



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 04:50 pm BST

PDB ID : 2E2I
Title : RNA polymerase II elongation complex in 5 mM Mg+2 with 2'-dGTP
Authors : Wang, D.; Bushnell, D.A.; Westover, K.D.; Kaplan, C.D.; Kornberg, R.D.
Deposited on : 2006-11-14
Resolution : 3.41 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

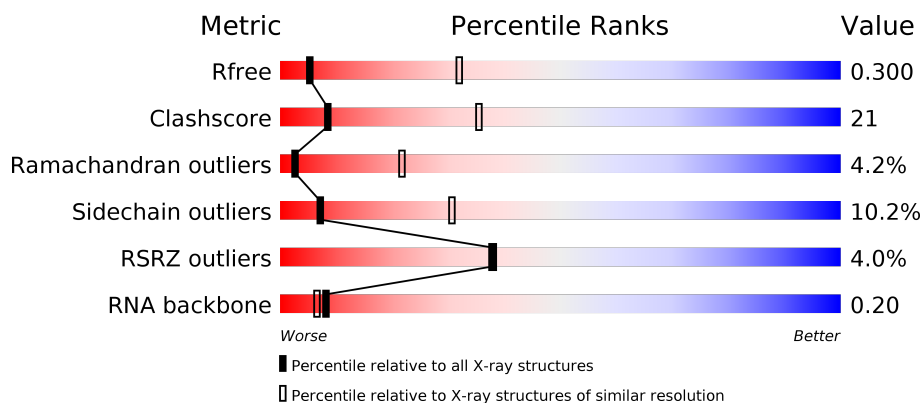
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)
RNA backbone	3102	1012 (3.88-2.96)

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

Mol	Chain	Length	Quality of chain
1	R	10	<div> <div>10%</div> <div>10% 20% 50% 20%</div> </div>
2	T	28	<div> <div>4%</div> <div>7% 75% 18%</div> </div>
3	N	14	<div> <div>7%</div> <div>7% 64% 29%</div> </div>
4	A	1733	<div> <div>4%</div> <div>51% 26% 19%</div> </div>

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

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 29722 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
1	R	10	Total	C	N	O	P	0	0	0
			216	98	45	64	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	28	Total	C	N	O	P	0	0	0
			564	270	102	165	27			

- 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
3	N	14	Total	C	N	O	P	0	0	0
			284	137	49	85	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1411	Total	C	N	O	S	0	0	0
			11098	6989	1944	2104	61			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1143	Total	C	N	O	S	0	0	0
			9092	5753	1595	1688	56			

- 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	213	Total	C	N	O	S	0	0	0
			1744	1107	308	318	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	86	Total	C	N	O	S	0	0	0
			697	445	118	131	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	134	Total	C	N	O	S	0	0	0
			1076	678	181	212	5			

- 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 polypeptide.

tide.

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

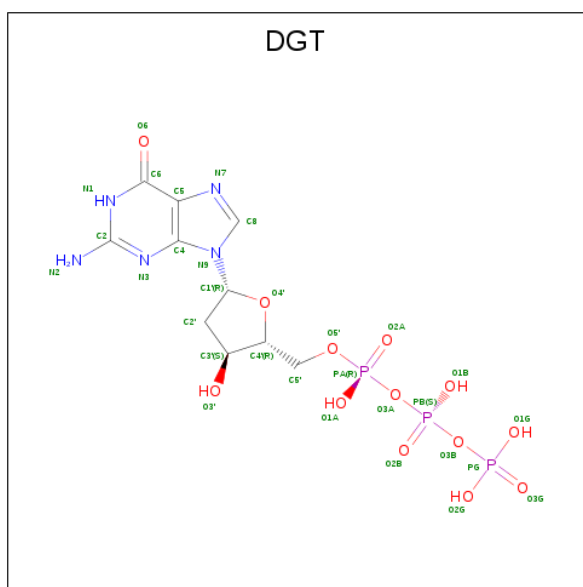
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

- Molecule 16 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).

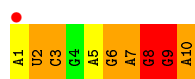


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
16	B	1	Total 62	C 20	N 10	O 26	P 6	0	1

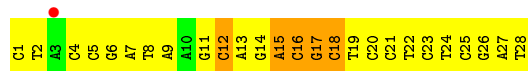
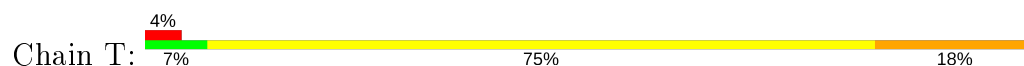
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

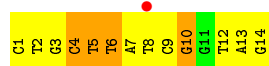
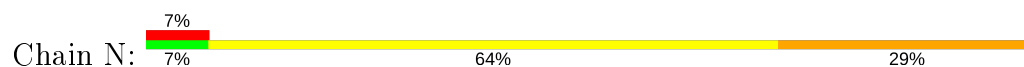
- Molecule 1: 5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3'



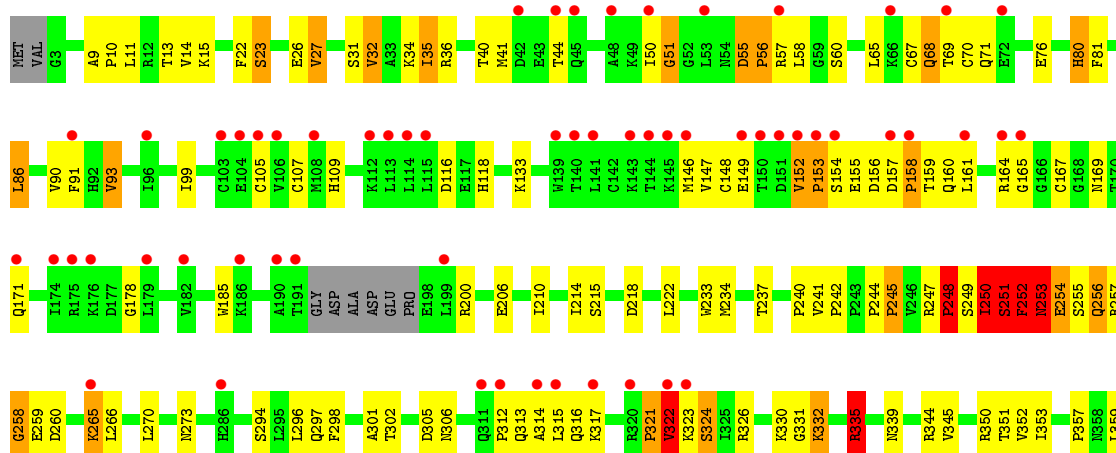
- Molecule 2: 28-MER DNA template strand



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



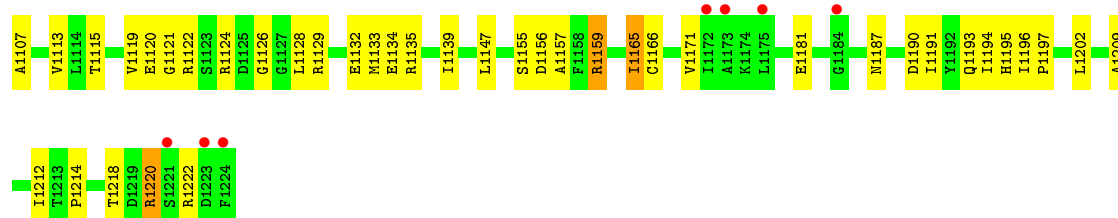
- Molecule 4: DNA-directed RNA polymerase II largest subunit





