



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:05 PM UTC

PDB ID : 4BXZ / pdb_00004bxz
Title : RNA Polymerase II-Bye1 complex
Authors : Kinkelin, K.; Wozniak, G.G.; Rothbart, S.B.; Lidschreiber, M.; Strahl, B.D.; Cramer, P.
Deposited on : 2013-07-16
Resolution : 4.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

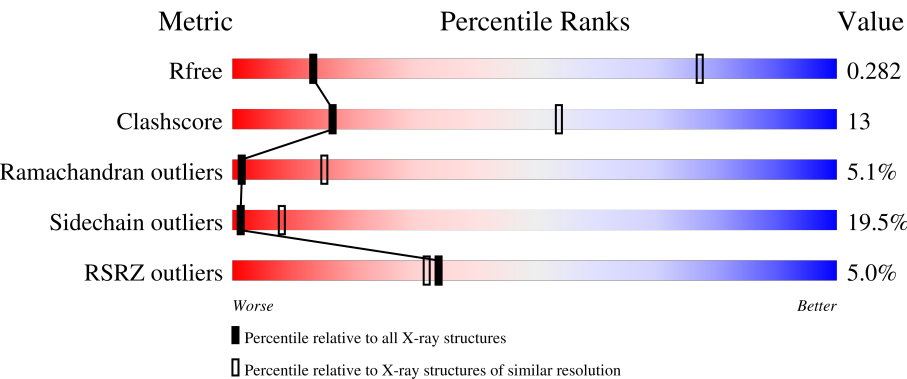
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
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 4.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1018 (5.66-3.94)
Clashscore	190562	1001 (5.60-3.98)
Ramachandran outliers	187476	1104 (5.70-3.90)
Sidechain outliers	187428	1085 (5.70-3.90)
RSRZ outliers	180081	1013 (5.66-3.94)

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	3% 40% 32% 8% 18%
2	B	1224	5% 49% 31% 9% 10%
3	C	318	43% 31% 8% 16%
4	D	221	5% 46% 28% 7% 20%
5	E	215	5% 54% 37% 7%

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Mol	Chain	Length	Quality of chain
6	F	155	2% 26% 25% . 46%
7	G	171	3% 60% 36% .
8	H	146	9% 42% 38% 10% . 9%
9	I	122	7% 54% 39% . . .
10	J	70	6% 44% 40% 6% . 7%
11	K	120	2% 62% 27% 8% .
12	L	70	14% 36% 20% 9% . 34%
13	X	594	4% 16% . 81%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 31509 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	1416	Total	C	N	O	S	0	0	0
			11140	7021	1946	2111	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1097	Total	C	N	O	S	0	0	0
			8720	5526	1523	1617	54			

- 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	177	Total	C	N	O	S	0	0	0
			1356	840	241	273	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1.

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 RPABC2.

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 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 RPABC3.

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 RPABC5.

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 RPABC4.

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 protein called TRANSCRIPTION FACTOR BYE1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	X	113	Total	C	N	O	0	0	0
			564	338	113	113			

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

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

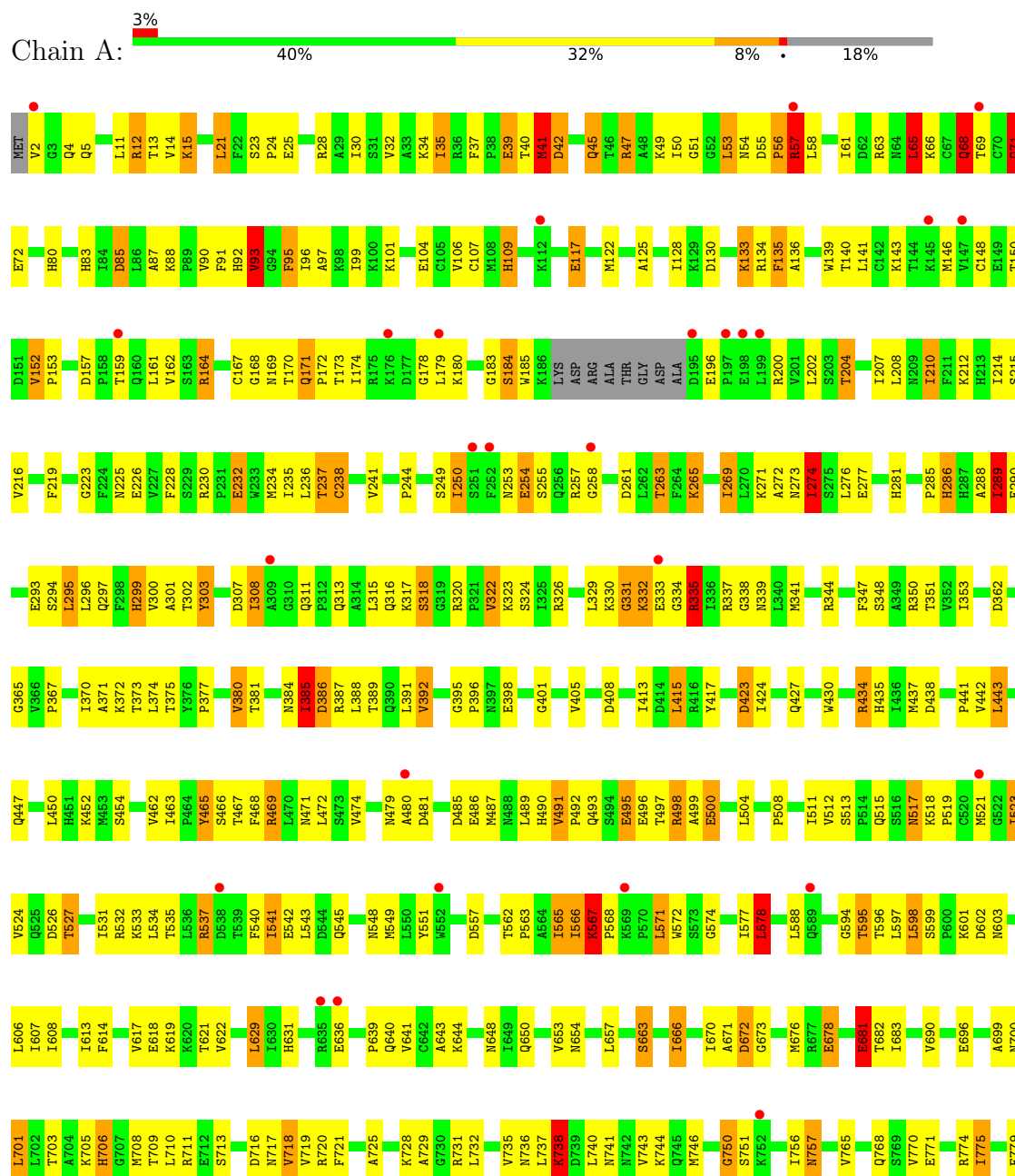
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

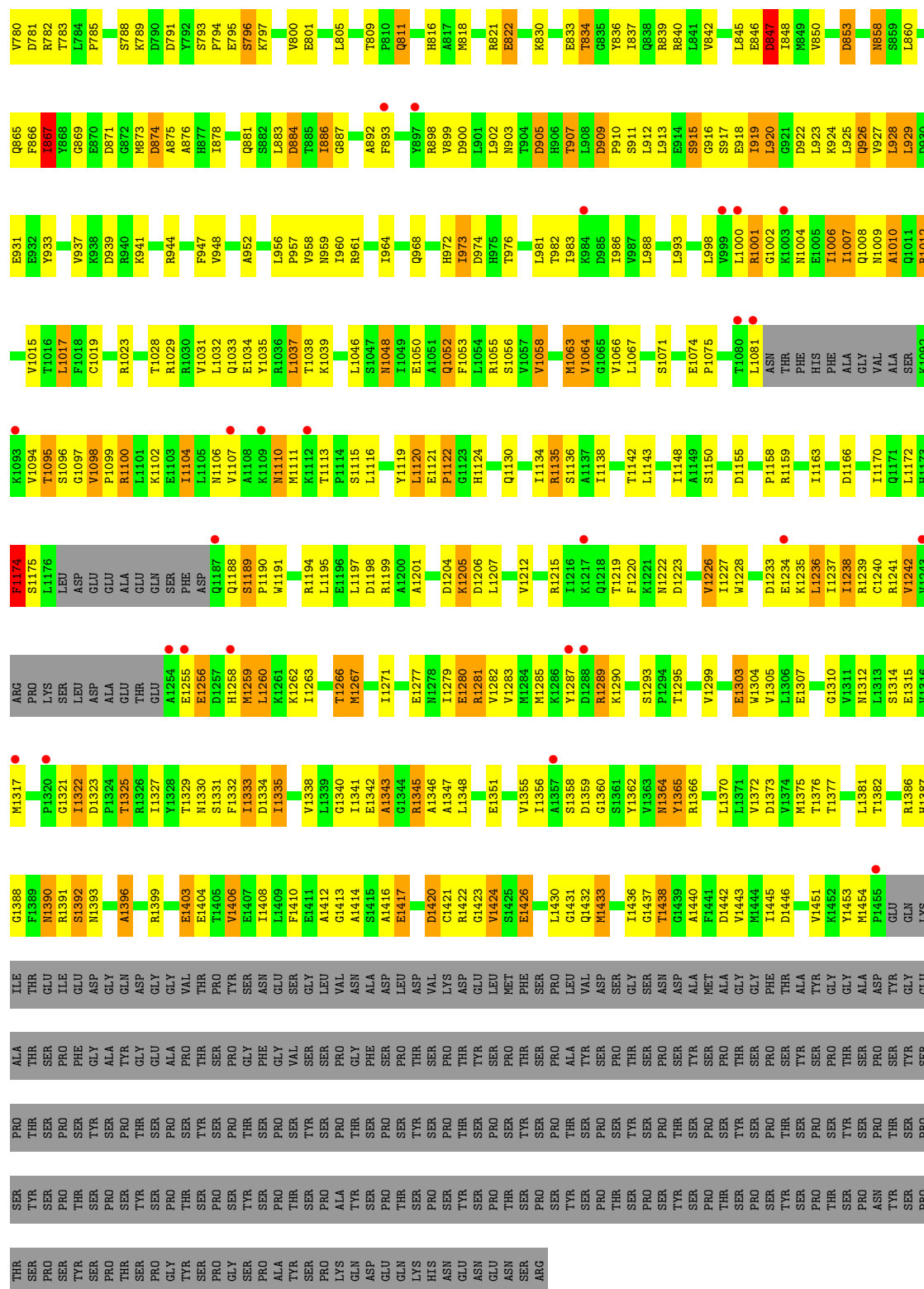
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

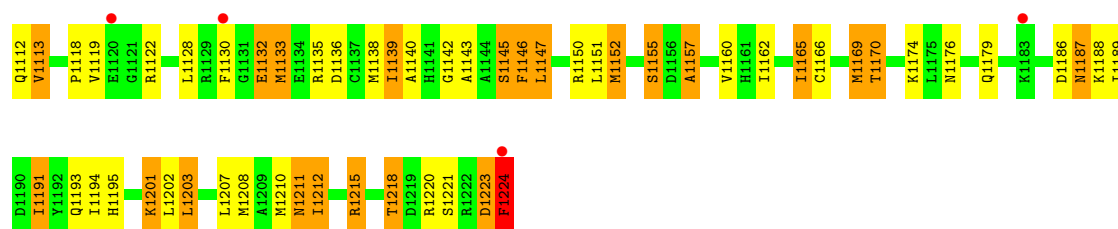
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



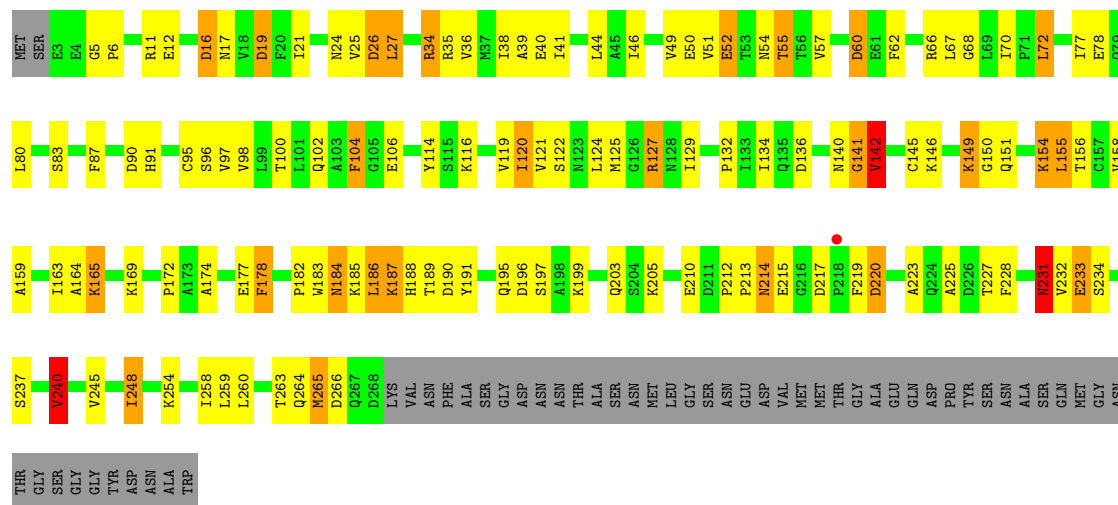






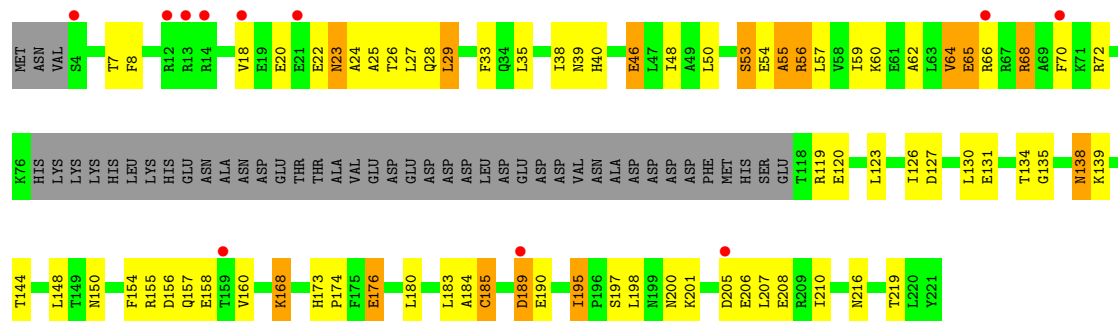
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C: 43% 31% 8% 16%



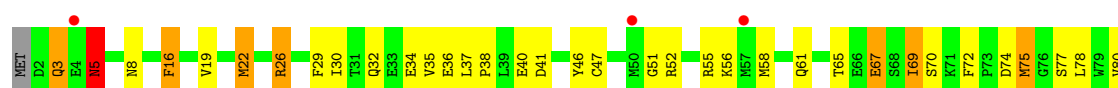
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

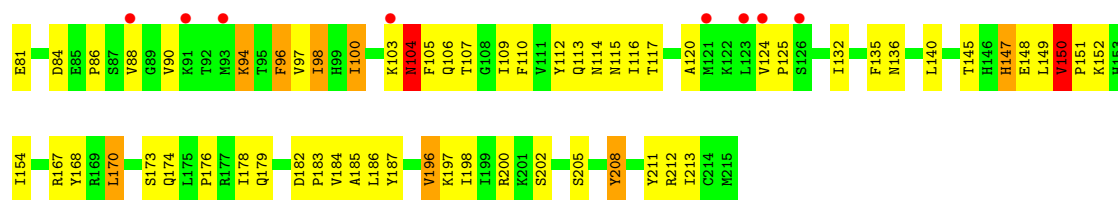
Chain D: 5% 46% 28% 7% 20%



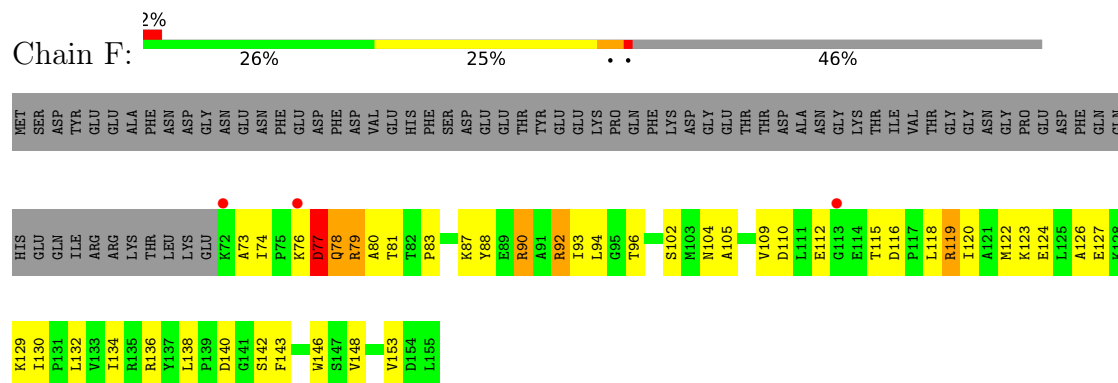
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1

Chain E: 5% 54% 37% 7%

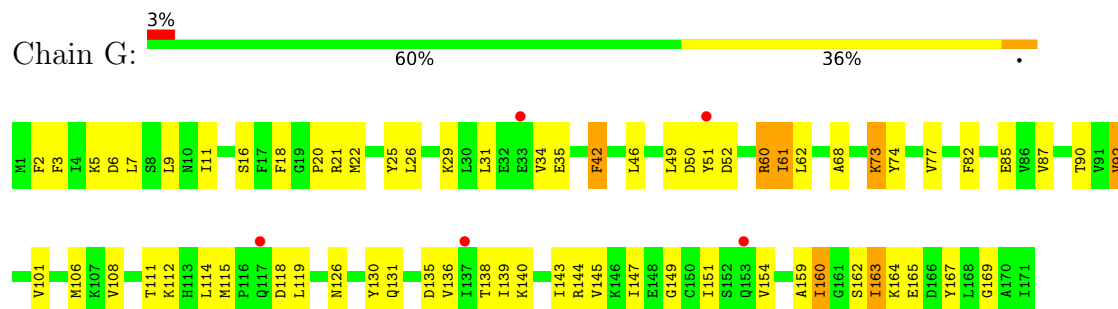




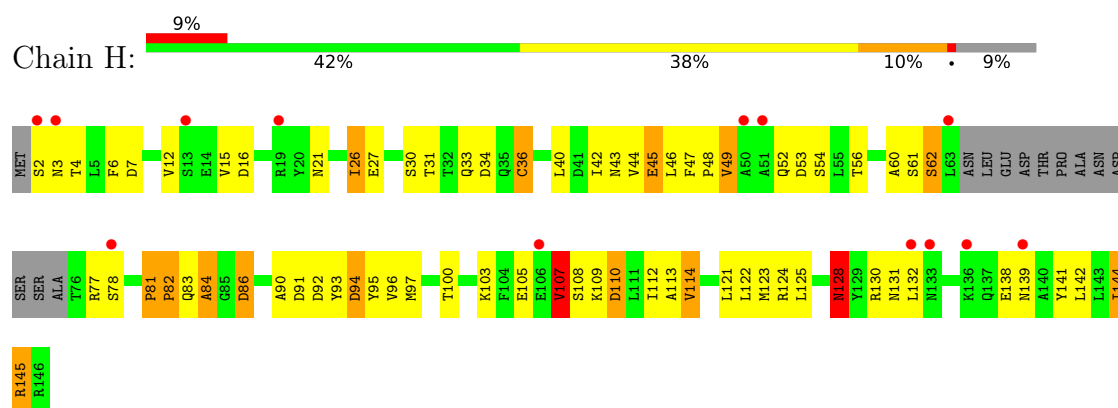
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2



