



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:47 AM UTC

PDB ID : 5C4J / pdb_00005c4j
Title : Crystal structure of a transcribing RNA Polymerase II complex reveals a complete transcription bubble
Authors : Barnes, C.O.; Calero, M.; Malik, I.; Spahr, H.; Zhang, Q.; Pullara, F.; Kaplan, C.D.; Calero, G.
Deposited on : 2015-06-18
Resolution : 4.00 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
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

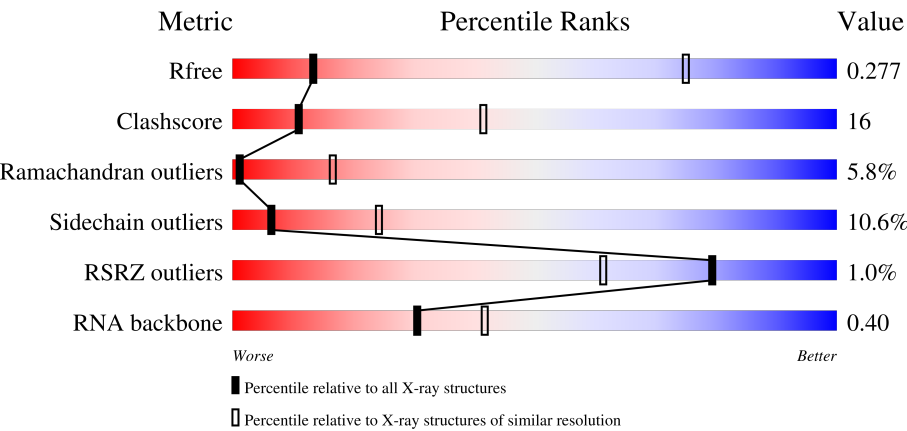
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)
RNA backbone	3983	1017 (4.84-3.10)

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	49% 27% 6% • 17%
2	B	1224	57% 31% 5% • 5%
3	C	318	51% 28% • 17%
4	E	215	63% 31% 5% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	9	
12	S	53	
13	U	53	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	ZN	C	402	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 30496 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	1432	Total	C	N	O	S	0	0	0
			11240	7079	1964	2136	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1157	Total	C	N	O	S	0	0	0
			9145	5776	1599	1714	56			

- 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
			2074	1304	345	412	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	212	Total	C	N	O	S	0	0	0
			1735	1102	306	316	11			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	143	Total	C	N	O	S	0	0	0
			1102	689	189	220	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	114	Total	C	N	O	S	0	0	0
			927	571	168	178	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	66	Total	C	N	O	S	0	0	0
			540	345	94	95	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	115	Total	C	N	O	S	0	0	0
			924	593	157	172	2			

- 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
			344	211	69	60	4			

- Molecule 11 is a RNA chain called RNA (5'-R(P*UP*CP*GP*AP*GP*AP*GP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	9	Total	C	N	O	P	0	0	0
			197	88	40	60	9			

- Molecule 12 is a DNA chain called NON-TEMPLATE STRAND DNA (38-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	S	38	Total	C	N	O	P	0	0	0
			782	371	142	231	38			

- Molecule 13 is a DNA chain called TEMPLATE STRAND DNA (38-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	U	38	Total	C	N	O	P	0	0	0
			771	366	144	223	38			

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

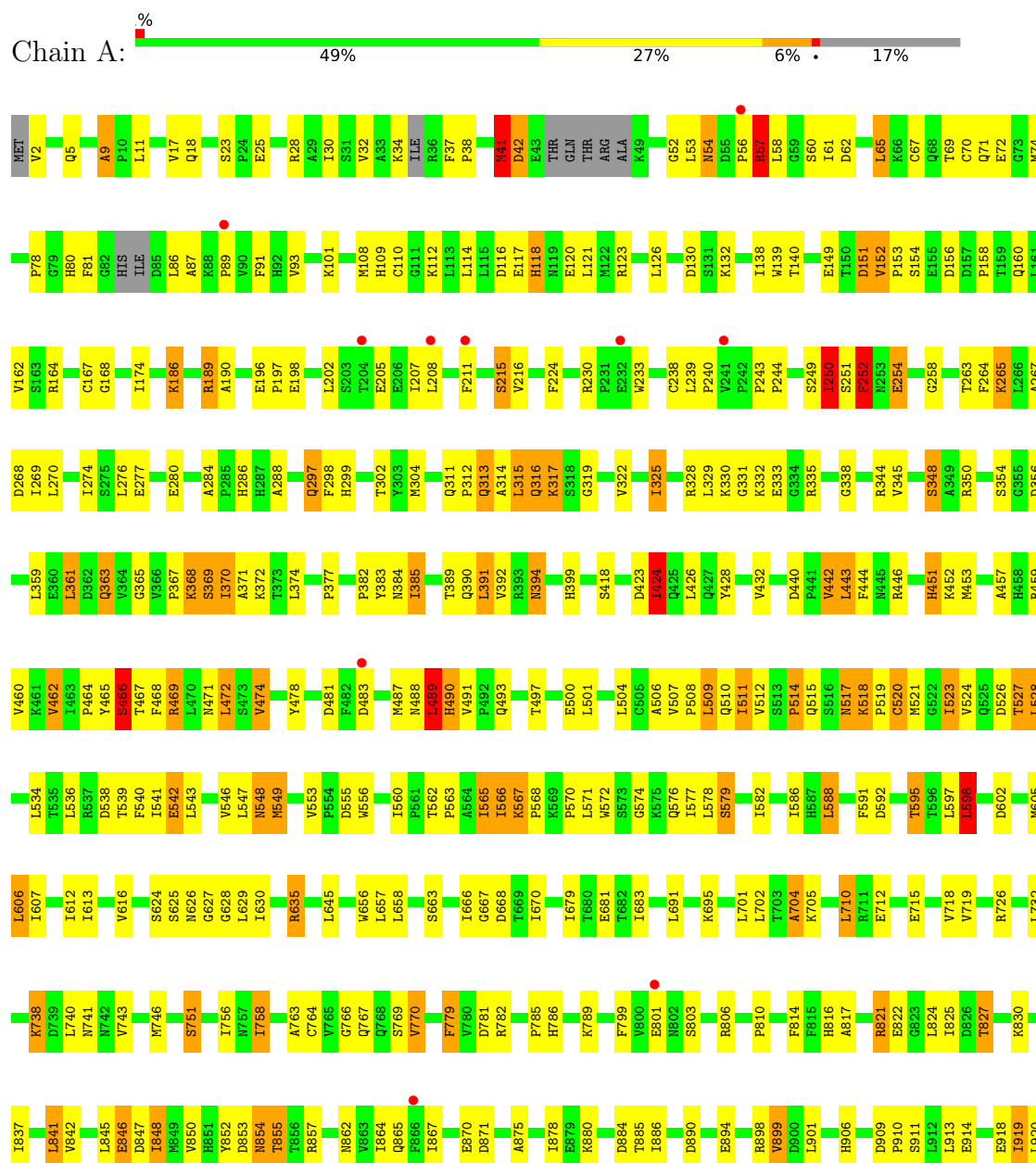
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

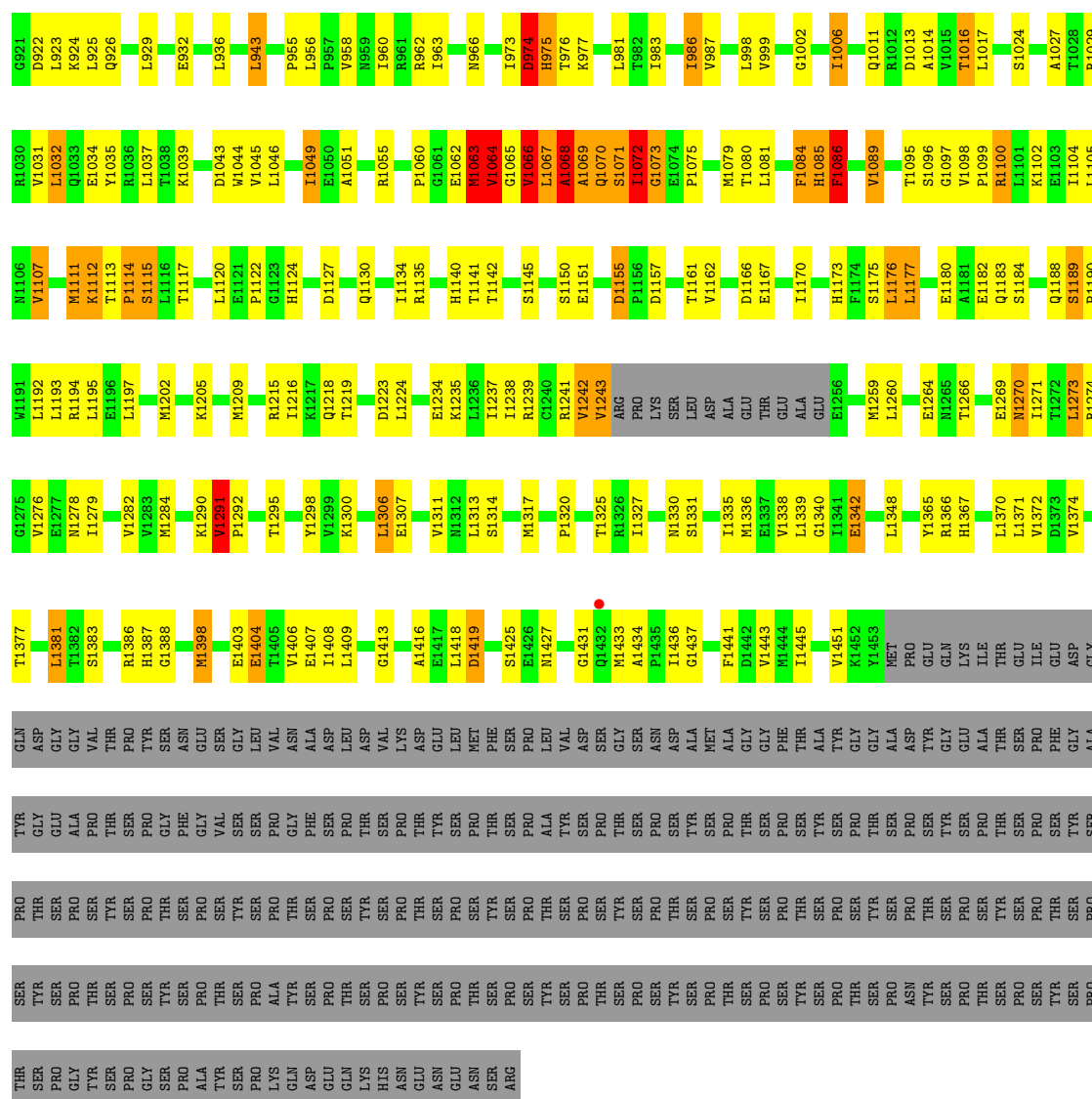
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	R	1	Total 1	Mg 1	0	0

3 Residue-property plots

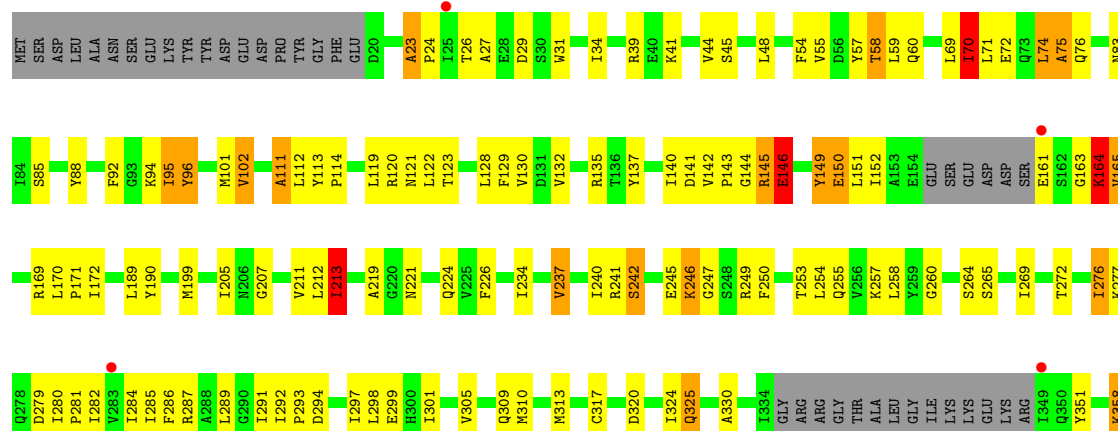
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

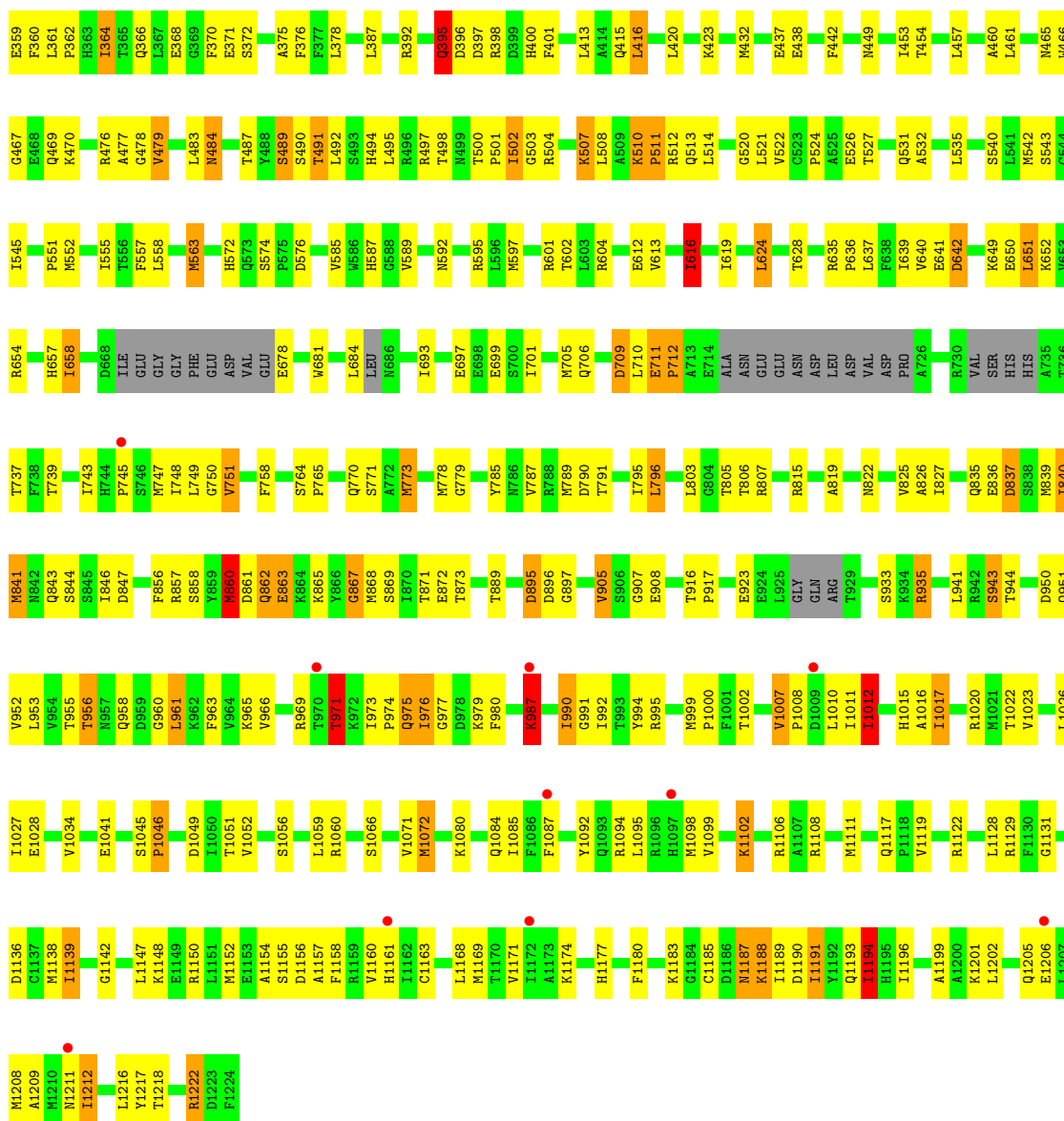
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



