Full wwPDB X-ray Structure Validation Report (i)

Oct 19, 2023 – 07:49 AM EDT

PDB ID	:	2NVQ
Title	:	RNA Polymerase II Elongation Complex in 150 mM Mg+2 with 2'dUTP
Authors	:	Wang, D.; Bushnell, D.A.; Westover, K.D.; Kaplan, C.D.; Kornberg, R.D.
Deposited on	:	2006-11-13
Resolution	:	2.90 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 (i) 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 (i)) were used in the production of this report:

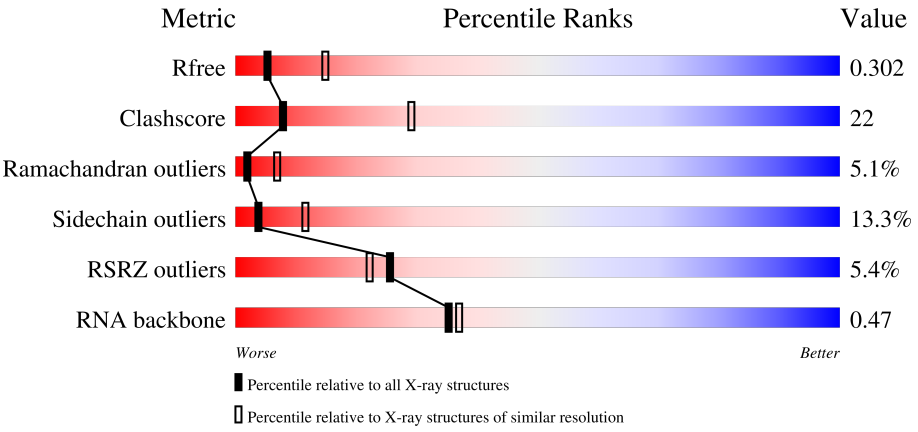
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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 <=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	10	10% 50% 30% 10%
2	T	28	25% 29% 36% 36%
3	N	14	36% 43% 57%
4	A	1733	5% 47% 26% 7% • 19%

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Mol	Chain	Length	Quality of chain
5	B	1224	4% 49% 34% 7% 9%
6	C	318	50% 27% 6% 16%
7	E	215	13% 60% 33% 7%
8	F	155	35% 17% 45%
9	H	146	8% 43% 36% 12% 9%
10	I	122	2% 56% 34% 5%
11	J	70	% 54% 31% 7% 7%
12	K	120	% 57% 35% 5%
13	L	70	3% 30% 21% 13% 34%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	DUT	T	29[B]	-	-	X	-
16	MG	A	2002[A]	-	-	-	X
16	MG	A	2002[B]	-	-	-	X

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 29425 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(*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	R	10	216	98	45	64	9	0	0	0

- Molecule 2 is a DNA chain called 28-MER DNA template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	T	28	566	271	104	164	27	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	N	14	284	137	49	85	13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	1405	11043	6965	1936	2081	61	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	B	1114	8861	5610	1549	1647	55	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	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	85	Total	C	N	O	S	0	0	0
			688	439	116	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.

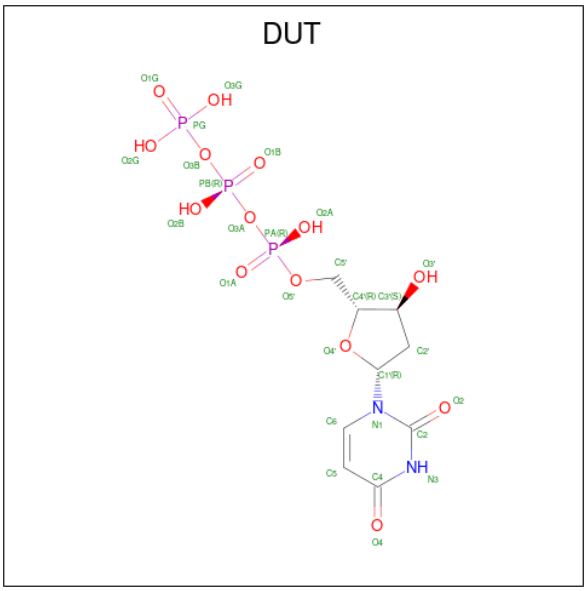
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- 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 DEOXYURIDINE-5'-TRIPHOSPHATE (three-letter code: DUT) (formula: $C_9H_{15}N_2O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	T	1	Total	C	N	O	P	0	1
			56	18	4	28	6		

- Molecule 15 is ZINC ION (three-letter code: 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 (three-letter code: MG) (formula: Mg).

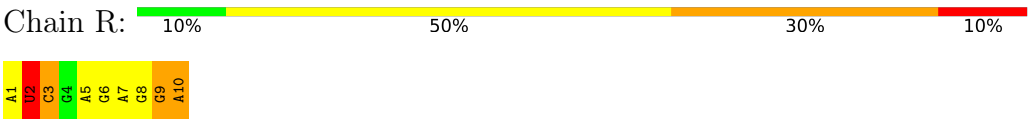
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	2	Total Mg 3 3	0	1

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.

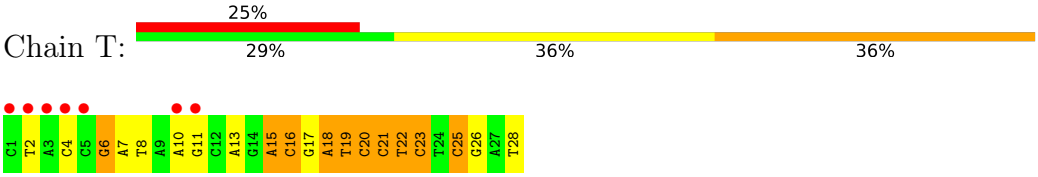
• Molecule 1: 5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3'

Chain R:



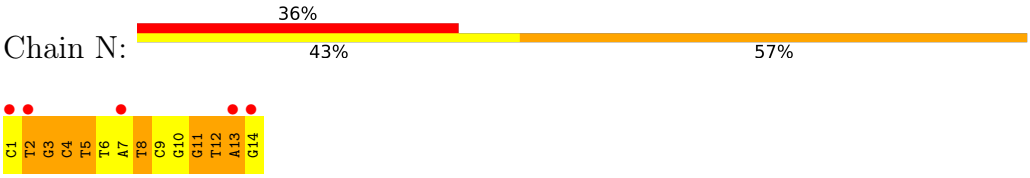
• Molecule 2: 28-MER DNA template strand

Chain T:



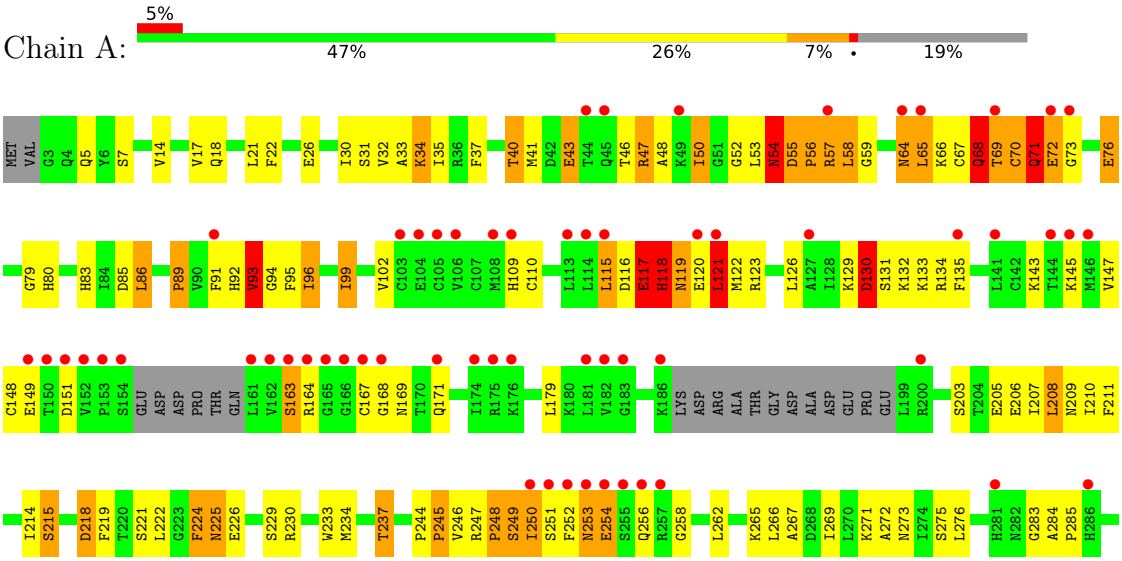
• Molecule 3: 5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3'

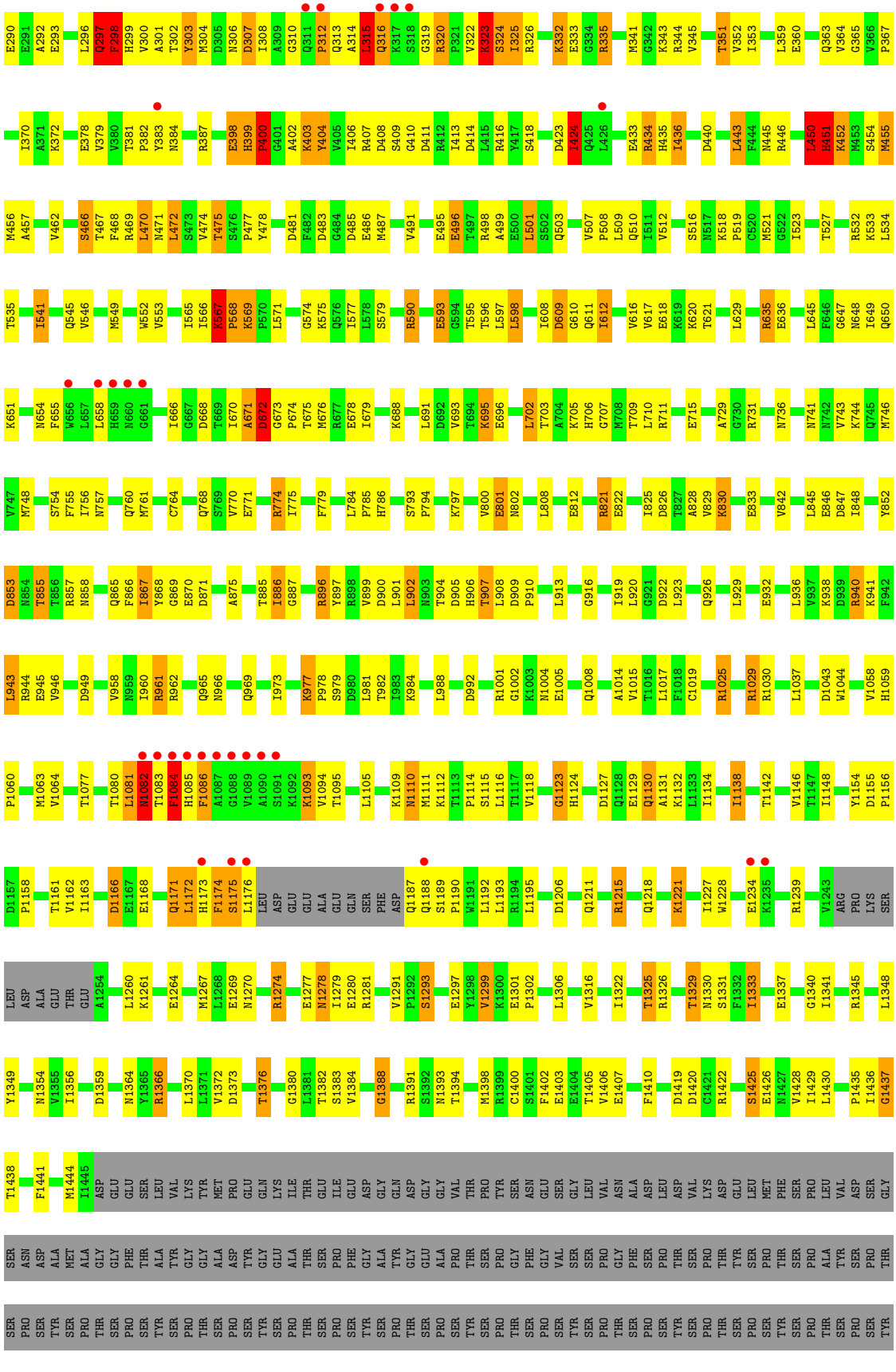
Chain N:

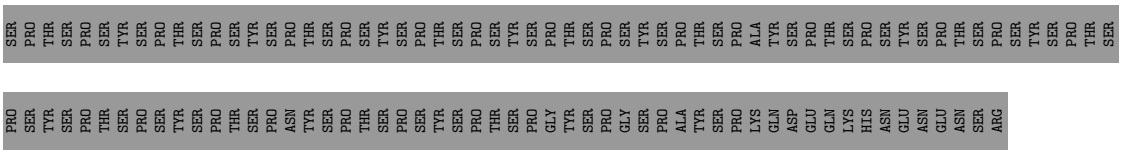


• Molecule 4: DNA-directed RNA polymerase II largest subunit

Chain A:

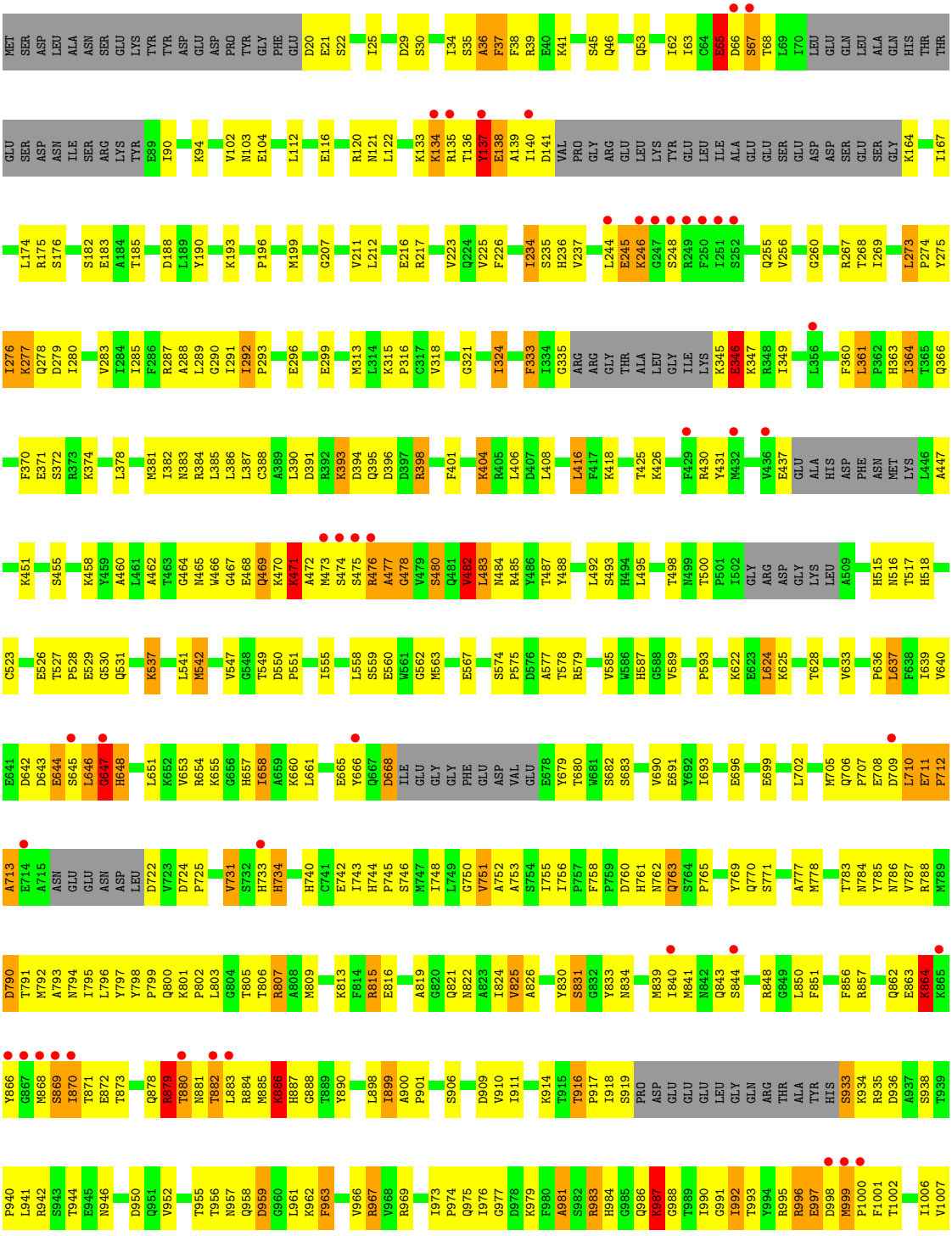


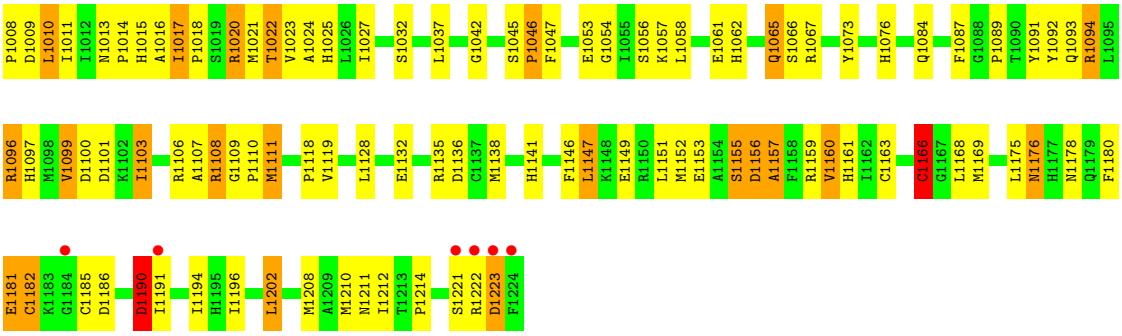




• Molecule 5: DNA-directed RNA polymerase II 140 kDa polypeptide

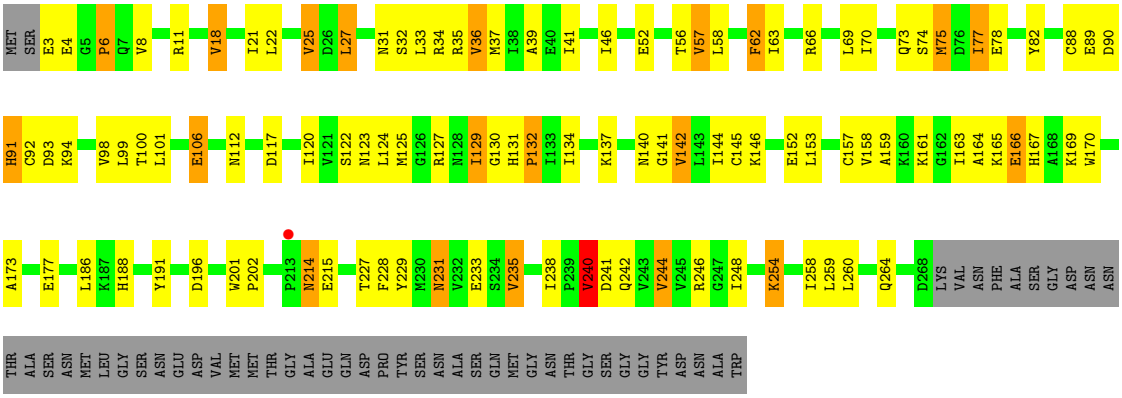
Chain B:





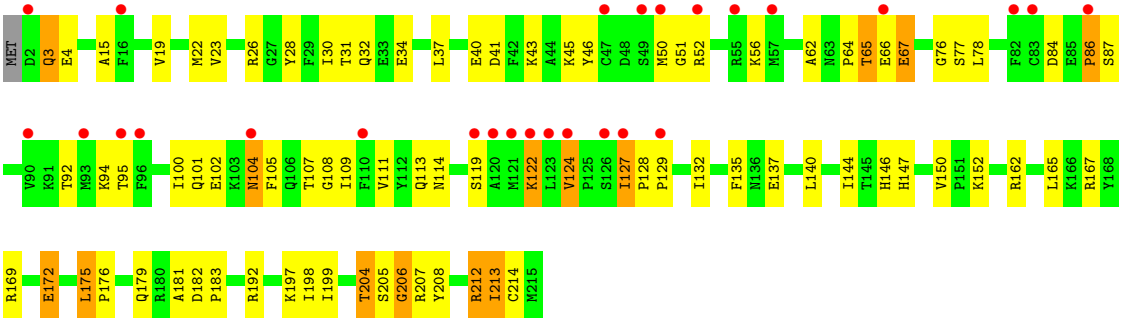
• Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide

Chain C:



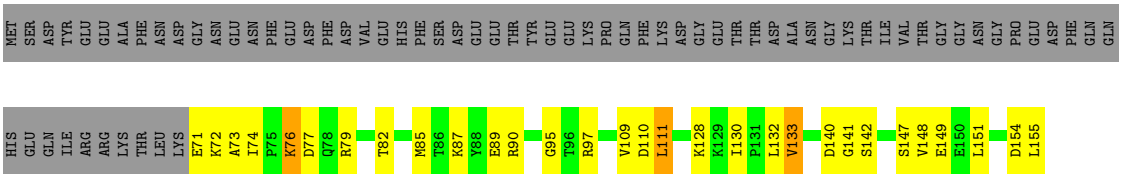
• Molecule 7: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

Chain E:



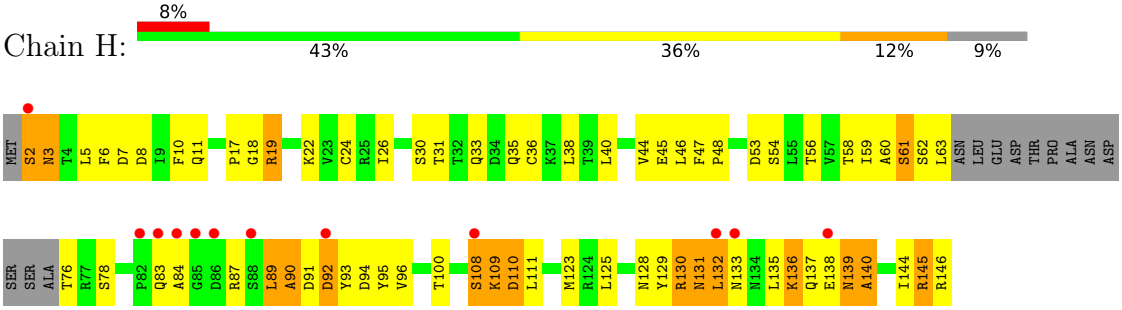
• Molecule 8: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

Chain F:



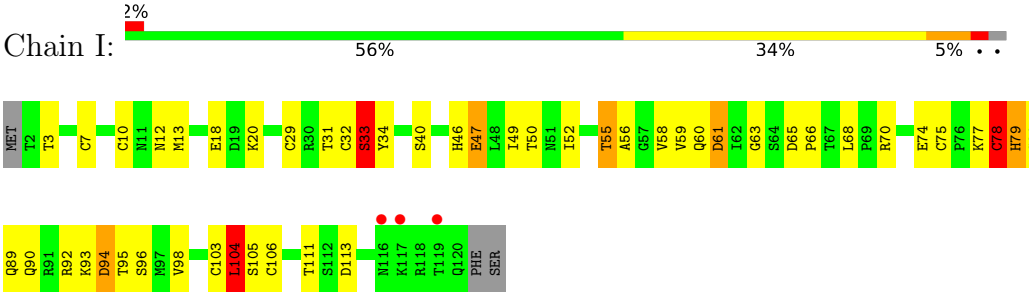
• Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

Chain H:



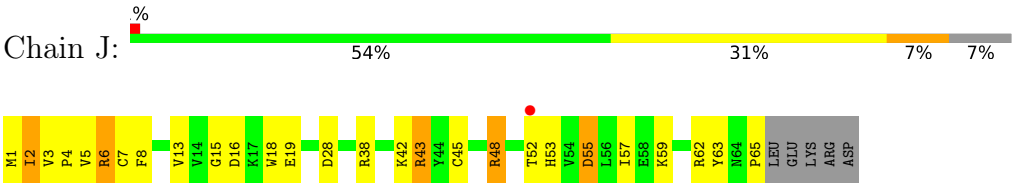
• Molecule 10: DNA-directed RNA polymerase II subunit 9

Chain I:



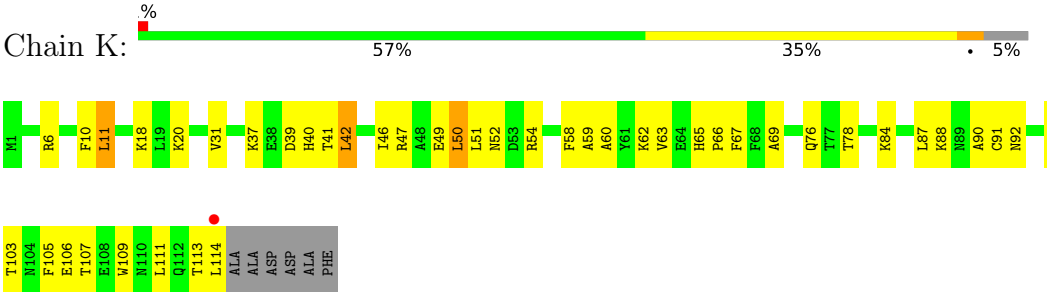
• Molecule 11: DNA-directed RNA polymerases I/II/III subunit 10

Chain J:



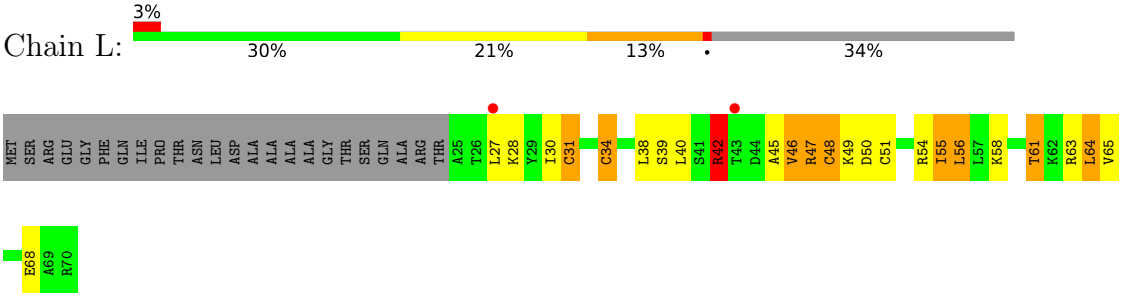
• Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K:



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

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	170.65Å 222.76Å 195.28Å 90.00° 101.31° 90.00°	Depositor
Resolution (Å)	48.45 – 2.90 48.14 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.7 (48.45-2.90) 92.7 (48.14-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.229 , 0.283 0.263 , 0.302	Depositor DCC
R_{free} test set	4429 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å^2)	59.7	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 28.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	29425	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, DUT

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	1.30	1/243 (0.4%)	2.35	19/378 (5.0%)
2	T	1.23	0/634	1.97	30/975 (3.1%)
3	N	1.30	0/317	2.06	26/488 (5.3%)
4	A	0.75	0/11241	0.79	1/15199 (0.0%)
5	B	0.86	2/9033 (0.0%)	0.87	6/12181 (0.0%)
6	C	0.83	2/2133 (0.1%)	0.84	0/2891
7	E	0.65	0/1788	0.69	0/2406
8	F	0.69	0/700	0.74	0/945
9	H	0.67	0/1086	0.79	0/1470
10	I	0.78	1/989 (0.1%)	0.85	2/1331 (0.2%)
11	J	0.89	0/541	0.88	0/727
12	K	0.78	0/937	0.82	0/1265
13	L	0.93	1/365 (0.3%)	1.08	1/485 (0.2%)
All	All	0.81	7/30007 (0.0%)	0.92	85/40741 (0.2%)

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	11
5	B	0	8
6	C	0	2
All	All	0	21

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	34	CYS	CB-SG	-6.03	1.72	1.82
6	C	88	CYS	CB-SG	-5.95	1.72	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	1	A	N9-C4	5.93	1.41	1.37
5	B	529	GLU	CG-CD	5.91	1.60	1.51
5	B	1087	PHE	CE2-CZ	5.37	1.47	1.37
6	C	78	GLU	CG-CD	5.10	1.59	1.51
10	I	7	CYS	CB-SG	-5.03	1.73	1.81

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	18	DA	O4'-C4'-C3'	-10.86	99.48	106.00
2	T	16	DC	O4'-C1'-N1	9.82	114.87	108.00
1	R	8	G	C4'-C3'-C2'	-9.14	93.46	102.60
3	N	1	DC	O4'-C1'-N1	8.83	114.18	108.00
1	R	8	G	O4'-C1'-N9	-8.56	101.35	108.20
3	N	5	DT	O4'-C1'-N1	8.49	113.94	108.00
3	N	5	DT	P-O3'-C3'	8.39	129.77	119.70
1	R	8	G	O5'-P-OP2	-8.35	98.19	105.70
3	N	6	DT	O4'-C1'-N1	8.28	113.79	108.00
3	N	4	DC	O4'-C1'-N1	8.17	113.72	108.00
13	L	31	CYS	CA-CB-SG	8.12	128.61	114.00
1	R	6	G	O4'-C1'-N9	7.89	114.51	108.20
2	T	16	DC	C1'-O4'-C4'	-7.85	102.25	110.10
2	T	20	DC	O4'-C4'-C3'	-7.84	101.30	106.00
1	R	9	G	O4'-C1'-N9	-7.79	101.97	108.20
3	N	11	DG	O4'-C4'-C3'	-7.67	101.40	106.00
2	T	21	DC	O4'-C4'-C3'	-7.51	101.49	106.00
2	T	21	DC	C4'-C3'-C2'	-7.43	96.42	103.10
1	R	3	C	O4'-C1'-N1	7.01	113.81	108.20
2	T	11	DG	O4'-C1'-N9	7.00	112.90	108.00
2	T	18	DA	C4'-C3'-C2'	-6.99	96.81	103.10
10	I	78	CYS	CA-CB-SG	6.93	126.48	114.00
5	B	1100	ASP	CB-CG-OD1	6.92	124.53	118.30
3	N	12	DT	C6-C5-C7	-6.92	118.75	122.90
1	R	8	G	C1'-O4'-C4'	-6.84	104.43	109.90
3	N	14	DG	O4'-C1'-N9	6.84	112.79	108.00
3	N	11	DG	P-O3'-C3'	6.77	127.82	119.70
2	T	25	DC	O4'-C1'-N1	6.75	112.72	108.00
2	T	6	DG	P-O3'-C3'	6.72	127.76	119.70
2	T	2	DT	O4'-C1'-N1	6.65	112.65	108.00
2	T	21	DC	C1'-O4'-C4'	-6.63	103.47	110.10
1	R	9	G	C5-C6-N1	6.61	114.80	111.50
1	R	8	G	C5-C6-N1	6.56	114.78	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	7	DA	O4'-C1'-N9	6.56	112.59	108.00
2	T	13	DA	O4'-C1'-N9	6.53	112.57	108.00
2	T	21	DC	N3-C4-C5	6.49	124.50	121.90
2	T	23	DC	O4'-C1'-N1	6.42	112.49	108.00
1	R	8	G	N1-C6-O6	-6.38	116.07	119.90
1	R	6	G	C4'-C3'-C2'	-6.37	96.23	102.60
3	N	2	DT	P-O3'-C3'	6.33	127.29	119.70
3	N	13	DA	O4'-C1'-N9	6.29	112.40	108.00
2	T	4	DC	O4'-C1'-N1	6.16	112.31	108.00
3	N	3	DG	N3-C4-C5	-6.10	125.55	128.60
1	R	10	A	C5'-C4'-O4'	6.09	116.41	109.10
2	T	15	DA	P-O3'-C3'	6.05	126.96	119.70
3	N	8	DT	P-O3'-C3'	6.02	126.92	119.70
2	T	21	DC	N1-C2-O2	5.89	122.44	118.90
2	T	21	DC	C6-N1-C2	5.89	122.66	120.30
3	N	7	DA	P-O3'-C3'	5.82	126.68	119.70
3	N	5	DT	C1'-O4'-C4'	-5.80	104.30	110.10
1	R	2	U	O4'-C1'-N1	5.78	112.82	108.20
3	N	12	DT	P-O3'-C3'	5.76	126.62	119.70
2	T	8	DT	C4-C5-C7	5.74	122.44	119.00
5	B	1020	ARG	NE-CZ-NH2	-5.74	117.43	120.30
5	B	492	LEU	CB-CG-CD1	-5.70	101.30	111.00
2	T	19	DT	C5-C4-O4	-5.69	120.92	124.90
3	N	2	DT	C6-C5-C7	-5.63	119.52	122.90
3	N	2	DT	O4'-C1'-N1	5.63	111.94	108.00
3	N	1	DC	C1'-O4'-C4'	-5.57	104.53	110.10
2	T	23	DC	P-O3'-C3'	-5.52	113.07	119.70
2	T	22	DT	O4'-C4'-C3'	-5.49	102.30	104.50
1	R	9	G	N9-C1'-C2'	-5.45	106.00	112.00
2	T	18	DA	N1-C2-N3	-5.43	126.59	129.30
2	T	18	DA	P-O5'-C5'	-5.40	112.26	120.90
1	R	3	C	P-O3'-C3'	-5.35	113.28	119.70
2	T	10	DA	O4'-C1'-N9	5.34	111.74	108.00
3	N	6	DT	C6-C5-C7	-5.34	119.70	122.90
10	I	78	CYS	N-CA-CB	5.32	120.17	110.60
3	N	1	DC	O4'-C1'-C2'	-5.30	101.66	105.90
5	B	668	ASP	CB-CG-OD2	5.28	123.05	118.30
2	T	10	DA	P-O3'-C3'	5.25	126.00	119.70
4	A	748	MET	CG-SD-CE	5.22	108.56	100.20
3	N	3	DG	C8-N9-C4	-5.22	104.31	106.40
3	N	3	DG	P-O3'-C3'	5.21	125.95	119.70
5	B	722	ASP	CB-CG-OD2	5.19	122.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	3	DG	N3-C4-N9	5.16	129.09	126.00
1	R	5	A	O4'-C1'-N9	5.15	112.32	108.20
1	R	8	G	O4'-C4'-C3'	-5.12	98.88	104.00
2	T	28	DT	C6-C5-C7	-5.09	119.85	122.90
3	N	1	DC	P-O3'-C3'	5.09	125.80	119.70
5	B	1166	CYS	CA-CB-SG	5.07	123.13	114.00
1	R	3	C	N1-C1'-C2'	-5.06	106.44	112.00
2	T	20	DC	N3-C4-C5	5.05	123.92	121.90
2	T	16	DC	O4'-C4'-C3'	-5.04	102.48	104.50
1	R	7	A	N9-C1'-C2'	-5.01	106.48	112.00

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1082	ASN	Peptide
4	A	115	LEU	Peptide
4	A	117	GLU	Peptide
4	A	218	ASP	Peptide
4	A	297	GLN	Peptide
4	A	298	PHE	Peptide
4	A	400	PRO	Peptide
4	A	402	ALA	Peptide
4	A	450	LEU	Peptide
4	A	671	ALA	Peptide
4	A	85	ASP	Peptide
5	B	1155	SER	Peptide
5	B	137	TYR	Peptide
5	B	138	GLU	Peptide
5	B	36	ALA	Peptide
5	B	478	GLY	Peptide
5	B	647	GLY	Peptide
5	B	886	LYS	Peptide
5	B	981	ALA	Peptide
6	C	3	GLU	Peptide
6	C	4	GLU	Peptide

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	R	216	0	109	4	0
2	T	566	0	316	21	0
3	N	284	0	161	8	0
4	A	11043	0	11133	534	0
5	B	8861	0	8884	458	0
6	C	2095	0	2051	91	0
7	E	1752	0	1776	56	0
8	F	688	0	707	19	0
9	H	1068	0	1040	52	0
10	I	971	0	927	32	0
11	J	532	0	542	38	0
12	K	919	0	929	43	0
13	L	363	0	386	14	0
14	T	56	0	22	16	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	3	0	0	0	0
All	All	29425	0	28983	1261	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 22.