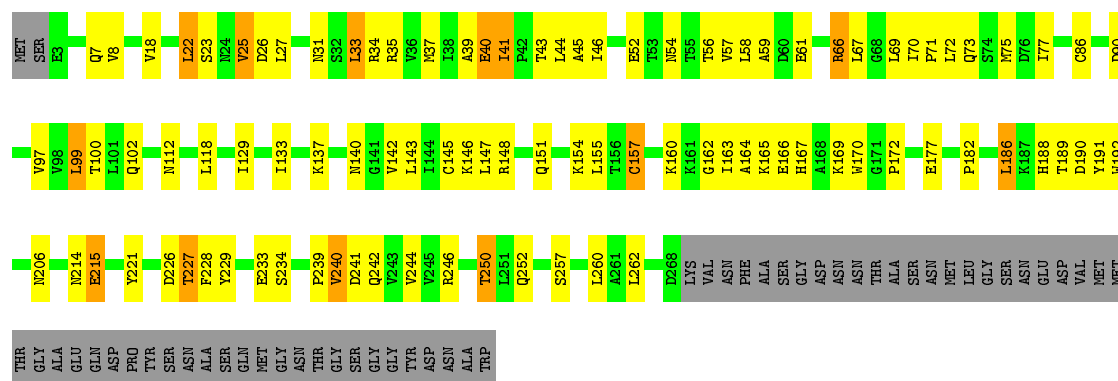
- Chain B:





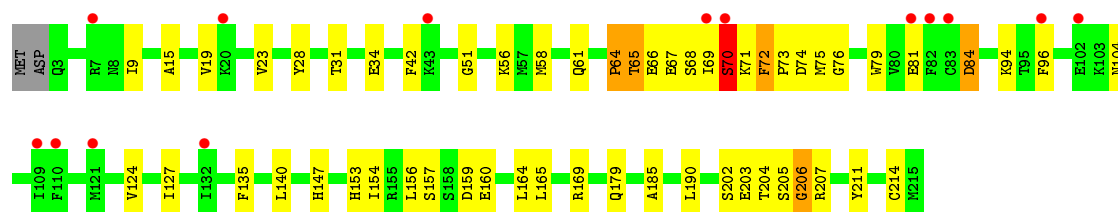
• Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide

Chain C: 53% 26% 16%



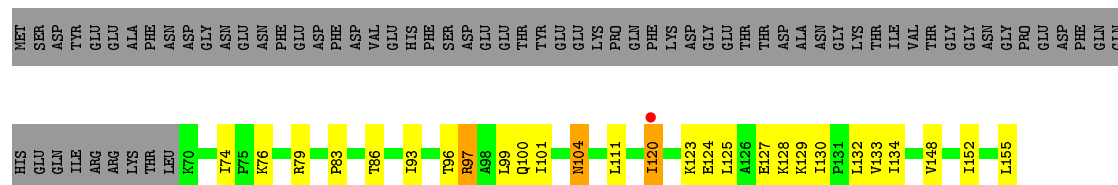
• Molecule 7: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

Chain E: 7% 73% 23%



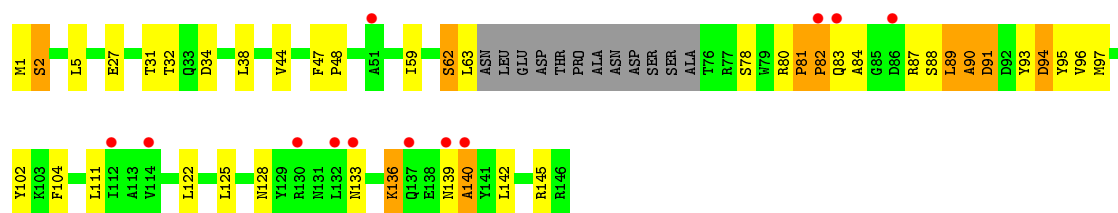
• Molecule 8: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

Chain F: 38% 15% 45%



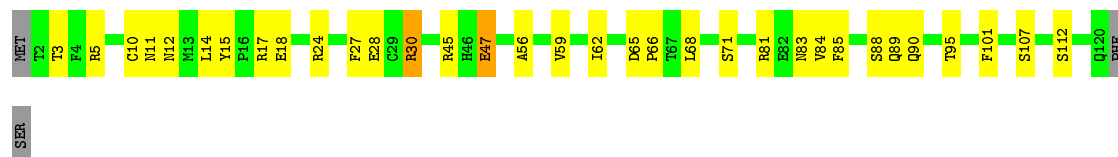
• Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

Chain H: 8% 63% 22% 7% 8%



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

Chain I: 70% 25% . .



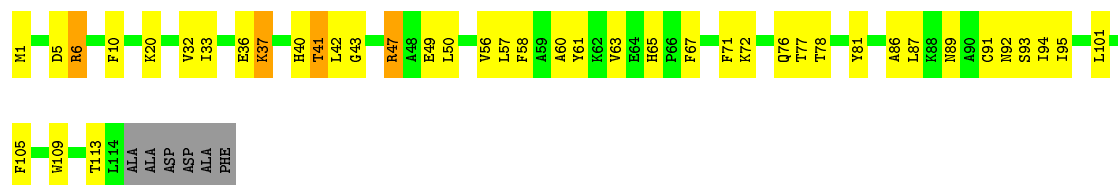
- Molecule 11: DNA-directed RNA polymerases I/II/III subunit 10

Chain J: 56% 24% 11% 7% .



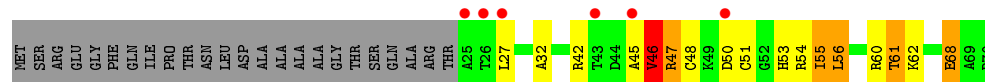
- Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K: 60% 32% 5% .



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

Chain L: 9% 41% 16% 7% 34% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.68Å 223.52Å 193.94Å 90.00° 100.54° 90.00°	Depositor
Resolution (Å)	50.00 – 3.41 49.77 – 3.41	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-3.41) 98.0 (49.77-3.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.266 , 0.316 0.257 , 0.300	Depositor DCC
R_{free} test set	4732 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	92.7	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 72.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	29722	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, DGT

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	1.15	0/243	1.89	10/378 (2.6%)
2	T	0.87	0/631	1.67	12/970 (1.2%)
3	N	0.81	0/317	1.53	9/488 (1.8%)
4	A	0.65	3/11294 (0.0%)	0.74	3/15270 (0.0%)
5	B	0.80	4/9268 (0.0%)	0.87	9/12496 (0.1%)
6	C	0.74	1/2133 (0.0%)	0.79	1/2891 (0.0%)
7	E	0.51	0/1780	0.64	0/2395
8	F	0.55	0/709	0.69	0/956
9	H	0.51	0/1094	0.66	0/1480
10	I	0.60	0/989	0.66	0/1331
11	J	0.85	1/541 (0.2%)	0.91	0/727
12	K	0.72	1/937 (0.1%)	0.72	0/1265
13	L	0.81	2/365 (0.5%)	0.91	0/485
All	All	0.71	12/30301 (0.0%)	0.84	44/41132 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	7
5	B	0	11
7	E	0	1
11	J	0	2
All	All	0	21

