120.78	111.36
8	H	81	PRO	N-CA-C	8.64	121.24	110.70
1	A	54	ASN	CA-CB-CG	8.45	121.05	112.60
1	A	42	ASP	CA-CB-CG	8.30	120.90	112.60
1	A	56	PRO	CA-C-N	8.29	137.38	121.54
1	A	56	PRO	C-N-CA	8.29	137.38	121.54
2	B	296	GLU	N-CA-C	-8.24	101.00	112.45
1	A	341	MET	CA-C-N	8.21	128.64	121.58
1	A	341	MET	C-N-CA	8.21	128.64	121.58
1	A	34	LYS	CA-C-N	8.10	136.27	121.70
1	A	34	LYS	C-N-CA	8.10	136.27	121.70
2	B	1184	GLY	CA-C-N	7.88	136.59	121.54
2	B	1184	GLY	C-N-CA	7.88	136.59	121.54
1	A	194	ALA	CA-C-N	7.85	135.83	121.70
1	A	194	ALA	C-N-CA	7.85	135.83	121.70
1	A	411	ASP	CA-C-N	7.76	132.74	122.42
1	A	411	ASP	C-N-CA	7.76	132.74	122.42
1	A	64	ASN	N-CA-C	-7.75	100.29	110.53
1	A	1403	GLU	CA-C-N	-7.63	111.18	122.86
1	A	1403	GLU	C-N-CA	-7.63	111.18	122.86
1	A	495	GLU	CA-C-N	7.57	130.74	120.44
1	A	495	GLU	C-N-CA	7.57	130.74	120.44
1	A	886	ILE	N-CA-C	7.33	117.42	110.30
2	B	628	THR	CA-C-N	7.29	135.47	121.54
2	B	628	THR	C-N-CA	7.29	135.47	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	87	LYS	CA-C-N	7.29	130.65	120.29
6	F	87	LYS	C-N-CA	7.29	130.65	120.29
2	B	340	ALA	CA-C-N	7.29	135.46	121.54
2	B	340	ALA	C-N-CA	7.29	135.46	121.54
10	J	9	SER	N-CA-C	7.26	118.88	110.97
2	B	339	THR	CA-C-N	7.23	135.35	121.54
2	B	339	THR	C-N-CA	7.23	135.35	121.54
8	H	128	ASN	CA-C-N	7.18	130.49	120.29
8	H	128	ASN	C-N-CA	7.18	130.49	120.29
2	B	681	TRP	N-CA-C	-7.18	103.39	111.14
1	A	1117	THR	CB-CA-C	7.15	123.25	111.23
1	A	1112	LYS	N-CA-C	7.13	118.84	111.14
7	G	34	VAL	N-CA-C	7.13	117.64	110.23
1	A	1403	GLU	N-CA-C	7.05	125.83	110.80
1	A	35	ILE	N-CA-CB	7.03	123.44	111.50
7	G	2	PHE	CA-CB-CG	6.99	120.79	113.80
2	B	1121	GLY	CA-C-N	6.99	129.95	120.38
2	B	1121	GLY	C-N-CA	6.99	129.95	120.38
1	A	1138	ILE	N-CA-C	6.97	117.54	111.90
1	A	399	HIS	N-CA-CB	6.95	122.74	110.37
2	B	736	THR	N-CA-C	-6.92	103.41	112.41
2	B	703	ILE	N-CA-C	6.85	118.92	108.71
4	D	53	SER	CA-C-N	6.81	129.30	120.44
4	D	53	SER	C-N-CA	6.81	129.30	120.44
2	B	1219	ASP	CA-CB-CG	6.81	119.41	112.60
1	A	311	GLN	N-CA-C	6.79	124.81	109.81
1	A	1445	ILE	N-CA-CB	6.79	118.12	110.72
1	A	445	ASN	CA-CB-CG	6.65	119.25	112.60
1	A	622	VAL	N-CA-CB	-6.61	104.65	112.39
2	B	1181	GLU	N-CA-C	6.61	124.89	110.80
1	A	1266	THR	N-CA-C	-6.61	103.77	110.97
2	B	320	ASP	CA-CB-CG	6.56	119.16	112.60
1	A	897	TYR	N-CA-C	6.55	121.49	112.90
1	A	1419	ASP	CA-C-N	6.54	129.35	120.38
1	A	1419	ASP	C-N-CA	6.54	129.35	120.38
4	D	26	THR	CA-C-N	6.54	131.69	122.08
4	D	26	THR	C-N-CA	6.54	131.69	122.08
1	A	143	LYS	CA-C-N	6.54	129.04	120.28
1	A	143	LYS	C-N-CA	6.54	129.04	120.28
1	A	411	ASP	N-CA-C	6.53	119.84	110.24
2	B	916	THR	CB-CA-C	6.50	118.20	109.42
4	D	188	ALA	N-CA-C	-6.49	104.25	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	48	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	334	GLY	CA-C-N	6.42	133.79	121.54
1	A	334	GLY	C-N-CA	6.42	133.79	121.54
1	A	219	PHE	CA-CB-CG	6.39	120.19	113.80
1	A	47	ARG	CA-C-N	6.37	133.72	121.54
1	A	47	ARG	C-N-CA	6.37	133.72	121.54
2	B	338	GLY	CA-C-N	6.36	133.15	121.70
2	B	338	GLY	C-N-CA	6.36	133.15	121.70
1	A	672	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	826	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	223	GLY	CA-C-N	6.26	133.50	121.54
1	A	223	GLY	C-N-CA	6.26	133.50	121.54
2	B	1136	ASP	CA-CB-CG	6.25	118.85	112.60
1	A	998	LEU	N-CA-C	6.25	119.33	109.96
12	L	44	ASP	CA-C-N	6.25	133.48	121.54
12	L	44	ASP	C-N-CA	6.25	133.48	121.54
1	A	1395	GLY	N-CA-C	6.25	118.67	111.36
2	B	1188	LYS	CA-C-N	6.24	133.21	121.97
2	B	1188	LYS	C-N-CA	6.24	133.21	121.97
2	B	1009	ASP	N-CA-C	-6.22	104.75	112.90
4	D	173	HIS	CB-CA-C	6.21	118.39	109.26
2	B	1122	ARG	CA-C-N	6.21	128.51	120.44
2	B	1122	ARG	C-N-CA	6.21	128.51	120.44
7	G	65	ASP	CA-CB-CG	6.21	118.81	112.60
2	B	902	GLY	CA-C-N	6.17	128.84	120.63
2	B	902	GLY	C-N-CA	6.17	128.84	120.63
2	B	732	SER	N-CA-C	6.16	116.70	108.38
1	A	346	ASP	CA-CB-CG	6.15	118.75	112.60
1	A	472	LEU	N-CA-C	6.14	118.77	111.71
3	C	135	GLN	CA-C-N	6.10	130.39	121.31
3	C	135	GLN	C-N-CA	6.10	130.39	121.31
2	B	472	ALA	CA-C-N	6.09	133.18	121.54
2	B	472	ALA	C-N-CA	6.09	133.18	121.54
3	C	135	GLN	N-CA-C	-6.09	106.45	114.31
4	D	23	ASN	CA-CB-CG	6.09	118.69	112.60
2	B	1177	HIS	N-CA-C	-6.09	105.61	113.16
4	D	169	SER	N-CA-C	-6.08	106.47	114.31
2	B	1156	ASP	N-CA-C	6.06	123.70	110.80
5	E	171	LYS	N-CA-C	-6.06	100.42	110.17
2	B	529	GLU	N-CA-C	-6.05	99.84	109.76
2	B	294	ASP	CA-CB-CG	6.04	118.64	112.60
9	I	9	ASP	CA-CB-CG	6.04	118.64	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	642	ASP	N-CA-C	-6.03	104.78	111.71
2	B	825	VAL	N-CA-C	6.02	116.60	108.17
11	K	53	ASP	CA-CB-CG	6.02	118.62	112.60
2	B	903	VAL	N-CA-C	6.02	117.50	109.37
2	B	198	ASP	CA-C-N	6.01	130.75	120.72
2	B	198	ASP	C-N-CA	6.01	130.75	120.72
2	B	45	SER	CA-C-N	6.00	129.13	120.79
2	B	45	SER	C-N-CA	6.00	129.13	120.79
1	A	157	ASP	N-CA-C	5.98	118.56	110.31
1	A	496	GLU	CA-C-N	5.97	128.20	120.44
1	A	496	GLU	C-N-CA	5.97	128.20	120.44
1	A	5	GLN	N-CA-C	5.95	119.33	110.52
2	B	591	ARG	N-CA-C	5.93	117.74	111.28
1	A	794	PRO	CA-C-N	5.92	128.21	120.28
1	A	794	PRO	C-N-CA	5.92	128.21	120.28
4	D	51	ASN	CA-CB-CG	5.91	118.51	112.60
8	H	16	ASP	N-CA-C	5.90	121.48	108.73
2	B	1017	ILE	N-CA-C	5.90	121.62	108.88
2	B	629	ASP	CA-CB-CG	5.89	118.49	112.60
3	C	183	TRP	N-CA-C	-5.89	99.68	109.46
8	H	36	CYS	N-CA-C	5.88	118.25	109.25
1	A	325	ILE	N-CA-C	-5.88	104.78	110.72
7	G	141	SER	N-CA-C	5.88	118.53	110.24
10	J	64	ASN	N-CA-C	5.87	122.78	109.81
8	H	85	GLY	N-CA-C	-5.87	105.70	112.50
1	A	193	ASP	CA-C-N	5.86	132.24	121.70
1	A	193	ASP	C-N-CA	5.86	132.24	121.70
2	B	222	ILE	N-CA-C	5.85	116.30	108.11
2	B	908	GLU	N-CA-C	-5.83	104.32	112.25
1	A	478	TYR	CA-C-N	5.82	132.65	121.54
1	A	478	TYR	C-N-CA	5.82	132.65	121.54
3	C	108	GLU	N-CA-C	-5.81	105.03	111.36
1	A	23	SER	N-CA-C	-5.81	102.73	109.93
8	H	83	GLN	CA-C-N	5.80	131.78	120.99
8	H	83	GLN	C-N-CA	5.80	131.78	120.99
1	A	268	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	54	ASN	CA-C-N	5.79	135.93	121.80
1	A	54	ASN	C-N-CA	5.79	135.93	121.80
1	A	1436	ILE	N-CA-CB	-5.79	103.42	111.41
2	B	188	ASP	CA-CB-CG	5.79	118.39	112.60
7	G	33	GLU	CA-C-N	5.78	128.34	120.77
7	G	33	GLU	C-N-CA	5.78	128.34	120.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1404	GLU	N-CA-C	5.78	119.89	112.26
4	D	220	LEU	CA-C-N	5.77	132.09	121.70
4	D	220	LEU	C-N-CA	5.77	132.09	121.70
8	H	128	ASN	CA-CB-CG	5.76	118.36	112.60
9	I	52	ILE	N-CA-CB	5.74	118.59	111.41
1	A	791	ASP	CA-CB-CG	5.73	118.33	112.60
1	A	222	LEU	N-CA-C	-5.72	103.14	110.53
1	A	666	ILE	N-CA-CB	5.72	119.52	110.54
1	A	485	ASP	CA-CB-CG	5.71	118.31	112.60
9	I	93	LYS	CA-C-N	5.70	128.23	120.54
9	I	93	LYS	C-N-CA	5.70	128.23	120.54
1	A	285	PRO	CA-C-N	5.68	132.40	121.54
1	A	285	PRO	C-N-CA	5.68	132.40	121.54
3	C	24	ASN	CA-CB-CG	5.68	118.28	112.60
8	H	20	TYR	CA-C-N	5.68	127.89	120.28
8	H	20	TYR	C-N-CA	5.68	127.89	120.28
1	A	677	ARG	CA-C-N	5.67	127.88	120.28
1	A	677	ARG	C-N-CA	5.67	127.88	120.28
4	D	158	GLU	CA-C-N	5.67	127.88	120.28
4	D	158	GLU	C-N-CA	5.67	127.88	120.28
11	K	113	THR	CA-C-N	5.67	131.90	121.70
11	K	113	THR	C-N-CA	5.67	131.90	121.70
1	A	462	VAL	N-CA-CB	5.65	116.69	110.53
1	A	398	GLU	CA-C-O	-5.64	115.15	121.81
9	I	13	MET	N-CA-C	5.64	117.82	110.43
3	C	62	PHE	CA-C-N	5.63	127.66	120.56
3	C	62	PHE	C-N-CA	5.63	127.66	120.56
2	B	343	ILE	CA-C-N	5.63	132.30	121.54
2	B	343	ILE	C-N-CA	5.63	132.30	121.54