All (1261) 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)
5:B:647:GLY:HA3	5:B:648:HIS:CB	1.51	1.34
5:B:800:GLN:HB3	11:J:52:THR:CG2	1.58	1.32
4:A:1364:ASN:ND2	4:A:1366:ARG:HG2	1.51	1.25
4:A:672:ASP:OD2	4:A:736:ASN:ND2	1.73	1.21
4:A:116:ASP:CB	4:A:117:GLU:HB2	1.73	1.17
5:B:906:SER:HB3	5:B:946:ASN:HB2	1.25	1.16
4:A:399:HIS:CB	4:A:400:PRO:HD3	1.74	1.16
5:B:647:GLY:HA3	5:B:648:HIS:HB2	1.21	1.16
2:T:18:DA:N1	14:T:29[B]:DUT:O2	1.78	1.15
4:A:399:HIS:HB3	4:A:400:PRO:CD	1.76	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:800:GLN:HB3	11:J:52:THR:HG22	1.28	1.13
4:A:399:HIS:HB3	4:A:400:PRO:HD3	1.14	1.13
4:A:1029:ARG:HG2	4:A:1029:ARG:HH11	1.13	1.13
4:A:672:ASP:CG	4:A:675:THR:OG1	1.87	1.13
4:A:672:ASP:OD1	4:A:674:PRO:HG2	1.49	1.12
4:A:672:ASP:HB3	4:A:675:THR:CB	1.80	1.12
4:A:1123:GLY:HA3	4:A:1124:HIS:HB2	1.19	1.11
4:A:590:ARG:HG3	4:A:590:ARG:HH11	1.16	1.10
5:B:1094:ARG:HH11	5:B:1094:ARG:CG	1.65	1.09
5:B:345:LYS:HA	5:B:347:LYS:H	0.97	1.08
4:A:116:ASP:HB3	4:A:117:GLU:HB2	1.29	1.08
5:B:647:GLY:HA3	5:B:648:HIS:HB3	1.30	1.08
5:B:1094:ARG:HG2	5:B:1094:ARG:NH1	1.54	1.08
4:A:567:LYS:HB2	4:A:568:PRO:HD2	1.36	1.08
4:A:672:ASP:HB3	4:A:675:THR:HB	1.13	1.08
4:A:249:SER:O	4:A:250:ILE:HG13	1.55	1.06
4:A:116:ASP:CA	4:A:117:GLU:HB2	1.84	1.06
4:A:672:ASP:CB	4:A:675:THR:HB	1.85	1.05
5:B:800:GLN:HB3	11:J:52:THR:HG21	1.31	1.03
2:T:18:DA:C2	14:T:29[B]:DUT:O2	2.11	1.02
4:A:565:ILE:HG23	4:A:567:LYS:CE	1.88	1.02
4:A:913:LEU:HD11	4:A:981:LEU:O	1.59	1.01
4:A:567:LYS:HB3	9:H:96:VAL:H	1.22	1.01
4:A:399:HIS:CG	4:A:400:PRO:HD3	1.95	1.00
5:B:709:ASP:O	5:B:710:LEU:HD23	1.60	1.00
5:B:647:GLY:CA	5:B:648:HIS:CB	2.36	1.00
5:B:708:GLU:O	5:B:712:PRO:HD3	1.60	1.00
4:A:53:LEU:HG	4:A:54:ASN:H	1.27	1.00
2:T:18:DA:N6	14:T:29[B]:DUT:HN3	1.60	0.99
5:B:801:LYS:O	11:J:52:THR:HG23	1.60	0.99
4:A:323:LYS:HG2	4:A:324:SER:H	1.26	0.99
4:A:567:LYS:CB	4:A:568:PRO:HD2	1.93	0.99
4:A:299:HIS:O	4:A:301:ALA:N	1.94	0.99
4:A:315:LEU:HG	4:A:320:ARG:HH21	1.28	0.98
11:J:3:VAL:HG21	11:J:18:TRP:HB2	1.43	0.98
5:B:313:MET:HE1	5:B:390:LEU:HG	1.45	0.98
4:A:565:ILE:HG23	4:A:567:LYS:HE3	1.02	0.98
4:A:472:LEU:O	4:A:475:THR:HB	1.63	0.97
4:A:672:ASP:CB	4:A:675:THR:CB	2.42	0.97
6:C:235:VAL:HG11	11:J:6:ARG:HH21	1.29	0.97
4:A:93:VAL:HG13	4:A:301:ALA:HB1	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:18:DA:H61	14:T:29[B]:DUT:HN3	1.12	0.96
4:A:116:ASP:HB3	4:A:117:GLU:CB	1.94	0.96
6:C:167:HIS:HD2	6:C:169:LYS:H	1.13	0.96
5:B:345:LYS:HA	5:B:347:LYS:N	1.80	0.96
4:A:56:PRO:O	4:A:57:ARG:HG3	1.65	0.94
7:E:64:PRO:HD3	7:E:76:GLY:HA2	1.49	0.93
4:A:609:ASP:O	4:A:611:GLN:N	2.01	0.92
4:A:1161:THR:HG22	4:A:1163:ILE:H	1.34	0.92
5:B:647:GLY:CA	5:B:648:HIS:HB3	1.98	0.92
4:A:1364:ASN:HD21	4:A:1366:ARG:HG2	1.34	0.91
5:B:313:MET:CE	5:B:390:LEU:HG	1.99	0.91
4:A:1110:ASN:H	4:A:1110:ASN:HD22	1.18	0.91
5:B:1084:GLN:HE22	6:C:191:TYR:HA	1.36	0.91
4:A:590:ARG:HG3	4:A:590:ARG:NH1	1.78	0.90
4:A:56:PRO:C	4:A:57:ARG:HG3	1.90	0.90
6:C:56:THR:HG22	6:C:57:VAL:H	1.35	0.90
5:B:744:HIS:HD2	5:B:746:SER:H	1.15	0.90
4:A:110:CYS:HB3	4:A:167:CYS:SG	2.12	0.89
4:A:116:ASP:HA	4:A:117:GLU:HB2	1.52	0.89
4:A:943:LEU:O	4:A:945:GLU:N	2.05	0.89
4:A:68:GLN:O	4:A:68:GLN:NE2	2.05	0.88
4:A:868:TYR:CE1	4:A:1064:VAL:HG11	2.08	0.88
4:A:672:ASP:OD1	4:A:675:THR:OG1	1.89	0.88
4:A:565:ILE:CG2	4:A:567:LYS:HE3	1.98	0.87
4:A:129:LYS:O	4:A:130:ASP:HB2	1.73	0.87
4:A:1364:ASN:HD22	4:A:1366:ARG:HG2	1.37	0.87
5:B:710:LEU:O	5:B:711:GLU:HB3	1.72	0.86
4:A:1029:ARG:HH11	4:A:1029:ARG:CG	1.88	0.86
4:A:218:ASP:HB2	4:A:219:PHE:HB2	1.55	0.86
5:B:260:GLY:O	5:B:267:ARG:HD3	1.76	0.85
4:A:567:LYS:HB3	9:H:96:VAL:N	1.90	0.85
6:C:52:GLU:HA	13:L:64:LEU:HD22	1.59	0.85
4:A:265:LYS:HG2	4:A:303:TYR:HB2	1.57	0.85
5:B:1094:ARG:HH11	5:B:1094:ARG:HG2	0.74	0.85
2:T:18:DA:N1	14:T:29[B]:DUT:C2	2.40	0.84
4:A:1364:ASN:ND2	4:A:1366:ARG:CG	2.40	0.84
5:B:763:GLN:HG2	5:B:765:PRO:HD2	1.60	0.84
5:B:957:ASN:HD22	5:B:959:ASP:HB2	1.43	0.83
11:J:3:VAL:HG21	11:J:18:TRP:CB	2.08	0.83
4:A:567:LYS:HG3	4:A:568:PRO:HD2	1.61	0.83
5:B:140:ILE:HB	5:B:141:ASP:HB2	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:324:SER:O	4:A:326:ARG:N	2.12	0.83
5:B:805:THR:HG21	5:B:815:ARG:HH21	1.44	0.83
4:A:134:ARG:HD3	4:A:221:SER:O	1.79	0.82
4:A:218:ASP:H	4:A:219:PHE:HB3	1.43	0.82
4:A:399:HIS:CB	4:A:400:PRO:CD	2.40	0.82
4:A:855:THR:HG21	4:A:857:ARG:HE	1.44	0.82
12:K:65:HIS:HD2	12:K:67:PHE:H	1.25	0.82
13:L:46:VAL:HG12	13:L:47:ARG:H	1.42	0.82
4:A:306:ASN:HD21	4:A:313:GLN:HB2	1.45	0.82
4:A:590:ARG:HH11	4:A:590:ARG:CG	1.93	0.81
10:I:103:CYS:O	10:I:105:SER:N	2.13	0.81
5:B:90:ILE:CD1	5:B:134:LYS:HG2	2.10	0.81
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.62	0.81
7:E:175:LEU:HD12	7:E:176:PRO:HD2	1.63	0.81
4:A:65:LEU:HD23	4:A:65:LEU:H	1.46	0.81
5:B:287:ARG:NH1	5:B:324:ILE:O	2.14	0.81
4:A:672:ASP:CB	4:A:675:THR:OG1	2.29	0.80
4:A:754:SER:H	4:A:757:ASN:HD22	1.30	0.80
4:A:1444:MET:HB2	8:F:133:VAL:HG12	1.64	0.80
4:A:567:LYS:CG	4:A:568:PRO:HD2	2.10	0.80
5:B:1084:GLN:NE2	6:C:191:TYR:HA	1.97	0.80
5:B:744:HIS:CD2	5:B:746:SER:H	1.99	0.80
5:B:63:ILE:O	5:B:67:SER:HB3	1.81	0.79
4:A:249:SER:O	4:A:250:ILE:CG1	2.30	0.79
5:B:176:SER:O	5:B:182:SER:HB3	1.82	0.79
5:B:363:HIS:O	5:B:364:ILE:HB	1.83	0.79
4:A:961:ARG:HG2	4:A:961:ARG:HH11	1.48	0.79
4:A:253:ASN:H	4:A:253:ASN:HD22	1.31	0.79
5:B:906:SER:HB3	5:B:946:ASN:CB	2.10	0.79
4:A:565:ILE:HG12	4:A:567:LYS:HZ1	1.48	0.78
4:A:269:ILE:HG22	4:A:299:HIS:HB2	1.66	0.78
5:B:476:ARG:O	5:B:478:GLY:N	2.17	0.78
4:A:855:THR:CG2	4:A:857:ARG:HE	1.96	0.78
5:B:1006:ILE:HD11	11:J:43:ARG:HB2	1.65	0.78
4:A:1131:ALA:HA	4:A:1134:ILE:HD12	1.66	0.78
4:A:332:LYS:O	4:A:333:GLU:HG2	1.82	0.77
4:A:596:THR:O	4:A:598:LEU:N	2.17	0.77
5:B:800:GLN:CB	11:J:52:THR:HG21	2.14	0.77
5:B:882:THR:HB	5:B:934:LYS:O	1.83	0.77
5:B:167:ILE:HG22	5:B:167:ILE:O	1.84	0.77
5:B:1107:ALA:O	5:B:1108:ARG:HB3	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:973:ILE:HG23	5:B:974:PRO:HD2	1.66	0.77
7:E:108:GLY:HA3	7:E:132:ILE:HG22	1.65	0.77
5:B:879:ARG:NE	5:B:879:ARG:H	1.83	0.77
5:B:825:VAL:HG23	5:B:1010:LEU:HB3	1.65	0.76
5:B:864:LYS:HG2	5:B:871:THR:HG23	1.67	0.76
4:A:483:ASP:HA	5:B:988:GLY:HA2	1.66	0.76
4:A:567:LYS:HB2	4:A:568:PRO:CD	2.13	0.76
5:B:102:VAL:HG23	5:B:112:LEU:HB2	1.66	0.76
4:A:378:GLU:OE2	4:A:434:ARG:HD3	1.86	0.76
4:A:901:LEU:HA	4:A:907:THR:HG23	1.68	0.76
4:A:961:ARG:HG2	4:A:961:ARG:NH1	1.99	0.76
5:B:211:VAL:CG2	5:B:483:LEU:HD13	2.15	0.76
5:B:137:TYR:O	5:B:138:GLU:HB2	1.85	0.76
4:A:208:LEU:O	4:A:208:LEU:HD22	1.86	0.75
5:B:906:SER:CB	5:B:946:ASN:HB2	2.13	0.75
5:B:1163:CYS:SG	5:B:1166:CYS:N	2.56	0.75
4:A:868:TYR:HE1	4:A:1064:VAL:HG11	1.49	0.75
7:E:3:GLN:HG2	7:E:4:GLU:H	1.51	0.75
5:B:398:ARG:HB3	5:B:398:ARG:NH1	2.02	0.74
5:B:984:HIS:CE1	5:B:1025:HIS:HA	2.22	0.74
4:A:31:SER:OG	4:A:83:HIS:HD2	1.71	0.74
5:B:223:VAL:O	5:B:384:ARG:NH2	2.20	0.74
6:C:98:VAL:H	6:C:122:SER:HB2	1.51	0.74
4:A:567:LYS:HG3	4:A:568:PRO:CD	2.18	0.74
4:A:1364:ASN:HD21	4:A:1366:ARG:HH11	1.34	0.74
5:B:30:SER:O	5:B:34:ILE:HD12	1.88	0.74
5:B:225:VAL:HG11	5:B:385:LEU:HA	1.69	0.74
5:B:797:TYR:O	11:J:1:MET:HG2	1.86	0.74
4:A:47:ARG:HA	4:A:47:ARG:CZ	2.18	0.74
5:B:269:ILE:HD11	5:B:386:LEU:HD21	1.69	0.73
4:A:1029:ARG:HG2	4:A:1029:ARG:NH1	1.94	0.73
4:A:1123:GLY:HA3	4:A:1124:HIS:CB	2.08	0.73
5:B:278:GLN:HG2	5:B:279:ASP:H	1.52	0.73
5:B:426:LYS:HE2	5:B:430:ARG:HH22	1.52	0.73
4:A:5:GLN:O	5:B:1159:ARG:NH2	2.22	0.73
4:A:298:PHE:C	4:A:298:PHE:CD2	2.59	0.73
4:A:471:ASN:O	4:A:474:VAL:HG12	1.88	0.73
5:B:647:GLY:CA	5:B:648:HIS:HB2	2.11	0.73
4:A:298:PHE:HD2	4:A:299:HIS:HA	1.52	0.73
11:J:3:VAL:CG2	11:J:18:TRP:HB2	2.17	0.72
5:B:25:ILE:HG23	5:B:29:ASP:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:216:GLU:OE1	5:B:537:LYS:HE2	1.90	0.72
5:B:1160:VAL:HG11	5:B:1169:MET:HG2	1.71	0.72
4:A:567:LYS:CB	4:A:568:PRO:CD	2.66	0.72
4:A:1333:ILE:O	4:A:1337:GLU:HG3	1.89	0.72
4:A:399:HIS:CG	4:A:400:PRO:CD	2.72	0.72
5:B:801:LYS:O	11:J:52:THR:CG2	2.35	0.72
5:B:899:ILE:HD11	5:B:911:ILE:HA	1.72	0.72
7:E:65:THR:HB	7:E:67:GLU:HB2	1.71	0.72
5:B:346:GLU:HA	5:B:349:ILE:CD1	2.20	0.72
5:B:979:LYS:HE2	5:B:987:LYS:HG2	1.72	0.72
4:A:1364:ASN:HD22	4:A:1366:ARG:CG	2.01	0.72
4:A:1110:ASN:H	4:A:1110:ASN:ND2	1.86	0.72
12:K:65:HIS:CD2	12:K:66:PRO:HD2	2.25	0.72
4:A:666:ILE:CD1	5:B:1027:ILE:HG12	2.20	0.72
5:B:515:HIS:H	5:B:518:HIS:CD2	2.08	0.71
7:E:22:MET:CE	7:E:26:ARG:HH21	2.03	0.71
5:B:800:GLN:CB	11:J:52:THR:HG22	2.14	0.71
5:B:364:ILE:HD13	5:B:585:VAL:HG13	1.71	0.71
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.72	0.71
12:K:65:HIS:CD2	12:K:67:PHE:H	2.08	0.71
5:B:426:LYS:HE2	5:B:430:ARG:NH2	2.06	0.71
5:B:864:LYS:HB3	5:B:872:GLU:H	1.55	0.71
5:B:952:VAL:HG22	5:B:966:VAL:HG13	1.73	0.71
12:K:40:HIS:HE1	12:K:63:VAL:HG22	1.56	0.70
5:B:1211:ASN:O	5:B:1212:ILE:HG13	1.91	0.70
4:A:1063:MET:SD	4:A:1436:ILE:HG13	2.31	0.70
5:B:879:ARG:H	5:B:879:ARG:CZ	2.05	0.70
5:B:955:THR:HG22	5:B:956:THR:H	1.57	0.70
5:B:1175:LEU:O	5:B:1176:ASN:HB3	1.90	0.70
4:A:741:ASN:HD22	4:A:744:LYS:H	1.39	0.70
4:A:1345:ARG:HG3	4:A:1376:THR:HG21	1.74	0.70
5:B:705:MET:H	5:B:710:LEU:HD12	1.55	0.70
4:A:399:HIS:CD2	4:A:400:PRO:HD3	2.26	0.69
12:K:102:LYS:O	12:K:106:GLU:HG3	1.91	0.69
5:B:976:ILE:HG23	5:B:977:GLY:N	2.06	0.69
6:C:11:ARG:HD3	6:C:21:ILE:HD11	1.75	0.69
4:A:553:VAL:HG13	4:A:648:ASN:ND2	2.08	0.69
4:A:800:VAL:O	4:A:802:ASN:N	2.25	0.69
4:A:1161:THR:HG22	4:A:1163:ILE:N	2.06	0.69
6:C:56:THR:HG22	6:C:57:VAL:N	2.08	0.69
9:H:47:PHE:HB3	9:H:95:TYR:HD1	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:19:VAL:O	7:E:23:VAL:HG23	1.92	0.69
13:L:40:LEU:HD11	13:L:49:LYS:HE2	1.73	0.69
13:L:46:VAL:HG12	13:L:47:ARG:N	2.07	0.68
4:A:298:PHE:HA	4:A:299:HIS:O	1.92	0.68
4:A:596:THR:C	4:A:598:LEU:H	1.94	0.68
2:T:18:DA:N1	14:T:29[B]:DUT:N3	2.42	0.68
4:A:31:SER:OG	4:A:83:HIS:CD2	2.46	0.68
5:B:802:PRO:HB3	5:B:1091:TYR:CG	2.29	0.68
4:A:535:THR:HG21	4:A:617:VAL:H	1.59	0.68
4:A:553:VAL:HG13	4:A:648:ASN:HD22	1.58	0.68
4:A:568:PRO:O	4:A:569:LYS:CB	2.41	0.68
4:A:219:PHE:HE1	4:A:226:GLU:HA	1.59	0.68
4:A:208:LEU:HD22	4:A:208:LEU:C	2.14	0.68
5:B:1006:ILE:HG22	5:B:1007:VAL:N	2.07	0.68
4:A:319:GLY:HA2	4:A:320:ARG:NH1	2.09	0.67
9:H:26:ILE:HG22	9:H:40:LEU:HB3	1.75	0.67
6:C:242:GLN:HB3	6:C:246:ARG:HE	1.59	0.67
4:A:593:GLU:OE2	4:A:593:GLU:HA	1.94	0.67
5:B:712:PRO:O	5:B:713:ALA:HB3	1.94	0.67
4:A:761:MET:HG3	5:B:1021:MET:HG2	1.75	0.67
12:K:40:HIS:HE1	12:K:63:VAL:CG2	2.07	0.67
14:T:29[A]:DUT:H5'2	14:T:29[A]:DUT:O1B	1.94	0.67
5:B:1023:VAL:O	5:B:1027:ILE:HG13	1.94	0.67
4:A:251:SER:HB3	4:A:258:GLY:HA3	1.75	0.67
4:A:901:LEU:H	4:A:926:GLN:NE2	1.93	0.67
4:A:1123:GLY:CA	4:A:1124:HIS:HB2	2.13	0.67
5:B:37:PHE:O	5:B:38:PHE:HB2	1.93	0.67
5:B:63:ILE:O	5:B:67:SER:CB	2.43	0.67
5:B:624:LEU:HD12	5:B:625:LYS:N	2.10	0.67
4:A:351:THR:HG22	4:A:352:VAL:H	1.59	0.66
4:A:351:THR:HG21	4:A:466:SER:O	1.94	0.66
4:A:423:ASP:OD2	4:A:424:ILE:N	2.20	0.66
4:A:116:ASP:CA	4:A:117:GLU:CB	2.63	0.66
4:A:407:ARG:HD2	4:A:413:ILE:HD11	1.77	0.66
5:B:1156:ASP:O	5:B:1157:ALA:HB3	1.96	0.66
5:B:90:ILE:HD13	5:B:134:LYS:HG2	1.77	0.66
4:A:707:GLY:HA3	4:A:1281:ARG:HG3	1.77	0.66
5:B:957:ASN:ND2	5:B:959:ASP:HB2	2.10	0.66
11:J:48:ARG:HG3	11:J:48:ARG:HH11	1.61	0.66
4:A:943:LEU:O	4:A:946:VAL:N	2.27	0.65
4:A:869:GLY:O	7:E:204:THR:HG21	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:276:LEU:HD11	4:A:292:ALA:HB1	1.77	0.65
4:A:1383:SER:O	4:A:1388:GLY:HA3	1.96	0.65
5:B:848:ARG:HH22	5:B:996:ARG:NH1	1.94	0.65
10:I:32:CYS:SG	10:I:33:SER:N	2.69	0.65
9:H:109:LYS:NZ	9:H:111:LEU:HD12	2.12	0.65
5:B:346:GLU:HA	5:B:349:ILE:HD12	1.79	0.65
5:B:879:ARG:O	5:B:882:THR:HG22	1.97	0.65
4:A:679:ILE:HG23	4:A:729:ALA:HB1	1.78	0.65
5:B:256:VAL:HG11	5:B:382:ILE:HD13	1.77	0.65
4:A:116:ASP:HA	4:A:117:GLU:CB	2.18	0.65
5:B:984:HIS:CD2	5:B:1024:ALA:HB3	2.31	0.65
6:C:258:ILE:CD1	12:K:42:LEU:HD21	2.26	0.64
10:I:63:GLY:HA3	10:I:104:LEU:HD11	1.77	0.64
4:A:117:GLU:C	4:A:118:HIS:O	2.34	0.64
4:A:68:GLN:O	4:A:70:CYS:N	2.26	0.64
4:A:117:GLU:H	4:A:118:HIS:CA	2.10	0.64
5:B:549:THR:HG22	5:B:550:ASP:H	1.62	0.64
5:B:1007:VAL:HG13	5:B:1008:PRO:HD2	1.78	0.64
4:A:47:ARG:HA	4:A:47:ARG:NE	2.12	0.64
4:A:117:GLU:H	4:A:118:HIS:C	2.00	0.64
5:B:398:ARG:CB	5:B:398:ARG:HH11	2.11	0.64
5:B:800:GLN:CB	11:J:52:THR:CG2	2.55	0.64
5:B:911:ILE:HD11	5:B:941:LEU:HD12	1.80	0.64
5:B:223:VAL:HG13	5:B:384:ARG:HH21	1.63	0.64
5:B:976:ILE:CG2	5:B:977:GLY:N	2.60	0.63
4:A:265:LYS:C	4:A:267:ALA:H	2.01	0.63
9:H:47:PHE:HB3	9:H:95:TYR:CD1	2.33	0.63
4:A:323:LYS:HG2	4:A:324:SER:N	2.06	0.63
2:T:15:DA:H2"	2:T:16:DC:O5'	1.98	0.63
4:A:567:LYS:HD3	9:H:95:TYR:CG	2.33	0.63
7:E:77:SER:HB3	7:E:105:PHE:HA	1.79	0.63
9:H:93:TYR:CD2	9:H:145:ARG:HB3	2.34	0.63
4:A:65:LEU:HD23	4:A:65:LEU:N	2.14	0.63
5:B:211:VAL:HG23	5:B:483:LEU:HD13	1.80	0.63
6:C:167:HIS:CD2	6:C:169:LYS:H	2.05	0.63
5:B:807:ARG:HG3	5:B:807:ARG:HH11	1.64	0.63
9:H:24:CYS:HB2	9:H:44:VAL:HG21	1.81	0.63
4:A:34:LYS:HE2	4:A:57:ARG:HH21	1.63	0.63
5:B:1190:ASP:O	5:B:1191:ILE:HG13	1.99	0.63
7:E:62:ALA:HB3	7:E:78:LEU:HD22	1.80	0.63
4:A:636:GLU:OE2	4:A:962:ARG:HD2	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:399:HIS:NE2	4:A:462:VAL:HG11	2.14	0.62
6:C:31:ASN:OD1	6:C:34:ARG:NH1	2.32	0.62
6:C:142:VAL:H	11:J:16:ASP:HB3	1.64	0.62
4:A:1084:PHE:CZ	4:A:1093:LYS:HA	2.33	0.62
5:B:136:THR:O	5:B:137:TYR:C	2.34	0.62
3:N:4:DC:H2"	3:N:5:DT:OP2	1.99	0.62
4:A:345:VAL:HG22	5:B:1128:LEU:O	1.99	0.62
13:L:30:ILE:O	13:L:56:LEU:HA	1.99	0.62
4:A:423:ASP:CG	4:A:424:ILE:H	2.01	0.62
4:A:635:ARG:HH11	4:A:635:ARG:HA	1.63	0.62
5:B:995:ARG:HB3	5:B:997:GLU:OE2	1.99	0.62
6:C:70:ILE:HD11	6:C:144:ILE:CD1	2.30	0.62
5:B:911:ILE:HD11	5:B:941:LEU:HA	1.80	0.62
9:H:137:GLN:C	9:H:139:ASN:H	2.03	0.62
4:A:218:ASP:H	4:A:219:PHE:CB	2.11	0.62
5:B:712:PRO:O	5:B:713:ALA:CB	2.47	0.62
6:C:33:LEU:HG	6:C:37:MET:HE3	1.82	0.62
9:H:2:SER:CB	9:H:3:ASN:HB2	2.28	0.62
4:A:381:THR:HG21	4:A:383:TYR:CD1	2.35	0.62
4:A:1325:THR:HG22	4:A:1326:ARG:HG3	1.80	0.62
4:A:72:GLU:HB3	4:A:76:GLU:CG	2.30	0.62
5:B:1013:ASN:OD1	5:B:1014:PRO:HD2	1.99	0.62
4:A:249:SER:C	4:A:250:ILE:CG1	2.66	0.62
5:B:710:LEU:O	5:B:711:GLU:CB	2.47	0.62
4:A:1129:GLU:HA	4:A:1132:LYS:HE3	1.82	0.61
5:B:293:PRO:HG2	5:B:296:GLU:HB2	1.81	0.61
5:B:976:ILE:O	5:B:990:ILE:O	2.17	0.61
4:A:673:GLY:N	4:A:674:PRO:HD2	2.15	0.61
3:N:2:DT:H1'	3:N:3:DG:N7	2.15	0.61
4:A:565:ILE:HG12	4:A:567:LYS:NZ	2.15	0.61
6:C:73:GLN:HE21	6:C:74:SER:H	1.48	0.61
4:A:323:LYS:CG	4:A:324:SER:H	2.09	0.61
4:A:22:PHE:HB2	5:B:1211:ASN:OD1	1.99	0.61
4:A:315:LEU:HG	4:A:320:ARG:NH2	2.09	0.61
12:K:91:CYS:O	12:K:95:ILE:HG13	2.00	0.61
4:A:351:THR:HG22	4:A:352:VAL:N	2.15	0.61
5:B:1152:MET:O	5:B:1157:ALA:HB2	2.00	0.61
10:I:98:VAL:HG11	10:I:113:ASP:HB2	1.82	0.61
10:I:78:CYS:C	10:I:80:SER:H	2.04	0.61
4:A:56:PRO:C	4:A:57:ARG:CG	2.67	0.61
5:B:753:ALA:HA	5:B:756:ILE:HD12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:72:LYS:HD3	8:F:142:SER:HB3	1.83	0.61
5:B:35:SER:HB3	5:B:39:ARG:HH21	1.64	0.61
4:A:866:PHE:C	4:A:867:ILE:HG13	2.20	0.61
5:B:516:ASN:H	5:B:516:ASN:HD22	1.48	0.61
4:A:115:LEU:O	4:A:122:MET:HG2	2.01	0.60
4:A:901:LEU:HD22	4:A:919:ILE:HG22	1.83	0.60
5:B:398:ARG:HB3	5:B:398:ARG:HH11	1.64	0.60
5:B:711:GLU:CG	5:B:711:GLU:O	2.50	0.60
4:A:247:ARG:N	4:A:248:PRO:HD3	2.16	0.60
5:B:280:ILE:HB	5:B:285:ILE:HD11	1.83	0.60
5:B:465:ASN:HA	5:B:476:ARG:HA	1.83	0.60
4:A:1189:SER:OG	4:A:1190:PRO:HD2	2.01	0.60
5:B:476:ARG:C	5:B:478:GLY:H	2.05	0.60
6:C:173:ALA:O	6:C:233:GLU:O	2.18	0.60
12:K:47:ARG:HD2	12:K:60:ALA:HA	1.82	0.60
4:A:962:ARG:HA	4:A:965:GLN:HE21	1.67	0.60
5:B:20:ASP:CG	5:B:21:GLU:H	2.05	0.60
5:B:487:THR:OG1	5:B:777:ALA:O	2.20	0.60
4:A:115:LEU:HD12	4:A:122:MET:HE2	1.84	0.60
5:B:706:GLN:O	5:B:710:LEU:HB2	2.02	0.60
5:B:841:MET:HE3	5:B:990:ILE:HD11	1.83	0.60
4:A:1080:THR:HG22	4:A:1081:LEU:N	2.17	0.59
5:B:955:THR:HG22	5:B:956:THR:N	2.18	0.59
7:E:28:TYR:HA	7:E:64:PRO:HA	1.84	0.59
9:H:2:SER:CA	9:H:3:ASN:HB2	2.32	0.59
4:A:65:LEU:H	4:A:65:LEU:CD2	2.16	0.59
4:A:828:ALA:HB2	5:B:530:GLY:HA2	1.84	0.59
5:B:886:LYS:HB3	5:B:887:HIS:HA	1.82	0.59
4:A:117:GLU:H	4:A:118:HIS:CB	2.15	0.59
4:A:961:ARG:HH11	4:A:961:ARG:CG	2.14	0.59
5:B:882:THR:HG23	5:B:883:LEU:H	1.68	0.59
4:A:1174:PHE:C	4:A:1174:PHE:CD1	2.76	0.59
5:B:879:ARG:NE	5:B:879:ARG:N	2.51	0.59
7:E:94:LYS:HE2	7:E:94:LYS:HA	1.84	0.59
4:A:828:ALA:CB	5:B:530:GLY:HA2	2.32	0.59
4:A:870:GLU:HG2	7:E:208:TYR:CD2	2.38	0.59
4:A:1441:PHE:CZ	8:F:89:GLU:HA	2.38	0.59
4:A:668:ASP:HB3	4:A:743:VAL:HG23	1.85	0.58
5:B:848:ARG:HA	6:C:69:LEU:HD21	1.84	0.58
7:E:41:ASP:O	7:E:45:LYS:HG2	2.03	0.58
4:A:115:LEU:HD22	4:A:119:ASN:HD22	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:218:ASP:O	4:A:221:SER:HB2	2.03	0.58
4:A:218:ASP:CB	4:A:219:PHE:HB2	2.29	0.58
5:B:287:ARG:HD3	5:B:292:ILE:HA	1.85	0.58
5:B:313:MET:HE2	5:B:390:LEU:HG	1.81	0.58
10:I:63:GLY:CA	10:I:104:LEU:HD11	2.34	0.58
4:A:64:ASN:HB3	4:A:66:LYS:HG2	1.84	0.58
4:A:452:LYS:HD3	4:A:510:GLN:OE1	2.03	0.58
5:B:802:PRO:HB3	5:B:1091:TYR:CD2	2.39	0.58
4:A:299:HIS:HA	4:A:302:THR:HG22	1.84	0.58
5:B:986:GLN:NE2	5:B:1022:THR:HG21	2.18	0.58
6:C:166:GLU:HG2	12:K:10:PHE:CZ	2.38	0.58
5:B:624:LEU:HD12	5:B:624:LEU:C	2.24	0.58
4:A:167:CYS:O	4:A:169:ASN:N	2.37	0.58
4:A:102:VAL:HG12	4:A:211:PHE:HE1	1.68	0.58
4:A:423:ASP:O	4:A:424:ILE:HB	2.04	0.58
4:A:1435:PRO:O	4:A:1436:ILE:HD12	2.03	0.58
5:B:869:SER:O	5:B:870:ILE:HG13	2.03	0.58
10:I:103:CYS:C	10:I:105:SER:H	2.05	0.58
4:A:273:ASN:HA	4:A:296:LEU:HD12	1.85	0.58
5:B:1149:GLU:HA	5:B:1153:GLU:OE2	2.04	0.57
6:C:73:GLN:HE21	6:C:75:MET:H	1.51	0.57
4:A:672:ASP:HB2	4:A:736:ASN:OD1	2.04	0.57
4:A:853:ASP:OD1	4:A:855:THR:HG22	2.03	0.57
4:A:93:VAL:CG1	4:A:301:ALA:HB1	2.27	0.57
4:A:1029:ARG:CG	4:A:1029:ARG:NH1	2.54	0.57
4:A:1174:PHE:C	4:A:1174:PHE:HD1	2.07	0.57
5:B:277:LYS:HZ1	5:B:335:GLY:H	1.52	0.57
4:A:53:LEU:HG	4:A:54:ASN:N	2.09	0.57
5:B:834:ASN:HB3	5:B:840:ILE:HD12	1.86	0.57
5:B:345:LYS:N	5:B:346:GLU:HG3	2.20	0.57
6:C:73:GLN:HE21	6:C:74:SER:N	2.03	0.57
6:C:242:GLN:HE21	6:C:246:ARG:HE	1.52	0.57
9:H:84:ALA:HA	9:H:87:ARG:HB2	1.85	0.57
5:B:370:PHE:O	5:B:372:SER:N	2.37	0.57
4:A:364:VAL:O	4:A:364:VAL:HG13	2.04	0.57
4:A:567:LYS:CG	4:A:568:PRO:CD	2.80	0.57
4:A:756:ILE:O	4:A:760:GLN:HG3	2.03	0.57
5:B:886:LYS:HB3	5:B:887:HIS:CA	2.34	0.57
5:B:291:ILE:HD12	5:B:291:ILE:H	1.68	0.57
4:A:276:LEU:CD1	4:A:292:ALA:HB1	2.34	0.57
7:E:175:LEU:CD1	7:E:176:PRO:HD2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1160:VAL:HG12	5:B:1161:HIS:H	1.70	0.57
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.87	0.57