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	J	10	CYS	CB-SG	7.21	1.94	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	86	CYS	CB-SG	-6.58	1.71	1.82
5	B	302	CYS	CB-SG	-6.13	1.71	1.82
12	K	91	CYS	CB-SG	-6.02	1.72	1.82
5	B	147	LEU	C-O	5.98	1.34	1.23
5	B	1029	CYS	CB-SG	-5.83	1.72	1.81
4	A	795	GLU	CG-CD	5.73	1.60	1.51
5	B	488	TYR	CE1-CZ	5.55	1.45	1.38
13	L	68	GLU	CB-CG	5.33	1.62	1.52
4	A	1020	CYS	CB-SG	-5.18	1.73	1.81
4	A	1400	CYS	CB-SG	-5.08	1.73	1.81
13	L	68	GLU	CG-CD	5.06	1.59	1.51

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	18	DC	O4'-C4'-C3'	-16.51	96.09	106.00
2	T	28	DT	C1'-O4'-C4'	-12.85	97.25	110.10
2	T	18	DC	C4'-C3'-C2'	-12.19	92.13	103.10
1	R	9	G	C5'-C4'-C3'	-9.98	100.04	116.00
2	T	18	DC	C1'-O4'-C4'	-8.74	101.36	110.10
2	T	28	DT	O4'-C1'-N1	8.53	113.97	108.00
1	R	9	G	P-O3'-C3'	-8.45	109.56	119.70
3	N	5	DT	C1'-O4'-C4'	-8.29	101.81	110.10
2	T	18	DC	O4'-C1'-N1	7.58	113.31	108.00
2	T	15	DA	P-O3'-C3'	7.43	128.62	119.70
3	N	10	DG	P-O3'-C3'	7.10	128.22	119.70
5	B	492	LEU	CA-CB-CG	-7.07	99.04	115.30
5	B	69	LEU	CA-CB-CG	6.82	130.99	115.30
5	B	485	ARG	NE-CZ-NH2	-6.64	116.98	120.30
3	N	6	DT	C1'-O4'-C4'	-6.40	103.70	110.10
1	R	6	G	N1-C6-O6	-6.29	116.12	119.90
3	N	5	DT	O4'-C1'-N1	6.14	112.30	108.00
2	T	16	DC	O4'-C1'-N1	6.12	112.28	108.00
2	T	18	DC	C4'-C3'-O3'	6.08	124.90	109.70
1	R	9	G	C8-N9-C4	-6.05	103.98	106.40
1	R	9	G	N9-C1'-C2'	-6.04	105.36	112.00
4	A	839	ARG	NE-CZ-NH1	6.03	123.31	120.30
5	B	1010	LEU	CB-CG-CD1	-5.98	100.83	111.00
4	A	821	ARG	NE-CZ-NH1	-5.91	117.34	120.30
3	N	3	DG	C5-C6-O6	-5.90	125.06	128.60
1	R	10	A	C3'-C2'-C1'	5.79	106.13	101.50
1	R	8	G	C5-C6-O6	-5.71	125.17	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	10	A	O4'-C1'-N9	5.57	112.66	108.20
5	B	118	ARG	NE-CZ-NH2	-5.56	117.52	120.30
6	C	58	LEU	CA-CB-CG	5.55	128.06	115.30
2	T	12	DC	P-O3'-C3'	5.46	126.26	119.70
1	R	9	G	C2'-C3'-O3'	5.43	122.40	113.70
4	A	1116	LEU	CA-CB-CG	5.43	127.78	115.30
3	N	5	DT	C5-C4-O4	-5.38	121.14	124.90
5	B	119	LEU	CA-CB-CG	-5.34	103.03	115.30
1	R	8	G	P-O3'-C3'	-5.22	113.43	119.70
3	N	14	DG	C5-C6-O6	-5.20	125.48	128.60
5	B	795	ILE	CG1-CB-CG2	-5.18	99.99	111.40
5	B	807	ARG	NE-CZ-NH2	-5.13	117.74	120.30
3	N	4	DC	P-O3'-C3'	5.12	125.85	119.70
5	B	807	ARG	NE-CZ-NH1	5.11	122.85	120.30
2	T	18	DC	C5'-C4'-C3'	5.07	123.23	114.10
3	N	5	DT	P-O3'-C3'	5.04	125.75	119.70
2	T	17	DG	N1-C6-O6	5.04	122.92	119.90

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1175	SER	Peptide
4	A	248	PRO	Peptide
4	A	250	ILE	Peptide
4	A	251	SER	Peptide
4	A	252	PHE	Peptide
4	A	254	GLU	Peptide
4	A	460	VAL	Peptide
5	B	141	ASP	Peptide
5	B	143	PRO	Peptide
5	B	145	ARG	Peptide
5	B	502	ILE	Peptide
5	B	503	GLY	Peptide
5	B	504	ARG	Peptide
5	B	506	GLY	Peptide
5	B	508	LEU	Peptide
5	B	636	PRO	Peptide
5	B	71	LEU	Peptide
5	B	89	GLU	Peptide
7	E	70	SER	Peptide
11	J	3	VAL	Peptide

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Mol	Chain	Res	Type	Group
11	J	4	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	216	0	109	13	0
2	T	564	0	316	88	0
3	N	284	0	161	19	0
4	A	11098	0	11174	428	0
5	B	9092	0	9135	504	0
6	C	2095	0	2051	95	0
7	E	1744	0	1772	46	0
8	F	697	0	720	19	0
9	H	1076	0	1052	32	0
10	I	971	0	928	16	0
11	J	532	0	542	48	0
12	K	919	0	929	37	0
13	L	363	0	388	6	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
16	B	62	0	24	2	0
All	All	29722	0	29301	1225	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 21.