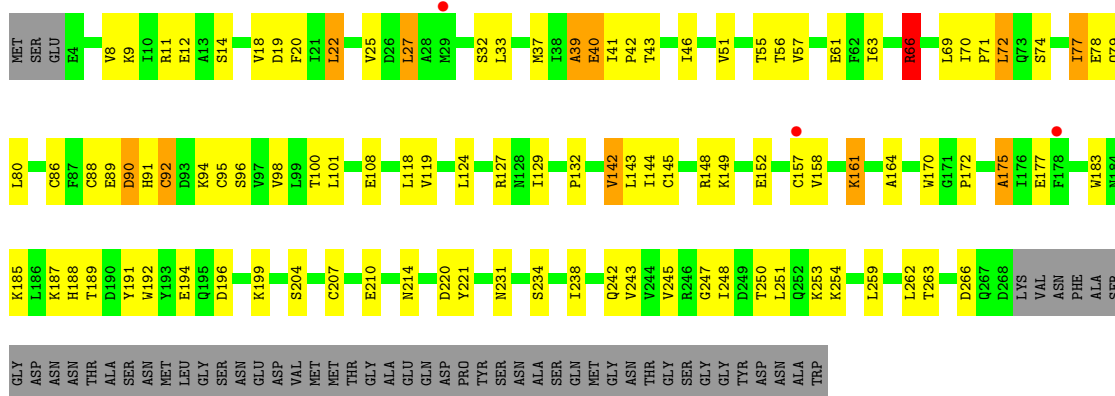


• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

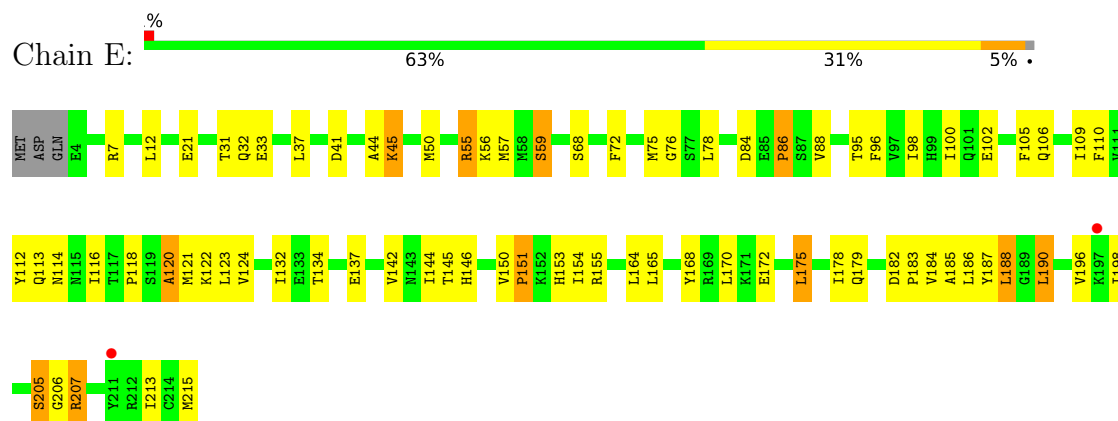




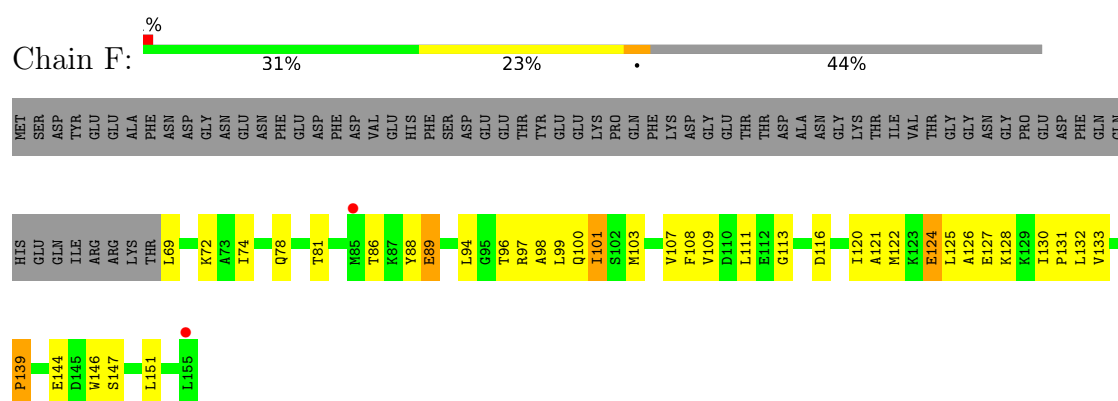
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



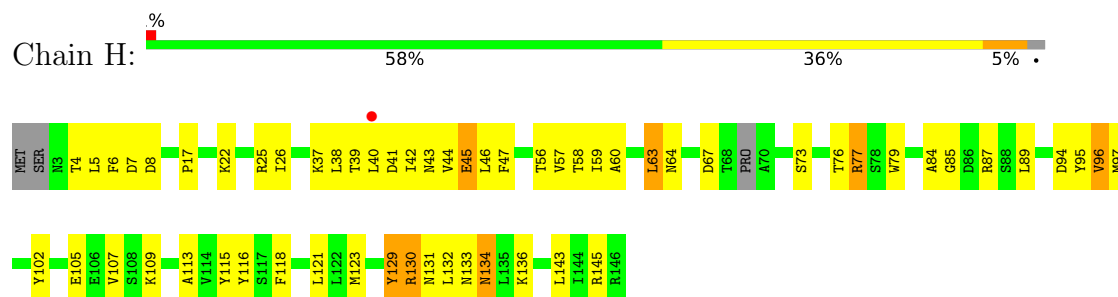
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



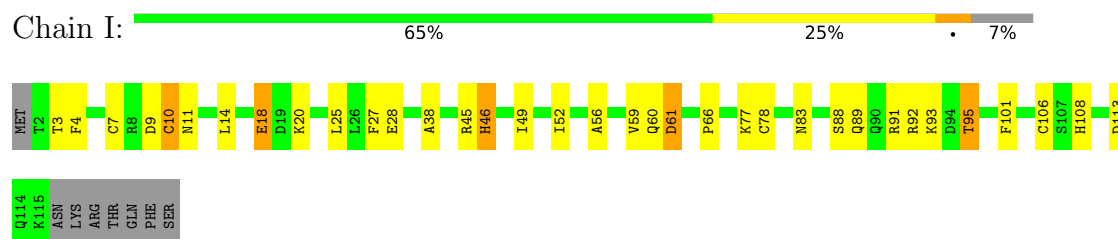
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



- 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

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	280.71 Å 223.38 Å 156.42 Å 90.00° 98.14° 90.00°	Depositor
Resolution (Å)	174.08 – 4.00 174.08 – 4.00	Depositor EDS
% Data completeness (in resolution range)	97.7 (174.08-4.00) 97.7 (174.08-4.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 4.00 Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.212 , 0.271 0.230 , 0.277	Depositor DCC
R_{free} test set	2689 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å ²)	155.3	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 213.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	30496	wwPDB-VP
Average B, all atoms (Å ²)	231.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: ZN, MG

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	0.81	2/11441 (0.0%)	1.48	105/15470 (0.7%)
2	B	0.80	2/9320 (0.0%)	1.42	61/12568 (0.5%)
3	C	0.79	0/2112	1.33	8/2866 (0.3%)
4	E	0.77	0/1771	1.42	9/2383 (0.4%)
5	F	0.76	0/717	1.42	5/967 (0.5%)
6	H	0.78	0/1120	1.37	7/1513 (0.5%)
7	I	0.71	0/945	1.38	4/1273 (0.3%)
8	J	0.78	0/549	1.43	6/738 (0.8%)
9	K	0.72	0/942	1.33	4/1272 (0.3%)
10	L	0.72	0/346	1.31	0/457
11	R	0.41	0/221	0.69	0/343
12	S	0.45	0/876	1.35	9/1351 (0.7%)
13	U	0.44	0/864	1.32	8/1328 (0.6%)
All	All	0.77	4/31224 (0.0%)	1.42	226/42529 (0.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1072	ILE	CA-C	6.37	1.60	1.52
2	B	527	THR	CA-C	5.67	1.58	1.52
1	A	1068	ALA	CA-C	5.19	1.59	1.52
2	B	161	GLU	N-CA	5.15	1.56	1.46

All (226) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	74	LEU	N-CA-C	12.36	128.54	112.72
5	F	96	THR	N-CA-C	10.79	123.13	111.36
4	E	55	ARG	N-CA-C	10.75	124.08	111.71
6	H	132	LEU	N-CA-C	10.36	123.63	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	U	25	DT	P-O3'-C3'	9.44	134.36	120.20
4	E	205	SER	N-CA-C	9.12	125.58	113.72
12	S	10	DG	P-O3'-C3'	9.12	133.88	120.20
4	E	122	LYS	N-CA-C	9.08	121.26	111.36
13	U	27	DG	P-O3'-C3'	8.96	133.64	120.20
7	I	18	GLU	N-CA-C	8.81	124.44	112.90
13	U	35	DG	P-O3'-C3'	8.59	133.09	120.20
13	U	17	DC	P-O3'-C3'	8.39	132.79	120.20
1	A	864	ILE	N-CA-C	-8.27	103.76	111.45
2	B	149	TYR	CA-C-N	8.12	136.31	121.70
2	B	149	TYR	C-N-CA	8.12	136.31	121.70
1	A	1071	SER	N-CA-C	-8.02	101.82	112.72
1	A	244	PRO	N-CA-C	7.99	120.45	110.70
1	A	1331	SER	CA-C-N	7.86	131.85	120.38
1	A	1331	SER	C-N-CA	7.86	131.85	120.38
6	H	134	ASN	N-CA-CB	7.77	122.53	109.87
1	A	1063	MET	CA-C-N	7.71	135.86	121.97
1	A	1063	MET	C-N-CA	7.71	135.86	121.97
1	A	151	ASP	CA-C-N	7.62	135.41	121.70
1	A	151	ASP	C-N-CA	7.62	135.41	121.70
2	B	70	ILE	N-CA-C	7.61	118.76	108.11
1	A	974	ASP	CA-C-N	7.58	135.35	121.70
1	A	974	ASP	C-N-CA	7.58	135.35	121.70
5	F	98	ALA	N-CA-C	-7.27	103.35	111.28
2	B	164	LYS	CA-C-N	7.20	134.93	121.97
2	B	164	LYS	C-N-CA	7.20	134.93	121.97
1	A	1291	VAL	CB-CA-C	7.10	116.29	109.33
12	S	12	DA	P-O3'-C3'	7.09	130.84	120.20
1	A	1071	SER	CA-C-N	7.02	134.60	121.97
1	A	1071	SER	C-N-CA	7.02	134.60	121.97
1	A	1066	VAL	CA-C-N	6.99	134.88	121.54
1	A	1066	VAL	C-N-CA	6.99	134.88	121.54
1	A	1086	PHE	CA-CB-CG	6.88	120.69	113.80
2	B	976	ILE	N-CA-CB	6.76	119.22	110.57
13	U	14	DA	P-O3'-C3'	6.73	130.29	120.20
2	B	141	ASP	N-CA-C	6.70	119.36	109.24
2	B	145	ARG	CA-C-N	6.59	133.56	121.70
2	B	145	ARG	C-N-CA	6.59	133.56	121.70
2	B	368	GLU	N-CA-C	6.51	118.96	111.02
2	B	1152	MET	N-CA-C	6.49	114.10	108.78
9	K	70	ARG	N-CA-C	6.47	119.00	108.26
1	A	1177	LEU	N-CA-C	6.45	119.38	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1311	VAL	N-CA-C	6.44	116.14	106.42
2	B	1122	ARG	CA-C-N	6.43	129.14	120.65
2	B	1122	ARG	C-N-CA	6.43	129.14	120.65
6	H	39	THR	N-CA-C	-6.34	98.08	108.41
5	F	98	ALA	N-CA-CB	6.33	119.42	110.12
12	S	28	DG	P-O3'-C3'	6.31	129.67	120.20
1	A	60	SER	N-CA-C	6.26	118.86	110.35
1	A	424	ILE	CA-C-N	6.25	128.98	120.54
1	A	424	ILE	C-N-CA	6.25	128.98	120.54
1	A	1167	GLU	N-CA-C	-6.22	107.53	114.62
2	B	860	MET	N-CA-C	6.22	118.83	108.20
2	B	511	PRO	CA-C-N	6.21	131.06	121.19
2	B	511	PRO	C-N-CA	6.21	131.06	121.19
2	B	943	SER	CA-C-N	6.19	129.05	120.63
2	B	943	SER	C-N-CA	6.19	129.05	120.63
1	A	1073	GLY	CA-C-N	6.19	128.55	120.26
1	A	1073	GLY	C-N-CA	6.19	128.55	120.26
1	A	69	THR	CB-CA-C	6.16	120.63	111.89
3	C	77	ILE	N-CA-C	6.15	116.32	110.42
1	A	842	VAL	N-CA-C	6.08	117.56	110.62
2	B	1211	ASN	CA-C-N	6.06	132.88	121.97
2	B	1211	ASN	C-N-CA	6.06	132.88	121.97
1	A	1089	VAL	CA-C-N	6.05	128.67	120.38
1	A	1089	VAL	C-N-CA	6.05	128.67	120.38
8	J	63	TYR	N-CA-C	-6.04	100.15	109.76
1	A	297	GLN	N-CA-C	-6.03	104.82	111.82
1	A	93	VAL	N-CA-C	6.00	117.46	110.62
2	B	359	GLU	N-CA-C	5.98	119.40	111.75
7	I	18	GLU	N-CA-CB	-5.96	101.38	110.33
1	A	459	ARG	CA-C-N	5.96	128.72	120.49
1	A	459	ARG	C-N-CA	5.96	128.72	120.49
1	A	121	LEU	N-CA-C	-5.96	106.05	113.55
2	B	616	ILE	N-CA-C	5.95	116.43	108.11
1	A	1451	VAL	CA-C-N	5.93	128.50	120.38
1	A	1451	VAL	C-N-CA	5.93	128.50	120.38
1	A	779	PHE	N-CA-C	-5.92	102.56	110.55
1	A	109	HIS	CA-C-N	5.90	132.80	121.54
1	A	109	HIS	C-N-CA	5.90	132.80	121.54
1	A	1069	ALA	N-CA-C	-5.87	105.12	112.93
2	B	991	GLY	CA-C-N	5.86	132.53	121.97
2	B	991	GLY	C-N-CA	5.86	132.53	121.97
12	S	11	DG	P-O3'-C3'	5.85	128.97	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	276	ILE	CA-C-N	5.84	130.03	120.63
2	B	276	ILE	C-N-CA	5.84	130.03	120.63
6	H	77	ARG	N-CA-C	5.82	123.19	110.80
8	J	61	LEU	N-CA-C	5.79	117.59	111.28
2	B	190	TYR	CA-C-N	5.75	128.45	120.29
2	B	190	TYR	C-N-CA	5.75	128.45	120.29
1	A	126	LEU	CA-C-N	5.74	128.24	120.38
1	A	126	LEU	C-N-CA	5.74	128.24	120.38
2	B	1017	ILE	N-CA-C	5.72	121.23	108.88
4	E	120	ALA	N-CA-C	-5.71	105.03	112.23
1	A	1387	HIS	N-CA-C	5.71	117.37	111.03
1	A	451	HIS	CA-C-N	5.70	128.19	120.38
1	A	451	HIS	C-N-CA	5.70	128.19	120.38
1	A	1443	VAL	N-CA-CB	5.70	116.74	110.53
2	B	1194	ILE	N-CA-C	5.68	118.13	108.86
2	B	498	THR	N-CA-C	5.67	118.39	107.44
12	S	4	DG	P-O3'-C3'	5.67	128.71	120.20
1	A	91	PHE	CA-CB-CG	5.66	119.46	113.80
2	B	371	GLU	N-CA-C	5.66	117.60	110.24
2	B	1139	ILE	N-CA-C	-5.64	105.60	110.74
7	I	61	ASP	N-CA-C	-5.63	105.75	113.30
9	K	110	ASN	CA-C-N	5.59	127.78	120.28
9	K	110	ASN	C-N-CA	5.59	127.78	120.28
1	A	1331	SER	N-CA-C	5.58	117.56	108.63
1	A	252	PHE	CA-CB-CG	5.58	119.38	113.80
2	B	751	VAL	CA-C-N	5.53	128.46	120.38
2	B	751	VAL	C-N-CA	5.53	128.46	120.38
13	U	25	DT	C4'-C3'-O3'	5.53	118.29	110.00
1	A	9	ALA	N-CA-C	5.52	115.94	109.60
8	J	16	ASP	CA-C-N	5.51	128.43	120.38
8	J	16	ASP	C-N-CA	5.51	128.43	120.38
1	A	1084	PHE	CA-C-N	5.51	132.06	121.54
1	A	1084	PHE	C-N-CA	5.51	132.06	121.54
4	E	165	LEU	N-CA-C	-5.49	106.54	113.18
12	S	15	DC	O4'-C1'-N1	5.46	116.59	108.40
13	U	35	DG	N9-C1'-C2'	5.45	121.67	113.50
1	A	62	ASP	CA-C-N	5.44	128.11	120.28
1	A	62	ASP	C-N-CA	5.44	128.11	120.28
12	S	13	DA	P-O5'-C5'	5.43	128.15	120.00
2	B	75	ALA	N-CA-C	5.43	117.93	109.52
1	A	1006	ILE	N-CA-CB	5.42	116.52	110.51
2	B	1188	LYS	CA-C-N	5.41	127.96	121.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1188	LYS	C-N-CA	5.41	127.96	121.84
1	A	489	LEU	CA-C-N	5.41	131.87	121.54
1	A	489	LEU	C-N-CA	5.41	131.87	121.54
2	B	1189	ILE	N-CA-C	-5.41	107.55	112.96
1	A	1102	LYS	N-CA-C	-5.38	105.49	111.36
1	A	1029	ARG	CA-C-N	5.37	127.79	120.54
1	A	1029	ARG	C-N-CA	5.37	127.79	120.54
2	B	916	THR	CB-CA-C	5.37	116.13	110.17
1	A	1180	GLU	N-CA-C	5.36	117.00	110.41
2	B	102	VAL	N-CA-C	5.36	115.61	108.11
6	H	136	LYS	CA-C-N	5.36	131.34	121.70
6	H	136	LYS	C-N-CA	5.36	131.34	121.70
1	A	705	LYS	N-CA-C	5.33	117.21	110.33
7	I	91	ARG	N-CA-C	5.33	117.42	108.73
8	J	15	GLY	CA-C-N	5.33	127.42	120.28
8	J	15	GLY	C-N-CA	5.33	127.42	120.28
3	C	66	ARG	CA-C-N	5.32	127.72	120.54
3	C	66	ARG	C-N-CA	5.32	127.72	120.54
1	A	848	ILE	CB-CA-C	5.32	118.46	111.33
2	B	370	PHE	CA-C-N	5.29	128.60	120.82
2	B	370	PHE	C-N-CA	5.29	128.60	120.82
2	B	557	PHE	CA-CB-CG	5.28	119.08	113.80
1	A	189	ARG	CA-C-N	5.27	131.61	121.54
1	A	189	ARG	C-N-CA	5.27	131.61	121.54
1	A	74	MET	N-CA-C	-5.27	106.92	113.55
1	A	224	PHE	N-CA-C	5.26	117.11	110.33
1	A	497	THR	CA-C-N	5.25	127.75	120.29
1	A	497	THR	C-N-CA	5.25	127.75	120.29
1	A	1188	GLN	CA-C-N	5.24	131.14	121.70
1	A	1188	GLN	C-N-CA	5.24	131.14	121.70
1	A	313	GLN	CA-C-N	5.24	128.98	120.60
1	A	313	GLN	C-N-CA	5.24	128.98	120.60
2	B	491	THR	CA-C-N	5.24	127.25	120.44
2	B	491	THR	C-N-CA	5.24	127.25	120.44
13	U	35	DG	P-O5'-C5'	5.24	127.85	120.00
1	A	372	LYS	N-CA-C	-5.23	107.44	113.88
2	B	856	PHE	CA-CB-CG	5.23	119.03	113.80
2	B	971	THR	N-CA-C	5.23	117.98	107.41
1	A	514	PRO	CA-C-N	5.22	128.05	120.79
1	A	514	PRO	C-N-CA	5.22	128.05	120.79
1	A	526	ASP	CA-CB-CG	5.21	117.81	112.60
2	B	847	ASP	CA-CB-CG	5.21	117.81	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	867	GLY	CA-C-N	5.21	131.07	121.70
2	B	867	GLY	C-N-CA	5.21	131.07	121.70
1	A	488	ASN	CA-CB-CG	5.20	117.80	112.60
2	B	213	ILE	CB-CA-C	5.18	117.89	111.15
12	S	14	DG	P-O3'-C3'	5.18	127.96	120.20
12	S	28	DG	N9-C1'-C2'	5.18	121.26	113.50
2	B	790	ASP	CA-C-N	5.17	128.18	120.31
2	B	790	ASP	C-N-CA	5.17	128.18	120.31
1	A	466	SER	N-CA-C	5.17	121.82	110.80
1	A	1443	VAL	N-CA-C	5.17	115.71	108.89
1	A	264	PHE	CA-CB-CG	5.16	118.96	113.80
6	H	131	ASN	N-CA-C	5.16	116.15	108.31
1	A	460	VAL	N-CA-C	5.16	116.88	109.51
2	B	372	SER	N-CA-C	-5.15	106.26	112.54
4	E	114	ASN	CA-C-N	5.13	128.96	121.31
4	E	114	ASN	C-N-CA	5.13	128.96	121.31
3	C	204	SER	CA-C-N	5.13	127.67	120.28
3	C	204	SER	C-N-CA	5.13	127.67	120.28
1	A	288	ALA	CA-C-N	5.13	127.70	120.42
1	A	288	ALA	C-N-CA	5.13	127.70	120.42
2	B	1102	LYS	CA-C-N	5.13	128.24	120.75
2	B	1102	LYS	C-N-CA	5.13	128.24	120.75
5	F	89	GLU	CA-C-N	5.13	128.51	120.82
5	F	89	GLU	C-N-CA	5.13	128.51	120.82
3	C	39	ALA	N-CA-C	5.12	119.40	111.56
1	A	487	MET	CA-C-N	5.11	129.81	121.74
1	A	487	MET	C-N-CA	5.11	129.81	121.74
1	A	487	MET	N-CA-C	5.10	117.72	109.40
3	C	207	CYS	CA-C-N	5.10	127.37	120.38
3	C	207	CYS	C-N-CA	5.10	127.37	120.38
1	A	1064	VAL	N-CA-C	5.10	119.95	109.34
2	B	597	MET	CA-C-N	5.09	127.35	120.38
2	B	597	MET	C-N-CA	5.09	127.35	120.38
4	E	96	PHE	CA-C-N	5.08	127.16	120.60
4	E	96	PHE	C-N-CA	5.08	127.16	120.60
1	A	884	ASP	CA-C-N	5.08	127.85	120.79
1	A	884	ASP	C-N-CA	5.08	127.85	120.79
1	A	517	ASN	CA-CB-CG	5.07	117.67	112.60
1	A	384	ASN	CA-CB-CG	5.06	117.66	112.60
1	A	1278	ASN	CA-C-N	5.06	127.39	120.35
1	A	1278	ASN	C-N-CA	5.06	127.39	120.35
1	A	1114	PRO	CA-C-N	5.05	131.18	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1114	PRO	C-N-CA	5.05	131.18	121.54
1	A	121	LEU	CA-C-N	5.04	127.45	120.29
1	A	121	LEU	C-N-CA	5.04	127.45	120.29
2	B	658	ILE	N-CA-CB	5.03	116.10	110.62
1	A	41	MET	CA-C-N	5.03	131.14	121.54
1	A	41	MET	C-N-CA	5.03	131.14	121.54
9	K	33	ILE	N-CA-C	5.02	115.26	107.28
1	A	1085	HIS	CA-C-N	5.01	131.12	121.54
1	A	1085	HIS	C-N-CA	5.01	131.12	121.54
1	A	316	GLN	CA-C-N	5.01	131.12	121.54
1	A	316	GLN	C-N-CA	5.01	131.12	121.54
1	A	345	VAL	N-CA-C	5.01	116.57	108.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11240	0	11270	301	0
2	B	9145	0	9117	276	0
3	C	2074	0	2020	165	0
4	E	1735	0	1762	84	0
5	F	705	0	731	53	0
6	H	1102	0	1035	59	0
7	I	927	0	886	36	0
8	J	540	0	554	26	0
9	K	924	0	934	76	0
10	L	344	0	366	27	0
11	R	197	0	96	6	0
12	S	782	0	429	7	0
13	U	771	0	425	6	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	2	0	0	2	0
14	I	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	J	1	0	0	0	0
14	L	1	0	0	1	0
15	R	1	0	0	0	0
All	All	30496	0	29625	991	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 16.