4:A:436:ILE:HD11	4:A:491:VAL:HG11	1.87	0.56
4:A:590:ARG:NH2	4:A:621:THR:OG1	2.37	0.56
5:B:784:ASN:OD1	5:B:788:ARG:HD2	2.05	0.56
5:B:840:ILE:HB	5:B:1011:ILE:HB	1.87	0.56
5:B:1182:CYS:SG	5:B:1185:CYS:HB3	2.44	0.56
4:A:253:ASN:O	4:A:254:GLU:HB2	2.05	0.56
13:L:28:LYS:HB2	13:L:39:SER:HB2	1.87	0.56
5:B:831:SER:HB2	5:B:833:TYR:HD1	1.70	0.56
7:E:40:GLU:HA	7:E:43:LYS:HZ2	1.70	0.56
10:I:10:CYS:SG	10:I:32:CYS:HB3	2.45	0.56
5:B:705:MET:N	5:B:710:LEU:HD12	2.21	0.56
5:B:783:THR:HG22	11:J:63:TYR:HE1	1.69	0.56
5:B:793:ALA:HB3	5:B:856:PHE:HB2	1.87	0.56
6:C:131:HIS:O	6:C:132:PRO:C	2.42	0.56
4:A:37:PHE:HB2	4:A:52:GLY:HA3	1.86	0.56
10:I:75:CYS:HB3	10:I:78:CYS:O	2.05	0.56
3:N:12:DT:H5"	7:E:119:SER:CB	2.35	0.56
4:A:549:MET:SD	4:A:577:ILE:CD1	2.94	0.56
4:A:55:ASP:H	4:A:56:PRO:HD2	1.70	0.56
5:B:122:LEU:HD22	5:B:958:GLN:HB2	1.86	0.56
5:B:274:PRO:O	5:B:275:TYR:HB2	2.06	0.56
5:B:637:LEU:HD13	5:B:740:HIS:HB3	1.88	0.56
4:A:885:THR:O	4:A:940:ARG:HD2	2.04	0.56
7:E:111:VAL:HG12	7:E:137:GLU:HG2	1.88	0.56
4:A:901:LEU:H	4:A:926:GLN:HE21	1.53	0.56
5:B:25:ILE:HD12	5:B:653:VAL:HG23	1.88	0.56
5:B:41:LYS:O	5:B:45:SER:HB3	2.06	0.56
5:B:515:HIS:HD2	5:B:517:THR:OG1	1.89	0.56
7:E:28:TYR:CE1	7:E:78:LEU:HD13	2.41	0.56
4:A:870:GLU:HB2	7:E:204:THR:HG21	1.86	0.56
5:B:850:LEU:HD21	5:B:1009:ASP:HB3	1.88	0.56
5:B:487:THR:HG22	5:B:488:TYR:N	2.20	0.55
5:B:523:CYS:HB2	5:B:750:GLY:N	2.22	0.55
5:B:639:ILE:CD1	5:B:691:GLU:HB2	2.33	0.55
6:C:235:VAL:HG11	11:J:6:ARG:NH2	2.12	0.55
4:A:58:LEU:C	4:A:58:LEU:HD23	2.27	0.55
4:A:399:HIS:CE1	4:A:462:VAL:HG11	2.40	0.55
5:B:516:ASN:H	5:B:516:ASN:ND2	2.04	0.55
7:E:56:LYS:HB2	7:E:84:ASP:OD1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:172:GLU:HG3	7:E:213:ILE:HD12	1.88	0.55
7:E:197:LYS:HE3	7:E:199:ILE:HD11	1.88	0.55
5:B:245:GLU:HG2	5:B:246:LYS:N	2.22	0.55
5:B:862:GLN:HG2	5:B:963:PHE:HB2	1.89	0.55
5:B:909:ASP:O	5:B:940:PRO:HA	2.06	0.55
6:C:233:GLU:OE1	11:J:43:ARG:NH2	2.40	0.55
4:A:306:ASN:O	4:A:307:ASP:HB3	2.07	0.55
6:C:56:THR:CG2	6:C:57:VAL:H	2.13	0.55
5:B:778:MET:HG2	5:B:794:ASN:HB3	1.87	0.55
4:A:72:GLU:HB3	4:A:76:GLU:HG3	1.89	0.55
4:A:672:ASP:OD1	4:A:674:PRO:CG	2.40	0.55
4:A:875:ALA:HB2	4:A:1366:ARG:HD2	1.88	0.55
5:B:711:GLU:O	5:B:711:GLU:HG3	2.06	0.55
6:C:36:VAL:HG23	12:K:41:THR:HG21	1.89	0.55
4:A:246:VAL:HG12	4:A:246:VAL:O	2.07	0.55
4:A:1211:GLN:O	4:A:1215:ARG:HB2	2.06	0.55
5:B:807:ARG:HH11	5:B:807:ARG:CG	2.20	0.55
5:B:986:GLN:HE21	5:B:1022:THR:HG21	1.71	0.55
7:E:40:GLU:HA	7:E:43:LYS:NZ	2.21	0.55
4:A:304:MET:O	4:A:326:ARG:HB2	2.06	0.55
5:B:770:GLN:OE1	5:B:983:ARG:HA	2.05	0.55
5:B:976:ILE:CG2	5:B:977:GLY:H	2.20	0.55
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.87	0.55
6:C:99:LEU:HB2	6:C:157:CYS:HB2	1.89	0.55
6:C:166:GLU:HG2	12:K:10:PHE:HZ	1.71	0.55
14:T:29[A]:DUT:O1B	14:T:29[A]:DUT:H4'	2.07	0.54
4:A:707:GLY:CA	4:A:1281:ARG:HG3	2.37	0.54
5:B:451:LYS:HG2	5:B:455:SER:HB2	1.88	0.54
5:B:1002:THR:HG22	5:B:1006:ILE:N	2.21	0.54
10:I:32:CYS:O	10:I:33:SER:HB2	2.06	0.54
4:A:35:ILE:O	4:A:35:ILE:HG22	2.06	0.54
4:A:326:ARG:HG2	4:A:1406:VAL:HG21	1.89	0.54
4:A:477:PRO:HG3	4:A:521:MET:HE3	1.89	0.54
5:B:212:LEU:HD23	5:B:480:SER:HB2	1.87	0.54
6:C:66:ARG:NH2	11:J:3:VAL:O	2.40	0.54
9:H:129:TYR:HA	9:H:131:ASN:ND2	2.23	0.54
14:T:29[A]:DUT:O1B	14:T:29[A]:DUT:C5'	2.55	0.54
4:A:443:LEU:HD12	5:B:1146:PHE:CZ	2.42	0.54
4:A:474:VAL:HG22	4:A:478:TYR:CE1	2.43	0.54
4:A:58:LEU:HG	4:A:58:LEU:O	2.07	0.54
4:A:1025:ARG:HA	4:A:1030:ARG:HH11	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1277:GLU:O	4:A:1278:ASN:HB2	2.06	0.54
5:B:1006:ILE:CD1	11:J:43:ARG:HB2	2.36	0.54
5:B:1099:VAL:C	5:B:1103:ILE:HD11	2.27	0.54
6:C:57:VAL:HG11	11:J:57:ILE:HD12	1.88	0.54
5:B:886:LYS:HD2	5:B:890:TYR:OH	2.07	0.54
5:B:1084:GLN:OE1	5:B:1084:GLN:N	2.41	0.54
9:H:2:SER:HB2	9:H:3:ASN:HB2	1.88	0.54
9:H:22:LYS:HD2	9:H:45:GLU:OE1	2.07	0.54
12:K:10:PHE:CD1	12:K:11:LEU:HD13	2.43	0.54
4:A:372:LYS:HA	4:A:435:HIS:CD2	2.43	0.54
4:A:403:LYS:HB2	4:A:404:TYR:CD1	2.42	0.54
5:B:62:ILE:HD12	5:B:418:LYS:HG3	1.89	0.54
10:I:78:CYS:SG	10:I:106:CYS:N	2.81	0.54
2:T:16:DC:H2'	2:T:17:DG:H8	1.71	0.54
4:A:70:CYS:O	4:A:72:GLU:HG2	2.08	0.54
4:A:1082:ASN:H	4:A:1082:ASN:ND2	2.06	0.54
4:A:1138:ILE:HG21	4:A:1316:VAL:HG13	1.89	0.54
5:B:1017:ILE:H	5:B:1018:PRO:HD3	1.73	0.54
11:J:5:VAL:HG12	11:J:6:ARG:HG3	1.89	0.54
2:T:20:DC:H2'	2:T:21:DC:O4'	2.08	0.54
5:B:886:LYS:CB	5:B:887:HIS:HA	2.37	0.54
4:A:92:HIS:HE1	5:B:1210:MET:O	1.91	0.54
4:A:467:THR:HG23	5:B:976:ILE:HG23	1.90	0.54
4:A:477:PRO:HG3	4:A:521:MET:CE	2.38	0.54
5:B:401:PHE:HA	5:B:404:LYS:HG3	1.90	0.54
5:B:475:SER:C	5:B:477:ALA:H	2.11	0.54
5:B:515:HIS:N	5:B:518:HIS:CD2	2.76	0.54
12:K:40:HIS:CE1	12:K:63:VAL:CG2	2.90	0.54
4:A:575:LYS:HD3	4:A:612:ILE:HD11	1.90	0.54
5:B:278:GLN:CG	5:B:279:ASP:H	2.16	0.54
5:B:361:LEU:HD11	5:B:381:MET:CE	2.38	0.53
12:K:65:HIS:CD2	12:K:66:PRO:CD	2.91	0.53
4:A:1435:PRO:C	4:A:1436:ILE:HD12	2.28	0.53
5:B:563:MET:HE1	5:B:587:HIS:HB2	1.90	0.53
5:B:578:THR:OG1	5:B:593:PRO:HG3	2.08	0.53
4:A:93:VAL:HG13	4:A:301:ALA:CB	2.28	0.53
5:B:363:HIS:O	5:B:364:ILE:CB	2.53	0.53
4:A:848:ILE:HD13	4:A:858:ASN:HB3	1.90	0.53
4:A:1333:ILE:O	4:A:1333:ILE:HD13	2.08	0.53
5:B:1135:ARG:HG3	5:B:1147:LEU:HD21	1.91	0.53
4:A:901:LEU:HB2	4:A:926:GLN:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1130:GLN:HE21	4:A:1134:ILE:HD11	1.73	0.53
5:B:292:ILE:H	5:B:293:PRO:HD2	1.74	0.53
5:B:1002:THR:HG22	5:B:1006:ILE:H	1.73	0.53
7:E:30:ILE:HG23	7:E:34:GLU:OE1	2.08	0.53
4:A:360:GLU:HB2	4:A:363:GLN:HG3	1.91	0.53
6:C:100:THR:HG22	6:C:101:LEU:N	2.22	0.53
2:T:16:DC:C6	2:T:17:DG:C8	2.97	0.53
4:A:381:THR:HG22	4:A:383:TYR:H	1.74	0.53
5:B:563:MET:HA	5:B:589:VAL:O	2.09	0.53
5:B:643:ASP:O	5:B:644:GLU:HB3	2.09	0.53
6:C:167:HIS:HD2	6:C:169:LYS:N	1.95	0.53
10:I:78:CYS:O	10:I:80:SER:N	2.40	0.53
4:A:871:ASP:OD1	4:A:1366:ARG:NH2	2.41	0.53
4:A:901:LEU:HA	4:A:907:THR:CG2	2.38	0.53
4:A:1329:THR:HG22	4:A:1331:SER:N	2.24	0.53
5:B:515:HIS:N	5:B:518:HIS:HD2	2.07	0.53
5:B:872:GLU:HG2	5:B:916:THR:HB	1.90	0.53
5:B:1013:ASN:C	5:B:1015:HIS:H	2.12	0.53
4:A:746:MET:HG2	5:B:1015:HIS:CE1	2.44	0.52
2:T:18:DA:H2'	2:T:19:DT:C6	2.43	0.52
4:A:102:VAL:HG12	4:A:211:PHE:CE1	2.44	0.52
4:A:451:HIS:HB3	4:A:454:SER:H	1.74	0.52
4:A:871:ASP:HB3	7:E:205:SER:HB3	1.90	0.52
7:E:3:GLN:HG2	7:E:4:GLU:N	2.21	0.52
4:A:1410:PHE:HD2	5:B:1212:ILE:HD11	1.75	0.52
5:B:898:LEU:HB2	13:L:58:LYS:HE3	1.92	0.52
6:C:92:CYS:SG	6:C:94:LYS:HB2	2.50	0.52
9:H:26:ILE:CG2	9:H:40:LEU:HB3	2.39	0.52
4:A:567:LYS:NZ	9:H:95:TYR:CZ	2.75	0.52
4:A:1436:ILE:O	4:A:1438:THR:N	2.43	0.52
5:B:315:LYS:N	5:B:316:PRO:HD2	2.24	0.52
5:B:346:GLU:HA	5:B:349:ILE:HD13	1.91	0.52
9:H:129:TYR:C	9:H:131:ASN:H	2.11	0.52
4:A:1110:ASN:HD22	4:A:1110:ASN:N	1.90	0.52
4:A:1195:LEU:HD11	4:A:1267:MET:CE	2.40	0.52
5:B:1111:MET:HE2	5:B:1118:PRO:N	2.25	0.52
10:I:103:CYS:C	10:I:105:SER:N	2.60	0.52
4:A:313:GLN:HG2	4:A:322:VAL:HG22	1.91	0.52
4:A:1425:SER:O	4:A:1429:ILE:HG13	2.10	0.52
9:H:131:ASN:O	9:H:133:ASN:N	2.42	0.52
4:A:58:LEU:HB2	4:A:80:HIS:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:534:LEU:O	4:A:574:GLY:HA3	2.10	0.52
4:A:568:PRO:O	4:A:569:LYS:HB2	2.09	0.52
4:A:786:HIS:HE1	5:B:742:GLU:OE1	1.93	0.52
5:B:211:VAL:HG21	5:B:483:LEU:HD13	1.88	0.52
7:E:135:PHE:HB3	7:E:140:LEU:HD11	1.91	0.52
3:N:8:DT:H2"	3:N:9:DC:OP2	2.09	0.52
4:A:55:ASP:O	4:A:57:ARG:N	2.43	0.52
4:A:297:GLN:HG3	4:A:298:PHE:N	2.25	0.52
5:B:1006:ILE:CG2	5:B:1007:VAL:N	2.73	0.52
1:R:2:U:H2'	1:R:3:C:H6	1.74	0.52
5:B:801:LYS:HG2	11:J:52:THR:O	2.09	0.52
11:J:45:CYS:O	11:J:48:ARG:HG3	2.10	0.52
4:A:57:ARG:HB3	4:A:68:GLN:HB3	1.92	0.52
4:A:896:ARG:HD2	4:A:897:TYR:CE1	2.45	0.52
4:A:365:GLY:O	4:A:468:PHE:HA	2.10	0.51
6:C:22:LEU:CD2	6:C:25:VAL:HG21	2.39	0.51
4:A:590:ARG:NH2	4:A:620:LYS:HB2	2.26	0.51
4:A:821:ARG:O	4:A:825:ILE:HG12	2.10	0.51
4:A:1348:LEU:HG	4:A:1372:VAL:HG22	1.91	0.51
7:E:100:ILE:HG23	7:E:105:PHE:HB2	1.91	0.51
9:H:128:ASN:O	9:H:131:ASN:OD1	2.27	0.51
5:B:102:VAL:HG12	5:B:103:ASN:N	2.24	0.51
5:B:957:ASN:ND2	5:B:959:ASP:H	2.09	0.51
9:H:100:THR:HG23	9:H:138:GLU:HA	1.91	0.51
5:B:1212:ILE:O	5:B:1214:PRO:HD3	2.11	0.51
9:H:89:LEU:C	9:H:91:ASP:H	2.13	0.51
1:R:3:C:H42	2:T:26:DG:H1	1.57	0.51
4:A:34:LYS:HE2	4:A:57:ARG:NH2	2.26	0.51
4:A:353:ILE:HD13	4:A:487:MET:HE3	1.92	0.51
5:B:287:ARG:HA	5:B:291:ILE:O	2.10	0.51
5:B:770:GLN:HG2	5:B:983:ARG:O	2.11	0.51
5:B:807:ARG:HG3	5:B:807:ARG:NH1	2.24	0.51
4:A:117:GLU:CA	4:A:118:HIS:O	2.59	0.51
5:B:542:MET:HE3	5:B:636:PRO:HG2	1.91	0.51
5:B:640:VAL:HG22	5:B:651:LEU:CD2	2.41	0.51
5:B:863:GLU:OE1	5:B:962:LYS:HB3	2.11	0.51
6:C:248:ILE:HG12	12:K:101:LEU:HD12	1.92	0.51
4:A:56:PRO:O	4:A:57:ARG:CG	2.51	0.51
5:B:794:ASN:N	5:B:794:ASN:HD22	2.07	0.51
5:B:844:SER:O	5:B:848:ARG:HG3	2.11	0.51
6:C:165:LYS:O	12:K:6:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:709:THR:HG21	10:I:93:LYS:O	2.11	0.51
5:B:879:ARG:NE	5:B:879:ARG:CA	2.74	0.51
12:K:49:GLU:HA	12:K:52:ASN:ND2	2.25	0.51
4:A:130:ASP:O	4:A:132:LYS:N	2.35	0.51
4:A:135:PHE:HD1	4:A:222:LEU:HB2	1.75	0.51
5:B:193:LYS:NZ	11:J:65:PRO:HG3	2.26	0.51
5:B:235:SER:OG	5:B:236:HIS:ND1	2.39	0.51
5:B:857:ARG:HH21	5:B:942:ARG:NH2	2.09	0.51
5:B:1107:ALA:O	5:B:1108:ARG:CB	2.58	0.51
4:A:549:MET:SD	4:A:577:ILE:HD11	2.50	0.51
5:B:785:TYR:CD1	5:B:785:TYR:C	2.83	0.51
5:B:803:LEU:HG	5:B:822:ASN:ND2	2.26	0.51
5:B:1073:TYR:N	5:B:1073:TYR:CD1	2.79	0.51
8:F:111:LEU:HD12	8:F:111:LEU:H	1.76	0.51
4:A:800:VAL:C	4:A:802:ASN:H	2.14	0.50
4:A:1110:ASN:ND2	4:A:1110:ASN:N	2.52	0.50
5:B:906:SER:CB	5:B:946:ASN:CB	2.83	0.50
9:H:63:LEU:C	9:H:90:ALA:H	2.14	0.50
4:A:320:ARG:CZ	4:A:320:ARG:H	2.24	0.50
4:A:323:LYS:O	4:A:324:SER:CB	2.59	0.50
5:B:884:ARG:O	5:B:936:ASP:HB3	2.12	0.50
6:C:46:ILE:HA	6:C:159:ALA:HA	1.92	0.50
9:H:44:VAL:HG12	9:H:44:VAL:O	2.10	0.50
12:K:40:HIS:CE1	12:K:63:VAL:HG21	2.46	0.50
12:K:62:LYS:HG3	12:K:62:LYS:O	2.10	0.50
4:A:71:GLN:O	4:A:73:GLY:N	2.44	0.50
5:B:665:GLU:O	5:B:668:ASP:HB3	2.10	0.50
6:C:167:HIS:CD2	6:C:169:LYS:HB3	2.46	0.50
7:E:144:ILE:O	7:E:150:VAL:HG21	2.11	0.50
4:A:535:THR:HG22	4:A:616:VAL:HA	1.93	0.50
4:A:754:SER:N	4:A:757:ASN:HD22	2.04	0.50
5:B:745:PRO:HB2	5:B:1047:PHE:CD1	2.47	0.50
7:E:15:ALA:O	7:E:19:VAL:HG23	2.12	0.50
9:H:5:LEU:HD12	9:H:60:ALA:O	2.11	0.50
4:A:541:ILE:HG13	4:A:546:VAL:HG22	1.94	0.50
4:A:567:LYS:O	4:A:569:LYS:N	2.45	0.50
4:A:647:GLY:O	4:A:651:LYS:HG3	2.11	0.50
4:A:800:VAL:O	4:A:800:VAL:HG12	2.11	0.50
5:B:120:ARG:HG2	5:B:955:THR:HG21	1.93	0.50
11:J:42:LYS:HG3	11:J:43:ARG:H	1.77	0.50
12:K:47:ARG:HH11	12:K:47:ARG:HB3	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:117:GLU:N	4:A:118:HIS:C	2.64	0.50
4:A:276:LEU:HD11	4:A:292:ALA:CB	2.42	0.50
4:A:381:THR:HG23	4:A:382:PRO:HD2	1.92	0.50
5:B:843:GLN:HB2	5:B:993:THR:HB	1.94	0.50
4:A:32:VAL:O	4:A:57:ARG:NH1	2.44	0.50
4:A:71:GLN:C	4:A:73:GLY:H	2.16	0.50
4:A:826:ASP:HA	4:A:829:VAL:HB	1.93	0.50
4:A:244:PRO:HB2	4:A:245:PRO:CD	2.42	0.50
4:A:496:GLU:HB2	8:F:95:GLY:HA3	1.94	0.50
4:A:779:PHE:CE2	5:B:517:THR:HG22	2.47	0.50
6:C:163:ILE:HD12	6:C:165:LYS:HB2	1.93	0.50
4:A:775:ILE:O	4:A:797:LYS:HE2	2.12	0.49
5:B:464:GLY:HA3	5:B:478:GLY:HA2	1.94	0.49
5:B:981:ALA:O	5:B:1093:GLN:N	2.31	0.49
9:H:139:ASN:O	9:H:140:ALA:HB3	2.12	0.49
2:T:18:DA:H2	14:T:29[B]:DUT:O2	1.86	0.49
4:A:203:SER:O	4:A:207:ILE:HG13	2.12	0.49
4:A:367:PRO:HG2	4:A:370:ILE:HG13	1.93	0.49
4:A:754:SER:H	4:A:757:ASN:ND2	2.05	0.49
4:A:1444:MET:O	8:F:133:VAL:N	2.42	0.49
5:B:62:ILE:HG23	5:B:418:LYS:HG3	1.93	0.49
5:B:558:LEU:C	5:B:560:GLU:H	2.16	0.49
4:A:552:TRP:NE1	4:A:655:PHE:CD1	2.81	0.49
5:B:873:THR:O	5:B:914:LYS:HG3	2.12	0.49
9:H:56:THR:O	9:H:144:ILE:HA	2.12	0.49
9:H:83:GLN:HG3	12:K:54:ARG:HB3	1.95	0.49
11:J:3:VAL:CG2	11:J:18:TRP:CB	2.83	0.49
2:T:18:DA:H61	14:T:29[B]:DUT:C4	2.24	0.49
4:A:219:PHE:HZ	4:A:230:ARG:HD3	1.78	0.49
4:A:793:SER:HB2	4:A:794:PRO:HD2	1.95	0.49
5:B:416:LEU:HD12	5:B:466:TRP:CZ2	2.47	0.49
5:B:488:TYR:CE2	5:B:813:LYS:HB2	2.48	0.49
5:B:567:GLU:H	5:B:567:GLU:CD	2.16	0.49
4:A:290:GLU:OE1	4:A:293:GLU:HG3	2.13	0.49
4:A:455:MET:O	5:B:1141:HIS:HE1	1.95	0.49
4:A:1015:VAL:CG1	4:A:1019:CYS:SG	3.00	0.49
5:B:185:THR:OG1	5:B:188:ASP:OD2	2.29	0.49
5:B:979:LYS:CE	5:B:987:LYS:HG2	2.42	0.49
5:B:1168:LEU:HD22	5:B:1208:MET:HE2	1.94	0.49
4:A:64:ASN:HB3	4:A:66:LYS:CG	2.43	0.49
5:B:190:TYR:CZ	5:B:196:PRO:HG3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:287:ARG:O	5:B:289:LEU:N	2.46	0.49
5:B:526:GLU:HG3	5:B:771:SER:HB3	1.94	0.49
5:B:975:GLN:HG2	5:B:976:ILE:H	1.78	0.49
6:C:112:ASN:ND2	6:C:146:LYS:HG2	2.27	0.49
13:L:42:ARG:HD2	13:L:42:ARG:H	1.77	0.49
5:B:234:ILE:HD13	5:B:234:ILE:H	1.76	0.49
6:C:57:VAL:HG12	6:C:58:LEU:HD23	1.93	0.49
10:I:10:CYS:SG	10:I:31:THR:HB	2.52	0.49
4:A:770:VAL:HA	4:A:822:GLU:OE1	2.13	0.49
5:B:882:THR:HG23	5:B:883:LEU:N	2.28	0.49
6:C:260:LEU:HG	6:C:264:GLN:HE22	1.78	0.49
7:E:109:ILE:HD13	7:E:109:ILE:N	2.28	0.49
9:H:92:ASP:OD2	9:H:92:ASP:N	2.45	0.49
4:A:91:PHE:HD2	4:A:297:GLN:OE1	1.96	0.49
4:A:470:LEU:HD21	4:A:487:MET:HE3	1.93	0.49
4:A:1340:GLY:HA2	7:E:183:PRO:HD2	1.94	0.49
5:B:911:ILE:HD11	5:B:941:LEU:CA	2.43	0.49
5:B:1111:MET:HE2	5:B:1118:PRO:CD	2.43	0.49
9:H:7:ASP:O	9:H:8:ASP:HB2	2.12	0.49
4:A:89:PRO:HG2	4:A:205:GLU:HG3	1.93	0.48
4:A:871:ASP:HB3	7:E:204:THR:HG23	1.93	0.48
10:I:55:THR:HG23	10:I:58:VAL:HG21	1.94	0.48
4:A:693:VAL:O	4:A:696:GLU:HB3	2.14	0.48
4:A:855:THR:HG23	4:A:857:ARG:HG3	1.94	0.48
5:B:696:GLU:O	5:B:699:GLU:HB2	2.13	0.48
4:A:335:ARG:NH1	5:B:1202:LEU:HD12	2.28	0.48
4:A:1111:MET:HG3	4:A:1114:PRO:HG3	1.94	0.48
4:A:1356:ILE:O	4:A:1359:ASP:HB3	2.13	0.48
5:B:645:SER:C	5:B:647:GLY:H	2.17	0.48
5:B:1037:LEU:HD13	5:B:1062:HIS:HB3	1.94	0.48
6:C:27:LEU:HA	6:C:228:PHE:CZ	2.48	0.48
8:F:109:VAL:HG22	8:F:110:ASP:N	2.28	0.48
4:A:148:CYS:HB3	4:A:169:ASN:H	1.78	0.48
5:B:574:SER:N	5:B:575:PRO:HD3	2.28	0.48
5:B:783:THR:HG21	11:J:59:LYS:HB3	1.96	0.48
6:C:70:ILE:HD11	6:C:144:ILE:HD12	1.94	0.48
3:N:12:DT:H5"	7:E:119:SER:HB2	1.95	0.48
4:A:306:ASN:O	4:A:307:ASP:CB	2.61	0.48
5:B:744:HIS:HD2	5:B:746:SER:N	1.97	0.48
4:A:1166:ASP:O	4:A:1168:GLU:N	2.47	0.48
5:B:918:ILE:HG13	5:B:935:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:238:ILE:HG22	6:C:242:GLN:HB2	1.95	0.48
5:B:291:ILE:HD12	5:B:291:ILE:N	2.28	0.48
6:C:186:LEU:HB3	6:C:188:HIS:CD2	2.48	0.48
9:H:40:LEU:HD13	9:H:123:MET:HG3	1.95	0.48
4:A:1002:GLY:O	4:A:1008:GLN:NE2	2.47	0.48
6:C:73:GLN:HE21	6:C:75:MET:N	2.12	0.48
4:A:695:LYS:HA	4:A:695:LYS:HD2	1.56	0.48
4:A:1080:THR:CG2	4:A:1081:LEU:N	2.77	0.48
5:B:1045:SER:O	5:B:1046:PRO:C	2.52	0.48
6:C:22:LEU:HD21	6:C:25:VAL:HG21	1.95	0.48
4:A:414:ASP:OD1	4:A:416:ARG:HG2	2.14	0.48
4:A:1004:ASN:O	4:A:1008:GLN:HG2	2.13	0.48
5:B:577:ALA:HB1	5:B:589:VAL:HB	1.95	0.48
5:B:1016:ALA:HB1	5:B:1020:ARG:NH1	2.29	0.48
6:C:77:ILE:HD12	6:C:161:LYS:HG3	1.96	0.48
4:A:672:ASP:OD1	4:A:675:THR:N	2.47	0.47
5:B:1054:GLY:HA2	5:B:1057:LYS:NZ	2.29	0.47
4:A:1329:THR:CG2	4:A:1331:SER:H	2.26	0.47
5:B:841:MET:O	5:B:993:THR:HA	2.14	0.47
5:B:998:ASP:OD1	6:C:35:ARG:NH2	2.47	0.47
14:T:29[B]:DUT:H6	14:T:29[B]:DUT:O1A	2.13	0.47
4:A:381:THR:CG2	4:A:382:PRO:HD2	2.45	0.47
4:A:919:ILE:O	4:A:922:ASP:HB2	2.14	0.47
5:B:22:SER:O	5:B:654:ARG:HD2	2.14	0.47
9:H:137:GLN:HB3	9:H:139:ASN:HB2	1.96	0.47
4:A:26:GLU:O	4:A:30:ILE:HB	2.14	0.47
4:A:457:ALA:HB2	4:A:501:LEU:HD13	1.97	0.47
4:A:1154:TYR:HE1	10:I:18:GLU:HG3	1.79	0.47
5:B:752:ALA:O	5:B:755:ILE:HG12	2.14	0.47
5:B:805:THR:HG22	5:B:809:MET:SD	2.54	0.47
5:B:881:ASN:HB2	5:B:933:SER:OG	2.14	0.47
5:B:1135:ARG:NH2	5:B:1136:ASP:OD1	2.47	0.47
5:B:1180:PHE:O	5:B:1181:GLU:HG2	2.15	0.47
4:A:507:VAL:HB	4:A:508:PRO:HD3	1.95	0.47
4:A:842:VAL:HG11	5:B:1136:ASP:OD2	2.15	0.47
5:B:660:LYS:HE2	5:B:679:TYR:CD1	2.49	0.47
5:B:794:ASN:C	5:B:795:ILE:HD12	2.35	0.47
6:C:6:PRO:HB2	12:K:101:LEU:HD23	1.96	0.47
6:C:259:LEU:HD12	6:C:259:LEU:HA	1.77	0.47
4:A:95:PHE:O	4:A:96:ILE:C	2.52	0.47
4:A:117:GLU:O	4:A:123:ARG:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1193:LEU:HB2	4:A:1260:LEU:HD11	1.96	0.47
5:B:53:GLN:HG2	5:B:547:VAL:HG13	1.95	0.47
5:B:378:LEU:O	5:B:382:ILE:HG12	2.15	0.47
5:B:745:PRO:O	5:B:748:ILE:HG12	2.15	0.47
5:B:900:ALA:HB3	13:L:61:THR:HG23	1.96	0.47
5:B:1094:ARG:CG	5:B:1094:ARG:NH1	2.38	0.47
7:E:64:PRO:CD	7:E:76:GLY:HA2	2.33	0.47
7:E:172:GLU:CG	7:E:213:ILE:HD12	2.45	0.47
10:I:46:HIS:O	10:I:47:GLU:O	2.33	0.47
11:J:1:MET:O	11:J:2:ILE:HB	2.13	0.47
4:A:800:VAL:HG13	4:A:812:GLU:HG2	1.96	0.47
5:B:778:MET:HB3	5:B:796:LEU:HD13	1.95	0.47
4:A:896:ARG:HB3	4:A:897:TYR:CD1	2.49	0.47
4:A:1410:PHE:CD2	5:B:1212:ILE:HD11	2.49	0.47
5:B:821:GLN:HB2	5:B:851:PHE:CE2	2.50	0.47
8:F:140:ASP:OD1	8:F:141:GLY:N	2.48	0.47
14:T:29[B]:DUT:C3'	14:T:29[B]:DUT:C6	2.93	0.47
4:A:64:ASN:O	4:A:66:LYS:N	2.48	0.47
4:A:312:PRO:O	4:A:313:GLN:NE2	2.48	0.47
4:A:320:ARG:H	4:A:320:ARG:NE	2.13	0.47
4:A:455:MET:O	5:B:1141:HIS:CE1	2.68	0.47
5:B:550:ASP:OD1	5:B:551:PRO:HD2	2.15	0.47
6:C:69:LEU:HD12	6:C:69:LEU:N	2.30	0.47
4:A:67:CYS:C	4:A:68:GLN:HG3	2.35	0.46
4:A:746:MET:HG2	5:B:1015:HIS:HE1	1.80	0.46
5:B:406:LEU:HD12	5:B:633:VAL:HG22	1.97	0.46
5:B:470:LYS:O	5:B:471:LYS:HG3	2.15	0.46
5:B:562:GLY:O	5:B:563:MET:HB3	2.15	0.46
5:B:890:TYR:CE2	5:B:910:VAL:HG21	2.50	0.46
5:B:1175:LEU:O	5:B:1176:ASN:CB	2.63	0.46
1:R:9:G:H2'	1:R:10:A:C8	2.50	0.46
4:A:14:VAL:HB	4:A:1430:LEU:HD13	1.97	0.46
4:A:17:VAL:HB	4:A:1419:ASP:HB3	1.97	0.46
4:A:43:GLU:OE1	4:A:46:THR:HB	2.16	0.46
4:A:55:ASP:O	4:A:58:LEU:N	2.48	0.46
4:A:253:ASN:O	4:A:254:GLU:CB	2.63	0.46
4:A:443:LEU:HD23	4:A:443:LEU:HA	1.73	0.46
4:A:495:GLU:O	4:A:498:ARG:HG3	2.14	0.46
5:B:798:TYR:OH	6:C:62:PHE:HE2	1.99	0.46
7:E:86:PRO:O	7:E:114:ASN:HB2	2.15	0.46
12:K:46:ILE:O	12:K:50:LEU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:298:PHE:O	4:A:298:PHE:CG	2.68	0.46
4:A:324:SER:C	4:A:326:ARG:N	2.69	0.46
4:A:650:GLN:O	4:A:654:ASN:HB2	2.16	0.46
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.49	0.46
7:E:100:ILE:O	7:E:101:GLN:C	2.52	0.46
4:A:499:ALA:O	4:A:503:GLN:HG2	2.14	0.46
5:B:680:THR:O	5:B:683:SER:HB2	2.15	0.46
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.48	0.46
4:A:116:ASP:HB3	4:A:117:GLU:HB3	1.87	0.46
4:A:523:ILE:HG23	4:A:527:THR:HB	1.97	0.46
4:A:532:ARG:HG3	4:A:616:VAL:HG11	1.98	0.46
4:A:1158:PRO:HB3	4:A:1188:GLN:OE1	2.16	0.46
4:A:1188:GLN:HB3	4:A:1189:SER:H	1.59	0.46
5:B:237:VAL:HG11	5:B:255:GLN:HE21	1.81	0.46
9:H:109:LYS:HZ2	9:H:111:LEU:HD12	1.81	0.46
4:A:596:THR:C	4:A:598:LEU:N	2.61	0.46
4:A:808:LEU:HD12	4:A:808:LEU:N	2.30	0.46
5:B:1106:ARG:HG2	5:B:1107:ALA:N	2.31	0.46
14:T:29[B]:DUT:C6	14:T:29[B]:DUT:H3'	2.46	0.46