All (1225) 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:69:LEU:HG	5:B:70:ILE:CG2	1.32	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:19:DT:H2'	2:T:20:DC:C6	1.41	1.51
5:B:142:VAL:CG1	5:B:144:GLY:HA3	1.43	1.45
5:B:142:VAL:HG13	5:B:144:GLY:CA	1.57	1.34
5:B:69:LEU:CA	5:B:70:ILE:HB	1.58	1.28
5:B:70:ILE:N	5:B:89:GLU:HG3	1.53	1.24
6:C:66:ARG:NH2	11:J:2:ILE:HG13	1.54	1.21
4:A:255:SER:HA	4:A:256:GLN:CB	1.72	1.18
5:B:341:LEU:HB3	5:B:342:GLY:HA2	1.19	1.16
2:T:18:DC:H5''	2:T:19:DT:OP1	1.44	1.16
2:T:19:DT:C2'	2:T:20:DC:C6	2.30	1.15
4:A:253:ASN:HA	4:A:255:SER:HB3	1.29	1.14
5:B:69:LEU:HG	5:B:70:ILE:HG21	1.22	1.13
5:B:504:ARG:HG2	5:B:505:ASP:H	1.00	1.13
5:B:341:LEU:CB	5:B:342:GLY:HA2	1.78	1.12
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.29	1.12
5:B:89:GLU:HA	5:B:90:ILE:HB	1.32	1.12
4:A:567:LYS:HB2	4:A:568:PRO:HD2	1.19	1.11
5:B:69:LEU:CG	5:B:70:ILE:CG2	2.27	1.11
5:B:142:VAL:CG2	5:B:143:PRO:HD2	1.80	1.10
4:A:253:ASN:CA	4:A:255:SER:HB3	1.80	1.10
6:C:66:ARG:HH21	11:J:2:ILE:CG1	1.63	1.09
5:B:287:ARG:HD3	5:B:292:ILE:HA	1.34	1.09
4:A:256:GLN:N	4:A:257:ARG:HA	1.59	1.08
5:B:69:LEU:HA	5:B:70:ILE:CB	1.73	1.08
4:A:567:LYS:CB	4:A:568:PRO:HD2	1.83	1.08
5:B:636:PRO:HB2	5:B:637:LEU:HA	1.10	1.08
5:B:143:PRO:HB2	5:B:144:GLY:HA2	1.29	1.07
5:B:145:ARG:HB2	5:B:146:GLU:HB2	1.26	1.07
5:B:142:VAL:HG22	5:B:143:PRO:CD	1.83	1.07
5:B:502:ILE:N	5:B:502:ILE:HD12	1.68	1.07
4:A:1356:ILE:HG13	4:A:1368:MET:HE2	1.37	1.07
5:B:955:THR:HG22	5:B:956:THR:H	1.20	1.06
2:T:20:DC:C2'	2:T:21:DC:H5''	1.86	1.06
4:A:255:SER:CA	4:A:256:GLN:HB2	1.79	1.05
4:A:1364:ASN:ND2	4:A:1366:ARG:HG2	1.69	1.05
5:B:636:PRO:HB2	5:B:637:LEU:CA	1.87	1.03
5:B:69:LEU:HG	5:B:70:ILE:HG22	1.06	1.03
5:B:334:ILE:HA	5:B:335:GLY:C	1.79	1.02
5:B:88:TYR:CD2	5:B:136:THR:HG23	1.93	1.02
5:B:89:GLU:H	5:B:89:GLU:CD	1.55	1.01
6:C:57:VAL:HG11	11:J:60:PHE:HB3	1.40	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:504:ARG:CG	5:B:505:ASP:H	1.74	1.00
4:A:255:SER:HA	4:A:256:GLN:HB2	0.99	0.99
2:T:18:DC:H2''	2:T:19:DT:H5'	1.42	0.99
5:B:145:ARG:HB2	5:B:146:GLU:CB	1.92	0.99
5:B:341:LEU:HB3	5:B:342:GLY:CA	1.93	0.98
2:T:18:DC:C2'	2:T:19:DT:H5'	1.93	0.97
5:B:504:ARG:HG2	5:B:505:ASP:N	1.78	0.97
5:B:69:LEU:CG	5:B:70:ILE:HG22	1.93	0.97
4:A:253:ASN:N	4:A:255:SER:HB3	1.80	0.97
2:T:19:DT:H2''	2:T:20:DC:H5'	1.43	0.96
4:A:153:PRO:HD2	4:A:154:SER:HA	1.46	0.95
5:B:89:GLU:CA	5:B:90:ILE:HB	1.96	0.95
11:J:8:PHE:H	11:J:49:MET:HE3	1.31	0.95
4:A:868:TYR:HE1	4:A:1064:VAL:HG11	1.29	0.94
4:A:1364:ASN:HD22	4:A:1366:ARG:HG2	1.32	0.94
5:B:70:ILE:N	5:B:89:GLU:CG	2.30	0.94
2:T:19:DT:H2'	2:T:20:DC:C5	2.02	0.94
5:B:635:ARG:HB2	5:B:636:PRO:HD2	1.52	0.92
5:B:72:GLU:OE2	5:B:73:GLN:HB2	1.70	0.92
5:B:71:LEU:HD13	5:B:71:LEU:O	1.69	0.92
4:A:1118:VAL:HG23	4:A:1306:LEU:HB2	1.51	0.92
2:T:27:DA:N1	4:A:252:PHE:CE1	2.38	0.92
5:B:69:LEU:HA	5:B:70:ILE:HB	0.92	0.91
5:B:899:ILE:HG21	5:B:949:VAL:HG21	1.51	0.91
4:A:316:GLN:HB3	4:A:317:LYS:HB2	1.51	0.91
5:B:143:PRO:HB2	5:B:144:GLY:CA	2.01	0.90
6:C:66:ARG:CG	6:C:66:ARG:HH11	1.84	0.90
2:T:20:DC:H2'	2:T:21:DC:C5'	2.02	0.89
5:B:976:ILE:O	5:B:990:ILE:HB	1.71	0.89
5:B:287:ARG:HG3	5:B:287:ARG:HH11	1.37	0.89
5:B:70:ILE:CA	5:B:89:GLU:HG3	2.03	0.89
5:B:848:ARG:HH22	5:B:996:ARG:NH1	1.71	0.89
4:A:565:ILE:HG23	4:A:567:LYS:HE3	1.55	0.88
5:B:69:LEU:CB	5:B:70:ILE:HB	2.02	0.88
2:T:19:DT:H2''	2:T:20:DC:C5'	2.02	0.88
2:T:18:DC:H3'	2:T:19:DT:H72	1.56	0.88
2:T:27:DA:N1	4:A:252:PHE:CZ	2.42	0.88
11:J:35:ALA:O	11:J:39:LEU:HD12	1.73	0.88
4:A:1017:LEU:HD12	7:E:206:GLY:H	1.38	0.87
4:A:446:ARG:HB2	4:A:487:MET:HE3	1.56	0.87
5:B:798:TYR:HE2	11:J:2:ILE:HG22	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1406:VAL:HA	4:A:1409:LEU:HD12	1.57	0.87
5:B:69:LEU:CA	5:B:70:ILE:CB	2.43	0.86
4:A:1118:VAL:HG12	4:A:1327:ILE:HD12	1.56	0.86
4:A:107:CYS:HA	4:A:171:GLN:HE21	1.39	0.86
6:C:66:ARG:NH2	11:J:2:ILE:HG23	1.91	0.86
5:B:139:ALA:N	5:B:140:ILE:HA	1.88	0.85
