



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:07 PM UTC

PDB ID : 2E2J / pdb_00002e2j
Title : RNA polymerase II elongation complex in 5 mM Mg+2 with GMPCPP
Authors : Wang, D.; Bushnell, D.A.; Westover, K.D.; Kaplan, C.D.; Kornberg, R.D.
Deposited on : 2006-11-14
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

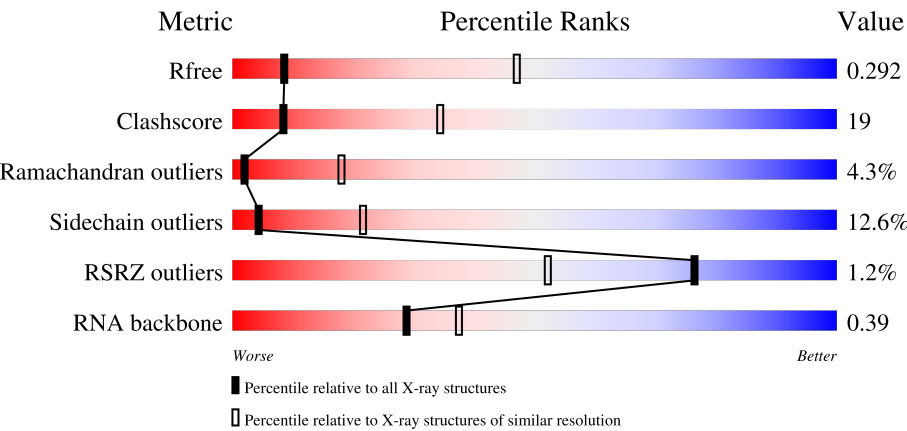
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	9	11% 67%11%11%11%
2	T	27	4% 70%30%
3	N	13	92%8%
4	A	1733	% 48%26%6%20%

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Mol	Chain	Length	Quality of chain
5	B	1224	
6	C	318	
7	E	215	
8	F	155	
9	H	146	
10	I	122	
11	J	70	
12	K	120	
13	L	70	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29206 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 RNA chain called 5'-R(P*AP*UP*CP*GP*AP*GP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	9	Total	C	N	O	P	0	0	0
			199	88	40	62	9			

- Molecule 2 is a DNA chain called 27-MER DNA template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	27	Total	C	N	O	P	0	0	0
			546	261	102	157	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	13	Total	C	N	O	P	0	0	0
			266	127	44	82	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase II largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1395	Total	C	N	O	S	0	0	0
			10969	6917	1923	2068	61			

- Molecule 5 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1105	Total	C	N	O	S	0	0	0
			8782	5560	1537	1630	55			

- Molecule 6 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	86	Total	C	N	O	S	0	0	0
			696	445	118	130	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

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

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit 9.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

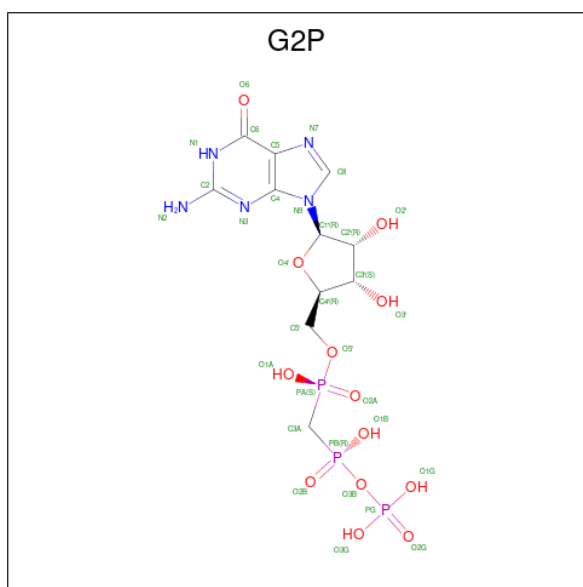
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypep-

tide.

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

- Molecule 14 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: G2P) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	T	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

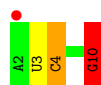
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	2	Total 2	Mg 2	0	0

3 Residue-property plots [i](#)

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: 5'-R(P*AP*UP*CP*GP*AP*GP*AP*GP*G)-3'



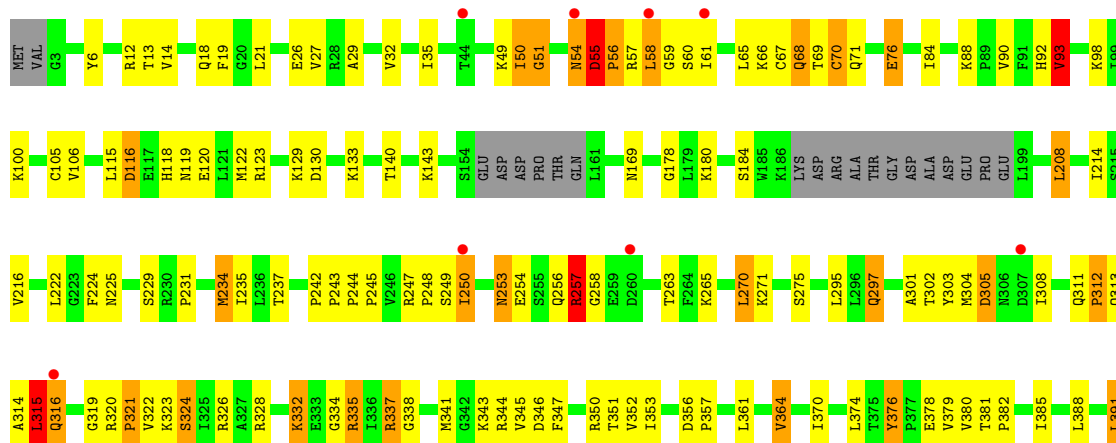
- Molecule 2: 27-MER DNA template strand



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



- Molecule 4: DNA-directed RNA polymerase II largest subunit

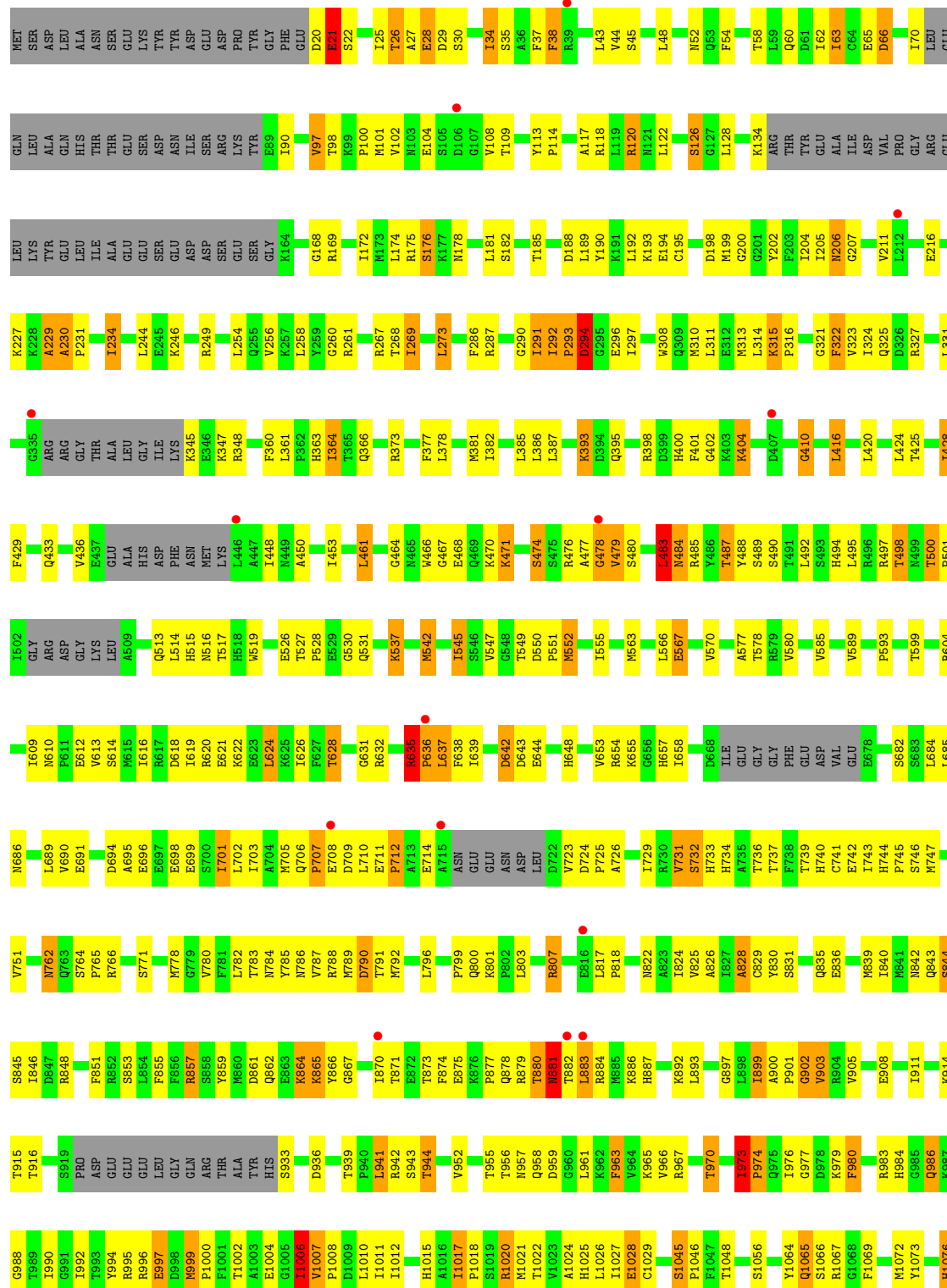




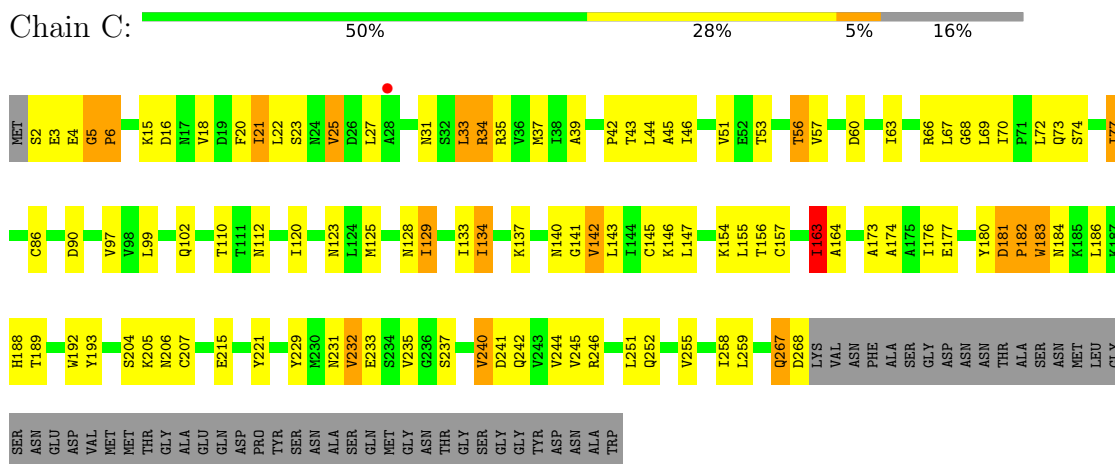
SER
PRO
GLY
SER
LEU
PRO
ALA
TYR
SER
PRO
GLY
LYS
GLN
ASP
GLU
GLN
LYS
HIS
ASN
GLU
ASN
GLU
SER
ARG

● Molecule 5: DNA-directed RNA polymerase II 140 kDa polypeptide

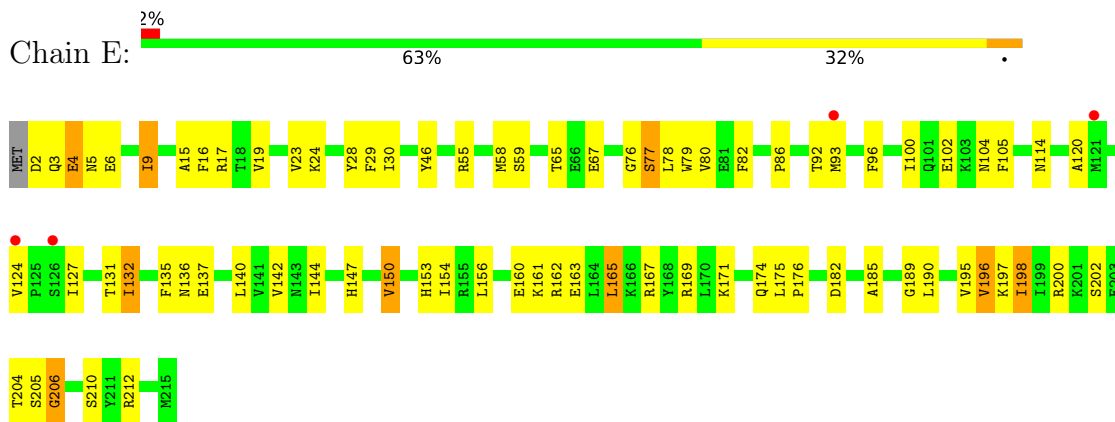
Chain B: 



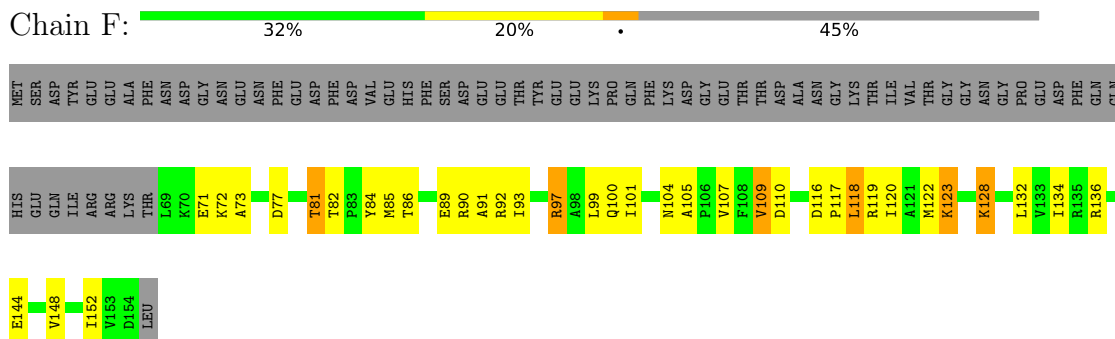
- Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide



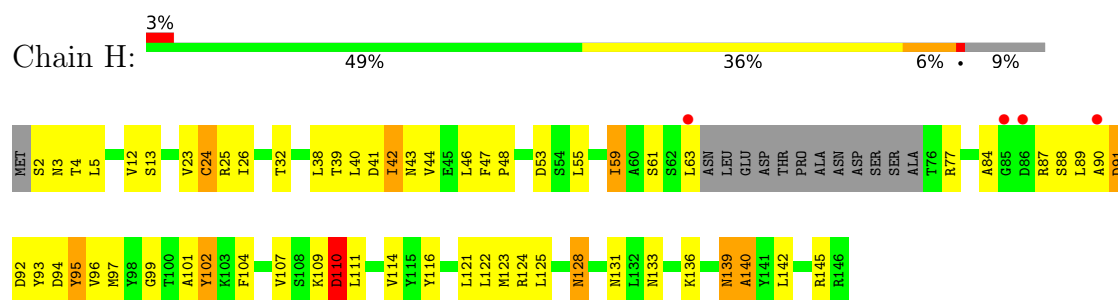
- Molecule 7: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide



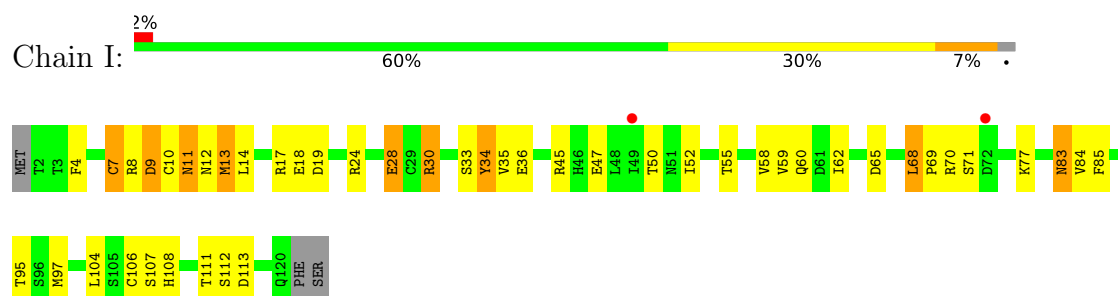
- Molecule 8: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



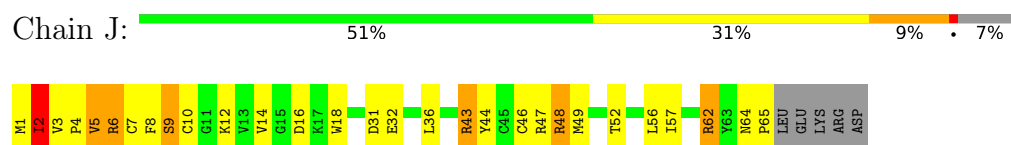
- Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



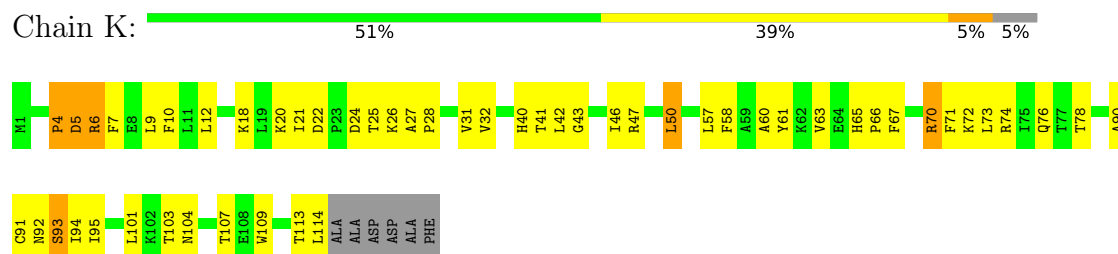
- Molecule 10: DNA-directed RNA polymerase II subunit 9