4:A:949:ASP:OD1	4:A:949:ASP:N	2.45	0.46
6:C:254:LYS:HD3	12:K:42:LEU:HD13	1.98	0.46
4:A:323:LYS:O	4:A:324:SER:HB3	2.16	0.46
5:B:140:ILE:H	5:B:141:ASP:C	2.19	0.46
5:B:273:LEU:HD21	5:B:360:PHE:CD1	2.51	0.46
7:E:124:VAL:HA	7:E:132:ILE:HD11	1.97	0.46
11:J:5:VAL:O	11:J:6:ARG:O	2.33	0.46
14:T:29[B]:DUT:H6	14:T:29[B]:DUT:H3'	1.97	0.46
4:A:847:ASP:OD2	4:A:858:ASN:HB2	2.16	0.46
4:A:1105:LEU:HB3	4:A:1384:VAL:CG2	2.46	0.46
5:B:1110:PRO:O	5:B:1119:VAL:HG13	2.16	0.46
4:A:423:ASP:CG	4:A:424:ILE:N	2.68	0.46
4:A:567:LYS:HD3	9:H:95:TYR:CD1	2.50	0.46
4:A:1118:VAL:HB	4:A:1306:LEU:HB2	1.98	0.46
5:B:1168:LEU:HB3	5:B:1208:MET:HE1	1.98	0.46
1:R:2:U:H2'	1:R:3:C:C6	2.51	0.45
4:A:130:ASP:C	4:A:132:LYS:H	2.18	0.45
4:A:671:ALA:O	4:A:672:ASP:O	2.35	0.45
4:A:1156:PRO:O	4:A:1158:PRO:HD3	2.16	0.45
5:B:25:ILE:HD12	5:B:653:VAL:CG2	2.46	0.45
5:B:658:ILE:HA	5:B:661:LEU:HD12	1.97	0.45
5:B:956:THR:HB	13:L:46:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1076:HIS:CG	12:K:40:HIS:CD2	3.04	0.45
5:B:1156:ASP:O	5:B:1157:ALA:CB	2.61	0.45
12:K:51:LEU:CD1	12:K:59:ALA:HB3	2.46	0.45
12:K:92:ASN:HA	12:K:95:ILE:HD12	1.98	0.45
4:A:608:ILE:C	4:A:609:ASP:O	2.53	0.45
4:A:800:VAL:HA	4:A:812:GLU:HG2	1.97	0.45
4:A:1171:GLN:H	4:A:1171:GLN:HG3	1.50	0.45
4:A:1192:LEU:HD11	4:A:1239:ARG:HB3	1.99	0.45
4:A:1277:GLU:O	4:A:1278:ASN:CB	2.64	0.45
4:A:120:GLU:O	4:A:121:LEU:HB2	2.15	0.45
4:A:711:ARG:NH1	10:I:95:THR:O	2.50	0.45
5:B:651:LEU:HD11	5:B:707:PRO:HG3	1.98	0.45
3:N:11:DG:H1'	3:N:12:DT:H5'	1.98	0.45
4:A:253:ASN:CG	4:A:254:GLU:H	2.19	0.45
4:A:575:LYS:HB3	4:A:612:ILE:HG12	1.98	0.45
5:B:1155:SER:O	5:B:1156:ASP:O	2.34	0.45
7:E:127:ILE:HD13	7:E:127:ILE:H	1.82	0.45
4:A:99:ILE:HD11	4:A:234:MET:CB	2.47	0.45
4:A:115:LEU:HD21	4:A:145:LYS:HE3	1.99	0.45
4:A:249:SER:C	4:A:250:ILE:HG12	2.35	0.45
7:E:192:ARG:O	7:E:192:ARG:HG3	2.16	0.45
9:H:6:PHE:CG	9:H:7:ASP:N	2.84	0.45
9:H:89:LEU:O	9:H:91:ASP:N	2.50	0.45
9:H:108:SER:O	9:H:110:ASP:N	2.50	0.45
4:A:1341:ILE:HG22	7:E:182:ASP:OD2	2.16	0.45
5:B:465:ASN:OD1	5:B:476:ARG:HB2	2.15	0.45
5:B:643:ASP:OD2	5:B:644:GLU:N	2.50	0.45
5:B:1106:ARG:HG2	5:B:1108:ARG:H	1.82	0.45
5:B:1111:MET:CE	5:B:1118:PRO:HA	2.47	0.45
6:C:124:LEU:O	6:C:127:ARG:HG2	2.17	0.45
4:A:446:ARG:HB2	4:A:487:MET:SD	2.57	0.45
4:A:826:ASP:N	4:A:826:ASP:OD1	2.49	0.45
4:A:848:ILE:HG21	4:A:1370:LEU:HD11	1.98	0.45
4:A:852:TYR:CE2	4:A:1060:PRO:HB2	2.52	0.45
5:B:102:VAL:HG22	5:B:112:LEU:HD22	1.99	0.45
6:C:70:ILE:HD11	6:C:144:ILE:HD11	1.99	0.45
6:C:241:ASP:HB3	12:K:109:TRP:CE2	2.51	0.45
4:A:567:LYS:HB2	9:H:95:TYR:HA	1.99	0.45
4:A:897:TYR:CD2	4:A:936:LEU:HD13	2.52	0.45
4:A:1341:ILE:HD13	4:A:1380:GLY:HA2	1.98	0.45
4:A:1436:ILE:O	4:A:1437:GLY:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:211:VAL:O	5:B:480:SER:HA	2.17	0.45
5:B:276:ILE:HD13	5:B:277:LYS:HE3	1.98	0.45
6:C:124:LEU:CD2	6:C:129:ILE:HG22	2.46	0.45
4:A:343:LYS:HE2	5:B:1151:LEU:HG	1.98	0.45
4:A:450:LEU:O	4:A:450:LEU:CD1	2.64	0.45
4:A:474:VAL:O	4:A:478:TYR:HD1	1.99	0.45
5:B:527:THR:OG1	5:B:528:PRO:HD2	2.16	0.45
2:T:16:DC:H2'	2:T:17:DG:C8	2.50	0.45
4:A:115:LEU:HD12	4:A:122:MET:CE	2.46	0.45
4:A:403:LYS:O	4:A:404:TYR:O	2.35	0.45
4:A:474:VAL:HG22	4:A:478:TYR:HE1	1.82	0.45
4:A:901:LEU:HD23	4:A:907:THR:HG22	1.98	0.45
5:B:226:PHE:HA	5:B:395:GLN:HG3	1.98	0.45
5:B:283:VAL:CG2	5:B:321:GLY:HA3	2.47	0.45
5:B:802:PRO:HB3	5:B:1091:TYR:CD1	2.51	0.45
5:B:890:TYR:CZ	5:B:910:VAL:HG21	2.52	0.45
6:C:152:GLU:HG2	6:C:153:LEU:N	2.32	0.45
7:E:127:ILE:N	7:E:128:PRO:HD3	2.32	0.45
4:A:50:ILE:O	4:A:56:PRO:HD3	2.16	0.44
4:A:571:LEU:HD22	9:H:46:LEU:HD11	1.98	0.44
4:A:1148:ILE:HD13	10:I:49:ILE:HD12	1.98	0.44
4:A:1172:LEU:HD23	4:A:1172:LEU:H	1.82	0.44
8:F:132:LEU:O	8:F:148:VAL:HG23	2.16	0.44
4:A:265:LYS:HE3	4:A:302:THR:HG23	1.99	0.44
4:A:298:PHE:HA	4:A:299:HIS:C	2.35	0.44
4:A:299:HIS:CA	4:A:302:THR:HG22	2.47	0.44
5:B:102:VAL:CG2	5:B:112:LEU:HB2	2.42	0.44
5:B:798:TYR:CD2	11:J:4:PRO:HG3	2.53	0.44
12:K:84:LYS:O	12:K:88:LYS:HG3	2.16	0.44
4:A:99:ILE:HD13	4:A:234:MET:HE3	1.99	0.44
4:A:115:LEU:HD13	4:A:119:ASN:ND2	2.31	0.44
4:A:265:LYS:C	4:A:267:ALA:N	2.69	0.44
4:A:456:MET:HE2	4:A:510:GLN:HB2	1.98	0.44
5:B:393:LYS:HE3	5:B:393:LYS:HA	1.99	0.44
5:B:637:LEU:HD11	5:B:693:ILE:HG13	2.00	0.44
5:B:654:ARG:H	5:B:657:HIS:HD2	1.65	0.44
5:B:911:ILE:CD1	5:B:941:LEU:HA	2.47	0.44
8:F:71:GLU:HA	8:F:72:LYS:HA	1.84	0.44
12:K:46:ILE:HG22	12:K:50:LEU:HD12	1.99	0.44
4:A:86:LEU:CB	4:A:237:THR:O	2.66	0.44
4:A:353:ILE:HD13	4:A:487:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1349:TYR:HA	4:A:1372:VAL:HG21	1.98	0.44
5:B:793:ALA:C	5:B:794:ASN:HD22	2.21	0.44
6:C:99:LEU:N	6:C:99:LEU:HD22	2.32	0.44
6:C:123:ASN:ND2	6:C:125:MET:HG3	2.32	0.44
10:I:68:LEU:HD13	10:I:84:VAL:HG11	1.98	0.44
4:A:1115:SER:HB3	4:A:1330:ASN:ND2	2.32	0.44
5:B:416:LEU:HD11	5:B:460:ALA:CB	2.47	0.44
5:B:542:MET:HE1	5:B:743:ILE:HG13	2.00	0.44
5:B:1096:ARG:O	5:B:1097:HIS:CB	2.66	0.44
7:E:213:ILE:HG12	7:E:214:CYS:H	1.82	0.44
11:J:53:HIS:HE1	11:J:55:ASP:OD1	2.01	0.44
4:A:40:THR:HG22	4:A:54:ASN:HD21	1.82	0.44
4:A:404:TYR:HA	4:A:413:ILE:O	2.17	0.44
4:A:568:PRO:O	4:A:569:LYS:HB3	2.17	0.44
4:A:645:LEU:O	4:A:649:ILE:HG13	2.18	0.44
5:B:333:PHE:HD1	5:B:333:PHE:O	2.00	0.44
5:B:826:ALA:O	5:B:1011:ILE:HA	2.18	0.44
5:B:1190:ASP:C	5:B:1191:ILE:HG13	2.38	0.44
8:F:73:ALA:O	8:F:74:ILE:HG13	2.18	0.44
4:A:1059:HIS:CE1	8:F:87:LYS:H	2.36	0.44
4:A:1279:ILE:O	4:A:1279:ILE:HG22	2.18	0.44
5:B:167:ILE:O	5:B:167:ILE:CG2	2.52	0.44
12:K:113:THR:O	12:K:114:LEU:CB	2.65	0.44
4:A:43:GLU:HG3	4:A:50:ILE:HG12	1.99	0.44
4:A:55:ASP:N	4:A:56:PRO:HD2	2.33	0.44
5:B:383:ASN:HD21	5:B:387:LEU:HD22	1.81	0.44
5:B:788:ARG:NH1	5:B:790:ASP:OD1	2.49	0.44
4:A:313:GLN:HG3	4:A:314:ALA:H	1.82	0.44
4:A:830:LYS:HE2	4:A:1082:ASN:ND2	2.33	0.44
4:A:902:LEU:HG	4:A:926:GLN:HG3	2.00	0.44
5:B:318:VAL:HG21	10:I:13:MET:HE2	1.99	0.44
5:B:515:HIS:H	5:B:518:HIS:HD2	1.56	0.44
5:B:950:ASP:HB3	5:B:967:ARG:HG2	1.99	0.44
4:A:132:LYS:HB3	4:A:132:LYS:HE2	1.85	0.43
4:A:273:ASN:C	4:A:275:SER:H	2.20	0.43
4:A:670:ILE:HD12	5:B:1067:ARG:NH1	2.33	0.43
5:B:702:LEU:HD12	5:B:702:LEU:HA	1.81	0.43
5:B:879:ARG:HB3	5:B:880:THR:H	1.55	0.43
5:B:1160:VAL:HG12	5:B:1161:HIS:N	2.33	0.43
13:L:42:ARG:HD2	13:L:42:ARG:N	2.33	0.43
3:N:12:DT:H2"	3:N:13:DA:OP2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:230:ARG:HG3	4:A:233:TRP:CZ3	2.52	0.43
4:A:567:LYS:CB	9:H:95:TYR:HA	2.48	0.43
4:A:771:GLU:N	4:A:822:GLU:OE1	2.39	0.43
4:A:984:LYS:O	4:A:988:LEU:HB3	2.18	0.43
5:B:65:GLU:HB3	5:B:66:ASP:H	1.54	0.43
5:B:645:SER:O	5:B:647:GLY:N	2.49	0.43
5:B:991:GLY:O	5:B:992:ILE:HB	2.17	0.43
5:B:1017:ILE:H	5:B:1018:PRO:CD	2.31	0.43
6:C:69:LEU:HB3	11:J:6:ARG:HD2	2.00	0.43
6:C:82:TYR:CE2	6:C:161:LYS:HD3	2.53	0.43
9:H:2:SER:N	9:H:3:ASN:HB2	2.33	0.43
9:H:38:LEU:HD13	9:H:125:LEU:HD13	1.99	0.43
9:H:93:TYR:HD2	9:H:145:ARG:HB3	1.82	0.43
12:K:107:THR:O	12:K:111:LEU:HG	2.19	0.43
4:A:315:LEU:HB3	4:A:316:GLN:H	1.55	0.43
5:B:431:TYR:CE2	5:B:447:ALA:HB3	2.53	0.43
5:B:760:ASP:OD1	5:B:760:ASP:N	2.48	0.43
5:B:1084:GLN:HG2	6:C:201:TRP:CH2	2.53	0.43
5:B:1099:VAL:O	5:B:1103:ILE:CD1	2.66	0.43
5:B:762:ASN:OD1	5:B:984:HIS:HD2	2.01	0.43
5:B:785:TYR:CD1	5:B:786:ASN:N	2.87	0.43
5:B:839:MET:HE1	5:B:1010:LEU:HD21	1.99	0.43
11:J:38:ARG:HE	11:J:38:ARG:HB2	1.69	0.43
4:A:341:MET:HB3	5:B:1132:GLU:HB3	2.00	0.43
4:A:904:THR:HG23	4:A:905:ASP:OD1	2.18	0.43
4:A:1043:ASP:N	4:A:1043:ASP:OD1	2.51	0.43
5:B:839:MET:CE	5:B:1010:LEU:HD21	2.48	0.43
5:B:955:THR:HG23	13:L:54:ARG:O	2.18	0.43
5:B:1096:ARG:O	5:B:1097:HIS:HB2	2.19	0.43
7:E:147:HIS:HB3	7:E:150:VAL:HG23	2.00	0.43
8:F:71:GLU:HA	8:F:72:LYS:O	2.19	0.43
10:I:94:ASP:OD2	10:I:94:ASP:N	2.51	0.43
4:A:272:ALA:HA	4:A:275:SER:HB3	2.00	0.43
4:A:298:PHE:CD2	4:A:298:PHE:O	2.71	0.43
4:A:666:ILE:HD11	5:B:1027:ILE:HG12	2.00	0.43
4:A:1293:SER:HB2	4:A:1299:VAL:CG2	2.48	0.43
5:B:798:TYR:N	5:B:799:PRO:HD3	2.33	0.43
5:B:806:THR:HG23	5:B:1045:SER:HA	2.00	0.43
5:B:911:ILE:HD11	5:B:941:LEU:CB	2.49	0.43
5:B:1016:ALA:HB1	5:B:1020:ARG:HH12	1.83	0.43
5:B:1106:ARG:NH2	5:B:1109:GLY:H	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:32:GLN:O	7:E:32:GLN:HG3	2.18	0.43
9:H:10:PHE:HA	9:H:30:SER:HA	2.00	0.43
4:A:224:PHE:HD2	4:A:229:SER:O	2.01	0.43
8:F:85:MET:O	8:F:155:LEU:HD21	2.19	0.43
4:A:151:ASP:CG	4:A:163:SER:HA	2.38	0.43
4:A:673:GLY:N	4:A:674:PRO:CD	2.81	0.43
4:A:845:LEU:O	4:A:848:ILE:HG12	2.19	0.43
4:A:900:ASP:HA	4:A:926:GLN:NE2	2.33	0.43
4:A:1171:GLN:O	4:A:1174:PHE:CD2	2.71	0.43
5:B:1001:PHE:CZ	5:B:1073:TYR:HB2	2.54	0.43
5:B:1013:ASN:C	5:B:1015:HIS:N	2.72	0.43
12:K:37:LYS:HA	12:K:69:ALA:HB1	2.01	0.43
12:K:39:ASP:HB2	12:K:40:HIS:H	1.65	0.43
2:T:17:DG:N3	2:T:17:DG:H2'	2.34	0.43
4:A:341:MET:HE2	4:A:1425:SER:HB3	2.01	0.43
4:A:1004:ASN:CG	7:E:167:ARG:HD2	2.39	0.43
5:B:1032:SER:HB3	5:B:1089:PRO:HG2	2.00	0.43
9:H:24:CYS:HB2	9:H:44:VAL:CG2	2.48	0.43
12:K:10:PHE:CE1	12:K:11:LEU:HD13	2.54	0.43
12:K:49:GLU:C	12:K:51:LEU:H	2.20	0.43
5:B:916:THR:HA	5:B:917:PRO:HD2	1.90	0.43
9:H:17:PRO:O	9:H:19:ARG:N	2.51	0.43
4:A:7:SER:OG	5:B:1161:HIS:HE1	2.01	0.42
4:A:43:GLU:HG2	4:A:50:ILE:HG23	2.01	0.42
4:A:398:GLU:O	4:A:399:HIS:O	2.36	0.42
5:B:470:LYS:C	5:B:472:ALA:H	2.22	0.42
5:B:493:SER:HA	5:B:751:VAL:HG11	2.01	0.42
5:B:1111:MET:HE3	5:B:1118:PRO:HA	2.00	0.42
8:F:76:LYS:HA	8:F:79:ARG:HD3	2.01	0.42
9:H:137:GLN:C	9:H:139:ASN:N	2.70	0.42
4:A:516:SER:HB2	4:A:518:LYS:HG2	2.01	0.42
4:A:779:PHE:CE1	4:A:785:PRO:HD3	2.53	0.42
4:A:784:LEU:HB3	4:A:786:HIS:HD2	1.85	0.42
4:A:1400:CYS:O	4:A:1405:THR:HG23	2.18	0.42
4:A:1428:VAL:HG21	5:B:1135:ARG:HD2	2.01	0.42
5:B:813:LYS:HA	5:B:816:GLU:OE1	2.18	0.42
4:A:35:ILE:HA	4:A:52:GLY:O	2.19	0.42
5:B:398:ARG:NH1	5:B:398:ARG:CB	2.72	0.42
5:B:474:SER:C	5:B:476:ARG:N	2.70	0.42
5:B:558:LEU:O	5:B:560:GLU:N	2.53	0.42
5:B:758:PHE:HB3	5:B:761:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:883:LEU:N	5:B:883:LEU:HD23	2.34	0.42
5:B:956:THR:HA	5:B:961:LEU:O	2.19	0.42
6:C:8:VAL:HG11	12:K:105:PHE:HD1	1.85	0.42
7:E:113:GLN:HA	7:E:137:GLU:HG3	2.01	0.42
4:A:709:THR:HG22	4:A:711:ARG:H	1.85	0.42
4:A:800:VAL:C	4:A:802:ASN:N	2.70	0.42
5:B:778:MET:O	5:B:819:ALA:HB1	2.19	0.42
6:C:18:VAL:CG2	6:C:240:VAL:HB	2.49	0.42
6:C:201:TRP:HA	6:C:202:PRO:HD3	1.79	0.42
2:T:22:DT:H2'	2:T:23:DC:C6	2.54	0.42
4:A:206:GLU:O	4:A:210:ILE:HG12	2.19	0.42
4:A:384:ASN:O	4:A:387:ARG:N	2.52	0.42
4:A:424:ILE:O	4:A:424:ILE:HG22	2.20	0.42
4:A:828:ALA:HB1	5:B:530:GLY:HA2	2.02	0.42
4:A:1064:VAL:O	4:A:1064:VAL:HG12	2.19	0.42
4:A:1301:GLU:HA	4:A:1302:PRO:HD3	1.89	0.42
5:B:174:LEU:O	5:B:175:ARG:HB3	2.18	0.42
5:B:870:ILE:HG22	5:B:870:ILE:O	2.19	0.42
6:C:22:LEU:HD23	6:C:22:LEU:O	2.19	0.42
6:C:70:ILE:CD1	6:C:144:ILE:HD11	2.49	0.42
7:E:22:MET:HE2	7:E:26:ARG:HH21	1.84	0.42
8:F:72:LYS:O	8:F:73:ALA:HB3	2.20	0.42
13:L:58:LYS:O	13:L:58:LYS:HG2	2.20	0.42
4:A:672:ASP:OD2	4:A:736:ASN:CG	2.52	0.42
4:A:966:ASN:HB3	4:A:1044:TRP:HH2	1.84	0.42
4:A:1116:LEU:HD22	4:A:1329:THR:OG1	2.20	0.42
5:B:36:ALA:HB2	5:B:661:LEU:HD22	2.02	0.42
5:B:116:GLU:HG2	5:B:120:ARG:HD3	2.00	0.42
5:B:471:LYS:O	5:B:476:ARG:HD3	2.18	0.42
6:C:244:VAL:HG21	12:K:105:PHE:CE1	2.54	0.42
4:A:265:LYS:CG	4:A:303:TYR:HB2	2.40	0.42
4:A:323:LYS:HZ3	4:A:324:SER:N	2.18	0.42
4:A:351:THR:CG2	4:A:352:VAL:N	2.82	0.42
4:A:535:THR:HG21	4:A:617:VAL:N	2.32	0.42
4:A:1187:GLN:HG3	4:A:1188:GLN:H	1.84	0.42
4:A:1206:ASP:N	4:A:1274:ARG:HH12	2.18	0.42
5:B:458:LYS:O	5:B:462:ALA:N	2.52	0.42
4:A:909:ASP:HA	4:A:910:PRO:HD2	1.84	0.42
4:A:1373:ASP:HA	4:A:1376:THR:HG22	2.02	0.42
5:B:848:ARG:HD2	11:J:8:PHE:O	2.20	0.42
5:B:1065:GLN:HE21	5:B:1065:GLN:HB2	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:111:THR:HG23	10:I:113:ASP:H	1.85	0.42
11:J:48:ARG:HH11	11:J:48:ARG:CG	2.29	0.42
2:T:22:DT:H2'	2:T:23:DC:H6	1.85	0.42
4:A:886:ILE:HG22	4:A:887:GLY:N	2.35	0.42
4:A:1084:PHE:HZ	4:A:1093:LYS:HA	1.79	0.42
5:B:787:VAL:O	5:B:787:VAL:HG12	2.19	0.42
6:C:73:GLN:NE2	6:C:74:SER:H	2.15	0.42
6:C:99:LEU:N	6:C:99:LEU:CD2	2.83	0.42
9:H:135:LEU:C	9:H:137:GLN:H	2.22	0.42
12:K:58:PHE:HB3	12:K:76:GLN:HB3	2.01	0.42
4:A:132:LYS:NZ	4:A:133:LYS:HE3	2.35	0.42
4:A:1174:PHE:CD1	4:A:1175:SER:HB2	2.55	0.42
5:B:1111:MET:HE2	5:B:1118:PRO:CA	2.50	0.42
8:F:97:ARG:HD3	8:F:130:ILE:HG23	2.01	0.42
4:A:276:LEU:HD11	4:A:292:ALA:O	2.20	0.41
5:B:622:LYS:HE2	10:I:59:VAL:HG11	2.02	0.41
5:B:654:ARG:H	5:B:657:HIS:CD2	2.38	0.41
5:B:744:HIS:CD2	5:B:746:SER:OG	2.73	0.41
5:B:769:TYR:CD2	5:B:769:TYR:N	2.87	0.41
5:B:911:ILE:HD11	5:B:941:LEU:CD1	2.48	0.41
6:C:231:ASN:HD22	6:C:231:ASN:C	2.23	0.41
6:C:242:GLN:HB3	6:C:246:ARG:NE	2.32	0.41
7:E:102:GLU:C	7:E:104:ASN:H	2.23	0.41
14:T:29[B]:DUT:H6	14:T:29[B]:DUT:C3'	2.49	0.41
4:A:1017:LEU:HB2	7:E:206:GLY:N	2.35	0.41
5:B:273:LEU:HD11	5:B:285:ILE:HD12	2.02	0.41
5:B:796:LEU:HD12	5:B:796:LEU:HA	1.67	0.41
5:B:910:VAL:HG13	5:B:938:SER:HB3	2.02	0.41
6:C:106:GLU:OE2	6:C:106:GLU:HA	2.19	0.41
4:A:148:CYS:HB3	4:A:167:CYS:O	2.20	0.41
4:A:512:VAL:HA	4:A:519:PRO:HA	2.01	0.41
5:B:1053:GLU:O	5:B:1057:LYS:HE3	2.19	0.41
5:B:1058:LEU:HA	5:B:1061:GLU:OE2	2.19	0.41
7:E:122:LYS:HE3	7:E:122:LYS:HA	2.02	0.41
9:H:44:VAL:HG13	9:H:48:PRO:HA	2.02	0.41
4:A:68:GLN:C	4:A:70:CYS:H	2.18	0.41
4:A:92:HIS:O	4:A:94:GLY:N	2.53	0.41
4:A:399:HIS:HB3	4:A:400:PRO:HD2	1.85	0.41
4:A:579:SER:OG	4:A:612:ILE:HG23	2.21	0.41
4:A:676:MET:SD	4:A:679:ILE:HD12	2.61	0.41
4:A:761:MET:CG	5:B:1021:MET:HG2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:896:ARG:NH2	4:A:1030:ARG:HH21	2.17	0.41
4:A:1086:PHE:H	4:A:1086:PHE:HD1	1.69	0.41
5:B:176:SER:O	5:B:182:SER:CB	2.62	0.41
5:B:273:LEU:O	5:B:276:ILE:HG22	2.20	0.41
5:B:475:SER:C	5:B:477:ALA:N	2.72	0.41
5:B:712:PRO:HD2	5:B:733:HIS:CE1	2.55	0.41
13:L:48:CYS:HB3	13:L:51:CYS:H	1.85	0.41
4:A:215:SER:HB3	4:A:218:ASP:OD2	2.21	0.41
4:A:406:ILE:HD11	4:A:433:GLU:OE2	2.21	0.41
4:A:702:LEU:HD22	4:A:702:LEU:HA	1.85	0.41
4:A:1407:GLU:OE1	4:A:1407:GLU:N	2.47	0.41
5:B:795:ILE:HD12	5:B:795:ILE:N	2.36	0.41
6:C:98:VAL:C	6:C:99:LEU:HD22	2.40	0.41
4:A:33:ALA:O	4:A:83:HIS:CD2	2.73	0.41
4:A:71:GLN:HB2	4:A:72:GLU:H	1.69	0.41
4:A:731:ARG:HG3	4:A:755:PHE:CE1	2.55	0.41
5:B:386:LEU:C	5:B:388:CYS:H	2.23	0.41
5:B:886:LYS:CB	5:B:887:HIS:CA	2.96	0.41
5:B:1007:VAL:HG13	5:B:1008:PRO:CD	2.49	0.41
2:T:25:DC:H5"	5:B:482:VAL:HG11	2.02	0.41
4:A:65:LEU:O	4:A:65:LEU:HG	2.21	0.41
4:A:284:ALA:HA	4:A:285:PRO:HD3	1.89	0.41
4:A:715:GLU:OE2	4:A:774:ARG:NH1	2.51	0.41
4:A:855:THR:HG21	4:A:857:ARG:NE	2.21	0.41
5:B:360:PHE:HE2	5:B:374:LYS:HB3	1.84	0.41
5:B:815:ARG:HE	5:B:815:ARG:HB3	1.71	0.41
6:C:244:VAL:HG21	12:K:105:PHE:CZ	2.56	0.41
4:A:1155:ASP:OD2	4:A:1161:THR:HG23	2.20	0.41
5:B:135:ARG:HH11	5:B:137:TYR:HA	1.85	0.41
5:B:784:ASN:HB3	11:J:63:TYR:CZ	2.55	0.41
5:B:984:HIS:CD2	5:B:1024:ALA:CB	3.03	0.41
6:C:41:ILE:HD13	6:C:41:ILE:HG21	1.78	0.41
7:E:198:ILE:CD1	7:E:212:ARG:HG3	2.50	0.41
4:A:58:LEU:O	4:A:58:LEU:CG	2.68	0.41
4:A:265:LYS:O	4:A:267:ALA:N	2.52	0.41
4:A:409:SER:O	4:A:411:ASP:N	2.54	0.41
4:A:899:VAL:HB	4:A:929:LEU:HD13	2.02	0.41
4:A:901:LEU:HB2	4:A:926:GLN:CG	2.51	0.41
4:A:1293:SER:HB2	4:A:1299:VAL:HG21	2.02	0.41
5:B:487:THR:CG2	5:B:488:TYR:N	2.83	0.41
5:B:640:VAL:HG22	5:B:651:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1002:THR:CG2	5:B:1006:ILE:H	2.33	0.41
6:C:134:ILE:HD12	6:C:141:GLY:H	1.85	0.41
6:C:238:ILE:CG2	6:C:242:GLN:HB2	2.51	0.41
10:I:77:LYS:O	10:I:79:HIS:N	2.54	0.41
4:A:567:LYS:HG3	4:A:568:PRO:CG	2.51	0.41
4:A:830:LYS:HE2	4:A:1082:ASN:HD22	1.85	0.41
4:A:1015:VAL:HG12	4:A:1019:CYS:SG	2.60	0.41
5:B:318:VAL:HG21	10:I:13:MET:CE	2.51	0.41
5:B:744:HIS:HA	5:B:745:PRO:HD3	1.85	0.41
5:B:885:MET:HB3	5:B:886:LYS:H	1.68	0.41
5:B:1006:ILE:HG22	5:B:1007:VAL:H	1.83	0.41
6:C:177:GLU:HG3	6:C:231:ASN:HB3	2.03	0.41
6:C:229:TYR:CD1	6:C:229:TYR:N	2.89	0.41
10:I:55:THR:HG23	10:I:58:VAL:CG2	2.50	0.41
4:A:705:LYS:O	4:A:706:HIS:C	2.60	0.40
4:A:1105:LEU:HD22	4:A:1384:VAL:HG21	2.03	0.40
4:A:1345:ARG:HG2	4:A:1372:VAL:CG1	2.51	0.40
5:B:136:THR:O	5:B:137:TYR:O	2.39	0.40
5:B:709:ASP:C	5:B:710:LEU:HD23	2.35	0.40
6:C:74:SER:O	6:C:77:ILE:HB	2.22	0.40
8:F:128:LYS:HD3	8:F:149:GLU:O	2.21	0.40
9:H:146:ARG:HA	9:H:146:ARG:HD3	1.97	0.40
10:I:96:SER:OG	10:I:98:VAL:HG23	2.21	0.40
4:A:265:LYS:HD3	4:A:322:VAL:HG21	2.03	0.40
4:A:351:THR:C	4:A:486:GLU:HG3	2.41	0.40
4:A:1402:PHE:CD2	4:A:1403:GLU:HB2	2.56	0.40
5:B:724:ASP:OD1	5:B:725:PRO:HD2	2.20	0.40
5:B:1153:GLU:OE2	5:B:1153:GLU:N	2.50	0.40
6:C:91:HIS:ND1	6:C:158:VAL:HG11	2.36	0.40
7:E:128:PRO:HA	7:E:129:PRO:C	2.41	0.40
12:K:87:LEU:O	12:K:90:ALA:HB3	2.21	0.40
4:A:1138:ILE:H	4:A:1138:ILE:HG13	1.77	0.40
4:A:1215:ARG:NE	4:A:1218:GLN:HE21	2.19	0.40
4:A:1227:ILE:HG22	4:A:1228:TRP:N	2.36	0.40
5:B:850:LEU:CD2	5:B:1009:ASP:HB3	2.51	0.40
5:B:996:ARG:HH22	6:C:173:ALA:HB3	1.85	0.40
5:B:1106:ARG:CG	5:B:1107:ALA:N	2.85	0.40
6:C:63:ILE:HA	6:C:66:ARG:HG3	2.02	0.40
7:E:179:GLN:C	7:E:181:ALA:N	2.73	0.40
8:F:147:SER:O	8:F:151:LEU:HD12	2.22	0.40
10:I:65:ASP:HA	10:I:66:PRO:HD3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:6:DG:N2	3:N:10:DG:N2	2.70	0.40
2:T:7:DA:OP2	2:T:7:DA:H2'	2.21	0.40
4:A:59:GLY:HA2	4:A:67:CYS:SG	2.62	0.40
4:A:303:TYR:HD2	4:A:304:MET:HG3	1.86	0.40
4:A:343:LYS:NZ	5:B:1156:ASP:HB2	2.37	0.40
4:A:545:GLN:O	4:A:549:MET:HG3	2.21	0.40
4:A:779:PHE:CZ	5:B:517:THR:HA	2.56	0.40
5:B:705:MET:CE	5:B:742:GLU:HG2	2.52	0.40
5:B:711:GLU:H	5:B:712:PRO:HD3	1.87	0.40
5:B:762:ASN:HD22	5:B:762:ASN:HA	1.64	0.40
5:B:1046:PRO:HB2	5:B:1047:PHE:H	1.80	0.40
5:B:1221:SER:C	5:B:1223:ASP:H	2.24	0.40
10:I:56:ALA:HB3	10:I:89:GLN:HG3	2.02	0.40
10:I:59:VAL:O	10:I:61:ASP:N	2.54	0.40
4:A:247:ARG:HD3	4:A:262:LEU:HD23	2.03	0.40
4:A:977:LYS:HA	4:A:978:PRO:HD3	1.98	0.40
5:B:121:ASN:HA	5:B:207:GLY:HA3	2.04	0.40
5:B:216:GLU:HB3	5:B:500:THR:HG23	2.02	0.40
5:B:278:GLN:CG	5:B:279:ASP:N	2.84	0.40
5:B:796:LEU:HB3	5:B:799:PRO:HG3	2.04	0.40
9:H:60:ALA:O	9:H:61:SER:CB	2.69	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
4	A	1395/1733 (80%)	1153 (83%)	158 (11%)	84 (6%)	1 4
5	B	1096/1224 (90%)	938 (86%)	108 (10%)	50 (5%)	2 9
6	C	264/318 (83%)	229 (87%)	27 (10%)	8 (3%)	4 17
7	E	212/215 (99%)	177 (84%)	28 (13%)	7 (3%)	4 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	F	83/155 (54%)	71 (86%)	11 (13%)	1 (1%)	13 40
9	H	129/146 (88%)	94 (73%)	22 (17%)	13 (10%)	0 1
10	I	117/122 (96%)	94 (80%)	14 (12%)	9 (8%)	1 2
11	J	63/70 (90%)	58 (92%)	2 (3%)	3 (5%)	2 8
12	K	112/120 (93%)	104 (93%)	8 (7%)	0	100 100
13	L	44/70 (63%)	28 (64%)	10 (23%)	6 (14%)	0 0
All	All	3515/4173 (84%)	2946 (84%)	388 (11%)	181 (5%)	2 7