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

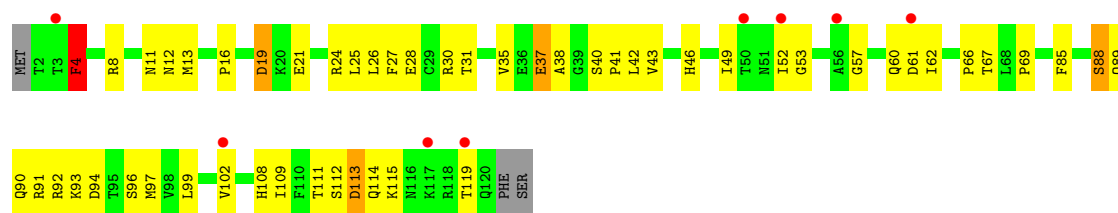


• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3

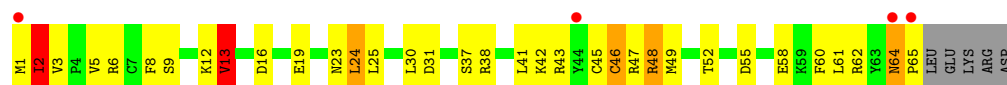
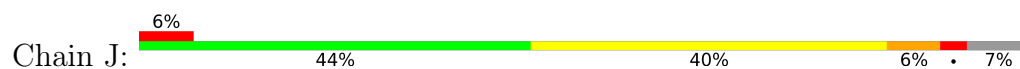


• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

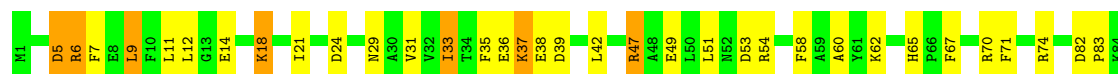




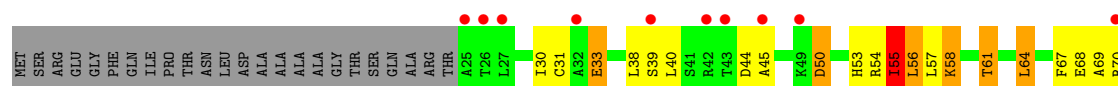
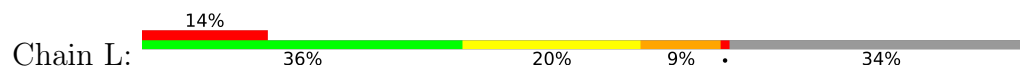
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5



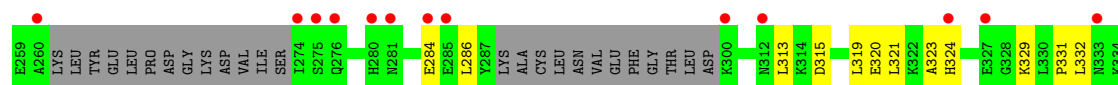
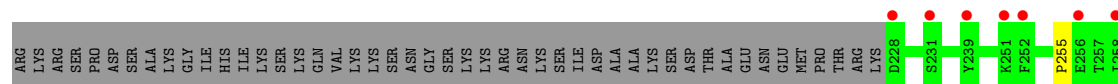
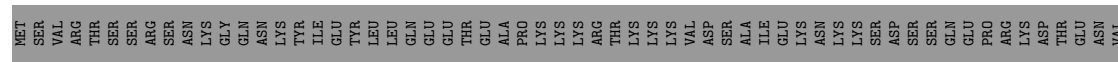
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11



• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4



• Molecule 13: TRANSCRIPTION FACTOR BYE1



ILE HIS	ILE	ASP	SER	L336	Y336	SER
	PRO	GLY	ILE	N337	N337	ILE
LYS	LYS	LEU	GLU	N338	N338	GLN
ARG	VAL	THR	THR	N339	N339	THR
TYR	GLU	GLU	HIS	N345	N345	HIS
LYS	GLY	ARG	ALA	P346	P346	ALA
ASP	LEU	LEU	ILE	D347	D347	ILE
PHE	PRO	THR	SER	N362	N362	SER
TYR	THR	THR	LYS	V365	V365	GLU
ILE	VAL	THR	PRO	GLU	GLU	VAL
VAL	ALA	ALA	PRO	VAL	VAL	PRO
SER	ALA	ALA	SER	PRO	PRO	PRO
LYS	PRO	PRO	THR	ASP	ASP	ASP
GLY	TYR	TYR	ILE	LYS	LYS	LYS
GLY	LEU	LEU	ILE	PRO	PRO	PRO
GLU	LYS	LYS	ASN	MET	MET	TYR
ILE	GLU	GLU	GLU	TYR	TYR	VAL
PRO	ILE	ILE	GLU	VAL	VAL	VAL
GLU	GLU	CYS	SER	LYS	LYS	LYS
ILE	ILE	TYR	ASN	HIS	HIS	THR
LEU	LEU	SER	CYS	LYS	LYS	LYS
ASP	ALA	ALA	GLY	GLY	GLY	GLY
ILE	ILE	ILE	PHE	ASP	ASP	ASP
GLY	VAL	VAL	LEU	GLU	GLU	GLU
SER	TYR	TYR	PRO	LEU	LEU	LEU
SER	TYR	TYR	ILE	GLY	GLY	ILE
HIS	GLN	GLN	GLY	ASP	ASP	ASP
ASN	LEU	LEU	LEU	ILE	ILE	ILE
ASP	PHE	PHE	GLY	GLU	GLU	GLU
GLU	PRO	PRO	LEU	ALA	ALA	ALA
ARG	SER	SER	GLU	GLU	GLU	GLU
SER	ASN	ASN	PHE	PRO	PRO	PRO
GLY	ASP	ASP	THR	GLN	GLN	GLN
PHE	ARG	ARG	TYR	GLY	GLY	GLY
SER	GLU	GLU	TYR	ASP	ASP	ASP
SER	SER	SER	ILE	ILE	ILE	ILE
ARG	LYS	LYS	ASN	LEU	LEU	LEU
MET	TYR	TYR	TYR	TYR	TYR	TYR
LYS	THR	THR	ILE	SER	SER	SER
SER	PHE	PHE	GLY	LYS	LYS	LYS
ASP	ALA	ALA	ALA	ASP	ASP	ASP
GLU	VAL	VAL	SER	GLU	GLU	GLU
THR	THR	THR	GLN	THR	THR	THR
LEU	VAL	VAL	LYS	ARG	ARG	ARG
PHE	ASP	ASP	LEU	LEU	LEU	LEU
ALA	SER	SER	ARG	HIS	HIS	HIS
PHE	LEU	LEU	ASP	ASN	ASN	ASN
VAL	GLU	GLU	ILE	ILE	ILE	ILE
VAL	VAL	VAL	PHE	ASP	ASP	ASP
VAL	LYS	LYS	LYS	ILE	ILE	ILE
GLN	ARG	ARG	GLU	ASP	ASP	ASP
GLU	ILE	ILE	ALA	SER	SER	SER
PHE	GLY	GLY	ILE	ASP	ASP	ASP

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	220.55Å 392.09Å 279.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 4.80 49.63 – 4.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.63-4.80) 99.8 (49.63-4.80)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 4.86Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.191 , 0.253 0.218 , 0.282	Depositor DCC
R_{free} test set	1172 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	151.9	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 349.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.039 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	31509	wwPDB-VP
Average B, all atoms (Å ²)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% 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	0.92	6/11339 (0.1%)	1.57	154/15334 (1.0%)
2	B	0.90	1/8889 (0.0%)	1.52	104/11987 (0.9%)
3	C	0.88	0/2133	1.46	24/2891 (0.8%)
4	D	0.88	0/1365	1.64	17/1837 (0.9%)
5	E	0.85	0/1788	1.51	27/2406 (1.1%)
6	F	0.93	0/691	1.53	9/933 (1.0%)
7	G	0.81	0/1368	1.43	4/1844 (0.2%)
8	H	0.94	0/1086	1.51	18/1470 (1.2%)
9	I	0.85	0/989	1.44	15/1331 (1.1%)
10	J	0.90	0/541	1.44	1/727 (0.1%)
11	K	0.85	0/938	1.50	10/1267 (0.8%)
12	L	0.96	0/365	1.54	2/485 (0.4%)
13	X	1.09	0/561	1.88	11/780 (1.4%)
All	All	0.90	7/32053 (0.0%)	1.54	396/43292 (0.9%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	ARG	CA-C	6.75	1.61	1.52
1	A	274	ILE	CA-C	6.12	1.59	1.52
1	A	858	ASN	CA-C	6.03	1.60	1.52
1	A	244	PRO	CA-C	5.73	1.57	1.52
1	A	491	VAL	CA-C	5.21	1.57	1.53
2	B	968	VAL	CA-C	5.09	1.58	1.52
1	A	250	ILE	CA-C	5.08	1.57	1.52