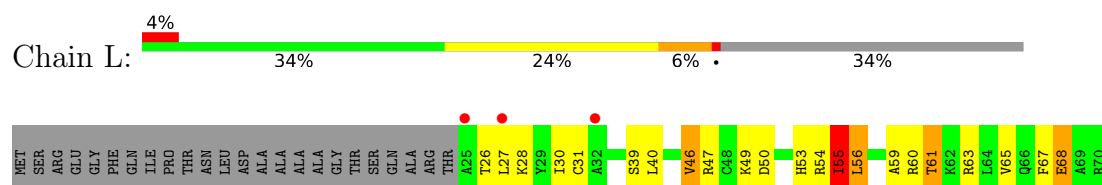
- Molecule 11: DNA-directed RNA polymerases I/II/III subunit 10



- Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide



- Molecule 13: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.14Å 222.02Å 194.65Å 90.00° 101.36° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50 50.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	94.5 (50.00-3.50) 94.6 (50.00-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.242 , 0.306 0.242 , 0.292	Depositor DCC
R_{free} test set	2511 reflections (2.83%)	wwPDB-VP
Wilson B-factor (Å ²)	101.1	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	29206	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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, G2P

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	R	0.70	0/223	1.26	1/345 (0.3%)
2	T	0.41	0/612	1.07	2/941 (0.2%)
3	N	0.37	0/296	1.08	2/453 (0.4%)
4	A	0.75	1/11163 (0.0%)	1.02	23/15091 (0.2%)
5	B	0.78	1/8952 (0.0%)	1.02	20/12071 (0.2%)
6	C	0.73	0/2139	0.99	3/2899 (0.1%)
7	E	0.68	0/1788	0.93	2/2406 (0.1%)
8	F	0.67	0/708	0.91	0/956
9	H	0.69	0/1086	0.95	4/1470 (0.3%)
10	I	0.79	0/989	0.96	2/1331 (0.2%)
11	J	0.78	0/541	0.98	0/727
12	K	0.74	0/937	0.99	0/1265
13	L	0.86	0/365	0.98	0/485
All	All	0.75	2/29799 (0.0%)	1.01	59/40440 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	3
5	B	0	4
6	C	0	1
9	H	1	1
11	J	0	1
All	All	1	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	250	ILE	CA-CB	7.40	1.61	1.54
5	B	882	THR	CA-CB	5.16	1.61	1.53

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	882	THR	N-CA-C	7.97	119.75	111.14
6	C	5	GLY	CA-C-N	7.55	129.28	119.84
6	C	5	GLY	C-N-CA	7.55	129.28	119.84
1	R	10	G	C5'-C4'-C3'	-7.05	105.42	116.00
4	A	513	SER	CA-C-N	6.99	127.58	119.47
4	A	513	SER	C-N-CA	6.99	127.58	119.47
5	B	1045	SER	CA-C-N	6.80	126.59	119.05
5	B	1045	SER	C-N-CA	6.80	126.59	119.05
5	B	296	GLU	N-CA-C	-6.75	104.86	113.23
6	C	163	ILE	N-CA-C	6.73	118.49	108.46
10	I	68	LEU	CA-C-N	6.65	128.15	119.84
10	I	68	LEU	C-N-CA	6.65	128.15	119.84
4	A	404	TYR	N-CA-C	6.61	118.83	110.24
9	H	92	ASP	N-CA-C	-6.47	105.25	113.02
4	A	888	GLY	N-CA-C	6.46	121.04	112.65
2	T	25	DG	C1'-O4'-C4'	-6.30	100.25	109.70
4	A	247	ARG	CA-C-N	6.20	127.58	119.84
4	A	247	ARG	C-N-CA	6.20	127.58	119.84
5	B	1006	ILE	CB-CA-C	-6.08	104.64	111.45
4	A	463	ILE	CA-C-N	5.96	125.93	120.21
4	A	463	ILE	C-N-CA	5.96	125.93	120.21
5	B	273	LEU	CA-C-N	5.95	125.89	119.76
5	B	273	LEU	C-N-CA	5.95	125.89	119.76
4	A	1311	VAL	N-CA-C	5.87	116.46	107.77
5	B	1007	VAL	N-CA-C	-5.83	104.41	109.19
5	B	410	GLY	CA-C-N	5.83	127.12	119.84
5	B	410	GLY	C-N-CA	5.83	127.12	119.84
3	N	12	DG	O4'-C1'-N9	5.83	117.14	108.40
5	B	66	ASP	N-CA-C	-5.82	105.84	113.17
4	A	242	PRO	CA-C-N	5.78	126.33	120.38
4	A	242	PRO	C-N-CA	5.78	126.33	120.38
4	A	376	TYR	CA-C-N	5.76	127.05	119.84
4	A	376	TYR	C-N-CA	5.76	127.05	119.84
4	A	886	ILE	N-CA-C	5.76	115.95	110.42
9	H	91	ASP	N-CA-C	5.69	117.50	107.61
4	A	55	ASP	CA-C-N	5.58	126.81	119.84
4	A	55	ASP	C-N-CA	5.58	126.81	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	624	SER	N-CA-C	-5.47	107.17	112.97
5	B	269	ILE	CB-CA-C	-5.46	105.03	111.09
5	B	635	ARG	C-N-CD	-5.41	102.81	125.00
4	A	567	LYS	CA-C-N	5.34	126.52	119.84
4	A	567	LYS	C-N-CA	5.34	126.52	119.84
4	A	455	MET	CB-CG-SD	-5.26	96.93	112.70
2	T	25	DG	O4'-C1'-N9	5.20	116.20	108.40
4	A	88	LYS	CA-C-N	5.20	126.34	119.84
4	A	88	LYS	C-N-CA	5.20	126.34	119.84
9	H	99	GLY	N-CA-C	5.14	118.72	111.42
5	B	881	ASN	CA-C-N	5.12	127.40	120.44
5	B	881	ASN	C-N-CA	5.12	127.40	120.44
3	N	12	DG	C3'-C2'-C1'	-5.11	93.93	101.60
4	A	725	ALA	N-CA-C	-5.10	107.61	113.88
5	B	723	VAL	N-CA-C	5.07	115.20	108.11
5	B	616	ILE	CB-CA-C	-5.05	104.17	111.19
7	E	182	ASP	CA-C-N	5.04	125.06	119.32
7	E	182	ASP	C-N-CA	5.04	125.06	119.32
5	B	973	ILE	CA-C-N	5.03	126.12	119.84
5	B	973	ILE	C-N-CA	5.03	126.12	119.84
9	H	59	ILE	N-CA-C	5.02	116.20	111.48
5	B	734	HIS	N-CA-C	5.02	118.53	111.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	H	110	ASP	CA