All (181) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	54	ASN
4	A	55	ASP
4	A	56	PRO
4	A	65	LEU
4	A	69	THR
4	A	93	VAL
4	A	118	HIS
4	A	121	LEU
4	A	130	ASP
4	A	131	SER
4	A	168	GLY
4	A	250	ILE
4	A	254	GLU
4	A	300	VAL
4	A	315	LEU
4	A	323	LYS
4	A	324	SER
4	A	399	HIS
4	A	451	HIS
4	A	567	LYS
4	A	593	GLU
4	A	597	LEU
4	A	609	ASP
4	A	610	GLY
4	A	672	ASP
4	A	846	GLU
4	A	923	LEU
4	A	944	ARG
4	A	1123	GLY

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Mol	Chain	Res	Type
4	A	1166	ASP
4	A	1221	LYS
5	B	65	GLU
5	B	67	SER
5	B	137	TYR
5	B	469	GLN
5	B	477	ALA
5	B	484	ASN
5	B	531	GLN
5	B	648	HIS
5	B	711	GLU
5	B	713	ALA
5	B	731	VAL
5	B	879	ARG
5	B	1046	PRO
5	B	1156	ASP
7	E	50	MET
7	E	172	GLU
9	H	3	ASN
9	H	61	SER
9	H	62	SER
9	H	108	SER
9	H	109	LYS
9	H	131	ASN
9	H	132	LEU
10	I	33	SER
10	I	47	GLU
10	I	60	GLN
10	I	79	HIS
10	I	104	LEU
13	L	64	LEU
4	A	68	GLN
4	A	76	GLU
4	A	79	GLY
4	A	117	GLU
4	A	119	ASN
4	A	214	ILE
4	A	215	SER
4	A	266	LEU
4	A	283	GLY
4	A	297	GLN
4	A	307	ASP