All (396) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	4	PHE	CA-CB-CG	11.03	124.83	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	5	ASN	N-CA-C	-8.91	102.56	113.97
1	A	517	ASN	CA-CB-CG	8.86	121.46	112.60
4	D	189	ASP	CA-CB-CG	8.50	121.10	112.60
1	A	56	PRO	CA-C-N	8.50	137.77	121.54
1	A	56	PRO	C-N-CA	8.50	137.77	121.54
1	A	1392	SER	CA-C-N	8.44	131.94	120.54
1	A	1392	SER	C-N-CA	8.44	131.94	120.54
13	X	321	LEU	N-CA-C	-8.32	102.32	114.39
1	A	1039	LYS	N-CA-C	-7.85	102.81	111.36
2	B	1130	PHE	N-CA-C	-7.79	98.05	109.11
4	D	189	ASP	N-CA-C	-7.69	101.64	111.02
1	A	134	ARG	N-CA-C	-7.64	103.03	111.36
1	A	381	THR	CB-CA-C	7.64	120.38	108.84
1	A	237	THR	N-CA-C	-7.53	105.00	114.56
11	K	71	PHE	CA-CB-CG	7.46	121.26	113.80
2	B	1169	MET	CA-C-N	7.33	130.41	120.44
2	B	1169	MET	C-N-CA	7.33	130.41	120.44
2	B	296	GLU	N-CA-C	-7.32	102.94	112.68
1	A	219	PHE	CA-CB-CG	7.22	121.02	113.80
1	A	1312	ASN	CA-C-N	7.21	130.26	120.38
1	A	1312	ASN	C-N-CA	7.21	130.26	120.38
1	A	1406	VAL	CA-C-N	7.13	130.71	120.79
1	A	1406	VAL	C-N-CA	7.13	130.71	120.79
13	X	286	LEU	N-CA-C	-7.10	103.74	113.18
8	H	83	GLN	CA-C-N	7.09	135.09	121.54
8	H	83	GLN	C-N-CA	7.09	135.09	121.54
2	B	784	ASN	CA-C-N	7.08	135.07	121.54
2	B	784	ASN	C-N-CA	7.08	135.07	121.54
13	X	255	PRO	N-CA-CB	7.07	110.67	103.25
3	C	62	PHE	CA-CB-CG	7.06	120.86	113.80
1	A	858	ASN	CA-C-N	7.05	135.18	122.06
1	A	858	ASN	C-N-CA	7.05	135.18	122.06
2	B	198	ASP	CA-C-N	7.05	130.04	120.38
2	B	198	ASP	C-N-CA	7.05	130.04	120.38
1	A	269	ILE	N-CA-C	-7.03	104.92	111.45
3	C	104	PHE	CA-CB-CG	7.02	120.82	113.80
2	B	1146	PHE	N-CA-C	-7.01	102.70	112.45
7	G	2	PHE	CA-CB-CG	6.99	120.78	113.80
1	A	598	LEU	N-CA-C	-6.95	104.83	113.38
2	B	1049	ASP	N-CA-C	-6.95	105.34	114.31
8	H	90	ALA	N-CA-C	-6.91	96.50	108.52
1	A	408	ASP	CA-CB-CG	6.90	119.50	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	853	ASP	CA-C-N	6.90	132.68	122.74
1	A	853	ASP	C-N-CA	6.90	132.68	122.74
2	B	890	TYR	CA-C-N	6.87	130.41	120.38
2	B	890	TYR	C-N-CA	6.87	130.41	120.38
6	F	90	ARG	CA-C-N	6.82	130.10	120.28
6	F	90	ARG	C-N-CA	6.82	130.10	120.28
2	B	575	PRO	CA-C-N	6.78	131.45	120.60
2	B	575	PRO	C-N-CA	6.78	131.45	120.60
1	A	892	ALA	CA-C-N	6.75	129.21	120.44
1	A	892	ALA	C-N-CA	6.75	129.21	120.44
5	E	147	HIS	CA-C-N	6.75	129.21	120.44
5	E	147	HIS	C-N-CA	6.75	129.21	120.44
2	B	1136	ASP	CA-CB-CG	6.74	119.34	112.60
2	B	1187	ASN	CA-C-N	6.72	134.38	121.54
2	B	1187	ASN	C-N-CA	6.72	134.38	121.54
4	D	59	ILE	N-CA-C	-6.71	103.69	111.00
2	B	1211	ASN	CA-CB-CG	6.71	119.31	112.60
8	H	128	ASN	CA-C-N	6.67	129.11	120.44
8	H	128	ASN	C-N-CA	6.67	129.11	120.44
1	A	150	THR	N-CA-C	-6.67	104.09	111.36
2	B	911	ILE	N-CA-C	-6.66	107.01	113.53
6	F	77	ASP	N-CA-C	-6.64	98.80	109.96
1	A	12	ARG	CA-C-N	6.61	132.03	120.87
1	A	12	ARG	C-N-CA	6.61	132.03	120.87
8	H	92	ASP	CA-C-N	6.60	131.72	121.76
8	H	92	ASP	C-N-CA	6.60	131.72	121.76
2	B	736	THR	N-CA-C	-6.56	105.44	113.50
5	E	96	PHE	CA-CB-CG	6.50	120.30	113.80
2	B	1224	PHE	CA-CB-CG	6.49	120.29	113.80
2	B	732	SER	CA-C-N	6.48	131.53	120.72
2	B	732	SER	C-N-CA	6.48	131.53	120.72
1	A	351	THR	CA-C-N	6.46	129.34	120.35
1	A	351	THR	C-N-CA	6.46	129.34	120.35
3	C	60	ASP	CA-CB-CG	6.45	119.05	112.60
1	A	887	GLY	N-CA-C	6.43	120.77	112.54
2	B	628	THR	N-CA-C	-6.43	104.13	114.09
2	B	1186	ASP	CA-CB-CG	6.42	119.02	112.60
3	C	26	ASP	CA-CB-CG	6.41	119.01	112.60
3	C	178	PHE	CA-CB-CG	6.41	120.20	113.80
2	B	834	ASN	CA-CB-CG	6.38	118.98	112.60
13	X	331	PRO	N-CA-CB	6.37	109.94	103.25
2	B	1201	LYS	CA-C-N	6.36	128.71	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	LYS	C-N-CA	6.36	128.71	120.44
1	A	296	LEU	CA-C-N	6.31	129.36	120.28
1	A	296	LEU	C-N-CA	6.31	129.36	120.28
2	B	846	ILE	CA-C-N	6.29	129.00	120.38
2	B	846	ILE	C-N-CA	6.29	129.00	120.38
4	D	189	ASP	CA-C-N	6.23	128.54	120.44
4	D	189	ASP	C-N-CA	6.23	128.54	120.44
2	B	600	LEU	CA-C-N	6.22	128.91	120.38
2	B	600	LEU	C-N-CA	6.22	128.91	120.38
1	A	271	LYS	N-CA-C	-6.21	104.19	110.97
2	B	20	ASP	CA-C-N	6.19	128.86	120.38
2	B	20	ASP	C-N-CA	6.19	128.86	120.38
1	A	1010	ALA	CA-C-N	6.17	128.84	120.44
1	A	1010	ALA	C-N-CA	6.17	128.84	120.44
5	E	173	SER	CA-C-N	6.15	133.28	121.54
5	E	173	SER	C-N-CA	6.15	133.28	121.54
2	B	694	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	1446	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	56	PRO	N-CA-C	-6.10	106.88	114.20
1	A	308	ILE	CA-C-N	6.09	130.34	120.60
1	A	308	ILE	C-N-CA	6.09	130.34	120.60
6	F	87	LYS	CA-C-N	6.09	130.99	120.58
6	F	87	LYS	C-N-CA	6.09	130.99	120.58
2	B	67	SER	CA-C-N	6.08	129.75	121.05
2	B	67	SER	C-N-CA	6.08	129.75	121.05
2	B	307	ASP	CA-C-N	6.07	128.41	120.28
2	B	307	ASP	C-N-CA	6.07	128.41	120.28
1	A	95	PHE	CA-C-N	6.06	130.24	120.30
1	A	95	PHE	C-N-CA	6.06	130.24	120.30
2	B	34	ILE	N-CA-C	-6.05	104.84	110.53
2	B	304	ASP	CA-CB-CG	6.04	118.64	112.60
4	D	195	ILE	N-CA-CB	6.03	119.65	111.21
1	A	781	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	423	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	169	ASN	CA-C-N	6.00	129.64	120.82
1	A	169	ASN	C-N-CA	6.00	129.64	120.82
1	A	438	ASP	CA-C-N	6.00	130.68	122.34
1	A	438	ASP	C-N-CA	6.00	130.68	122.34
13	X	346	PRO	N-CA-CB	5.99	110.09	103.26
2	B	968	VAL	CA-C-N	5.98	131.86	122.17
2	B	968	VAL	C-N-CA	5.98	131.86	122.17
9	I	52	ILE	N-CA-CB	5.96	119.37	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	491	THR	CA-C-N	5.95	128.26	120.28
2	B	491	THR	C-N-CA	5.95	128.26	120.28
2	B	642	ASP	CA-C-N	5.95	130.21	120.63
2	B	642	ASP	C-N-CA	5.95	130.21	120.63
9	I	60	GLN	N-CA-C	-5.94	104.89	111.36
1	A	249	SER	CA-C-N	5.93	127.22	121.65
1	A	249	SER	C-N-CA	5.93	127.22	121.65
3	C	240	VAL	CA-C-N	5.92	128.54	120.54
3	C	240	VAL	C-N-CA	5.92	128.54	120.54
2	B	555	ILE	CA-C-N	5.92	128.13	120.44
2	B	555	ILE	C-N-CA	5.92	128.13	120.44
1	A	1420	ASP	CA-C-N	5.91	132.82	121.54
1	A	1420	ASP	C-N-CA	5.91	132.82	121.54
1	A	313	GLN	N-CA-C	-5.90	106.06	113.20
10	J	5	VAL	N-CA-C	-5.87	101.09	108.84
1	A	1365	TYR	CA-C-N	5.86	128.41	120.38
1	A	1365	TYR	C-N-CA	5.86	128.41	120.38
1	A	578	LEU	CA-C-N	5.86	128.71	120.28
1	A	578	LEU	C-N-CA	5.86	128.71	120.28
2	B	738	PHE	CA-CB-CG	5.85	119.65	113.80
4	D	176	GLU	CA-C-N	5.85	127.93	120.56
4	D	176	GLU	C-N-CA	5.85	127.93	120.56
2	B	836	GLU	CA-C-N	5.84	132.69	121.54
2	B	836	GLU	C-N-CA	5.84	132.69	121.54
1	A	526	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	537	ARG	CA-C-N	5.82	128.08	120.28
1	A	537	ARG	C-N-CA	5.82	128.08	120.28
11	K	24	ASP	CA-C-N	5.80	127.99	120.44
11	K	24	ASP	C-N-CA	5.80	127.99	120.44
1	A	24	PRO	CA-C-N	5.77	130.35	120.71
1	A	24	PRO	C-N-CA	5.77	130.35	120.71
1	A	341	MET	CA-C-N	5.77	126.16	122.18
1	A	341	MET	C-N-CA	5.77	126.16	122.18
2	B	386	LEU	CA-C-N	5.77	128.01	120.28
2	B	386	LEU	C-N-CA	5.77	128.01	120.28
1	A	317	LYS	CA-C-N	5.74	132.50	121.54
1	A	317	LYS	C-N-CA	5.74	132.50	121.54
1	A	296	LEU	N-CA-C	-5.72	104.96	111.14
2	B	999	MET	N-CA-C	5.72	116.17	109.60
1	A	853	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	1012	ARG	CA-C-N	5.70	127.84	120.44
1	A	1012	ARG	C-N-CA	5.70	127.84	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1066	VAL	CA-C-N	5.69	127.91	120.28
1	A	1066	VAL	C-N-CA	5.69	127.91	120.28
2	B	709	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	524	VAL	CA-C-N	5.69	132.40	121.54
1	A	524	VAL	C-N-CA	5.69	132.40	121.54
8	H	132	LEU	CA-C-N	5.68	128.16	120.44
8	H	132	LEU	C-N-CA	5.68	128.16	120.44
9	I	108	HIS	CA-C-N	5.68	128.18	120.63
9	I	108	HIS	C-N-CA	5.68	128.18	120.63
1	A	495	GLU	CA-C-N	5.67	130.28	120.58
1	A	495	GLU	C-N-CA	5.67	130.28	120.58
6	F	143	PHE	N-CA-C	5.67	117.41	108.96
1	A	244	PRO	N-CA-C	5.67	117.61	110.70
4	D	150	ASN	CA-CB-CG	5.66	118.26	112.60
6	F	120	ILE	CA-C-N	5.65	128.41	120.28
6	F	120	ILE	C-N-CA	5.65	128.41	120.28
2	B	1170	THR	CA-C-N	5.64	132.13	121.97
2	B	1170	THR	C-N-CA	5.64	132.13	121.97
7	G	163	ILE	N-CA-C	-5.63	107.25	112.43
13	X	284	GLU	N-CA-C	-5.63	106.41	113.28
8	H	21	ASN	CA-CB-CG	5.63	118.23	112.60
5	E	103	LYS	CA-C-N	5.61	132.26	121.54
5	E	103	LYS	C-N-CA	5.61	132.26	121.54
1	A	485	ASP	CA-CB-CG	5.61	118.21	112.60
2	B	896	ASP	N-CA-C	-5.61	106.33	112.72
7	G	118	ASP	CA-CB-CG	5.61	118.21	112.60
3	C	231	ASN	CA-CB-CG	5.57	118.17	112.60
2	B	998	ASP	CA-CB-CG	5.55	118.16	112.60
2	B	454	THR	CA-C-N	5.54	127.64	120.44
2	B	454	THR	C-N-CA	5.54	127.64	120.44
1	A	135	PHE	N-CA-C	-5.53	105.17	111.14
1	A	133	LYS	CA-C-N	5.52	128.13	120.29
1	A	133	LYS	C-N-CA	5.52	128.13	120.29
1	A	122	MET	N-CA-C	-5.50	105.36	111.36
9	I	66	PRO	CA-C-N	5.49	127.91	120.38
9	I	66	PRO	C-N-CA	5.49	127.91	120.38
4	D	54	GLU	N-CA-C	-5.49	104.72	111.75
5	E	125	PRO	CA-C-N	5.47	128.37	120.38
5	E	125	PRO	C-N-CA	5.47	128.37	120.38
9	I	41	PRO	CA-C-N	5.47	129.69	122.30
9	I	41	PRO	C-N-CA	5.47	129.69	122.30
8	H	62	SER	N-CA-C	5.47	115.34	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	X	321	LEU	CA-C-N	5.47	130.45	122.08
13	X	321	LEU	C-N-CA	5.47	130.45	122.08
1	A	491	VAL	N-CA-C	5.46	112.53	107.56
2	B	1113	VAL	CA-C-N	5.45	129.06	120.89
2	B	1113	VAL	C-N-CA	5.45	129.06	120.89
11	K	39	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	867	ILE	N-CA-C	-5.43	100.83	108.27
3	C	165	LYS	N-CA-C	-5.43	105.52	111.82
13	X	345	ASN	CA-C-N	5.43	125.51	119.32
13	X	345	ASN	C-N-CA	5.43	125.51	119.32
1	A	847	ASP	CA-C-N	5.40	127.81	120.63
1	A	847	ASP	C-N-CA	5.40	127.81	120.63
2	B	394	ASP	CA-C-N	5.40	128.51	120.95
2	B	394	ASP	C-N-CA	5.40	128.51	120.95
1	A	874	ASP	CA-C-N	5.38	131.82	121.54
1	A	874	ASP	C-N-CA	5.38	131.82	121.54
3	C	225	ALA	N-CA-C	5.38	117.52	108.96
4	D	205	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	130	ASP	CA-C-N	5.38	127.75	120.38
1	A	130	ASP	C-N-CA	5.38	127.75	120.38
3	C	78	GLU	CB-CG-CD	5.38	121.74	112.60
4	D	39	ASN	N-CA-C	-5.38	100.41	108.96
1	A	1212	VAL	CA-C-N	5.37	125.90	119.94
1	A	1212	VAL	C-N-CA	5.37	125.90	119.94
2	B	66	ASP	CA-C-N	5.37	131.80	121.54
2	B	66	ASP	C-N-CA	5.37	131.80	121.54
1	A	289	ILE	N-CA-C	-5.36	105.16	111.00
11	K	92	ASN	CA-C-N	5.35	127.45	120.28
11	K	92	ASN	C-N-CA	5.35	127.45	120.28
1	A	1055	ARG	N-CA-C	-5.34	105.03	112.45
1	A	1110	ASN	CA-C-N	5.34	128.68	121.05
1	A	1110	ASN	C-N-CA	5.34	128.68	121.05
1	A	1360	GLY	CA-C-N	5.33	128.66	120.82
1	A	1360	GLY	C-N-CA	5.33	128.66	120.82
9	I	112	SER	CA-C-N	5.33	128.66	120.82
9	I	112	SER	C-N-CA	5.33	128.66	120.82
8	H	3	ASN	CA-C-N	5.33	129.25	121.31
8	H	3	ASN	C-N-CA	5.33	129.25	121.31
1	A	1174	PHE	CA-C-N	5.32	127.95	120.28
1	A	1174	PHE	C-N-CA	5.32	127.95	120.28
3	C	34	ARG	CA-C-N	5.32	127.68	120.44
3	C	34	ARG	C-N-CA	5.32	127.68	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	148	GLU	CA-C-N	5.32	127.94	120.28
5	E	148	GLU	C-N-CA	5.32	127.94	120.28
13	X	324	HIS	N-CA-C	-5.31	106.93	113.41
1	A	648	ASN	CA-CB-CG	5.31	117.91	112.60
1	A	452	LYS	N-CA-C	-5.31	105.49	111.28
1	A	499	ALA	N-CA-C	-5.31	105.54	112.23
2	B	248	SER	CA-C-N	5.31	131.68	121.54
2	B	248	SER	C-N-CA	5.31	131.68	121.54
5	E	150	VAL	N-CA-C	5.30	113.71	107.77
1	A	480	ALA	CA-C-N	5.30	130.17	121.58
1	A	480	ALA	C-N-CA	5.30	130.17	121.58
4	D	64	VAL	CA-C-N	5.30	127.81	120.29
4	D	64	VAL	C-N-CA	5.30	127.81	120.29
1	A	408	ASP	CA-C-N	5.28	130.38	121.14
1	A	408	ASP	C-N-CA	5.28	130.38	121.14
1	A	39	GLU	CA-C-N	5.28	131.62	121.54
1	A	39	GLU	C-N-CA	5.28	131.62	121.54
2	B	1002	THR	N-CA-C	-5.27	103.43	110.55
5	E	29	PHE	CA-C-N	5.27	129.42	122.51
5	E	29	PHE	C-N-CA	5.27	129.42	122.51
2	B	431	TYR	N-CA-C	-5.27	105.61	111.36
2	B	629	ASP	CA-CB-CG	5.27	117.87	112.60
4	D	200	ASN	CA-C-N	5.26	127.86	120.28
4	D	200	ASN	C-N-CA	5.26	127.86	120.28
1	A	398	GLU	N-CA-C	-5.26	102.70	110.48
3	C	155	LEU	CA-C-N	5.26	129.09	121.26
3	C	155	LEU	C-N-CA	5.26	129.09	121.26
1	A	884	ASP	CA-C-N	5.26	127.75	120.29
1	A	884	ASP	C-N-CA	5.26	127.75	120.29
1	A	893	PHE	CA-C-N	5.26	127.32	120.28
1	A	893	PHE	C-N-CA	5.26	127.32	120.28
2	B	628	THR	CB-CA-C	5.25	118.26	109.80
2	B	428	ILE	N-CA-C	-5.25	105.42	110.72
1	A	1034	GLU	CB-CG-CD	5.24	121.51	112.60
1	A	1334	ASP	CA-CB-CG	5.24	117.84	112.60
2	B	835	GLN	CA-C-N	5.24	129.85	122.46
2	B	835	GLN	C-N-CA	5.24	129.85	122.46
9	I	19	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	853	ASP	N-CA-C	-5.23	106.73	113.01
2	B	1049	ASP	CA-CB-CG	5.23	117.83	112.60
9	I	112	SER	N-CA-C	-5.23	106.90	113.28
1	A	1420	ASP	CA-CB-CG	5.22	117.82	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	159	ALA	N-CA-C	5.22	115.43	108.38
8	H	145	ARG	CA-C-N	5.22	131.09	121.70
8	H	145	ARG	C-N-CA	5.22	131.09	121.70
2	B	998	ASP	CA-C-N	5.22	128.08	120.51
2	B	998	ASP	C-N-CA	5.22	128.08	120.51
1	A	1205	LYS	N-CA-C	-5.21	106.51	112.92
1	A	1390	ASN	CA-CB-CG	5.21	117.81	112.60
5	E	97	VAL	CA-C-N	5.21	127.82	120.42
5	E	97	VAL	C-N-CA	5.21	127.82	120.42
1	A	204	THR	CA-C-N	5.21	127.52	120.44
1	A	204	THR	C-N-CA	5.21	127.52	120.44
5	E	16	PHE	CA-C-N	5.21	127.26	120.28
5	E	16	PHE	C-N-CA	5.21	127.26	120.28
9	I	93	LYS	CA-C-N	5.21	127.26	120.28
9	I	93	LYS	C-N-CA	5.21	127.26	120.28
1	A	750	GLY	CA-C-N	5.21	131.48	121.54
1	A	750	GLY	C-N-CA	5.21	131.48	121.54
1	A	41	MET	CA-C-N	5.20	131.48	121.54
1	A	41	MET	C-N-CA	5.20	131.48	121.54
1	A	1143	LEU	CA-C-N	5.18	127.23	120.28
1	A	1143	LEU	C-N-CA	5.18	127.23	120.28
1	A	1071	SER	N-CA-C	-5.17	106.89	114.39
3	C	212	PRO	N-CA-C	5.17	117.01	110.70
5	E	94	LYS	CA-C-N	5.17	127.16	120.44
5	E	94	LYS	C-N-CA	5.17	127.16	120.44
1	A	1205	LYS	CA-C-N	5.17	131.41	121.54
1	A	1205	LYS	C-N-CA	5.17	131.41	121.54
2	B	734	HIS	CA-C-N	5.17	128.19	120.90
2	B	734	HIS	C-N-CA	5.17	128.19	120.90
3	C	248	ILE	CA-C-N	5.16	127.15	120.44
3	C	248	ILE	C-N-CA	5.16	127.15	120.44
2	B	609	ILE	N-CA-C	-5.16	101.96	108.93
1	A	847	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	1226	VAL	CA-C-N	5.16	130.21	122.58
1	A	1226	VAL	C-N-CA	5.16	130.21	122.58
2	B	228	LYS	CA-C-N	5.15	131.38	121.54
2	B	228	LYS	C-N-CA	5.15	131.38	121.54
2	B	1033	LYS	CA-C-N	5.15	127.05	120.56
2	B	1033	LYS	C-N-CA	5.15	127.05	120.56
3	C	237	SER	CA-C-N	5.15	127.81	123.33
3	C	237	SER	C-N-CA	5.15	127.81	123.33
8	H	7	ASP	CA-CB-CG	5.14	117.74	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	681	GLU	CA-C-N	5.13	127.15	120.28
1	A	681	GLU	C-N-CA	5.13	127.15	120.28
8	H	45	GLU	N-CA-C	-5.12	105.39	110.97
11	K	5	ASP	CA-C-N	5.12	131.32	121.54
11	K	5	ASP	C-N-CA	5.12	131.32	121.54
2	B	286	PHE	CA-CB-CG	5.11	118.91	113.80
2	B	294	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	602	ASP	CA-CB-CG	5.11	117.71	112.60
3	C	141	GLY	CA-C-N	5.10	131.16	121.97
3	C	141	GLY	C-N-CA	5.10	131.16	121.97
1	A	1343	ALA	N-CA-C	-5.10	107.22	113.50
2	B	963	PHE	CA-CB-CG	5.09	118.89	113.80
1	A	1063	MET	CA-C-N	5.09	131.13	121.97
1	A	1063	MET	C-N-CA	5.09	131.13	121.97
1	A	331	GLY	CA-C-N	5.09	131.26	121.54
1	A	331	GLY	C-N-CA	5.09	131.26	121.54
5	E	5	ASN	CA-C-N	5.09	127.10	120.28
5	E	5	ASN	C-N-CA	5.09	127.10	120.28
2	B	828	ALA	N-CA-C	5.08	117.72	109.24
1	A	212	LYS	CA-C-N	5.08	127.59	120.28
1	A	212	LYS	C-N-CA	5.08	127.59	120.28
3	C	54	ASN	CA-CB-CG	5.07	117.67	112.60
2	B	1223	ASP	CA-C-N	5.07	130.83	121.70
2	B	1223	ASP	C-N-CA	5.07	130.83	121.70
1	A	648	ASN	CA-C-N	5.06	127.03	120.70
1	A	648	ASN	C-N-CA	5.06	127.03	120.70
5	E	32	GLN	CA-C-N	5.06	128.00	120.31
5	E	32	GLN	C-N-CA	5.06	128.00	120.31
1	A	25	GLU	CA-C-N	5.06	127.32	120.44
1	A	25	GLU	C-N-CA	5.06	127.32	120.44
2	B	978	ASP	CA-CB-CG	5.05	117.65	112.60
11	K	83	PRO	CA-C-N	5.05	127.46	120.29
11	K	83	PRO	C-N-CA	5.05	127.46	120.29
1	A	833	GLU	CA-C-N	5.04	127.04	120.28
1	A	833	GLU	C-N-CA	5.04	127.04	120.28
1	A	1266	THR	CA-C-N	5.04	127.35	120.54
1	A	1266	THR	C-N-CA	5.04	127.35	120.54
2	B	221	ASN	CA-CB-CG	5.04	117.64	112.60
2	B	1078	GLY	CA-C-N	5.03	129.41	121.56
2	B	1078	GLY	C-N-CA	5.03	129.41	121.56
3	C	265	MET	N-CA-C	-5.03	105.87	111.36
1	A	1099	PRO	CA-C-N	5.03	127.02	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1099	PRO	C-N-CA	5.03	127.02	120.28
4	D	23	ASN	CA-CB-CG	5.03	117.63	112.60
2	B	1003	ALA	CA-C-N	5.03	128.72	120.63
2	B	1003	ALA	C-N-CA	5.03	128.72	120.63
2	B	1084	GLN	CA-C-N	5.03	128.03	120.69
2	B	1084	GLN	C-N-CA	5.03	128.03	120.69
8	H	94	ASP	CA-CB-CG	5.02	117.62	112.60
6	F	126	ALA	N-CA-C	-5.02	105.45	111.03
1	A	731	ARG	CA-C-N	5.02	127.28	120.65
1	A	731	ARG	C-N-CA	5.02	127.28	120.65
12	L	54	ARG	CA-C-N	5.02	131.01	121.97
12	L	54	ARG	C-N-CA	5.02	131.01	121.97
2	B	296	GLU	CA-C-N	5.01	126.87	120.56
2	B	296	GLU	C-N-CA	5.01	126.87	120.56
2	B	839	MET	N-CA-C	5.01	116.66	108.55
5	E	34	GLU	CA-C-N	5.00	126.83	120.72
5	E	34	GLU	C-N-CA	5.00	126.83	120.72

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	11140	0	11218	367	0
2	B	8720	0	8745	231	0
3	C	2095	0	2051	71	0
4	D	1356	0	1319	33	0
5	E	1752	0	1776	48	0
6	F	679	0	701	21	0
7	G	1340	0	1357	30	0
8	H	1068	0	1040	30	0
9	I	971	0	930	26	0
10	J	532	0	543	17	0
11	K	920	0	929	27	0
12	L	363	0	386	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	X	564	0	239	4	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	31509	0	31234	807	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 13.