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1392	SER	Peptide
4	A	257	ARG	Peptide
4	A	258	GLY	Peptide
5	B	1065	GLN	Peptide
5	B	293	PRO	Peptide
5	B	478	GLY	Peptide
5	B	828	ALA	Peptide
6	C	20	PHE	Peptide
9	H	110	ASP	Peptide
11	J	4	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	199	0	98	4	0
2	T	546	0	304	5	0
3	N	266	0	149	0	0
4	A	10969	0	11067	437	0
5	B	8782	0	8816	435	0
6	C	2101	0	2056	93	0
7	E	1752	0	1776	50	0
8	F	696	0	720	34	0
9	H	1068	0	1040	52	0
10	I	971	0	927	29	0
11	J	532	0	542	43	0
12	K	919	0	929	41	0
13	L	363	0	386	10	0
14	T	32	0	14	1	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	A	2	0	0	0	0
All	All	29206	0	28824	1108	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1108) 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)
9:H:109:LYS:HB3	9:H:110:ASP:CA	1.54	1.34
9:H:109:LYS:CB	9:H:110:ASP:HA	1.49	1.31
4:A:399:HIS:CB	4:A:400:PRO:HD3	1.65	1.27
5:B:635:ARG:CG	5:B:636:PRO:HD2	1.65	1.24
4:A:567:LYS:CB	4:A:568:PRO:HD2	1.73	1.18
5:B:637:LEU:CD2	5:B:742:GLU:OE2	1.93	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:567:LYS:HB2	4:A:568:PRO:CD	1.74	1.15
7:E:3:GLN:HA	7:E:4:GLU:HB2	1.28	1.15
4:A:399:HIS:HB3	4:A:400:PRO:CD	1.76	1.14
4:A:899:VAL:HB	4:A:929:LEU:HD11	1.31	1.11
11:J:64:ASN:HB3	11:J:65:PRO:HD3	1.29	1.11
4:A:315:LEU:HB2	4:A:316:GLN:CA	1.81	1.10
5:B:636:PRO:HB2	5:B:637:LEU:HB3	1.34	1.09
5:B:637:LEU:HD23	5:B:742:GLU:OE2	1.52	1.09
4:A:315:LEU:HB2	4:A:316:GLN:HA	1.08	1.08
4:A:399:HIS:CG	4:A:400:PRO:HD3	1.89	1.07
4:A:399:HIS:HB3	4:A:400:PRO:HD3	1.09	1.05
4:A:315:LEU:CB	4:A:316:GLN:HA	1.84	1.05
4:A:455:MET:SD	5:B:1137:CYS:HB2	1.97	1.05
5:B:864:LYS:HB2	5:B:865:LYS:HA	1.38	1.03
4:A:353:ILE:HD13	4:A:487:MET:HE3	1.37	1.02
5:B:637:LEU:HD22	5:B:742:GLU:HA	1.42	1.00
5:B:636:PRO:CB	5:B:637:LEU:HB3	1.91	1.00
4:A:1364:ASN:ND2	4:A:1366:ARG:HG2	1.76	0.99
5:B:636:PRO:HB2	5:B:637:LEU:CB	1.93	0.97
5:B:635:ARG:HG3	5:B:636:PRO:HD2	1.44	0.97
4:A:668:ASP:HB3	4:A:743:VAL:HG23	1.47	0.95
5:B:292:ILE:H	5:B:293:PRO:HD2	1.29	0.95
4:A:315:LEU:CB	4:A:316:GLN:CA	2.41	0.95
5:B:205:ILE:HG22	5:B:206:ASN:ND2	1.82	0.94
5:B:635:ARG:CB	5:B:636:PRO:HD2	2.00	0.92
5:B:636:PRO:CB	5:B:637:LEU:CA	2.48	0.92
4:A:567:LYS:HB3	9:H:96:VAL:H	1.34	0.91
4:A:351:THR:HG22	4:A:352:VAL:N	1.86	0.90
5:B:269:ILE:HD11	5:B:386:LEU:HD21	1.52	0.90
5:B:636:PRO:HB3	5:B:637:LEU:HA	1.54	0.89
6:C:66:ARG:NH2	11:J:3:VAL:O	2.06	0.89
4:A:1364:ASN:HD21	4:A:1366:ARG:HH11	1.16	0.89
5:B:216:GLU:HB3	5:B:500:THR:HG23	1.54	0.86
5:B:824:ILE:HG12	11:J:48:ARG:HH12	1.40	0.86
5:B:636:PRO:CB	5:B:637:LEU:HA	2.05	0.85
5:B:848:ARG:HH22	5:B:996:ARG:NH1	1.72	0.85
4:A:1015:VAL:HG12	4:A:1019:CYS:SG	2.14	0.85
5:B:25:ILE:HD11	5:B:653:VAL:HB	1.57	0.85
4:A:633:VAL:HG11	4:A:645:LEU:HD22	1.58	0.85
4:A:455:MET:SD	5:B:1137:CYS:CB	2.65	0.84
4:A:1242:VAL:HG12	4:A:1243:VAL:H	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:72:LYS:HG3	8:F:73:ALA:H	1.41	0.84
5:B:549:THR:HG22	5:B:550:ASP:H	1.43	0.83
5:B:865:LYS:CG	5:B:866:TYR:HA	2.09	0.82
5:B:37:PHE:O	5:B:38:PHE:HB2	1.76	0.82
5:B:635:ARG:O	5:B:636:PRO:O	1.97	0.82
6:C:123:ASN:ND2	6:C:125:MET:HG2	1.95	0.82
4:A:573:SER:H	4:A:576:GLN:HG3	1.45	0.82
5:B:995:ARG:HB3	5:B:997:GLU:OE2	1.80	0.82
4:A:1161:THR:HG22	4:A:1163:ILE:H	1.43	0.81
4:A:518:LYS:HB2	4:A:519:PRO:HD2	1.62	0.81
4:A:1338:VAL:HG12	4:A:1339:LEU:HD23	1.60	0.81
12:K:26:LYS:HA	12:K:27:ALA:HB3	1.60	0.81
10:I:111:THR:HG22	10:I:113:ASP:H	1.45	0.81
5:B:635:ARG:CB	5:B:636:PRO:CD	2.58	0.81
10:I:59:VAL:HG12	10:I:60:GLN:H	1.44	0.81
4:A:1370:LEU:O	4:A:1374:VAL:HG23	1.80	0.80
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.63	0.80
4:A:351:THR:CG2	4:A:352:VAL:N	2.42	0.80
5:B:636:PRO:CB	5:B:637:LEU:CB	2.55	0.80
7:E:198:ILE:HD11	7:E:212:ARG:HG3	1.64	0.80
4:A:873:MET:HG2	4:A:957:PRO:HG3	1.64	0.80
5:B:635:ARG:HG2	5:B:636:PRO:HD2	1.62	0.79
4:A:666:ILE:HG23	5:B:1026:LEU:HB3	1.64	0.79
4:A:824:LEU:HD21	5:B:765:PRO:HB3	1.64	0.79
9:H:84:ALA:HA	9:H:87:ARG:HB2	1.64	0.79
5:B:865:LYS:CB	5:B:866:TYR:HA	2.14	0.78
4:A:567:LYS:HB2	4:A:568:PRO:HD2	0.84	0.78
5:B:857:ARG:HG3	5:B:857:ARG:HH11	1.49	0.77
4:A:1394:THR:HG21	4:A:1398:MET:HE3	1.65	0.77
6:C:45:ALA:HA	6:C:72:LEU:HD12	1.65	0.77
7:E:3:GLN:HB3	7:E:5:ASN:H	1.50	0.76
4:A:1364:ASN:ND2	4:A:1366:ARG:CG	2.48	0.76
5:B:325:GLN:HE22	10:I:12:ASN:ND2	1.84	0.76
12:K:6:ARG:HH11	12:K:6:ARG:HB3	1.51	0.76
4:A:467:THR:HG23	5:B:976:ILE:HG23	1.68	0.75
4:A:858:ASN:C	4:A:858:ASN:HD22	1.94	0.75
5:B:286:PHE:HB3	5:B:297:ILE:HD12	1.67	0.75
5:B:1147:LEU:O	5:B:1147:LEU:HD22	1.86	0.75
5:B:780:VAL:HG12	5:B:817:LEU:HD23	1.68	0.75
8:F:109:VAL:HG11	8:F:123:LYS:HG2	1.68	0.75
5:B:1028:GLU:HG2	5:B:1090:THR:HG23	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.69	0.74
5:B:824:ILE:HG12	11:J:48:ARG:NH1	2.03	0.74
11:J:3:VAL:HG21	11:J:18:TRP:HB2	1.68	0.74
5:B:313:MET:HE3	5:B:386:LEU:HD22	1.68	0.74
4:A:672:ASP:HB3	4:A:675:THR:OG1	1.88	0.73
4:A:477:PRO:HG3	4:A:521:MET:HE2	1.69	0.73
6:C:2:SER:N	6:C:3:GLU:HB3	2.02	0.73
4:A:567:LYS:NZ	9:H:43:ASN:HB3	2.02	0.73
5:B:200:GLY:HA2	5:B:202:TYR:CE2	2.24	0.72
5:B:292:ILE:N	5:B:293:PRO:HD2	2.04	0.72
5:B:778:MET:HE1	5:B:1094:ARG:HH11	1.52	0.72
4:A:875:ALA:HB2	4:A:1366:ARG:HD2	1.71	0.72
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.71	0.72
4:A:399:HIS:CG	4:A:400:PRO:CD	2.68	0.72
4:A:628:GLY:O	4:A:632:VAL:HG23	1.89	0.72
4:A:794:PRO:HD2	4:A:795:GLU:OE2	1.90	0.72
5:B:1159:ARG:HD3	5:B:1193:GLN:HG3	1.72	0.71
5:B:637:LEU:HD13	5:B:741:CYS:O	1.89	0.71
6:C:255:VAL:O	6:C:258:ILE:HG22	1.90	0.71
5:B:851:PHE:HB3	5:B:1094:ARG:HD2	1.72	0.71
11:J:8:PHE:H	11:J:49:MET:HE3	1.53	0.71
5:B:636:PRO:HB3	5:B:637:LEU:CA	2.19	0.71
9:H:109:LYS:CB	9:H:110:ASP:CA	2.30	0.71
6:C:69:LEU:HD12	11:J:6:ARG:HD3	1.74	0.70
5:B:292:ILE:H	5:B:293:PRO:CD	2.04	0.70
6:C:99:LEU:HB2	6:C:157:CYS:HB2	1.73	0.70
5:B:619:ILE:HG13	10:I:65:ASP:HB2	1.71	0.70
4:A:208:LEU:O	4:A:208:LEU:HD22	1.91	0.70
13:L:55:ILE:O	13:L:56:LEU:HB2	1.90	0.70
4:A:666:ILE:HG23	5:B:1026:LEU:CB	2.22	0.70
5:B:29:ASP:HB3	5:B:658:ILE:HD13	1.74	0.70
5:B:839:MET:HE3	5:B:1010:LEU:HD21	1.72	0.70
11:J:10:CYS:SG	11:J:43:ARG:HD2	2.31	0.70
4:A:265:LYS:NZ	4:A:322:VAL:HB	2.07	0.69
4:A:353:ILE:HD13	4:A:487:MET:CE	2.16	0.69
4:A:21:LEU:HD12	4:A:229:SER:HB2	1.74	0.69
4:A:573:SER:O	4:A:576:GLN:HB2	1.92	0.69
4:A:1441:PHE:CZ	8:F:89:GLU:HA	2.28	0.68
5:B:654:ARG:H	5:B:657:HIS:HD2	1.39	0.68
5:B:859:TYR:OH	5:B:941:LEU:HD23	1.93	0.68
6:C:51:VAL:HG22	6:C:155:LEU:CD2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1364:ASN:HD22	4:A:1366:ARG:CG	2.07	0.68
10:I:34:TYR:HE2	10:I:36:GLU:HG3	1.59	0.68
5:B:800:GLN:HG2	11:J:52:THR:HG22	1.76	0.68
5:B:1187:ASN:HD21	5:B:1190:ASP:H	1.42	0.68
5:B:635:ARG:O	5:B:636:PRO:C	2.37	0.67
4:A:1273:LEU:O	4:A:1274:ARG:HB3	1.93	0.67
5:B:1084:GLN:NE2	6:C:192:TRP:H	1.91	0.67
4:A:265:LYS:HZ2	4:A:322:VAL:HB	1.59	0.67
5:B:839:MET:CE	5:B:1010:LEU:HD21	2.24	0.67
6:C:67:LEU:HA	6:C:70:ILE:HD12	1.77	0.67
10:I:34:TYR:CE2	10:I:36:GLU:HG3	2.30	0.67
9:H:47:PHE:HB3	9:H:95:TYR:HD1	1.58	0.67
4:A:821:ARG:O	4:A:825:ILE:HG12	1.94	0.67
9:H:47:PHE:HB3	9:H:95:TYR:CD1	2.30	0.67
11:J:3:VAL:HG21	11:J:18:TRP:CB	2.24	0.67
4:A:482:PHE:CD1	5:B:836:GLU:HB2	2.30	0.67
5:B:494:HIS:HD2	5:B:497:ARG:NH1	1.93	0.67
5:B:1076:HIS:CD2	12:K:40:HIS:NE2	2.62	0.67
7:E:3:GLN:CA	7:E:4:GLU:HB2	2.17	0.67
4:A:1394:THR:CG2	4:A:1398:MET:HE3	2.24	0.67
9:H:63:LEU:C	9:H:90:ALA:HB3	2.20	0.67
4:A:855:THR:CG2	4:A:857:ARG:HE	2.08	0.66
6:C:142:VAL:H	11:J:16:ASP:HB3	1.59	0.66
5:B:211:VAL:O	5:B:480:SER:HA	1.95	0.66
5:B:325:GLN:HE22	10:I:12:ASN:HD21	1.42	0.66
5:B:803:LEU:H	5:B:822:ASN:HD21	1.42	0.66
5:B:986:GLN:HE21	5:B:1022:THR:HG21	1.58	0.66
11:J:64:ASN:HB3	11:J:65:PRO:CD	2.17	0.66
4:A:1189:SER:OG	4:A:1190:PRO:HD2	1.94	0.66
4:A:315:LEU:CB	4:A:316:GLN:C	2.68	0.66
4:A:446:ARG:HG2	4:A:447:GLN:N	2.09	0.66
5:B:911:ILE:HD11	5:B:941:LEU:HG	1.76	0.66
9:H:109:LYS:HD2	9:H:111:LEU:HG	1.77	0.66
5:B:464:GLY:HA2	5:B:479:VAL:O	1.95	0.66
5:B:287:ARG:NH1	5:B:324:ILE:O	2.29	0.65
5:B:955:THR:HG22	5:B:956:THR:N	2.09	0.65
4:A:457:ALA:O	4:A:507:VAL:HG23	1.96	0.65
4:A:901:LEU:H	4:A:926:GLN:NE2	1.94	0.65
5:B:258:LEU:HB2	5:B:385:LEU:HD21	1.77	0.65
6:C:112:ASN:ND2	6:C:146:LYS:HG2	2.10	0.65
6:C:183:TRP:H	6:C:183:TRP:CD1	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:424:ILE:HD12	4:A:424:ILE:O	1.97	0.65
4:A:1017:LEU:HB2	7:E:205:SER:HA	1.76	0.65
5:B:20:ASP:O	5:B:22:SER:N	2.30	0.65
7:E:19:VAL:O	7:E:23:VAL:HG23	1.97	0.65
4:A:315:LEU:HB2	4:A:316:GLN:C	2.21	0.65
5:B:287:ARG:NH2	5:B:294:ASP:OD2	2.30	0.65
5:B:744:HIS:HD2	5:B:746:SER:OG	1.79	0.65
4:A:55:ASP:H	4:A:56:PRO:HD2	1.62	0.64
4:A:399:HIS:CD2	4:A:400:PRO:HD3	2.31	0.64
4:A:888:GLY:O	4:A:940:ARG:NH2	2.31	0.64
5:B:848:ARG:NH2	5:B:996:ARG:NH1	2.44	0.64
6:C:56:THR:HG21	6:C:145:CYS:SG	2.38	0.64
7:E:6:GLU:O	7:E:9:ILE:HG22	1.98	0.64
9:H:40:LEU:HD13	9:H:123:MET:HE3	1.80	0.64
4:A:658:LEU:HD13	5:B:831:SER:HA	1.80	0.64
6:C:145:CYS:SG	6:C:146:LYS:N	2.71	0.64
11:J:52:THR:HG22	11:J:52:THR:O	1.98	0.64
4:A:672:ASP:H	4:A:736:ASN:HD21	1.46	0.64
4:A:871:ASP:OD1	4:A:1366:ARG:NH2	2.31	0.64
4:A:645:LEU:O	4:A:649:ILE:HG13	1.98	0.64
4:A:392:VAL:HG13	4:A:415:LEU:HD11	1.80	0.63
4:A:545:GLN:HB3	4:A:549:MET:HE3	1.79	0.63
5:B:744:HIS:CD2	5:B:746:SER:OG	2.51	0.63
5:B:999:MET:HG2	5:B:1007:VAL:HG13	1.78	0.63
6:C:133:ILE:HD11	6:C:237:SER:HA	1.78	0.63
5:B:393:LYS:HE3	5:B:393:LYS:HA	1.81	0.63
9:H:5:LEU:HD22	9:H:133:ASN:O	1.97	0.63
5:B:378:LEU:O	5:B:382:ILE:HG12	1.97	0.63
5:B:402:GLY:HA2	5:B:695:ALA:HB3	1.81	0.63
5:B:487:THR:CG2	5:B:488:TYR:N	2.61	0.63
5:B:711:GLU:O	5:B:711:GLU:HG3	1.99	0.63
6:C:57:VAL:HG23	11:J:57:ILE:HD11	1.80	0.63
5:B:612:GLU:O	5:B:632:ARG:NH2	2.31	0.63
5:B:1002:THR:CG2	5:B:1006:ILE:HG12	2.29	0.63
5:B:957:ASN:O	5:B:959:ASP:N	2.31	0.63
11:J:48:ARG:HH21	11:J:49:MET:HE1	1.63	0.63
11:J:8:PHE:N	11:J:49:MET:HE3	2.15	0.62
4:A:466:SER:O	5:B:1103:ILE:HD12	1.99	0.62
6:C:43:THR:HG22	6:C:44:LEU:N	2.14	0.62
2:T:21:DT:OP1	4:A:344:ARG:NH1	2.27	0.62
5:B:1096:ARG:HH11	5:B:1096:ARG:HG2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:26:LYS:CA	12:K:27:ALA:HB3	2.29	0.62
1:R:10:G:O2'	4:A:446:ARG:NH2	2.33	0.62
5:B:1084:GLN:HE22	6:C:192:TRP:H	1.47	0.62
6:C:99:LEU:HD13	6:C:120:ILE:HA	1.81	0.62
10:I:8:ARG:O	10:I:9:ASP:HB2	1.98	0.62
5:B:428:ILE:HD11	5:B:448:ILE:HG12	1.82	0.62
4:A:504:LEU:HD11	8:F:91:ALA:CB	2.29	0.62
5:B:796:LEU:O	5:B:799:PRO:HD3	1.99	0.62
6:C:128:ASN:O	6:C:129:ILE:HD12	2.00	0.62
10:I:59:VAL:HG12	10:I:60:GLN:N	2.13	0.62
5:B:639:ILE:HA	5:B:740:HIS:HB3	1.81	0.62
5:B:865:LYS:HG2	5:B:866:TYR:HA	1.81	0.62
4:A:765:VAL:HG22	4:A:800:VAL:HB	1.81	0.61
4:A:913:LEU:HD12	4:A:915:SER:H	1.65	0.61
4:A:565:ILE:HG23	4:A:567:LYS:HG2	1.82	0.61
8:F:93:ILE:HD11	8:F:134:ILE:HD11	1.82	0.61
4:A:793:SER:HB2	4:A:794:PRO:CD	2.30	0.61
5:B:636:PRO:HB3	5:B:637:LEU:HB3	1.78	0.61
6:C:46:ILE:HD12	6:C:157:CYS:HB3	1.83	0.61
5:B:114:PRO:HG3	5:B:181:LEU:HD21	1.80	0.61
4:A:779:PHE:CE1	4:A:785:PRO:HD3	2.35	0.61
4:A:1134:ILE:O	4:A:1138:ILE:HG12	2.00	0.61
4:A:451:HIS:HB2	4:A:454:SER:HB2	1.83	0.61
5:B:708:GLU:O	5:B:709:ASP:HB2	2.00	0.61
5:B:784:ASN:OD1	5:B:788:ARG:HD2	2.01	0.61
7:E:28:TYR:CE1	7:E:78:LEU:HD13	2.35	0.61
8:F:118:LEU:O	8:F:118:LEU:HD12	2.01	0.61
5:B:542:MET:SD	5:B:747:MET:HE2	2.40	0.61
4:A:12:ARG:HB3	5:B:1218:THR:HG22	1.82	0.61
4:A:350:ARG:HB2	5:B:1128:LEU:HD11	1.83	0.61
4:A:596:THR:C	4:A:598:LEU:H	2.07	0.61
4:A:910:PRO:HA	4:A:916:GLY:HA3	1.82	0.61
5:B:864:LYS:CB	5:B:865:LYS:HA	2.14	0.60
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.36	0.60
4:A:76:GLU:OE2	5:B:1159:ARG:NH1	2.34	0.60
5:B:999:MET:HG2	5:B:1008:PRO:HD2	1.84	0.60
12:K:6:ARG:HB3	12:K:6:ARG:NH1	2.16	0.60
12:K:63:VAL:HG23	12:K:63:VAL:O	2.01	0.60
4:A:853:ASP:OD1	4:A:855:THR:HG22	2.00	0.60
7:E:15:ALA:O	7:E:19:VAL:HG23	2.02	0.60
9:H:38:LEU:HD13	9:H:125:LEU:HD13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:92:HIS:HE1	5:B:1211:ASN:HB3	1.67	0.60
4:A:596:THR:O	4:A:598:LEU:N	2.35	0.60
4:A:981:LEU:HD21	4:A:1039:LYS:HA	1.84	0.60
4:A:407:ARG:HD3	4:A:413:ILE:HD11	1.84	0.59
4:A:1341:ILE:HD13	4:A:1379:GLY:O	2.02	0.59
5:B:310:MET:O	5:B:313:MET:HB2	2.02	0.59
5:B:1002:THR:HG21	5:B:1006:ILE:HG12	1.83	0.59
6:C:186:LEU:HB3	6:C:188:HIS:CD2	2.37	0.59
4:A:382:PRO:HD3	4:A:428:TYR:CE2	2.36	0.59
4:A:1004:ASN:ND2	7:E:167:ARG:HD2	2.17	0.59
5:B:637:LEU:HD22	5:B:742:GLU:CA	2.27	0.59
12:K:4:PRO:O	12:K:5:ASP:C	2.44	0.59
4:A:546:VAL:O	4:A:550:LEU:HD22	2.01	0.59
10:I:45:ARG:HE	10:I:47:GLU:HG3	1.66	0.59
4:A:645:LEU:HD11	4:A:649:ILE:HD11	1.84	0.59
4:A:765:VAL:HG13	4:A:802:ASN:O	2.01	0.59
4:A:567:LYS:HZ1	9:H:43:ASN:HB3	1.64	0.59
5:B:25:ILE:HG23	5:B:29:ASP:HB2	1.83	0.59
5:B:992:ILE:CD1	12:K:67:PHE:HE2	2.16	0.59
7:E:3:GLN:HA	7:E:4:GLU:CB	2.19	0.59
5:B:976:ILE:O	5:B:990:ILE:HB	2.03	0.59
5:B:642:ASP:C	5:B:644:GLU:H	2.10	0.59
4:A:778:GLY:HA3	5:B:516:ASN:HB2	1.85	0.58
5:B:744:HIS:CD2	5:B:746:SER:H	2.20	0.58
4:A:896:ARG:HD2	4:A:897:TYR:CE1	2.38	0.58
5:B:635:ARG:HG3	5:B:635:ARG:HH11	1.68	0.58
6:C:252:GLN:HG3	12:K:95:ILE:HG23	1.84	0.58
5:B:322:PHE:O	5:B:322:PHE:CD1	2.56	0.58
7:E:100:ILE:HG23	7:E:105:PHE:HB2	1.85	0.58
4:A:58:LEU:HD21	4:A:243:PRO:HB3	1.86	0.58
4:A:1424:VAL:HG13	4:A:1436:ILE:HD11	1.83	0.58
6:C:67:LEU:HA	6:C:70:ILE:CD1	2.33	0.58
4:A:672:ASP:H	4:A:736:ASN:ND2	2.02	0.58
4:A:858:ASN:ND2	4:A:860:LEU:H	2.01	0.58
5:B:956:THR:HA	5:B:961:LEU:O	2.02	0.58
5:B:884:ARG:O	5:B:936:ASP:HB3	2.02	0.58
6:C:182:PRO:HB2	6:C:207:CYS:SG	2.44	0.58
4:A:407:ARG:HH11	4:A:413:ILE:HD11	1.69	0.58
4:A:754:SER:H	4:A:757:ASN:HD22	1.51	0.58
5:B:955:THR:CG2	5:B:956:THR:N	2.66	0.58
9:H:47:PHE:CB	9:H:95:TYR:HD1	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:95:TYR:HE2	9:H:97:MET:CG	2.15	0.58
4:A:1436:ILE:O	4:A:1438:THR:N	2.37	0.58
5:B:60:GLN:O	5:B:63:ILE:HG22	2.02	0.58
4:A:1409:LEU:HD13	5:B:1207:LEU:HD21	1.86	0.58
5:B:778:MET:CE	5:B:853:SER:HB3	2.34	0.58
5:B:269:ILE:CD1	5:B:386:LEU:HD21	2.32	0.58
4:A:315:LEU:HB3	4:A:316:GLN:C	2.29	0.57
5:B:784:ASN:CG	5:B:788:ARG:HD2	2.29	0.57
4:A:1436:ILE:O	4:A:1437:GLY:C	2.46	0.57
5:B:635:ARG:HB2	5:B:636:PRO:CD	2.32	0.57
5:B:114:PRO:CG	5:B:181:LEU:HD21	2.34	0.57
5:B:1117:GLN:HE21	5:B:1199:ALA:HB2	1.69	0.57
6:C:134:ILE:HG23	6:C:141:GLY:H	1.68	0.57
4:A:599:SER:C	4:A:601:LYS:H	2.13	0.57
4:A:648:ASN:O	4:A:652:VAL:HG23	2.05	0.57
5:B:373:ARG:HA	5:B:566:LEU:HD23	1.86	0.57
5:B:1002:THR:HG23	5:B:1004:GLU:H	1.69	0.57
4:A:1400:CYS:SG	4:A:1409:LEU:HG	2.45	0.57
5:B:801:LYS:O	11:J:52:THR:HG23	2.04	0.57
7:E:202:SER:OG	7:E:204:THR:HG22	2.05	0.57
8:F:101:ILE:HD13	8:F:120:ILE:HG22	1.86	0.57
5:B:479:VAL:O	5:B:480:SER:HB3	2.05	0.57
4:A:256:GLN:CA	4:A:257:ARG:HB3	2.35	0.57
4:A:741:ASN:HD22	4:A:744:LYS:H	1.52	0.57
6:C:242:GLN:O	6:C:246:ARG:HB2	2.05	0.57
6:C:133:ILE:CD1	6:C:237:SER:HA	2.35	0.56
11:J:56:LEU:O	11:J:57:ILE:C	2.48	0.56
4:A:1100:ARG:HH21	4:A:1351:GLU:HG3	1.71	0.56
5:B:227:LYS:N	5:B:395:GLN:OE1	2.37	0.56
4:A:14:VAL:H	4:A:1432:GLN:HE22	1.54	0.56
5:B:621:GLU:O	5:B:622:LYS:HG2	2.05	0.56
6:C:43:THR:CG2	6:C:44:LEU:N	2.68	0.56
10:I:19:ASP:HB3	10:I:24:ARG:H	1.71	0.56
4:A:483:ASP:HA	5:B:988:GLY:HA2	1.87	0.56
4:A:497:THR:CG2	5:B:1146:PHE:HD1	2.18	0.56
4:A:896:ARG:HB3	4:A:897:TYR:HD1	1.70	0.56
5:B:287:ARG:HG2	5:B:292:ILE:HD13	1.87	0.56
5:B:654:ARG:H	5:B:657:HIS:CD2	2.22	0.56
4:A:14:VAL:H	4:A:1432:GLN:NE2	2.04	0.56
6:C:186:LEU:HB3	6:C:188:HIS:HD2	1.71	0.56
4:A:256:GLN:HA	4:A:257:ARG:CB	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:848:ILE:HD12	4:A:864:ILE:HG13	1.88	0.56
5:B:256:VAL:HG11	5:B:382:ILE:HD13	1.87	0.56
5:B:613:VAL:HG22	5:B:628:THR:HG23	1.87	0.56
5:B:1115:THR:HB	5:B:1117:GLN:HG3	1.86	0.56
7:E:29:PHE:C	7:E:30:ILE:HG13	2.31	0.56
4:A:1428:VAL:HG21	5:B:1135:ARG:HD2	1.87	0.56
8:F:72:LYS:HG3	8:F:73:ALA:N	2.16	0.56
4:A:924:LYS:O	4:A:927:VAL:HG12	2.05	0.56
5:B:709:ASP:C	5:B:711:GLU:H	2.14	0.56
5:B:803:LEU:N	5:B:822:ASN:HD21	2.04	0.56
6:C:181:ASP:OD2	6:C:186:LEU:HD13	2.05	0.56
4:A:106:VAL:HG11	4:A:214:ILE:HD11	1.87	0.56
4:A:590:ARG:HH21	4:A:621:THR:HA	1.71	0.56
4:A:1161:THR:HG22	4:A:1162:VAL:N	2.20	0.56
5:B:1152:MET:O	5:B:1157:ALA:HB2	2.06	0.56
10:I:30:ARG:HD2	10:I:30:ARG:N	2.20	0.56
5:B:216:GLU:HB3	5:B:500:THR:CG2	2.29	0.55
11:J:48:ARG:HH21	11:J:49:MET:CE	2.18	0.55
4:A:370:ILE:HG22	4:A:374:LEU:CD1	2.36	0.55
4:A:507:VAL:HB	4:A:508:PRO:HD3	1.87	0.55
5:B:477:ALA:O	5:B:479:VAL:N	2.38	0.55
7:E:2:ASP:O	7:E:3:GLN:HB2	2.06	0.55
5:B:862:GLN:HG2	5:B:963:PHE:HB2	1.88	0.55
9:H:91:ASP:HA	9:H:93:TYR:HD1	1.70	0.55
4:A:407:ARG:HG2	4:A:430:TRP:CZ2	2.41	0.55