All (991) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:151:PRO:HD2	4:E:153:HIS:CE1	1.30	1.65
7:I:56:ALA:HB2	7:I:89:GLN:CD	1.35	1.52
4:E:151:PRO:CD	4:E:153:HIS:HE1	1.24	1.50
7:I:56:ALA:CB	7:I:89:GLN:OE1	1.64	1.46
3:C:221:TYR:CB	6:H:46:LEU:HD22	1.44	1.43
1:A:53:LEU:HD23	1:A:54:ASN:N	1.45	1.30
7:I:56:ALA:CB	7:I:89:GLN:CD	2.03	1.29
1:A:116:ASP:OD1	1:A:164:ARG:CG	1.78	1.29
3:C:221:TYR:CA	6:H:46:LEU:CD2	2.10	1.29
1:A:116:ASP:OD1	1:A:164:ARG:HG2	1.17	1.28
3:C:221:TYR:HA	6:H:46:LEU:CD2	1.60	1.28
3:C:8:VAL:HG23	9:K:108:GLU:OE1	1.26	1.27
3:C:70:ILE:HD12	3:C:142:VAL:CG1	1.66	1.23
7:I:56:ALA:CB	7:I:89:GLN:NE2	2.03	1.20
3:C:88:CYS:SG	3:C:91:HIS:O	2.00	1.18
3:C:221:TYR:CA	6:H:46:LEU:HD21	1.72	1.17
3:C:259:LEU:HG	9:K:91:CYS:SG	1.85	1.16
3:C:70:ILE:HD12	3:C:142:VAL:HG11	1.23	1.16
3:C:221:TYR:HB3	6:H:46:LEU:CD2	1.77	1.15
7:I:56:ALA:HB3	7:I:89:GLN:OE1	1.45	1.15
3:C:91:HIS:CD2	3:C:96:SER:CB	2.31	1.14
1:A:870:GLU:O	4:E:205:SER:HB2	1.48	1.12
6:H:41:ASP:O	6:H:42:ILE:HG13	1.49	1.12
10:L:57:LEU:HD23	10:L:59:ALA:N	1.63	1.12
3:C:221:TYR:CA	6:H:46:LEU:HD22	1.75	1.10
7:I:56:ALA:HB2	7:I:89:GLN:NE2	1.65	1.10
3:C:118:LEU:HD11	3:C:132:PRO:HG3	1.27	1.08
1:A:1067:LEU:O	1:A:1069:ALA:N	1.86	1.08
3:C:70:ILE:CD1	3:C:142:VAL:HG11	1.83	1.07
7:I:56:ALA:CB	7:I:89:GLN:HE22	1.65	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:56:ALA:HB2	7:I:89:GLN:OE1	1.34	1.07
3:C:8:VAL:CG2	9:K:108:GLU:OE1	2.03	1.05
2:B:289:LEU:CD2	2:B:375:ALA:HB2	1.85	1.05
4:E:151:PRO:CD	4:E:153:HIS:CE1	2.11	1.04
2:B:285:ILE:HD13	2:B:378:LEU:HD11	1.37	1.04
9:K:75:ILE:HD13	9:K:83:PRO:HB2	1.06	1.04
9:K:94:ILE:O	9:K:98:LEU:HD13	1.58	1.03
5:F:94:LEU:HD12	5:F:121:ALA:CB	1.89	1.02
3:C:91:HIS:CD2	3:C:96:SER:OG	2.12	1.02
6:H:22:LYS:O	6:H:43:ASN:ND2	1.92	1.01
9:K:75:ILE:CD1	9:K:83:PRO:HB2	1.91	1.01
10:L:57:LEU:HD23	10:L:59:ALA:H	0.87	1.00
9:K:19:LEU:HD21	9:K:35:PHE:CE2	1.97	1.00
5:F:94:LEU:CD1	5:F:121:ALA:HB3	1.91	1.00
3:C:262:LEU:HD22	9:K:88:LYS:NZ	1.77	0.99
3:C:43:THR:HG21	3:C:172:PRO:HG3	1.42	0.99
2:B:282:ILE:O	2:B:285:ILE:HG22	1.63	0.98
2:B:130:VAL:HG23	2:B:132:VAL:HG23	1.42	0.98
5:F:97:ARG:HG3	5:F:101:ILE:HD12	1.44	0.97
3:C:100:THR:OG1	3:C:119:VAL:HG23	1.64	0.97
8:J:20:SER:O	8:J:24:LEU:HG	1.64	0.97
3:C:43:THR:CG2	3:C:172:PRO:HG3	1.94	0.96
4:E:178:ILE:HD11	4:E:182:ASP:OD1	1.66	0.95
9:K:75:ILE:HD13	9:K:83:PRO:CB	1.96	0.95
3:C:221:TYR:HB3	6:H:46:LEU:HD22	0.96	0.94
3:C:71:PRO:C	3:C:72:LEU:HD12	1.93	0.94
4:E:110:PHE:HE2	4:E:116:ILE:HD11	1.32	0.94
3:C:70:ILE:CD1	3:C:142:VAL:CG1	2.42	0.94
9:K:11:LEU:HD23	9:K:12:LEU:N	1.83	0.94
10:L:57:LEU:CD2	10:L:59:ALA:H	1.79	0.94
3:C:78:GLU:N	3:C:78:GLU:OE1	2.01	0.93
3:C:221:TYR:CB	6:H:46:LEU:CD2	2.29	0.93
1:A:53:LEU:HD23	1:A:54:ASN:H	1.33	0.93
4:E:184:VAL:O	4:E:188:LEU:HD13	1.66	0.93
3:C:70:ILE:HD12	3:C:142:VAL:HG12	1.49	0.93
3:C:259:LEU:CG	9:K:91:CYS:SG	2.56	0.92
2:B:285:ILE:HD13	2:B:378:LEU:CD1	2.00	0.91
3:C:91:HIS:CD2	3:C:96:SER:HB2	2.03	0.91
5:F:94:LEU:HD12	5:F:121:ALA:HB1	1.52	0.91
4:E:151:PRO:O	4:E:153:HIS:ND1	2.02	0.91
1:A:565:ILE:HD11	1:A:571:LEU:H	1.36	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:125:LEU:HD12	5:F:126:ALA:N	1.85	0.91
7:I:56:ALA:HB1	7:I:89:GLN:HE22	1.33	0.90
2:B:44:VAL:HG23	2:B:48:LEU:HD11	1.51	0.90
8:J:30:LEU:HD13	8:J:34:THR:OG1	1.72	0.89
3:C:251:LEU:HD22	9:K:98:LEU:HD21	1.54	0.89
3:C:221:TYR:HA	6:H:46:LEU:HD21	0.90	0.89
5:F:130:ILE:CG2	5:F:132:LEU:HD13	2.03	0.89
6:H:6:PHE:CZ	6:H:8:ASP:HB2	2.06	0.88
6:H:6:PHE:O	6:H:7:ASP:OD1	1.92	0.88
10:L:33:GLU:OE2	10:L:53:HIS:CD2	2.26	0.88
3:C:91:HIS:NE2	3:C:96:SER:OG	2.05	0.88
4:E:151:PRO:CG	4:E:153:HIS:CE1	2.57	0.88
1:A:354:SER:HB2	1:A:469:ARG:HD3	1.55	0.87
2:B:360:PHE:CE1	2:B:361:LEU:HD13	2.09	0.87
9:K:91:CYS:O	9:K:94:ILE:HG22	1.74	0.87
1:A:1067:LEU:HD23	1:A:1068:ALA:H	1.38	0.87
5:F:86:THR:HG22	5:F:89:GLU:OE1	1.74	0.86
2:B:289:LEU:HD23	2:B:375:ALA:HB2	1.56	0.86
1:A:565:ILE:HD11	1:A:571:LEU:N	1.91	0.86
5:F:94:LEU:CD1	5:F:121:ALA:CB	2.49	0.86
2:B:74:LEU:HD12	2:B:75:ALA:H	1.41	0.86
1:A:116:ASP:OD1	1:A:164:ARG:HG3	1.71	0.85
3:C:92:CYS:SG	14:C:402:ZN:ZN	1.64	0.85
3:C:92:CYS:HG	14:C:402:ZN:ZN	0.56	0.85
3:C:262:LEU:HD22	9:K:88:LYS:HZ3	1.40	0.85
3:C:9:LYS:HA	9:K:108:GLU:OE2	1.77	0.84
2:B:254:LEU:HD12	2:B:272:THR:O	1.76	0.84
2:B:44:VAL:HG23	2:B:48:LEU:CD1	2.06	0.84
5:F:94:LEU:HD11	5:F:121:ALA:HB3	1.58	0.84
9:K:45:LEU:HD13	9:K:94:ILE:CD1	2.07	0.83
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.60	0.82
5:F:131:PRO:C	5:F:132:LEU:HD12	2.04	0.82
4:E:110:PHE:CE2	4:E:116:ILE:HD11	2.14	0.82
3:C:92:CYS:O	3:C:96:SER:OG	1.98	0.82
2:B:69:LEU:CD1	2:B:432:MET:HE2	2.10	0.81
2:B:285:ILE:CD1	2:B:378:LEU:HD11	2.10	0.81
1:A:53:LEU:CD2	1:A:54:ASN:N	2.39	0.81
3:C:118:LEU:HD12	3:C:118:LEU:O	1.81	0.81
4:E:179:GLN:HB3	4:E:215:MET:HE2	1.63	0.81
8:J:43:ARG:O	8:J:46:CYS:SG	2.38	0.80
4:E:151:PRO:HG2	4:E:153:HIS:CE1	2.17	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:75:ILE:HD12	9:K:75:ILE:O	1.81	0.80
3:C:91:HIS:CE1	3:C:96:SER:OG	2.34	0.80
7:I:18:GLU:HG3	7:I:20:LYS:CD	2.11	0.80
1:A:845:LEU:HB3	1:A:1065:GLY:O	1.81	0.80
3:C:100:THR:OG1	3:C:119:VAL:CG2	2.29	0.80
2:B:44:VAL:CG2	2:B:48:LEU:HD11	2.11	0.79
5:F:97:ARG:HA	5:F:100:GLN:HB2	1.64	0.79
1:A:152:VAL:HG12	1:A:160:GLN:O	1.83	0.79
3:C:145:CYS:HA	8:J:2:ILE:HD11	1.64	0.78
2:B:254:LEU:CD2	2:B:361:LEU:HD11	2.13	0.78
3:C:91:HIS:NE2	3:C:96:SER:CB	2.46	0.78
3:C:259:LEU:HD21	9:K:91:CYS:HB3	1.65	0.78
4:E:118:PRO:HA	4:E:121:MET:HB2	1.65	0.78
1:A:311:GLN:HB2	1:A:312:PRO:HD2	1.66	0.78
1:A:1067:LEU:C	1:A:1069:ALA:H	1.88	0.78
7:I:18:GLU:HG3	7:I:20:LYS:HD3	1.65	0.77
2:B:149:TYR:HA	2:B:150:GLU:HB2	1.65	0.77
2:B:387:LEU:CD2	2:B:392:ARG:HB2	2.15	0.77
5:F:99:LEU:HD23	5:F:103:MET:HG2	1.65	0.77
7:I:78:CYS:SG	7:I:106:CYS:HB3	2.24	0.77
1:A:1071:SER:O	1:A:1072:ILE:HG13	1.85	0.76
1:A:870:GLU:O	4:E:205:SER:CB	2.32	0.76
2:B:282:ILE:O	2:B:285:ILE:CG2	2.31	0.76
3:C:144:ILE:O	8:J:2:ILE:HD13	1.85	0.76
1:A:467:THR:HG23	1:A:469:ARG:HH12	1.49	0.76
2:B:289:LEU:HD23	2:B:291:ILE:HD13	1.67	0.76
10:L:64:LEU:HD12	10:L:64:LEU:O	1.84	0.76
2:B:142:VAL:HB	2:B:143:PRO:HD2	1.66	0.75
3:C:27:LEU:H	3:C:27:LEU:HD23	1.51	0.75
4:E:78:LEU:HD11	4:E:109:ILE:HG12	1.68	0.75
1:A:712:GLU:HG3	7:I:93:LYS:HE2	1.68	0.75
2:B:130:VAL:CG2	2:B:132:VAL:HG23	2.14	0.75
1:A:78:PRO:HB3	2:B:1201:LYS:HD2	1.69	0.75
3:C:145:CYS:HA	8:J:2:ILE:CD1	2.17	0.74
10:L:34:CYS:SG	14:L:101:ZN:ZN	1.76	0.74
5:F:86:THR:HG23	5:F:89:GLU:H	1.52	0.74
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.51	0.74
1:A:566:ILE:HB	6:H:96:VAL:HG23	1.69	0.74
4:E:144:ILE:CD1	4:E:183:PRO:HB2	2.18	0.74
9:K:11:LEU:HD23	9:K:12:LEU:H	1.50	0.73
2:B:26:THR:HG22	2:B:27:ALA:N	2.03	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:88:VAL:HB	4:E:116:ILE:HG12	1.70	0.72
9:K:45:LEU:HD13	9:K:94:ILE:HD11	1.69	0.72
2:B:69:LEU:HD12	2:B:432:MET:HE2	1.70	0.72
2:B:213:ILE:HD11	2:B:497:ARG:HB3	1.71	0.72
2:B:254:LEU:HD23	2:B:361:LEU:HD11	1.71	0.72
5:F:94:LEU:HD12	5:F:121:ALA:HB3	1.57	0.72
6:H:40:LEU:HD23	6:H:41:ASP:N	2.03	0.72
1:A:252:PHE:HZ	11:R:2:U:C1'	2.02	0.72
9:K:94:ILE:O	9:K:98:LEU:CD1	2.36	0.72
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.72	0.72
4:E:151:PRO:HG2	4:E:198:ILE:CG2	2.21	0.71
1:A:37:PHE:H	1:A:52:GLY:HA3	1.55	0.71
3:C:259:LEU:CD1	9:K:91:CYS:SG	2.78	0.71
3:C:33:LEU:O	3:C:33:LEU:HD23	1.90	0.71
3:C:91:HIS:CG	3:C:96:SER:OG	2.44	0.71
1:A:1342:GLU:HB3	4:E:151:PRO:HG3	1.72	0.70
3:C:91:HIS:NE2	3:C:96:SER:HB2	2.04	0.70
1:A:770:VAL:HG23	1:A:822:GLU:HG3	1.73	0.70
2:B:74:LEU:HD12	2:B:75:ALA:N	2.06	0.70
1:A:963:ILE:HD13	1:A:1049:ILE:HG13	1.72	0.70
2:B:101:MET:HG2	2:B:111:ALA:HA	1.73	0.70
4:E:124:VAL:HG13	4:E:132:ILE:HB	1.73	0.70
1:A:53:LEU:HD23	1:A:53:LEU:C	2.17	0.70
3:C:221:TYR:N	6:H:46:LEU:CD2	2.53	0.70
1:A:443:LEU:HG	1:A:501:LEU:HD21	1.74	0.70
2:B:360:PHE:CZ	2:B:361:LEU:HD13	2.26	0.70
3:C:70:ILE:O	3:C:72:LEU:CD1	2.40	0.70
2:B:285:ILE:CD1	2:B:378:LEU:CD1	2.66	0.70
10:L:30:ILE:CG2	10:L:57:LEU:HB3	2.22	0.70
9:K:87:LEU:C	9:K:87:LEU:HD23	2.17	0.70
10:L:57:LEU:CD2	10:L:59:ALA:N	2.46	0.70
6:H:96:VAL:HG12	6:H:143:LEU:HA	1.75	0.69
1:A:446:ARG:HB3	1:A:478:TYR:HD2	1.57	0.69
7:I:78:CYS:SG	7:I:106:CYS:CB	2.81	0.69
10:L:57:LEU:CD2	10:L:59:ALA:HA	2.23	0.69
3:C:33:LEU:HD23	3:C:33:LEU:C	2.18	0.69
1:A:1170:ILE:HD11	1:A:1239:ARG:HH11	1.57	0.69
8:J:36:LEU:HA	8:J:41:LEU:HD12	1.75	0.69
1:A:252:PHE:CE2	11:R:2:U:H4'	2.28	0.68
1:A:738:LYS:HE3	3:C:194:GLU:HA	1.73	0.68
5:F:130:ILE:HG23	5:F:132:LEU:HD13	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:11:LEU:O	9:K:37:LYS:HG3	1.92	0.68
9:K:19:LEU:HD21	9:K:35:PHE:CD2	2.27	0.68
3:C:33:LEU:HD21	3:C:37:MET:SD	2.33	0.68
4:E:185:ALA:O	4:E:190:LEU:HD23	1.93	0.68
5:F:99:LEU:HD23	5:F:99:LEU:C	2.18	0.68
10:L:30:ILE:HG22	10:L:57:LEU:HB3	1.74	0.68
4:E:206:GLY:O	4:E:207:ARG:HG2	1.94	0.68
2:B:69:LEU:HD12	2:B:69:LEU:O	1.93	0.68
1:A:1067:LEU:HD23	1:A:1068:ALA:N	2.08	0.68
1:A:1155:ASP:HB3	1:A:1162:VAL:HG23	1.76	0.68
2:B:654:ARG:H	2:B:657:HIS:HD2	1.42	0.68
1:A:369:SER:O	1:A:371:ALA:N	2.28	0.67
3:C:262:LEU:HD23	3:C:262:LEU:O	1.94	0.67
1:A:855:THR:CG2	1:A:857:ARG:HE	2.07	0.67
2:B:137:TYR:CE1	2:B:151:LEU:HD13	2.28	0.67
3:C:262:LEU:HD23	3:C:262:LEU:C	2.20	0.67
2:B:387:LEU:C	2:B:387:LEU:HD23	2.19	0.67
3:C:57:VAL:HG21	8:J:60:PHE:HB3	1.76	0.67
9:K:21:ILE:HA	9:K:33:ILE:HG22	1.77	0.67
2:B:955:THR:HG22	2:B:956:THR:H	1.60	0.67
3:C:72:LEU:HD12	3:C:72:LEU:N	2.10	0.67
12:S:14:DG:H4'	12:S:15:DC:H5'	1.76	0.67
1:A:515:GLN:NE2	1:A:1075:PRO:HD3	2.09	0.67
1:A:1434:ALA:HB1	1:A:1436:ILE:HD13	1.76	0.67
2:B:416:LEU:HD22	2:B:466:TRP:CE3	2.29	0.67
1:A:348:SER:HB3	2:B:1128:LEU:HB2	1.76	0.67
4:E:188:LEU:N	4:E:188:LEU:HD12	2.10	0.67
1:A:252:PHE:HZ	11:R:2:U:H1'	1.60	0.66
1:A:367:PRO:HB3	9:K:2:ASN:ND2	2.11	0.66
2:B:387:LEU:HD23	2:B:392:ARG:HB2	1.77	0.66
5:F:130:ILE:HG22	5:F:132:LEU:HD13	1.77	0.66
3:C:27:LEU:HD23	3:C:27:LEU:N	2.11	0.66
4:E:37:LEU:HD21	4:E:45:LYS:NZ	2.11	0.66
1:A:810:PRO:HB3	2:B:745:PRO:HB3	1.76	0.66
2:B:397:ASP:HB3	2:B:400:HIS:HB2	1.77	0.66
1:A:53:LEU:HD23	1:A:54:ASN:CA	2.26	0.66
4:E:190:LEU:N	4:E:190:LEU:HD22	2.10	0.66
9:K:91:CYS:O	9:K:94:ILE:CG2	2.44	0.66
6:H:40:LEU:HD23	6:H:40:LEU:C	2.21	0.66
6:H:44:VAL:O	6:H:45:GLU:C	2.37	0.66
1:A:382:PRO:HD3	1:A:428:TYR:HE1	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:MET:HE1	2:B:1015:HIS:HA	1.78	0.65
7:I:56:ALA:HB3	7:I:89:GLN:CD	2.03	0.65
2:B:254:LEU:CD2	2:B:361:LEU:CD1	2.74	0.65
2:B:841:MET:HB3	2:B:846:ILE:HD11	1.77	0.65
3:C:51:VAL:HB	10:L:65:VAL:CG2	2.26	0.65
9:K:12:LEU:N	9:K:12:LEU:HD12	2.10	0.65
9:K:87:LEU:HD23	9:K:87:LEU:O	1.95	0.65
1:A:1071:SER:HB3	1:A:1367:HIS:CD2	2.31	0.65
3:C:27:LEU:H	3:C:27:LEU:CD2	2.09	0.65
2:B:858:SER:HA	2:B:966:VAL:O	1.96	0.65
1:A:974:ASP:HA	1:A:975:HIS:HB2	1.77	0.65
2:B:511:PRO:HD2	2:B:512:ARG:HG3	1.78	0.65
3:C:33:LEU:CD2	3:C:37:MET:SD	2.85	0.65
3:C:262:LEU:CD2	9:K:88:LYS:NZ	2.58	0.65
8:J:30:LEU:HD13	8:J:34:THR:HG1	1.60	0.65
2:B:1084:GLN:HE22	3:C:191:TYR:HA	1.61	0.65
1:A:855:THR:HG21	1:A:857:ARG:HE	1.62	0.64
3:C:22:LEU:HD23	3:C:25:VAL:HG21	1.79	0.64
1:A:846:GLU:O	1:A:1066:VAL:HG12	1.97	0.64
1:A:335:ARG:HE	2:B:1202:LEU:HD23	1.61	0.64
4:E:151:PRO:O	4:E:153:HIS:CE1	2.49	0.64
3:C:80:LEU:HD12	3:C:94:LYS:O	1.98	0.64
2:B:526:GLU:HG2	2:B:771:SER:HB2	1.80	0.64
3:C:259:LEU:HD21	9:K:91:CYS:CB	2.28	0.64
8:J:10:CYS:SG	8:J:11:GLY:N	2.70	0.64
2:B:26:THR:HG22	2:B:27:ALA:H	1.62	0.63
4:E:187:TYR:C	4:E:188:LEU:HD12	2.23	0.63
2:B:826:ALA:HB3	2:B:1011:ILE:HG12	1.81	0.63
2:B:387:LEU:HD23	2:B:387:LEU:O	1.99	0.63
3:C:262:LEU:HD22	9:K:88:LYS:HZ1	1.62	0.63
3:C:9:LYS:CA	9:K:108:GLU:OE2	2.46	0.63
1:A:781:ASP:HB2	1:A:789:LYS:HG2	1.79	0.63
2:B:289:LEU:HD21	2:B:375:ALA:HB2	1.78	0.63
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.81	0.63
4:E:188:LEU:HB2	4:E:190:LEU:HD21	1.81	0.63
1:A:451:HIS:CD2	1:A:453:MET:HB2	2.34	0.62
1:A:1063:MET:O	1:A:1066:VAL:HG13	1.99	0.62
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.80	0.62
6:H:44:VAL:HA	6:H:47:PHE:O	1.99	0.62
1:A:1182:GLU:HB2	1:A:1183:GLN:HB3	1.81	0.62
2:B:542:MET:HB3	2:B:636:PRO:HD2	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.81	0.62
3:C:66:ARG:NH2	8:J:2:ILE:HG22	2.14	0.62
2:B:867:GLY:HA3	2:B:869:SER:H	1.63	0.62
2:B:1142:GLY:HA3	5:F:88:TYR:CE2	2.34	0.62
4:E:179:GLN:HA	4:E:215:MET:HG2	1.81	0.62
4:E:182:ASP:OD1	4:E:184:VAL:HG22	2.00	0.62
1:A:1016:THR:HB	4:E:206:GLY:HA3	1.82	0.62
2:B:26:THR:CG2	2:B:27:ALA:H	2.13	0.62
10:L:43:THR:O	10:L:44:ASP:OD1	2.16	0.62
3:C:70:ILE:HD13	3:C:142:VAL:HG11	1.78	0.61
6:H:43:ASN:ND2	6:H:44:VAL:H	1.98	0.61
2:B:254:LEU:HD22	2:B:361:LEU:CD1	2.30	0.61
2:B:1080:LYS:HE3	3:C:188:HIS:HB2	1.82	0.61
1:A:1070:GLN:C	1:A:1072:ILE:H	2.09	0.61
1:A:1111:MET:HG3	1:A:1112:LYS:H	1.65	0.61
2:B:72:GLU:OE1	2:B:74:LEU:HD23	1.99	0.61
2:B:309:GLN:HE21	2:B:392:ARG:HH21	1.49	0.61
2:B:358:LYS:HA	2:B:366:GLN:HB2	1.82	0.61
2:B:74:LEU:HB3	2:B:85:SER:HA	1.83	0.61
3:C:221:TYR:HB3	6:H:46:LEU:CG	2.30	0.61
7:I:56:ALA:CA	7:I:89:GLN:OE1	2.45	0.61
10:L:57:LEU:CD2	10:L:59:ALA:CA	2.78	0.61
1:A:89:PRO:HD2	1:A:205:GLU:HG2	1.82	0.61
2:B:642:ASP:HA	2:B:649:LYS:HG2	1.83	0.61
4:E:37:LEU:HD11	4:E:45:LYS:NZ	2.16	0.61
4:E:144:ILE:HD12	4:E:183:PRO:HB2	1.82	0.61
5:F:130:ILE:CG2	5:F:132:LEU:CD1	2.78	0.61
8:J:30:LEU:HD12	8:J:31:ASP:O	2.01	0.61
1:A:901:LEU:H	1:A:926:GLN:NE2	1.99	0.61
5:F:99:LEU:HD23	5:F:99:LEU:O	2.02	0.60
1:A:824:LEU:HD21	2:B:765:PRO:HB3	1.82	0.60
2:B:542:MET:HG2	2:B:747:MET:HB3	1.84	0.60
1:A:472:LEU:HD22	2:B:835:GLN:HE22	1.67	0.60
2:B:221:ASN:HB3	2:B:242:SER:HA	1.83	0.60
1:A:974:ASP:HB3	1:A:976:THR:H	1.66	0.60
3:C:259:LEU:HD11	9:K:91:CYS:SG	2.42	0.60
12:S:10:DG:H1	13:U:31:DC:H42	1.47	0.60
5:F:111:LEU:HG	5:F:113:GLY:H	1.66	0.60
6:H:116:TYR:HB2	6:H:123:MET:HB3	1.83	0.60
1:A:252:PHE:HE2	11:R:2:U:H4'	1.64	0.60
1:A:489:LEU:HG	1:A:490:HIS:H	1.67	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:91:HIS:CG	3:C:92:CYS:H	2.20	0.60
1:A:81:PHE:HE2	2:B:1209:ALA:HB2	1.66	0.59
3:C:32:SER:CB	9:K:45:LEU:HD23	2.32	0.59
4:E:144:ILE:CD1	4:E:183:PRO:CB	2.80	0.59
5:F:86:THR:HG22	5:F:89:GLU:CD	2.28	0.59
2:B:26:THR:CG2	2:B:27:ALA:N	2.65	0.59
3:C:43:THR:HG1	3:C:170:TRP:CD1	2.20	0.59
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.84	0.59
4:E:37:LEU:HD21	4:E:45:LYS:HZ3	1.66	0.59
2:B:170:LEU:HD12	2:B:171:PRO:HD2	1.84	0.59
10:L:64:LEU:HD12	10:L:64:LEU:C	2.28	0.59
1:A:446:ARG:HB3	1:A:478:TYR:CD2	2.38	0.59
3:C:66:ARG:NH1	8:J:2:ILE:CG2	2.65	0.59
1:A:359:LEU:HD22	1:A:363:GLN:HB3	1.84	0.59
3:C:77:ILE:HG13	3:C:161:LYS:HE3	1.83	0.59
4:E:187:TYR:HB3	4:E:188:LEU:HD12	1.85	0.59
3:C:66:ARG:CZ	8:J:2:ILE:HG22	2.32	0.59
3:C:89:GLU:O	3:C:90:ASP:OD1	2.20	0.59
9:K:65:HIS:CD2	9:K:67:PHE:HB2	2.38	0.59
9:K:45:LEU:HD13	9:K:94:ILE:HD12	1.84	0.58
1:A:850:VAL:HG23	1:A:1064:VAL:HG21	1.86	0.58
3:C:92:CYS:SG	3:C:95:CYS:SG	3.01	0.58