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Mol	Chain	Res	Type
4	A	312	PRO
4	A	404	TYR
4	A	408	ASP
4	A	410	GLY
4	A	424	ILE
4	A	568	PRO
4	A	569	LYS
4	A	853	ASP
4	A	943	LEU
4	A	1278	ASN
4	A	1437	GLY
5	B	288	ALA
5	B	471	LYS
5	B	473	MET
5	B	864	LYS
5	B	870	ILE
5	B	888	GLY
5	B	987	LYS
7	E	206	GLY
9	H	18	GLY
9	H	54	SER
9	H	90	ALA
10	I	3	THR
11	J	2	ILE
11	J	6	ARG
13	L	45	ALA
4	A	40	THR
4	A	48	ALA
4	A	72	GLU
4	A	149	GLU
4	A	248	PRO
4	A	308	ILE
4	A	310	GLY
4	A	958	VAL
4	A	1083	THR
4	A	1093	LYS
5	B	37	PHE
5	B	104	GLU
5	B	290	GLY
5	B	364	ILE
5	B	371	GLU
5	B	476	ARG

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Mol	Chain	Res	Type
5	B	559	SER
5	B	644	GLU
5	B	647	GLY
5	B	712	PRO
5	B	992	ILE
5	B	1223	ASP
6	C	227	THR
7	E	51	GLY
8	F	154	ASP
9	H	130	ARG
9	H	136	LYS
4	A	71	GLN
4	A	109	HIS
4	A	126	LEU
4	A	249	SER
4	A	332	LYS
4	A	400	PRO
4	A	418	SER
4	A	979	SER
4	A	1014	ALA
4	A	1084	PHE
5	B	139	ALA
5	B	248	SER
5	B	467	GLY
5	B	646	LEU
5	B	734	HIS
5	B	1190	ASP
6	C	90	ASP
6	C	214	ASN
10	I	78	CYS
13	L	56	LEU
4	A	325	ILE
4	A	801	GLU
4	A	1081	LEU
5	B	346	GLU
5	B	480	SER
5	B	1017	ILE
5	B	1108	ARG
5	B	1157	ALA
6	C	130	GLY
6	C	142	VAL
6	C	240	VAL

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Mol	Chain	Res	Type
7	E	124	VAL
9	H	140	ALA
13	L	42	ARG
13	L	46	VAL
13	L	55	ILE
4	A	225	ASN
4	A	1127	ASP
5	B	483	LEU
5	B	901	PRO
6	C	6	PRO
6	C	132	PRO
7	E	3	GLN
7	E	86	PRO
10	I	20	LYS
10	I	34	TYR
11	J	15	GLY
4	A	96	ILE
4	A	245	PRO
5	B	1042	GLY
4	A	89	PRO
4	A	99	ILE
5	B	292	ILE
5	B	482	VAL
4	A	916	GLY
4	A	1388	GLY
5	B	824	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	A	1225/1520 (81%)	1052 (86%)	173 (14%)	3 10
5	B	967/1061 (91%)	851 (88%)	116 (12%)	5 15
6	C	234/274 (85%)	205 (88%)	29 (12%)	4 14
7	E	196/197 (100%)	172 (88%)	24 (12%)	5 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	F	75/137 (55%)	69 (92%)	6 (8%)	12 33
9	H	117/128 (91%)	96 (82%)	21 (18%)	2 5
10	I	113/116 (97%)	96 (85%)	17 (15%)	3 9
11	J	60/65 (92%)	52 (87%)	8 (13%)	4 11
12	K	99/102 (97%)	90 (91%)	9 (9%)	9 28
13	L	40/57 (70%)	27 (68%)	13 (32%)	0 0
All	All	3126/3657 (86%)	2710 (87%)	416 (13%)	4 11

All (416) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	18	GLN
4	A	21	LEU
4	A	34	LYS
4	A	41	MET
4	A	43	GLU
4	A	47	ARG
4	A	50	ILE
4	A	54	ASN
4	A	57	ARG
4	A	58	LEU
4	A	64	ASN
4	A	68	GLN
4	A	69	THR
4	A	70	CYS
4	A	71	GLN
4	A	86	LEU
4	A	93	VAL
4	A	118	HIS
4	A	121	LEU
4	A	130	ASP
4	A	143	LYS
4	A	147	VAL
4	A	163	SER
4	A	164	ARG
4	A	171	GLN
4	A	179	LEU
4	A	208	LEU
4	A	209	ASN
4	A	224	PHE

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Mol	Chain	Res	Type
4	A	225	ASN
4	A	237	THR
4	A	252	PHE
4	A	253	ASN
4	A	256	GLN
4	A	271	LYS
4	A	298	PHE
4	A	303	TYR
4	A	315	LEU
4	A	316	GLN
4	A	320	ARG
4	A	323	LYS
4	A	325	ILE
4	A	335	ARG
4	A	344	ARG
4	A	351	THR
4	A	359	LEU
4	A	379	VAL
4	A	398	GLU
4	A	403	LYS
4	A	424	ILE
4	A	434	ARG
4	A	436	ILE
4	A	440	ASP
4	A	443	LEU
4	A	445	ASN
4	A	450	LEU
4	A	451	HIS
4	A	452	LYS
4	A	455	MET
4	A	466	SER
4	A	469	ARG
4	A	470	LEU
4	A	472	LEU
4	A	475	THR
4	A	481	ASP
4	A	485	ASP
4	A	496	GLU
4	A	501	LEU
4	A	509	LEU
4	A	533	LYS
4	A	541	ILE

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Mol	Chain	Res	Type
4	A	566	ILE
4	A	567	LYS
4	A	590	ARG
4	A	595	THR
4	A	598	LEU
4	A	612	ILE
4	A	618	GLU
4	A	629	LEU
4	A	635	ARG
4	A	658	LEU
4	A	672	ASP
4	A	678	GLU
4	A	688	LYS
4	A	691	LEU
4	A	695	LYS
4	A	702	LEU
4	A	703	THR
4	A	710	LEU
4	A	764	CYS
4	A	768	GLN
4	A	774	ARG
4	A	801	GLU
4	A	821	ARG
4	A	830	LYS
4	A	833	GLU
4	A	855	THR
4	A	865	GLN
4	A	867	ILE
4	A	886	ILE
4	A	896	ARG
4	A	902	LEU
4	A	906	HIS
4	A	907	THR
4	A	908	LEU
4	A	920	LEU
4	A	932	GLU
4	A	938	LYS
4	A	940	ARG
4	A	941	LYS
4	A	960	ILE
4	A	961	ARG
4	A	969	GLN

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Mol	Chain	Res	Type
4	A	973	ILE
4	A	977	LYS
4	A	982	THR
4	A	992	ASP
4	A	1001	ARG
4	A	1005	GLU
4	A	1025	ARG
4	A	1029	ARG
4	A	1037	LEU
4	A	1058	VAL
4	A	1077	THR
4	A	1082	ASN
4	A	1084	PHE
4	A	1085	HIS
4	A	1086	PHE
4	A	1094	VAL
4	A	1095	THR
4	A	1109	LYS
4	A	1110	ASN
4	A	1112	LYS
4	A	1130	GLN
4	A	1138	ILE
4	A	1142	THR
4	A	1146	VAL
4	A	1162	VAL
4	A	1171	GLN
4	A	1172	LEU
4	A	1173	HIS
4	A	1174	PHE
4	A	1175	SER
4	A	1176	LEU
4	A	1215	ARG
4	A	1221	LYS
4	A	1234	GLU
4	A	1261	LYS
4	A	1264	GLU
4	A	1269	GLU
4	A	1270	ASN
4	A	1274	ARG
4	A	1280	GLU
4	A	1291	VAL
4	A	1293	SER

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Mol	Chain	Res	Type
4	A	1297	GLU
4	A	1299	VAL
4	A	1322	ILE
4	A	1325	THR
4	A	1329	THR
4	A	1333	ILE
4	A	1354	ASN
4	A	1366	ARG
4	A	1376	THR
4	A	1382	THR
4	A	1391	ARG
4	A	1393	ASN
4	A	1394	THR
4	A	1398	MET
4	A	1420	ASP
4	A	1422	ARG
4	A	1425	SER
4	A	1426	GLU
5	B	46	GLN
5	B	65	GLU
5	B	68	THR
5	B	94	LYS
5	B	133	LYS
5	B	134	LYS
5	B	137	TYR
5	B	164	LYS
5	B	183	GLU
5	B	199	MET
5	B	217	ARG
5	B	234	ILE
5	B	244	LEU
5	B	245	GLU
5	B	246	LYS
5	B	268	THR
5	B	273	LEU
5	B	276	ILE
5	B	277	LYS
5	B	299	GLU
5	B	324	ILE
5	B	333	PHE
5	B	346	GLU
5	B	361	LEU

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Mol	Chain	Res	Type
5	B	366	GLN
5	B	391	ASP
5	B	393	LYS
5	B	394	ASP
5	B	396	ASP
5	B	398	ARG
5	B	404	LYS
5	B	408	LEU
5	B	416	LEU
5	B	425	THR
5	B	437	GLU
5	B	468	GLU
5	B	469	GLN
5	B	471	LYS
5	B	482	VAL
5	B	485	ARG
5	B	495	LEU
5	B	498	THR
5	B	537	LYS
5	B	541	LEU
5	B	542	MET
5	B	555	ILE
5	B	579	ARG
5	B	624	LEU
5	B	628	THR
5	B	637	LEU
5	B	642	ASP
5	B	646	LEU
5	B	655	LYS
5	B	658	ILE
5	B	666	TYR
5	B	682	SER
5	B	690	VAL
5	B	710	LEU
5	B	731	VAL
5	B	734	HIS
5	B	751	VAL
5	B	763	GLN
5	B	790	ASP
5	B	791	THR
5	B	792	MET
5	B	807	ARG

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Mol	Chain	Res	Type
5	B	815	ARG
5	B	825	VAL
5	B	831	SER
5	B	864	LYS
5	B	866	TYR
5	B	868	MET
5	B	869	SER
5	B	878	GLN
5	B	879	ARG
5	B	880	THR
5	B	882	THR
5	B	886	LYS
5	B	899	ILE
5	B	916	THR
5	B	919	SER
5	B	933	SER
5	B	944	THR
5	B	959	ASP
5	B	963	PHE
5	B	967	ARG
5	B	969	ARG
5	B	983	ARG
5	B	987	LYS
5	B	996	ARG
5	B	997	GLU
5	B	999	MET
5	B	1010	LEU
5	B	1022	THR
5	B	1065	GLN
5	B	1092	TYR
5	B	1094	ARG
5	B	1096	ARG
5	B	1099	VAL
5	B	1101	ASP
5	B	1103	ILE
5	B	1111	MET
5	B	1138	MET
5	B	1147	LEU
5	B	1160	VAL
5	B	1166	CYS
5	B	1176	ASN
5	B	1178	ASN

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Mol	Chain	Res	Type
5	B	1181	GLU
5	B	1182	CYS
5	B	1186	ASP
5	B	1190	ASP
5	B	1194	ILE
5	B	1196	ILE
5	B	1202	LEU
5	B	1222	ARG
6	C	18	VAL
6	C	25	VAL
6	C	27	LEU
6	C	32	SER
6	C	36	VAL
6	C	57	VAL
6	C	62	PHE
6	C	75	MET
6	C	77	ILE
6	C	89	GLU
6	C	91	HIS
6	C	93	ASP
6	C	106	GLU
6	C	117	ASP
6	C	120	ILE
6	C	129	ILE
6	C	137	LYS
6	C	140	ASN
6	C	145	CYS
6	C	166	GLU
6	C	170	TRP
6	C	196	ASP
6	C	214	ASN
6	C	215	GLU
6	C	231	ASN
6	C	235	VAL
6	C	240	VAL
6	C	244	VAL
6	C	254	LYS
7	E	31	THR
7	E	37	LEU
7	E	46	TYR
7	E	52	ARG
7	E	65	THR

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Mol	Chain	Res	Type
7	E	66	GLU
7	E	67	GLU
7	E	87	SER
7	E	92	THR
7	E	95	THR
7	E	104	ASN
7	E	107	THR
7	E	122	LYS
7	E	127	ILE
7	E	146	HIS
7	E	152	LYS
7	E	162	ARG
7	E	165	LEU
7	E	169	ARG
7	E	175	LEU
7	E	204	THR
7	E	207	ARG
7	E	212	ARG
7	E	213	ILE
8	F	76	LYS
8	F	77	ASP
8	F	82	THR
8	F	90	ARG
8	F	111	LEU
8	F	133	VAL
9	H	2	SER
9	H	11	GLN
9	H	19	ARG
9	H	31	THR
9	H	33	GLN
9	H	35	GLN
9	H	36	CYS
9	H	53	ASP
9	H	58	THR
9	H	59	ILE
9	H	76	THR
9	H	78	SER
9	H	89	LEU
9	H	92	ASP
9	H	94	ASP
9	H	110	ASP
9	H	130	ARG

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Mol	Chain	Res	Type
9	H	132	LEU
9	H	136	LYS
9	H	139	ASN
9	H	145	ARG
10	I	12	ASN
10	I	29	CYS
10	I	33	SER
10	I	40	SER
10	I	50	THR
10	I	52	ILE
10	I	55	THR
10	I	61	ASP
10	I	70	ARG
10	I	74	GLU
10	I	78	CYS
10	I	83	ASN
10	I	84	VAL
10	I	90	GLN
10	I	92	ARG
10	I	94	ASP
10	I	104	LEU
11	J	7	CYS
11	J	13	VAL
11	J	19	GLU
11	J	28	ASP
11	J	43	ARG
11	J	48	ARG
11	J	55	ASP
11	J	62	ARG
12	K	11	LEU
12	K	18	LYS
12	K	20	LYS
12	K	31	VAL
12	K	42	LEU
12	K	50	LEU
12	K	78	THR
12	K	101	LEU
12	K	103	THR
13	L	27	LEU
13	L	31	CYS
13	L	34	CYS
13	L	38	LEU

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Mol	Chain	Res	Type
13	L	42	ARG
13	L	47	ARG
13	L	48	CYS
13	L	50	ASP
13	L	55	ILE
13	L	61	THR
13	L	63	ARG
13	L	65	VAL
13	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	4	GLN
4	A	18	GLN
4	A	54	ASN
4	A	64	ASN
4	A	83	HIS
4	A	92	HIS
4	A	119	ASN
4	A	225	ASN
4	A	253	ASN
4	A	282	ASN
4	A	297	GLN
4	A	299	HIS
4	A	313	GLN
4	A	339	ASN
4	A	445	ASN
4	A	503	GLN
4	A	517	ASN
4	A	584	ASN
4	A	631	HIS
4	A	648	ASN
4	A	741	ASN
4	A	757	ASN
4	A	768	GLN
4	A	786	HIS
4	A	926	GLN
4	A	965	GLN
4	A	969	GLN
4	A	996	ASN
4	A	1009	ASN