6	F	154	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	218	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	60	SER	N-CA-C	5.57	118.31	109.50
2	B	1013	ASN	N-CA-C	5.57	116.83	109.93
1	A	505	CYS	N-CA-C	5.56	119.38	112.59
1	A	1132	LYS	CA-C-N	5.55	127.72	120.28
1	A	1132	LYS	C-N-CA	5.55	127.72	120.28
1	A	523	ILE	CB-CA-C	5.54	118.35	111.15
2	B	478	GLY	CA-C-N	5.54	127.53	120.56
2	B	478	GLY	C-N-CA	5.54	127.53	120.56
1	A	174	ILE	N-CA-C	5.53	116.55	108.58
9	I	119	THR	CB-CA-C	5.53	116.63	109.28
1	A	1376	THR	N-CA-C	5.53	118.14	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	818	PRO	N-CA-C	5.51	118.93	111.22
3	C	40	GLU	N-CA-C	5.50	120.67	113.30
3	C	266	ASP	CA-C-N	5.50	127.91	120.38
3	C	266	ASP	C-N-CA	5.50	127.91	120.38
2	B	1153	GLU	CB-CG-CD	5.48	121.91	112.60
2	B	1155	SER	CA-C-N	5.47	132.00	121.54
2	B	1155	SER	C-N-CA	5.47	132.00	121.54
7	G	117	GLN	CA-C-N	5.46	127.59	120.28
7	G	117	GLN	C-N-CA	5.46	127.59	120.28
1	A	1315	GLU	N-CA-C	5.45	118.05	111.40
4	D	163	VAL	CA-C-N	5.44	127.92	120.46
4	D	163	VAL	C-N-CA	5.44	127.92	120.46
1	A	963	ILE	N-CA-CB	5.44	116.91	110.55
5	E	95	THR	CA-C-N	5.44	127.51	120.44
5	E	95	THR	C-N-CA	5.44	127.51	120.44
3	C	265	MET	CA-C-N	5.43	127.56	120.28
3	C	265	MET	C-N-CA	5.43	127.56	120.28
1	A	399	HIS	CA-CB-CG	-5.42	108.38	113.80
1	A	890	ASP	CA-C-N	5.41	127.80	120.44
1	A	890	ASP	C-N-CA	5.41	127.80	120.44
7	G	131	GLN	N-CA-C	5.41	117.72	108.90
2	B	906	SER	N-CA-C	5.40	122.31	110.80
9	I	94	ASP	CA-C-N	5.39	131.84	121.54
9	I	94	ASP	C-N-CA	5.39	131.84	121.54
1	A	70	CYS	N-CA-C	-5.39	101.51	109.86
1	A	319	GLY	CA-C-N	5.38	128.52	120.83
1	A	319	GLY	C-N-CA	5.38	128.52	120.83
3	C	222	LYS	CA-C-N	5.36	128.72	121.05
3	C	222	LYS	C-N-CA	5.36	128.72	121.05
10	J	16	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	310	GLY	CA-C-N	5.36	134.87	121.80
1	A	310	GLY	C-N-CA	5.36	134.87	121.80
1	A	44	THR	N-CA-C	-5.35	104.65	110.91
1	A	1269	GLU	N-CA-C	5.35	118.27	111.69
1	A	331	GLY	CA-C-N	5.34	131.75	121.54
1	A	331	GLY	C-N-CA	5.34	131.75	121.54
2	B	208	SER	N-CA-C	5.34	118.64	110.20
4	D	18	VAL	CA-C-N	5.34	131.32	121.70
4	D	18	VAL	C-N-CA	5.34	131.32	121.70
1	A	1001	ARG	N-CA-C	5.34	119.93	113.41
2	B	433	GLN	CA-C-N	5.33	127.42	120.28
2	B	433	GLN	C-N-CA	5.33	127.42	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	466	SER	N-CA-C	5.33	120.72	113.37
2	B	943	SER	CA-C-N	5.32	127.36	120.44
2	B	943	SER	C-N-CA	5.32	127.36	120.44
1	A	626	ASN	N-CA-C	5.32	117.50	111.11
1	A	1257	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	511	ILE	N-CA-C	5.32	115.76	110.23
1	A	875	ALA	CA-C-N	5.31	127.40	120.28
1	A	875	ALA	C-N-CA	5.31	127.40	120.28
1	A	33	ALA	CA-C-N	5.30	130.12	122.44
1	A	33	ALA	C-N-CA	5.30	130.12	122.44
2	B	733	HIS	CA-C-N	5.30	127.69	120.54
2	B	733	HIS	C-N-CA	5.30	127.69	120.54
3	C	56	THR	N-CA-C	5.30	117.36	110.53
1	A	1424	VAL	CA-C-N	5.29	127.62	120.38
1	A	1424	VAL	C-N-CA	5.29	127.62	120.38
5	E	5	ASN	CA-C-N	5.29	128.10	120.38
5	E	5	ASN	C-N-CA	5.29	128.10	120.38
1	A	1072	ILE	N-CA-C	-5.28	107.62	111.90
2	B	1156	ASP	CA-C-N	5.28	131.62	121.54
2	B	1156	ASP	C-N-CA	5.28	131.62	121.54
1	A	408	ASP	N-CA-C	-5.28	105.53	111.28
1	A	1447	GLU	CB-CG-CD	5.27	121.56	112.60
8	H	130	ARG	CA-C-N	5.27	127.61	120.44
8	H	130	ARG	C-N-CA	5.27	127.61	120.44
1	A	78	PRO	N-CA-C	-5.27	103.84	111.22
3	C	178	PHE	CA-CB-CG	5.26	119.06	113.80
2	B	1159	ARG	N-CA-C	5.25	117.29	107.99
2	B	1180	PHE	CA-CB-CG	-5.25	108.55	113.80
2	B	791	THR	N-CA-C	-5.25	101.59	109.15
2	B	707	PRO	CA-C-N	5.24	128.69	120.82
2	B	707	PRO	C-N-CA	5.24	128.69	120.82
4	D	196	PRO	CA-C-N	5.24	127.31	120.28
4	D	196	PRO	C-N-CA	5.24	127.31	120.28
2	B	366	GLN	N-CA-C	-5.24	105.75	113.61
8	H	137	GLN	CA-C-N	5.23	127.81	120.28
8	H	137	GLN	C-N-CA	5.23	127.81	120.28
2	B	68	THR	CB-CA-C	5.22	116.22	109.80
2	B	1139	ILE	CA-C-N	5.22	127.28	120.28
2	B	1139	ILE	C-N-CA	5.22	127.28	120.28
7	G	64	THR	N-CA-C	5.22	117.88	111.82
7	G	18	PHE	CA-CB-CG	5.22	119.02	113.80
1	A	1231	ASP	CA-C-N	5.21	127.53	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1231	ASP	C-N-CA	5.21	127.53	120.44
1	A	174	ILE	N-CA-CB	5.21	116.40	110.72
1	A	535	THR	N-CA-C	5.21	118.66	112.72
5	E	21	GLU	CA-C-N	5.21	127.21	120.44
5	E	21	GLU	C-N-CA	5.21	127.21	120.44
1	A	1295	THR	CB-CA-C	5.20	120.76	110.42
2	B	417	PHE	CA-C-N	5.20	127.19	120.44
2	B	417	PHE	C-N-CA	5.20	127.19	120.44
1	A	1237	ILE	N-CA-C	5.19	116.20	108.46
1	A	818	MET	CA-C-N	5.19	125.74	119.98
1	A	818	MET	C-N-CA	5.19	125.74	119.98
9	I	115	LYS	N-CA-C	-5.19	107.01	113.55
1	A	627	GLY	CA-C-N	5.18	131.57	121.41
1	A	627	GLY	C-N-CA	5.18	131.57	121.41
1	A	602	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	871	ASP	CA-CB-CG	5.18	117.78	112.60
8	H	131	ASN	CA-CB-CG	5.17	117.77	112.60
1	A	234	MET	N-CA-C	-5.17	106.92	113.18
1	A	1435	PRO	CA-C-N	5.17	129.91	123.14
1	A	1435	PRO	C-N-CA	5.17	129.91	123.14
2	B	880	THR	CA-C-N	5.17	131.41	121.54
2	B	880	THR	C-N-CA	5.17	131.41	121.54
2	B	648	HIS	CA-C-N	5.16	129.28	122.42
2	B	648	HIS	C-N-CA	5.16	129.28	122.42
2	B	752	ALA	N-CA-C	5.16	116.98	111.36
2	B	628	THR	N-CA-C	-5.16	106.15	112.90
12	L	49	LYS	CA-C-N	5.16	131.39	121.54
12	L	49	LYS	C-N-CA	5.16	131.39	121.54
3	C	100	THR	CB-CA-C	5.15	119.21	109.37
2	B	998	ASP	N-CA-C	-5.15	107.13	113.41
3	C	262	LEU	CA-C-N	5.15	127.18	120.28
3	C	262	LEU	C-N-CA	5.15	127.18	120.28
3	C	45	ALA	CA-C-N	5.15	127.48	120.63
3	C	45	ALA	C-N-CA	5.15	127.48	120.63
11	K	43	GLY	CA-C-N	5.15	127.69	120.28
11	K	43	GLY	C-N-CA	5.15	127.69	120.28
1	A	123	ARG	CA-C-N	5.14	127.43	120.44
1	A	123	ARG	C-N-CA	5.14	127.43	120.44
2	B	693	ILE	N-CA-C	5.14	114.98	107.37
2	B	1011	ILE	N-CA-CB	5.14	118.68	112.10
4	D	10	THR	N-CA-C	5.14	119.39	113.18
2	B	378	LEU	CA-C-N	5.12	125.67	119.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	378	LEU	C-N-CA	5.12	125.67	119.98
1	A	867	ILE	CB-CA-C	5.12	118.37	110.28
3	C	96	SER	N-CA-C	5.12	116.85	109.07
2	B	41	LYS	N-CA-C	5.12	118.67	112.23
11	K	24	ASP	CA-C-N	5.11	127.38	120.44
11	K	24	ASP	C-N-CA	5.11	127.38	120.44
7	G	106	MET	N-CA-C	5.10	118.05	110.14
2	B	1065	GLN	CB-CA-C	5.10	117.91	110.26
8	H	131	ASN	N-CA-C	-5.10	105.64	111.14
3	C	207	CYS	CA-C-N	5.09	127.06	120.44
3	C	207	CYS	C-N-CA	5.09	127.06	120.44
6	F	83	PRO	CA-C-N	5.09	130.77	122.07
6	F	83	PRO	C-N-CA	5.09	130.77	122.07
1	A	614	PHE	CA-CB-CG	5.08	118.88	113.80
1	A	55	ASP	N-CA-CB	5.07	119.39	110.37
5	E	123	LEU	CA-C-N	5.07	124.38	120.33
5	E	123	LEU	C-N-CA	5.07	124.38	120.33
1	A	893	PHE	N-CA-C	-5.07	105.45	110.97
1	A	781	ASP	CA-CB-CG	5.06	117.66	112.60
2	B	713	ALA	N-CA-C	5.06	117.21	110.53
2	B	199	MET	N-CA-C	5.06	118.71	112.54
3	C	120	ILE	N-CA-CB	5.06	116.76	111.00
1	A	240	PRO	CA-C-N	5.05	126.03	122.60
1	A	240	PRO	C-N-CA	5.05	126.03	122.60
1	A	832	ALA	CA-C-N	5.05	127.00	120.44
1	A	832	ALA	C-N-CA	5.05	127.00	120.44
2	B	684	LEU	CA-C-N	5.03	127.03	120.28
2	B	684	LEU	C-N-CA	5.03	127.03	120.28
3	C	87	PHE	N-CA-C	5.03	119.51	113.17
2	B	882	THR	N-CA-C	5.03	116.45	111.07
1	A	797	LYS	N-CA-C	5.03	118.56	112.93
2	B	996	ARG	N-CA-C	5.03	118.18	111.75
5	E	173	SER	CA-C-N	5.02	130.33	120.99
5	E	173	SER	C-N-CA	5.02	130.33	120.99
1	A	644	LYS	CA-C-N	5.01	127.25	120.38
1	A	644	LYS	C-N-CA	5.01	127.25	120.38
2	B	186	GLU	CA-C-N	5.01	127.00	120.28
2	B	186	GLU	C-N-CA	5.01	127.00	120.28
1	A	329	LEU	CA-C-N	5.01	128.21	121.05
1	A	329	LEU	C-N-CA	5.01	128.21	121.05
1	A	1424	VAL	N-CA-C	-5.00	105.62	110.42

There are no chirality outliers.