All (807) 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)
3:C:83:SER:HA	3:C:95:CYS:HB2	1.36	1.05
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.38	1.04
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.46	0.97
1:A:821:ARG:HG2	2:B:514:LEU:H	1.31	0.95
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.53	0.89
1:A:51:GLY:HA2	1:A:56:PRO:HB3	1.53	0.89
1:A:465:TYR:HB3	2:B:976:ILE:HG21	1.53	0.89
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.53	0.89
2:B:900:ALA:HB3	12:L:61:THR:HG23	1.54	0.89
4:D:183:LEU:HD23	7:G:144:ARG:HE	1.38	0.88
1:A:1121:GLU:HB3	1:A:1124:HIS:NE2	1.90	0.86
1:A:49:LYS:HD3	1:A:54:ASN:HB3	1.57	0.85
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.14	0.83
2:B:35:SER:HB3	2:B:39:ARG:HE	1.43	0.82
8:H:81:PRO:HB2	8:H:82:PRO:HD3	1.62	0.81
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.61	0.81
5:E:147:HIS:HD2	5:E:149:LEU:H	1.28	0.81
1:A:332:LYS:H	1:A:337:ARG:HB2	1.46	0.80
3:C:83:SER:HA	3:C:95:CYS:CB	2.12	0.80
2:B:866:TYR:CD2	2:B:870:ILE:HB	2.17	0.79
1:A:208:LEU:HD12	1:A:235:ILE:HB	1.64	0.79
1:A:329:LEU:HD22	2:B:1203:LEU:HD12	1.64	0.79
2:B:570:VAL:HB	2:B:573:GLN:HB3	1.66	0.78
4:D:62:ALA:HB1	7:G:50:ASP:H	1.48	0.77
1:A:225:ASN:HD22	1:A:228:PHE:H	1.33	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:PRO:HA	3:C:24:ASN:HB3	1.68	0.76
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.67	0.75
2:B:843:GLN:HB2	2:B:993:THR:HB	1.67	0.75
1:A:106:VAL:HG21	1:A:214:ILE:HG12	1.68	0.75
1:A:316:GLN:HB2	1:A:322:VAL:HG22	1.69	0.75
1:A:517:ASN:HD21	1:A:1362:TYR:HE2	1.33	0.75
2:B:702:LEU:HD13	9:I:67:THR:HA	1.67	0.74
2:B:346:GLU:H	2:B:349:ILE:HD12	1.53	0.74
1:A:567:LYS:HB3	8:H:96:VAL:H	1.52	0.73
1:A:1396:ALA:HA	1:A:1399:ARG:HH21	1.52	0.73
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.71	0.73
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.71	0.72
1:A:265:LYS:HD2	1:A:322:VAL:HG11	1.72	0.72
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.72	0.72
2:B:1001:PHE:CE2	3:C:178:PHE:HB3	2.25	0.72
2:B:706:GLN:HB2	2:B:709:ASP:HB2	1.72	0.72
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.55	0.72
8:H:105:GLU:HB3	8:H:113:ALA:HB3	1.70	0.72
9:I:85:PHE:HB2	9:I:99:LEU:HD22	1.72	0.72
2:B:642:ASP:HA	2:B:649:LYS:HA	1.73	0.71
12:L:55:ILE:HD12	12:L:56:LEU:H	1.55	0.71
1:A:285:PRO:HB2	1:A:288:ALA:HB3	1.73	0.71
1:A:367:PRO:HD2	1:A:370:ILE:HD12	1.72	0.70
2:B:624:LEU:HD22	2:B:626:ILE:HG13	1.72	0.70
11:K:38:GLU:HG3	11:K:42:LEU:HD22	1.71	0.70
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.73	0.70
1:A:535:THR:HG21	1:A:617:VAL:HG23	1.73	0.70
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.31	0.70
2:B:282:ILE:HA	2:B:285:ILE:HD12	1.74	0.70
1:A:1377:THR:HG22	5:E:176:PRO:HB3	1.74	0.70
3:C:177:GLU:HB3	3:C:231:ASN:HB3	1.72	0.69
1:A:1333:ILE:HD13	1:A:1333:ILE:H	1.57	0.69
1:A:1006:ILE:HD11	5:E:167:ARG:HB2	1.73	0.69
1:A:1279:ILE:HA	1:A:1310:GLY:HA3	1.75	0.69
3:C:11:ARG:HH12	3:C:205:LYS:HE3	1.58	0.69
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.57	0.69
1:A:269:ILE:HG13	1:A:299:HIS:HB3	1.74	0.69
1:A:1423:GLY:H	1:A:1426:GLU:HG3	1.57	0.68
2:B:558:LEU:HB3	2:B:563:MET:HG3	1.74	0.68
2:B:293:PRO:HB2	9:I:11:ASN:HD22	1.58	0.68
1:A:1002:GLY:HA3	1:A:1007:ILE:CG2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:GLN:HB2	1:A:322:VAL:CG2	2.24	0.67
8:H:33:GLN:HB3	8:H:36:CYS:HB2	1.76	0.67
1:A:1228:TRP:HB3	1:A:1238:ILE:HG23	1.76	0.67
2:B:778:MET:HG2	2:B:794:ASN:HB3	1.76	0.67
1:A:35:ILE:HG21	1:A:241:VAL:HG21	1.77	0.66
4:D:120:GLU:HA	4:D:123:LEU:HD12	1.78	0.66
1:A:1081:LEU:HD22	1:A:1096:SER:HB2	1.77	0.66
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.77	0.66
1:A:387:ARG:HH12	1:A:434:ARG:NH1	1.93	0.66
2:B:1160:VAL:HG11	2:B:1201:LYS:HG3	1.76	0.66
3:C:46:ILE:HD12	3:C:46:ILE:H	1.61	0.65
3:C:186:LEU:HB3	3:C:188:HIS:HD2	1.60	0.65
13:X:319:LEU:HA	13:X:345:ASN:HA	1.78	0.65
1:A:793:SER:HB2	1:A:796:SER:HB2	1.78	0.65
3:C:55:THR:HB	3:C:151:GLN:HA	1.78	0.65
1:A:565:ILE:HG13	8:H:97:MET:HG2	1.77	0.65
4:D:68:ARG:HB2	4:D:72:ARG:HH21	1.62	0.65
2:B:797:TYR:HE1	2:B:971:THR:HG23	1.62	0.64
1:A:370:ILE:HD11	2:B:1103:ILE:HD11	1.79	0.64
2:B:992:ILE:HG12	2:B:993:THR:N	2.12	0.64
1:A:335:ARG:HA	1:A:339:ASN:HB2	1.80	0.64
2:B:664:THR:HG1	2:B:678:GLU:N	1.95	0.64
1:A:830:LYS:O	1:A:834:THR:HB	1.97	0.64
1:A:709:THR:HG23	9:I:94:ASP:HA	1.80	0.64
1:A:28:ARG:HH12	1:A:85:ASP:HB3	1.63	0.63
1:A:299:HIS:HA	1:A:302:THR:HB	1.80	0.63
1:A:497:THR:HG23	2:B:1146:PHE:HD1	1.64	0.63
1:A:531:ILE:HG21	1:A:622:VAL:HG11	1.78	0.63
2:B:866:TYR:HD2	2:B:870:ILE:HB	1.62	0.63
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.24	0.63
1:A:1189:SER:HB3	1:A:1241:ARG:HB3	1.79	0.63
2:B:224:GLN:HE21	2:B:403:LYS:HD3	1.64	0.63
6:F:109:VAL:HG21	6:F:124:GLU:HA	1.80	0.63
2:B:1132:GLU:HB2	2:B:1133:MET:HE3	1.81	0.62
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.81	0.62
11:K:12:LEU:HA	11:K:37:LYS:HG3	1.81	0.62
1:A:788:SER:HB3	9:I:69:PRO:HG3	1.81	0.62
2:B:425:THR:HA	2:B:428:ILE:HD12	1.81	0.62
6:F:81:THR:HB	6:F:136:ARG:HH11	1.64	0.62
1:A:741:ASN:HD22	1:A:744:LYS:H	1.46	0.62
1:A:12:ARG:HD2	2:B:1218:THR:HB	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:LEU:HG	1:A:613:ILE:HD13	1.80	0.62
4:D:56:ARG:HB2	4:D:148:LEU:HB3	1.82	0.62
4:D:207:LEU:HA	4:D:210:ILE:HD12	1.81	0.62
1:A:2:VAL:HG23	2:B:1157:ALA:HB1	1.80	0.62
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.29	0.62
3:C:220:ASP:HB3	3:C:223:ALA:HB2	1.82	0.62
8:H:44:VAL:HG22	8:H:49:VAL:H	1.64	0.61
1:A:332:LYS:HE2	2:B:1132:GLU:HG3	1.81	0.61
2:B:38:PHE:C	2:B:40:GLU:H	2.09	0.61
2:B:1033:LYS:O	2:B:1037:LEU:HG	2.01	0.61
3:C:83:SER:CA	3:C:95:CYS:HB2	2.20	0.61
1:A:1260:LEU:HA	1:A:1263:ILE:HD12	1.82	0.61
2:B:904:ARG:HG3	2:B:948:ILE:HG13	1.83	0.61
5:E:47:CYS:HB3	5:E:51:GLY:HA2	1.81	0.61
10:J:42:LYS:HG3	10:J:43:ARG:H	1.65	0.61
9:I:4:PHE:HE2	9:I:13:MET:HG3	1.66	0.61
1:A:1386:ARG:HA	1:A:1390:ASN:HB2	1.82	0.60
2:B:334:ILE:HG21	2:B:352:ALA:HB2	1.84	0.60
2:B:515:HIS:HB3	2:B:518:HIS:CE1	2.36	0.60
1:A:12:ARG:HG2	1:A:13:THR:H	1.67	0.60
1:A:881:GLN:NE2	1:A:960:ILE:H	1.98	0.60
1:A:919:ILE:HG13	1:A:925:LEU:HD13	1.83	0.60
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.82	0.60
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.84	0.60
2:B:992:ILE:HG12	2:B:993:THR:H	1.67	0.60
3:C:187:LYS:HB2	3:C:219:PHE:HE1	1.67	0.60
12:L:31:CYS:SG	12:L:55:ILE:HD11	2.42	0.59
2:B:806:THR:HG23	2:B:1046:PRO:HD3	1.85	0.59
5:E:178:ILE:HB	5:E:212:ARG:HB3	1.84	0.59
7:G:18:PHE:HA	7:G:22:MET:HE2	1.85	0.59
2:B:1174:LYS:HD2	2:B:1179:GLN:HB2	1.85	0.59
5:E:3:GLN:HG2	5:E:5:ASN:HD22	1.68	0.59
2:B:640:VAL:HG22	2:B:651:LEU:HG	1.83	0.59
1:A:738:LYS:HB2	1:A:740:LEU:HG	1.85	0.58
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.83	0.58
1:A:774:ARG:HG3	1:A:797:LYS:HD3	1.85	0.58
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.86	0.58
2:B:114:PRO:HG3	2:B:181:LEU:HG	1.83	0.58
6:F:105:ALA:HA	7:G:16:SER:HA	1.86	0.58
1:A:672:ASP:HB3	1:A:736:ASN:HD21	1.69	0.58
2:B:296:GLU:O	2:B:300:HIS:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:512:ARG:HA	2:B:534:GLY:HA3	1.86	0.58
2:B:778:MET:HB2	2:B:1094:ARG:HG2	1.86	0.58
3:C:259:LEU:HD21	11:K:91:CYS:HB3	1.86	0.58
4:D:154:PHE:HA	4:D:219:THR:HB	1.85	0.58
4:D:154:PHE:HB2	4:D:160:VAL:HG22	1.86	0.58
1:A:497:THR:CG2	2:B:1146:PHE:HD1	2.16	0.58
5:E:147:HIS:NE2	5:E:149:LEU:HD12	2.19	0.58
2:B:281:PRO:HD2	2:B:284:ILE:HD13	1.86	0.57
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.40	0.57
1:A:1124:HIS:CD2	1:A:1130:GLN:HG2	2.39	0.57
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.86	0.57
1:A:1063:MET:HB2	2:B:1140:ALA:HA	1.86	0.57
1:A:1148:ILE:HG23	9:I:49:ILE:HB	1.87	0.57
8:H:47:PHE:CD2	8:H:95:TYR:HD2	2.23	0.57
1:A:912:LEU:HD22	1:A:1033:GLN:HA	1.85	0.57
2:B:603:LEU:HB3	2:B:609:ILE:H	1.70	0.57
2:B:780:VAL:HG13	2:B:795:ILE:HD11	1.87	0.57
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.87	0.57
2:B:1065:GLN:HB3	2:B:1069:PHE:O	2.05	0.57
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.86	0.57
1:A:265:LYS:HB3	1:A:303:TYR:HB2	1.87	0.56
1:A:899:VAL:HB	1:A:929:LEU:HG	1.86	0.56
2:B:843:GLN:HG3	11:K:6:ARG:HH21	1.69	0.56
1:A:101:LYS:HA	1:A:139:TRP:HE1	1.68	0.56
1:A:170:THR:HB	1:A:185:TRP:HD1	1.70	0.56
1:A:512:VAL:HG12	1:A:876:ALA:HB1	1.85	0.56
2:B:976:ILE:HD11	2:B:992:ILE:HA	1.87	0.56
3:C:98:VAL:HG22	3:C:158:VAL:HG13	1.86	0.56
5:E:19:VAL:HG11	5:E:80:VAL:HG11	1.87	0.56
5:E:147:HIS:CD2	5:E:149:LEU:H	2.16	0.56
11:K:58:PHE:CZ	11:K:60:ALA:HB3	2.40	0.56
1:A:385:ILE:HG23	1:A:386:ASP:H	1.71	0.56
3:C:50:GLU:HB3	3:C:156:THR:HB	1.87	0.56
1:A:14:VAL:HB	1:A:1430:LEU:HD13	1.87	0.56
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.87	0.56
5:E:16:PHE:HB2	5:E:58:MET:HE3	1.88	0.56
1:A:353:ILE:HD13	1:A:487:MET:HE3	1.87	0.56
1:A:1102:LYS:O	1:A:1106:ASN:HB2	2.05	0.56
2:B:276:ILE:HG23	2:B:335:GLY:H	1.70	0.56
2:B:657:HIS:HA	2:B:660:LYS:HD2	1.88	0.56
1:A:91:PHE:HD1	1:A:99:ILE:HD13	1.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001:ARG:HB3	6:F:80:ALA:HA	1.86	0.55
2:B:115:GLN:HE21	2:B:119:LEU:HD21	1.70	0.55
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.88	0.55
1:A:348:SER:HB2	2:B:1128:LEU:HB2	1.88	0.55
1:A:881:GLN:HB2	1:A:956:LEU:HB2	1.88	0.55
1:A:185:TRP:CZ3	1:A:200:ARG:HB2	2.42	0.55
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.89	0.55
10:J:8:PHE:H	10:J:49:MET:HE3	1.71	0.55
1:A:441:PRO:HG2	1:A:498:ARG:HB2	1.88	0.55
1:A:202:LEU:HB3	1:A:207:ILE:HD11	1.89	0.55
1:A:1138:ILE:HG13	1:A:1282:VAL:HG21	1.89	0.55
7:G:149:GLY:HA3	7:G:160:ILE:HD12	1.88	0.55
2:B:559:SER:HA	2:B:563:MET:HB2	1.89	0.55
1:A:387:ARG:HH12	1:A:434:ARG:HH11	1.55	0.55
2:B:879:ARG:O	2:B:934:LYS:HB2	2.06	0.55
3:C:12:GLU:HB2	3:C:19:ASP:HB2	1.88	0.55
3:C:102:GLN:HE21	3:C:154:LYS:HG3	1.71	0.55
5:E:61:GLN:HE21	5:E:105:PHE:HE1	1.56	0.55
7:G:114:LEU:HD12	7:G:162:SER:HB3	1.89	0.54
1:A:15:LYS:HE3	1:A:15:LYS:HA	1.88	0.54
1:A:821:ARG:HG2	2:B:514:LEU:N	2.12	0.54
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.88	0.54
3:C:46:ILE:HD13	3:C:67:LEU:O	2.08	0.54
1:A:330:LYS:O	1:A:334:GLY:HA3	2.06	0.54
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.90	0.54
2:B:515:HIS:CD2	2:B:516:ASN:H	2.26	0.54
2:B:641:GLU:C	2:B:643:ASP:H	2.15	0.54
5:E:168:TYR:HB3	5:E:170:LEU:HD12	1.89	0.54
1:A:185:TRP:HZ3	1:A:200:ARG:HB2	1.73	0.54
1:A:335:ARG:HG2	2:B:1203:LEU:HB2	1.88	0.54
2:B:216:GLU:HA	2:B:406:LEU:HD23	1.90	0.54
2:B:911:ILE:CG2	2:B:966:VAL:HG11	2.38	0.54
12:L:40:LEU:HB3	12:L:44:ASP:HB3	1.89	0.54
1:A:153:PRO:HA	1:A:161:LEU:HA	1.89	0.53
1:A:1219:THR:HG21	1:A:1271:ILE:HG12	1.90	0.53
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.90	0.53
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.90	0.53
7:G:163:ILE:HB	7:G:169:GLY:HA2	1.89	0.53
1:A:367:PRO:HA	1:A:463:ILE:O	2.09	0.53
2:B:52:ASN:HA	2:B:177:LYS:HG3	1.91	0.53
4:D:155:ARG:H	4:D:219:THR:HB	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:VAL:HB	1:A:800:VAL:HB	1.90	0.53
1:A:1115:SER:H	1:A:1330:ASN:HB3	1.74	0.53
3:C:91:HIS:CE1	3:C:158:VAL:HG21	2.42	0.53
2:B:453:ILE:HG22	2:B:457:LEU:HD11	1.91	0.53
4:D:66:ARG:HG3	7:G:51:TYR:HB2	1.89	0.53
10:J:58:GLU:HA	10:J:61:LEU:HD12	1.91	0.53
1:A:55:ASP:C	1:A:57:ARG:H	2.17	0.53
1:A:183:GLY:O	1:A:184:SER:HB2	2.08	0.53
1:A:1335:ILE:HG21	1:A:1347:ALA:HB2	1.91	0.53
3:C:187:LYS:HB2	3:C:219:PHE:CE1	2.43	0.53
2:B:893:LEU:HG	2:B:899:ILE:HG13	1.91	0.53
1:A:1001:ARG:CD	6:F:83:PRO:HD3	2.38	0.53
2:B:283:VAL:HG23	2:B:284:ILE:HD12	1.91	0.53
1:A:1235:LYS:HD2	1:A:1237:ILE:HD11	1.89	0.53
2:B:654:ARG:H	2:B:657:HIS:HD2	1.56	0.52
7:G:60:ARG:NH2	7:G:62:LEU:HA	2.23	0.52
1:A:276:LEU:HD22	1:A:293:GLU:HA	1.90	0.52
3:C:102:GLN:HG3	3:C:154:LYS:HG3	1.91	0.52
2:B:881:ASN:HB2	2:B:933:SER:HB2	1.90	0.52
10:J:48:ARG:O	10:J:52:THR:HG22	2.09	0.52
1:A:15:LYS:HA	1:A:15:LYS:CE	2.39	0.52
1:A:1433:MET:HE1	6:F:92:ARG:HD2	1.91	0.52
2:B:291:ILE:HG22	2:B:297:ILE:HG13	1.91	0.52
2:B:614:SER:HB2	2:B:697:GLU:HB2	1.91	0.52
13:X:313:LEU:C	13:X:315:ASP:H	2.17	0.52
1:A:148:CYS:O	1:A:168:GLY:HA2	2.10	0.52
2:B:204:ILE:HA	2:B:208:SER:O	2.10	0.52
4:D:168:LYS:HE3	4:D:174:PRO:HA	1.90	0.52
1:A:563:PRO:HB3	1:A:572:TRP:CE2	2.45	0.52
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.91	0.52
1:A:1009:ASN:HD22	1:A:1012:ARG:HH11	1.57	0.52
1:A:117:GLU:CD	1:A:117:GLU:H	2.18	0.52
1:A:913:LEU:HD22	1:A:1032:LEU:HD13	1.91	0.52
2:B:225:VAL:HG11	2:B:385:LEU:HA	1.92	0.52
7:G:9:LEU:HD22	7:G:34:VAL:HG23	1.91	0.52
1:A:614:PHE:HB3	8:H:122:LEU:HD21	1.92	0.52
2:B:283:VAL:HG11	2:B:318:VAL:HA	1.92	0.52
2:B:637:LEU:HD12	2:B:693:ILE:HD13	1.90	0.52
2:B:944:THR:HB	2:B:1122:ARG:NH2	2.25	0.52
2:B:1142:GLY:HA3	6:F:88:TYR:HE1	1.75	0.52
3:C:100:THR:HG22	3:C:119:VAL:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:165:LYS:HE2	11:K:9:LEU:HD22	1.91	0.52
10:J:24:LEU:HD21	10:J:38:ARG:HD2	1.90	0.52
1:A:332:LYS:N	1:A:337:ARG:HB2	2.20	0.51
2:B:979:LYS:HE2	2:B:987:LYS:HB2	1.91	0.51
1:A:738:LYS:H	1:A:738:LYS:HE2	1.76	0.51
1:A:873:MET:HG3	1:A:1056:SER:HB3	1.92	0.51
1:A:845:LEU:HA	1:A:848:ILE:HD12	1.93	0.51
2:B:125:SER:HA	2:B:171:PRO:HA	1.93	0.51
2:B:532:ALA:HA	2:B:535:LEU:HD12	1.91	0.51
9:I:4:PHE:CE2	9:I:13:MET:HG3	2.44	0.51
1:A:939:ASP:OD2	1:A:1023:ARG:HD2	2.11	0.51
1:A:1347:ALA:O	1:A:1351:GLU:HB2	2.11	0.51
5:E:135:PHE:HE1	5:E:186:LEU:HB3	1.75	0.51
7:G:25:TYR:CE2	7:G:29:LYS:HD3	2.46	0.51
1:A:11:LEU:HD13	2:B:1193:GLN:HE21	1.74	0.51
1:A:230:ARG:HB3	1:A:232:GLU:HG2	1.92	0.51
1:A:690:VAL:HG22	1:A:718:VAL:HG22	1.92	0.51
1:A:708:MET:SD	1:A:713:SER:HA	2.50	0.51
1:A:779:PHE:CZ	1:A:785:PRO:HD3	2.46	0.51
1:A:1119:TYR:HA	1:A:1305:VAL:HG22	1.93	0.51
10:J:6:ARG:HG2	10:J:13:VAL:HA	1.92	0.51
1:A:333:GLU:HA	1:A:338:GLY:HA3	1.92	0.51
1:A:973:ILE:HG12	1:A:1037:LEU:HA	1.92	0.51
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.92	0.51
2:B:1001:PHE:HB3	2:B:1007:VAL:HG23	1.93	0.51
3:C:16:ASP:HA	3:C:234:SER:HB3	1.92	0.51
1:A:898:ARG:HD3	1:A:933:TYR:CG	2.46	0.51
1:A:1004:ASN:HD21	1:A:1007:ILE:HG13	1.74	0.51
1:A:1063:MET:HG3	2:B:1139:ILE:HG22	1.92	0.51
2:B:304:ASP:CG	2:B:305:VAL:H	2.18	0.51
2:B:806:THR:HG22	2:B:808:ALA:H	1.76	0.51
1:A:92:HIS:HE2	1:A:1410:PHE:HE2	1.59	0.51
1:A:867:ILE:HD11	1:A:1010:ALA:HB1	1.91	0.51
1:A:1120:LEU:HD22	1:A:1304:TRP:HB2	1.92	0.51
1:A:1150:SER:H	9:I:46:HIS:HB3	1.75	0.51
2:B:361:LEU:HG	2:B:363:HIS:CE1	2.46	0.51
2:B:416:LEU:HD11	2:B:460:ALA:HB3	1.92	0.51
5:E:151:PRO:HG3	5:E:200:ARG:HG3	1.93	0.51
1:A:395:GLY:O	1:A:401:GLY:HA3	2.11	0.51
2:B:651:LEU:HD21	2:B:707:PRO:HB3	1.92	0.51
1:A:171:GLN:HG3	1:A:172:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:114:VAL:HG22	8:H:125:LEU:HB3	1.92	0.51
1:A:523:ILE:HG23	1:A:527:THR:HB	1.93	0.50
2:B:1135:ARG:HG3	2:B:1147:LEU:HD11	1.93	0.50
1:A:162:VAL:HG12	1:A:164:ARG:H	1.77	0.50
1:A:706:HIS:HB2	13:X:362:ASN:O	2.10	0.50
1:A:1189:SER:CB	1:A:1242:VAL:H	2.25	0.50
1:A:1433:MET:HE3	2:B:1145:SER:OG	2.11	0.50
2:B:487:THR:HG23	2:B:490:SER:HB3	1.94	0.50
2:B:950:ASP:HB3	2:B:967:ARG:HB3	1.92	0.50
3:C:50:GLU:HG2	12:L:64:LEU:HD12	1.93	0.50
1:A:471:ASN:O	1:A:474:VAL:HG12	2.11	0.50
1:A:743:VAL:HA	1:A:746:MET:HE3	1.92	0.50
2:B:620:ARG:HD2	9:I:62:ILE:HD11	1.93	0.50
1:A:1134:ILE:HG22	1:A:1138:ILE:HD13	1.94	0.50
2:B:554:ILE:HG21	2:B:626:ILE:HG21	1.93	0.50
1:A:65:LEU:HB3	1:A:71:GLN:CB	2.42	0.50
1:A:512:VAL:HG13	1:A:631:HIS:CE1	2.47	0.50
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.30	0.50
3:C:142:VAL:H	10:J:16:ASP:HB3	1.76	0.50
3:C:145:CYS:HA	10:J:2:ILE:HD12	1.94	0.50
1:A:608:ILE:HB	1:A:613:ILE:HD11	1.93	0.50
5:E:202:SER:HB3	5:E:205:SER:OG	2.12	0.50
1:A:850:VAL:HG23	1:A:1064:VAL:HG21	1.94	0.50
3:C:98:VAL:H	3:C:122:SER:HB3	1.76	0.50
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.94	0.50
1:A:353:ILE:HA	1:A:468:PHE:O	2.12	0.50
1:A:362:ASP:HB3	1:A:508:PRO:HD3	1.94	0.50
2:B:408:LEU:HD11	2:B:545:ILE:HD13	1.93	0.50
3:C:196:ASP:HB3	3:C:199:LYS:HB2	1.93	0.50
1:A:1006:ILE:CD1	5:E:167:ARG:HB2	2.42	0.50
1:A:1134:ILE:O	1:A:1138:ILE:HG12	2.12	0.49
8:H:81:PRO:HB2	8:H:82:PRO:CD	2.38	0.49
1:A:922:ASP:HB3	1:A:925:LEU:HB2	1.94	0.49
1:A:986:ILE:HG12	1:A:1031:VAL:HG11	1.94	0.49
1:A:1412:ALA:HA	1:A:1417:GLU:HB2	1.94	0.49
2:B:1208:MET:C	2:B:1210:MET:H	2.19	0.49
1:A:294:SER:HA	1:A:297:GLN:HB3	1.94	0.49
2:B:545:ILE:HG13	2:B:633:VAL:HG13	1.95	0.49
2:B:893:LEU:HD23	2:B:898:LEU:HA	1.94	0.49
1:A:690:VAL:HG11	1:A:794:PRO:HD3	1.95	0.49
2:B:36:ALA:HA	2:B:39:ARG:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:791:THR:HA	2:B:858:SER:H	1.78	0.49
1:A:1135:ARG:HG3	1:A:1136:SER:H	1.77	0.49
2:B:115:GLN:O	2:B:119:LEU:HG	2.12	0.49
7:G:92:VAL:HG12	7:G:140:LYS:NZ	2.26	0.49
9:I:19:ASP:HB3	9:I:24:ARG:HG3	1.95	0.49
2:B:867:GLY:C	2:B:869:SER:H	2.21	0.49
6:F:77:ASP:O	6:F:78:GLN:HB2	2.12	0.49
6:F:112:GLU:HB2	6:F:123:LYS:HE2	1.95	0.49
1:A:619:LYS:HD2	1:A:750:GLY:HA3	1.95	0.49
1:A:757:ASN:HD22	1:A:757:ASN:H	1.59	0.49
1:A:1008:GLN:HB3	1:A:1012:ARG:NH2	2.28	0.49
1:A:1332:PHE:HA	1:A:1335:ILE:HG13	1.95	0.49
2:B:284:ILE:HG13	2:B:324:ILE:HG21	1.95	0.49
1:A:867:ILE:HD12	5:E:208:TYR:HD1	1.78	0.49
1:A:1422:ARG:HH12	2:B:1224:PHE:HB2	1.76	0.49
1:A:51:GLY:CA	1:A:56:PRO:HB3	2.34	0.49
1:A:350:ARG:HB2	2:B:1128:LEU:HD11	1.94	0.49
2:B:1080:LYS:HB2	3:C:188:HIS:HB3	1.94	0.49
5:E:56:LYS:HD2	5:E:84:ASP:HB2	1.95	0.49
9:I:27:PHE:CE2	9:I:38:ALA:HA	2.48	0.49
1:A:1100:ARG:HE	1:A:1104:ILE:HD11	1.77	0.49
11:K:7:PHE:C	11:K:9:LEU:H	2.21	0.49
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.95	0.48
1:A:1404:GLU:O	1:A:1408:ILE:HD12	2.13	0.48
1:A:347:PHE:HB3	1:A:491:VAL:HB	1.95	0.48
8:H:82:PRO:C	8:H:84:ALA:H	2.21	0.48
1:A:1198:ASP:HB3	1:A:1201:ALA:HB3	1.95	0.48
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.95	0.48
1:A:405:VAL:HG23	1:A:415:LEU:HD11	1.96	0.48
1:A:973:ILE:HD11	1:A:1038:THR:HG23	1.95	0.48
1:A:1386:ARG:HG3	1:A:1387:HIS:CE1	2.48	0.48
8:H:81:PRO:CB	8:H:82:PRO:HD3	2.40	0.48
11:K:58:PHE:HE2	11:K:74:ARG:HB3	1.78	0.48
1:A:107:CYS:HA	1:A:171:GLN:OE1	2.14	0.48
1:A:725:ALA:HA	1:A:728:LYS:HG2	1.94	0.48
2:B:613:VAL:HG13	2:B:627:PHE:O	2.14	0.48
8:H:30:SER:HB3	8:H:36:CYS:HB3	1.94	0.48
2:B:885:MET:HA	2:B:936:ASP:HB3	1.95	0.48
3:C:70:ILE:HG12	3:C:142:VAL:HG11	1.94	0.48
7:G:61:ILE:HG13	7:G:68:ALA:HB2	1.96	0.48
1:A:551:TYR:HB2	11:K:58:PHE:HZ	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:ALA:HB1	9:I:114:GLN:HB2	1.95	0.48
1:A:1002:GLY:HA3	1:A:1007:ILE:HG22	1.95	0.48
2:B:795:ILE:HG22	2:B:854:LEU:HB2	1.95	0.48
8:H:56:THR:O	8:H:144:ILE:HA	2.14	0.48
12:L:53:HIS:HB3	12:L:55:ILE:HG12	1.95	0.48
1:A:537:ARG:HH12	8:H:122:LEU:HG	1.79	0.48
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.96	0.48
2:B:666:TYR:C	2:B:668:ASP:H	2.22	0.48
2:B:797:TYR:HB2	2:B:852:ARG:O	2.13	0.48
2:B:604:ARG:HG2	2:B:611:PRO:HA	1.95	0.48
2:B:862:GLN:HB2	2:B:864:LYS:HE3	1.95	0.48
3:C:174:ALA:HB3	3:C:233:GLU:HB3	1.96	0.48