4:A:814:PHE:CE1	5:B:514:LEU:HD21	2.41	0.55
4:A:1015:VAL:CG1	4:A:1019:CYS:SG	2.91	0.55
5:B:20:ASP:O	5:B:21:GLU:C	2.48	0.55
5:B:875:GLU:O	5:B:877:PRO:HD3	2.06	0.55
5:B:973:ILE:CG2	5:B:974:PRO:HD2	2.37	0.55
5:B:1084:GLN:CD	5:B:1084:GLN:H	2.15	0.55
5:B:826:ALA:O	5:B:1011:ILE:HA	2.06	0.55
11:J:64:ASN:CB	11:J:65:PRO:HD3	2.12	0.55
4:A:364:VAL:O	4:A:364:VAL:HG13	2.06	0.55
4:A:1282:VAL:HG22	4:A:1308:THR:HG23	1.89	0.55
6:C:56:THR:HG22	6:C:57:VAL:H	1.70	0.55
4:A:244:PRO:HB2	4:A:245:PRO:HD3	1.89	0.55
4:A:381:THR:OG1	4:A:382:PRO:HD2	2.07	0.55
5:B:205:ILE:HG22	5:B:206:ASN:HD21	1.68	0.55
5:B:620:ARG:HD2	10:I:68:LEU:HD11	1.87	0.55
4:A:14:VAL:HB	4:A:1432:GLN:HE22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:507:VAL:O	4:A:510:GLN:HB2	2.07	0.54
4:A:840:ARG:HG2	4:A:1402:PHE:HZ	1.72	0.54
5:B:118:ARG:HA	5:B:207:GLY:HA2	1.88	0.54
4:A:1373:ASP:O	4:A:1377:THR:HG23	2.07	0.54
12:K:24:ASP:OD2	12:K:74:ARG:NH1	2.40	0.54
4:A:527:THR:HG21	4:A:650:GLN:HG2	1.89	0.54
4:A:1236:LEU:C	4:A:1237:ILE:HG13	2.33	0.54
6:C:241:ASP:HB3	12:K:109:TRP:CE2	2.43	0.54
4:A:401:GLY:C	4:A:435:HIS:CD2	2.86	0.54
4:A:855:THR:HG21	4:A:857:ARG:HE	1.72	0.54
4:A:1105:LEU:HD23	4:A:1384:VAL:HG21	1.89	0.54
10:I:111:THR:HG22	10:I:112:SER:N	2.22	0.54
4:A:1059:HIS:HB3	8:F:86:THR:HB	1.88	0.54
4:A:1161:THR:HG22	4:A:1163:ILE:N	2.20	0.54
12:K:57:LEU:HD12	12:K:76:GLN:HG2	1.90	0.54
4:A:302:THR:HA	4:A:305:ASP:O	2.06	0.54
4:A:981:LEU:CD2	4:A:1039:LYS:HA	2.38	0.54
5:B:174:LEU:HD21	5:B:204:ILE:HD11	1.89	0.54
5:B:230:ALA:H	5:B:231:PRO:HD2	1.73	0.54
5:B:515:HIS:HD2	5:B:517:THR:OG1	1.91	0.54
5:B:638:PHE:O	5:B:740:HIS:HB2	2.08	0.54
5:B:861:ASP:OD1	5:B:914:LYS:HE2	2.08	0.54
5:B:980:PHE:N	5:B:980:PHE:CD1	2.75	0.54
6:C:33:LEU:O	6:C:37:MET:HB2	2.07	0.54
7:E:176:PRO:O	7:E:212:ARG:HA	2.06	0.54
7:E:144:ILE:O	7:E:150:VAL:HG21	2.08	0.54
9:H:101:ALA:HB2	9:H:116:TYR:CE2	2.43	0.54
13:L:28:LYS:HB2	13:L:39:SER:HA	1.89	0.54
4:A:573:SER:H	4:A:576:GLN:CG	2.18	0.54
4:A:759:ALA:O	4:A:763:ALA:HB3	2.08	0.54
4:A:814:PHE:O	4:A:817:ALA:HB3	2.08	0.54
13:L:60:ARG:HG3	13:L:61:THR:H	1.73	0.54
4:A:455:MET:HE1	5:B:1138:MET:SD	2.48	0.54
4:A:1410:PHE:HD2	5:B:1212:ILE:HD11	1.72	0.54
5:B:65:GLU:N	5:B:65:GLU:OE1	2.41	0.54
5:B:899:ILE:HD11	5:B:911:ILE:HA	1.89	0.54
8:F:85:MET:HE2	8:F:93:ILE:HG13	1.90	0.54
5:B:189:LEU:HA	5:B:192:LEU:HD12	1.90	0.54
5:B:690:VAL:HG12	5:B:691:GLU:N	2.22	0.54
5:B:1076:HIS:ND1	5:B:1076:HIS:N	2.56	0.54
12:K:65:HIS:CD2	12:K:66:PRO:HD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:58:LEU:CD2	4:A:59:GLY:H	2.21	0.53
4:A:351:THR:CG2	4:A:352:VAL:H	2.22	0.53
4:A:568:PRO:HD3	9:H:94:ASP:O	2.08	0.53
4:A:889:SER:HB2	4:A:892:ALA:H	1.73	0.53
4:A:1242:VAL:HG12	4:A:1243:VAL:N	2.17	0.53
4:A:1434:ALA:O	4:A:1436:ILE:N	2.41	0.53
5:B:487:THR:H	5:B:490:SER:HB3	1.73	0.53
5:B:840:ILE:HB	5:B:1011:ILE:HB	1.90	0.53
6:C:51:VAL:HG22	6:C:155:LEU:HD22	1.90	0.53
4:A:449:SER:OG	5:B:1134:GLU:OE2	2.26	0.53
4:A:886:ILE:HD11	4:A:943:LEU:HB3	1.88	0.53
5:B:287:ARG:HA	5:B:291:ILE:O	2.09	0.53
9:H:38:LEU:HD11	9:H:123:MET:HE2	1.89	0.53
10:I:55:THR:HG23	10:I:58:VAL:HG21	1.90	0.53
5:B:857:ARG:HG3	5:B:857:ARG:NH1	2.19	0.53
12:K:61:TYR:HA	12:K:72:LYS:O	2.08	0.53
4:A:855:THR:HG23	4:A:857:ARG:HE	1.74	0.53
5:B:731:VAL:O	5:B:732:SER:HB2	2.09	0.53
4:A:208:LEU:HD22	4:A:208:LEU:C	2.30	0.53
4:A:583:PRO:O	4:A:610:GLY:HA3	2.09	0.53
5:B:292:ILE:N	5:B:293:PRO:CD	2.67	0.53
5:B:778:MET:HE3	5:B:853:SER:HB3	1.91	0.53
8:F:84:TYR:CE1	8:F:152:ILE:HD12	2.44	0.53
8:F:85:MET:CE	8:F:93:ILE:HG13	2.39	0.53
4:A:58:LEU:HD22	4:A:59:GLY:H	1.74	0.53
4:A:256:GLN:HA	4:A:257:ARG:HB3	1.90	0.53
4:A:332:LYS:C	4:A:334:GLY:H	2.17	0.53
5:B:25:ILE:HG22	5:B:26:THR:N	2.23	0.53
5:B:120:ARG:HB3	5:B:955:THR:HG21	1.91	0.53
5:B:229:ALA:HB1	5:B:231:PRO:HD2	1.89	0.53
5:B:321:GLY:O	5:B:323:VAL:N	2.42	0.53
4:A:467:THR:HG23	5:B:976:ILE:CG2	2.37	0.53
5:B:176:SER:O	5:B:182:SER:CB	2.57	0.53
5:B:230:ALA:HA	5:B:261:ARG:NH1	2.23	0.53
5:B:315:LYS:N	5:B:316:PRO:HD2	2.24	0.53
5:B:799:PRO:HB3	5:B:818:PRO:HG2	1.90	0.53
4:A:896:ARG:HB3	4:A:897:TYR:CD1	2.43	0.53
5:B:361:LEU:HD21	5:B:377:PHE:HD2	1.74	0.53
4:A:855:THR:HG21	4:A:857:ARG:HH21	1.73	0.52
4:A:1328:TYR:OH	4:A:1351:GLU:OE1	2.20	0.52
5:B:286:PHE:CB	5:B:297:ILE:HD12	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:351:THR:HG23	5:B:1103:ILE:HD13	1.92	0.52
5:B:1076:HIS:CD2	12:K:40:HIS:CD2	2.98	0.52
4:A:528:LEU:HA	4:A:531:ILE:HG22	1.91	0.52
5:B:260:GLY:O	5:B:267:ARG:HD3	2.10	0.52
8:F:89:GLU:O	8:F:93:ILE:HG12	2.09	0.52
9:H:128:ASN:O	9:H:131:ASN:OD1	2.28	0.52
4:A:344:ARG:HA	5:B:1129:ARG:HA	1.92	0.52
4:A:875:ALA:HA	4:A:878:ILE:HD12	1.91	0.52
5:B:637:LEU:CD2	5:B:742:GLU:HA	2.29	0.52
4:A:897:TYR:HD2	4:A:936:LEU:HD13	1.74	0.52
5:B:1065:GLN:NE2	5:B:1069:PHE:H	2.08	0.52
6:C:2:SER:N	6:C:3:GLU:CB	2.71	0.52
9:H:109:LYS:HB2	9:H:111:LEU:HB2	1.92	0.52
4:A:642:CYS:O	4:A:645:LEU:HB3	2.09	0.52
5:B:519:TRP:HZ2	5:B:705:MET:HE1	1.73	0.52
5:B:788:ARG:NH1	5:B:790:ASP:OD1	2.43	0.52
4:A:434:ARG:HH21	4:A:437:MET:HG3	1.75	0.52
4:A:315:LEU:CD1	4:A:319:GLY:O	2.58	0.52
4:A:942:PHE:C	4:A:942:PHE:CD2	2.88	0.52
5:B:230:ALA:H	5:B:231:PRO:CD	2.22	0.52
10:I:4:PHE:CE1	10:I:13:MET:HE2	2.45	0.52
4:A:140:THR:HA	4:A:143:LYS:HE3	1.92	0.52
4:A:549:MET:HE1	4:A:656:TRP:HD1	1.75	0.52
5:B:168:GLY:H	5:B:450:ALA:HB1	1.75	0.52
4:A:1312:ASN:O	4:A:1316:VAL:HG23	2.10	0.51
5:B:470:LYS:O	5:B:471:LYS:HG3	2.10	0.51
4:A:69:THR:O	4:A:71:GLN:HG3	2.10	0.51
4:A:98:LYS:HB3	4:A:234:MET:HE1	1.92	0.51
4:A:507:VAL:O	4:A:508:PRO:C	2.52	0.51
4:A:567:LYS:HZ3	9:H:43:ASN:HB3	1.73	0.51
5:B:682:SER:O	5:B:686:ASN:ND2	2.42	0.51
5:B:1076:HIS:HD2	12:K:40:HIS:CE1	2.29	0.51
4:A:129:LYS:O	4:A:130:ASP:HB2	2.10	0.51
4:A:399:HIS:O	4:A:401:GLY:N	2.43	0.51
4:A:401:GLY:H	4:A:435:HIS:HD2	1.57	0.51
4:A:1206:ASP:HB2	4:A:1274:ARG:HH12	1.75	0.51
6:C:259:LEU:HD13	12:K:91:CYS:HB3	1.90	0.51
4:A:351:THR:HG21	4:A:466:SER:O	2.11	0.51
4:A:1410:PHE:CD2	5:B:1212:ILE:HD11	2.44	0.51
6:C:97:VAL:HG21	6:C:129:ILE:CG2	2.41	0.51
7:E:135:PHE:HB3	7:E:140:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:482:PHE:HD1	5:B:836:GLU:HB2	1.76	0.51
4:A:467:THR:HG22	5:B:1099:VAL:HG11	1.92	0.51
4:A:870:GLU:HB2	7:E:204:THR:HG21	1.93	0.51
5:B:955:THR:HG23	13:L:54:ARG:O	2.10	0.51
6:C:184:ASN:ND2	6:C:189:THR:O	2.44	0.51
4:A:12:ARG:HB3	5:B:1218:THR:CG2	2.41	0.51
4:A:370:ILE:HG22	4:A:374:LEU:HD12	1.93	0.51
5:B:1160:VAL:HG12	5:B:1161:HIS:H	1.76	0.51
6:C:102:GLN:HG2	6:C:154:LYS:CD	2.40	0.51
6:C:251:LEU:O	6:C:255:VAL:HG23	2.11	0.51
5:B:979:LYS:C	5:B:980:PHE:CD1	2.89	0.51
6:C:43:THR:CG2	6:C:44:LEU:H	2.23	0.51
9:H:139:ASN:O	9:H:140:ALA:HB3	2.11	0.51
4:A:512:VAL:HA	4:A:519:PRO:HA	1.93	0.50
4:A:979:SER:OG	4:A:980:ASP:N	2.45	0.50
4:A:1017:LEU:HB2	7:E:206:GLY:H	1.75	0.50
5:B:549:THR:HG22	5:B:550:ASP:N	2.21	0.50
5:B:642:ASP:O	5:B:644:GLU:N	2.44	0.50
7:E:65:THR:C	7:E:67:GLU:H	2.18	0.50
4:A:224:PHE:CZ	4:A:231:PRO:HG3	2.47	0.50
4:A:563:PRO:HG2	4:A:566:ILE:HG12	1.94	0.50
4:A:1192:LEU:HD11	4:A:1239:ARG:HB3	1.92	0.50
5:B:800:GLN:CG	11:J:52:THR:HG22	2.41	0.50
5:B:986:GLN:HA	5:B:986:GLN:OE1	2.11	0.50
6:C:180:TYR:O	6:C:180:TYR:CD1	2.64	0.50
8:F:109:VAL:CG1	8:F:110:ASP:N	2.74	0.50
4:A:678:GLU:HA	4:A:681:GLU:HG2	1.92	0.50
5:B:100:PRO:HG3	5:B:172:ILE:HG13	1.93	0.50
5:B:286:PHE:HB3	5:B:297:ILE:CD1	2.37	0.50
10:I:8:ARG:O	10:I:9:ASP:CB	2.59	0.50
4:A:567:LYS:HB3	9:H:96:VAL:N	2.15	0.50
4:A:1364:ASN:HD21	4:A:1366:ARG:HG2	1.67	0.50
5:B:635:ARG:HB2	5:B:636:PRO:HD3	1.94	0.50
9:H:110:ASP:O	9:H:128:ASN:CG	2.55	0.50
11:J:1:MET:H3	11:J:56:LEU:HD12	1.76	0.50
11:J:7:CYS:HA	11:J:49:MET:HG2	1.94	0.50
5:B:1096:ARG:HH11	5:B:1096:ARG:CG	2.23	0.50
13:L:60:ARG:HG3	13:L:61:THR:N	2.26	0.50
4:A:907:THR:HG22	4:A:908:LEU:N	2.27	0.50
4:A:1021:LEU:HD11	4:A:1025:ARG:NH1	2.26	0.50
4:A:1118:VAL:HA	4:A:1327:ILE:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:73:GLN:HE21	6:C:74:SER:N	2.08	0.50
4:A:345:VAL:HG12	5:B:1155:SER:HB2	1.93	0.50
4:A:828:ALA:CB	5:B:530:GLY:HA2	2.41	0.50
4:A:901:LEU:HD22	4:A:919:ILE:HG22	1.93	0.50
5:B:1076:HIS:HD2	12:K:40:HIS:NE2	2.06	0.50
5:B:1079:LYS:HE3	6:C:188:HIS:CE1	2.47	0.50
9:H:95:TYR:HE2	9:H:97:MET:HG3	1.77	0.50
11:J:6:ARG:HA	11:J:12:LYS:O	2.12	0.50
4:A:446:ARG:HH21	4:A:485:ASP:CG	2.20	0.50
5:B:487:THR:HG22	5:B:489:SER:N	2.27	0.50
5:B:789:MET:HE3	5:B:965:LYS:HB3	1.93	0.50
5:B:1096:ARG:HG2	5:B:1096:ARG:NH1	2.27	0.50
5:B:515:HIS:CD2	5:B:517:THR:H	2.30	0.50
12:K:7:PHE:CD1	12:K:7:PHE:C	2.89	0.50
4:A:896:ARG:HD2	4:A:897:TYR:HE1	1.76	0.49
5:B:705:MET:HE2	5:B:745:PRO:HB3	1.94	0.49
5:B:1017:ILE:H	5:B:1018:PRO:HD3	1.78	0.49
5:B:1017:ILE:HD12	5:B:1026:LEU:HD21	1.94	0.49
6:C:31:ASN:O	6:C:35:ARG:HG3	2.12	0.49
9:H:109:LYS:HB2	9:H:111:LEU:N	2.26	0.49
4:A:1364:ASN:HD21	4:A:1366:ARG:NH1	1.97	0.49
4:A:1436:ILE:O	4:A:1439:GLY:N	2.40	0.49
5:B:294:ASP:OD2	5:B:294:ASP:N	2.34	0.49
4:A:809:THR:HB	4:A:810:PRO:HD2	1.94	0.49
5:B:900:ALA:O	5:B:902:GLY:N	2.45	0.49
6:C:16:ASP:O	6:C:233:GLU:HA	2.12	0.49
5:B:864:LYS:HB2	5:B:865:LYS:CA	2.25	0.49
5:B:1073:TYR:CE2	5:B:1080:LYS:HG3	2.48	0.49
5:B:1106:ARG:HG3	5:B:1107:ALA:N	2.27	0.49
7:E:198:ILE:HD12	7:E:198:ILE:H	1.78	0.49
7:E:136:ASN:OD1	7:E:137:GLU:N	2.45	0.49
4:A:376:TYR:CZ	4:A:498:ARG:HD2	2.48	0.49
4:A:523:ILE:HG23	4:A:527:THR:HB	1.95	0.49
4:A:451:HIS:HB3	4:A:453:MET:N	2.28	0.49
4:A:800:VAL:HG12	4:A:802:ASN:H	1.78	0.49
4:A:464:PRO:HG2	12:K:67:PHE:CD1	2.47	0.49
4:A:907:THR:HG22	4:A:908:LEU:H	1.78	0.49
6:C:22:LEU:CD2	6:C:25:VAL:HG21	2.42	0.49
10:I:106:CYS:SG	10:I:108:HIS:HB3	2.53	0.49
1:R:3:U:H2'	1:R:4:C:H6	1.77	0.49
4:A:351:THR:HG23	5:B:1103:ILE:CD1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:457:ALA:HB3	4:A:506:ALA:HA	1.95	0.49
4:A:1393:ASN:O	4:A:1393:ASN:CG	2.56	0.49
5:B:120:ARG:HA	5:B:963:PHE:HE2	1.78	0.49
5:B:498:THR:HB	5:B:537:LYS:O	2.13	0.49
5:B:635:ARG:HG3	5:B:635:ARG:NH1	2.28	0.49
4:A:901:LEU:HB2	4:A:926:GLN:HG2	1.95	0.48
4:A:960:ILE:O	4:A:961:ARG:C	2.55	0.48
5:B:636:PRO:HB3	5:B:743:ILE:HG12	1.95	0.48
5:B:637:LEU:HD21	5:B:742:GLU:OE2	2.04	0.48
5:B:984:HIS:CE1	5:B:1025:HIS:HA	2.48	0.48
4:A:504:LEU:HD11	8:F:91:ALA:HB1	1.95	0.48
4:A:549:MET:O	4:A:550:LEU:C	2.54	0.48
4:A:1425:SER:O	4:A:1429:ILE:HD12	2.12	0.48
4:A:830:LYS:HG3	4:A:1098:VAL:HG21	1.96	0.48
5:B:1146:PHE:CZ	5:B:1150:ARG:HG3	2.48	0.48
8:F:81:THR:HG1	8:F:144:GLU:CD	2.20	0.48
11:J:1:MET:H1	11:J:56:LEU:HB2	1.78	0.48
2:T:20:DC:H2'	2:T:21:DT:O4'	2.13	0.48
4:A:760:GLN:HE21	4:A:765:VAL:HA	1.77	0.48
5:B:527:THR:OG1	5:B:528:PRO:HD2	2.12	0.48
5:B:545:ILE:HG23	5:B:631:GLY:HA2	1.95	0.48
5:B:840:ILE:HG12	5:B:992:ILE:HG22	1.95	0.48
5:B:44:VAL:HG11	5:B:495:LEU:HD13	1.96	0.48
5:B:101:MET:HE2	5:B:169:ARG:HH22	1.79	0.48
5:B:992:ILE:HD11	12:K:67:PHE:CE2	2.47	0.48
5:B:1072:MET:O	5:B:1081:LEU:HB2	2.13	0.48
7:E:153:HIS:O	7:E:154:ILE:HD13	2.14	0.48
8:F:97:ARG:HD2	8:F:101:ILE:CD1	2.44	0.48
12:K:12:LEU:HD12	12:K:12:LEU:H	1.78	0.48
4:A:332:LYS:H	4:A:337:ARG:HB3	1.79	0.48
5:B:996:ARG:HG3	5:B:1007:VAL:HG21	1.95	0.48
5:B:1002:THR:HG23	5:B:1004:GLU:N	2.28	0.48
7:E:161:LYS:HD2	7:E:195:VAL:HG23	1.94	0.48
13:L:40:LEU:HD11	13:L:49:LYS:HE2	1.95	0.48
4:A:512:VAL:O	4:A:512:VAL:HG13	2.12	0.48
4:A:1193:LEU:HD21	4:A:1267:MET:HE2	1.94	0.48
7:E:93:MET:HE3	7:E:120:ALA:HB1	1.96	0.48
4:A:1100:ARG:NH2	4:A:1351:GLU:HG3	2.28	0.48
5:B:992:ILE:HD11	12:K:67:PHE:HE2	1.77	0.48
5:B:999:MET:HE3	5:B:999:MET:HA	1.96	0.48
4:A:477:PRO:HG3	4:A:521:MET:CE	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:599:SER:OG	4:A:614:PHE:CD1	2.66	0.48
4:A:1161:THR:CG2	4:A:1162:VAL:N	2.76	0.48
5:B:325:GLN:NE2	10:I:12:ASN:ND2	2.58	0.48
5:B:1084:GLN:OE1	5:B:1084:GLN:N	2.47	0.48
5:B:1200:ALA:O	5:B:1201:LYS:C	2.56	0.48
10:I:28:GLU:HB3	10:I:35:VAL:HG22	1.95	0.48
1:R:3:U:H2'	1:R:4:C:C6	2.49	0.48
4:A:378:GLU:OE1	4:A:434:ARG:HD3	2.14	0.48
4:A:741:ASN:C	4:A:741:ASN:ND2	2.71	0.48
5:B:887:HIS:HB2	5:B:908:GLU:OE2	2.13	0.48
5:B:1084:GLN:CD	5:B:1084:GLN:N	2.72	0.48
4:A:1277:GLU:O	4:A:1278:ASN:HB2	2.14	0.47
5:B:314:LEU:O	5:B:315:LYS:C	2.55	0.47
5:B:893:LEU:HD22	5:B:897:GLY:O	2.13	0.47
5:B:1107:ALA:O	5:B:1108:ARG:CB	2.62	0.47
4:A:768:GLN:HG2	4:A:816:HIS:HA	1.94	0.47
4:A:1063:MET:SD	4:A:1436:ILE:HG12	2.54	0.47
4:A:1097:GLY:C	4:A:1099:PRO:HD2	2.39	0.47
5:B:461:LEU:O	5:B:480:SER:OG	2.29	0.47
11:J:9:SER:OG	11:J:48:ARG:NH2	2.47	0.47
4:A:55:ASP:O	4:A:58:LEU:N	2.37	0.47
5:B:195:CYS:CB	5:B:782:LEU:HD22	2.44	0.47
5:B:567:GLU:H	5:B:567:GLU:CD	2.22	0.47
5:B:1073:TYR:N	5:B:1073:TYR:CD1	2.82	0.47
6:C:43:THR:HG23	6:C:74:SER:OG	2.14	0.47
9:H:25:ARG:HD2	9:H:39:THR:HG22	1.96	0.47
11:J:43:ARG:HG3	11:J:46:CYS:SG	2.54	0.47
12:K:46:ILE:HG22	12:K:50:LEU:HD12	1.97	0.47
4:A:913:LEU:CD1	4:A:915:SER:H	2.26	0.47
5:B:636:PRO:HB3	5:B:637:LEU:CB	2.34	0.47
6:C:5:GLY:HA3	6:C:6:PRO:HD2	1.65	0.47
6:C:56:THR:HG23	6:C:147:LEU:HD23	1.95	0.47
4:A:802:ASN:HD21	5:B:729:ILE:H	1.63	0.47
5:B:401:PHE:HA	5:B:404:LYS:HG3	1.95	0.47
5:B:624:LEU:C	5:B:624:LEU:HD12	2.39	0.47
5:B:701:ILE:HG13	5:B:740:HIS:CE1	2.50	0.47
4:A:120:GLU:HA	4:A:123:ARG:HD3	1.96	0.47
4:A:1118:VAL:O	4:A:1305:VAL:HG13	2.15	0.47
4:A:1242:VAL:CG1	4:A:1243:VAL:H	2.21	0.47
4:A:543:LEU:O	4:A:544:ASP:C	2.57	0.47
5:B:28:GLU:C	5:B:30:SER:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:955:THR:CG2	5:B:956:THR:H	2.27	0.47
2:T:15:DC:H2''	2:T:16:DG:O5'	2.15	0.47
4:A:1154:TYR:HD1	4:A:1191:TRP:CH2	2.33	0.47
4:A:1441:PHE:CE2	8:F:89:GLU:HA	2.49	0.47
5:B:321:GLY:C	5:B:323:VAL:H	2.22	0.47
5:B:637:LEU:HD22	5:B:742:GLU:OE2	2.01	0.47
5:B:899:ILE:HD11	5:B:911:ILE:HG12	1.97	0.47
5:B:976:ILE:HG23	5:B:977:GLY:N	2.30	0.47
8:F:109:VAL:HG13	8:F:110:ASP:N	2.30	0.47
14:T:3000:G2P:O3G	5:B:1020:ARG:NH1	2.48	0.47
4:A:847:ASP:OD2	4:A:858:ASN:HB2	2.15	0.47
5:B:487:THR:HG23	5:B:488:TYR:H	1.78	0.47
5:B:37:PHE:O	5:B:38:PHE:CB	2.54	0.47
5:B:402:GLY:CA	5:B:695:ALA:HB3	2.43	0.47
5:B:864:LYS:HB3	5:B:871:THR:HG23	1.95	0.47
5:B:892:LYS:HG2	5:B:903:VAL:HG11	1.97	0.47
5:B:1002:THR:HG22	5:B:1006:ILE:H	1.80	0.47
9:H:41:ASP:HB3	9:H:121:LEU:HD22	1.96	0.47
5:B:361:LEU:HD21	5:B:377:PHE:CD2	2.50	0.46
5:B:500:THR:HA	5:B:501:PRO:HD3	1.50	0.46
5:B:865:LYS:CB	5:B:866:TYR:CA	2.89	0.46
6:C:60:ASP:HB3	13:L:67:PHE:CE1	2.50	0.46
4:A:1193:LEU:C	4:A:1193:LEU:HD12	2.41	0.46
5:B:709:ASP:O	5:B:711:GLU:N	2.48	0.46
6:C:186:LEU:CB	6:C:188:HIS:HD2	2.28	0.46
12:K:70:ARG:O	12:K:70:ARG:HG3	2.16	0.46
13:L:30:ILE:C	13:L:56:LEU:HD23	2.40	0.46
4:A:256:GLN:HB3	4:A:257:ARG:HB3	1.97	0.46
4:A:335:ARG:HD2	5:B:1202:LEU:HD12	1.98	0.46
5:B:363:HIS:O	5:B:364:ILE:HB	2.16	0.46
7:E:46:TYR:CE2	7:E:58:MET:HA	2.49	0.46
7:E:65:THR:C	7:E:67:GLU:N	2.73	0.46
4:A:746:MET:HG2	5:B:1015:HIS:CE1	2.50	0.46
4:A:1209:MET:O	4:A:1212:VAL:HB	2.15	0.46
5:B:550:ASP:OD1	5:B:551:PRO:HD2	2.15	0.46
5:B:636:PRO:HB2	5:B:637:LEU:CA	2.26	0.46
5:B:701:ILE:HD11	5:B:703:ILE:HD11	1.97	0.46
5:B:952:VAL:HG22	5:B:966:VAL:HG13	1.97	0.46
6:C:102:GLN:HG2	6:C:154:LYS:HD2	1.98	0.46
13:L:68:GLU:OE1	13:L:68:GLU:O	2.34	0.46
4:A:347:PHE:HB2	5:B:1150:ARG:HH22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:993:LEU:HD23	4:A:1022:LEU:HD21	1.98	0.46
4:A:1356:ILE:HG22	4:A:1361:SER:O	2.15	0.46
5:B:113:TYR:O	5:B:114:PRO:C	2.59	0.46
5:B:363:HIS:HD2	5:B:585:VAL:HG22	1.80	0.46
7:E:198:ILE:HD12	7:E:198:ILE:N	2.30	0.46
4:A:115:LEU:HD22	4:A:119:ASN:HB2	1.98	0.46
4:A:511:ILE:O	4:A:519:PRO:HA	2.16	0.46
5:B:865:LYS:HB2	5:B:866:TYR:HA	1.96	0.46
11:J:32:GLU:CD	11:J:32:GLU:H	2.22	0.46
4:A:55:ASP:N	4:A:56:PRO:HD2	2.30	0.46
10:I:71:SER:H	10:I:83:ASN:ND2	2.14	0.46
4:A:740:LEU:HD21	6:C:193:TYR:CE2	2.51	0.46
5:B:308:TRP:HA	5:B:311:LEU:HD12	1.98	0.46
5:B:400:HIS:CE1	5:B:517:THR:HG21	2.51	0.46
8:F:82:THR:HG22	8:F:84:TYR:HB2	1.97	0.46
4:A:90:VAL:HG11	4:A:297:GLN:HA	1.98	0.46
5:B:654:ARG:N	5:B:657:HIS:HD2	2.10	0.46
5:B:1064:TYR:N	5:B:1064:TYR:CD1	2.83	0.46
6:C:67:LEU:HD11	6:C:155:LEU:HD13	1.98	0.46
8:F:81:THR:OG1	8:F:144:GLU:OE1	2.30	0.46
4:A:19:PHE:O	4:A:1416:ALA:HA	2.16	0.46
4:A:315:LEU:HD13	4:A:319:GLY:O	2.16	0.46
4:A:567:LYS:CB	4:A:568:PRO:CD	2.52	0.46
4:A:875:ALA:HB2	4:A:1366:ARG:CD	2.44	0.46
4:A:913:LEU:HD13	4:A:914:GLU:H	1.81	0.46
8:F:97:ARG:HD2	8:F:101:ILE:HG13	1.97	0.46
4:A:57:ARG:C	4:A:68:GLN:HG2	2.41	0.45
4:A:353:ILE:HD12	4:A:482:PHE:CE2	2.51	0.45
6:C:57:VAL:CG2	11:J:57:ILE:HD11	2.44	0.45
4:A:67:CYS:O	4:A:70:CYS:HB3	2.16	0.45
4:A:590:ARG:NH2	4:A:621:THR:HA	2.30	0.45
4:A:1058:VAL:HG12	4:A:1062:GLU:HG3	1.98	0.45
5:B:26:THR:O	5:B:27:ALA:C	2.59	0.45
5:B:762:ASN:ND2	5:B:1022:THR:HA	2.31	0.45
8:F:116:ASP:OD2	8:F:117:PRO:HD2	2.16	0.45
9:H:24:CYS:HB2	9:H:44:VAL:CG2	2.46	0.45
4:A:754:SER:N	4:A:757:ASN:HD22	2.13	0.45