There are no planarity outliers.

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	260	0
2	B	8859	0	8901	168	0
3	C	2095	0	2051	64	0
4	D	1434	0	1460	24	0
5	E	1752	0	1776	29	0
6	F	679	0	701	17	0
7	G	1340	0	1357	31	0
8	H	1068	0	1040	26	0
9	I	971	0	927	24	0
10	J	532	0	542	19	0
11	K	920	0	929	29	0
12	L	363	0	386	6	0
13	N	207	0	114	3	0
14	P	90	0	44	0	0
15	T	365	0	204	5	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	31858	0	31665	611	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 10.

All (611) 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:867:ILE:CG1	1:A:867:ILE:CD1	1.82	1.56
1:A:53:LEU:HD23	1:A:54:ASN:H	1.10	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:THR:HG21	1:A:857:ARG:HE	1.18	1.06
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.51	0.91
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.52	0.91
7:G:1:MET:HE1	7:G:80:LYS:O	1.70	0.90
4:D:40:HIS:HB3	7:G:73:LYS:HE3	1.52	0.90
5:E:31:THR:HG23	5:E:34:GLU:HB2	1.55	0.88
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.56	0.86
3:C:98:VAL:H	3:C:122:SER:HB3	1.40	0.84
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.59	0.83
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.60	0.83
3:C:147:LEU:HB3	3:C:151:GLN:HB2	1.61	0.81
3:C:66:ARG:NH2	10:J:3:VAL:O	2.14	0.80
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.44	0.80
1:A:53:LEU:HD23	1:A:54:ASN:N	1.94	0.80
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.62	0.80
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.64	0.80
1:A:433:GLU:OE1	2:B:1108:ARG:NH2	2.15	0.79
3:C:148:ARG:H	3:C:151:GLN:HG3	1.48	0.78
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.66	0.78
3:C:46:ILE:HD12	3:C:46:ILE:H	1.49	0.77
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.67	0.76
3:C:163:ILE:HD12	3:C:165:LYS:HB2	1.65	0.76
4:D:203:SER:HB3	4:D:206:GLU:HB2	1.68	0.76
2:B:839:MET:HE1	2:B:980:PHE:HB2	1.68	0.75
1:A:1329:THR:HG22	1:A:1331:SER:H	1.51	0.75
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.27	0.75
7:G:1:MET:SD	7:G:2:PHE:N	2.58	0.75
2:B:313:MET:HE2	2:B:386:LEU:HD22	1.69	0.74
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.71	0.73
8:H:82:PRO:C	8:H:84:ALA:H	1.97	0.72
1:A:53:LEU:CD2	1:A:54:ASN:H	1.98	0.72
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	1.89	0.72
3:C:32:SER:O	3:C:36:VAL:HG23	1.88	0.72
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.70	0.72
10:J:48:ARG:O	10:J:52:THR:HG23	1.89	0.72
2:B:296:GLU:O	2:B:300:HIS:HD2	1.73	0.71
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.72	0.71
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.71	0.71
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.73	0.71
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.23	0.71
2:B:705:MET:H	2:B:710:LEU:HD12	1.55	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:620:ARG:HE	9:I:89:GLN:HE22	1.39	0.70
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.57	0.70
4:D:40:HIS:HB3	7:G:73:LYS:CE	2.20	0.70
1:A:37:PHE:HD2	1:A:52:GLY:HA3	1.58	0.68
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.28	0.68
1:A:1433:MET:HE3	7:G:63:PRO:HB3	1.74	0.68
1:A:492:PRO:HB3	1:A:497:THR:HG22	1.73	0.68
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.76	0.68
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.74	0.67
1:A:383:TYR:HB3	6:F:115:THR:HG22	1.76	0.67
1:A:254:GLU:HB3	2:B:935:ARG:HH21	1.59	0.67
1:A:64:ASN:O	1:A:65:LEU:HB3	1.94	0.66
3:C:100:THR:HG22	3:C:119:VAL:HG12	1.77	0.66
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.61	0.66
2:B:918:ILE:HD13	2:B:935:ARG:HH12	1.60	0.66
4:D:18:VAL:HG22	4:D:19:GLU:HA	1.76	0.66
4:D:167:LEU:HB3	4:D:177:VAL:HG22	1.78	0.66
12:L:28:LYS:HB2	12:L:39:SER:HA	1.78	0.65
1:A:855:THR:CG2	1:A:857:ARG:HE	2.04	0.65
7:G:131:GLN:HG3	7:G:136:VAL:HG22	1.78	0.65
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.78	0.64
12:L:61:THR:HG21	12:L:63:ARG:HE	1.61	0.64
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.78	0.64
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.79	0.64
2:B:839:MET:CE	2:B:980:PHE:HB2	2.27	0.64
11:K:87:LEU:O	11:K:91:CYS:HB2	1.98	0.64
7:G:34:VAL:O	7:G:37:SER:HB3	1.98	0.64
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.63	0.63
1:A:1348:LEU:O	1:A:1352:VAL:HG23	1.97	0.63
1:A:37:PHE:CD2	1:A:52:GLY:HA3	2.34	0.63
1:A:915:SER:HB2	1:A:919:ILE:HD13	1.81	0.63
4:D:176:GLU:OE2	4:D:197:SER:HB2	1.99	0.63
1:A:1162:VAL:HG11	9:I:41:PRO:HG3	1.81	0.63
1:A:315:LEU:HA	1:A:321:PRO:HA	1.81	0.63
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.63	0.62
1:A:63:ARG:HA	1:A:74:MET:HG3	1.82	0.62
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.82	0.62
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.82	0.62
2:B:806:THR:HG22	2:B:808:ALA:H	1.65	0.62
10:J:1:MET:HG3	10:J:60:PHE:CE2	2.31	0.61
2:B:100:PRO:HG3	2:B:172:ILE:HD12	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:38:LEU:HD11	8:H:123:MET:HE2	1.83	0.61
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.83	0.61
13:N:2:DA:H61	15:T:16:DT:H3	1.48	0.60
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.83	0.60
2:B:996:ARG:HG2	2:B:1007:VAL:HG11	1.83	0.60
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.35	0.59
1:A:1393:ASN:H	1:A:1393:ASN:HD22	1.50	0.59
2:B:882:THR:C	2:B:884:ARG:H	2.10	0.59
3:C:46:ILE:HD13	3:C:67:LEU:O	2.01	0.59
5:E:185:ALA:HA	5:E:190:LEU:HD12	1.84	0.59
6:F:76:LYS:HA	6:F:79:ARG:CD	2.30	0.59
1:A:1266:THR:HG23	1:A:1270:ASN:HD22	1.68	0.59
1:A:866:PHE:O	1:A:867:ILE:HD12	2.03	0.59
1:A:1141:THR:HG23	1:A:1205:LYS:HD3	1.83	0.59
1:A:140:THR:HA	1:A:143:LYS:HE2	1.84	0.59
7:G:138:THR:HG22	7:G:139:ILE:H	1.67	0.59
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.85	0.58
3:C:20:PHE:HE2	3:C:22:LEU:HD13	1.67	0.58
1:A:629:LEU:O	1:A:633:VAL:HG23	2.02	0.58
1:A:586:ILE:HD11	1:A:637:LYS:HG2	1.85	0.58
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.84	0.58
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.86	0.58
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.85	0.58
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.84	0.58
1:A:982:THR:HB	1:A:985:ASP:H	1.69	0.58
2:B:1169:MET:HE1	2:B:1204:PHE:HB2	1.86	0.58
10:J:48:ARG:HH21	10:J:49:MET:HE1	1.68	0.58
2:B:755:ILE:HG23	2:B:809:MET:HE2	1.86	0.58
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.36	0.57
1:A:855:THR:HG21	1:A:857:ARG:NE	2.03	0.57
2:B:713:ALA:HA	2:B:733:HIS:NE2	2.19	0.57
9:I:72:ASP:O	9:I:81:ARG:HG2	2.03	0.57
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.86	0.57
1:A:1095:THR:HG23	1:A:1113:THR:HG23	1.86	0.57
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.87	0.57
1:A:1442:ASP:HB2	6:F:137:TYR:HE1	1.70	0.57
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.85	0.57
1:A:1418:LEU:HD23	2:B:1222:ARG:HD3	1.87	0.57
1:A:475:THR:HG21	2:B:836:GLU:OE2	2.05	0.57
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.87	0.57
1:A:492:PRO:CB	1:A:497:THR:HG22	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.86	0.57
2:B:758:PHE:CE1	2:B:1044:ALA:HA	2.40	0.57
3:C:40:GLU:OE2	3:C:254:LYS:HE3	2.05	0.57
1:A:219:PHE:HA	1:A:222:LEU:HD12	1.87	0.56
3:C:148:ARG:N	3:C:151:GLN:HG3	2.19	0.56
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.86	0.56
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.88	0.56
2:B:344:LYS:HB3	2:B:347:LYS:HB2	1.86	0.56
4:D:7:THR:HG21	7:G:5:LYS:HZ1	1.70	0.56
2:B:210:LYS:HD3	2:B:482:VAL:HG23	1.87	0.56
3:C:100:THR:HG22	3:C:119:VAL:CG1	2.36	0.56
1:A:1154:TYR:CE1	9:I:18:GLU:HG3	2.40	0.56
11:K:107:THR:O	11:K:111:LEU:HG	2.05	0.56
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.06	0.56