1:A:973:ILE:HD11	1:A:1038:THR:H	1.79	0.47
1:A:1048:ASN:O	1:A:1052:GLN:HB2	2.13	0.47
2:B:1169:MET:HE3	2:B:1169:MET:H	1.79	0.47
3:C:125:MET:HB2	3:C:127:ARG:HE	1.79	0.47
1:A:1111:MET:HE2	1:A:1333:ILE:HD11	1.96	0.47
2:B:121:ASN:HB2	2:B:963:PHE:CE2	2.48	0.47
2:B:901:PRO:HD3	2:B:952:VAL:HB	1.96	0.47
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.94	0.47
2:B:249:ARG:O	2:B:251:ILE:HG13	2.15	0.47
8:H:112:ILE:HD12	8:H:128:ASN:HA	1.95	0.47
4:D:25:ALA:C	4:D:27:LEU:H	2.23	0.47
5:E:145:THR:HG21	5:E:187:TYR:CG	2.49	0.47
8:H:12:VAL:HB	8:H:52:GLN:H	1.79	0.47
8:H:100:THR:HA	8:H:138:GLU:HA	1.96	0.47
1:A:903:ASN:HD22	1:A:905:ASP:H	1.61	0.47
2:B:168:GLY:H	2:B:450:ALA:HB1	1.78	0.47
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.95	0.47
1:A:541:ILE:HG21	1:A:549:MET:HE1	1.96	0.47
1:A:909:ASP:C	1:A:911:SER:H	2.22	0.47
1:A:1386:ARG:HD3	1:A:1403:GLU:HB3	1.96	0.47
5:E:72:PHE:HB3	5:E:75:MET:HB2	1.96	0.47
11:K:33:ILE:HD13	11:K:87:LEU:HD22	1.97	0.47
1:A:869:GLY:C	1:A:871:ASP:H	2.23	0.47
1:A:1386:ARG:HG3	1:A:1387:HIS:NE2	2.30	0.47
2:B:498:THR:HB	2:B:537:LYS:O	2.14	0.47
3:C:11:ARG:HD3	3:C:21:ILE:HD11	1.96	0.47
3:C:182:PRO:HD2	3:C:210:GLU:CD	2.40	0.47
4:D:29:LEU:HB3	7:G:82:PHE:CZ	2.49	0.47
6:F:116:ASP:HB3	6:F:119:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:VAL:HG22	1:A:153:PRO:HD2	1.97	0.47
1:A:350:ARG:HD2	2:B:1128:LEU:HD21	1.96	0.47
1:A:907:THR:OG1	1:A:920:LEU:HG	2.14	0.47
5:E:80:VAL:HG22	5:E:109:ILE:HB	1.97	0.47
11:K:18:LYS:HD3	11:K:38:GLU:HG2	1.96	0.47
1:A:1035:TYR:HB3	1:A:1037:LEU:HG	1.97	0.47
9:I:40:SER:C	9:I:42:LEU:H	2.22	0.47
1:A:377:PRO:HD3	1:A:493:GLN:CD	2.40	0.47
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.97	0.47
1:A:511:ILE:HD11	1:A:643:ALA:HB2	1.96	0.47
1:A:1009:ASN:HA	1:A:1012:ARG:HD2	1.97	0.47
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.96	0.47
5:E:26:ARG:HH22	5:E:107:THR:HG21	1.79	0.47
1:A:255:SER:H	2:B:935:ARG:HH21	1.61	0.46
1:A:347:PHE:HE2	1:A:375:THR:HG23	1.80	0.46
1:A:903:ASN:ND2	1:A:905:ASP:H	2.13	0.46
1:A:1333:ILE:H	1:A:1333:ILE:CD1	2.21	0.46
2:B:297:ILE:O	2:B:301:ILE:HD12	2.15	0.46
2:B:880:THR:HB	2:B:934:LYS:HD2	1.96	0.46
2:B:956:THR:HG23	2:B:960:GLY:HA2	1.96	0.46
3:C:185:LYS:HD3	3:C:213:PRO:HA	1.96	0.46
5:E:77:SER:O	5:E:105:PHE:HB3	2.16	0.46
1:A:427:GLN:HB2	1:A:430:TRP:NE1	2.30	0.46
1:A:443:LEU:HD11	2:B:1138:MET:SD	2.55	0.46
1:A:497:THR:HG23	2:B:1146:PHE:CD1	2.49	0.46
1:A:1197:LEU:O	1:A:1236:LEU:HD13	2.15	0.46
3:C:68:GLY:HA3	12:L:69:ALA:HB1	1.97	0.46
1:A:671:ALA:HB3	1:A:676:MET:HG2	1.97	0.46
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.80	0.46
2:B:1162:ILE:HG12	2:B:1194:ILE:HG12	1.96	0.46
1:A:809:THR:HB	2:B:730:ARG:HG2	1.97	0.46
1:A:1116:LEU:HD13	1:A:1329:THR:HB	1.98	0.46
4:D:62:ALA:HA	4:D:65:GLU:HB2	1.98	0.46
9:I:102:VAL:HG13	9:I:109:ILE:HG13	1.97	0.46
1:A:28:ARG:HG3	1:A:238:CYS:SG	2.55	0.46
1:A:91:PHE:H	1:A:297:GLN:HE22	1.63	0.46
1:A:172:PRO:HB2	1:A:183:GLY:HA2	1.97	0.46
1:A:537:ARG:HG2	8:H:121:LEU:HD23	1.98	0.46
2:B:615:MET:HG2	2:B:626:ILE:HG12	1.96	0.46
10:J:42:LYS:HG3	10:J:43:ARG:N	2.30	0.46
2:B:698:GLU:HA	2:B:701:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1023:VAL:HG13	2:B:1026:LEU:HD12	1.97	0.46
4:D:57:LEU:HD23	4:D:60:LYS:HD3	1.97	0.46
1:A:125:ALA:HA	1:A:128:ILE:HD12	1.98	0.46
1:A:285:PRO:HD2	1:A:289:ILE:HD12	1.97	0.46
1:A:941:LYS:HA	1:A:944:ARG:HB2	1.98	0.46
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.98	0.46
2:B:899:ILE:O	2:B:952:VAL:HG21	2.15	0.46
2:B:980:PHE:CD1	2:B:1094:ARG:HA	2.51	0.46
5:E:35:VAL:C	5:E:37:LEU:H	2.24	0.46
9:I:111:THR:HB	9:I:113:ASP:HB2	1.98	0.46
1:A:42:ASP:CG	1:A:47:ARG:HA	2.41	0.46
1:A:540:PHE:HB3	1:A:571:LEU:HG	1.98	0.46
3:C:120:ILE:HG21	3:C:124:LEU:HD21	1.98	0.46
3:C:183:TRP:HB2	3:C:185:LYS:HE2	1.97	0.46
1:A:179:LEU:HD22	1:A:297:GLN:HG3	1.98	0.46
1:A:1343:ALA:HB2	5:E:150:VAL:HG13	1.97	0.46
2:B:345:LYS:C	2:B:347:LYS:H	2.24	0.46
2:B:1142:GLY:HA3	6:F:88:TYR:CE1	2.51	0.46
5:E:196:VAL:HG23	5:E:212:ARG:HB2	1.98	0.46
11:K:65:HIS:HD2	11:K:67:PHE:H	1.63	0.46
1:A:1000:LEU:HB3	1:A:1007:ILE:HG23	1.98	0.46
2:B:221:ASN:OD1	2:B:242:SER:HA	2.15	0.46
2:B:944:THR:HB	2:B:1122:ARG:HH21	1.81	0.46
3:C:146:LYS:CB	10:J:61:LEU:HD11	2.46	0.46
4:D:190:GLU:HG3	7:G:167:TYR:CG	2.51	0.46
5:E:78:LEU:HD21	5:E:109:ILE:HD12	1.96	0.46
1:A:68:GLN:HE22	1:A:80:HIS:HB2	1.80	0.45
2:B:523:CYS:HA	2:B:524:PRO:HD3	1.80	0.45
2:B:590:HIS:HD2	2:B:592:ASN:H	1.64	0.45
2:B:1187:ASN:HB3	2:B:1191:ILE:HD11	1.98	0.45
4:D:29:LEU:HB2	4:D:33:PHE:O	2.15	0.45
1:A:500:GLU:CD	1:A:1438:THR:HG21	2.41	0.45
3:C:184:ASN:HB2	3:C:191:TYR:OH	2.17	0.45
7:G:60:ARG:HH21	7:G:62:LEU:HG	1.78	0.45
10:J:41:LEU:HD13	10:J:47:ARG:HA	1.97	0.45
1:A:35:ILE:HB	1:A:83:HIS:O	2.16	0.45
1:A:551:TYR:CE2	11:K:62:LYS:HG2	2.52	0.45
5:E:55:ARG:HA	5:E:58:MET:HB3	1.99	0.45
1:A:596:THR:C	1:A:598:LEU:H	2.25	0.45
3:C:263:THR:HA	3:C:266:ASP:HB2	1.98	0.45
1:A:1158:PRO:HB3	1:A:1188:GLN:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1220:PHE:HZ	1:A:1267:MET:HG2	1.81	0.45
3:C:91:HIS:HB2	3:C:96:SER:OG	2.16	0.45
5:E:38:PRO:HD2	5:E:41:ASP:HB2	1.98	0.45
7:G:34:VAL:HG11	7:G:74:TYR:CE2	2.52	0.45
1:A:1121:GLU:HG3	1:A:1122:PRO:HD2	1.98	0.45
2:B:364:ILE:HD11	2:B:377:PHE:CD2	2.51	0.45
2:B:1055:ILE:HA	2:B:1058:LEU:HD12	1.99	0.45
4:D:7:THR:HA	7:G:7:LEU:HD23	1.98	0.45
9:I:109:ILE:HD12	9:I:109:ILE:H	1.82	0.45
11:K:49:GLU:HB2	11:K:94:ILE:HD11	1.97	0.45
1:A:41:MET:HA	1:A:49:LYS:HG2	1.99	0.45
1:A:90:VAL:HG11	1:A:300:VAL:HB	1.98	0.45
1:A:534:LEU:O	1:A:574:GLY:HA3	2.17	0.45
1:A:956:LEU:HD11	1:A:1017:LEU:HD23	1.99	0.45
2:B:898:LEU:HD21	2:B:964:VAL:HG11	1.99	0.45
3:C:104:PHE:CE1	3:C:150:GLY:HA2	2.52	0.45
1:A:563:PRO:HG2	1:A:566:ILE:HG23	1.98	0.45
1:A:830:LYS:HD3	1:A:1098:VAL:HG21	1.99	0.45
1:A:1376:THR:HG22	5:E:212:ARG:HH22	1.82	0.45
2:B:541:LEU:HD11	2:B:754:SER:HB2	1.99	0.45
2:B:882:THR:HG1	2:B:933:SER:N	2.15	0.45
4:D:33:PHE:CZ	7:G:42:PHE:HA	2.51	0.45
2:B:542:MET:HB2	2:B:747:MET:HB3	1.99	0.45
1:A:135:PHE:HD2	1:A:223:GLY:H	1.65	0.44
1:A:143:LYS:O	1:A:146:MET:HG3	2.17	0.44
1:A:986:ILE:HG21	1:A:1028:THR:HA	1.99	0.44
11:K:82:ASP:HB3	11:K:85:ASP:HB2	1.99	0.44
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.99	0.44
1:A:780:VAL:O	1:A:782:ARG:HD3	2.18	0.44
1:A:866:PHE:C	1:A:867:ILE:HG13	2.42	0.44
1:A:65:LEU:HB3	1:A:71:GLN:HB2	1.99	0.44
1:A:959:ASN:OD1	1:A:961:ARG:HB3	2.17	0.44
2:B:90:ILE:HA	2:B:133:LYS:O	2.18	0.44
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.98	0.44
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.98	0.44
7:G:6:ASP:C	7:G:73:LYS:HZ1	2.26	0.44
1:A:272:ALA:HB2	1:A:295:LEU:HD23	1.99	0.44
1:A:850:VAL:CG2	1:A:1064:VAL:HG21	2.48	0.44
1:A:1258:HIS:O	1:A:1262:LYS:HG3	2.18	0.44
1:A:1289:ARG:HD3	1:A:1290:LYS:H	1.83	0.44
3:C:254:LYS:HB3	11:K:42:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:198:LEU:HA	4:D:201:LYS:HB2	1.98	0.44
5:E:197:LYS:HG3	5:E:211:TYR:CE1	2.52	0.44
1:A:12:ARG:HB3	2:B:1218:THR:HG22	2.00	0.44
1:A:55:ASP:HA	1:A:58:LEU:H	1.81	0.44
2:B:971:THR:HG22	2:B:973:ILE:HD13	2.00	0.44
1:A:512:VAL:HG13	1:A:631:HIS:HE1	1.81	0.44
1:A:873:MET:HE3	1:A:957:PRO:HG3	2.00	0.44
5:E:98:ILE:H	5:E:98:ILE:HG13	1.62	0.44
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.53	0.44
2:B:270:LYS:HA	2:B:281:PRO:HA	1.99	0.44
2:B:274:PRO:O	2:B:275:TYR:HB2	2.17	0.44
2:B:620:ARG:HG3	9:I:57:GLY:O	2.18	0.44
1:A:768:GLN:HG2	1:A:816:HIS:HA	2.00	0.44
1:A:1081:LEU:HD11	1:A:1358:SER:O	2.18	0.44
1:A:1340:GLY:H	5:E:183:PRO:HD2	1.83	0.44
3:C:97:VAL:O	3:C:159:ALA:HB3	2.18	0.44
1:A:663:SER:CB	2:B:1085:ILE:HA	2.48	0.43
8:H:40:LEU:HD13	8:H:123:MET:HG3	2.00	0.43
1:A:405:VAL:HG12	1:A:413:ILE:HD12	2.00	0.43
2:B:573:GLN:O	2:B:575:PRO:HD3	2.18	0.43
2:B:839:MET:O	2:B:990:ILE:HA	2.17	0.43
2:B:844:SER:HB2	2:B:995:ARG:HA	1.99	0.43
1:A:277:GLU:HG2	1:A:281:HIS:CD2	2.54	0.43
1:A:594:GLY:HA3	1:A:601:LYS:HD3	2.00	0.43
1:A:709:THR:HG22	1:A:711:ARG:H	1.83	0.43
1:A:1317:MET:O	1:A:1322:ILE:HD11	2.19	0.43
2:B:1166:CYS:HA	2:B:1215:ARG:HD3	2.00	0.43
11:K:38:GLU:OE1	11:K:42:LEU:HD13	2.17	0.43
1:A:207:ILE:HA	1:A:210:ILE:HD12	2.01	0.43
1:A:467:THR:HG21	2:B:977:GLY:HA3	2.01	0.43
1:A:512:VAL:HA	1:A:519:PRO:HA	2.00	0.43
1:A:729:ALA:HA	1:A:732:LEU:HD12	2.00	0.43
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.18	0.43
2:B:900:ALA:HA	12:L:58:LYS:HD3	2.01	0.43
3:C:114:TYR:CD1	3:C:140:ASN:HB3	2.53	0.43
1:A:95:PHE:HB3	1:A:234:MET:SD	2.58	0.43
1:A:269:ILE:CG1	1:A:299:HIS:HB3	2.45	0.43
1:A:1015:VAL:HG11	1:A:1053:PHE:CZ	2.54	0.43
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.99	0.43
2:B:724:ASP:HB3	2:B:727:LYS:HB2	2.00	0.43
3:C:163:ILE:CD1	3:C:165:LYS:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:100:ILE:O	5:E:104:ASN:HA	2.19	0.43
6:F:118:LEU:O	6:F:122:MET:HG3	2.18	0.43
10:J:42:LYS:HE3	10:J:43:ARG:HD3	1.98	0.43
1:A:527:THR:HG21	1:A:650:GLN:HG2	2.00	0.43
1:A:588:LEU:HD22	1:A:629:LEU:HD23	2.00	0.43
1:A:706:HIS:CD2	1:A:1135:ARG:HH22	2.35	0.43
1:A:774:ARG:O	1:A:775:ILE:C	2.61	0.43
1:A:899:VAL:HG22	1:A:1029:ARG:HD2	2.01	0.43
2:B:515:HIS:HB3	2:B:518:HIS:ND1	2.34	0.43
8:H:62:SER:HA	8:H:141:TYR:HE2	1.83	0.43
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.48	0.43
2:B:118:ARG:HA	2:B:207:GLY:HA2	2.01	0.43
2:B:414:ALA:O	2:B:418:LYS:HB2	2.18	0.43
2:B:864:LYS:HB2	2:B:872:GLU:OE1	2.18	0.43
3:C:169:LYS:HE2	12:L:70:ARG:HG3	2.00	0.43
3:C:215:GLU:C	3:C:217:ASP:H	2.26	0.43
5:E:26:ARG:NH2	5:E:107:THR:HG21	2.33	0.43
1:A:333:GLU:H	1:A:338:GLY:HA3	1.84	0.43
1:A:1189:SER:HB3	1:A:1242:VAL:H	1.82	0.43
6:F:132:LEU:O	6:F:148:VAL:HG13	2.18	0.43
1:A:88:LYS:HB2	1:A:276:LEU:HD21	2.00	0.43
1:A:392:VAL:HA	1:A:415:LEU:HD21	2.01	0.43
1:A:492:PRO:HB3	1:A:497:THR:HG22	2.01	0.43
2:B:486:TYR:CD1	2:B:1096:ARG:HD2	2.54	0.43
2:B:905:VAL:HB	2:B:941:LEU:HD22	2.01	0.43
3:C:220:ASP:HB3	3:C:223:ALA:CB	2.48	0.43
5:E:90:VAL:HA	5:E:120:ALA:HB2	2.00	0.43
6:F:76:LYS:O	6:F:79:ARG:HD3	2.18	0.43
11:K:18:LYS:HG2	11:K:36:GLU:O	2.18	0.43
1:A:531:ILE:HG13	1:A:578:LEU:HD11	2.00	0.43
1:A:696:GLU:HA	1:A:701:LEU:HD12	2.01	0.43
1:A:1170:ILE:O	1:A:1174:PHE:HB2	2.18	0.43
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	2.00	0.43
2:B:118:ARG:HH11	2:B:788:ARG:NH1	2.17	0.43
2:B:637:LEU:HD23	2:B:742:GLU:HA	2.00	0.43
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.19	0.43
4:D:56:ARG:NH2	4:D:57:LEU:HD21	2.34	0.43
4:D:144:THR:HG22	4:D:148:LEU:HD12	1.99	0.43
4:D:185:CYS:SG	4:D:190:GLU:HG2	2.59	0.43
1:A:371:ALA:O	1:A:435:HIS:HB3	2.19	0.42
1:A:1342:GLU:HG3	5:E:198:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:427:ASP:HA	2:B:430:ARG:HB2	2.01	0.42
2:B:590:HIS:HD2	2:B:592:ASN:N	2.17	0.42
2:B:879:ARG:HB3	2:B:883:LEU:HG	2.00	0.42
4:D:33:PHE:HZ	7:G:42:PHE:HA	1.82	0.42
4:D:66:ARG:HG3	7:G:51:TYR:CB	2.48	0.42
5:E:67:GLU:C	5:E:69:ILE:H	2.27	0.42
8:H:15:VAL:HA	8:H:26:ILE:HG13	2.01	0.42
1:A:924:LYS:HA	1:A:927:VAL:HB	2.02	0.42
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	2.00	0.42
2:B:765:PRO:O	2:B:769:TYR:HD1	2.02	0.42
1:A:1355:VAL:HA	1:A:1358:SER:OG	2.18	0.42
2:B:842:ASN:HD22	2:B:845:SER:N	2.18	0.42
2:B:893:LEU:HD11	2:B:910:VAL:HB	2.01	0.42
4:D:120:GLU:O	4:D:123:LEU:HB2	2.18	0.42
6:F:127:GLU:HB3	6:F:129:LYS:HE3	2.00	0.42
1:A:232:GLU:HG2	1:A:232:GLU:H	1.70	0.42
1:A:1386:ARG:HA	1:A:1390:ASN:CB	2.49	0.42
3:C:17:ASN:HA	3:C:232:VAL:O	2.20	0.42
7:G:101:VAL:HG21	7:G:145:VAL:HG11	2.01	0.42
9:I:88:SER:C	9:I:90:GLN:H	2.27	0.42
1:A:443:LEU:HD12	2:B:1146:PHE:CE2	2.53	0.42
1:A:1163:ILE:HD13	1:A:1194:ARG:HD2	2.01	0.42
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	2.02	0.42
3:C:245:VAL:HG13	11:K:102:LYS:HD3	2.00	0.42
3:C:248:ILE:HG23	11:K:98:LEU:HD22	2.01	0.42
4:D:66:ARG:HG2	4:D:70:PHE:CE2	2.54	0.42
9:I:26:LEU:HB3	9:I:35:VAL:CG1	2.49	0.42
1:A:140:THR:HA	1:A:143:LYS:NZ	2.34	0.42
1:A:588:LEU:HD23	1:A:607:ILE:HD12	2.00	0.42
1:A:1166:ASP:CG	1:A:1239:ARG:HD2	2.45	0.42
2:B:322:PHE:HZ	9:I:30:ARG:HB2	1.84	0.42
1:A:497:THR:CG2	2:B:1146:PHE:CD1	3.01	0.42
1:A:519:PRO:HD3	1:A:631:HIS:ND1	2.34	0.42
1:A:678:GLU:O	1:A:681:GLU:HB3	2.20	0.42
2:B:534:GLY:O	2:B:537:LYS:HE2	2.19	0.42
2:B:797:TYR:CD1	2:B:852:ARG:HB3	2.54	0.42
2:B:1106:ARG:NH1	2:B:1118:PRO:HB3	2.35	0.42
11:K:35:PHE:O	11:K:70:ARG:HA	2.20	0.42
1:A:97:ALA:O	1:A:101:LYS:HG2	2.18	0.42
5:E:22:MET:O	5:E:26:ARG:HB2	2.20	0.42
7:G:9:LEU:HD23	7:G:11:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:130:TYR:O	7:G:136:VAL:HA	2.20	0.42
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.67	0.42
1:A:567:LYS:HD2	1:A:568:PRO:HD3	2.01	0.42
1:A:770:VAL:HG13	1:A:822:GLU:HG3	2.02	0.42
1:A:867:ILE:HG12	1:A:1000:LEU:HD11	2.02	0.42
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	2.02	0.42
2:B:756:ILE:HG21	2:B:767:ASN:OD1	2.20	0.42
3:C:169:LYS:NZ	12:L:69:ALA:HB3	2.34	0.42
1:A:490:HIS:HB3	2:B:1150:ARG:NH1	2.35	0.42
1:A:548:ASN:HA	11:K:60:ALA:HB1	2.02	0.42
1:A:1387:HIS:HA	1:A:1391:ARG:HG2	2.00	0.42
2:B:364:ILE:HG21	2:B:373:ARG:HB3	2.01	0.42
2:B:394:ASP:HB2	9:I:91:ARG:HD2	2.01	0.42
8:H:43:ASN:OD1	8:H:45:GLU:HB3	2.20	0.42
1:A:672:ASP:HB2	3:C:195:GLN:HE22	1.84	0.41
1:A:789:LYS:HG3	9:I:67:THR:HB	2.01	0.41
1:A:847:ASP:HA	1:A:1424:VAL:HG23	2.02	0.41
1:A:1280:GLU:HB3	1:A:1281:ARG:H	1.71	0.41
1:A:1289:ARG:HB2	1:A:1303:GLU:HG2	2.02	0.41
1:A:1423:GLY:N	1:A:1426:GLU:HG3	2.30	0.41
2:B:123:THR:HG23	2:B:205:ILE:HA	2.02	0.41
2:B:552:MET:HA	2:B:555:ILE:HB	2.02	0.41
3:C:60:ASP:HB3	12:L:67:PHE:CE2	2.55	0.41
7:G:112:LYS:HA	7:G:115:MET:HE3	2.01	0.41
11:K:70:ARG:HE	11:K:70:ARG:HB3	1.67	0.41
1:A:353:ILE:HG21	1:A:487:MET:HE3	2.02	0.41
13:X:320:GLU:HA	13:X:323:ALA:HB3	2.02	0.41
1:A:54:ASN:C	1:A:56:PRO:HD3	2.45	0.41
1:A:782:ARG:HB3	1:A:789:LYS:HA	2.01	0.41
1:A:1364:ASN:HD22	1:A:1365:TYR:N	2.18	0.41
2:B:227:LYS:HG2	2:B:236:HIS:CD2	2.56	0.41
2:B:327:ARG:HG2	2:B:331:LEU:HD13	2.01	0.41
1:A:92:HIS:NE2	1:A:1410:PHE:HE2	2.17	0.41
1:A:101:LYS:HA	1:A:139:TRP:NE1	2.34	0.41
1:A:548:ASN:HD21	11:K:47:ARG:HH21	1.68	0.41
1:A:641:VAL:O	1:A:644:LYS:HB3	2.20	0.41
1:A:683:ILE:HD13	1:A:801:GLU:HG3	2.02	0.41
1:A:883:LEU:H	1:A:952:ALA:HB1	1.85	0.41
1:A:886:ILE:HG23	1:A:944:ARG:HG3	2.02	0.41
2:B:580:VAL:O	2:B:586:TRP:HD1	2.04	0.41
2:B:705:MET:H	2:B:710:LEU:HD12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1003:ALA:O	3:C:177:GLU:HA	2.21	0.41
6:F:74:ILE:HG13	6:F:142:SER:HB2	2.01	0.41
10:J:43:ARG:HG3	10:J:45:CYS:SG	2.61	0.41
1:A:273:ASN:HD22	1:A:274:ILE:HD12	1.84	0.41
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.20	0.41
1:A:1343:ALA:O	1:A:1346:ALA:HB3	2.20	0.41
2:B:210:LYS:HA	2:B:210:LYS:HD2	1.84	0.41
2:B:286:PHE:CD2	2:B:297:ILE:HG23	2.55	0.41
2:B:800:GLN:HB2	2:B:821:GLN:HA	2.01	0.41
2:B:1078:GLY:HA3	3:C:27:LEU:HD11	2.02	0.41
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.55	0.41
2:B:580:VAL:HG13	2:B:624:LEU:HB3	2.01	0.41
4:D:130:LEU:O	4:D:134:THR:HB	2.20	0.41
5:E:154:ILE:O	5:E:196:VAL:HA	2.20	0.41
7:G:31:LEU:O	7:G:35:GLU:HB3	2.21	0.41
1:A:65:LEU:HB3	1:A:71:GLN:HB3	2.02	0.41
1:A:344:ARG:HA	2:B:1128:LEU:O	2.20	0.41
1:A:374:LEU:HB3	1:A:491:VAL:HG21	2.03	0.41
1:A:571:LEU:HD22	8:H:46:LEU:HD11	2.02	0.41
3:C:104:PHE:HE1	3:C:150:GLY:HA2	1.85	0.41
8:H:2:SER:HA	8:H:62:SER:HB3	2.02	0.41
1:A:608:ILE:H	1:A:613:ILE:CD1	2.32	0.41
1:A:717:ASN:O	1:A:720:ARG:HB2	2.21	0.41
1:A:1190:PRO:HG2	1:A:1191:TRP:CD1	2.55	0.41
2:B:653:VAL:HG13	2:B:689:LEU:HB3	2.02	0.41
2:B:1006:ILE:H	2:B:1006:ILE:HG13	1.62	0.41
3:C:149:LYS:HB3	3:C:150:GLY:H	1.58	0.41
1:A:21:LEU:HD12	1:A:1414:ALA:HA	2.02	0.41
1:A:874:ASP:HA	1:A:1058:VAL:HG13	2.03	0.41
1:A:1323:ASP:C	1:A:1325:THR:H	2.28	0.41
2:B:579:ARG:HA	2:B:589:VAL:HG12	2.02	0.41
2:B:799:PRO:HD2	10:J:1:MET:H3	1.86	0.41
2:B:852:ARG:HH22	12:L:70:ARG:C	2.29	0.41
8:H:84:ALA:C	8:H:86:ASP:H	2.27	0.41
8:H:105:GLU:HG2	8:H:107:VAL:HG13	2.03	0.41
9:I:16:PRO:HB3	9:I:25:LEU:HD11	2.02	0.41
10:J:41:LEU:HD22	10:J:46:CYS:HB2	2.03	0.41
1:A:91:PHE:CE1	1:A:99:ILE:HG21	2.56	0.41
1:A:465:TYR:HB3	2:B:976:ILE:CG2	2.37	0.41
1:A:928:LEU:HA	1:A:931:GLU:OE2	2.21	0.41
1:A:1031:VAL:O	1:A:1035:TYR:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1121:GLU:HB2	1:A:1321:GLY:C	2.46	0.41
1:A:1431:GLY:HA3	2:B:1152:MET:HG3	2.02	0.41
2:B:793:ALA:O	2:B:855:PHE:HA	2.20	0.41
2:B:878:GLN:HA	2:B:885:MET:HE1	2.03	0.41
4:D:23:ASN:HB3	7:G:82:PHE:HD1	1.85	0.41
7:G:106:MET:HE3	7:G:108:VAL:HG22	2.03	0.41
1:A:531:ILE:HD11	1:A:578:LEU:HD21	2.03	0.40
1:A:811:GLN:H	1:A:811:GLN:HG3	1.52	0.40
1:A:840:ARG:HH12	1:A:1102:LYS:HG3	1.87	0.40
1:A:1095:THR:HB	1:A:1100:ARG:HB2	2.02	0.40
4:D:8:PHE:H	7:G:5:LYS:HE3	1.85	0.40
1:A:133:LYS:HA	1:A:136:ALA:HB3	2.03	0.40
1:A:737:LEU:HA	1:A:738:LYS:HE2	2.04	0.40
1:A:1130:GLN:HG3	1:A:1134:ILE:HD11	2.02	0.40
1:A:1191:TRP:HB3	1:A:1260:LEU:HD22	2.02	0.40
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	2.03	0.40
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	2.02	0.40
2:B:188:ASP:O	2:B:192:LEU:HB2	2.21	0.40
2:B:486:TYR:CE1	2:B:1096:ARG:HD2	2.57	0.40
5:E:88:VAL:HB	5:E:116:ILE:HG12	2.02	0.40
5:E:176:PRO:HD2	5:E:211:TYR:O	2.21	0.40
6:F:130:ILE:HG22	6:F:132:LEU:H	1.85	0.40
1:A:567:LYS:HE3	8:H:46:LEU:HD12	2.02	0.40
1:A:865:GLN:HA	5:E:208:TYR:OH	2.21	0.40
1:A:913:LEU:HD12	1:A:915:SER:OG	2.22	0.40
1:A:1413:GLY:HA3	2:B:1212:ILE:HG12	2.03	0.40
2:B:92:PHE:HZ	2:B:428:ILE:HD13	1.86	0.40
4:D:35:LEU:O	4:D:46:GLU:HA	2.19	0.40
4:D:53:SER:C	4:D:55:ALA:N	2.80	0.40
5:E:136:ASN:O	5:E:140:LEU:HD12	2.21	0.40
1:A:53:LEU:HD22	1:A:263:THR:HG22	2.04	0.40
1:A:700:ASN:O	9:I:115:LYS:HD2	2.21	0.40
3:C:72:LEU:HA	3:C:132:PRO:HA	2.03	0.40
3:C:169:LYS:HZ2	12:L:69:ALA:HB3	1.85	0.40
4:D:24:ALA:C	4:D:26:THR:H	2.29	0.40
6:F:90:ARG:HG2	6:F:94:LEU:CD1	2.52	0.40
11:K:38:GLU:HG3	11:K:42:LEU:CD2	2.47	0.40
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	2.02	0.40
1:A:365:GLY:HA3	1:A:469:ARG:HG3	2.04	0.40
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.36	0.40
1:A:1194:ARG:HG3	1:A:1237:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.04	0.40
5:E:112:TYR:CD2	5:E:115:ASN:HA	2.57	0.40
6:F:79:ARG:HG2	6:F:146:TRP:CZ2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1406/1733 (81%)	1111 (79%)	218 (16%)	77 (6%)	1	15
2	B	1075/1224 (88%)	861 (80%)	155 (14%)	59 (6%)	1	15
3	C	264/318 (83%)	208 (79%)	47 (18%)	9 (3%)	3	20
4	D	173/221 (78%)	144 (83%)	18 (10%)	11 (6%)	1	13
5	E	212/215 (99%)	176 (83%)	30 (14%)	6 (3%)	4	24
6	F	82/155 (53%)	69 (84%)	11 (13%)	2 (2%)	4	27
7	G	169/171 (99%)	143 (85%)	22 (13%)	4 (2%)	4	27
8	H	129/146 (88%)	96 (74%)	17 (13%)	16 (12%)	0	4
9	I	117/122 (96%)	96 (82%)	18 (15%)	3 (3%)	4	25
10	J	63/70 (90%)	46 (73%)	14 (22%)	3 (5%)	2	16
11	K	113/120 (94%)	94 (83%)	18 (16%)	1 (1%)	14	49
12	L	44/70 (63%)	25 (57%)	13 (30%)	6 (14%)	0	3
13	X	107/594 (18%)	83 (78%)	20 (19%)	4 (4%)	2	19
All	All	3954/5159 (77%)	3152 (80%)	601 (15%)	201 (5%)	1	15