2:T:19:DT:C2'	2:T:20:DC:H6	1.80	0.85
5:B:1159:ARG:HD3	5:B:1193:GLN:HG3	1.59	0.85
5:B:1084:GLN:HE22	6:C:191:TYR:HA	1.39	0.85
5:B:879:ARG:O	5:B:882:THR:HG22	1.76	0.85
5:B:145:ARG:CB	5:B:146:GLU:HB2	2.07	0.84
4:A:51:GLY:HA2	4:A:56:PRO:HG3	1.57	0.84
5:B:1084:GLN:NE2	6:C:191:TYR:HA	1.92	0.84
5:B:141:ASP:O	5:B:142:VAL:HB	1.76	0.84
2:T:18:DC:C5'	2:T:19:DT:OP1	2.22	0.84
5:B:763:GLN:HG2	5:B:765:PRO:HD2	1.58	0.84
6:C:45:ALA:HA	6:C:72:LEU:HD12	1.57	0.84
7:E:67:GLU:CB	7:E:68:SER:HA	2.08	0.84
5:B:69:LEU:CG	5:B:70:ILE:HG21	1.98	0.83
3:N:1:DC:H4'	3:N:2:DT:OP1	1.76	0.83
5:B:502:ILE:N	5:B:502:ILE:CD1	2.41	0.83
2:T:19:DT:H2'	2:T:20:DC:H6	1.02	0.83
5:B:338:GLY:HA2	5:B:340:ALA:H	1.43	0.83
4:A:450:LEU:H	4:A:450:LEU:HD12	1.44	0.83
5:B:70:ILE:HG23	5:B:70:ILE:O	1.79	0.83
8:F:97:ARG:HD2	8:F:101:ILE:HD11	1.59	0.83
5:B:88:TYR:CE2	5:B:136:THR:HG23	2.13	0.82
6:C:73:GLN:HE21	6:C:75:MET:H	1.27	0.82
7:E:65:THR:HA	7:E:66:GLU:C	2.00	0.82
5:B:334:ILE:HA	5:B:335:GLY:O	1.77	0.82
7:E:72:PHE:H	7:E:73:PRO:HA	1.43	0.82
4:A:1323:ASP:OD1	4:A:1325:THR:HG22	1.80	0.82
2:T:20:DC:C2'	2:T:21:DC:C5'	2.56	0.82
4:A:256:GLN:N	4:A:257:ARG:CA	2.42	0.81
3:N:7:DA:C2'	3:N:8:DT:H71	2.09	0.81
4:A:901:LEU:H	4:A:926:GLN:HE21	1.28	0.81
4:A:754:SER:H	4:A:757:ASN:HD22	1.24	0.81
5:B:136:THR:HB	5:B:137:TYR:HA	1.61	0.81
5:B:25:ILE:HD11	5:B:653:VAL:HB	1.61	0.81
4:A:256:GLN:H	4:A:257:ARG:HA	1.46	0.81
1:R:8:G:N2	2:T:22:DT:N3	2.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:142:VAL:CG1	5:B:144:GLY:CA	2.31	0.80
5:B:504:ARG:CG	5:B:505:ASP:N	2.36	0.79
6:C:43:THR:HG22	6:C:44:LEU:H	1.46	0.79
5:B:142:VAL:HG22	5:B:143:PRO:HD2	0.89	0.79
5:B:378:LEU:O	5:B:378:LEU:HG	1.79	0.79
4:A:316:GLN:HB3	4:A:317:LYS:CB	2.12	0.79
6:C:66:ARG:NH1	11:J:5:VAL:HG23	1.97	0.79
2:T:14:DG:C2	2:T:15:DA:N6	2.49	0.79
2:T:20:DC:H2''	2:T:21:DC:H5''	1.64	0.79
4:A:253:ASN:N	4:A:255:SER:CB	2.44	0.79
4:A:885:THR:O	4:A:940:ARG:HG3	1.82	0.79
5:B:287:ARG:HG3	5:B:287:ARG:NH1	1.95	0.79
5:B:71:LEU:O	5:B:71:LEU:CD1	2.30	0.79
4:A:1105:LEU:HD23	4:A:1384:VAL:HG21	1.65	0.78
6:C:66:ARG:NH2	11:J:2:ILE:CG2	2.46	0.78
4:A:90:VAL:HG13	4:A:297:GLN:NE2	1.98	0.78
4:A:401:GLY:O	4:A:435:HIS:CD2	2.37	0.78
5:B:802:PRO:HB3	5:B:1091:TYR:CD1	2.18	0.78
5:B:798:TYR:CE2	11:J:2:ILE:HG22	2.18	0.78
5:B:89:GLU:N	5:B:89:GLU:CD	2.30	0.78
5:B:1187:ASN:HD21	5:B:1190:ASP:HB3	1.48	0.78
3:N:8:DT:H2''	3:N:9:DC:O5'	1.82	0.78
6:C:66:ARG:CZ	11:J:2:ILE:HG21	2.14	0.77
5:B:726:ALA:HB1	5:B:1051:THR:HG21	1.65	0.77
6:C:182:PRO:HG3	6:C:206:ASN:O	1.84	0.77
3:N:7:DA:H2''	3:N:8:DT:H71	1.66	0.77
9:H:81:PRO:CB	9:H:82:PRO:HD2	2.14	0.77
2:T:20:DC:H2'	2:T:21:DC:H5'	1.66	0.77
5:B:72:GLU:OE2	5:B:73:GLN:CB	2.32	0.77
5:B:766:ARG:NH2	5:B:1020:ARG:HD3	1.99	0.76
6:C:99:LEU:HD12	6:C:118:LEU:HD22	1.67	0.76
6:C:66:ARG:CZ	11:J:2:ILE:CG2	2.63	0.76
6:C:69:LEU:HD12	11:J:6:ARG:HD3	1.67	0.76
4:A:153:PRO:CD	4:A:154:SER:HA	2.15	0.76
5:B:955:THR:HG22	5:B:956:THR:N	2.00	0.76
11:J:3:VAL:HG21	11:J:18:TRP:HB2	1.68	0.76
4:A:567:LYS:HB2	4:A:568:PRO:CD	2.09	0.75
5:B:344:LYS:HA	5:B:345:LYS:HB3	1.68	0.75
4:A:351:THR:HG22	4:A:352:VAL:N	2.02	0.75
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.21	0.75
4:A:1356:ILE:HG13	4:A:1368:MET:CE	2.15	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:66:ARG:HH21	11:J:2:ILE:HG13	0.70	0.74
2:T:25:DC:H2'	2:T:26:DG:O5'	1.86	0.74
4:A:868:TYR:CE1	4:A:1064:VAL:HG11	2.19	0.74
4:A:445:ASN:HB3	4:A:455:MET:HG2	1.69	0.74
5:B:329:THR:HA	5:B:332:ASP:HB3	1.70	0.74
5:B:955:THR:HG23	13:L:54:ARG:O	1.86	0.74
5:B:654:ARG:H	5:B:657:HIS:HD2	1.33	0.74
5:B:862:GLN:HG2	5:B:963:PHE:HB2	1.68	0.74
2:T:18:DC:H2'	2:T:19:DT:C6	2.22	0.74
5:B:72:GLU:CD	5:B:73:GLN:N	2.41	0.73
5:B:744:HIS:HD2	5:B:746:SER:H	1.36	0.73
13:L:60:ARG:HG3	13:L:61:THR:H	1.51	0.73
6:C:165:LYS:O	12:K:6:ARG:NH1	2.21	0.73
5:B:70:ILE:HA	5:B:89:GLU:CG	2.18	0.73
4:A:875:ALA:HB2	4:A:1366:ARG:HD2	1.71	0.73
7:E:75:MET:CB	7:E:76:GLY:HA2	2.19	0.72