2:B:882:THR:HG21	2:B:935:ARG:HA	1.87	0.56
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.88	0.55
1:A:464:PRO:HD2	11:K:67:PHE:HD2	1.71	0.55
1:A:35:ILE:HG13	1:A:56:PRO:HG2	1.88	0.55
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.88	0.55
3:C:125:MET:HE3	3:C:125:MET:HA	1.88	0.55
2:B:486:TYR:HB3	2:B:1096:ARG:NH2	2.21	0.55
12:L:61:THR:HG21	12:L:63:ARG:NE	2.21	0.55
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.06	0.55
2:B:168:GLY:H	2:B:450:ALA:HB1	1.71	0.55
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.89	0.55
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.89	0.55
1:A:35:ILE:HG22	1:A:84:ILE:CG2	2.37	0.54
1:A:216:VAL:O	1:A:220:THR:HB	2.06	0.54
1:A:34:LYS:HB3	1:A:83:HIS:CE1	2.42	0.54
1:A:514:PRO:HG2	1:A:1067:LEU:HD11	1.90	0.54
2:B:780:VAL:HG21	10:J:56:LEU:HD13	1.90	0.54
2:B:1201:LYS:HD3	2:B:1205:GLN:OE1	2.07	0.54
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.89	0.54
2:B:1168:LEU:HB2	2:B:1170:THR:OG1	2.07	0.54
2:B:1185:CYS:HA	4:D:17:LYS:HD3	1.90	0.54
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.88	0.54
1:A:55:ASP:N	1:A:56:PRO:HD3	2.22	0.54
1:A:55:ASP:H	1:A:56:PRO:HD3	1.72	0.54
1:A:1433:MET:CE	7:G:63:PRO:HB3	2.38	0.54
1:A:1159:ARG:HE	1:A:1174:PHE:HE2	1.55	0.54
2:B:128:LEU:HD21	2:B:170:LEU:HB2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ASP:HB3	1:A:45:GLN:HA	1.89	0.54
1:A:56:PRO:CD	1:A:58:LEU:HG	2.38	0.54
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.90	0.53
3:C:265:MET:HE1	11:K:19:LEU:HB2	1.89	0.53
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.42	0.53
1:A:569:LYS:HG2	1:A:571:LEU:HD13	1.91	0.53
2:B:1100:ASP:OD2	11:K:1:MET:HB3	2.08	0.53
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.90	0.53
2:B:126:SER:OG	2:B:172:ILE:HD11	2.09	0.53
8:H:89:LEU:C	8:H:91:ASP:H	2.16	0.53
7:G:111:THR:HG22	7:G:113:HIS:H	1.73	0.53
11:K:12:LEU:HA	11:K:37:LYS:HG3	1.91	0.53
1:A:187:LYS:HE3	1:A:198:GLU:HB2	1.90	0.53
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.90	0.53
6:F:128:LYS:HB3	6:F:149:GLU:HA	1.91	0.53
1:A:354:SER:O	1:A:469:ARG:HA	2.09	0.53
1:A:534:LEU:O	1:A:574:GLY:HA3	2.09	0.53
10:J:48:ARG:HE	10:J:49:MET:CE	2.21	0.53
2:B:101:MET:HA	2:B:112:LEU:H	1.74	0.53
2:B:1181:GLU:HG3	2:B:1188:LYS:HG2	1.90	0.53
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.57	0.52
3:C:22:LEU:HD22	3:C:230:MET:HE1	1.91	0.52
8:H:23:VAL:HG11	8:H:121:LEU:HD22	1.90	0.52
1:A:562:THR:O	1:A:576:GLN:NE2	2.42	0.52
1:A:497:THR:HG23	2:B:1146:PHE:HD1	1.74	0.52
1:A:524:VAL:HG12	1:A:525:GLN:H	1.72	0.52
1:A:1451:VAL:O	1:A:1454:MET:HE2	2.10	0.52
1:A:344:ARG:HB3	2:B:1118:PRO:HB2	1.92	0.52
6:F:128:LYS:HD3	6:F:148:VAL:O	2.08	0.52
7:G:26:LEU:HD13	7:G:56:ILE:HD11	1.92	0.52
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.92	0.52
2:B:745:PRO:O	2:B:748:ILE:HG12	2.10	0.52
3:C:52:GLU:HA	12:L:64:LEU:HD22	1.91	0.52
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.92	0.52
1:A:347:PHE:HE1	1:A:375:THR:HG22	1.74	0.52
1:A:1386:ARG:HE	1:A:1403:GLU:HG2	1.75	0.52
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.91	0.52
1:A:41:MET:CB	1:A:49:LYS:HA	2.40	0.52
1:A:857:ARG:HD3	1:A:861:GLY:O	2.10	0.52
5:E:135:PHE:HB3	5:E:140:LEU:HD21	1.91	0.52
2:B:428:ILE:HG22	2:B:432:MET:HE2	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.40	0.51
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.25	0.51
11:K:57:LEU:HB2	11:K:76:GLN:HG2	1.92	0.51
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.93	0.51
1:A:541:ILE:HG21	1:A:549:MET:CE	2.40	0.51
2:B:1106:ARG:HG3	2:B:1107:ALA:N	2.25	0.51
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.93	0.51
7:G:119:LEU:HD21	7:G:137:ILE:HD12	1.91	0.51
13:N:2:DA:H2''	13:N:3:DA:OP2	2.11	0.51
1:A:873:MET:C	1:A:1058:VAL:HG22	2.36	0.51
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.93	0.51
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.92	0.51
7:G:8:SER:HB2	7:G:71:ASN:HD21	1.75	0.51
9:I:14:LEU:HB3	9:I:27:PHE:HB3	1.92	0.51
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.92	0.51
7:G:1:MET:CE	7:G:80:LYS:O	2.52	0.51
7:G:142:ARG:HB3	7:G:171:ILE:HD12	1.92	0.51
1:A:1004:ASN:CG	5:E:167:ARG:HD2	2.35	0.51
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.45	0.51
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.93	0.51
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.11	0.51
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.93	0.50
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.93	0.50
9:I:106:CYS:SG	9:I:108:HIS:HB3	2.52	0.50
1:A:449:SER:HA	1:A:454:SER:CB	2.41	0.50
2:B:343:ILE:O	2:B:344:LYS:HB2	2.11	0.50
1:A:1095:THR:HG21	1:A:1112:LYS:CB	2.41	0.50
9:I:50:THR:HG22	9:I:52:ILE:H	1.76	0.50
13:N:2:DA:N6	15:T:16:DT:H3	2.09	0.50
1:A:541:ILE:HG21	1:A:549:MET:HE1	1.93	0.50
2:B:870:ILE:HG22	2:B:917:PRO:HG2	1.94	0.50
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.93	0.50
6:F:94:LEU:HD22	6:F:122:MET:HG2	1.92	0.50
1:A:15:LYS:HG2	2:B:1220:ARG:HE	1.76	0.50
1:A:95:PHE:CE1	1:A:1414:ALA:HB2	2.47	0.50
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.47	0.50
1:A:847:ASP:HB3	1:A:1398:MET:HE1	1.92	0.50
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.94	0.50
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.93	0.50
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.94	0.50
3:C:46:ILE:H	3:C:46:ILE:CD1	2.22	0.50

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	2.12	0.50
4:D:13:ARG:NH1	4:D:18:VAL:H	2.10	0.50
4:D:27:LEU:HD12	4:D:173:HIS:HB2	1.94	0.50
1:A:35:ILE:HA	1:A:52:GLY:O	2.11	0.49
1:A:512:VAL:HA	1:A:519:PRO:HA	1.93	0.49
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.94	0.49
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.47	0.49
1:A:635:ARG:HH11	1:A:635:ARG:HA	1.78	0.49
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.93	0.49
1:A:1147:THR:HB	9:I:48:LEU:HD22	1.94	0.49
2:B:291:ILE:HD12	2:B:291:ILE:H	1.78	0.49
2:B:365:THR:HG21	2:B:370:PHE:CD1	2.48	0.49
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.42	0.49
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.42	0.49
1:A:1436:ILE:O	1:A:1437:GLY:C	2.56	0.49
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.93	0.49
2:B:841:MET:HG3	2:B:1010:LEU:HD12	1.94	0.49
5:E:100:ILE:HA	5:E:105:PHE:HD2	1.77	0.49
1:A:443:LEU:HD23	1:A:501:LEU:HD22	1.94	0.49
5:E:176:PRO:O	5:E:212:ARG:HA	2.13	0.49
1:A:194:ALA:HB2	1:A:197:PRO:HB3	1.94	0.49
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.46	0.49
4:D:159:THR:O	4:D:163:VAL:HG23	2.12	0.49
1:A:568:PRO:HG2	8:H:46:LEU:HD12	1.95	0.49
1:A:868:TYR:CE1	1:A:1064:VAL:HB	2.48	0.49
2:B:1166:CYS:SG	2:B:1166:CYS:O	2.71	0.49
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.95	0.49
1:A:446:ARG:HB2	1:A:487:MET:SD	2.53	0.49
2:B:773:MET:CE	2:B:985:GLY:HA2	2.43	0.49
3:C:62:PHE:O	3:C:66:ARG:HG3	2.13	0.49
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.93	0.48
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.95	0.48
1:A:56:PRO:HD3	1:A:58:LEU:HG	1.95	0.48
1:A:566:ILE:HD11	8:H:98:TYR:HB2	1.93	0.48
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.47	0.48
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.96	0.48
2:B:980:PHE:CD1	2:B:1094:ARG:HA	2.48	0.48
8:H:125:LEU:HG	8:H:130:ARG:HH22	1.77	0.48
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.48	0.48
1:A:933:TYR:O	1:A:937:VAL:HG23	2.13	0.48
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:149:LYS:C	3:C:151:GLN:H	2.21	0.48
2:B:756:ILE:O	2:B:759:PRO:HD3	2.13	0.48
2:B:542:MET:HE1	2:B:743:ILE:HD12	1.96	0.48
5:E:26:ARG:HH22	5:E:133:GLU:CD	2.22	0.48