1:A:1063:MET:HB3	1:A:1066:VAL:HG13	1.84	0.58
2:B:213:ILE:HG22	2:B:479:VAL:H	1.68	0.58
2:B:291:ILE:HG22	2:B:297:ILE:HG12	1.85	0.58
4:E:151:PRO:HG2	4:E:198:ILE:HG23	1.86	0.58
1:A:9:ALA:HB3	2:B:1161:HIS:CD2	2.39	0.58
2:B:487:THR:H	2:B:490:SER:HB3	1.68	0.58
3:C:66:ARG:NH1	8:J:2:ILE:HG21	2.18	0.58
2:B:484:ASN:HD22	2:B:494:HIS:HD2	1.51	0.58
6:H:6:PHE:C	6:H:7:ASP:OD1	2.45	0.58
1:A:567:LYS:HB3	1:A:568:PRO:CD	2.34	0.58
4:E:118:PRO:HA	4:E:121:MET:CB	2.33	0.58
4:E:172:GLU:HG3	4:E:213:ILE:HD13	1.86	0.58
3:C:90:ASP:O	3:C:91:HIS:HB3	2.04	0.58
1:A:1014:ALA:HA	4:E:205:SER:OG	2.04	0.57
2:B:511:PRO:HD2	2:B:512:ARG:H	1.69	0.57
1:A:270:LEU:O	1:A:274:ILE:HG22	2.05	0.57
1:A:1067:LEU:CD2	1:A:1068:ALA:H	2.15	0.57
2:B:846:ILE:HG23	2:B:974:PRO:HD2	1.86	0.57
6:H:26:ILE:N	6:H:40:LEU:O	2.32	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:101:ILE:HG12	5:F:107:VAL:HG22	1.86	0.57
2:B:144:GLY:HA2	2:B:146:GLU:HB2	1.85	0.57
2:B:170:LEU:HA	2:B:457:LEU:HD13	1.86	0.57
2:B:980:PHE:CE2	2:B:990:ILE:HD11	2.40	0.57
2:B:310:MET:HA	2:B:313:MET:HE2	1.85	0.57
1:A:28:ARG:HH22	1:A:34:LYS:HA	1.68	0.57
1:A:845:LEU:HD12	1:A:1065:GLY:O	2.04	0.57
4:E:12:LEU:HD21	4:E:55:ARG:HH11	1.68	0.57
1:A:467:THR:HG21	2:B:976:ILE:HG22	1.86	0.57
1:A:546:VAL:HG21	1:A:572:TRP:CD1	2.40	0.57
3:C:91:HIS:CG	3:C:92:CYS:N	2.73	0.57
9:K:94:ILE:HG12	9:K:98:LEU:HD13	1.87	0.57
1:A:1013:ASP:O	4:E:205:SER:OG	2.22	0.57
2:B:129:PHE:O	2:B:130:VAL:HG13	2.04	0.57
3:C:262:LEU:HD21	9:K:88:LYS:HE2	1.86	0.57
2:B:770:GLN:HA	2:B:773:MET:HG3	1.87	0.56
6:H:63:LEU:HB2	6:H:89:LEU:HD22	1.87	0.56
1:A:58:LEU:HG	1:A:80:HIS:O	2.05	0.56
2:B:241:ARG:HH21	12:S:20:DC:H41	1.53	0.56
4:E:144:ILE:HD13	4:E:183:PRO:CB	2.35	0.56
2:B:130:VAL:HG22	2:B:165:VAL:HG23	1.87	0.56
1:A:841:LEU:O	1:A:845:LEU:HD23	2.06	0.56
4:E:41:ASP:O	4:E:45:LYS:HG3	2.04	0.56
1:A:151:ASP:HA	1:A:152:VAL:HB	1.86	0.56
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.87	0.56
2:B:466:TRP:HE1	2:B:479:VAL:HG21	1.70	0.56
2:B:520:GLY:H	2:B:748:ILE:HG23	1.71	0.56
3:C:263:THR:O	3:C:266:ASP:HB3	2.05	0.56
1:A:330:LYS:HG3	1:A:1406:VAL:HG23	1.88	0.56
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.88	0.56
2:B:532:ALA:HA	2:B:535:LEU:HD12	1.88	0.56
2:B:654:ARG:H	2:B:657:HIS:CD2	2.24	0.56
2:B:863:GLU:HB3	2:B:961:LEU:HD22	1.88	0.56
3:C:55:THR:HB	3:C:152:GLU:H	1.71	0.56
4:E:31:THR:HG22	4:E:32:GLN:N	2.21	0.56
9:K:19:LEU:CD2	9:K:35:PHE:CE2	2.81	0.56
4:E:144:ILE:HD13	4:E:183:PRO:HB3	1.86	0.55
1:A:1150:SER:HB3	7:I:46:HIS:HB2	1.88	0.55
2:B:999:MET:HG2	2:B:1007:VAL:HG13	1.88	0.55
7:I:56:ALA:N	7:I:89:GLN:OE1	2.38	0.55
1:A:30:ILE:HA	2:B:1183:LYS:O	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:GLU:HA	1:A:338:GLY:HA3	1.88	0.55
1:A:523:ILE:HG23	1:A:527:THR:HG23	1.88	0.55
2:B:130:VAL:HG23	2:B:132:VAL:CG2	2.27	0.55
2:B:364:ILE:HG22	2:B:585:VAL:HG13	1.89	0.55
2:B:502:ILE:HG22	2:B:503:GLY:H	1.71	0.55
4:E:44:ALA:O	4:E:45:LYS:HG3	2.06	0.55
4:E:151:PRO:HG2	4:E:198:ILE:HG21	1.88	0.55
2:B:137:TYR:CD1	2:B:151:LEU:HD13	2.41	0.55
2:B:282:ILE:C	2:B:285:ILE:HG22	2.30	0.55
2:B:286:PHE:CG	2:B:297:ILE:HG23	2.41	0.55
3:C:245:VAL:HA	3:C:248:ILE:HD12	1.89	0.55
2:B:492:LEU:HA	2:B:495:LEU:HD12	1.89	0.55
1:A:467:THR:HG23	1:A:469:ARG:NH1	2.21	0.55
5:F:74:ILE:HD12	5:F:144:GLU:HG3	1.89	0.55
2:B:289:LEU:HD23	2:B:291:ILE:CD1	2.36	0.54
2:B:510:LYS:HB2	2:B:511:PRO:HA	1.88	0.54
2:B:999:MET:HE3	2:B:1008:PRO:HG2	1.88	0.54
2:B:1158:PHE:HE2	2:B:1201:LYS:HD3	1.71	0.54
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.89	0.54
2:B:149:TYR:CA	2:B:150:GLU:HB2	2.37	0.54
4:E:21:GLU:OE2	4:E:146:HIS:HE1	1.90	0.54
2:B:872:GLU:HA	2:B:917:PRO:HD3	1.89	0.54
12:S:10:DG:H1'	12:S:11:DG:H5'	1.90	0.54
1:A:602:ASP:HB3	1:A:616:VAL:HG23	1.90	0.54
1:A:1013:ASP:O	4:E:205:SER:O	2.26	0.54
1:A:1313:LEU:HD23	1:A:1338:VAL:HG11	1.89	0.54
2:B:113:TYR:HB3	2:B:114:PRO:HD2	1.89	0.54
2:B:130:VAL:CG2	2:B:132:VAL:CG2	2.85	0.54
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.88	0.54
2:B:806:THR:HG23	2:B:1046:PRO:HD3	1.90	0.54
5:F:130:ILE:HG22	5:F:132:LEU:CD1	2.37	0.54
1:A:252:PHE:CZ	11:R:2:U:H1'	2.40	0.54
1:A:483:ASP:HB3	2:B:837:ASP:HB3	1.90	0.54
5:F:125:LEU:O	5:F:126:ALA:C	2.50	0.54
1:A:32:VAL:HB	1:A:57:ARG:HB3	1.90	0.53
1:A:61:ILE:HG21	1:A:250:ILE:HG13	1.89	0.53
10:L:60:ARG:HG2	10:L:61:THR:N	2.23	0.53
1:A:53:LEU:CD2	1:A:54:ASN:H	2.16	0.53
1:A:515:GLN:HE22	1:A:1075:PRO:HD3	1.73	0.53
3:C:101:LEU:HD23	3:C:101:LEU:C	2.34	0.53
1:A:534:LEU:O	1:A:539:THR:HG21	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1383:SER:HB2	1:A:1388:GLY:HA3	1.91	0.53
2:B:305:VAL:O	2:B:305:VAL:HG12	2.08	0.53
6:H:4:THR:HG21	6:H:7:ASP:OD1	2.07	0.53
7:I:83:ASN:HD21	7:I:101:PHE:HD2	1.55	0.53
9:K:20:LYS:HZ1	9:K:36:GLU:HG3	1.73	0.53
1:A:845:LEU:CB	1:A:1065:GLY:O	2.56	0.53
2:B:637:LEU:HB2	2:B:693:ILE:HD13	1.90	0.53
8:J:56:LEU:O	8:J:57:ILE:C	2.51	0.53
1:A:314:ALA:HB1	1:A:322:VAL:HG12	1.89	0.53
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.91	0.53
2:B:140:ILE:O	2:B:140:ILE:HG13	2.09	0.53
3:C:100:THR:HG1	3:C:119:VAL:HG23	1.70	0.53
4:E:55:ARG:HE	4:E:84:ASP:HA	1.73	0.53
4:E:118:PRO:HA	4:E:121:MET:CG	2.39	0.53
6:H:56:THR:HB	6:H:145:ARG:HB3	1.91	0.53
1:A:240:PRO:HB2	2:B:1209:ALA:HA	1.89	0.53
3:C:43:THR:OG1	3:C:170:TRP:HB3	2.08	0.53
3:C:55:THR:HG22	3:C:55:THR:O	2.08	0.53
1:A:315:LEU:HD12	1:A:316:GLN:H	1.74	0.53
2:B:164:LYS:O	2:B:165:VAL:HG22	2.08	0.53
2:B:420:LEU:HD23	2:B:453:ILE:HA	1.89	0.53
2:B:510:LYS:HD2	2:B:513:GLN:HB2	1.90	0.53
3:C:66:ARG:CZ	8:J:2:ILE:CG2	2.86	0.53
3:C:118:LEU:HD11	3:C:132:PRO:CG	2.18	0.53
2:B:260:GLY:HA2	2:B:264:SER:HB3	1.91	0.53
2:B:1171:VAL:HG21	2:B:1191:ILE:HG12	1.90	0.53
10:L:30:ILE:HG21	10:L:57:LEU:HD22	1.90	0.53
1:A:18:GLN:HB3	1:A:1418:LEU:HG	1.90	0.53
1:A:298:PHE:O	1:A:302:THR:HG22	2.08	0.53
2:B:1002:THR:HG22	2:B:1072:MET:HE2	1.90	0.53
3:C:118:LEU:CD1	3:C:132:PRO:HG3	2.19	0.53
9:K:42:LEU:O	9:K:46:ILE:HG12	2.08	0.53
1:A:446:ARG:HG3	1:A:446:ARG:HH11	1.73	0.52
1:A:591:PHE:HA	1:A:595:THR:HG21	1.91	0.52
5:F:122:MET:O	5:F:125:LEU:HG	2.08	0.52
1:A:53:LEU:CD2	1:A:54:ASN:CG	2.82	0.52
1:A:565:ILE:CD1	1:A:571:LEU:H	2.14	0.52
1:A:1107:VAL:HG12	1:A:1383:SER:HA	1.90	0.52
2:B:415:GLN:HE22	2:B:476:ARG:HH22	1.57	0.52
4:E:183:PRO:HA	4:E:186:LEU:HD12	1.89	0.52
1:A:377:PRO:HA	1:A:432:VAL:O	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:PHE:HB3	2:B:163:GLY:O	2.08	0.52
6:H:58:THR:HB	6:H:143:LEU:HB2	1.92	0.52
1:A:368:LYS:HA	1:A:462:VAL:HG12	1.91	0.52
1:A:464:PRO:HB2	9:K:4:PRO:HD3	1.92	0.52
2:B:860:MET:HB3	2:B:965:LYS:HG3	1.90	0.52
6:H:8:ASP:OD2	6:H:129:TYR:OH	2.17	0.52
1:A:963:ILE:HG22	1:A:1045:VAL:HG22	1.92	0.52
10:L:60:ARG:HG2	10:L:61:THR:O	2.09	0.52
1:A:489:LEU:CG	1:A:490:HIS:H	2.22	0.52
3:C:46:ILE:HG21	3:C:157:CYS:HB2	1.91	0.52
4:E:188:LEU:N	4:E:188:LEU:CD1	2.73	0.52
5:F:86:THR:HG22	5:F:89:GLU:CG	2.40	0.52
5:F:133:VAL:HG12	5:F:147:SER:HA	1.91	0.52
1:A:606:LEU:HB3	1:A:613:ILE:HB	1.90	0.52
1:A:919:ILE:O	1:A:922:ASP:HB2	2.10	0.52
2:B:773:MET:HE1	2:B:987:LYS:HB3	1.92	0.52
1:A:216:VAL:HG12	1:A:230:ARG:HH21	1.74	0.52
1:A:1035:TYR:HB3	1:A:1037:LEU:HD23	1.91	0.52
4:E:72:PHE:HB2	4:E:75:MET:SD	2.50	0.52
9:K:27:ALA:HB3	9:K:74:ARG:HH21	1.75	0.52
1:A:845:LEU:HA	1:A:848:ILE:HD12	1.91	0.52
1:A:901:LEU:H	1:A:926:GLN:HE22	1.58	0.52
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.92	0.52
9:K:12:LEU:N	9:K:12:LEU:CD1	2.73	0.52
2:B:1158:PHE:CE2	2:B:1160:VAL:HG13	2.45	0.52
3:C:72:LEU:CD1	3:C:72:LEU:N	2.73	0.52
4:E:151:PRO:CG	4:E:198:ILE:CG2	2.88	0.52
4:E:187:TYR:HB3	4:E:188:LEU:CD1	2.40	0.52
7:I:78:CYS:HG	7:I:106:CYS:CB	2.23	0.52
1:A:471:ASN:HB3	1:A:474:VAL:HG12	1.91	0.51
2:B:123:THR:HG23	2:B:205:ILE:HA	1.92	0.51
6:H:38:LEU:CD2	6:H:40:LEU:HB2	2.40	0.51
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.93	0.51
2:B:129:PHE:O	2:B:130:VAL:CG1	2.59	0.51
2:B:737:THR:O	7:I:66:PRO:HB2	2.11	0.51
3:C:80:LEU:HD11	3:C:95:CYS:HA	1.92	0.51
9:K:32:VAL:O	9:K:32:VAL:HG23	2.10	0.51
2:B:74:LEU:CD1	2:B:75:ALA:N	2.73	0.51
2:B:1171:VAL:CG2	2:B:1191:ILE:HG12	2.40	0.51
3:C:14:SER:HA	9:K:115:ALA:HB3	1.92	0.51
5:F:97:ARG:HG3	5:F:101:ILE:CD1	2.29	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:133:ASN:OD1	6:H:134:ASN:N	2.44	0.51
9:K:65:HIS:HD2	9:K:67:PHE:H	1.58	0.51
1:A:960:ILE:C	1:A:962:ARG:H	2.18	0.51
2:B:489:SER:HA	2:B:492:LEU:HD12	1.93	0.51
6:H:6:PHE:CE1	6:H:8:ASP:HB2	2.44	0.51
1:A:899:VAL:HB	1:A:929:LEU:HD13	1.93	0.51
2:B:955:THR:HG22	2:B:956:THR:N	2.25	0.51
2:B:1023:VAL:HA	2:B:1026:LEU:HD12	1.92	0.51
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.92	0.51
2:B:1142:GLY:HA3	5:F:88:TYR:HE2	1.71	0.51
2:B:706:GLN:HB3	2:B:709:ASP:HB2	1.93	0.51
6:H:41:ASP:O	6:H:42:ILE:CG1	2.40	0.51
1:A:542:GLU:CD	1:A:542:GLU:H	2.19	0.51
10:L:38:LEU:HD21	10:L:49:LYS:H	1.76	0.51
1:A:58:LEU:HD23	1:A:243:PRO:HA	1.93	0.51
1:A:1027:ALA:O	1:A:1031:VAL:HG23	2.10	0.51
2:B:540:SER:HA	2:B:750:GLY:HA2	1.93	0.51
3:C:46:ILE:HD12	3:C:46:ILE:H	1.76	0.51
5:F:130:ILE:HG23	5:F:132:LEU:CD1	2.38	0.51
1:A:11:LEU:HB2	2:B:1193:GLN:HG2	1.93	0.50
3:C:79:GLN:HG3	3:C:127:ARG:HH11	1.76	0.50
5:F:116:ASP:O	5:F:120:ILE:HG13	2.10	0.50
1:A:1117:THR:HG22	1:A:1307:GLU:HG2	1.93	0.50
2:B:779:GLY:HA2	2:B:796:LEU:HB2	1.94	0.50
10:L:60:ARG:NH1	10:L:61:THR:O	2.44	0.50
1:A:871:ASP:CG	1:A:1366:ARG:HH22	2.20	0.50
2:B:128:LEU:HD11	2:B:170:LEU:HB2	1.94	0.50
2:B:791:THR:O	2:B:857:ARG:HG3	2.12	0.50
2:B:974:PRO:HB3	2:B:980:PHE:HZ	1.75	0.50
3:C:79:GLN:HG3	3:C:127:ARG:NH1	2.26	0.50
4:E:182:ASP:OD1	4:E:184:VAL:CG2	2.59	0.50
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.92	0.50
2:B:269:ILE:H	2:B:317:CYS:HB3	1.75	0.50
2:B:298:LEU:O	2:B:301:ILE:N	2.45	0.50
6:H:43:ASN:HD21	6:H:45:GLU:HG2	1.77	0.50
1:A:361:LEU:HA	1:A:471:ASN:HD22	1.77	0.50
1:A:663:SER:HB2	2:B:1085:ILE:HA	1.94	0.50
4:E:151:PRO:HD2	4:E:153:HIS:HE1	0.39	0.50
5:F:99:LEU:CD2	5:F:103:MET:HG2	2.40	0.50
6:H:43:ASN:ND2	6:H:44:VAL:N	2.60	0.49
13:U:25:DT:H2''	13:U:26:DC:H5'	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1336:MET:HE2	1:A:1381:LEU:HB2	1.94	0.49
3:C:11:ARG:NH2	3:C:19:ASP:OD1	2.44	0.49
6:H:40:LEU:C	6:H:40:LEU:CD2	2.86	0.49
1:A:1161:THR:HG21	1:A:1239:ARG:NH1	2.27	0.49
2:B:44:VAL:HG23	2:B:48:LEU:HD12	1.92	0.49
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.93	0.49
2:B:1168:LEU:HD13	2:B:1208:MET:HE3	1.94	0.49
7:I:92:ARG:HB2	7:I:95:THR:HG23	1.94	0.49
2:B:511:PRO:CD	2:B:512:ARG:H	2.25	0.49
8:J:38:ARG:C	8:J:40:GLY:H	2.20	0.49
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.93	0.49
2:B:1158:PHE:CE2	2:B:1201:LYS:HD3	2.46	0.49
3:C:40:GLU:HG2	3:C:254:LYS:NZ	2.27	0.49
3:C:91:HIS:ND1	3:C:92:CYS:N	2.61	0.49
3:C:92:CYS:O	3:C:96:SER:N	2.45	0.49
4:E:190:LEU:N	4:E:190:LEU:CD2	2.75	0.49
5:F:99:LEU:C	5:F:99:LEU:CD2	2.85	0.49
12:S:26:DG:N3	12:S:27:DT:N3	2.60	0.49
1:A:1413:GLY:HA3	2:B:1212:ILE:HD12	1.94	0.49
2:B:31:TRP:HA	2:B:34:ILE:HD12	1.94	0.49
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.94	0.49
2:B:129:PHE:C	2:B:130:VAL:HG13	2.37	0.49
2:B:975:GLN:O	2:B:990:ILE:HD13	2.12	0.49
1:A:86:LEU:HD21	1:A:239:LEU:H	1.78	0.49
1:A:391:LEU:HA	1:A:394:ASN:HB2	1.94	0.49
1:A:1115:SER:O	1:A:1330:ASN:HB2	2.13	0.49
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.48	0.49
7:I:4:PHE:CE2	7:I:14:LEU:HB2	2.47	0.49
10:L:43:THR:C	10:L:44:ASP:OD1	2.55	0.49
2:B:867:GLY:HA3	2:B:869:SER:N	2.27	0.49
4:E:155:ARG:HA	4:E:196:VAL:HG12	1.95	0.49
2:B:552:MET:HA	2:B:555:ILE:HD12	1.95	0.49
3:C:88:CYS:SG	3:C:91:HIS:C	2.91	0.49
6:H:59:ILE:HD11	6:H:123:MET:HE1	1.94	0.49
9:K:33:ILE:HG13	9:K:73:LEU:HB3	1.96	0.48
9:K:87:LEU:C	9:K:87:LEU:CD2	2.86	0.48
9:K:91:CYS:C	9:K:94:ILE:HG22	2.37	0.48
1:A:986:ILE:HD11	1:A:1032:LEU:HD21	1.95	0.48
6:H:105:GLU:HB3	6:H:113:ALA:HB3	1.95	0.48
1:A:520:CYS:HB3	1:A:521:MET:HE2	1.96	0.48
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:185:LYS:HE3	3:C:220:ASP:HB2	1.95	0.48
3:C:262:LEU:C	3:C:262:LEU:CD2	2.86	0.48
5:F:109:VAL:HG11	5:F:124:GLU:HA	1.95	0.48
1:A:101:LYS:HG2	1:A:139:TRP:CD1	2.49	0.48
1:A:966:ASN:HB3	1:A:1044:TRP:HH2	1.78	0.48
10:L:30:ILE:CG2	10:L:57:LEU:HD22	2.43	0.48
2:B:524:PRO:HD2	2:B:749:LEU:HD23	1.95	0.48
2:B:1117:GLN:OE1	2:B:1199:ALA:HB2	2.14	0.48
12:S:33:DT:H3	13:U:8:DA:H61	1.61	0.48
1:A:216:VAL:HG12	1:A:230:ARG:NH2	2.28	0.48
1:A:579:SER:HA	1:A:582:ILE:HD12	1.96	0.48
2:B:293:PRO:O	2:B:297:ILE:HG13	2.14	0.48
2:B:294:ASP:O	2:B:298:LEU:HG	2.13	0.48
2:B:1174:LYS:HG2	2:B:1177:HIS:HB2	1.95	0.48
6:H:41:ASP:C	6:H:42:ILE:HG13	2.32	0.48
1:A:367:PRO:HB3	9:K:2:ASN:HD21	1.76	0.48
3:C:91:HIS:O	3:C:92:CYS:HB3	2.13	0.48
1:A:663:SER:CB	2:B:1085:ILE:HA	2.43	0.48
1:A:845:LEU:O	1:A:846:GLU:C	2.57	0.48
2:B:460:ALA:HB1	2:B:466:TRP:CE3	2.49	0.48
2:B:484:ASN:HD22	2:B:494:HIS:CD2	2.31	0.48
2:B:1016:ALA:O	2:B:1020:ARG:HG2	2.14	0.48
2:B:1160:VAL:HG23	2:B:1194:ILE:HG13	1.96	0.48
4:E:185:ALA:HA	4:E:190:LEU:HD23	1.95	0.48
1:A:1170:ILE:HD11	1:A:1239:ARG:NH1	2.25	0.48
3:C:33:LEU:C	3:C:33:LEU:CD2	2.86	0.48
1:A:392:VAL:HG11	1:A:424:ILE:HG21	1.96	0.47
1:A:880:LYS:HA	1:A:955:PRO:HA	1.96	0.47
1:A:1068:ALA:HA	1:A:1071:SER:HB2	1.95	0.47
2:B:640:VAL:HA	2:B:651:LEU:HA	1.96	0.47
7:I:77:LYS:HD2	7:I:108:HIS:HB2	1.95	0.47
1:A:53:LEU:CD2	1:A:53:LEU:C	2.86	0.47
3:C:127:ARG:HG3	3:C:129:ILE:HG22	1.95	0.47
1:A:846:GLU:O	1:A:848:ILE:N	2.47	0.47
1:A:1070:GLN:C	1:A:1073:GLY:H	2.22	0.47
1:A:1404:GLU:HB3	1:A:1407:GLU:HB2	1.97	0.47
2:B:387:LEU:CD2	2:B:387:LEU:C	2.86	0.47
2:B:601:ARG:HH21	2:B:639:ILE:HD11	1.80	0.47
1:A:280:GLU:HA	1:A:284:ALA:HB2	1.94	0.47
2:B:640:VAL:HG22	2:B:651:LEU:HB3	1.96	0.47
5:F:147:SER:O	5:F:151:LEU:HD12	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:56:ALA:HB3	7:I:89:GLN:NE2	2.16	0.47
1:A:715:GLU:HA	1:A:718:VAL:HG22	1.96	0.47
1:A:956:LEU:HD21	1:A:1017:LEU:HD23	1.97	0.47
3:C:221:TYR:HB3	6:H:46:LEU:CD1	2.44	0.47
1:A:356:ASP:HB3	1:A:359:LEU:HB2	1.97	0.47
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.97	0.47
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.95	0.47
9:K:56:VAL:HA	9:K:77:THR:HG22	1.96	0.47
1:A:1107:VAL:HG21	1:A:1381:LEU:HD23	1.96	0.47
3:C:262:LEU:CD2	9:K:88:LYS:HE2	2.45	0.47
5:F:131:PRO:O	5:F:132:LEU:HG	2.15	0.47
2:B:60:GLN:HE22	2:B:94:LYS:NZ	2.13	0.47
3:C:221:TYR:HB3	6:H:46:LEU:HD13	1.96	0.47
2:B:284:ILE:HG12	2:B:324:ILE:HD11	1.97	0.47
2:B:521:LEU:HA	2:B:543:SER:HB3	1.95	0.47
2:B:1060:ARG:HB2	2:B:1066:SER:HB3	1.96	0.47
4:E:168:TYR:HB2	4:E:170:LEU:HD12	1.97	0.47
6:H:118:PHE:HB2	6:H:121:LEU:HB2	1.96	0.47
9:K:31:VAL:HB	9:K:75:ILE:HD11	1.97	0.47
1:A:1095:THR:HG21	1:A:1112:LYS:HB3	1.96	0.46
1:A:446:ARG:HG2	1:A:478:TYR:HB3	1.97	0.46
1:A:817:ALA:HB1	2:B:524:PRO:HB2	1.98	0.46
1:A:853:ASP:C	1:A:855:THR:H	2.24	0.46
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.96	0.46
5:F:97:ARG:NH2	5:F:131:PRO:HG2	2.30	0.46
5:F:125:LEU:O	5:F:127:GLU:N	2.49	0.46