4:A:1015:VAL:HG12	4:A:1019:CYS:SG	2.29	0.72
4:A:157:ASP:HB3	4:A:158:PRO:HD3	1.71	0.72
5:B:71:LEU:HD22	5:B:72:GLU:HB2	1.70	0.72
4:A:1161:THR:HG22	4:A:1163:ILE:H	1.54	0.72
5:B:137:TYR:CD2	5:B:138:GLU:HG2	2.25	0.72
4:A:345:VAL:HG12	5:B:1155:SER:HB2	1.70	0.72
2:T:27:DA:N1	4:A:252:PHE:HE1	1.86	0.72
4:A:567:LYS:CB	4:A:568:PRO:CD	2.63	0.72
5:B:89:GLU:O	5:B:135:ARG:NH1	2.23	0.72
6:C:66:ARG:HG2	6:C:66:ARG:NH1	2.04	0.72
4:A:741:ASN:HD22	4:A:744:LYS:H	1.35	0.71
5:B:1077:THR:HG23	5:B:1079:LYS:H	1.53	0.71
4:A:351:THR:HG22	4:A:352:VAL:H	1.55	0.71
5:B:756:ILE:HG12	5:B:770:GLN:HG2	1.72	0.71
5:B:1106:ARG:HD3	5:B:1126:GLY:O	1.90	0.71
5:B:287:ARG:HD3	5:B:292:ILE:CA	2.16	0.71
6:C:112:ASN:ND2	6:C:146:LYS:HG2	2.05	0.71
2:T:22:DT:H2'	2:T:23:DC:O4'	1.89	0.71
4:A:249:SER:O	4:A:250:ILE:CG1	2.38	0.71
5:B:501:PRO:C	5:B:502:ILE:HD12	2.09	0.71
5:B:906:SER:HB3	5:B:946:ASN:HB2	1.70	0.71
5:B:88:TYR:HD2	5:B:136:THR:HG23	1.52	0.71
4:A:901:LEU:H	4:A:926:GLN:NE2	1.86	0.71
5:B:992:ILE:HD11	12:K:67:PHE:CE2	2.26	0.70
5:B:200:GLY:HA2	5:B:202:TYR:CE2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:834:THR:HG21	4:A:1077:THR:HA	1.73	0.70
5:B:1084:GLN:OE1	5:B:1084:GLN:N	2.23	0.70
5:B:955:THR:CG2	5:B:956:THR:H	2.01	0.70
5:B:89:GLU:HA	5:B:90:ILE:CB	2.14	0.70
6:C:242:GLN:HE21	6:C:246:ARG:HE	1.38	0.70
4:A:14:VAL:HB	4:A:1432:GLN:HE22	1.56	0.70
4:A:511:ILE:HG12	4:A:521:MET:CE	2.21	0.70
4:A:133:LYS:HG2	4:A:1391:ARG:HH21	1.55	0.70
4:A:849:MET:HE1	4:A:1061:GLY:HA2	1.73	0.70
4:A:518:LYS:HB2	4:A:519:PRO:HD2	1.74	0.70
5:B:542:MET:HG3	5:B:747:MET:CE	2.21	0.70
5:B:68:THR:O	5:B:69:LEU:HB3	1.92	0.70
6:C:66:ARG:HG2	6:C:66:ARG:HH11	1.54	0.70
5:B:345:LYS:H	5:B:348:ARG:H	1.40	0.70
5:B:72:GLU:OE1	5:B:72:GLU:CA	2.40	0.70
4:A:249:SER:O	4:A:250:ILE:HG13	1.92	0.70
7:E:185:ALA:HA	7:E:190:LEU:HD23	1.73	0.69
7:E:67:GLU:HA	7:E:67:GLU:OE1	1.92	0.69
4:A:302:THR:HA	4:A:305:ASP:O	1.91	0.69
5:B:70:ILE:HA	5:B:89:GLU:HG3	1.75	0.69
4:A:645:LEU:HD11	4:A:649:ILE:HD11	1.75	0.69
4:A:608:ILE:O	4:A:609:ASP:O	2.11	0.69
4:A:533:LYS:HE3	4:A:745:GLN:HE22	1.58	0.69
5:B:544:CYS:HB2	5:B:634:TYR:CE1	2.28	0.69
4:A:344:ARG:NH2	5:B:1120:GLU:HG3	2.08	0.68
5:B:145:ARG:HB2	5:B:146:GLU:CG	2.23	0.68
4:A:1134:ILE:O	4:A:1138:ILE:HG12	1.92	0.68
4:A:998:LEU:HD12	4:A:1001:ARG:HG3	1.74	0.68
4:A:1175:SER:OG	4:A:1176:LEU:C	2.31	0.68
7:E:67:GLU:HB3	7:E:69:ILE:HA	1.75	0.68
5:B:515:HIS:HD2	5:B:517:THR:OG1	1.76	0.68
5:B:519:TRP:HZ2	5:B:705:MET:HE1	1.56	0.68
5:B:72:GLU:OE1	5:B:72:GLU:HA	1.93	0.68
6:C:233:GLU:OE2	11:J:43:ARG:NH2	2.26	0.68
5:B:140:ILE:HG13	5:B:141:ASP:OD1	1.93	0.68
5:B:70:ILE:CA	5:B:89:GLU:CG	2.70	0.68
5:B:143:PRO:CB	5:B:144:GLY:HA2	2.15	0.67
5:B:69:LEU:C	5:B:89:GLU:CG	2.62	0.67
6:C:66:ARG:HH12	11:J:5:VAL:HG23	1.59	0.67
4:A:91:PHE:H	4:A:297:GLN:HE22	1.42	0.67
4:A:567:LYS:CG	4:A:568:PRO:HD2	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:401:GLY:C	4:A:435:HIS:CD2	2.68	0.67
4:A:55:ASP:H	4:A:56:PRO:HD2	1.57	0.67
5:B:142:VAL:HG11	5:B:144:GLY:HA3	1.68	0.67
2:T:15:DA:C2	2:T:16:DC:C5	2.83	0.67
5:B:519:TRP:HZ2	5:B:705:MET:CE	2.07	0.67
5:B:837:ASP:HB3	5:B:1020:ARG:NH2	2.10	0.67
3:N:7:DA:H2"	3:N:8:DT:C6	2.28	0.67
5:B:783:THR:O	5:B:783:THR:HG22	1.96	0.66
6:C:71:PRO:HB2	6:C:133:ILE:HD12	1.76	0.66
9:H:62:SER:OG	9:H:63:LEU:N	2.27	0.66
4:A:607:ILE:HG12	4:A:612:ILE:HG22	1.75	0.66
5:B:976:ILE:HG23	5:B:977:GLY:H	1.58	0.66
7:E:157:SER:OG	7:E:160:GLU:HG3	1.96	0.66
4:A:252:PHE:HA	4:A:253:ASN:OD1	1.95	0.66
1:R:8:G:N2	2:T:22:DT:H3	1.93	0.66
4:A:1064:VAL:HG12	4:A:1370:LEU:HD22	1.78	0.66
5:B:72:GLU:OE2	5:B:73:GLN:CG	2.43	0.66
4:A:251:SER:O	4:A:253:ASN:HB3	1.96	0.66
4:A:500:GLU:O	4:A:500:GLU:HG2	1.96	0.66
5:B:848:ARG:NH2	5:B:996:ARG:NH1	2.44	0.66
4:A:993:LEU:HD22	4:A:1046:LEU:HG	1.78	0.66
4:A:244:PRO:HB2	4:A:245:PRO:HD3	1.78	0.66
4:A:888:GLY:O	4:A:940:ARG:NH2	2.28	0.66
5:B:1032:SER:HB3	5:B:1089:PRO:HB2	1.78	0.66
4:A:381:THR:OG1	4:A:382:PRO:HD2	1.95	0.66