6:F:111:LEU:HD12	6:F:111:LEU:H	1.79	0.48
1:A:380:VAL:CG1	1:A:385:ILE:HG12	2.43	0.48
1:A:646:PHE:O	1:A:650:GLN:HG2	2.13	0.48
1:A:1172:LEU:C	1:A:1174:PHE:H	2.22	0.48
8:H:80:ARG:HG2	11:K:57:LEU:HD22	1.94	0.48
1:A:589:GLN:HG2	1:A:606:LEU:HD13	1.96	0.48
2:B:751:VAL:HG13	2:B:812:LEU:HD22	1.94	0.48
1:A:194:ALA:HA	1:A:195:ASP:C	2.39	0.48
1:A:870:GLU:HB2	5:E:204:THR:CG2	2.43	0.48
1:A:1445:ILE:HG13	7:G:61:ILE:HD11	1.96	0.48
2:B:341:LEU:HD12	2:B:343:ILE:H	1.78	0.48
5:E:15:ALA:O	5:E:19:VAL:HG23	2.13	0.48
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.95	0.48
9:I:101:PHE:HE1	9:I:112:SER:HB3	1.78	0.48
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.44	0.48
1:A:345:VAL:HG12	2:B:1155:SER:HB2	1.95	0.48
2:B:510:LYS:N	2:B:511:PRO:HD3	2.29	0.48
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.96	0.48
7:G:34:VAL:HG13	7:G:45:ILE:HG21	1.95	0.48
1:A:548:ASN:HD21	11:K:47:ARG:HE	1.62	0.47
3:C:84:ARG:HD3	11:K:11:LEU:HD21	1.96	0.47
9:I:83:ASN:HA	9:I:104:LEU:HG	1.96	0.47
1:A:1166:ASP:HA	1:A:1169:ILE:HD12	1.96	0.47
10:J:48:ARG:HE	10:J:49:MET:HE2	1.79	0.47
1:A:50:ILE:C	1:A:52:GLY:H	2.22	0.47
2:B:1198:TYR:CE1	2:B:1201:LYS:HE3	2.49	0.47
9:I:102:VAL:HG22	9:I:109:ILE:HG12	1.97	0.47
2:B:425:THR:HA	2:B:428:ILE:HD12	1.97	0.47
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.96	0.47
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.78	0.47
5:E:4:GLU:HB3	5:E:7:ARG:NE	2.29	0.47
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.96	0.47
1:A:1076:ALA:HA	1:A:1079:MET:HE2	1.97	0.47
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.95	0.47
2:B:613:VAL:HG22	2:B:628:THR:HA	1.96	0.47
2:B:710:LEU:C	2:B:733:HIS:HB3	2.40	0.47
2:B:1002:THR:HG22	2:B:1072:MET:HE2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:933:SER:O	2:B:935:ARG:N	2.47	0.47
1:A:862:ASN:HA	5:E:174:GLN:HA	1.96	0.47
1:A:464:PRO:HD2	11:K:67:PHE:CD2	2.50	0.47
2:B:102:VAL:HG13	2:B:112:LEU:HD22	1.97	0.47
3:C:56:THR:HG21	3:C:145:CYS:SG	2.55	0.47
4:D:54:GLU:O	4:D:58:VAL:HG23	2.15	0.47
1:A:353:ILE:HD12	1:A:482:PHE:CD1	2.51	0.46
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.78	0.46
2:B:130:VAL:HG23	2:B:167:ILE:HD13	1.96	0.46
2:B:800:GLN:HB3	10:J:52:THR:OG1	2.16	0.46
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.80	0.46
1:A:216:VAL:HG13	1:A:226:GLU:HB3	1.98	0.46
1:A:329:LEU:HD22	2:B:1203:LEU:HD12	1.97	0.46
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.97	0.46
1:A:549:MET:SD	1:A:577:ILE:HD11	2.55	0.46
1:A:579:SER:HA	1:A:582:ILE:HG13	1.97	0.46
2:B:315:LYS:N	2:B:316:PRO:HD2	2.31	0.46
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.98	0.46
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.42	0.46
1:A:1148:ILE:HA	9:I:49:ILE:HD12	1.96	0.46
1:A:12:ARG:NH1	2:B:1218:THR:OG1	2.49	0.46
1:A:35:ILE:HG21	1:A:241:VAL:HG21	1.98	0.46
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.81	0.46
2:B:857:ARG:NH1	2:B:945:GLU:OE2	2.48	0.46
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.79	0.46
7:G:100:GLU:HG3	7:G:109:PHE:HB2	1.98	0.46
10:J:64:ASN:HB2	10:J:65:PRO:HD3	1.98	0.46
1:A:105:CYS:SG	1:A:139:TRP:HA	2.56	0.46
1:A:1153:TYR:HB2	1:A:1192:LEU:HD23	1.98	0.46
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.98	0.46
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.97	0.46
1:A:565:ILE:O	1:A:570:PRO:HA	2.16	0.46
1:A:41:MET:HB3	1:A:49:LYS:HA	1.98	0.46
2:B:54:PHE:HA	2:B:58:THR:HB	1.97	0.46
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.97	0.46
7:G:92:VAL:HG21	7:G:102:GLN:HB2	1.97	0.46
8:H:40:LEU:HB2	8:H:123:MET:HG3	1.98	0.46
2:B:1082:MET:HA	3:C:189:THR:HA	1.98	0.46
3:C:92:CYS:SG	3:C:94:LYS:HB2	2.56	0.46
2:B:542:MET:HG3	2:B:747:MET:HB3	1.98	0.46
1:A:636:GLU:OE1	1:A:962:ARG:NH1	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1074:GLU:O	1:A:1077:THR:HB	2.15	0.45
2:B:295:GLY:H	2:B:298:LEU:HD12	1.81	0.45
2:B:487:THR:HG22	2:B:490:SER:HB3	1.98	0.45
2:B:622:LYS:HE3	9:I:59:VAL:HG22	1.99	0.45
6:F:109:VAL:HG12	6:F:124:GLU:HG2	1.98	0.45
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.98	0.45
1:A:1095:THR:HG21	1:A:1112:LYS:HB3	1.96	0.45
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.97	0.45
4:D:130:LEU:HD13	4:D:142:LYS:HG2	1.98	0.45
1:A:500:GLU:HG2	2:B:1143:ALA:HA	1.99	0.45
1:A:588:LEU:HD23	1:A:607:ILE:HD12	1.98	0.45
4:D:153:ARG:HG2	4:D:218:GLU:HG3	1.98	0.45
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.97	0.45
1:A:61:ILE:HG22	1:A:62:ASP:H	1.82	0.45
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.98	0.45
4:D:47:LEU:HD21	7:G:3:PHE:CD1	2.52	0.45
8:H:35:GLN:HE22	8:H:128:ASN:HD22	1.64	0.45
1:A:92:HIS:HB2	1:A:236:LEU:HD21	1.99	0.45
1:A:495:GLU:HG3	6:F:98:ALA:HB1	1.98	0.45
2:B:757:PRO:HG2	2:B:1028:GLU:HG3	1.98	0.45
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.98	0.45
3:C:181:ASP:CG	3:C:186:LEU:HD12	2.42	0.45
4:D:52:LEU:HG	4:D:182:SER:HB3	1.98	0.45
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.16	0.45
2:B:577:ALA:HB1	2:B:589:VAL:HB	1.98	0.45
1:A:381:THR:HG22	1:A:384:ASN:CG	2.42	0.45
5:E:97:VAL:HG13	5:E:127:ILE:HG12	1.99	0.45
2:B:757:PRO:HG3	2:B:983:ARG:CZ	2.47	0.45
5:E:23:VAL:HG12	5:E:28:TYR:HB2	1.99	0.45
11:K:65:HIS:HE1	11:K:67:PHE:CG	2.35	0.45
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.98	0.44
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.98	0.44
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.53	0.44
8:H:127:GLY:N	8:H:130:ARG:HH21	2.16	0.44
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.98	0.44
1:A:1187:GLN:HG3	1:A:1188:GLN:HG2	1.99	0.44
1:A:1280:GLU:O	1:A:1282:VAL:HG23	2.17	0.44
1:A:1379:GLY:HA2	5:E:177:ARG:O	2.17	0.44
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.99	0.44
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.99	0.44
2:B:652:LYS:HB3	2:B:689:LEU:HD23	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:10:DA:H2"	15:T:11:DG:C8	2.52	0.44
1:A:51:GLY:C	1:A:56:PRO:HB3	2.43	0.44
1:A:832:ALA:HB1	15:T:18:DT:H2"	2.00	0.44
1:A:1220:PHE:HE1	1:A:1271:ILE:HD11	1.83	0.44
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.99	0.44
5:E:19:VAL:O	5:E:23:VAL:HG23	2.17	0.44
8:H:82:PRO:C	8:H:84:ALA:N	2.72	0.44
1:A:62:ASP:HB3	1:A:64:ASN:O	2.17	0.44
1:A:1317:MET:HG3	1:A:1327:ILE:HG21	2.00	0.44
2:B:490:SER:HB2	2:B:775:LYS:HA	1.99	0.44
3:C:6:PRO:HB3	3:C:25:VAL:HG13	1.98	0.44
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.98	0.44
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.99	0.44
3:C:18:VAL:HG12	3:C:20:PHE:HD1	1.83	0.44
3:C:18:VAL:HG22	11:K:109:TRP:HZ3	1.82	0.44
3:C:252:GLN:HG2	11:K:95:ILE:HG23	2.00	0.44
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.99	0.44
1:A:531:ILE:HG21	1:A:622:VAL:HG11	1.99	0.44
1:A:767:GLN:HA	1:A:799:PHE:HA	1.98	0.44
2:B:908:GLU:HG3	2:B:943:SER:HA	2.00	0.44
2:B:952:VAL:HB	12:L:58:LYS:HB2	2.00	0.44
5:E:202:SER:OG	5:E:204:THR:HG22	2.18	0.44
12:L:68:GLU:HB2	12:L:70:ARG:HD2	2.00	0.44
1:A:242:PRO:HG3	2:B:1209:ALA:HB1	2.00	0.44
1:A:768:GLN:CG	1:A:816:HIS:HA	2.48	0.44
2:B:680:THR:O	2:B:683:SER:HB2	2.18	0.44
1:A:743:VAL:O	1:A:747:VAL:HG23	2.18	0.44
1:A:1342:GLU:OE2	5:E:212:ARG:NH1	2.51	0.44
2:B:282:ILE:HA	2:B:285:ILE:HD12	1.99	0.44
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.99	0.44
3:C:164:ALA:HA	3:C:167:HIS:O	2.18	0.44
3:C:238:ILE:HG23	3:C:242:GLN:HB2	2.00	0.44
5:E:118:PRO:O	5:E:122:LYS:HG2	2.18	0.44
8:H:16:ASP:HA	8:H:17:PRO:HD3	1.90	0.44
1:A:584:ASN:O	1:A:637:LYS:HE2	2.18	0.43
1:A:1329:THR:HG22	1:A:1331:SER:N	2.27	0.43
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.33	0.43
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	2.00	0.43