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Mol	Chain	Res	Type
4	A	1082	ASN
4	A	1110	ASN
4	A	1130	GLN
4	A	1218	GLN
4	A	1265	ASN
4	A	1364	ASN
4	A	1387	HIS
4	A	1393	ASN
4	A	1427	ASN
4	A	1432	GLN
5	B	121	ASN
5	B	206	ASN
5	B	215	GLN
5	B	255	GLN
5	B	325	GLN
5	B	366	GLN
5	B	383	ASN
5	B	395	GLN
5	B	415	GLN
5	B	484	ASN
5	B	513	GLN
5	B	515	HIS
5	B	516	ASN
5	B	518	HIS
5	B	657	HIS
5	B	733	HIS
5	B	744	HIS
5	B	762	ASN
5	B	794	ASN
5	B	822	ASN
5	B	887	HIS
5	B	957	ASN
5	B	984	HIS
5	B	1015	HIS
5	B	1025	HIS
5	B	1062	HIS
5	B	1076	HIS
5	B	1141	HIS
5	B	1161	HIS
6	C	73	GLN
6	C	112	ASN
6	C	123	ASN

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Mol	Chain	Res	Type
6	C	167	HIS
6	C	203	GLN
6	C	214	ASN
6	C	231	ASN
6	C	242	GLN
6	C	264	GLN
7	E	104	ASN
9	H	3	ASN
9	H	11	GLN
9	H	33	GLN
10	I	12	ASN
10	I	83	ASN
10	I	116	ASN
11	J	53	HIS
12	K	40	HIS
12	K	52	ASN
12	K	65	HIS
12	K	76	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	8/10 (80%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	U

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

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 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	DUT	T	29[A]	16	25,29,29	1.11	1 (4%)	37,45,45	1.79	7 (18%)
14	DUT	T	29[B]	16	25,29,29	1.12	1 (4%)	37,45,45	3.09	14 (37%)

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	DUT	T	29[A]	16	-	3/22/34/34	0/2/2/2
14	DUT	T	29[B]	16	-	4/22/34/34	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	29[B]	DUT	C2-N1	-2.49	1.34	1.38
14	T	29[A]	DUT	C2-N1	-2.49	1.34	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	29[B]	DUT	O4'-C4'-C5'	11.48	147.16	109.37
14	T	29[B]	DUT	O5'-C5'-C4'	7.74	135.64	108.99
14	T	29[B]	DUT	O2G-PG-O3B	-5.77	85.27	104.64
14	T	29[A]	DUT	C4-N3-C2	-5.27	119.63	126.58
14	T	29[A]	DUT	N3-C2-N1	4.50	120.86	114.89
14	T	29[B]	DUT	C2'-C1'-N1	-4.48	103.46	113.77
14	T	29[B]	DUT	O2G-PG-O1G	4.24	127.28	110.68
14	T	29[A]	DUT	O4'-C1'-N1	3.73	114.52	107.86
14	T	29[A]	DUT	C5-C4-N3	3.25	119.71	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	29[B]	DUT	C1'-N1-C2	3.23	124.00	117.64
14	T	29[B]	DUT	O3B-PG-O1G	-3.13	93.80	111.19
14	T	29[B]	DUT	N3-C2-N1	2.99	118.86	114.89
14	T	29[B]	DUT	C5'-C4'-C3'	-2.85	98.02	114.74
14	T	29[A]	DUT	O4-C4-C5	-2.76	120.31	125.16
14	T	29[B]	DUT	O3G-PG-O2G	2.62	117.64	107.64
14	T	29[A]	DUT	PB-O3B-PG	-2.58	123.97	132.83
14	T	29[B]	DUT	O3'-C3'-C2'	-2.54	101.81	110.90
14	T	29[A]	DUT	PB-O3A-PA	-2.32	124.87	132.83
14	T	29[B]	DUT	O4'-C1'-N1	2.10	111.61	107.86
14	T	29[B]	DUT	C6-N1-C2	-2.04	118.38	120.99
14	T	29[B]	DUT	C1'-N1-C6	-2.04	117.52	121.55

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	29[A]	DUT	C3'-C4'-C5'-O5'
14	T	29[B]	DUT	C4'-C5'-O5'-PA
14	T	29[B]	DUT	C5'-O5'-PA-O2A
14	T	29[B]	DUT	C5'-O5'-PA-O3A
14	T	29[A]	DUT	O4'-C4'-C5'-O5'
14	T	29[B]	DUT	O4'-C4'-C5'-O5'
14	T	29[A]	DUT	C4'-C5'-O5'-PA

There are no ring outliers.

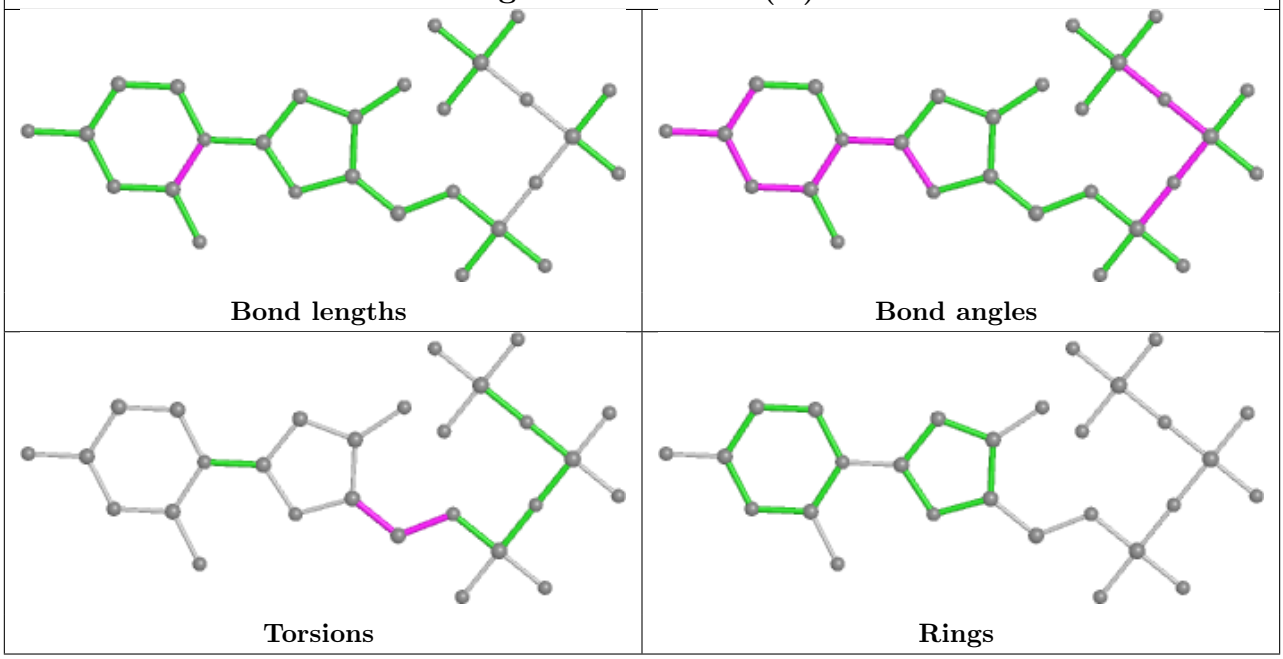
2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	29[A]	DUT	3	0
14	T	29[B]	DUT	13	0

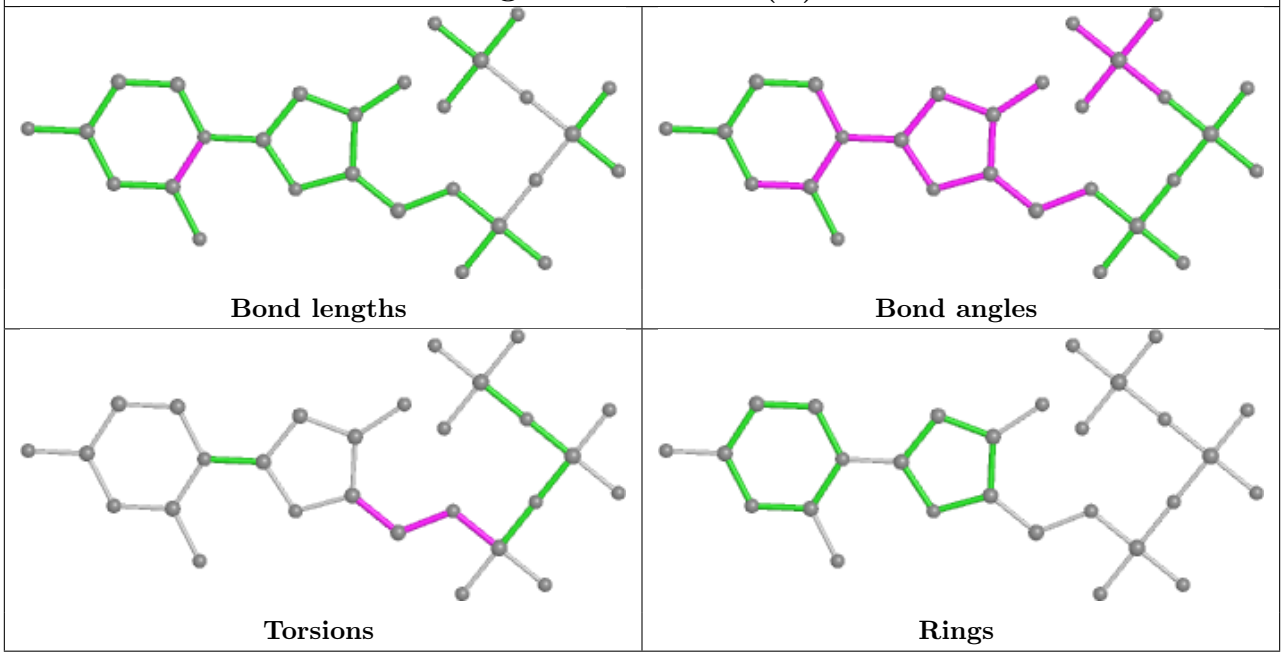
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand DUT T 29 (A)



Ligand DUT T 29 (B)



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, 95^{th} 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	10/10 (100%)	-0.51	0 100 100	30, 50, 93, 109	0
2	T	28/28 (100%)	0.59	7 (25%) 0 0	40, 108, 139, 145	0
3	N	14/14 (100%)	1.35	5 (35%) 0 0	73, 119, 144, 149	0
4	A	1405/1733 (81%)	0.34	88 (6%) 20 16	24, 56, 77, 131	0
5	B	1114/1224 (91%)	0.37	48 (4%) 35 31	28, 55, 84, 104	0
6	C	266/318 (83%)	-0.02	1 (0%) 92 93	40, 54, 73, 99	0
7	E	214/215 (99%)	0.58	27 (12%) 3 3	43, 64, 88, 91	0
8	F	85/155 (54%)	-0.11	0 100 100	44, 59, 81, 90	0
9	H	133/146 (91%)	0.58	12 (9%) 9 7	52, 66, 88, 94	0
10	I	119/122 (97%)	0.06	3 (2%) 57 55	37, 51, 84, 96	0
11	J	65/70 (92%)	0.17	1 (1%) 73 73	44, 56, 72, 81	0
12	K	114/120 (95%)	0.06	1 (0%) 84 84	45, 57, 73, 82	0
13	L	46/70 (65%)	0.45	2 (4%) 35 31	57, 87, 98, 101	0
All	All	3613/4225 (85%)	0.32	195 (5%) 25 22	24, 57, 85, 149	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	1087	ALA	7.8
4	A	1082	ASN	7.8
5	B	250	PHE	7.4
5	B	869	SER	7.4
4	A	1089	VAL	6.7
4	A	69	THR	6.5
5	B	883	LEU	6.4
4	A	65	LEU	6.3
5	B	866	TYR	6.3

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Mol	Chain	Res	Type	RSRZ
4	A	1085	HIS	6.3
7	E	93	MET	6.2
13	L	27	LEU	6.2
9	H	85	GLY	5.9
4	A	44	THR	5.7
5	B	1224	PHE	5.7
4	A	311	GLN	5.6
7	E	121	MET	5.4
4	A	1176	LEU	5.4
4	A	1091	SER	5.3
4	A	1083	THR	5.2
4	A	152	VAL	5.1
9	H	86	ASP	5.0
4	A	250	ILE	5.0
4	A	1090	ALA	4.9
9	H	132	LEU	4.8
4	A	150	THR	4.8
5	B	429	PHE	4.7
4	A	149	GLU	4.7
4	A	168	GLY	4.6
5	B	249	ARG	4.5
4	A	256	GLN	4.5
4	A	115	LEU	4.3
4	A	316	GLN	4.3
5	B	882	THR	4.3
7	E	83	CYS	4.2
5	B	1223	ASP	4.2
5	B	865	LYS	4.2
7	E	2	ASP	4.1
4	A	318	SER	4.1
7	E	126	SER	4.1
4	A	255	SER	4.0
7	E	50	MET	4.0
4	A	105	CYS	3.9
2	T	3	DA	3.9
5	B	474	SER	3.9
4	A	145	LYS	3.8
4	A	1088	GLY	3.8
4	A	286	HIS	3.8
5	B	647	GLY	3.8
4	A	182	VAL	3.8
4	A	113	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
3	N	14	DG	3.7
7	E	49	SER	3.7
4	A	174	ILE	3.7
4	A	165	GLY	3.7
5	B	868	MET	3.6
4	A	1175	SER	3.6
5	B	1222	ARG	3.6
4	A	1086	PHE	3.6
4	A	183	GLY	3.6
2	T	2	DT	3.6
4	A	153	PRO	3.5
5	B	666	TYR	3.5
4	A	1234	GLU	3.5
4	A	257	ARG	3.4
5	B	251	ILE	3.4
5	B	709	ASP	3.4
2	T	1	DC	3.4
4	A	1084	PHE	3.4
4	A	114	LEU	3.4
13	L	43	THR	3.4
7	E	96	PHE	3.3
7	E	119	SER	3.3
4	A	154	SER	3.3
4	A	141	LEU	3.3
7	E	123	LEU	3.2
9	H	84	ALA	3.2
4	A	1173	HIS	3.2
5	B	870	ILE	3.2
7	E	129	PRO	3.2
4	A	171	GLN	3.2
7	E	52	ARG	3.1
9	H	133	ASN	3.1
4	A	146	MET	3.1
7	E	104	ASN	3.0
4	A	164	ARG	3.0
4	A	176	LYS	3.0
9	H	82	PRO	3.0
5	B	252	SER	3.0
5	B	1184	GLY	3.0
4	A	317	LYS	3.0
4	A	109	HIS	3.0
7	E	124	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
7	E	122	LYS	2.9
7	E	86	PRO	2.9
4	A	49	LYS	2.9
4	A	144	THR	2.9
4	A	166	GLY	2.8
4	A	91	PHE	2.8
5	B	714	GLU	2.8
4	A	161	LEU	2.8
5	B	880	THR	2.7
5	B	645	SER	2.7
4	A	200	ARG	2.7
5	B	475	SER	2.7
5	B	246	LYS	2.7
7	E	90	VAL	2.7
4	A	1188	GLN	2.6
7	E	110	PHE	2.6
5	B	1221	SER	2.6
4	A	181	LEU	2.6
5	B	436	VAL	2.6
4	A	660	ASN	2.6
4	A	254	GLU	2.6
9	H	2	SER	2.6
4	A	162	VAL	2.6
5	B	733	HIS	2.6
5	B	134	LYS	2.6
4	A	45	GLN	2.5
2	T	4	DC	2.5
5	B	66	ASP	2.5
4	A	106	VAL	2.5
7	E	57	MET	2.5
9	H	108	SER	2.5
4	A	175	ARG	2.4
7	E	127	ILE	2.4
4	A	103	CYS	2.4
4	A	64	ASN	2.4
4	A	72	GLU	2.4
4	A	658	LEU	2.4
4	A	104	GLU	2.4
5	B	248	SER	2.4
7	E	55	ARG	2.4
9	H	83	GLN	2.4
5	B	244	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
4	A	120	GLU	2.3
4	A	659	HIS	2.3
10	I	119	THR	2.3
4	A	167	CYS	2.3
5	B	356	LEU	2.3
4	A	151	ASP	2.3
5	B	1000	PRO	2.3
5	B	1191	ILE	2.3
6	C	213	PRO	2.3
4	A	127	ALA	2.3
5	B	840	ILE	2.3
5	B	135	ARG	2.2
4	A	312	PRO	2.2
5	B	140	ILE	2.2
7	E	16	PHE	2.2
2	T	10	DA	2.2
4	A	57	ARG	2.2
10	I	117	LYS	2.2
5	B	247	GLY	2.2
5	B	844	SER	2.2
7	E	66	GLU	2.2
12	K	114	LEU	2.2
5	B	137	TYR	2.2
4	A	253	ASN	2.2
10	I	116	ASN	2.2
4	A	121	LEU	2.2
4	A	281	HIS	2.2
2	T	5	DC	2.2
5	B	867	GLY	2.2
9	H	92	ASP	2.2
7	E	47	CYS	2.2
4	A	108	MET	2.2
4	A	426	LEU	2.2
3	N	13	DA	2.2
5	B	67	SER	2.2
7	E	82	PHE	2.1
2	T	11	DG	2.1
3	N	7	DA	2.1
4	A	383	TYR	2.1
5	B	999	MET	2.1
4	A	251	SER	2.1
4	A	656	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
11	J	52	THR	2.1
5	B	476	ARG	2.1
7	E	120	ALA	2.1
9	H	88	SER	2.1
3	N	1	DC	2.1
4	A	661	GLY	2.0
5	B	432	MET	2.0
4	A	135	PHE	2.0
4	A	252	PHE	2.0
4	A	73	GLY	2.0
4	A	186	LYS	2.0
3	N	2	DT	2.0
9	H	138	GLU	2.0
7	E	95	THR	2.0
5	B	473	MET	2.0
5	B	998	ASP	2.0
4	A	163	SER	2.0
4	A	1235	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	MG	A	2002[A]	1/1	0.72	0.60	43,43,43,43	1
16	MG	A	2002[B]	1/1	0.72	0.60	33,33,33,33	1
14	DUT	T	29[A]	28/28	0.73	0.40	76,80,97,98	28
14	DUT	T	29[B]	28/28	0.73	0.40	70,73,79,80	28
15	ZN	A	1734	1/1	0.77	0.11	84,84,84,84	0

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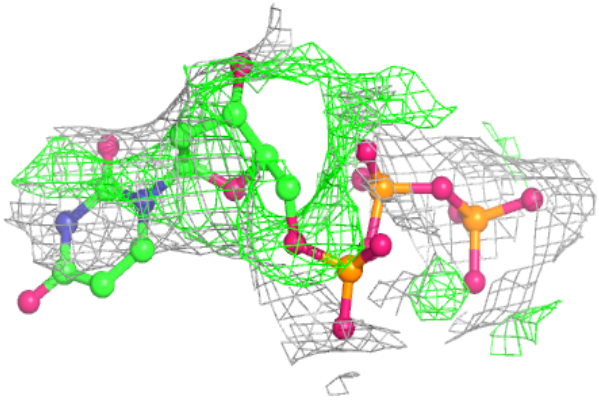
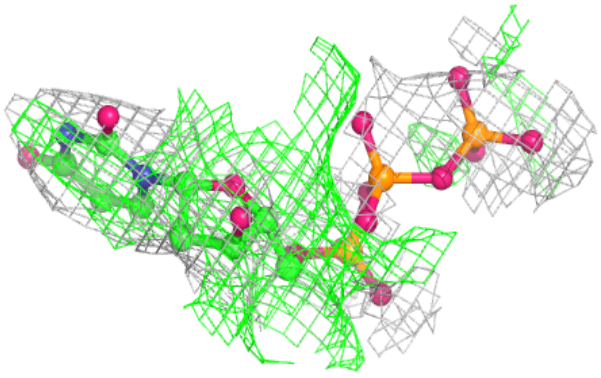
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	ZN	I	203	1/1	0.89	0.17	83,83,83,83	0
16	MG	A	2001	1/1	0.95	0.29	46,46,46,46	0
15	ZN	B	1307	1/1	0.96	0.05	80,80,80,80	0
15	ZN	C	319	1/1	0.96	0.13	48,48,48,48	0
15	ZN	I	204	1/1	0.97	0.07	57,57,57,57	0
15	ZN	A	1735	1/1	0.98	0.07	78,78,78,78	0
15	ZN	J	101	1/1	0.98	0.20	50,50,50,50	0
15	ZN	L	105	1/1	0.98	0.06	91,91,91,91	0

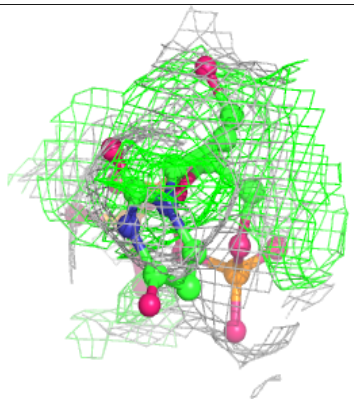
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DUT T 29 (A):

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

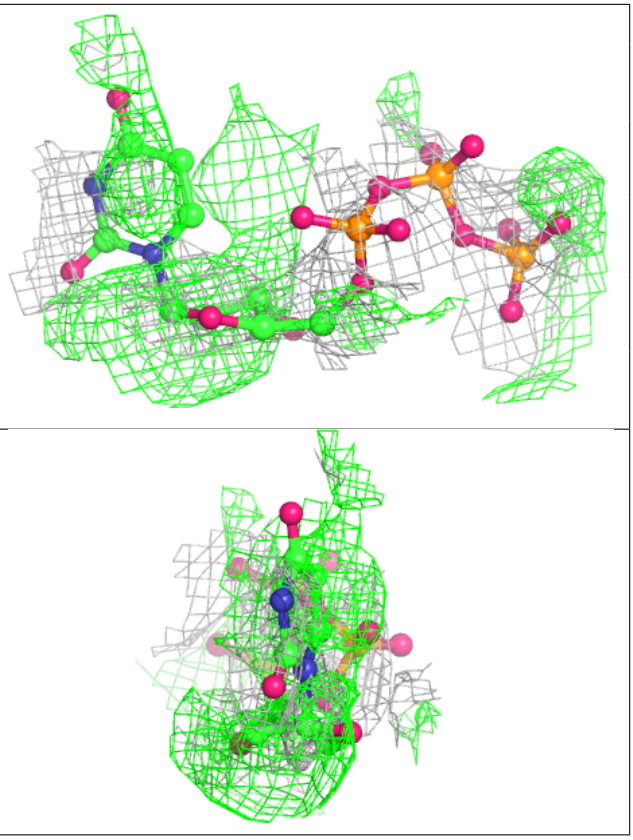






Electron density around DUT T 29 (B):

$2mF_o$-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.