5:B:984:HIS:CD2	5:B:1024:ALA:HB3	2.50	0.45
12:K:43:GLY:HA2	12:K:71:PHE:CZ	2.52	0.45
4:A:313:GLN:HG3	4:A:314:ALA:H	1.82	0.45
4:A:956:LEU:HD11	4:A:1017:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1305:VAL:HG12	4:A:1306:LEU:N	2.30	0.45
5:B:848:ARG:HH22	5:B:996:ARG:HH11	1.59	0.45
6:C:66:ARG:HH21	11:J:5:VAL:H	1.64	0.45
6:C:99:LEU:CD1	6:C:120:ILE:HA	2.46	0.45
10:I:69:PRO:HB2	10:I:85:PHE:CE2	2.51	0.45
12:K:47:ARG:HG3	12:K:60:ALA:HA	1.98	0.45
4:A:472:LEU:O	4:A:475:THR:HB	2.17	0.45
6:C:15:LYS:O	6:C:240:VAL:HG22	2.16	0.45
7:E:77:SER:HB2	7:E:105:PHE:HD2	1.81	0.45
9:H:59:ILE:HD13	9:H:142:LEU:HD12	1.99	0.45
4:A:1371:LEU:O	4:A:1372:VAL:C	2.60	0.45
5:B:706:GLN:O	5:B:707:PRO:O	2.35	0.45
6:C:137:LYS:HB3	6:C:137:LYS:HE3	1.78	0.45
2:T:26:DA:C6	2:T:27:DT:H72	2.51	0.45
4:A:338:GLY:HA2	5:B:1129:ARG:HH22	1.81	0.45
4:A:343:LYS:NZ	5:B:1156:ASP:OD2	2.49	0.45
5:B:807:ARG:HG3	5:B:807:ARG:HH11	1.82	0.45
5:B:1065:GLN:NE2	5:B:1067:ARG:H	2.15	0.45
6:C:180:TYR:O	6:C:181:ASP:HB3	2.16	0.45
8:F:107:VAL:HG12	8:F:109:VAL:H	1.81	0.45
12:K:90:ALA:O	12:K:94:ILE:HD12	2.16	0.45
4:A:18:GLN:HG2	4:A:1418:LEU:HD12	1.98	0.45
4:A:350:ARG:HG2	4:A:486:GLU:HG2	1.99	0.45
4:A:1098:VAL:N	4:A:1099:PRO:HD2	2.32	0.45
5:B:549:THR:HB	5:B:628:THR:HG21	1.99	0.45
5:B:785:TYR:CD1	5:B:785:TYR:C	2.94	0.45
5:B:1007:VAL:HG13	5:B:1008:PRO:HD2	1.97	0.45
6:C:173:ALA:O	6:C:174:ALA:HB3	2.17	0.45
4:A:380:VAL:HG22	4:A:430:TRP:H	1.82	0.45
5:B:70:ILE:O	5:B:70:ILE:HG22	2.16	0.45
5:B:483:LEU:O	5:B:484:ASN:HB2	2.17	0.45
5:B:484:ASN:ND2	5:B:490:SER:OG	2.50	0.45
5:B:766:ARG:HA	5:B:766:ARG:HD3	1.77	0.45
6:C:267:GLN:HA	6:C:267:GLN:OE1	2.17	0.45
7:E:79:TRP:HE1	7:E:96:PHE:HE1	1.64	0.45
10:I:7:CYS:HB2	10:I:14:LEU:HD21	1.99	0.45
5:B:273:LEU:HD21	5:B:360:PHE:CD1	2.51	0.45
6:C:4:GLU:HG3	6:C:5:GLY:H	1.81	0.45
9:H:26:ILE:HG22	9:H:40:LEU:HB3	1.99	0.45
4:A:26:GLU:O	4:A:29:ALA:N	2.45	0.44
4:A:626:ASN:HD21	4:A:880:LYS:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:775:ILE:HB	4:A:797:LYS:O	2.17	0.44
4:A:893:PHE:CD2	4:A:893:PHE:C	2.96	0.44
4:A:1059:HIS:ND1	8:F:86:THR:HA	2.32	0.44
4:A:1400:CYS:C	4:A:1402:PHE:H	2.25	0.44
5:B:193:LYS:HB3	5:B:787:VAL:HG11	1.99	0.44
5:B:526:GLU:HG3	5:B:771:SER:HB3	1.98	0.44
5:B:580:VAL:HG22	5:B:624:LEU:HB3	1.98	0.44
5:B:1065:GLN:HE21	5:B:1069:PHE:H	1.64	0.44
11:J:3:VAL:HG21	11:J:18:TRP:CG	2.52	0.44
4:A:599:SER:C	4:A:601:LYS:N	2.75	0.44
4:A:1189:SER:O	4:A:1241:ARG:HD3	2.18	0.44
6:C:2:SER:N	6:C:3:GLU:CA	2.80	0.44
6:C:123:ASN:HD21	6:C:125:MET:HG2	1.78	0.44
6:C:177:GLU:HB2	6:C:231:ASN:HB3	1.99	0.44
7:E:171:LYS:HE2	7:E:174:GLN:NE2	2.32	0.44
9:H:102:TYR:OH	9:H:122:LEU:HD22	2.17	0.44
11:J:32:GLU:O	11:J:36:LEU:HG	2.16	0.44
4:A:577:ILE:O	4:A:580:VAL:HG23	2.18	0.44
5:B:190:TYR:CE1	11:J:62:ARG:HG2	2.53	0.44
5:B:234:ILE:HD13	5:B:234:ILE:H	1.82	0.44
9:H:104:PHE:CZ	9:H:136:LYS:HA	2.52	0.44
10:I:59:VAL:CG1	10:I:60:GLN:H	2.24	0.44
4:A:909:ASP:C	4:A:911:SER:N	2.74	0.44
4:A:1006:ILE:HD11	7:E:163:GLU:HG3	1.99	0.44
4:A:1188:GLN:HB3	4:A:1189:SER:H	1.56	0.44
4:A:1305:VAL:CG1	4:A:1306:LEU:N	2.80	0.44
10:I:111:THR:CG2	10:I:112:SER:N	2.80	0.44
4:A:455:MET:HE2	4:A:455:MET:HB3	1.81	0.44
4:A:666:ILE:CG2	5:B:1026:LEU:HB2	2.47	0.44
4:A:1030:ARG:O	4:A:1031:VAL:C	2.61	0.44
5:B:578:THR:OG1	5:B:593:PRO:HG3	2.17	0.44
5:B:744:HIS:HD2	5:B:746:SER:H	1.63	0.44
5:B:973:ILE:HG22	5:B:974:PRO:HD2	1.99	0.44
5:B:1084:GLN:HE22	6:C:192:TRP:N	2.13	0.44
5:B:1136:ASP:HA	5:B:1139:ILE:HD12	1.99	0.44
6:C:229:TYR:CD1	6:C:229:TYR:N	2.86	0.44
4:A:326:ARG:HG3	4:A:1406:VAL:HG11	2.00	0.44
4:A:463:ILE:CB	4:A:464:PRO:HD2	2.47	0.44
4:A:852:TYR:O	4:A:853:ASP:HB3	2.18	0.44
4:A:1364:ASN:ND2	4:A:1366:ARG:HH11	1.98	0.44
5:B:1106:ARG:HD3	5:B:1127:GLY:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:28:TYR:HE1	7:E:78:LEU:HD13	1.82	0.44
7:E:167:ARG:HA	7:E:167:ARG:HD3	1.78	0.44
8:F:128:LYS:HD2	8:F:148:VAL:O	2.18	0.44
4:A:897:TYR:CD2	4:A:936:LEU:HD13	2.50	0.44
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.98	0.44
7:E:185:ALA:HA	7:E:190:LEU:HD23	1.99	0.44
1:R:10:G:HO2'	4:A:446:ARG:NH2	2.16	0.44
4:A:343:LYS:NZ	5:B:1197:PRO:HB3	2.32	0.44
4:A:370:ILE:HG22	4:A:374:LEU:HD11	2.00	0.44
4:A:857:ARG:HA	4:A:864:ILE:HG12	1.98	0.44
4:A:954:TRP:HA	4:A:955:PRO:HD2	1.86	0.44
5:B:48:LEU:O	5:B:52:ASN:ND2	2.50	0.44
10:I:104:LEU:HD23	10:I:104:LEU:HA	1.90	0.44
4:A:49:LYS:HZ2	4:A:60:SER:HA	1.83	0.44
4:A:116:ASP:C	4:A:118:HIS:H	2.25	0.44
4:A:361:LEU:HD22	4:A:646:PHE:CD1	2.53	0.44
4:A:382:PRO:N	4:A:428:TYR:HE2	2.16	0.44
4:A:660:ASN:OD1	5:B:1082:MET:HG3	2.16	0.44
4:A:785:PRO:HG3	5:B:698:GLU:HG2	1.99	0.44
5:B:58:THR:O	5:B:62:ILE:HG12	2.17	0.44
5:B:185:THR:OG1	5:B:188:ASP:OD2	2.36	0.44
5:B:327:ARG:O	5:B:331:LEU:HD12	2.18	0.44
5:B:684:LEU:CD2	5:B:689:LEU:HD12	2.48	0.44
5:B:881:ASN:HB2	5:B:933:SER:OG	2.18	0.44
5:B:1200:ALA:O	5:B:1203:LEU:N	2.51	0.44
7:E:131:THR:C	7:E:132:ILE:HG13	2.43	0.44
4:A:49:LYS:O	4:A:50:ILE:HG12	2.18	0.43
4:A:271:LYS:O	4:A:275:SER:HB2	2.18	0.43
4:A:311:GLN:HA	4:A:312:PRO:HD3	1.87	0.43
4:A:335:ARG:CD	5:B:1202:LEU:HD12	2.48	0.43
4:A:885:THR:O	4:A:940:ARG:HG3	2.18	0.43
4:A:901:LEU:H	4:A:926:GLN:HE21	1.66	0.43
5:B:707:PRO:HB2	5:B:708:GLU:H	1.61	0.43
6:C:31:ASN:C	6:C:33:LEU:N	2.75	0.43
4:A:18:GLN:HG2	4:A:1418:LEU:CD1	2.48	0.43
4:A:567:LYS:HE3	9:H:46:LEU:HD12	1.98	0.43
4:A:574:GLY:O	4:A:575:LYS:C	2.60	0.43
4:A:680:THR:C	4:A:682:THR:H	2.26	0.43
4:A:683:ILE:HG21	4:A:801:GLU:HG2	2.00	0.43
4:A:1198:ASP:O	4:A:1202:MET:HG2	2.18	0.43
5:B:97:VAL:HB	5:B:178:ASN:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:198:ASP:OD1	5:B:485:ARG:NH2	2.51	0.43
5:B:942:ARG:O	5:B:944:THR:N	2.51	0.43
6:C:74:SER:O	6:C:77:ILE:HB	2.18	0.43
8:F:100:GLN:O	8:F:105:ALA:HB3	2.19	0.43
9:H:23:VAL:HG21	9:H:121:LEU:HD21	1.99	0.43
5:B:54:PHE:HA	5:B:58:THR:HB	2.00	0.43
5:B:487:THR:HG22	5:B:489:SER:H	1.82	0.43
5:B:800:GLN:CB	11:J:52:THR:HG22	2.48	0.43
5:B:980:PHE:N	5:B:980:PHE:HD1	2.14	0.43
4:A:909:ASP:C	4:A:911:SER:H	2.26	0.43
4:A:1140:HIS:HB2	4:A:1276:VAL:O	2.17	0.43
5:B:900:ALA:HB3	13:L:61:THR:HG23	1.99	0.43
8:F:77:ASP:OD1	8:F:77:ASP:N	2.50	0.43
4:A:535:THR:HG21	4:A:617:VAL:H	1.83	0.43
4:A:828:ALA:HB2	5:B:530:GLY:HA2	2.00	0.43
4:A:1015:VAL:O	4:A:1018:PHE:N	2.51	0.43
5:B:487:THR:HG22	5:B:488:TYR:N	2.31	0.43
5:B:610:ASN:HB3	5:B:613:VAL:HG23	1.99	0.43
5:B:696:GLU:O	5:B:699:GLU:HB2	2.18	0.43
5:B:870:ILE:HG22	5:B:870:ILE:O	2.18	0.43
6:C:33:LEU:HD12	6:C:251:LEU:HD23	1.99	0.43
11:J:44:TYR:HA	11:J:47:ARG:HB2	2.01	0.43
4:A:535:THR:O	4:A:536:LEU:C	2.61	0.43
4:A:711:ARG:HG2	10:I:97:MET:HE3	2.00	0.43
4:A:774:ARG:HG3	4:A:797:LYS:HE3	2.01	0.43
4:A:1155:ASP:OD1	4:A:1162:VAL:HG23	2.18	0.43
5:B:552:MET:HA	5:B:555:ILE:HB	2.00	0.43
4:A:68:GLN:C	4:A:70:CYS:H	2.26	0.43
4:A:535:THR:HG23	4:A:575:LYS:HG2	2.00	0.43
5:B:577:ALA:HB1	5:B:589:VAL:CG1	2.49	0.43
6:C:63:ILE:O	6:C:66:ARG:N	2.52	0.43
4:A:93:VAL:HG22	4:A:301:ALA:HA	2.01	0.43
4:A:560:ILE:HD11	12:K:58:PHE:CD1	2.54	0.43
4:A:709:THR:HG22	4:A:710:LEU:N	2.34	0.43
4:A:834:THR:HG21	4:A:1077:THR:OG1	2.18	0.43
5:B:801:LYS:O	5:B:801:LYS:HG3	2.17	0.43
5:B:1021:MET:HE3	5:B:1021:MET:HB2	1.81	0.43
6:C:102:GLN:HG2	6:C:154:LYS:HD3	2.00	0.43
7:E:77:SER:CB	7:E:105:PHE:HD2	2.31	0.43
9:H:44:VAL:O	9:H:44:VAL:HG12	2.18	0.43
9:H:95:TYR:C	9:H:95:TYR:CD2	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:43:GLY:HA2	12:K:71:PHE:CE1	2.52	0.43
12:K:92:ASN:O	12:K:93:SER:C	2.61	0.43
4:A:746:MET:HG2	5:B:1015:HIS:HE1	1.83	0.43
4:A:802:ASN:HD21	5:B:729:ILE:N	2.16	0.43
4:A:1319:VAL:HG13	4:A:1320:PRO:HD2	2.01	0.43
5:B:254:LEU:HD23	5:B:381:MET:SD	2.59	0.43
5:B:690:VAL:HG12	5:B:691:GLU:H	1.82	0.43
5:B:842:ASN:HD22	5:B:845:SER:HB3	1.83	0.43
5:B:899:ILE:HG22	5:B:900:ALA:H	1.84	0.43
6:C:73:GLN:HE21	6:C:74:SER:H	1.67	0.43
5:B:363:HIS:HD2	5:B:585:VAL:CG2	2.32	0.43
6:C:34:ARG:NH1	6:C:35:ARG:HG2	2.34	0.43
4:A:1280:GLU:HB3	4:A:1281:ARG:H	1.54	0.42
5:B:604:ARG:HH21	5:B:614:SER:HA	1.84	0.42
5:B:796:LEU:HD23	5:B:799:PRO:HA	2.01	0.42
6:C:183:TRP:O	6:C:184:ASN:C	2.62	0.42
7:E:198:ILE:HD12	7:E:210:SER:O	2.18	0.42
10:I:30:ARG:HD2	10:I:30:ARG:H	1.84	0.42
4:A:434:ARG:NH2	4:A:437:MET:HG3	2.34	0.42
4:A:1021:LEU:O	4:A:1022:LEU:C	2.61	0.42
4:A:1116:LEU:HB2	4:A:1308:THR:OG1	2.18	0.42
4:A:1154:TYR:HD1	4:A:1191:TRP:CZ3	2.37	0.42
5:B:364:ILE:HD13	5:B:585:VAL:HG13	2.00	0.42
8:F:81:THR:O	8:F:82:THR:C	2.61	0.42
4:A:320:ARG:HB2	5:B:471:LYS:HE2	2.01	0.42
4:A:689:LYS:HG2	4:A:689:LYS:O	2.19	0.42
5:B:479:VAL:O	5:B:480:SER:CB	2.67	0.42
7:E:147:HIS:HB3	7:E:150:VAL:HG23	2.00	0.42
7:E:160:GLU:O	7:E:163:GLU:HB3	2.20	0.42
4:A:356:ASP:HA	4:A:357:PRO:HD2	1.74	0.42
5:B:800:GLN:HG2	11:J:52:THR:CG2	2.46	0.42
5:B:1119:VAL:O	5:B:1126:GLY:HA3	2.19	0.42
12:K:40:HIS:O	12:K:41:THR:C	2.63	0.42
4:A:51:GLY:HA2	4:A:56:PRO:HG3	2.01	0.42
4:A:93:VAL:HG23	4:A:304:MET:HE2	2.01	0.42
4:A:577:ILE:H	4:A:577:ILE:HG13	1.54	0.42
4:A:899:VAL:O	4:A:929:LEU:HD12	2.20	0.42
5:B:1102:LYS:O	5:B:1103:ILE:C	2.62	0.42
7:E:55:ARG:HB3	7:E:82:PHE:HB3	2.02	0.42
7:E:135:PHE:CD2	7:E:140:LEU:HD11	2.54	0.42
11:J:2:ILE:HD12	11:J:2:ILE:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:65:HIS:CD2	12:K:67:PHE:H	2.37	0.42
5:B:287:ARG:HG2	5:B:292:ILE:HA	2.02	0.42
5:B:899:ILE:H	5:B:899:ILE:HG13	1.69	0.42
6:C:176:ILE:HG12	6:C:232:VAL:HG13	2.02	0.42
12:K:7:PHE:HA	12:K:10:PHE:CE2	2.55	0.42
4:A:54:ASN:O	4:A:55:ASP:HB2	2.19	0.42
4:A:797:LYS:HE3	4:A:797:LYS:HB3	1.88	0.42
4:A:1366:ARG:HG2	4:A:1366:ARG:H	1.59	0.42
5:B:273:LEU:HD21	5:B:360:PHE:HD1	1.84	0.42
5:B:1072:MET:HE3	5:B:1087:PHE:CE1	2.53	0.42
5:B:1117:GLN:NE2	5:B:1199:ALA:HB2	2.34	0.42
6:C:204:SER:C	6:C:206:ASN:N	2.78	0.42
7:E:196:VAL:HG23	7:E:197:LYS:N	2.35	0.42
9:H:2:SER:O	9:H:3:ASN:HB2	2.20	0.42
4:A:343:LYS:HZ1	5:B:1197:PRO:HB3	1.85	0.42
4:A:347:PHE:HB2	5:B:1150:ARG:NH2	2.35	0.42
4:A:845:LEU:O	4:A:846:GLU:C	2.62	0.42
5:B:345:LYS:O	5:B:348:ARG:HG2	2.20	0.42
5:B:865:LYS:HB2	5:B:866:TYR:CA	2.49	0.42
5:B:994:TYR:HB2	5:B:999:MET:HE1	2.00	0.42
5:B:1190:ASP:O	5:B:1191:ILE:HG13	2.19	0.42
6:C:3:GLU:HB3	12:K:104:ASN:HD21	1.85	0.42
6:C:67:LEU:O	6:C:68:GLY:C	2.63	0.42
4:A:455:MET:CE	5:B:1138:MET:SD	3.08	0.42
4:A:901:LEU:HG	4:A:926:GLN:HE21	1.84	0.42
4:A:1118:VAL:HB	4:A:1306:LEU:HB2	2.01	0.42
5:B:174:LEU:HD11	5:B:204:ILE:HG13	2.02	0.42
6:C:181:ASP:HA	6:C:182:PRO:HD2	1.82	0.42
4:A:909:ASP:OD2	4:A:910:PRO:HD2	2.20	0.42
5:B:43:LEU:HD23	5:B:43:LEU:HA	1.88	0.42
5:B:118:ARG:HH22	5:B:194:GLU:CD	2.27	0.42
5:B:429:PHE:O	5:B:433:GLN:HG3	2.20	0.42
5:B:739:THR:OG1	5:B:740:HIS:N	2.53	0.42
5:B:1028:GLU:O	5:B:1029:CYS:C	2.63	0.42
4:A:475:THR:HG22	4:A:476:SER:N	2.35	0.41
4:A:648:ASN:OD1	4:A:648:ASN:N	2.53	0.41
4:A:811:GLN:O	4:A:812:GLU:C	2.62	0.41
4:A:1324:PRO:HB2	7:E:142:VAL:HG11	2.02	0.41
4:A:304:MET:O	4:A:305:ASP:HB2	2.20	0.41
4:A:346:ASP:H	5:B:1154:ALA:HB1	1.85	0.41
4:A:609:ASP:O	4:A:611:GLN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:645:LEU:CD1	4:A:649:ILE:HD11	2.50	0.41
4:A:1101:LEU:O	4:A:1105:LEU:HD12	2.20	0.41
5:B:1159:ARG:CD	5:B:1193:GLN:HG3	2.46	0.41
8:F:118:LEU:O	8:F:122:MET:HG3	2.20	0.41
12:K:32:VAL:HG22	12:K:74:ARG:HB2	2.02	0.41
4:A:256:GLN:CB	4:A:257:ARG:HB3	2.50	0.41
4:A:576:GLN:O	4:A:579:SER:HB2	2.21	0.41
4:A:668:ASP:HB3	4:A:743:VAL:CG2	2.33	0.41
4:A:741:ASN:HD22	4:A:741:ASN:C	2.27	0.41
4:A:902:LEU:H	4:A:902:LEU:HG	1.50	0.41
5:B:476:ARG:O	5:B:477:ALA:C	2.63	0.41
5:B:762:ASN:HD21	5:B:1022:THR:HA	1.85	0.41
5:B:846:ILE:HG23	5:B:974:PRO:HG2	2.02	0.41
5:B:874:PHE:CD2	5:B:914:LYS:HB3	2.54	0.41
5:B:1174:LYS:HB2	5:B:1179:GLN:O	2.20	0.41
6:C:37:MET:HB2	6:C:37:MET:HE3	1.92	0.41
2:T:17:DA:OP1	4:A:337:ARG:NH2	2.54	0.41
4:A:328:ARG:HD3	4:A:335:ARG:HH12	1.84	0.41
4:A:407:ARG:HG2	4:A:430:TRP:CE2	2.55	0.41
4:A:414:ASP:OD1	4:A:416:ARG:HG2	2.20	0.41
4:A:662:PHE:O	5:B:828:ALA:HA	2.19	0.41
4:A:913:LEU:HD12	4:A:915:SER:N	2.31	0.41
4:A:1332:PHE:CE1	4:A:1348:LEU:HD13	2.55	0.41
4:A:1389:PHE:C	4:A:1391:ARG:H	2.28	0.41
5:B:711:GLU:N	5:B:712:PRO:CD	2.84	0.41
5:B:724:ASP:C	5:B:726:ALA:H	2.27	0.41
5:B:855:PHE:N	5:B:970:THR:O	2.53	0.41
12:K:73:LEU:HD12	12:K:73:LEU:HA	1.82	0.41
4:A:986:ILE:HG21	4:A:1028:THR:HA	2.03	0.41
5:B:609:ILE:O	5:B:610:ASN:C	2.62	0.41
5:B:899:ILE:HD11	5:B:911:ILE:HG23	2.02	0.41
6:C:31:ASN:C	6:C:33:LEU:H	2.27	0.41
7:E:86:PRO:HB3	7:E:114:ASN:HD22	1.84	0.41
9:H:5:LEU:O	9:H:133:ASN:HB3	2.21	0.41
9:H:93:TYR:CD2	9:H:145:ARG:HB3	2.56	0.41
9:H:104:PHE:HD2	9:H:114:VAL:HG12	1.86	0.41
4:A:115:LEU:HB2	4:A:122:MET:HE3	2.02	0.41
4:A:562:THR:HG22	4:A:563:PRO:HD2	2.03	0.41
6:C:42:PRO:HA	6:C:163:ILE:HG23	2.02	0.41
8:F:132:LEU:O	8:F:148:VAL:HG23	2.20	0.41
12:K:20:LYS:HE3	12:K:22:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:321:PRO:HB2	4:A:322:VAL:H	1.55	0.41
5:B:416:LEU:HD23	5:B:420:LEU:HD12	2.02	0.41
5:B:800:GLN:HB3	11:J:52:THR:CG2	2.50	0.41
5:B:1024:ALA:O	5:B:1027:ILE:N	2.53	0.41
8:F:81:THR:HG21	8:F:136:ARG:HD3	2.02	0.41
9:H:42:ILE:HD12	9:H:95:TYR:CZ	2.56	0.41
9:H:44:VAL:HG13	9:H:48:PRO:HA	2.02	0.41
4:A:84:ILE:HD11	4:A:270:LEU:HG	2.03	0.41
4:A:619:LYS:O	4:A:623:GLY:N	2.49	0.41
4:A:1344:GLY:O	4:A:1345:ARG:C	2.62	0.41
5:B:800:GLN:HB3	11:J:52:THR:HG22	2.03	0.41
4:A:65:LEU:O	4:A:71:GLN:HA	2.21	0.41
4:A:848:ILE:HG22	4:A:1064:VAL:HG23	2.03	0.41
5:B:34:ILE:O	5:B:37:PHE:O	2.38	0.41
5:B:100:PRO:HA	5:B:126:SER:HB3	2.03	0.41
5:B:114:PRO:HB2	5:B:194:GLU:OE2	2.21	0.41
5:B:492:LEU:HB3	5:B:751:VAL:HG21	2.02	0.41
5:B:702:LEU:H	5:B:739:THR:HG23	1.84	0.41
5:B:1164:GLY:HA3	5:B:1190:ASP:HB3	2.03	0.41
6:C:120:ILE:H	6:C:120:ILE:HG13	1.74	0.41
6:C:235:VAL:HG21	11:J:6:ARG:HH21	1.86	0.41
7:E:24:LYS:HB3	7:E:30:ILE:HD12	2.02	0.41
9:H:24:CYS:HB2	9:H:44:VAL:HG23	2.02	0.41
9:H:109:LYS:HB3	9:H:110:ASP:HA	0.60	0.41
4:A:341:MET:HE2	4:A:843:LYS:NZ	2.36	0.41
4:A:503:GLN:HE21	8:F:90:ARG:HH21	1.69	0.41
4:A:623:GLY:C	4:A:625:SER:H	2.29	0.41
4:A:901:LEU:HD12	4:A:926:GLN:HG2	2.02	0.41
5:B:258:LEU:HD13	5:B:269:ILE:HG12	2.03	0.41
7:E:135:PHE:HD2	7:E:140:LEU:HD11	1.87	0.41
9:H:12:VAL:HB	9:H:53:ASP:H	1.86	0.41
9:H:38:LEU:HD12	9:H:124:ARG:O	2.21	0.41
9:H:123:MET:HE1	9:H:142:LEU:HD11	2.03	0.41
11:J:8:PHE:H	11:J:49:MET:CE	2.27	0.41
12:K:6:ARG:O	12:K:9:LEU:HG	2.21	0.41
12:K:12:LEU:HD12	12:K:12:LEU:N	2.35	0.41
12:K:65:HIS:CD2	12:K:65:HIS:C	2.99	0.41
4:A:401:GLY:N	4:A:435:HIS:HD2	2.18	0.40
4:A:756:ILE:O	4:A:760:GLN:HG3	2.20	0.40
4:A:1339:LEU:CD1	7:E:147:HIS:CD2	3.04	0.40
5:B:550:ASP:OD1	5:B:551:PRO:CD	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:653:VAL:HG22	5:B:689:LEU:HB3	2.03	0.40
5:B:1045:SER:HA	5:B:1046:PRO:HD3	1.85	0.40
6:C:46:ILE:H	6:C:46:ILE:HG12	1.71	0.40
10:I:33:SER:O	10:I:34:TYR:C	2.64	0.40
4:A:315:LEU:HD12	4:A:319:GLY:O	2.22	0.40
4:A:388:LEU:O	4:A:391:LEU:HB2	2.22	0.40
4:A:469:ARG:HB3	4:A:469:ARG:NH1	2.37	0.40
4:A:605:MET:HE3	4:A:614:PHE:O	2.21	0.40
4:A:837:ILE:HD13	4:A:837:ILE:HA	1.86	0.40
5:B:899:ILE:HG22	5:B:900:ALA:N	2.37	0.40
7:E:16:PHE:O	7:E:17:ARG:C	2.63	0.40
4:A:224:PHE:HD2	4:A:229:SER:O	2.04	0.40
4:A:455:MET:SD	5:B:1137:CYS:HB3	2.54	0.40
4:A:662:PHE:HB3	5:B:829:CYS:SG	2.61	0.40
4:A:730:GLY:C	4:A:732:LEU:H	2.30	0.40
5:B:28:GLU:C	5:B:30:SER:N	2.79	0.40
5:B:724:ASP:HA	5:B:725:PRO:HD3	1.98	0.40
5:B:843:GLN:O	5:B:844:SER:C	2.64	0.40
6:C:242:GLN:HA	6:C:245:VAL:HB	2.02	0.40
8:F:99:LEU:HD13	8:F:99:LEU:C	2.47	0.40
9:H:111:LEU:HD23	9:H:111:LEU:HA	1.93	0.40
4:A:443:LEU:HD23	4:A:443:LEU:HA	1.76	0.40
4:A:466:SER:O	5:B:1103:ILE:CD1	2.67	0.40
4:A:568:PRO:HB3	6:C:221:TYR:CE1	2.56	0.40
4:A:650:GLN:O	4:A:651:LYS:C	2.63	0.40
4:A:737:LEU:HD23	4:A:737:LEU:HA	1.94	0.40
4:A:1351:GLU:OE2	4:A:1351:GLU:HA	2.18	0.40
4:A:1393:ASN:O	4:A:1393:ASN:OD1	2.40	0.40
5:B:117:ALA:HA	5:B:122:LEU:HB2	2.04	0.40
5:B:839:MET:HB3	5:B:1012:ILE:HG22	2.02	0.40
9:H:95:TYR:C	9:H:95:TYR:HD2	2.30	0.40
11:J:1:MET:N	11:J:56:LEU:H	2.20	0.40
11:J:1:MET:O	11:J:2:ILE:HG22	2.22	0.40
4:A:1066:VAL:O	4:A:1067:LEU:C	2.63	0.40
5:B:899:ILE:CD1	5:B:911:ILE:HG23	2.51	0.40
5:B:1138:MET:HA	5:B:1138:MET:HE3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	1383/1733 (80%)	1136 (82%)	182 (13%)	65 (5%)	2	17
5	B	1087/1224 (89%)	918 (84%)	124 (11%)	45 (4%)	2	19
6	C	265/318 (83%)	222 (84%)	34 (13%)	9 (3%)	3	23
7	E	212/215 (99%)	180 (85%)	25 (12%)	7 (3%)	3	23
8	F	84/155 (54%)	73 (87%)	10 (12%)	1 (1%)	10	41
9	H	129/146 (88%)	101 (78%)	23 (18%)	5 (4%)	2	20
10	I	117/122 (96%)	95 (81%)	18 (15%)	4 (3%)	3	23
11	J	63/70 (90%)	56 (89%)	5 (8%)	2 (3%)	3	24
12	K	112/120 (93%)	97 (87%)	11 (10%)	4 (4%)	2	22
13	L	44/70 (63%)	25 (57%)	11 (25%)	8 (18%)	0	1
All	All	3496/4173 (84%)	2903 (83%)	443 (13%)	150 (4%)	2	18