9:K:75:ILE:CD1	9:K:83:PRO:CB	2.73	0.46
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.80	0.46
2:B:120:ARG:HB3	2:B:122:LEU:HD13	1.97	0.46
1:A:32:VAL:HG21	1:A:57:ARG:O	2.16	0.46
1:A:1043:ASP:HA	1:A:1046:LEU:HD12	1.98	0.46
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.80	0.46
3:C:145:CYS:HA	8:J:2:ILE:HD13	1.96	0.46
5:F:86:THR:CG2	5:F:89:GLU:HG3	2.45	0.46
6:H:5:LEU:HD22	6:H:133:ASN:O	2.15	0.46
3:C:88:CYS:SG	3:C:92:CYS:SG	3.14	0.46
5:F:97:ARG:O	5:F:101:ILE:N	2.28	0.46
5:F:125:LEU:HD12	5:F:125:LEU:C	2.39	0.46
5:F:146:TRP:HB3	5:F:151:LEU:HD11	1.97	0.46
1:A:265:LYS:HD3	1:A:302:THR:HG23	1.98	0.46
1:A:1063:MET:HB3	1:A:1066:VAL:CG1	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:ILE:H	2:B:364:ILE:HG13	1.62	0.46
2:B:681:TRP:HA	2:B:684:LEU:HD12	1.97	0.46
2:B:805:THR:HG21	2:B:815:ARG:HD3	1.98	0.46
6:H:102:TYR:CZ	6:H:115:TYR:HB3	2.51	0.46
1:A:365:GLY:HA3	1:A:469:ARG:HB3	1.98	0.46
1:A:451:HIS:HA	1:A:1070:GLN:HB2	1.98	0.46
1:A:452:LYS:HE2	1:A:510:GLN:HE22	1.80	0.46
1:A:534:LEU:O	1:A:574:GLY:HA3	2.16	0.46
1:A:667:GLY:HA2	1:A:670:ILE:HD12	1.98	0.46
1:A:738:LYS:HG3	1:A:740:LEU:HG	1.98	0.46
2:B:285:ILE:HD13	2:B:378:LEU:HD13	1.94	0.46
1:A:827:THR:HA	1:A:830:LYS:HB2	1.98	0.46
3:C:78:GLU:N	3:C:78:GLU:CD	2.73	0.46
5:F:99:LEU:O	5:F:103:MET:HG2	2.15	0.46
1:A:56:PRO:HD2	1:A:58:LEU:HD13	1.98	0.46
1:A:208:LEU:HA	1:A:211:PHE:HB2	1.98	0.46
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.98	0.46
4:E:31:THR:CG2	4:E:32:GLN:N	2.78	0.46
9:K:31:VAL:HB	9:K:75:ILE:CD1	2.45	0.46
1:A:855:THR:HG23	1:A:857:ARG:HE	1.79	0.45
1:A:1216:ILE:HA	1:A:1219:THR:HG22	1.98	0.45
1:A:1284:MET:HA	1:A:1306:LEU:HG	1.98	0.45
3:C:70:ILE:O	3:C:72:LEU:HD12	2.16	0.45
1:A:825:ILE:HD12	2:B:512:ARG:HB3	1.98	0.45
2:B:711:GLU:HB3	2:B:712:PRO:HD3	1.97	0.45
1:A:524:VAL:O	1:A:527:THR:HG22	2.16	0.45
1:A:1120:LEU:HB3	1:A:1124:HIS:HB2	1.98	0.45
2:B:1150:ARG:HA	2:B:1154:ALA:HB3	1.98	0.45
3:C:80:LEU:HD11	3:C:95:CYS:CA	2.46	0.45
4:E:56:LYS:O	4:E:57:MET:C	2.58	0.45
1:A:304:MET:HA	1:A:325:ILE:HD12	1.99	0.45
1:A:821:ARG:O	1:A:825:ILE:HG12	2.16	0.45
1:A:1398:MET:HA	1:A:1425:SER:HB3	1.97	0.45
2:B:803:LEU:H	2:B:822:ASN:HD21	1.64	0.45
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.98	0.45
2:B:975:GLN:HE21	2:B:976:ILE:H	1.64	0.45
5:F:131:PRO:C	5:F:132:LEU:CD1	2.85	0.45
7:I:18:GLU:HG3	7:I:20:LYS:HD2	1.94	0.45
7:I:59:VAL:C	7:I:61:ASP:H	2.25	0.45
8:J:6:ARG:HA	8:J:12:LYS:O	2.16	0.45
2:B:558:LEU:HD22	2:B:563:MET:HE3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ILE:HA	1:A:328:ARG:HD2	1.98	0.45
1:A:683:ILE:HG12	1:A:801:GLU:HG3	1.99	0.45
1:A:779:PHE:HB2	1:A:782:ARG:HG2	1.98	0.45
1:A:1336:MET:HG3	1:A:1381:LEU:HD13	1.97	0.45
2:B:69:LEU:CD1	2:B:432:MET:CE	2.91	0.45
2:B:827:ILE:HG13	2:B:1012:ILE:HD11	1.99	0.45
3:C:41:ILE:HD11	3:C:247:GLY:HA2	1.98	0.45
9:K:19:LEU:CD2	9:K:35:PHE:CD2	2.97	0.45
2:B:95:ILE:HD12	2:B:96:TYR:H	1.81	0.45
3:C:74:SER:HA	3:C:129:ILE:HG13	1.99	0.45
3:C:234:SER:HB2	3:C:243:VAL:HG21	1.98	0.45
6:H:6:PHE:HE1	6:H:57:VAL:HG23	1.81	0.45
7:I:49:ILE:HG23	7:I:92:ARG:HH22	1.82	0.45
10:L:33:GLU:OE2	10:L:53:HIS:HD2	1.93	0.45
2:B:285:ILE:HD11	2:B:360:PHE:CZ	2.52	0.45
2:B:469:GLN:HA	2:B:470:LYS:HA	1.68	0.45
4:E:56:LYS:O	4:E:59:SER:N	2.50	0.45
1:A:466:SER:HA	9:K:2:ASN:HD22	1.82	0.45
1:A:547:LEU:HD23	9:K:59:ALA:H	1.81	0.45
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.99	0.45
3:C:8:VAL:CB	9:K:108:GLU:OE1	2.64	0.45
3:C:91:HIS:CD2	3:C:158:VAL:CG1	3.00	0.45
7:I:25:LEU:HB3	7:I:38:ALA:HB2	1.99	0.45
1:A:382:PRO:HA	1:A:385:ILE:HD12	1.99	0.45
1:A:1111:MET:HB2	1:A:1114:PRO:HG3	1.99	0.45
3:C:51:VAL:HB	10:L:65:VAL:HG23	1.98	0.45
6:H:63:LEU:HD13	6:H:89:LEU:HD13	1.99	0.45
1:A:354:SER:HB2	1:A:469:ARG:CD	2.36	0.44
1:A:981:LEU:HD23	1:A:1039:LYS:HA	1.99	0.44
3:C:250:THR:HA	3:C:253:LYS:HE3	1.98	0.44
1:A:17:VAL:HG13	1:A:1419:ASP:HB2	1.99	0.44
1:A:758:ILE:H	1:A:758:ILE:HG13	1.60	0.44
1:A:974:ASP:HB3	1:A:977:LYS:H	1.83	0.44
2:B:604:ARG:HH22	2:B:697:GLU:CD	2.25	0.44
2:B:709:ASP:HB3	2:B:710:LEU:HD12	1.99	0.44
10:L:30:ILE:HB	10:L:59:ALA:HB2	1.99	0.44
1:A:635:ARG:HA	1:A:635:ARG:HE	1.81	0.44
2:B:324:ILE:HD13	2:B:330:ALA:HA	1.99	0.44
4:E:112:TYR:HE1	4:E:134:THR:HB	1.81	0.44
6:H:4:THR:HG22	6:H:6:PHE:H	1.81	0.44
9:K:18:LYS:HE3	9:K:38:GLU:HG2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:ILE:CD1	3:C:142:VAL:HG12	2.26	0.44
7:I:7:CYS:SG	7:I:9:ASP:O	2.75	0.44
10:L:51:CYS:C	10:L:53:HIS:H	2.26	0.44
1:A:117:GLU:O	1:A:118:HIS:C	2.61	0.44
1:A:252:PHE:CZ	11:R:2:U:H4'	2.53	0.44
1:A:514:PRO:HB3	1:A:875:ALA:HB3	1.99	0.44
1:A:1100:ARG:HE	1:A:1104:ILE:HD11	1.82	0.44
2:B:387:LEU:HD21	2:B:392:ARG:HB2	1.99	0.44
2:B:1171:VAL:HG11	2:B:1180:PHE:HD1	1.81	0.44
1:A:38:PRO:HB3	1:A:267:ALA:HB1	1.99	0.44
1:A:442:VAL:HG22	1:A:491:VAL:HG22	1.99	0.44
1:A:1051:ALA:O	1:A:1055:ARG:HB2	2.17	0.44
1:A:1194:ARG:CZ	1:A:1237:ILE:HG21	2.47	0.44
3:C:259:LEU:HG	9:K:91:CYS:HG	1.77	0.44
4:E:118:PRO:CA	4:E:121:MET:HB2	2.44	0.44
6:H:40:LEU:HD23	6:H:41:ASP:C	2.42	0.44
1:A:565:ILE:CD1	1:A:570:PRO:HA	2.47	0.44
1:A:691:LEU:HD11	1:A:695:LYS:HE3	1.99	0.44
1:A:1194:ARG:HH22	1:A:1235:LYS:HE2	1.83	0.44
2:B:70:ILE:HA	2:B:88:TYR:O	2.18	0.44
2:B:908:GLU:HA	2:B:941:LEU:HB3	1.99	0.44
13:U:22:DC:H2'	13:U:23:DT:C6	2.53	0.44
1:A:315:LEU:HB2	12:S:12:DA:H61	1.83	0.44
2:B:905:VAL:HB	2:B:941:LEU:HD22	1.99	0.44
2:B:170:LEU:HD12	2:B:171:PRO:CD	2.48	0.44
2:B:551:PRO:HB3	2:B:628:THR:HG21	1.99	0.44
4:E:86:PRO:HA	4:E:113:GLN:HB2	2.00	0.44
1:A:579:SER:HB2	1:A:612:ILE:H	1.83	0.43
1:A:1062:GLU:C	1:A:1064:VAL:H	2.26	0.43
1:A:1197:LEU:HD13	1:A:1209:MET:HE1	2.00	0.43
9:K:113:THR:HB	9:K:114:LEU:HB2	1.99	0.43
1:A:845:LEU:CG	1:A:1065:GLY:O	2.66	0.43
1:A:1124:HIS:CG	1:A:1130:GLN:HG2	2.54	0.43
2:B:286:PHE:CD2	2:B:297:ILE:HG23	2.53	0.43
2:B:778:MET:HG3	2:B:1094:ARG:HB3	2.00	0.43
2:B:1106:ARG:NH2	2:B:1111:MET:SD	2.91	0.43
3:C:11:ARG:HB3	3:C:12:GLU:OE1	2.18	0.43
5:F:108:PHE:CZ	5:F:131:PRO:HG3	2.53	0.43
7:I:14:LEU:HB3	7:I:27:PHE:HB3	1.99	0.43
1:A:528:LEU:HD13	1:A:751:SER:H	1.82	0.43
2:B:1129:ARG:HD3	13:U:21:DC:H5''	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LEU:HG	1:A:238:CYS:HA	2.01	0.43
1:A:553:VAL:HB	1:A:556:TRP:HB2	2.00	0.43
1:A:741:ASN:HA	3:C:192:TRP:HE1	1.84	0.43
3:C:74:SER:HB2	3:C:238:ILE:HG23	2.00	0.43
1:A:265:LYS:HD2	1:A:322:VAL:HG11	1.99	0.43
1:A:1135:ARG:HD2	1:A:1282:VAL:O	2.19	0.43
2:B:825:VAL:HG21	2:B:1092:TYR:CE1	2.54	0.43
8:J:14:VAL:HA	8:J:17:LYS:HG3	2.00	0.43
1:A:816:HIS:HE2	2:B:764:SER:H	1.67	0.43
1:A:1223:ASP:HA	1:A:1243:VAL:HG13	2.01	0.43
2:B:977:GLY:HA3	2:B:1099:VAL:CB	2.48	0.43
1:A:350:ARG:HB2	2:B:1128:LEU:HD11	2.00	0.43
1:A:562:THR:HG22	6:H:79:TRP:HD1	1.84	0.43
1:A:909:ASP:C	1:A:911:SER:H	2.27	0.43
1:A:1189:SER:HB2	1:A:1190:PRO:CD	2.49	0.43
2:B:253:THR:O	2:B:253:THR:HG23	2.19	0.43
2:B:305:VAL:O	2:B:305:VAL:CG1	2.67	0.43
2:B:1180:PHE:HB2	2:B:1188:LYS:HB2	2.01	0.43
1:A:512:VAL:HA	1:A:519:PRO:HA	2.00	0.43
1:A:824:LEU:HA	1:A:827:THR:HG22	2.01	0.43
1:A:886:ILE:HB	1:A:943:LEU:HD23	2.00	0.43
2:B:57:TYR:O	2:B:59:LEU:N	2.51	0.43
3:C:148:ARG:NH2	8:J:61:LEU:O	2.49	0.43
2:B:865:LYS:HA	2:B:871:THR:HG22	2.00	0.43
2:B:1163:CYS:HA	2:B:1191:ILE:HG13	2.01	0.43
6:H:4:THR:HG22	6:H:5:LEU:N	2.33	0.43
6:H:26:ILE:HD12	6:H:42:ILE:HB	2.00	0.43
1:A:377:PRO:HD3	1:A:493:GLN:NE2	2.34	0.43
1:A:548:ASN:HA	9:K:60:ALA:HB1	2.00	0.43
2:B:254:LEU:HD22	2:B:361:LEU:HD12	2.01	0.43
2:B:840:ILE:HG12	2:B:994:TYR:HE1	1.83	0.43
3:C:175:ALA:HB2	8:J:10:CYS:HB2	2.00	0.43
3:C:177:GLU:HB2	3:C:231:ASN:HB3	2.01	0.43
2:B:1169:MET:HG3	2:B:1205:GLN:HG3	2.01	0.42
3:C:66:ARG:NH1	8:J:2:ILE:HG22	2.31	0.42
1:A:70:CYS:HB2	2:B:1174:LYS:HD2	2.01	0.42
1:A:1290:LYS:HD3	1:A:1298:TYR:HB3	2.01	0.42
1:A:1292:PRO:HA	1:A:1298:TYR:HA	1.99	0.42
2:B:102:VAL:HB	2:B:112:LEU:HD13	2.01	0.42
2:B:119:LEU:HD22	2:B:789:MET:H	1.84	0.42
8:J:56:LEU:O	8:J:58:GLU:N	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:36:GLU:HA	9:K:36:GLU:OE1	2.18	0.42
1:A:857:ARG:NH2	5:F:139:PRO:HG2	2.34	0.42
1:A:1016:THR:HB	4:E:205:SER:O	2.19	0.42
2:B:246:LYS:HG2	2:B:249:ARG:HA	2.00	0.42
10:L:32:ALA:O	10:L:33:GLU:HB2	2.18	0.42
1:A:563:PRO:C	1:A:565:ILE:H	2.27	0.42
1:A:1066:VAL:O	1:A:1069:ALA:HB3	2.18	0.42
1:A:1175:SER:HA	1:A:1176:LEU:HA	1.78	0.42
1:A:1386:ARG:HH12	13:U:16:DA:H1'	1.84	0.42
1:A:1418:LEU:HD13	2:B:1222:ARG:HE	1.84	0.42
2:B:234:ILE:HG12	2:B:257:LYS:HD2	2.02	0.42
2:B:1071:VAL:HG13	3:C:189:THR:HG21	2.00	0.42
1:A:1317:MET:HG2	4:E:142:VAL:HG11	2.02	0.42
2:B:398:ARG:HH11	2:B:507:LYS:HD3	1.85	0.42
1:A:174:ILE:HG12	1:A:202:LEU:CD1	2.49	0.42
1:A:508:PRO:HA	1:A:511:ILE:HD12	2.01	0.42
1:A:1161:THR:HG21	1:A:1239:ARG:HH12	1.83	0.42
1:A:1320:PRO:HD3	4:E:7:ARG:HH21	1.85	0.42
2:B:487:THR:HG21	2:B:819:ALA:HB2	2.02	0.42
2:B:995:ARG:HD3	9:K:6:ARG:HH12	1.85	0.42
2:B:1071:VAL:HG22	2:B:1084:GLN:HG2	2.02	0.42
3:C:221:TYR:CG	6:H:46:LEU:HD22	2.40	0.42
1:A:2:VAL:N	2:B:1157:ALA:HB1	2.35	0.42
1:A:41:MET:HB3	1:A:42:ASP:H	1.59	0.42
1:A:588:LEU:HB3	1:A:607:ILE:HB	2.01	0.42
2:B:1017:ILE:HG22	2:B:1022:THR:HG23	2.01	0.42
3:C:183:TRP:CD1	3:C:210:GLU:HB3	2.55	0.42
1:A:369:SER:O	1:A:370:ILE:C	2.63	0.42
1:A:1140:HIS:HB2	1:A:1279:ILE:HB	2.02	0.42
2:B:57:TYR:HB2	2:B:58:THR:H	1.72	0.42
3:C:196:ASP:HB3	3:C:199:LYS:HB2	2.02	0.42
1:A:814:PHE:HA	1:A:817:ALA:HB3	2.01	0.42
2:B:119:LEU:HD22	2:B:789:MET:HB2	2.01	0.42
2:B:212:LEU:HA	2:B:479:VAL:O	2.20	0.42
2:B:242:SER:HB3	2:B:362:PRO:HD2	2.01	0.42
3:C:124:LEU:O	3:C:127:ARG:HG2	2.19	0.42
4:E:76:GLY:HA3	4:E:106:GLN:HB2	2.02	0.42
5:F:132:LEU:HD12	5:F:132:LEU:N	2.35	0.42
1:A:120:GLU:HA	1:A:123:ARG:HB3	2.02	0.41
1:A:598:LEU:HD23	6:H:25:ARG:HH22	1.84	0.41
1:A:1215:ARG:HG2	1:A:1273:LEU:HD23	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:789:MET:HG3	2:B:953:LEU:HD23	2.02	0.41
2:B:862:GLN:HB3	2:B:963:PHE:HD2	1.84	0.41
3:C:70:ILE:O	3:C:72:LEU:HD11	2.17	0.41
3:C:86:CYS:SG	3:C:92:CYS:SG	3.18	0.41
4:E:98:ILE:HG23	4:E:102:GLU:HG3	2.01	0.41
5:F:125:LEU:HD12	5:F:126:ALA:H	1.76	0.41
7:I:78:CYS:SG	7:I:106:CYS:SG	3.18	0.41
1:A:23:SER:HB3	1:A:233:TRP:CH2	2.55	0.41
2:B:224:GLN:HE21	2:B:396:ASP:HB3	1.86	0.41
3:C:259:LEU:HD11	9:K:91:CYS:CB	2.50	0.41
6:H:130:ARG:HB3	6:H:134:ASN:HB2	2.02	0.41
9:K:33:ILE:HD11	9:K:73:LEU:HD23	2.01	0.41
9:K:94:ILE:HG12	9:K:98:LEU:CD1	2.50	0.41
1:A:239:LEU:HD11	1:A:304:MET:CE	2.50	0.41
1:A:763:ALA:O	1:A:803:SER:HB2	2.20	0.41
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.35	0.41
2:B:254:LEU:CD1	2:B:272:THR:O	2.60	0.41
2:B:1158:PHE:HB3	2:B:1196:ILE:O	2.19	0.41
3:C:101:LEU:C	3:C:101:LEU:CD2	2.93	0.41
3:C:259:LEU:HD11	9:K:91:CYS:HB3	2.01	0.41
3:C:262:LEU:CD2	9:K:88:LYS:CE	2.97	0.41
4:E:88:VAL:HG11	4:E:110:PHE:HZ	1.84	0.41
8:J:30:LEU:CD1	8:J:31:ASP:O	2.67	0.41
1:A:453:MET:HG2	1:A:520:CYS:SG	2.60	0.41
1:A:960:ILE:HA	1:A:963:ILE:HD12	2.03	0.41
1:A:974:ASP:HA	1:A:975:HIS:CB	2.46	0.41
1:A:1340:GLY:HA2	4:E:182:ASP:OD2	2.20	0.41
2:B:563:MET:HE1	2:B:587:HIS:HB3	2.01	0.41
3:C:8:VAL:C	9:K:108:GLU:OE2	2.62	0.41
3:C:242:GLN:HA	3:C:245:VAL:HG12	2.03	0.41
4:E:110:PHE:CE2	4:E:116:ILE:CD1	2.96	0.41
1:A:1427:ASN:O	1:A:1431:GLY:N	2.53	0.41
2:B:54:PHE:HA	2:B:58:THR:HB	2.03	0.41
2:B:971:THR:HG21	3:C:61:GLU:HG3	2.01	0.41
2:B:1099:VAL:HA	2:B:1102:LYS:HB2	2.02	0.41
4:E:68:SER:HB3	4:E:75:MET:SD	2.60	0.41
7:I:9:ASP:O	7:I:10:CYS:C	2.63	0.41
2:B:237:VAL:HG12	2:B:255:GLN:HB2	2.02	0.41
2:B:299:GLU:HG3	2:B:572:HIS:NE2	2.35	0.41
2:B:895:ASP:C	2:B:897:GLY:H	2.28	0.41
2:B:979:LYS:HE2	2:B:1095:LEU:HD22	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:151:PRO:HB2	4:E:198:ILE:CG2	2.51	0.41
4:E:170:LEU:HD13	4:E:175:LEU:HD23	2.02	0.41
1:A:186:LYS:HG2	1:A:197:PRO:HB3	2.02	0.41
2:B:130:VAL:CG2	2:B:165:VAL:CG2	2.98	0.41
3:C:108:GLU:OE1	3:C:149:LYS:HE2	2.20	0.41
1:A:1269:GLU:O	1:A:1270:ASN:HB2	2.20	0.41
2:B:145:ARG:HA	2:B:146:GLU:CB	2.51	0.41
2:B:1034:VAL:HG22	2:B:1059:LEU:HD13	2.03	0.41
2:B:1187:ASN:HD22	2:B:1190:ASP:H	1.69	0.41
3:C:90:ASP:O	3:C:91:HIS:CB	2.67	0.41
3:C:221:TYR:CB	6:H:46:LEU:HD13	2.51	0.41
1:A:108:MET:HE1	1:A:174:ILE:HD11	2.02	0.41
1:A:344:ARG:HA	2:B:1129:ARG:HA	2.03	0.41
1:A:1151:GLU:HG2	7:I:45:ARG:HE	1.86	0.41
3:C:32:SER:HB2	9:K:45:LEU:HD23	2.01	0.41
3:C:43:THR:OG1	3:C:170:TRP:CB	2.67	0.41
3:C:56:THR:HG21	3:C:145:CYS:SG	2.61	0.41
4:E:37:LEU:HD21	4:E:45:LYS:HZ2	1.85	0.41
7:I:18:GLU:CG	7:I:20:LYS:HD3	2.45	0.41
10:L:47:ARG:HB3	10:L:54:ARG:HG2	2.03	0.41
1:A:71:GLN:HE22	2:B:1177:HIS:CD2	2.39	0.41
1:A:508:PRO:O	1:A:511:ILE:HB	2.21	0.41
1:A:540:PHE:HB3	1:A:571:LEU:HB3	2.02	0.41
1:A:767:GLN:HB2	1:A:799:PHE:HD1	1.86	0.41
2:B:135:ARG:CB	2:B:151:LEU:HD11	2.51	0.41
3:C:91:HIS:CD2	3:C:158:VAL:HG11	2.56	0.41
5:F:81:THR:OG1	5:F:146:TRP:NE1	2.53	0.41
1:A:785:PRO:HD2	1:A:786:HIS:HD2	1.85	0.40
2:B:29:ASP:HB3	2:B:658:ILE:HG21	2.02	0.40
2:B:245:GLU:N	2:B:246:LYS:HA	2.36	0.40
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.95	0.40
7:I:18:GLU:CG	7:I:20:LYS:HD2	2.51	0.40
1:A:565:ILE:HD12	1:A:565:ILE:C	2.46	0.40
1:A:837:ILE:HD11	1:A:1098:VAL:HG13	2.04	0.40
1:A:852:TYR:CE1	1:A:1060:PRO:HB2	2.56	0.40
1:A:1141:THR:HG22	1:A:1274:ARG:HB2	2.03	0.40
2:B:616:ILE:O	2:B:624:LEU:HA	2.21	0.40
4:E:145:THR:HA	4:E:150:VAL:HG11	2.03	0.40
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.87	0.40
1:A:1404:GLU:HB2	1:A:1408:ILE:HD12	2.03	0.40
2:B:287:ARG:HD3	2:B:325:GLN:HA	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:309:GLN:NE2	2:B:392:ARG:HH21	2.16	0.40
2:B:613:VAL:HG22	2:B:628:THR:HA	2.03	0.40
3:C:80:LEU:CD1	3:C:95:CYS:HA	2.50	0.40
4:E:116:ILE:CG2	4:E:120:ALA:HB3	2.52	0.40
1:A:506:ALA:O	1:A:509:LEU:HB2	2.21	0.40
1:A:549:MET:HE2	1:A:656:TRP:HB2	2.03	0.40
1:A:565:ILE:HA	6:H:97:MET:HA	2.03	0.40
1:A:1142:THR:O	1:A:1145:SER:HB3	2.21	0.40
2:B:825:VAL:HG21	2:B:1092:TYR:HE1	1.86	0.40
3:C:33:LEU:HD23	3:C:37:MET:SD	2.62	0.40
5:F:97:ARG:HH21	5:F:131:PRO:HG2	1.86	0.40
1:A:311:GLN:HB2	1:A:312:PRO:CD	2.46	0.40
1:A:704:ALA:HB2	1:A:710:LEU:HD12	2.04	0.40
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.51	0.40
3:C:43:THR:HG1	3:C:170:TRP:HD1	1.67	0.40
3:C:79:GLN:OE1	3:C:79:GLN:HA	2.21	0.40
6:H:26:ILE:O	6:H:40:LEU:N	2.31	0.40
9:K:37:LYS:N	9:K:37:LYS:HD3	2.37	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	1422/1733 (82%)	1129 (79%)	199 (14%)	94 (7%)	1	15
2	B	1141/1224 (93%)	919 (80%)	158 (14%)	64 (6%)	1	17
3	C	263/318 (83%)	226 (86%)	30 (11%)	7 (3%)	4	28
4	E	210/215 (98%)	186 (89%)	17 (8%)	7 (3%)	3	24
5	F	85/155 (55%)	72 (85%)	9 (11%)	4 (5%)	2	19
6	H	139/146 (95%)	97 (70%)	26 (19%)	16 (12%)	0	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	I	112/122 (92%)	88 (79%)	16 (14%)	8 (7%)	1	14
8	J	64/70 (91%)	49 (77%)	11 (17%)	4 (6%)	1	15
9	K	113/120 (94%)	99 (88%)	12 (11%)	2 (2%)	6	34
10	L	41/70 (59%)	31 (76%)	6 (15%)	4 (10%)	0	9
All	All	3590/4173 (86%)	2896 (81%)	484 (14%)	210 (6%)	1	16