4:A:457:ALA:HB3	4:A:506:ALA:HA	1.76	0.66
5:B:341:LEU:HB2	5:B:342:GLY:HA2	1.75	0.66
5:B:88:TYR:CE2	5:B:136:THR:CG2	2.78	0.66
4:A:1364:ASN:HD21	4:A:1366:ARG:NH1	1.93	0.66
4:A:534:LEU:O	4:A:574:GLY:HA3	1.96	0.66
5:B:114:PRO:HG3	5:B:181:LEU:HD11	1.78	0.66
4:A:1339:LEU:HD13	7:E:147:HIS:CD2	2.31	0.66
5:B:766:ARG:HH22	5:B:1020:ARG:HD3	1.57	0.65
5:B:287:ARG:NE	5:B:292:ILE:O	2.29	0.65
5:B:334:ILE:CA	5:B:335:GLY:C	2.62	0.65
12:K:65:HIS:HD2	12:K:67:PHE:H	1.44	0.65
5:B:341:LEU:CB	5:B:342:GLY:CA	2.62	0.65
5:B:70:ILE:O	5:B:71:LEU:CB	2.44	0.65
7:E:75:MET:HB2	7:E:76:GLY:HA2	1.78	0.65
5:B:25:ILE:HG22	5:B:29:ASP:HB2	1.78	0.65
5:B:980:PHE:O	5:B:981:ALA:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:164:ARG:HB3	4:A:165:GLY:HA2	1.79	0.65
5:B:125:SER:HB3	5:B:171:PRO:HA	1.79	0.65
5:B:70:ILE:CG2	5:B:70:ILE:O	2.45	0.65
7:E:202:SER:OG	7:E:204:THR:HG22	1.97	0.65
2:T:4:DC:H2''	2:T:5:DC:O5'	1.96	0.65
6:C:66:ARG:HE	11:J:2:ILE:HG12	1.61	0.65
5:B:216:GLU:HB3	5:B:500:THR:HG23	1.79	0.64
5:B:766:ARG:NH2	5:B:1020:ARG:CD	2.60	0.64
4:A:255:SER:CA	4:A:256:GLN:CB	2.55	0.64
4:A:535:THR:O	4:A:575:LYS:HE2	1.97	0.64
5:B:286:PHE:HB3	5:B:297:ILE:HD12	1.78	0.64
5:B:843:GLN:HA	5:B:846:ILE:HD12	1.79	0.64
11:J:8:PHE:N	11:J:49:MET:HE3	2.09	0.64
2:T:14:DG:N2	2:T:15:DA:H62	1.94	0.64
6:C:46:ILE:CG2	6:C:157:CYS:HB3	2.27	0.64
5:B:70:ILE:O	5:B:71:LEU:HG	1.98	0.64
6:C:66:ARG:HG3	6:C:66:ARG:HH11	1.62	0.64
5:B:502:ILE:HG22	5:B:503:GLY:N	2.12	0.64
5:B:70:ILE:H	5:B:89:GLU:HG3	1.60	0.64
5:B:71:LEU:O	5:B:88:TYR:N	2.30	0.64
7:E:67:GLU:HB2	7:E:68:SER:HA	1.80	0.64
5:B:327:ARG:O	5:B:330:ALA:HB3	1.97	0.64
6:C:27:LEU:HD12	6:C:228:PHE:HE2	1.62	0.64
2:T:8:DT:H2''	2:T:9:DA:O5'	1.97	0.64
10:I:68:LEU:HB3	10:I:84:VAL:HG13	1.79	0.63
4:A:690:VAL:HG22	4:A:718:VAL:HG13	1.79	0.63
5:B:69:LEU:C	5:B:89:GLU:HG2	2.18	0.63
3:N:7:DA:H2''	3:N:8:DT:C7	2.28	0.63
5:B:141:ASP:OD1	5:B:141:ASP:N	2.30	0.63
4:A:1152:ILE:HG12	4:A:1260:LEU:HD23	1.79	0.63
5:B:502:ILE:H	5:B:502:ILE:HD12	1.61	0.63
5:B:843:GLN:O	5:B:843:GLN:HG3	1.98	0.63
4:A:1364:ASN:HD21	4:A:1366:ARG:HH11	1.43	0.63
4:A:567:LYS:HG3	4:A:568:PRO:CD	2.29	0.63
5:B:46:GLN:OE1	5:B:408:LEU:HD21	1.99	0.63
4:A:637:LYS:HB3	4:A:641:VAL:HG11	1.81	0.63
5:B:635:ARG:CB	5:B:636:PRO:HD2	2.20	0.63
8:F:132:LEU:O	8:F:148:VAL:HG23	1.99	0.63
5:B:1016:ALA:CB	5:B:1020:ARG:HH21	2.11	0.63
5:B:69:LEU:CD1	5:B:70:ILE:HG21	2.29	0.63
5:B:71:LEU:HD13	5:B:71:LEU:C	2.19	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:874:ASP:CA	4:A:1058:VAL:HG23	2.29	0.62
4:A:1118:VAL:CG2	4:A:1306:LEU:HB2	2.29	0.62
5:B:634:TYR:CE1	5:B:692:TYR:CD1	2.87	0.62
4:A:23:SER:O	4:A:27:VAL:HG23	1.99	0.62
5:B:1084:GLN:NE2	6:C:192:TRP:H	1.98	0.62
4:A:741:ASN:ND2	4:A:744:LYS:H	1.96	0.62
5:B:542:MET:HG3	5:B:747:MET:HE3	1.81	0.62
5:B:58:THR:O	5:B:62:ILE:HG12	1.99	0.62
3:N:7:DA:H2''	3:N:8:DT:C5	2.35	0.62
4:A:901:LEU:HD22	4:A:919:ILE:HG22	1.81	0.62
4:A:330:LYS:HG2	4:A:331:GLY:H	1.65	0.61
5:B:889:THR:HG22	5:B:891:ASP:HB2	1.82	0.61
5:B:1084:GLN:HE22	6:C:192:TRP:H	1.46	0.61
10:I:15:TYR:CD1	10:I:30:ARG:HD3	2.35	0.61
6:C:241:ASP:HB3	12:K:109:TRP:CE2	2.35	0.61
4:A:32:VAL:O	4:A:57:ARG:HD2	2.00	0.61
6:C:18:VAL:CG2	6:C:240:VAL:HB	2.31	0.61
6:C:73:GLN:HE21	6:C:75:MET:N	1.95	0.61
5:B:515:HIS:H	5:B:518:HIS:CD2	2.19	0.61
6:C:46:ILE:HG23	6:C:157:CYS:HB3	1.82	0.61
7:E:15:ALA:O	7:E:19:VAL:HG23	2.00	0.61
9:H:38:LEU:HD13	9:H:125:LEU:HD13	1.83	0.61
3:N:12:DT:H2''	3:N:13:DA:C8	2.36	0.61
5:B:70:ILE:O	5:B:71:LEU:HB3	2.01	0.61
4:A:389:THR:OG1	4:A:426:LEU:HD12	2.01	0.61
4:A:955:PRO:O	4:A:956:LEU:HG	2.00	0.61
6:C:66:ARG:NH2	11:J:2:ILE:CG1	2.39	0.61
9:H:82:PRO:O	9:H:83:GLN:HB2	1.99	0.61
3:N:7:DA:C2'	3:N:8:DT:C7	2.78	0.61
5:B:72:GLU:OE2	5:B:73:GLN:HG3	2.01	0.60
5:B:975:GLN:HG2	5:B:976:ILE:H	1.66	0.60
7:E:67:GLU:HB3	7:E:68:SER:HA	1.81	0.60
9:H:81:PRO:HB2	9:H:82:PRO:HD2	1.82	0.60
2:T:8:DT:C2'	2:T:9:DA:C8	2.84	0.60
5:B:1017:ILE:H	5:B:1018:PRO:HD2	1.66	0.60