1:A:358:ASN:HB2	11:K:65:HIS:HD2	1.82	0.43
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.52	0.43
1:A:709:THR:HB	1:A:712:GLU:H	1.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:GLY:HA2	2:B:298:LEU:HB2	2.00	0.43
2:B:640:VAL:HG22	2:B:651:LEU:HG	1.99	0.43
2:B:705:MET:HE3	2:B:742:GLU:HG2	2.01	0.43
5:E:167:ARG:HD3	5:E:167:ARG:HA	1.83	0.43
7:G:81:PRO:HG3	7:G:106:MET:SD	2.57	0.43
1:A:458:HIS:NE2	1:A:478:TYR:OH	2.40	0.43
4:D:23:ASN:HA	4:D:28:GLN:O	2.18	0.43
1:A:982:THR:H	1:A:985:ASP:HB2	1.83	0.43
1:A:1364:ASN:OD1	1:A:1366:ARG:HG2	2.19	0.43
1:A:21:LEU:HD11	1:A:1414:ALA:HA	2.00	0.43
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.52	0.43
1:A:388:LEU:HA	1:A:391:LEU:HD12	2.00	0.43
11:K:51:LEU:HD13	11:K:59:ALA:HB3	2.01	0.43
1:A:185:TRP:HE3	1:A:185:TRP:H	1.65	0.43
1:A:745:GLN:HA	1:A:748:MET:HE3	1.99	0.43
1:A:933:TYR:HA	1:A:936:LEU:HD12	2.00	0.43
1:A:1403:GLU:HG3	15:T:17:DT:H5'	2.00	0.43
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.84	0.43
2:B:542:MET:HG2	2:B:747:MET:HE3	2.00	0.43
3:C:148:ARG:HD3	3:C:149:LYS:HG2	2.01	0.43
3:C:163:ILE:CD1	3:C:165:LYS:HB2	2.40	0.43
5:E:179:GLN:HA	5:E:215:MET:HB2	2.00	0.43
8:H:24:CYS:HB2	8:H:44:VAL:HG21	2.01	0.43
2:B:620:ARG:HE	9:I:89:GLN:NE2	2.10	0.43
4:D:27:LEU:CD1	4:D:173:HIS:HB2	2.47	0.43
1:A:51:GLY:HA2	1:A:56:PRO:HA	2.01	0.43
1:A:856:THR:HB	1:A:865:GLN:HB2	2.01	0.43
3:C:20:PHE:CE2	3:C:22:LEU:HD13	2.51	0.43
1:A:598:LEU:HD13	8:H:25:ARG:NH1	2.34	0.42
2:B:1166:CYS:O	2:B:1168:LEU:N	2.46	0.42
3:C:100:THR:HB	3:C:121:VAL:HG21	2.01	0.42
1:A:399:HIS:HB3	1:A:400:PRO:HD3	2.01	0.42
1:A:897:TYR:HB3	1:A:936:LEU:HD13	2.02	0.42
1:A:974:ASP:C	1:A:976:THR:H	2.27	0.42
2:B:641:GLU:HG3	2:B:652:LYS:HE2	2.00	0.42
3:C:10:ILE:HD12	11:K:108:GLU:HB3	2.01	0.42
4:D:13:ARG:HH12	4:D:18:VAL:H	1.67	0.42
3:C:175:ALA:HB2	10:J:10:CYS:HB2	2.02	0.42
1:A:106:VAL:HG21	1:A:214:ILE:HG12	2.02	0.42
1:A:596:THR:HB	1:A:598:LEU:H	1.85	0.42
2:B:35:SER:HA	2:B:811:TYR:HE1	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:PRO:HG2	2:B:234:ILE:HD12	2.00	0.42
2:B:278:GLN:HB2	2:B:337:ARG:HG2	2.01	0.42
2:B:405:ARG:HB3	2:B:631:GLY:HA3	2.01	0.42
2:B:880:THR:HB	2:B:934:LYS:HD2	2.01	0.42
5:E:43:LYS:O	5:E:47:CYS:HB2	2.20	0.42
7:G:154:VAL:HB	7:G:155:SER:H	1.68	0.42
1:A:1048:ASN:O	1:A:1052:GLN:HB2	2.18	0.42
8:H:100:THR:HG23	8:H:138:GLU:HA	2.02	0.42
10:J:9:SER:HB2	10:J:45:CYS:HB2	2.02	0.42
1:A:1372:VAL:O	1:A:1376:THR:HB	2.19	0.42
2:B:356:LEU:HA	2:B:360:PHE:HB3	2.01	0.42
2:B:764:SER:HB3	2:B:765:PRO:HD3	2.00	0.42
8:H:2:SER:N	8:H:61:SER:HG	2.18	0.42
9:I:34:TYR:HE2	9:I:36:GLU:HG2	1.85	0.42
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.19	0.42
1:A:871:ASP:CG	1:A:1366:ARG:HH22	2.26	0.42
1:A:1221:LYS:HB3	1:A:1222:ASN:H	1.68	0.42
2:B:711:GLU:HB2	2:B:712:PRO:HD3	2.01	0.42
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.50	0.42
11:K:51:LEU:HD12	11:K:51:LEU:HA	1.89	0.42
1:A:42:ASP:O	1:A:44:THR:N	2.53	0.42
1:A:200:ARG:NH2	1:A:206:GLU:OE2	2.52	0.42
7:G:45:ILE:HA	7:G:78:VAL:HG12	2.01	0.42
1:A:62:ASP:O	1:A:64:ASN:N	2.49	0.42
1:A:1031:VAL:HA	1:A:1035:TYR:CD2	2.55	0.42
2:B:21:GLU:O	2:B:656:GLY:HA3	2.19	0.42
2:B:35:SER:HA	2:B:811:TYR:CE1	2.54	0.42
2:B:101:MET:HB3	2:B:111:ALA:HA	2.00	0.42
2:B:398:ARG:HB2	2:B:398:ARG:HH11	1.84	0.42
2:B:766:ARG:NH2	2:B:1020:ARG:HH11	2.18	0.42
2:B:873:THR:O	2:B:914:LYS:HA	2.20	0.42
8:H:63:LEU:HB3	8:H:90:ALA:HB2	2.02	0.42
1:A:1168:GLU:O	1:A:1172:LEU:HG	2.19	0.42
2:B:254:LEU:HD23	2:B:381:MET:HE1	2.02	0.42
4:D:31:GLN:O	4:D:34:GLN:HB2	2.20	0.42
4:D:144:THR:HG21	7:G:46:LEU:HD13	2.02	0.42
9:I:111:THR:HG21	9:I:118:ARG:HD2	2.02	0.42
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.90	0.41
1:A:519:PRO:HD3	1:A:631:HIS:ND1	2.35	0.41
2:B:361:LEU:O	2:B:374:LYS:HE2	2.18	0.41
2:B:792:MET:HA	2:B:856:PHE:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:65:HIS:HE1	11:K:67:PHE:CD1	2.38	0.41
1:A:450:LEU:HA	1:A:838:GLN:NE2	2.36	0.41
1:A:1393:ASN:H	1:A:1393:ASN:ND2	2.16	0.41
3:C:73:GLN:O	3:C:129:ILE:HA	2.20	0.41
6:F:73:ALA:HB2	6:F:143:PHE:CZ	2.55	0.41
1:A:709:THR:HG22	1:A:711:ARG:H	1.84	0.41
1:A:1288:ASP:HA	1:A:1302:PRO:HB3	2.03	0.41
2:B:259:TYR:CE2	2:B:270:LYS:HB2	2.56	0.41
2:B:483:LEU:HD11	2:B:491:THR:HG23	2.01	0.41
2:B:996:ARG:CG	2:B:1007:VAL:HG11	2.50	0.41
3:C:255:VAL:HG21	11:K:94:ILE:HG21	2.00	0.41
8:H:105:GLU:HB3	8:H:113:ALA:HB3	2.03	0.41
1:A:104:GLU:HG3	1:A:174:ILE:HD12	2.01	0.41
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.56	0.41
1:A:75:ASN:HA	2:B:1116:ARG:HH12	1.85	0.41
1:A:151:ASP:HA	1:A:163:SER:HA	2.01	0.41
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.20	0.41
3:C:184:ASN:ND2	3:C:189:THR:O	2.54	0.41
4:D:194:LEU:HD22	7:G:86:VAL:HG11	2.02	0.41
1:A:774:ARG:HH21	1:A:797:LYS:HB2	1.86	0.41
1:A:1121:GLU:HB3	1:A:1124:HIS:CE1	2.55	0.41
2:B:497:ARG:HH22	2:B:775:LYS:HD3	1.85	0.41
3:C:177:GLU:HB2	3:C:231:ASN:HB3	2.03	0.41
5:E:135:PHE:HD2	5:E:140:LEU:HD22	1.85	0.41
7:G:13:LEU:HD23	7:G:13:LEU:HA	1.85	0.41
1:A:568:PRO:HB2	3:C:221:TYR:CE2	2.55	0.41
1:A:704:ALA:HB2	1:A:710:LEU:HA	2.03	0.41
8:H:36:CYS:HA	8:H:126:GLU:O	2.21	0.41
4:D:188:ALA:HB2	4:D:208:GLU:HG3	2.02	0.41
1:A:66:LYS:HD2	1:A:71:GLN:HB3	2.03	0.41
1:A:313:GLN:O	1:A:314:ALA:C	2.64	0.41
1:A:335:ARG:NH1	2:B:1206:GLU:OE2	2.54	0.41
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.55	0.41
1:A:697:ALA:HB2	1:A:702:LEU:HD13	2.03	0.41
1:A:1444:MET:HB2	1:A:1444:MET:HE2	1.59	0.41
2:B:33:VAL:HG12	2:B:681:TRP:HZ3	1.85	0.41
2:B:90:ILE:HD12	2:B:432:MET:SD	2.60	0.41
2:B:848:ARG:HD2	10:J:8:PHE:O	2.20	0.41
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.56	0.41
9:I:8:ARG:O	9:I:9:ASP:CG	2.64	0.41
10:J:45:CYS:O	10:J:48:ARG:HG3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:32:VAL:HG22	11:K:74:ARG:HG3	2.01	0.41
11:K:65:HIS:CE1	11:K:67:PHE:CG	3.09	0.41
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.56	0.41
1:A:1124:HIS:HB2	1:A:1130:GLN:HG2	2.03	0.41
1:A:1191:TRP:HZ3	9:I:43:VAL:HG21	1.86	0.41
2:B:102:VAL:HG22	2:B:112:LEU:HB2	2.02	0.41
3:C:15:LYS:O	3:C:240:VAL:HG22	2.21	0.41
3:C:77:ILE:HA	3:C:129:ILE:HD11	2.03	0.41
11:K:8:GLU:O	11:K:37:LYS:HD3	2.20	0.41
1:A:35:ILE:HG22	1:A:84:ILE:HG22	2.03	0.40
1:A:1317:MET:HE2	5:E:142:VAL:HG11	2.03	0.40
1:A:1356:ILE:HG23	1:A:1361:SER:HB2	2.03	0.40
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.21	0.40
2:B:69:LEU:O	2:B:90:ILE:N	2.54	0.40
2:B:291:ILE:HG22	2:B:297:ILE:HG13	2.03	0.40
2:B:620:ARG:HG3	9:I:62:ILE:HD11	2.03	0.40
2:B:1119:VAL:HG23	2:B:1126:GLY:HA2	2.03	0.40
1:A:37:PHE:CD2	1:A:52:GLY:CA	3.04	0.40
1:A:765:VAL:HG21	1:A:808:LEU:HD11	2.02	0.40
1:A:132:LYS:HE3	1:A:1411:GLU:OE1	2.21	0.40
1:A:1139:GLU:HB2	1:A:1282:VAL:HB	2.04	0.40
2:B:165:VAL:O	2:B:167:ILE:HD12	2.22	0.40
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.87	0.40
2:B:918:ILE:HG12	2:B:935:ARG:HH22	1.86	0.40
3:C:175:ALA:HB3	10:J:43:ARG:NH1	2.35	0.40
3:C:232:VAL:HG21	3:C:244:VAL:HG22	2.03	0.40
7:G:9:LEU:HD22	7:G:34:VAL:HG23	2.03	0.40
8:H:82:PRO:O	8:H:84:ALA:N	2.52	0.40
10:J:7:CYS:HA	10:J:49:MET:HE3	2.01	0.40
1:A:79:GLY:H	2:B:1201:LYS:HZ3	1.70	0.40
1:A:738:LYS:HA	8:H:19:ARG:HH12	1.85	0.40
1:A:1376:THR:HG23	5:E:212:ARG:NH2	2.32	0.40
2:B:1056:SER:HB3	2:B:1066:SER:HB2	2.02	0.40
3:C:148:ARG:HG3	3:C:149:LYS:H	1.87	0.40
8:H:89:LEU:O	8:H:91:ASP:N	2.55	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	1414/1732 (82%)	1230 (87%)	132 (9%)	52 (4%)	2	21
2	B	1095/1224 (90%)	959 (88%)	94 (9%)	42 (4%)	2	20
3	C	264/318 (83%)	245 (93%)	18 (7%)	1 (0%)	30	62
4	D	174/221 (79%)	149 (86%)	17 (10%)	8 (5%)	2	17
5	E	212/215 (99%)	194 (92%)	14 (7%)	4 (2%)	6	33