All (210) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	65	LEU
1	A	152	VAL
1	A	153	PRO
1	A	162	VAL
1	A	190	ALA
1	A	370	ILE
1	A	399	HIS
1	A	465	TYR
1	A	466	SER
1	A	629	LEU
1	A	751	SER
1	A	846	GLU
1	A	847	ASP
1	A	1064	VAL
1	A	1067	LEU
1	A	1068	ALA
1	A	1072	ILE
1	A	1111	MET
1	A	1270	ASN
1	A	1365	TYR
1	A	1416	ALA
2	B	45	SER
2	B	58	THR
2	B	150	GLU
2	B	165	VAL
2	B	242	SER
2	B	477	ALA
2	B	531	GLN
2	B	785	TYR
2	B	807	ARG
2	B	895	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	933	SER
2	B	987	LYS
2	B	992	ILE
2	B	1046	PRO
2	B	1212	ILE
3	C	90	ASP
3	C	92	CYS
3	C	142	VAL
3	C	161	LYS
4	E	207	ARG
6	H	64	ASN
6	H	67	ASP
6	H	94	ASP
8	J	6	ARG
1	A	42	ASP
1	A	87	ALA
1	A	110	CYS
1	A	168	GLY
1	A	249	SER
1	A	252	PHE
1	A	258	GLY
1	A	490	HIS
1	A	566	ILE
1	A	567	LYS
1	A	595	THR
1	A	624	SER
1	A	626	ASN
1	A	975	HIS
1	A	1016	THR
1	A	1079	MET
1	A	1084	PHE
1	A	1085	HIS
1	A	1097	GLY
1	A	1377	THR
1	A	1433	MET
1	A	1437	GLY
2	B	76	GLN
2	B	95	ILE
2	B	146	GLU
2	B	152	ILE
2	B	164	LYS
2	B	247	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	351	TYR
2	B	442	PHE
2	B	478	GLY
2	B	479	VAL
2	B	507	LYS
2	B	705	MET
2	B	907	GLY
2	B	935	ARG
2	B	1216	LEU
3	C	175	ALA
4	E	59	SER
5	F	128	LYS
6	H	73	SER
6	H	77	ARG
6	H	96	VAL
6	H	107	VAL
6	H	109	LYS
7	I	3	THR
8	J	2	ILE
8	J	49	MET
10	L	69	ALA
1	A	130	ASP
1	A	154	SER
1	A	186	LYS
1	A	286	HIS
1	A	331	GLY
1	A	423	ASP
1	A	517	ASN
1	A	543	LEU
1	A	704	ALA
1	A	1127	ASP
2	B	55	VAL
2	B	96	TYR
2	B	111	ALA
2	B	358	LYS
2	B	510	LYS
2	B	711	GLU
2	B	751	VAL
2	B	836	GLU
2	B	896	ASP
2	B	943	SER
2	B	951	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	E	45	LYS
4	E	50	MET
6	H	85	GLY
7	I	88	SER
7	I	113	ASP
10	L	38	LEU
10	L	39	SER
1	A	54	ASN
1	A	72	GLU
1	A	156	ASP
1	A	167	CYS
1	A	215	SER
1	A	317	LYS
1	A	319	GLY
1	A	332	LYS
1	A	369	SER
1	A	598	LEU
1	A	628	GLY
1	A	854	ASN
1	A	958	VAL
1	A	1086	PHE
1	A	1115	SER
1	A	1184	SER
1	A	1327	ILE
1	A	1403	GLU
2	B	41	LYS
2	B	219	ALA
2	B	265	SER
2	B	395	GLN
2	B	504	ARG
2	B	514	LEU
2	B	1041	GLU
2	B	1155	SER
2	B	1185	CYS
3	C	40	GLU
3	C	214	ASN
4	E	86	PRO
5	F	72	LYS
5	F	78	GLN
5	F	139	PRO
6	H	45	GLU
6	H	84	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	H	87	ARG
6	H	129	TYR
7	I	10	CYS
7	I	11	ASN
7	I	95	THR
8	J	57	ILE
1	A	5	GLN
1	A	67	CYS
1	A	118	HIS
1	A	251	SER
1	A	254	GLU
1	A	385	ILE
1	A	418	SER
1	A	424	ILE
1	A	1002	GLY
1	A	1063	MET
1	A	1122	PRO
1	A	1300	LYS
2	B	652	LYS
2	B	712	PRO
2	B	868	MET
2	B	1108	ARG
2	B	1156	ASP
4	E	151	PRO
4	E	164	LEU
7	I	60	GLN
9	K	41	THR
10	L	30	ILE
1	A	114	LEU
1	A	565	ILE
1	A	986	ILE
1	A	1107	VAL
2	B	23	ALA
2	B	250	PHE
2	B	467	GLY
6	H	60	ALA
6	H	76	THR
7	I	28	GLU
1	A	250	ILE
1	A	910	PRO
2	B	960	GLY
1	A	158	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	K	23	PRO
1	A	474	VAL
2	B	1012	ILE
2	B	1045	SER
6	H	17	PRO
1	A	627	GLY
1	A	1089	VAL
2	B	501	PRO
2	B	1131	GLY
2	B	1119	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1244/1520 (82%)	1053 (85%)	191 (15%)	2	15
2	B	991/1061 (93%)	879 (89%)	112 (11%)	5	22
3	C	230/274 (84%)	221 (96%)	9 (4%)	28	51
4	E	194/197 (98%)	186 (96%)	8 (4%)	27	49
5	F	77/137 (56%)	74 (96%)	3 (4%)	28	51
6	H	115/128 (90%)	112 (97%)	3 (3%)	40	61
7	I	108/116 (93%)	106 (98%)	2 (2%)	50	67
8	J	61/65 (94%)	59 (97%)	2 (3%)	33	56
9	K	99/102 (97%)	96 (97%)	3 (3%)	36	57
10	L	38/57 (67%)	36 (95%)	2 (5%)	20	44
All	All	3157/3657 (86%)	2822 (89%)	335 (11%)	6	24