All (201) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	47	ARG
1	A	57	ARG
1	A	65	LEU
1	A	71	GLN
1	A	93	VAL
1	A	164	ARG
1	A	323	LYS
1	A	331	GLY
1	A	332	LYS
1	A	335	ARG
1	A	385	ILE
1	A	424	ILE
1	A	462	VAL
1	A	466	SER
1	A	543	LEU
1	A	567	LYS
1	A	751	SER
1	A	775	ILE
1	A	875	ALA
1	A	1097	GLY
1	A	1223	ASP
1	A	1281	ARG
2	B	67	SER
2	B	108	VAL
2	B	177	LYS
2	B	229	ALA
2	B	249	ARG
2	B	266	ALA
2	B	364	ILE
2	B	367	LEU
2	B	731	VAL
2	B	734	HIS
2	B	785	TYR
2	B	880	THR
2	B	962	LYS
2	B	1041	GLU
2	B	1132	GLU
2	B	1157	ALA
2	B	1165	ILE
2	B	1188	LYS
3	C	40	GLU
3	C	197	SER

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Mol	Chain	Res	Type
3	C	240	VAL
4	D	18	VAL
5	E	104	ASN
5	E	174	GLN
6	F	78	GLN
7	G	20	PRO
8	H	84	ALA
8	H	128	ASN
10	J	2	ILE
12	L	55	ILE
13	X	332	LEU
13	X	335	LEU
13	X	336	VAL
1	A	41	MET
1	A	42	ASP
1	A	66	LYS
1	A	68	GLN
1	A	167	CYS
1	A	184	SER
1	A	286	HIS
1	A	318	SER
1	A	673	GLY
1	A	846	GLU
1	A	923	LEU
1	A	1206	ASP
1	A	1314	SER
1	A	1388	GLY
1	A	1403	GLU
1	A	1437	GLY
2	B	45	SER
2	B	55	VAL
2	B	245	GLU
2	B	251	ILE
2	B	275	TYR
2	B	369	GLY
2	B	447	ALA
2	B	667	GLN
2	B	711	GLU
2	B	712	PRO
2	B	751	VAL
2	B	772	ALA
2	B	1046	PRO