All (150) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	54	ASN
4	A	55	ASP
4	A	93	VAL
4	A	248	PRO
4	A	321	PRO
4	A	399	HIS
4	A	567	LYS
4	A	597	LEU
4	A	846	GLU
4	A	853	ASP
4	A	1036	ARG
4	A	1274	ARG
4	A	1435	PRO
4	A	1437	GLY

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Mol	Chain	Res	Type
5	B	21	GLU
5	B	229	ALA
5	B	483	LEU
5	B	484	ASN
5	B	531	GLN
5	B	636	PRO
5	B	707	PRO
5	B	731	VAL
5	B	958	GLN
7	E	59	SER
7	E	206	GLY
9	H	32	THR
9	H	110	ASP
10	I	34	TYR
11	J	2	ILE
13	L	53	HIS
13	L	55	ILE
4	A	50	ILE
4	A	76	GLU
4	A	257	ARG
4	A	312	PRO
4	A	315	LEU
4	A	323	LYS
4	A	424	ILE
4	A	583	PRO
4	A	593	GLU
4	A	609	ASP
4	A	922	ASP
4	A	1221	LYS
4	A	1314	SER
5	B	466	TRP
5	B	478	GLY
5	B	643	ASP
5	B	710	LEU
5	B	712	PRO
5	B	883	LEU
6	C	90	ASP
6	C	142	VAL
6	C	267	GLN
8	F	128	LYS
9	H	139	ASN
10	I	9	ASP