All (335) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	41	MET
1	A	57	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	65	LEU
1	A	112	LYS
1	A	132	LYS
1	A	138	ILE
1	A	140	THR
1	A	149	GLU
1	A	189	ARG
1	A	196	GLU
1	A	198	GLU
1	A	207	ILE
1	A	215	SER
1	A	250	ILE
1	A	254	GLU
1	A	263	THR
1	A	265	LYS
1	A	268	ASP
1	A	276	LEU
1	A	277	GLU
1	A	297	GLN
1	A	313	GLN
1	A	315	LEU
1	A	317	LYS
1	A	325	ILE
1	A	329	LEU
1	A	348	SER
1	A	361	LEU
1	A	363	GLN
1	A	368	LYS
1	A	374	LEU
1	A	383	TYR
1	A	389	THR
1	A	390	GLN
1	A	391	LEU
1	A	394	ASN
1	A	426	LEU
1	A	440	ASP
1	A	442	VAL
1	A	443	LEU
1	A	444	PHE
1	A	462	VAL
1	A	468	PHE
1	A	469	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	472	LEU
1	A	481	ASP
1	A	489	LEU
1	A	500	GLU
1	A	504	LEU
1	A	507	VAL
1	A	509	LEU
1	A	511	ILE
1	A	518	LYS
1	A	520	CYS
1	A	523	ILE
1	A	527	THR
1	A	528	LEU
1	A	536	LEU
1	A	538	ASP
1	A	541	ILE
1	A	542	GLU
1	A	548	ASN
1	A	549	MET
1	A	555	ASP
1	A	560	ILE
1	A	576	GLN
1	A	577	ILE
1	A	578	LEU
1	A	579	SER
1	A	586	ILE
1	A	588	LEU
1	A	592	ASP
1	A	597	LEU
1	A	598	LEU
1	A	605	MET
1	A	606	LEU
1	A	625	SER
1	A	630	ILE
1	A	635	ARG
1	A	645	LEU
1	A	657	LEU
1	A	658	LEU
1	A	666	ILE
1	A	668	ASP
1	A	679	ILE
1	A	681	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	701	LEU
1	A	702	LEU
1	A	710	LEU
1	A	719	VAL
1	A	732	LEU
1	A	738	LYS
1	A	743	VAL
1	A	756	ILE
1	A	758	ILE
1	A	764	CYS
1	A	769	SER
1	A	770	VAL
1	A	806	ARG
1	A	821	ARG
1	A	827	THR
1	A	841	LEU
1	A	854	ASN
1	A	855	THR
1	A	862	ASN
1	A	865	GLN
1	A	867	ILE
1	A	878	ILE
1	A	885	THR
1	A	890	ASP
1	A	894	GLU
1	A	898	ARG
1	A	899	VAL
1	A	906	HIS
1	A	913	LEU
1	A	914	GLU
1	A	918	GLU
1	A	919	ILE
1	A	920	LEU
1	A	923	LEU
1	A	924	LYS
1	A	925	LEU
1	A	932	GLU
1	A	936	LEU
1	A	943	LEU
1	A	973	ILE
1	A	974	ASP
1	A	983	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	987	VAL
1	A	998	LEU
1	A	999	VAL
1	A	1006	ILE
1	A	1011	GLN
1	A	1024	SER
1	A	1032	LEU
1	A	1034	GLU
1	A	1049	ILE
1	A	1064	VAL
1	A	1066	VAL
1	A	1070	GLN
1	A	1080	THR
1	A	1081	LEU
1	A	1086	PHE
1	A	1096	SER
1	A	1100	ARG
1	A	1105	LEU
1	A	1112	LYS
1	A	1113	THR
1	A	1134	ILE
1	A	1155	ASP
1	A	1157	ASP
1	A	1166	ASP
1	A	1173	HIS
1	A	1176	LEU
1	A	1177	LEU
1	A	1189	SER
1	A	1192	LEU
1	A	1193	LEU
1	A	1195	LEU
1	A	1202	MET
1	A	1205	LYS
1	A	1218	GLN
1	A	1224	LEU
1	A	1234	GLU
1	A	1238	ILE
1	A	1241	ARG
1	A	1242	VAL
1	A	1243	VAL
1	A	1259	MET
1	A	1260	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1264	GLU
1	A	1266	THR
1	A	1271	ILE
1	A	1273	LEU
1	A	1276	VAL
1	A	1291	VAL
1	A	1295	THR
1	A	1306	LEU
1	A	1314	SER
1	A	1325	THR
1	A	1342	GLU
1	A	1370	LEU
1	A	1371	LEU
1	A	1374	VAL
1	A	1381	LEU
1	A	1398	MET
1	A	1404	GLU
1	A	1409	LEU
1	A	1419	ASP
1	A	1445	ILE
2	B	39	ARG
2	B	70	ILE
2	B	71	LEU
2	B	83	ASN
2	B	92	PHE
2	B	146	GLU
2	B	172	ILE
2	B	189	LEU
2	B	199	MET
2	B	213	ILE
2	B	237	VAL
2	B	246	LYS
2	B	258	LEU
2	B	276	ILE
2	B	277	LYS
2	B	279	ASP
2	B	280	ILE
2	B	320	ASP
2	B	325	GLN
2	B	364	ILE
2	B	376	PHE
2	B	395	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	401	PHE
2	B	413	LEU
2	B	416	LEU
2	B	423	LYS
2	B	437	GLU
2	B	438	GLU
2	B	449	ASN
2	B	461	LEU
2	B	465	ASN
2	B	484	ASN
2	B	489	SER
2	B	491	THR
2	B	500	THR
2	B	502	ILE
2	B	508	LEU
2	B	522	VAL
2	B	545	ILE
2	B	563	MET
2	B	574	SER
2	B	576	ASP
2	B	589	VAL
2	B	592	ASN
2	B	595	ARG
2	B	602	THR
2	B	612	GLU
2	B	616	ILE
2	B	619	ILE
2	B	624	LEU
2	B	635	ARG
2	B	641	GLU
2	B	642	ASP
2	B	650	GLU
2	B	651	LEU
2	B	678	GLU
2	B	699	GLU
2	B	701	ILE
2	B	709	ASP
2	B	739	THR
2	B	743	ILE
2	B	758	PHE
2	B	773	MET
2	B	787	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	795	ILE
2	B	796	LEU
2	B	837	ASP
2	B	839	MET
2	B	840	ILE
2	B	841	MET
2	B	844	SER
2	B	860	MET
2	B	861	ASP
2	B	862	GLN
2	B	863	GLU
2	B	873	THR
2	B	889	THR
2	B	905	VAL
2	B	923	GLU
2	B	935	ARG
2	B	944	THR
2	B	950	ASP
2	B	956	THR
2	B	958	GLN
2	B	961	LEU
2	B	969	ARG
2	B	971	THR
2	B	973	ILE
2	B	975	GLN
2	B	987	LYS
2	B	990	ILE
2	B	1007	VAL
2	B	1010	LEU
2	B	1012	ILE
2	B	1027	ILE
2	B	1028	GLU
2	B	1049	ASP
2	B	1051	THR
2	B	1052	VAL
2	B	1072	MET
2	B	1087	PHE
2	B	1098	MET
2	B	1138	MET
2	B	1147	LEU
2	B	1148	LYS
2	B	1187	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1191	ILE
2	B	1194	ILE
2	B	1206	GLU
2	B	1217	TYR
2	B	1218	THR
2	B	1222	ARG
3	C	22	LEU
3	C	27	LEU
3	C	63	ILE
3	C	66	ARG
3	C	69	LEU
3	C	72	LEU
3	C	98	VAL
3	C	143	LEU
3	C	187	LYS
4	E	33	GLU
4	E	95	THR
4	E	123	LEU
4	E	137	GLU
4	E	154	ILE
4	E	175	LEU
4	E	188	LEU
4	E	190	LEU
5	F	69	LEU
5	F	101	ILE
5	F	124	GLU
6	H	37	LYS
6	H	63	LEU
6	H	130	ARG
7	I	46	HIS
7	I	52	ILE
8	J	25	LEU
8	J	41	LEU
9	K	12	LEU
9	K	16	GLU
9	K	38	GLU
10	L	28	LYS
10	L	46	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	71	GLN
1	A	119	ASN
1	A	171	GLN
1	A	306	ASN
1	A	316	GLN
1	A	363	GLN
1	A	390	GLN
1	A	435	HIS
1	A	479	ASN
1	A	493	GLN
1	A	515	GLN
1	A	548	ASN
1	A	589	GLN
1	A	760	GLN
1	A	768	GLN
1	A	865	GLN
1	A	881	GLN
1	A	926	GLN
1	A	965	GLN
1	A	1048	ASN
1	A	1070	GLN
1	A	1128	GLN
1	A	1130	GLN
1	A	1183	GLN
1	A	1188	GLN
1	A	1203	ASN
1	A	1211	GLN
1	A	1218	GLN
1	A	1354	ASN
1	A	1387	HIS
2	B	46	GLN
2	B	60	GLN
2	B	178	ASN
2	B	221	ASN
2	B	224	GLN
2	B	309	GLN
2	B	325	GLN
2	B	350	GLN
2	B	415	GLN
2	B	484	ASN
2	B	499	ASN
2	B	518	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	538	ASN
2	B	610	ASN
2	B	706	GLN
2	B	770	GLN
2	B	794	ASN
2	B	800	GLN
2	B	835	GLN
2	B	843	GLN
2	B	862	GLN
2	B	958	GLN
2	B	975	GLN
2	B	1040	ASN
2	B	1097	HIS
2	B	1177	HIS
3	C	17	ASN
3	C	54	ASN
3	C	112	ASN
3	C	123	ASN
3	C	131	HIS
3	C	214	ASN
3	C	231	ASN
4	E	8	ASN
4	E	54	GLN
4	E	99	HIS
4	E	146	HIS
6	H	43	ASN
6	H	52	GLN
7	I	11	ASN
7	I	12	ASN
7	I	83	ASN
9	K	2	ASN
9	K	29	ASN
9	K	52	ASN
9	K	65	HIS
9	K	89	ASN
9	K	92	ASN
9	K	110	ASN
10	L	53	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	7/9 (77%)	2 (28%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	6	G
11	R	8	G