6	F	82/155 (53%)	75 (92%)	6 (7%)	1 (1%)	10	41
7	G	169/171 (99%)	159 (94%)	7 (4%)	3 (2%)	6	34
8	H	129/146 (88%)	102 (79%)	20 (16%)	7 (5%)	1	14
9	I	117/122 (96%)	98 (84%)	16 (14%)	3 (3%)	4	27
10	J	63/70 (90%)	52 (82%)	6 (10%)	5 (8%)	1	8
11	K	113/120 (94%)	109 (96%)	3 (3%)	1 (1%)	14	47
12	L	44/70 (63%)	26 (59%)	11 (25%)	7 (16%)	0	2
All	All	3876/4564 (85%)	3398 (88%)	344 (9%)	134 (4%)	3	23

All (134) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	72	GLU
1	A	169	ASN
1	A	189	ARG
1	A	193	ASP
1	A	257	ARG
1	A	286	HIS
1	A	311	GLN
1	A	318	SER
1	A	332	LYS
1	A	335	ARG
1	A	410	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1403	GLU
1	A	1405	THR
2	B	341	LEU
2	B	344	LYS
2	B	473	MET
2	B	867	GLY
2	B	879	ARG
2	B	943	SER
2	B	1046	PRO
2	B	1157	ALA
2	B	1181	GLU
2	B	1185	CYS
4	D	18	VAL
4	D	199	ASN
8	H	90	ALA
9	I	9	ASP
10	J	6	ARG
10	J	55	ASP
12	L	53	HIS
1	A	43	GLU
1	A	47	ARG
1	A	54	ASN
1	A	58	LEU
1	A	76	GLU
1	A	178	GLY
1	A	195	ASP
1	A	224	PHE
1	A	465	TYR
1	A	628	GLY
1	A	1124	HIS
1	A	1175	SER
2	B	108	VAL
2	B	229	ALA
2	B	251	ILE
2	B	282	ILE
2	B	338	GLY
2	B	629	ASP
2	B	643	ASP
2	B	707	PRO
2	B	711	GLU
2	B	731	VAL
2	B	772	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	880	THR
2	B	1066	SER
2	B	1167	GLY
2	B	1175	LEU
2	B	1176	ASN
2	B	1190	ASP
3	C	215	GLU
4	D	16	LYS
4	D	137	ASN
5	E	45	LYS
7	G	154	VAL
8	H	81	PRO
8	H	82	PRO
8	H	83	GLN
9	I	95	THR
12	L	45	ALA
12	L	59	ALA
1	A	35	ILE
1	A	74	MET
1	A	131	SER
1	A	167	CYS
1	A	399	HIS
1	A	1281	ARG
2	B	67	SER
2	B	792	MET
2	B	883	LEU
2	B	1223	ASP
4	D	15	LEU
4	D	52	LEU
4	D	119	ARG
5	E	36	GLU
6	F	73	ALA
8	H	17	PRO
10	J	2	ILE
10	J	30	LEU
11	K	114	LEU
12	L	56	LEU
1	A	156	ASP
1	A	449	SER
1	A	525	GLN
1	A	567	LYS
1	A	569	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	870	GLU
1	A	975	HIS
1	A	1173	HIS
1	A	1438	THR
2	B	262	GLU
2	B	339	THR
2	B	340	ALA
2	B	751	VAL
2	B	942	ARG
4	D	11	ARG
5	E	104	ASN
5	E	137	GLU
7	G	2	PHE
8	H	60	ALA
8	H	128	ASN
12	L	26	THR
12	L	55	ILE
1	A	62	ASP
1	A	958	VAL
1	A	1122	PRO
1	A	1255	GLU
2	B	277	LYS
2	B	1155	SER
9	I	3	THR
10	J	29	GLU
12	L	50	ASP
1	A	73	GLY
1	A	333	GLU
2	B	343	ILE
2	B	619	ILE
2	B	902	GLY
2	B	1096	ARG
1	A	310	GLY
7	G	63	PRO
1	A	61	ILE
1	A	196	GLU
1	A	1437	GLY
1	A	1242	VAL

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%)	1047 (84%)	193 (16%)	2	15
2	B	966/1061 (91%)	811 (84%)	155 (16%)	2	14
3	C	234/274 (85%)	199 (85%)	35 (15%)	3	17
4	D	160/200 (80%)	126 (79%)	34 (21%)	1	6
5	E	196/197 (100%)	169 (86%)	27 (14%)	3	19
6	F	74/137 (54%)	68 (92%)	6 (8%)	11	35
7	G	152/152 (100%)	128 (84%)	24 (16%)	2	15
8	H	117/128 (91%)	102 (87%)	15 (13%)	4	21
9	I	113/116 (97%)	101 (89%)	12 (11%)	6	27
10	J	60/65 (92%)	49 (82%)	11 (18%)	2	10
11	K	99/102 (97%)	84 (85%)	15 (15%)	3	16
12	L	40/57 (70%)	25 (62%)	15 (38%)	0	1
All	All	3451/4008 (86%)	2909 (84%)	542 (16%)	2	15

All (542) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	12	ARG
1	A	13	THR
1	A	15	LYS
1	A	28	ARG
1	A	34	LYS
1	A	41	MET
1	A	62	ASP
1	A	64	ASN
1	A	65	LEU
1	A	90	VAL
1	A	93	VAL
1	A	106	VAL
1	A	157	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	159	THR
1	A	174	ILE
1	A	182	VAL
1	A	188	ASP
1	A	199	LEU
1	A	204	THR
1	A	208	LEU
1	A	220	THR
1	A	225	ASN
1	A	227	VAL
1	A	236	LEU
1	A	255	SER
1	A	256	GLN
1	A	261	ASP
1	A	270	LEU
1	A	274	ILE
1	A	277	GLU
1	A	279	LEU
1	A	289	ILE
1	A	290	GLU
1	A	295	LEU
1	A	307	ASP
1	A	313	GLN
1	A	316	GLN
1	A	322	VAL
1	A	324	SER
1	A	330	LYS
1	A	335	ARG
1	A	337	ARG
1	A	343	LYS
1	A	344	ARG
1	A	353	ILE
1	A	375	THR
1	A	381	THR
1	A	385	ILE
1	A	386	ASP
1	A	389	THR
1	A	393	ARG
1	A	394	ASN
1	A	398	GLU
1	A	408	ASP
1	A	411	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	423	ASP
1	A	425	GLN
1	A	427	GLN
1	A	431	LYS
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	461	LYS
1	A	463	ILE
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	500	GLU
1	A	505	CYS
1	A	517	ASN
1	A	518	LYS
1	A	524	VAL
1	A	532	ARG
1	A	566	ILE
1	A	571	LEU
1	A	577	ILE
1	A	582	ILE
1	A	589	GLN
1	A	593	GLU
1	A	596	THR
1	A	598	LEU
1	A	603	ASN
1	A	618	GLU
1	A	629	LEU
1	A	634	THR
1	A	666	ILE
1	A	670	ILE
1	A	672	ASP
1	A	691	LEU
1	A	702	LEU
1	A	711	ARG
1	A	738	LYS
1	A	740	LEU
1	A	756	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	768	GLN
1	A	769	SER
1	A	773	LYS
1	A	788	SER
1	A	795	GLU
1	A	821	ARG
1	A	826	ASP
1	A	827	THR
1	A	831	THR
1	A	834	THR
1	A	839	ARG
1	A	855	THR
1	A	867	ILE
1	A	878	ILE
1	A	896	ARG
1	A	904	THR
1	A	915	SER
1	A	919	ILE
1	A	920	LEU
1	A	926	GLN
1	A	929	LEU
1	A	948	VAL
1	A	960	ILE
1	A	964	ILE
1	A	973	ILE
1	A	976	THR
1	A	983	ILE
1	A	998	LEU
1	A	999	VAL
1	A	1001	ARG
1	A	1009	ASN
1	A	1015	VAL
1	A	1038	THR
1	A	1052	GLN
1	A	1058	VAL
1	A	1062	GLU
1	A	1067	LEU
1	A	1078	GLN
1	A	1096	SER
1	A	1100	ARG
1	A	1116	LEU
1	A	1118	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1120	LEU
1	A	1124	HIS
1	A	1133	LEU
1	A	1135	ARG
1	A	1142	THR
1	A	1170	ILE
1	A	1172	LEU
1	A	1173	HIS
1	A	1175	SER
1	A	1176	LEU
1	A	1192	LEU
1	A	1195	LEU
1	A	1208	THR
1	A	1218	GLN
1	A	1222	ASN
1	A	1234	GLU
1	A	1237	ILE
1	A	1242	VAL
1	A	1255	GLU
1	A	1257	ASP
1	A	1264	GLU
1	A	1273	LEU
1	A	1279	ILE
1	A	1288	ASP
1	A	1291	VAL
1	A	1293	SER
1	A	1295	THR
1	A	1297	GLU
1	A	1303	GLU
1	A	1308	THR
1	A	1315	GLU
1	A	1316	VAL
1	A	1325	THR
1	A	1327	ILE
1	A	1333	ILE
1	A	1336	MET
1	A	1341	ILE
1	A	1376	THR
1	A	1391	ARG
1	A	1393	ASN
1	A	1398	MET
1	A	1400	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1403	GLU
1	A	1405	THR
1	A	1424	VAL
1	A	1426	GLU
1	A	1433	MET
1	A	1438	THR
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1453	TYR
1	A	1454	MET
2	B	21	GLU
2	B	25	ILE
2	B	26	THR
2	B	46	GLN
2	B	56	ASP
2	B	63	ILE
2	B	94	LYS
2	B	101	MET
2	B	104	GLU
2	B	110	HIS
2	B	118	ARG
2	B	130	VAL
2	B	169	ARG
2	B	178	ASN
2	B	187	SER
2	B	217	ARG
2	B	218	SER
2	B	222	ILE
2	B	223	VAL
2	B	240	ILE
2	B	251	ILE
2	B	261	ARG
2	B	267	ARG
2	B	272	THR
2	B	276	ILE
2	B	277	LYS
2	B	278	GLN
2	B	280	ILE
2	B	298	LEU
2	B	324	ILE
2	B	325	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	337	ARG
2	B	339	THR
2	B	341	LEU
2	B	343	ILE
2	B	344	LYS
2	B	348	ARG
2	B	357	GLN
2	B	361	LEU
2	B	364	ILE
2	B	365	THR
2	B	367	LEU
2	B	393	LYS
2	B	395	GLN
2	B	398	ARG
2	B	408	LEU
2	B	412	LEU
2	B	416	LEU
2	B	423	LYS
2	B	426	LYS
2	B	430	ARG
2	B	436	VAL
2	B	446	LEU
2	B	448	ILE
2	B	453	ILE
2	B	469	GLN
2	B	470	LYS
2	B	482	VAL
2	B	485	ARG
2	B	487	THR
2	B	490	SER
2	B	502	ILE
2	B	513	GLN
2	B	531	GLN
2	B	538	ASN
2	B	545	ILE
2	B	547	VAL
2	B	549	THR
2	B	552	MET
2	B	554	ILE
2	B	563	MET
2	B	570	VAL
2	B	574	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	576	ASP
2	B	595	ARG
2	B	598	GLU
2	B	603	LEU
2	B	604	ARG
2	B	612	GLU
2	B	615	MET
2	B	616	ILE
2	B	620	ARG
2	B	624	LEU
2	B	628	THR
2	B	644	GLU
2	B	653	VAL
2	B	658	ILE
2	B	680	THR
2	B	703	ILE
2	B	730	ARG
2	B	734	HIS
2	B	737	THR
2	B	743	ILE
2	B	755	ILE
2	B	766	ARG
2	B	786	ASN
2	B	787	VAL
2	B	790	ASP
2	B	795	ILE
2	B	797	TYR
2	B	831	SER
2	B	835	GLN
2	B	839	MET
2	B	844	SER
2	B	870	ILE
2	B	871	THR
2	B	878	GLN
2	B	882	THR
2	B	889	THR
2	B	906	SER
2	B	908	GLU
2	B	934	LYS
2	B	942	ARG
2	B	944	THR
2	B	946	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	948	ILE
2	B	954	VAL
2	B	964	VAL
2	B	969	ARG
2	B	970	THR
2	B	975	GLN
2	B	986	GLN
2	B	997	GLU
2	B	1006	ILE
2	B	1007	VAL
2	B	1028	GLU
2	B	1034	VAL
2	B	1045	SER
2	B	1049	ASP
2	B	1060	ARG
2	B	1065	GLN
2	B	1072	MET
2	B	1094	ARG
2	B	1096	ARG
2	B	1106	ARG
2	B	1112	GLN
2	B	1120	GLU
2	B	1123	SER
2	B	1128	LEU
2	B	1138	MET
2	B	1147	LEU
2	B	1151	LEU
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1170	THR
2	B	1175	LEU
2	B	1179	GLN
2	B	1183	LYS
2	B	1188	LYS