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Mol	Chain	Res	Type
2	B	1113	VAL
2	B	1223	ASP
3	C	142	VAL
4	D	53	SER
4	D	56	ARG
4	D	119	ARG
4	D	135	GLY
4	D	184	ALA
5	E	36	GLU
7	G	154	VAL
8	H	6	PHE
8	H	81	PRO
8	H	82	PRO
8	H	94	ASP
8	H	108	SER
8	H	131	ASN
8	H	139	ASN
10	J	13	VAL
11	K	6	ARG
12	L	33	GLU
12	L	45	ALA
1	A	40	THR
1	A	322	VAL
1	A	396	PRO
1	A	639	PRO
1	A	738	LYS
1	A	858	ASN
1	A	981	LEU
1	A	1122	PRO
1	A	1236	LEU
1	A	1416	ALA
1	A	1421	CYS
2	B	40	GLU
2	B	305	VAL
2	B	511	PRO
2	B	608	ASP
2	B	649	LYS
2	B	725	PRO
2	B	907	GLY
2	B	982	SER
2	B	1066	SER
2	B	1102	LYS

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Mol	Chain	Res	Type
2	B	1215	ARG
3	C	90	ASP
4	D	40	HIS
4	D	55	ALA
4	D	138	ASN
5	E	3	GLN
5	E	75	MET
8	H	78	SER
8	H	110	ASP
9	I	61	ASP
9	I	88	SER
12	L	50	ASP
1	A	5	GLN
1	A	63	ARG
1	A	196	GLU
1	A	465	TYR
1	A	1396	ALA
1	A	1440	ALA
2	B	41	LYS
2	B	106	ASP
2	B	214	ALA
2	B	575	PRO
2	B	642	ASP
2	B	1119	VAL
3	C	214	ASN
4	D	22	GLU
6	F	73	ALA
8	H	60	ALA
8	H	77	ARG
13	X	329	LYS
1	A	4	GLN
1	A	45	GLN
1	A	109	HIS
1	A	117	GLU
1	A	253	ASN
1	A	958	VAL
1	A	1107	VAL
1	A	1255	GLU
2	B	1189	ILE
3	C	149	LYS
4	D	20	GLU
5	E	185	ALA

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Mol	Chain	Res	Type
7	G	52	ASP
8	H	109	LYS
12	L	39	SER
12	L	56	LEU
1	A	254	GLU
1	A	380	VAL
1	A	479	ASN
1	A	1256	GLU
1	A	1424	VAL
1	A	1454	MET
2	B	514	LEU
2	B	593	PRO
2	B	894	ASP
2	B	1108	ARG
2	B	1143	ALA
2	B	1155	SER
7	G	147	ILE
8	H	103	LYS
9	I	53	GLY
10	J	64	ASN
1	A	916	GLY
1	A	178	GLY
1	A	599	SER
2	B	168	GLY
2	B	436	VAL
3	C	5	GLY
8	H	107	VAL
1	A	910	PRO
1	A	1189	SER
1	A	1327	ILE
3	C	141	GLY
1	A	258	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1239/1520 (82%)	974 (79%)	265 (21%)	1	6
2	B	952/1061 (90%)	770 (81%)	182 (19%)	1	8
3	C	234/274 (85%)	190 (81%)	44 (19%)	1	9
4	D	140/200 (70%)	112 (80%)	28 (20%)	1	8
5	E	196/197 (100%)	164 (84%)	32 (16%)	2	12
6	F	74/137 (54%)	62 (84%)	12 (16%)	2	12
7	G	152/152 (100%)	126 (83%)	26 (17%)	2	11
8	H	117/128 (91%)	95 (81%)	22 (19%)	1	9
9	I	113/116 (97%)	99 (88%)	14 (12%)	4	18
10	J	60/65 (92%)	44 (73%)	16 (27%)	0	3
11	K	99/102 (97%)	83 (84%)	16 (16%)	2	12
12	L	40/57 (70%)	30 (75%)	10 (25%)	0	4
All	All	3416/4009 (85%)	2749 (80%)	667 (20%)	1	8

All (667) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	21	LEU
1	A	23	SER
1	A	30	ILE
1	A	32	VAL
1	A	34	LYS
1	A	37	PHE
1	A	39	GLU
1	A	41	MET
1	A	45	GLN
1	A	50	ILE
1	A	53	LEU
1	A	61	ILE
1	A	65	LEU
1	A	68	GLN
1	A	69	THR
1	A	71	GLN
1	A	72	GLU
1	A	85	ASP
1	A	93	VAL
1	A	96	ILE
1	A	104	GLU

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Mol	Chain	Res	Type
1	A	109	HIS
1	A	141	LEU
1	A	152	VAL
1	A	157	ASP
1	A	159	THR
1	A	171	GLN
1	A	173	THR
1	A	174	ILE
1	A	180	LYS
1	A	204	THR
1	A	210	ILE
1	A	215	SER
1	A	216	VAL
1	A	226	GLU
1	A	232	GLU
1	A	236	LEU
1	A	237	THR
1	A	238	CYS
1	A	250	ILE
1	A	254	GLU
1	A	257	ARG
1	A	261	ASP
1	A	263	THR
1	A	265	LYS
1	A	274	ILE
1	A	286	HIS
1	A	289	ILE
1	A	290	GLU
1	A	295	LEU
1	A	299	HIS
1	A	303	TYR
1	A	307	ASP
1	A	308	ILE
1	A	311	GLN
1	A	315	LEU
1	A	318	SER
1	A	320	ARG
1	A	324	SER
1	A	335	ARG
1	A	372	LYS
1	A	373	THR
1	A	384	ASN

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Mol	Chain	Res	Type
1	A	385	ILE
1	A	386	ASP
1	A	389	THR
1	A	392	VAL
1	A	415	LEU
1	A	417	TYR
1	A	423	ASP
1	A	434	ARG
1	A	437	MET
1	A	442	VAL
1	A	443	LEU
1	A	447	GLN
1	A	450	LEU
1	A	454	SER
1	A	469	ARG
1	A	472	LEU
1	A	481	ASP
1	A	486	GLU
1	A	489	LEU
1	A	495	GLU
1	A	496	GLU
1	A	498	ARG
1	A	500	GLU
1	A	504	LEU
1	A	513	SER
1	A	515	GLN
1	A	518	LYS
1	A	521	MET
1	A	523	ILE
1	A	527	THR
1	A	532	ARG
1	A	533	LYS
1	A	541	ILE
1	A	542	GLU
1	A	545	GLN
1	A	557	ASP
1	A	562	THR
1	A	565	ILE
1	A	566	ILE
1	A	567	LYS
1	A	571	LEU
1	A	577	ILE

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Mol	Chain	Res	Type
1	A	578	LEU
1	A	595	THR
1	A	597	LEU
1	A	618	GLU
1	A	621	THR
1	A	629	LEU
1	A	636	GLU
1	A	640	GLN
1	A	653	VAL
1	A	654	ASN
1	A	657	LEU
1	A	663	SER
1	A	666	ILE
1	A	670	ILE
1	A	672	ASP
1	A	678	GLU
1	A	681	GLU
1	A	682	THR
1	A	701	LEU
1	A	703	THR
1	A	705	LYS
1	A	706	HIS
1	A	710	LEU
1	A	716	ASP
1	A	718	VAL
1	A	719	VAL
1	A	721	PHE
1	A	735	VAL
1	A	738	LYS
1	A	756	ILE
1	A	757	ASN
1	A	771	GLU
1	A	783	THR
1	A	791	ASP
1	A	795	GLU
1	A	796	SER
1	A	805	LEU
1	A	811	GLN
1	A	818	MET
1	A	822	GLU
1	A	834	THR
1	A	837	ILE

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Mol	Chain	Res	Type
1	A	839	ARG
1	A	842	VAL
1	A	847	ASP
1	A	853	ASP
1	A	860	LEU
1	A	867	ILE
1	A	884	ASP
1	A	886	ILE
1	A	905	ASP
1	A	907	THR
1	A	909	ASP
1	A	915	SER
1	A	917	SER
1	A	918	GLU
1	A	919	ILE
1	A	920	LEU
1	A	926	GLN
1	A	928	LEU
1	A	929	LEU
1	A	937	VAL
1	A	947	PHE
1	A	948	VAL
1	A	964	ILE
1	A	968	GLN
1	A	972	HIS
1	A	973	ILE
1	A	974	ASP
1	A	976	THR
1	A	982	THR
1	A	983	ILE
1	A	988	LEU
1	A	998	LEU
1	A	1001	ARG
1	A	1006	ILE
1	A	1007	ILE
1	A	1017	LEU
1	A	1019	CYS
1	A	1037	LEU
1	A	1048	ASN
1	A	1050	GLU
1	A	1052	GLN
1	A	1058	VAL

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Mol	Chain	Res	Type
1	A	1064	VAL
1	A	1067	LEU
1	A	1094	VAL
1	A	1095	THR
1	A	1098	VAL
1	A	1100	ARG
1	A	1104	ILE
1	A	1110	ASN
1	A	1113	THR
1	A	1120	LEU
1	A	1135	ARG
1	A	1142	THR
1	A	1159	ARG
1	A	1172	LEU
1	A	1174	PHE
1	A	1175	SER
1	A	1195	LEU
1	A	1199	ARG
1	A	1204	ASP
1	A	1205	LYS
1	A	1207	LEU
1	A	1215	ARG
1	A	1222	ASN
1	A	1226	VAL
1	A	1227	ILE
1	A	1233	ASP
1	A	1234	GLU
1	A	1238	ILE
1	A	1240	CYS
1	A	1242	VAL
1	A	1256	GLU
1	A	1259	MET
1	A	1260	LEU
1	A	1266	THR
1	A	1267	MET
1	A	1277	GLU
1	A	1280	GLU
1	A	1283	VAL
1	A	1285	MET
1	A	1287	TYR
1	A	1289	ARG
1	A	1293	SER

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Mol	Chain	Res	Type
1	A	1295	THR
1	A	1299	VAL
1	A	1303	GLU
1	A	1307	GLU
1	A	1315	GLU
1	A	1322	ILE
1	A	1325	THR
1	A	1331	SER
1	A	1333	ILE
1	A	1335	ILE
1	A	1338	VAL
1	A	1341	ILE
1	A	1345	ARG
1	A	1356	ILE
1	A	1359	ASP
1	A	1364	ASN
1	A	1366	ARG
1	A	1370	LEU
1	A	1373	ASP
1	A	1375	MET
1	A	1381	LEU
1	A	1382	THR
1	A	1392	SER
1	A	1393	ASN
1	A	1417	GLU
1	A	1426	GLU
1	A	1433	MET
1	A	1438	THR
1	A	1442	ASP
1	A	1443	VAL
1	A	1445	ILE
1	A	1451	VAL
1	A	1453	TYR
2	B	20	ASP
2	B	21	GLU
2	B	25	ILE
2	B	33	VAL
2	B	44	VAL
2	B	46	GLN
2	B	50	SER
2	B	56	ASP
2	B	58	THR

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Mol	Chain	Res	Type
2	B	59	LEU
2	B	61	ASP
2	B	63	ILE
2	B	102	VAL
2	B	103	ASN
2	B	108	VAL
2	B	119	LEU
2	B	126	SER
2	B	128	LEU
2	B	130	VAL
2	B	131	ASP
2	B	167	ILE
2	B	177	LYS
2	B	189	LEU
2	B	192	LEU
2	B	194	GLU
2	B	211	VAL
2	B	223	VAL
2	B	232	SER
2	B	244	LEU
2	B	248	SER
2	B	251	ILE
2	B	254	LEU
2	B	261	ARG
2	B	268	THR
2	B	273	LEU
2	B	283	VAL
2	B	289	LEU
2	B	294	ASP
2	B	305	VAL
2	B	313	MET
2	B	324	ILE
2	B	329	THR
2	B	331	LEU
2	B	334	ILE
2	B	348	ARG
2	B	349	ILE
2	B	361	LEU
2	B	365	THR
2	B	367	LEU
2	B	376	PHE
2	B	382	ILE

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Mol	Chain	Res	Type
2	B	387	LEU
2	B	393	LYS
2	B	394	ASP
2	B	395	GLN
2	B	398	ARG
2	B	408	LEU
2	B	415	GLN
2	B	418	LYS
2	B	424	LEU
2	B	425	THR
2	B	429	PHE
2	B	430	ARG
2	B	436	VAL
2	B	448	ILE
2	B	452	THR
2	B	453	ILE
2	B	466	TRP
2	B	487	THR
2	B	491	THR
2	B	492	LEU
2	B	514	LEU
2	B	531	GLN
2	B	538	ASN
2	B	541	LEU
2	B	550	ASP
2	B	552	MET
2	B	563	MET
2	B	567	GLU
2	B	570	VAL
2	B	576	ASP
2	B	580	VAL
2	B	582	VAL
2	B	591	ARG
2	B	596	LEU
2	B	599	THR
2	B	602	THR
2	B	616	ILE
2	B	620	ARG
2	B	624	LEU
2	B	628	THR
2	B	635	ARG
2	B	644	GLU