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 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	1432/1733 (82%)	-0.23	11 (0%) 82 65	28, 216, 298, 382	0
2	B	1157/1224 (94%)	-0.13	14 (1%) 76 59	115, 221, 304, 366	0
3	C	265/318 (83%)	-0.24	3 (1%) 78 60	134, 213, 270, 315	0
4	E	212/215 (98%)	-0.29	2 (0%) 81 64	153, 232, 298, 322	0
5	F	87/155 (56%)	-0.09	2 (2%) 61 45	134, 193, 260, 341	0
6	H	143/146 (97%)	-0.35	1 (0%) 84 68	176, 258, 312, 334	0
7	I	114/122 (93%)	-0.36	0 100 100	177, 240, 306, 334	0
8	J	66/70 (94%)	-0.25	2 (3%) 52 38	125, 223, 286, 318	0
9	K	115/120 (95%)	-0.18	1 (0%) 81 64	131, 202, 271, 293	0
10	L	43/70 (61%)	0.01	1 (2%) 61 45	170, 228, 283, 364	0
11	R	9/9 (100%)	-0.33	0 100 100	285, 306, 337, 338	0
12	S	38/53 (71%)	0.13	0 100 100	338, 360, 380, 381	0
13	U	38/53 (71%)	0.17	0 100 100	275, 348, 378, 380	0
All	All	3719/4288 (86%)	-0.20	37 (0%) 79 61	28, 221, 309, 382	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	PRO	4.4
4	E	211	TYR	4.3
2	B	161	GLU	4.1
3	C	178	PHE	3.4
8	J	44	TYR	3.4
9	K	59	ALA	3.4
2	B	349	ILE	3.3
5	F	155	LEU	3.3
2	B	1087	PHE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1432	GLN	2.9
1	A	208	LEU	2.8
2	B	745	PRO	2.7
1	A	241	VAL	2.7
1	A	204	THR	2.7
2	B	970	THR	2.7
1	A	866	PHE	2.6
1	A	232	GLU	2.6
2	B	987	LYS	2.5
1	A	483	ASP	2.5
2	B	1172	ILE	2.5
2	B	1161	HIS	2.5
2	B	1009	ASP	2.5
1	A	801	GLU	2.4
2	B	283	VAL	2.4
2	B	25	ILE	2.2
6	H	40	LEU	2.2
8	J	4	PRO	2.2
1	A	56	PRO	2.1
5	F	85	MET	2.1
4	E	197	LYS	2.1
3	C	157	CYS	2.1
2	B	1097	HIS	2.1
2	B	1211	ASN	2.1
1	A	211	PHE	2.0
10	L	59	ALA	2.0
3	C	29	MET	2.0
2	B	1206	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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
15	MG	R	101	1/1	0.90	0.07	201,201,201,201	0
14	ZN	J	101	1/1	0.97	0.06	207,207,207,207	0
14	ZN	A	1801	1/1	0.98	0.13	205,205,205,205	0
14	ZN	C	401	1/1	0.99	0.05	226,226,226,226	0
14	ZN	C	402	1/1	0.99	0.03	186,186,186,186	0
14	ZN	I	202	1/1	0.99	0.02	213,213,213,213	0
14	ZN	A	1802	1/1	0.99	0.03	200,200,200,200	0
14	ZN	L	101	1/1	0.99	0.02	202,202,202,202	0
14	ZN	B	1301	1/1	0.99	0.04	214,214,214,214	0
14	ZN	I	201	1/1	1.00	0.04	201,201,201,201	0

6.5 Other polymers [i](#)

There are no such residues in this entry.