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Mol	Chain	Res	Type
10	I	11	ASN
10	I	77	LYS
13	L	47	ARG
13	L	63	ARG
4	A	66	LYS
4	A	68	GLN
4	A	253	ASN
4	A	254	GLU
4	A	418	SER
4	A	568	PRO
4	A	870	GLU
4	A	958	VAL
4	A	972	HIS
4	A	1388	GLY
5	B	38	PHE
5	B	294	ASP
5	B	322	PHE
5	B	468	GLU
5	B	474	SER
5	B	879	ARG
5	B	902	GLY
5	B	943	SER
5	B	986	GLN
5	B	1096	ARG
6	C	110	THR
7	E	165	LEU
11	J	6	ARG
12	K	70	ARG
13	L	46	VAL
13	L	50	ASP
4	A	56	PRO
4	A	178	GLY
4	A	305	ASP
4	A	324	SER
4	A	332	LYS
4	A	465	TYR
4	A	544	ASP
4	A	1016	THR
4	A	1054	LEU
4	A	1270	ASN
4	A	1396	ALA
4	A	1401	SER

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Mol	Chain	Res	Type
5	B	230	ALA
5	B	467	GLY
5	B	733	HIS
5	B	864	LYS
5	B	974	PRO
5	B	1017	ILE
6	C	6	PRO
6	C	181	ASP
6	C	205	LYS
7	E	4	GLU
7	E	124	VAL
9	H	128	ASN
12	K	4	PRO
12	K	5	ASP
12	K	28	PRO
13	L	59	ALA
4	A	591	PHE
4	A	700	ASN
4	A	961	ARG
5	B	90	ILE
5	B	176	SER
5	B	290	GLY
5	B	436	VAL
5	B	648	HIS
5	B	732	SER
5	B	880	THR
5	B	901	PRO
5	B	1178	ASN
5	B	1181	GLU
6	C	182	PRO
9	H	140	ALA
13	L	56	LEU
4	A	27	VAL
4	A	364	VAL
4	A	536	LEU
4	A	610	GLY
4	A	1107	VAL
4	A	1173	HIS
5	B	292	ILE
5	B	881	ASN
4	A	793	SER
4	A	1424	VAL

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Mol	Chain	Res	Type
4	A	51	GLY
5	B	410	GLY
4	A	1324	PRO
6	C	21	ILE
4	A	35	ILE
5	B	867	GLY
7	E	76	GLY
7	E	189	GLY
4	A	400	PRO
4	A	647	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	
4	A	1218/1520 (80%)	1060 (87%)	158 (13%)	4	21
5	B	959/1061 (90%)	833 (87%)	126 (13%)	4	20
6	C	235/274 (86%)	212 (90%)	23 (10%)	7	30
7	E	196/197 (100%)	179 (91%)	17 (9%)	9	33
8	F	76/137 (56%)	67 (88%)	9 (12%)	5	23
9	H	117/128 (91%)	104 (89%)	13 (11%)	6	25
10	I	113/116 (97%)	97 (86%)	16 (14%)	3	18
11	J	60/65 (92%)	52 (87%)	8 (13%)	4	20
12	K	99/102 (97%)	85 (86%)	14 (14%)	3	18
13	L	40/57 (70%)	32 (80%)	8 (20%)	1	7
All	All	3113/3657 (85%)	2721 (87%)	392 (13%)	4	21

All (392) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	6	TYR
4	A	13	THR
4	A	32	VAL

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Mol	Chain	Res	Type
4	A	58	LEU
4	A	61	ILE
4	A	70	CYS
4	A	93	VAL
4	A	100	LYS
4	A	105	CYS
4	A	116	ASP
4	A	133	LYS
4	A	169	ASN
4	A	180	LYS
4	A	184	SER
4	A	208	LEU
4	A	216	VAL
4	A	222	LEU
4	A	225	ASN
4	A	234	MET
4	A	235	ILE
4	A	237	THR
4	A	249	SER
4	A	250	ILE
4	A	253	ASN
4	A	257	ARG
4	A	263	THR
4	A	270	LEU
4	A	295	LEU
4	A	297	GLN
4	A	303	TYR
4	A	308	ILE
4	A	315	LEU
4	A	316	GLN
4	A	324	SER
4	A	335	ARG
4	A	337	ARG
4	A	379	VAL
4	A	385	ILE
4	A	391	LEU
4	A	403	LYS
4	A	409	SER
4	A	413	ILE
4	A	419	LYS
4	A	443	LEU
4	A	449	SER

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Mol	Chain	Res	Type
4	A	450	LEU
4	A	454	SER
4	A	463	ILE
4	A	466	SER
4	A	469	ARG
4	A	470	LEU
4	A	472	LEU
4	A	475	THR
4	A	485	ASP
4	A	496	GLU
4	A	501	LEU
4	A	509	LEU
4	A	527	THR
4	A	538	ASP
4	A	544	ASP
4	A	550	LEU
4	A	565	ILE
4	A	566	ILE
4	A	576	GLN
4	A	577	ILE
4	A	588	LEU
4	A	596	THR
4	A	597	LEU
4	A	599	SER
4	A	612	ILE
4	A	618	GLU
4	A	634	THR
4	A	648	ASN
4	A	679	ILE
4	A	702	LEU
4	A	732	LEU
4	A	735	VAL
4	A	740	LEU
4	A	741	ASN
4	A	756	ILE
4	A	765	VAL
4	A	795	GLU
4	A	801	GLU
4	A	803	SER
4	A	806	ARG
4	A	821	ARG
4	A	830	LYS

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Mol	Chain	Res	Type
4	A	831	THR
4	A	837	ILE
4	A	838	GLN
4	A	855	THR
4	A	856	THR
4	A	858	ASN
4	A	867	ILE
4	A	871	ASP
4	A	880	LYS
4	A	885	THR
4	A	886	ILE
4	A	889	SER
4	A	902	LEU
4	A	908	LEU
4	A	913	LEU
4	A	918	GLU
4	A	920	LEU
4	A	929	LEU
4	A	949	ASP
4	A	964	ILE
4	A	969	GLN
4	A	982	THR
4	A	996	ASN
4	A	1017	LEU
4	A	1034	GLU
4	A	1058	VAL
4	A	1067	LEU
4	A	1094	VAL
4	A	1095	THR
4	A	1110	ASN
4	A	1117	THR
4	A	1118	VAL
4	A	1120	LEU
4	A	1129	GLU
4	A	1135	ARG
4	A	1142	THR
4	A	1146	VAL
4	A	1159	ARG
4	A	1176	LEU
4	A	1187	GLN
4	A	1193	LEU
4	A	1221	LYS