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Mol	Chain	Res	Type
2	B	652	LYS
2	B	653	VAL
2	B	658	ILE
2	B	666	TYR
2	B	684	LEU
2	B	694	ASP
2	B	708	GLU
2	B	711	GLU
2	B	727	LYS
2	B	754	SER
2	B	755	ILE
2	B	771	SER
2	B	785	TYR
2	B	791	THR
2	B	792	MET
2	B	795	ILE
2	B	825	VAL
2	B	836	GLU
2	B	840	ILE
2	B	842	ASN
2	B	844	SER
2	B	855	PHE
2	B	860	MET
2	B	863	GLU
2	B	865	LYS
2	B	870	ILE
2	B	878	GLN
2	B	879	ARG
2	B	880	THR
2	B	891	ASP
2	B	895	ASP
2	B	903	VAL
2	B	905	VAL
2	B	909	ASP
2	B	916	THR
2	B	935	ARG
2	B	956	THR
2	B	959	ASP
2	B	966	VAL
2	B	970	THR
2	B	973	ILE
2	B	975	GLN

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Mol	Chain	Res	Type
2	B	976	ILE
2	B	986	GLN
2	B	987	LYS
2	B	996	ARG
2	B	999	MET
2	B	1006	ILE
2	B	1007	VAL
2	B	1012	ILE
2	B	1017	ILE
2	B	1022	THR
2	B	1026	LEU
2	B	1034	VAL
2	B	1045	SER
2	B	1049	ASP
2	B	1050	ILE
2	B	1052	VAL
2	B	1055	ILE
2	B	1059	LEU
2	B	1071	VAL
2	B	1072	MET
2	B	1077	THR
2	B	1084	GLN
2	B	1087	PHE
2	B	1094	ARG
2	B	1101	ASP
2	B	1112	GLN
2	B	1133	MET
2	B	1139	ILE
2	B	1145	SER
2	B	1147	LEU
2	B	1151	LEU
2	B	1152	MET
2	B	1155	SER
2	B	1165	ILE
2	B	1170	THR
2	B	1176	ASN
2	B	1191	ILE
2	B	1195	HIS
2	B	1202	LEU
2	B	1203	LEU
2	B	1207	LEU
2	B	1211	ASN

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Mol	Chain	Res	Type
2	B	1212	ILE
2	B	1218	THR
2	B	1220	ARG
2	B	1221	SER
2	B	1224	PHE
3	C	16	ASP
3	C	19	ASP
3	C	25	VAL
3	C	26	ASP
3	C	27	LEU
3	C	34	ARG
3	C	35	ARG
3	C	36	VAL
3	C	38	ILE
3	C	49	VAL
3	C	51	VAL
3	C	52	GLU
3	C	55	THR
3	C	57	VAL
3	C	66	ARG
3	C	72	LEU
3	C	80	LEU
3	C	87	PHE
3	C	106	GLU
3	C	120	ILE
3	C	121	VAL
3	C	127	ARG
3	C	129	ILE
3	C	134	ILE
3	C	136	ASP
3	C	142	VAL
3	C	154	LYS
3	C	155	LEU
3	C	184	ASN
3	C	186	LEU
3	C	187	LYS
3	C	189	THR
3	C	190	ASP
3	C	203	GLN
3	C	214	ASN
3	C	220	ASP
3	C	227	THR

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Mol	Chain	Res	Type
3	C	231	ASN
3	C	233	GLU
3	C	240	VAL
3	C	258	ILE
3	C	260	LEU
3	C	264	GLN
3	C	265	MET
4	D	28	GLN
4	D	29	LEU
4	D	38	ILE
4	D	46	GLU
4	D	48	ILE
4	D	50	LEU
4	D	64	VAL
4	D	65	GLU
4	D	68	ARG
4	D	126	ILE
4	D	127	ASP
4	D	131	GLU
4	D	138	ASN
4	D	139	LYS
4	D	156	ASP
4	D	157	GLN
4	D	158	GLU
4	D	168	LYS
4	D	173	HIS
4	D	176	GLU
4	D	180	LEU
4	D	185	CYS
4	D	189	ASP
4	D	195	ILE
4	D	197	SER
4	D	206	GLU
4	D	208	GLU
4	D	216	ASN
5	E	5	ASN
5	E	8	ASN
5	E	22	MET
5	E	26	ARG
5	E	30	ILE
5	E	40	GLU
5	E	46	TYR

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Mol	Chain	Res	Type
5	E	52	ARG
5	E	65	THR
5	E	67	GLU
5	E	69	ILE
5	E	70	SER
5	E	74	ASP
5	E	81	GLU
5	E	94	LYS
5	E	96	PHE
5	E	98	ILE
5	E	100	ILE
5	E	104	ASN
5	E	106	GLN
5	E	110	PHE
5	E	114	ASN
5	E	117	THR
5	E	150	VAL
5	E	152	LYS
5	E	170	LEU
5	E	179	GLN
5	E	182	ASP
5	E	184	VAL
5	E	196	VAL
5	E	208	TYR
5	E	213	ILE
6	F	77	ASP
6	F	79	ARG
6	F	92	ARG
6	F	96	THR
6	F	102	SER
6	F	104	ASN
6	F	110	ASP
6	F	115	THR
6	F	119	ARG
6	F	138	LEU
6	F	140	ASP
6	F	153	VAL
7	G	3	PHE
7	G	21	ARG
7	G	26	LEU
7	G	42	PHE
7	G	46	LEU

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Mol	Chain	Res	Type
7	G	49	LEU
7	G	60	ARG
7	G	61	ILE
7	G	73	LYS
7	G	77	VAL
7	G	85	GLU
7	G	87	VAL
7	G	90	THR
7	G	92	VAL
7	G	111	THR
7	G	119	LEU
7	G	126	ASN
7	G	131	GLN
7	G	135	ASP
7	G	138	THR
7	G	139	ILE
7	G	143	ILE
7	G	151	ILE
7	G	160	ILE
7	G	164	LYS
7	G	165	GLU
8	H	4	THR
8	H	16	ASP
8	H	26	ILE
8	H	27	GLU
8	H	31	THR
8	H	34	ASP
8	H	36	CYS
8	H	42	ILE
8	H	49	VAL
8	H	53	ASP
8	H	54	SER
8	H	61	SER
8	H	86	ASP
8	H	91	ASP
8	H	107	VAL
8	H	110	ASP
8	H	114	VAL
8	H	124	ARG
8	H	128	ASN
8	H	130	ARG
8	H	142	LEU

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Mol	Chain	Res	Type
8	H	144	ILE
9	I	4	PHE
9	I	8	ARG
9	I	12	ASN
9	I	21	GLU
9	I	28	GLU
9	I	31	THR
9	I	37	GLU
9	I	43	VAL
9	I	89	GLN
9	I	92	ARG
9	I	96	SER
9	I	97	MET
9	I	113	ASP
9	I	119	THR
10	J	2	ILE
10	J	3	VAL
10	J	9	SER
10	J	12	LYS
10	J	13	VAL
10	J	19	GLU
10	J	23	ASN
10	J	24	LEU
10	J	25	LEU
10	J	30	LEU
10	J	31	ASP
10	J	37	SER
10	J	46	CYS
10	J	48	ARG
10	J	55	ASP
10	J	62	ARG
11	K	5	ASP
11	K	9	LEU
11	K	11	LEU
11	K	14	GLU
11	K	18	LYS
11	K	21	ILE
11	K	29	ASN
11	K	31	VAL
11	K	33	ILE
11	K	37	LYS
11	K	47	ARG

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Mol	Chain	Res	Type
11	K	51	LEU
11	K	53	ASP
11	K	54	ARG
11	K	85	ASP
11	K	92	ASN
12	L	30	ILE
12	L	33	GLU
12	L	38	LEU
12	L	50	ASP
12	L	55	ILE
12	L	57	LEU
12	L	58	LYS
12	L	61	THR
12	L	64	LEU
12	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	68	GLN
1	A	75	ASN
1	A	83	HIS
1	A	119	ASN
1	A	209	ASN
1	A	225	ASN
1	A	273	ASN
1	A	281	HIS
1	A	297	GLN
1	A	299	HIS
1	A	316	GLN
1	A	358	ASN
1	A	363	GLN
1	A	397	ASN
1	A	399	HIS
1	A	445	ASN
1	A	447	GLN
1	A	471	ASN
1	A	488	ASN
1	A	517	ASN
1	A	545	GLN
1	A	548	ASN

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Mol	Chain	Res	Type
1	A	589	GLN
1	A	626	ASN
1	A	631	HIS
1	A	654	ASN
1	A	698	GLN
1	A	741	ASN
1	A	757	ASN
1	A	767	GLN
1	A	786	HIS
1	A	881	GLN
1	A	903	ASN
1	A	1008	GLN
1	A	1009	ASN
1	A	1048	ASN
1	A	1128	GLN
1	A	1188	GLN
1	A	1232	ASN
1	A	1312	ASN
1	A	1330	ASN
1	A	1354	ASN
1	A	1364	ASN
1	A	1387	HIS
2	B	103	ASN
2	B	110	HIS
2	B	115	GLN
2	B	121	ASN
2	B	178	ASN
2	B	206	ASN
2	B	215	GLN
2	B	224	GLN
2	B	300	HIS
2	B	325	GLN
2	B	366	GLN
2	B	465	ASN
2	B	481	GLN
2	B	484	ASN
2	B	499	ASN
2	B	515	HIS
2	B	516	ASN
2	B	538	ASN
2	B	590	HIS
2	B	592	ASN

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Mol	Chain	Res	Type
2	B	657	HIS
2	B	744	HIS
2	B	770	GLN
2	B	784	ASN
2	B	786	ASN
2	B	842	ASN
2	B	843	GLN
2	B	862	GLN
2	B	1025	HIS
2	B	1062	HIS
2	B	1161	HIS
2	B	1178	ASN
2	B	1179	GLN
2	B	1193	GLN
2	B	1211	ASN
3	C	24	ASN
3	C	54	ASN
3	C	91	HIS
3	C	102	GLN
3	C	112	ASN
3	C	167	HIS
3	C	184	ASN
3	C	195	GLN
3	C	203	GLN
3	C	231	ASN
4	D	41	GLN
5	E	5	ASN
5	E	61	GLN
5	E	63	ASN
5	E	147	HIS
7	G	57	GLN
7	G	102	GLN
7	G	122	ASN
8	H	133	ASN
9	I	11	ASN
9	I	12	ASN
9	I	51	ASN
9	I	83	ASN
11	K	29	ASN
11	K	44	ASN
11	K	65	HIS
11	K	76	GLN

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Mol	Chain	Res	Type
11	K	92	ASN
11	K	104	ASN
11	K	112	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	1

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	3.44

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	1416/1733 (81%)	0.35	52 (3%) 45 38	118, 185, 242, 274	0
2	B	1097/1224 (89%)	0.45	57 (5%) 33 31	111, 200, 254, 282	0
3	C	266/318 (83%)	0.24	1 (0%) 88 77	139, 193, 237, 271	0
4	D	177/221 (80%)	0.63	11 (6%) 26 28	149, 199, 250, 261	0
5	E	214/215 (99%)	0.49	11 (5%) 33 32	153, 223, 267, 279	0
6	F	84/155 (54%)	0.32	3 (3%) 46 39	113, 165, 217, 239	0
7	G	171/171 (100%)	0.26	5 (2%) 53 43	157, 188, 230, 261	0
8	H	133/146 (91%)	0.65	13 (9%) 13 17	185, 229, 254, 261	0
9	I	119/122 (97%)	0.60	8 (6%) 24 26	185, 233, 264, 271	0
10	J	65/70 (92%)	0.31	4 (6%) 26 28	148, 173, 225, 245	0
11	K	115/120 (95%)	0.33	2 (1%) 69 55	140, 182, 230, 246	0
12	L	46/70 (65%)	1.02	10 (21%) 2 6	153, 242, 260, 266	0
13	X	113/594 (19%)	1.25	25 (22%) 2 6	232, 271, 294, 295	0
All	All	4016/5159 (77%)	0.43	202 (5%) 34 32	111, 196, 260, 295	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	335	GLY	6.9
4	D	4	SER	6.6
7	G	51	TYR	4.6
13	X	260	ALA	4.6
13	X	228	ASP	4.4
1	A	57	ARG	4.4
2	B	134	LYS	4.4
13	X	333	ASN	4.3
2	B	715	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	159	THR	4.2
5	E	121	MET	4.2
1	A	1080	THR	4.1
12	L	26	THR	4.1
2	B	1130	PHE	4.1
11	K	115	ALA	4.1
2	B	246	LYS	4.0
2	B	70	ILE	4.0
13	X	280	HIS	4.0
2	B	882	THR	3.8
13	X	347	ASP	3.8
6	F	113	GLY	3.7
1	A	1254	ALA	3.7
1	A	1455	PRO	3.6
2	B	436	VAL	3.6
1	A	1243	VAL	3.6
8	H	132	LEU	3.6
1	A	1187	GLN	3.5
8	H	136	LYS	3.5
12	L	32	ALA	3.5
2	B	591	ARG	3.4
9	I	119	THR	3.4
12	L	25	ALA	3.4
11	K	114	LEU	3.3
2	B	108	VAL	3.3
9	I	117	LYS	3.2
8	H	78	SER	3.2
5	E	123	LEU	3.2
9	I	52	ILE	3.2
2	B	509	ALA	3.2
1	A	145	LYS	3.2
2	B	408	LEU	3.1
2	B	726	ALA	3.1
2	B	736	THR	3.1
2	B	250	PHE	3.1
1	A	1109	LYS	3.1
4	D	205	ASP	3.1
2	B	467	GLY	3.0
6	F	72	LYS	3.0
13	X	231	SER	3.0
4	D	18	VAL	2.9
10	J	1	MET	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	243	ALA	2.9
13	X	285	GLU	2.9
1	A	176	LYS	2.9
5	E	103	LYS	2.9
4	D	70	PHE	2.9
8	H	106	GLU	2.9
8	H	50	ALA	2.8
8	H	63	LEU	2.8
2	B	251	ILE	2.8
1	A	897	TYR	2.8
2	B	919	SER	2.8
1	A	195	ASP	2.8
1	A	589	GLN	2.8
1	A	752	LYS	2.8
1	A	1317	MET	2.8
2	B	248	SER	2.8
2	B	881	ASN	2.7
1	A	2	VAL	2.7
4	D	12	ARG	2.7
1	A	552	TRP	2.7
13	X	256	GLU	2.7
4	D	66	ARG	2.7
2	B	164	LYS	2.7
1	A	893	PHE	2.7
2	B	1120	GLU	2.7
9	I	3	THR	2.7
12	L	27	LEU	2.7
2	B	649	LYS	2.6
5	E	124	VAL	2.6
9	I	61	ASP	2.6
1	A	480	ALA	2.6
2	B	813	LYS	2.6
2	B	883	LEU	2.6
2	B	918	ILE	2.6
13	X	252	PHE	2.5
1	A	1234	GLU	2.5
7	G	117	GLN	2.5
13	X	276	GLN	2.5
13	X	284	GLU	2.5
5	E	50	MET	2.5
13	X	274	ILE	2.5
2	B	345	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
12	L	49	LYS	2.5
1	A	198	GLU	2.5
1	A	1003	LYS	2.5
10	J	65	PRO	2.5
1	A	1287	TYR	2.5
1	A	1112	LYS	2.5
1	A	1258	HIS	2.5
1	A	69	THR	2.4
2	B	478	GLY	2.4
13	X	258	ILE	2.4
2	B	461	LEU	2.4
1	A	538	ASP	2.4
4	D	189	ASP	2.4
9	I	102	VAL	2.4
2	B	680	THR	2.4
1	A	251	SER	2.4
1	A	999	VAL	2.4
8	H	133	ASN	2.4
2	B	725	PRO	2.3
7	G	137	ILE	2.3
4	D	14	ARG	2.3
1	A	333	GLU	2.3
5	E	57	MET	2.3
1	A	199	LEU	2.3
8	H	51	ALA	2.3
13	X	365	VAL	2.3
5	E	93	MET	2.3
5	E	126	SER	2.3
2	B	712	PRO	2.3
1	A	636	GLU	2.3
1	A	309	ALA	2.3
1	A	252	PHE	2.3
2	B	545	ILE	2.3
2	B	584	GLY	2.3
1	A	569	LYS	2.3
2	B	1183	LYS	2.3
1	A	1107	VAL	2.3
1	A	1255	GLU	2.3
1	A	147	VAL	2.3
4	D	13	ARG	2.3
13	X	339	ASN	2.2
13	X	251	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	314	LEU	2.2
2	B	642	ASP	2.2
2	B	958	GLN	2.2
2	B	553	PRO	2.2
3	C	218	PRO	2.2
1	A	1081	LEU	2.2
8	H	139	ASN	2.2
2	B	267	ARG	2.2
1	A	179	LEU	2.2
2	B	264	SER	2.2
1	A	1093	LYS	2.2
5	E	4	GLU	2.2
2	B	33	VAL	2.2
5	E	88	VAL	2.2
12	L	42	ARG	2.2
1	A	197	PRO	2.2
13	X	312	ASN	2.2
4	D	159	THR	2.2
5	E	91	LYS	2.2
13	X	275	SER	2.2
12	L	70	ARG	2.2
1	A	258	GLY	2.1
1	A	112	LYS	2.1
13	X	337	ASN	2.1
12	L	43	THR	2.1
8	H	2	SER	2.1
1	A	1217	LYS	2.1
10	J	64	ASN	2.1
13	X	281	ASN	2.1
2	B	98	THR	2.1
4	D	21	GLU	2.1
2	B	227	LYS	2.1
13	X	346	PRO	2.1
1	A	635	ARG	2.1
2	B	249	ARG	2.1
7	G	153	GLN	2.1
1	A	1357	ALA	2.1
9	I	56	ALA	2.1
10	J	44	TYR	2.1
13	X	300	LYS	2.1
2	B	870	ILE	2.1
1	A	1288	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	347	LYS	2.1
8	H	3	ASN	2.1
12	L	45	ALA	2.1
8	H	13	SER	2.1
6	F	76	LYS	2.1
13	X	239	TYR	2.1
2	B	1224	PHE	2.1
2	B	437	GLU	2.1
12	L	39	SER	2.1
2	B	533	CYS	2.0
9	I	50	THR	2.0
2	B	132	VAL	2.0
2	B	619	ILE	2.0
2	B	658	ILE	2.0
13	X	324	HIS	2.0
1	A	1320	PRO	2.0
2	B	561	TRP	2.0
13	X	327	GLU	2.0
1	A	1000	LEU	2.0
2	B	645	SER	2.0
2	B	646	LEU	2.0
1	A	521	MET	2.0
7	G	33	GLU	2.0
8	H	19	ARG	2.0
1	A	984	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	A	2458	1/1	0.69	0.19	130,130,130,130	0
14	ZN	L	1071	1/1	0.94	0.07	266,266,266,266	0
14	ZN	I	1121	1/1	0.98	0.09	230,230,230,230	0
14	ZN	A	2456	1/1	0.99	0.06	181,181,181,181	0
14	ZN	I	1122	1/1	0.99	0.02	245,245,245,245	0
14	ZN	B	2225	1/1	1.00	0.04	96,96,96,96	0
14	ZN	J	1066	1/1	1.00	0.06	192,192,192,192	0
14	ZN	C	1269	1/1	1.00	0.07	140,140,140,140	0
14	ZN	A	2457	1/1	1.00	0.06	105,105,105,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.