2	B	1189	ILE
2	B	1191	ILE
2	B	1201	LYS
2	B	1202	LEU
2	B	1212	ILE
3	C	3	GLU
3	C	11	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	23	SER
3	C	25	VAL
3	C	27	LEU
3	C	48	SER
3	C	52	GLU
3	C	53	THR
3	C	54	ASN
3	C	55	THR
3	C	56	THR
3	C	78	GLU
3	C	79	GLN
3	C	83	SER
3	C	100	THR
3	C	108	GLU
3	C	113	VAL
3	C	121	VAL
3	C	122	SER
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	147	LEU
3	C	148	ARG
3	C	151	GLN
3	C	186	LEU
3	C	215	GLU
3	C	232	VAL
3	C	235	VAL
3	C	238	ILE
3	C	240	VAL
3	C	259	LEU
3	C	260	LEU
3	C	268	ASP
4	D	5	THR
4	D	6	SER
4	D	7	THR
4	D	9	GLN
4	D	10	THR
4	D	11	ARG
4	D	12	ARG
4	D	18	VAL
4	D	22	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	27	LEU
4	D	35	LEU
4	D	40	HIS
4	D	41	GLN
4	D	52	LEU
4	D	65	GLU
4	D	67	ARG
4	D	119	ARG
4	D	123	LEU
4	D	126	ILE
4	D	127	ASP
4	D	134	THR
4	D	139	LYS
4	D	156	ASP
4	D	165	GLN
4	D	177	VAL
4	D	182	SER
4	D	187	THR
4	D	193	THR
4	D	197	SER
4	D	201	LYS
4	D	206	GLU
4	D	218	GLU
4	D	219	THR
4	D	221	TYR
5	E	3	GLN
5	E	9	ILE
5	E	30	ILE
5	E	31	THR
5	E	37	LEU
5	E	49	SER
5	E	57	MET
5	E	69	ILE
5	E	72	PHE
5	E	92	THR
5	E	100	ILE
5	E	114	ASN
5	E	115	ASN
5	E	122	LYS
5	E	127	ILE
5	E	131	THR
5	E	140	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	150	VAL
5	E	154	ILE
5	E	166	LYS
5	E	171	LYS
5	E	173	SER
5	E	191	LYS
5	E	192	ARG
5	E	196	VAL
5	E	202	SER
5	E	204	THR
6	F	79	ARG
6	F	82	THR
6	F	86	THR
6	F	93	ILE
6	F	115	THR
6	F	152	ILE
7	G	11	ILE
7	G	13	LEU
7	G	22	MET
7	G	24	GLN
7	G	26	LEU
7	G	39	THR
7	G	61	ILE
7	G	64	THR
7	G	65	ASP
7	G	90	THR
7	G	93	SER
7	G	96	GLN
7	G	106	MET
7	G	114	LEU
7	G	118	ASP
7	G	131	GLN
7	G	133	SER
7	G	138	THR
7	G	143	ILE
7	G	151	ILE
7	G	154	VAL
7	G	155	SER
7	G	162	SER
7	G	171	ILE
8	H	14	GLU
8	H	26	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	31	THR
8	H	34	ASP
8	H	42	ILE
8	H	76	THR
8	H	77	ARG
8	H	89	LEU
8	H	91	ASP
8	H	103	LYS
8	H	106	GLU
8	H	112	ILE
8	H	130	ARG
8	H	138	GLU
8	H	146	ARG
9	I	8	ARG
9	I	17	ARG
9	I	31	THR
9	I	35	VAL
9	I	51	ASN
9	I	62	ILE
9	I	74	GLU
9	I	81	ARG
9	I	83	ASN
9	I	84	VAL
9	I	94	ASP
9	I	111	THR
10	J	2	ILE
10	J	3	VAL
10	J	6	ARG
10	J	12	LYS
10	J	13	VAL
10	J	14	VAL
10	J	16	ASP
10	J	22	LEU
10	J	23	ASN
10	J	52	THR
10	J	59	LYS
11	K	11	LEU
11	K	18	LYS
11	K	20	LYS
11	K	25	THR
11	K	29	ASN
11	K	31	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	37	LYS
11	K	41	THR
11	K	47	ARG
11	K	51	LEU
11	K	91	CYS
11	K	92	ASN
11	K	101	LEU
11	K	107	THR
11	K	114	LEU
12	L	27	LEU
12	L	28	LYS
12	L	33	GLU
12	L	38	LEU
12	L	43	THR
12	L	44	ASP
12	L	46	VAL
12	L	47	ARG
12	L	51	CYS
12	L	55	ILE
12	L	58	LYS
12	L	61	THR
12	L	65	VAL
12	L	66	GLN
12	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	253	ASN
1	A	311	GLN
1	A	339	ASN
1	A	363	GLN
1	A	399	HIS
1	A	425	GLN
1	A	445	ASN
1	A	548	ASN
1	A	589	GLN
1	A	640	GLN
1	A	648	ASN
1	A	742	ASN
1	A	811	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	838	GLN
1	A	851	HIS
1	A	862	ASN
1	A	877	HIS
1	A	953	ASN
1	A	968	GLN
1	A	975	HIS
1	A	994	GLN
1	A	1009	ASN
1	A	1078	GLN
1	A	1106	ASN
1	A	1128	GLN
1	A	1270	ASN
1	A	1390	ASN
1	A	1393	ASN
2	B	110	HIS
2	B	178	ASN
2	B	300	HIS
2	B	383	ASN
2	B	433	GLN
2	B	465	ASN
2	B	587	HIS
2	B	842	ASN
2	B	1025	HIS
2	B	1062	HIS
2	B	1084	GLN
2	B	1117	GLN
2	B	1176	ASN
2	B	1195	HIS
3	C	7	GLN
3	C	102	GLN
3	C	131	HIS
3	C	135	GLN
3	C	184	ASN
3	C	224	GLN
4	D	37	GLN
4	D	143	ASN
5	E	5	ASN
5	E	54	GLN
7	G	71	ASN
7	G	131	GLN
7	G	158	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	35	GLN
8	H	52	GLN
8	H	83	GLN
8	H	131	ASN
8	H	137	GLN
9	I	60	GLN
9	I	83	ASN
9	I	89	GLN
9	I	108	HIS
9	I	114	GLN
9	I	120	GLN
11	K	76	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	3/5 (60%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is 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	1.00	1 (5%)	25,30,33	2.31	9 (36%)

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	-	4/7/21/22	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	22	BRU	C6-C5	2.13	1.38	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	N3-C2-N1	4.89	121.26	114.89
15	T	22	BRU	C5-C4-N3	4.76	118.81	113.34
15	T	22	BRU	O4-C4-C5	-3.93	120.79	125.80
15	T	22	BRU	C6-N1-C2	-3.77	117.55	121.30
15	T	22	BRU	O2-C2-N3	-3.75	114.58	121.49
15	T	22	BRU	C4-N3-C2	-3.68	122.52	127.34
15	T	22	BRU	C1'-N1-C2	2.93	123.39	117.66
15	T	22	BRU	C6-C5-C4	-2.87	117.76	120.67
15	T	22	BRU	O4'-C1'-N1	2.37	112.07	107.86

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	22	BRU	O4'-C4'-C5'-O5'
15	T	22	BRU	C3'-C4'-C5'-O5'
15	T	22	BRU	C2'-C1'-N1-C2
15	T	22	BRU	C2'-C1'-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	934:LYS	C	935:ARG	N	4.93
1	B	351:TYR	C	352:ALA	N	3.22

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%)	-0.30	18 (1%) 75 50	48, 96, 156, 222	0
2	B	1115/1224 (91%)	-0.05	29 (2%) 57 33	51, 114, 178, 210	0
3	C	266/318 (83%)	-0.41	0 100 100	71, 100, 140, 168	0
4	D	178/221 (80%)	-0.06	10 (5%) 30 17	75, 112, 164, 183	0
5	E	214/215 (99%)	-0.12	0 100 100	75, 130, 176, 189	0
6	F	84/155 (54%)	-0.67	1 (1%) 76 52	51, 75, 104, 120	0
7	G	171/171 (100%)	-0.26	0 100 100	67, 95, 136, 154	0
8	H	133/146 (91%)	0.31	5 (3%) 44 24	109, 137, 176, 195	0
9	I	119/122 (97%)	0.11	4 (3%) 48 27	109, 138, 177, 196	0
10	J	65/70 (92%)	-0.24	1 (1%) 72 47	75, 97, 132, 146	0
11	K	115/120 (95%)	-0.53	1 (0%) 81 58	66, 97, 136, 155	0
12	L	46/70 (65%)	0.77	4 (8%) 16 10	91, 157, 173, 180	0
13	N	10/14 (71%)	1.25	2 (20%) 3 3	192, 220, 260, 264	0
14	P	4/5 (80%)	-0.02	0 100 100	110, 121, 141, 167	0
15	T	17/26 (65%)	1.12	2 (11%) 9 6	122, 191, 266, 267	0
All	All	3959/4609 (85%)	-0.17	77 (1%) 66 41	48, 106, 172, 267	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	446	LEU	6.0
1	A	1243	VAL	5.1
2	B	709	ASP	5.1
1	A	1080	THR	4.7
12	L	27	LEU	4.6
2	B	509	ALA	4.5
8	H	63	LEU	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	L	26	THR	4.5
2	B	882	THR	4.4
15	T	24	DG	4.0
10	J	65	PRO	3.9
2	B	502	ILE	3.8
2	B	883	LEU	3.8
2	B	134	LYS	3.7
2	B	1224	PHE	3.6
2	B	708	GLU	3.6
2	B	70	ILE	3.5
1	A	251	SER	3.5
4	D	25	ALA	3.5
4	D	3	VAL	3.5
11	K	114	LEU	3.3
4	D	76	LYS	3.2
2	B	251	ILE	3.1
12	L	25	ALA	3.1
1	A	1173	HIS	3.0
2	B	164	LYS	3.0
13	N	8	DT	3.0
2	B	476	ARG	2.9
4	D	24	ALA	2.9
4	D	221	TYR	2.8
9	I	120	GLN	2.8
4	D	173	HIS	2.8
1	A	1187	GLN	2.8
12	L	28	LYS	2.7
1	A	56	PRO	2.7
8	H	90	ALA	2.6
1	A	1176	LEU	2.6
2	B	243	ALA	2.6
2	B	340	ALA	2.6
8	H	132	LEU	2.6
1	A	186	LYS	2.6
8	H	82	PRO	2.6
1	A	194	ALA	2.5
13	N	7	DC	2.5
2	B	1049	ASP	2.5
2	B	246	LYS	2.5
1	A	57	ARG	2.4
2	B	343	ILE	2.4
2	B	715	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	190	ALA	2.4
9	I	93	LYS	2.4
1	A	51	GLY	2.3
6	F	72	LYS	2.3
4	D	187	THR	2.3
2	B	249	ARG	2.3
1	A	310	GLY	2.3
2	B	1222	ARG	2.3
2	B	710	LEU	2.2
4	D	17	LYS	2.2
2	B	353	LYS	2.2
2	B	933	SER	2.2
4	D	10	THR	2.2
1	A	1257	ASP	2.2
2	B	958	GLN	2.2
15	T	7	DT	2.1
1	A	1321	GLY	2.1
1	A	1254	ALA	2.1
2	B	341	LEU	2.1
2	B	477	ALA	2.1
9	I	116	ASN	2.1
8	H	136	LYS	2.1
2	B	342	GLY	2.1
2	B	791	THR	2.1
1	A	252	PHE	2.0
1	A	142	CYS	2.0
9	I	119	THR	2.0
4	D	13	ARG	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	BRU	T	22	20/21	0.92	0.10	144,154,161,166	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
16	ZN	L	1071	1/1	0.98	0.04	154,154,154,154	0
16	ZN	I	1122	1/1	0.99	0.03	178,178,178,178	0
16	ZN	B	2225	1/1	1.00	0.03	74,74,74,74	0
16	ZN	C	1269	1/1	1.00	0.02	83,83,83,83	0
16	ZN	I	1121	1/1	1.00	0.03	115,115,115,115	0
16	ZN	A	2456	1/1	1.00	0.02	133,133,133,133	0
16	ZN	J	1066	1/1	1.00	0.03	83,83,83,83	0
16	ZN	A	2457	1/1	1.00	0.03	64,64,64,64	0
17	MG	A	2458	1/1	1.00	0.02	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.