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Mol	Chain	Res	Type
4	A	1223	ASP
4	A	1259	MET
4	A	1262	LYS
4	A	1264	GLU
4	A	1276	VAL
4	A	1280	GLU
4	A	1281	ARG
4	A	1288	ASP
4	A	1291	VAL
4	A	1295	THR
4	A	1299	VAL
4	A	1308	THR
4	A	1316	VAL
4	A	1322	ILE
4	A	1325	THR
4	A	1329	THR
4	A	1333	ILE
4	A	1335	ILE
4	A	1350	LYS
4	A	1351	GLU
4	A	1366	ARG
4	A	1370	LEU
4	A	1372	VAL
4	A	1376	THR
4	A	1384	VAL
4	A	1385	THR
4	A	1393	ASN
4	A	1394	THR
4	A	1404	GLU
5	B	21	GLU
5	B	26	THR
5	B	28	GLU
5	B	34	ILE
5	B	35	SER
5	B	45	SER
5	B	63	ILE
5	B	66	ASP
5	B	97	VAL
5	B	98	THR
5	B	102	VAL
5	B	104	GLU
5	B	108	VAL

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Mol	Chain	Res	Type
5	B	109	THR
5	B	120	ARG
5	B	126	SER
5	B	128	LEU
5	B	134	LYS
5	B	175	ARG
5	B	199	MET
5	B	206	ASN
5	B	234	ILE
5	B	244	LEU
5	B	246	LYS
5	B	249	ARG
5	B	268	THR
5	B	291	ILE
5	B	294	ASP
5	B	315	LYS
5	B	347	LYS
5	B	364	ILE
5	B	366	GLN
5	B	387	LEU
5	B	393	LYS
5	B	398	ARG
5	B	404	LYS
5	B	416	LEU
5	B	424	LEU
5	B	425	THR
5	B	428	ILE
5	B	453	ILE
5	B	461	LEU
5	B	471	LYS
5	B	474	SER
5	B	479	VAL
5	B	483	LEU
5	B	487	THR
5	B	498	THR
5	B	500	THR
5	B	513	GLN
5	B	537	LYS
5	B	542	MET
5	B	545	ILE
5	B	547	VAL
5	B	552	MET

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Mol	Chain	Res	Type
5	B	563	MET
5	B	567	GLU
5	B	570	VAL
5	B	599	THR
5	B	618	ASP
5	B	624	LEU
5	B	626	ILE
5	B	628	THR
5	B	635	ARG
5	B	637	LEU
5	B	642	ASP
5	B	655	LYS
5	B	685	LEU
5	B	694	ASP
5	B	701	ILE
5	B	714	GLU
5	B	736	THR
5	B	737	THR
5	B	762	ASN
5	B	764	SER
5	B	783	THR
5	B	786	ASN
5	B	790	ASP
5	B	791	THR
5	B	792	MET
5	B	807	ARG
5	B	825	VAL
5	B	835	GLN
5	B	844	SER
5	B	857	ARG
5	B	865	LYS
5	B	873	THR
5	B	878	GLN
5	B	880	THR
5	B	883	LEU
5	B	886	LYS
5	B	899	ILE
5	B	903	VAL
5	B	905	VAL
5	B	915	THR
5	B	916	THR
5	B	939	THR

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Mol	Chain	Res	Type
5	B	941	LEU
5	B	944	THR
5	B	963	PHE
5	B	967	ARG
5	B	970	THR
5	B	973	ILE
5	B	980	PHE
5	B	983	ARG
5	B	997	GLU
5	B	999	MET
5	B	1006	ILE
5	B	1020	ARG
5	B	1028	GLU
5	B	1048	THR
5	B	1076	HIS
5	B	1082	MET
5	B	1084	GLN
5	B	1096	ARG
5	B	1099	VAL
5	B	1102	LYS
5	B	1113	VAL
5	B	1132	GLU
5	B	1147	LEU
5	B	1160	VAL
5	B	1194	ILE
5	B	1196	ILE
5	B	1202	LEU
5	B	1218	THR
5	B	1220	ARG
6	C	18	VAL
6	C	21	ILE
6	C	23	SER
6	C	25	VAL
6	C	27	LEU
6	C	33	LEU
6	C	34	ARG
6	C	53	THR
6	C	56	THR
6	C	77	ILE
6	C	86	CYS
6	C	129	ILE
6	C	134	ILE

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Mol	Chain	Res	Type
6	C	140	ASN
6	C	143	LEU
6	C	156	THR
6	C	163	ILE
6	C	183	TRP
6	C	215	GLU
6	C	232	VAL
6	C	240	VAL
6	C	244	VAL
6	C	268	ASP
7	E	9	ILE
7	E	77	SER
7	E	80	VAL
7	E	92	THR
7	E	102	GLU
7	E	104	ASN
7	E	127	ILE
7	E	132	ILE
7	E	150	VAL
7	E	156	LEU
7	E	162	ARG
7	E	165	LEU
7	E	169	ARG
7	E	175	LEU
7	E	196	VAL
7	E	198	ILE
7	E	200	ARG
8	F	71	GLU
8	F	81	THR
8	F	92	ARG
8	F	97	ARG
8	F	104	ASN
8	F	109	VAL
8	F	118	LEU
8	F	119	ARG
8	F	123	LYS
9	H	4	THR
9	H	13	SER
9	H	24	CYS
9	H	42	ILE
9	H	55	LEU
9	H	61	SER

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Mol	Chain	Res	Type
9	H	77	ARG
9	H	88	SER
9	H	89	LEU
9	H	95	TYR
9	H	102	TYR
9	H	107	VAL
9	H	110	ASP
10	I	7	CYS
10	I	10	CYS
10	I	11	ASN
10	I	13	MET
10	I	17	ARG
10	I	18	GLU
10	I	28	GLU
10	I	30	ARG
10	I	50	THR
10	I	52	ILE
10	I	62	ILE
10	I	70	ARG
10	I	83	ASN
10	I	84	VAL
10	I	95	THR
10	I	107	SER
11	J	2	ILE
11	J	5	VAL
11	J	9	SER
11	J	14	VAL
11	J	31	ASP
11	J	43	ARG
11	J	48	ARG
11	J	62	ARG
12	K	6	ARG
12	K	18	LYS
12	K	21	ILE
12	K	25	THR
12	K	31	VAL
12	K	42	LEU
12	K	50	LEU
12	K	78	THR
12	K	93	SER
12	K	101	LEU
12	K	103	THR

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Mol	Chain	Res	Type
12	K	107	THR
12	K	113	THR
12	K	114	LEU
13	L	26	THR
13	L	27	LEU
13	L	31	CYS
13	L	46	VAL
13	L	55	ILE
13	L	61	THR
13	L	65	VAL
13	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	68	GLN
4	A	83	HIS
4	A	313	GLN
4	A	316	GLN
4	A	390	GLN
4	A	425	GLN
4	A	435	HIS
4	A	503	GLN
4	A	584	ASN
4	A	626	ASN
4	A	736	ASN
4	A	741	ASN
4	A	757	ASN
4	A	760	GLN
4	A	767	GLN
4	A	768	GLN
4	A	858	ASN
4	A	906	HIS
4	A	926	GLN
4	A	975	HIS
4	A	1011	GLN
4	A	1078	GLN
4	A	1171	GLN
4	A	1218	GLN
4	A	1364	ASN
4	A	1432	GLN
5	B	52	ASN

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Mol	Chain	Res	Type
5	B	103	ASN
5	B	121	ASN
5	B	178	ASN
5	B	206	ASN
5	B	363	HIS
5	B	366	GLN
5	B	383	ASN
5	B	484	ASN
5	B	515	HIS
5	B	516	ASN
5	B	657	HIS
5	B	667	GLN
5	B	686	ASN
5	B	734	HIS
5	B	744	HIS
5	B	762	ASN
5	B	767	ASN
5	B	822	ASN
5	B	842	ASN
5	B	862	GLN
5	B	878	GLN
5	B	957	ASN
5	B	958	GLN
5	B	984	HIS
5	B	986	GLN
5	B	1015	HIS
5	B	1025	HIS
5	B	1065	GLN
5	B	1076	HIS
5	B	1084	GLN
5	B	1117	GLN
5	B	1161	HIS
5	B	1178	ASN
5	B	1187	ASN
6	C	17	ASN
6	C	73	GLN
6	C	112	ASN
6	C	123	ASN
6	C	188	HIS
6	C	203	GLN
6	C	224	GLN
6	C	231	ASN

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Mol	Chain	Res	Type
6	C	242	GLN
6	C	252	GLN
7	E	32	GLN
7	E	61	GLN
7	E	101	GLN
7	E	114	ASN
7	E	147	HIS
8	F	100	GLN
8	F	104	ASN
9	H	11	GLN
9	H	33	GLN
9	H	35	GLN
9	H	134	ASN
10	I	12	ASN
10	I	46	HIS
10	I	60	GLN
10	I	83	ASN
10	I	108	HIS
10	I	116	ASN
10	I	120	GLN
12	K	52	ASN
12	K	65	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	8/9 (88%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	4	C
1	R	10	G

There are no RNA pucker outliers to report.

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

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 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	G2P	T	3000	-	30,34,34	1.08	1 (3%)	46,54,54	1.78	9 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	G2P	T	3000	-	-	5/19/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	3000	G2P	PB-O3B	2.79	1.61	1.58

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	3000	G2P	C5-C4-N3	-5.32	119.93	128.39
14	T	3000	G2P	C2-N3-C4	4.58	120.19	112.30
14	T	3000	G2P	PB-O3B-PG	-4.16	117.54	132.45
14	T	3000	G2P	N9-C4-N3	3.30	132.56	125.95
14	T	3000	G2P	C2-N1-C6	-2.85	119.94	125.11
14	T	3000	G2P	O6-C6-C5	-2.36	120.30	126.53
14	T	3000	G2P	C5-C6-N1	2.26	119.01	113.25
14	T	3000	G2P	C3'-C2'-C1'	2.03	105.30	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	3000	G2P	C4'-O4'-C1'	2.02	113.92	109.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

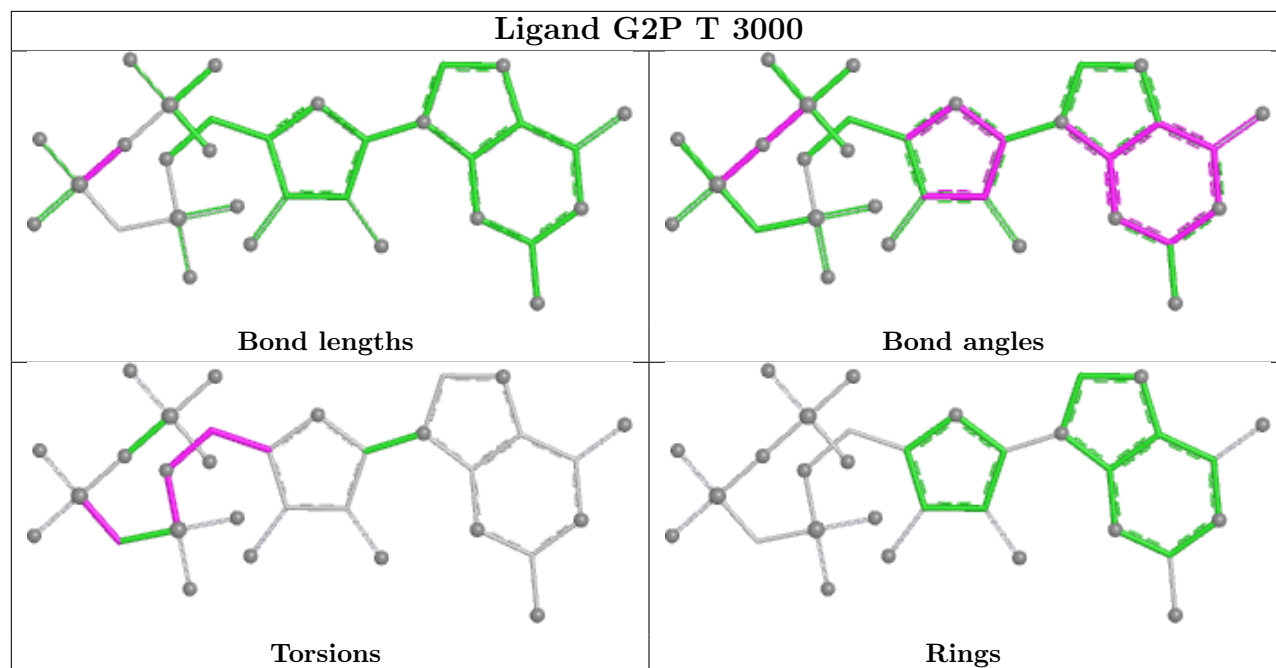
Mol	Chain	Res	Type	Atoms
14	T	3000	G2P	O4'-C4'-C5'-O5'
14	T	3000	G2P	C3'-C4'-C5'-O5'
14	T	3000	G2P	C4'-C5'-O5'-PA
14	T	3000	G2P	PA-C3A-PB-O2B
14	T	3000	G2P	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	3000	G2P	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	R	9/9 (100%)	0.46	1 (11%) 10 7	98, 111, 151, 169	0
2	T	27/27 (100%)	0.67	1 (3%) 45 25	100, 203, 234, 238	0
3	N	13/13 (100%)	0.68	0 100 100	197, 219, 252, 258	0
4	A	1395/1733 (80%)	0.00	12 (0%) 81 58	61, 99, 161, 173	0
5	B	1105/1224 (90%)	-0.01	15 (1%) 73 48	64, 94, 139, 155	0
6	C	267/318 (83%)	-0.27	1 (0%) 88 72	74, 89, 122, 144	0
7	E	214/215 (99%)	0.08	4 (1%) 66 41	79, 116, 155, 159	0
8	F	86/155 (55%)	-0.12	0 100 100	75, 105, 145, 156	0
9	H	133/146 (91%)	0.20	4 (3%) 52 30	100, 118, 146, 148	0
10	I	119/122 (97%)	0.09	2 (1%) 69 43	84, 103, 123, 142	0
11	J	65/70 (92%)	-0.33	0 100 100	69, 87, 107, 112	0
12	K	114/120 (95%)	-0.27	0 100 100	73, 95, 112, 115	0
13	L	46/70 (65%)	0.64	3 (6%) 25 15	102, 147, 159, 163	0
All	All	3593/4222 (85%)	-0.01	43 (1%) 76 52	61, 99, 157, 258	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	335	GLY	4.9
4	A	44	THR	3.9
5	B	882	THR	3.9
1	R	2	A	3.8
5	B	883	LEU	3.6
9	H	86	ASP	3.4
5	B	636	PRO	3.2
5	B	870	ILE	3.1
7	E	121	MET	3.1

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Mol	Chain	Res	Type	RSRZ
4	A	58	LEU	3.1
5	B	212	LEU	2.9
13	L	27	LEU	2.8
4	A	260	ASP	2.7
9	H	63	LEU	2.7
5	B	708	GLU	2.6
5	B	816	GLU	2.6
7	E	93	MET	2.6
5	B	106	ASP	2.5
4	A	307	ASP	2.5
4	A	1315	GLU	2.5
2	T	3	DC	2.5
5	B	39	ARG	2.5
9	H	85	GLY	2.5
5	B	407	ASP	2.4
4	A	61	ILE	2.4
7	E	126	SER	2.3
10	I	49	ILE	2.3
4	A	54	ASN	2.3
6	C	28	ALA	2.3
10	I	72	ASP	2.3
13	L	32	ALA	2.2
4	A	1081	LEU	2.2
4	A	250	ILE	2.2
5	B	446	LEU	2.2
4	A	316	GLN	2.1
13	L	25	ALA	2.1
5	B	1211	ASN	2.1
4	A	455	MET	2.1
5	B	478	GLY	2.1
9	H	90	ALA	2.1
7	E	124	VAL	2.0
4	A	1108	ALA	2.0
5	B	715	ALA	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 ⓘ

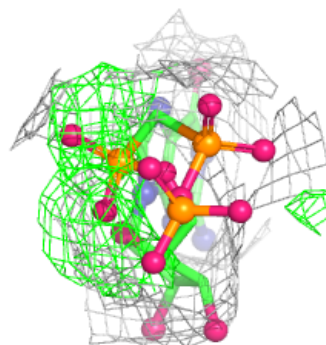
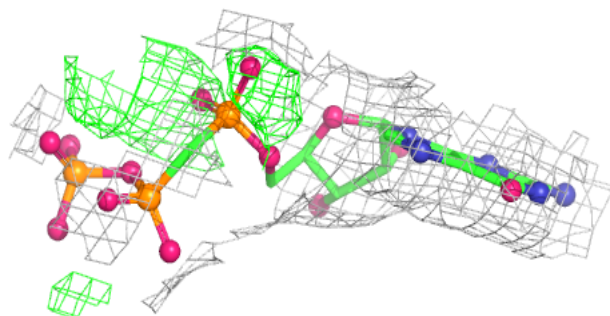
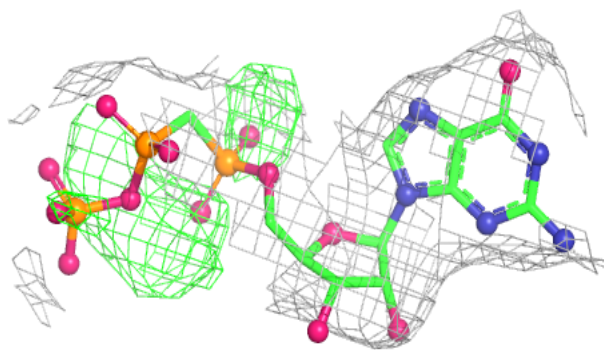
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
14	G2P	T	3000	32/32	0.85	0.11	125,129,158,158	0
16	MG	A	2002	1/1	0.86	0.22	76,76,76,76	0
15	ZN	A	1734	1/1	0.96	0.09	165,165,165,165	0
16	MG	A	2001	1/1	0.97	0.04	67,67,67,67	0
15	ZN	L	105	1/1	0.98	0.05	146,146,146,146	0
15	ZN	B	1307	1/1	0.99	0.02	138,138,138,138	0
15	ZN	A	1735	1/1	0.99	0.06	153,153,153,153	0
15	ZN	J	101	1/1	1.00	0.02	77,77,77,77	0
15	ZN	C	319	1/1	1.00	0.02	90,90,90,90	0
15	ZN	I	203	1/1	1.00	0.03	101,101,101,101	0
15	ZN	I	204	1/1	1.00	0.02	90,90,90,90	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around G2P T 3000:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.