5:B:678:GLU:O	5:B:678:GLU:HG2	2.01	0.60
5:B:89:GLU:CB	5:B:90:ILE:HB	2.31	0.60
2:T:18:DC:H2''	2:T:19:DT:C5'	2.26	0.60
2:T:19:DT:H2''	2:T:20:DC:O4'	2.01	0.60
2:T:27:DA:N1	4:A:252:PHE:HZ	1.96	0.60
4:A:858:ASN:HD22	4:A:858:ASN:C	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:778:MET:HE2	5:B:1094:ARG:HG2	1.84	0.60
5:B:464:GLY:HA2	5:B:479:VAL:O	2.01	0.60
5:B:550:ASP:OD1	5:B:551:PRO:HD2	2.01	0.60
4:A:1333:ILE:O	4:A:1337:GLU:HG3	2.02	0.60
3:N:4:DC:H2''	3:N:5:DT:OP2	2.02	0.60
2:T:19:DT:C2'	2:T:20:DC:H5'	2.26	0.60
5:B:256:VAL:HG11	5:B:382:ILE:HD13	1.83	0.60
3:N:7:DA:H2'	3:N:8:DT:H71	1.82	0.60
4:A:915:SER:O	4:A:919:ILE:HG12	2.02	0.60
5:B:744:HIS:CD2	5:B:746:SER:OG	2.54	0.59
5:B:344:LYS:HB3	5:B:345:LYS:O	2.02	0.59
4:A:996:ASN:HA	4:A:998:LEU:HD23	1.83	0.59
9:H:139:ASN:O	9:H:140:ALA:HB3	2.02	0.59
4:A:805:LEU:O	4:A:805:LEU:HG	2.02	0.59
2:T:18:DC:H3'	2:T:19:DT:C7	2.32	0.59
4:A:567:LYS:HG3	4:A:568:PRO:HG2	1.83	0.59
4:A:834:THR:HG21	4:A:1077:THR:CA	2.33	0.59
4:A:399:HIS:HB3	4:A:400:PRO:HD3	1.84	0.59
5:B:847:ASP:HB3	6:C:167:HIS:CE1	2.38	0.59
9:H:63:LEU:C	9:H:90:ALA:HB3	2.23	0.59
4:A:1174:PHE:HB3	4:A:1175:SER:HB3	1.85	0.59
4:A:351:THR:HG21	4:A:466:SER:O	2.03	0.59
4:A:34:LYS:HD3	4:A:36:ARG:HH22	1.67	0.59
4:A:608:ILE:O	4:A:609:ASP:C	2.41	0.59
4:A:351:THR:HG23	5:B:1103:ILE:HG12	1.83	0.59
12:K:65:HIS:CD2	12:K:67:PHE:HB2	2.37	0.59
13:L:32:ALA:HB3	13:L:55:ILE:HD12	1.85	0.59
5:B:136:THR:HB	5:B:137:TYR:CA	2.33	0.59
5:B:211:VAL:O	5:B:480:SER:HA	2.03	0.59
7:E:135:PHE:HB3	7:E:140:LEU:HD11	1.84	0.59
5:B:287:ARG:CG	5:B:287:ARG:HH11	2.11	0.59
5:B:507:LYS:O	5:B:508:LEU:HB2	2.01	0.59
5:B:732:SER:HB2	5:B:734:HIS:CD2	2.38	0.59
4:A:326:ARG:HG3	4:A:1406:VAL:HG11	1.85	0.58
6:C:67:LEU:HD11	6:C:155:LEU:HD13	1.85	0.58
5:B:411:PRO:HA	5:B:414:ALA:HB3	1.84	0.58
4:A:215:SER:HB3	4:A:218:ASP:CG	2.24	0.58
4:A:573:SER:O	4:A:576:GLN:HB2	2.04	0.58
4:A:675:THR:O	4:A:679:ILE:HG13	2.04	0.58
5:B:72:GLU:OE1	5:B:72:GLU:C	2.42	0.58
4:A:1116:LEU:HD13	4:A:1329:THR:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:248:SER:O	5:B:249:ARG:HB2	2.01	0.58
5:B:370:PHE:HD2	5:B:373:ARG:HG3	1.68	0.58
12:K:81:TYR:HE2	12:K:86:ALA:HB2	1.68	0.58
5:B:139:ALA:N	5:B:140:ILE:CA	2.63	0.58
5:B:142:VAL:HG13	5:B:144:GLY:HA3	0.66	0.58
4:A:1422:ARG:HH21	5:B:1220:ARG:HD2	1.68	0.58
4:A:618:GLU:HG3	4:A:620:LYS:H	1.69	0.58
5:B:834:ASN:HB3	5:B:840:ILE:HD12	1.86	0.58
5:B:977:GLY:H	5:B:1099:VAL:HG21	1.69	0.58
5:B:1073:TYR:N	5:B:1073:TYR:CD1	2.70	0.58
5:B:361:LEU:O	5:B:363:HIS:O	2.22	0.58
5:B:504:ARG:HD2	5:B:505:ASP:N	2.18	0.58
5:B:610:ASN:HB3	5:B:613:VAL:HG23	1.86	0.58
4:A:1339:LEU:CD1	7:E:147:HIS:CD2	2.87	0.58
7:E:64:PRO:HB3	7:E:75:MET:HG3	1.86	0.58
4:A:148:CYS:SG	4:A:167:CYS:HB3	2.44	0.58
4:A:874:ASP:HA	4:A:1058:VAL:HG23	1.86	0.57
5:B:1106:ARG:HG3	5:B:1107:ALA:N	2.18	0.57
4:A:255:SER:C	4:A:257:ARG:HA	2.23	0.57
4:A:549:MET:SD	4:A:577:ILE:HD13	2.44	0.57
5:B:89:GLU:HB2	5:B:90:ILE:O	2.04	0.57
5:B:1084:GLN:HE22	6:C:192:TRP:N	2.02	0.57
9:H:47:PHE:HB3	9:H:95:TYR:HD1	1.69	0.57
4:A:622:VAL:HG22	4:A:622:VAL:O	2.04	0.57
11:J:2:ILE:HG23	11:J:3:VAL:O	2.04	0.57
4:A:672:ASP:H	4:A:736:ASN:HD21	1.52	0.57
5:B:839:MET:CE	5:B:980:PHE:HB2	2.34	0.57
11:J:32:GLU:O	11:J:36:LEU:HD23	2.04	0.57
4:A:767:GLN:HG3	4:A:768:GLN:N	2.20	0.57
5:B:71:LEU:C	5:B:71:LEU:CD1	2.71	0.57
4:A:483:ASP:HA	5:B:988:GLY:HA2	1.87	0.57
6:C:147:LEU:HB3	6:C:151:GLN:HB2	1.87	0.57
2:T:16:DC:H2'	2:T:17:DG:C8	2.40	0.57
2:T:18:DC:C3'	2:T:19:DT:H5'	2.34	0.57
4:A:55:ASP:O	4:A:57:ARG:N	2.38	0.57
5:B:176:SER:O	5:B:182:SER:HB3	2.04	0.57
4:A:466:SER:HB3	5:B:1103:ILE:HD11	1.87	0.57
4:A:793:SER:HB2	4:A:794:PRO:HD2	1.86	0.57
5:B:287:ARG:NH1	5:B:324:ILE:O	2.38	0.57
6:C:66:ARG:NE	11:J:2:ILE:HG21	2.19	0.57
4:A:240:PRO:HG2	5:B:1209:ALA:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:195:CYS:HB3	5:B:782:LEU:HD22	1.86	0.57
4:A:1128:GLN:HB3	4:A:1304:TRP:NE1	2.20	0.57
5:B:504:ARG:C	5:B:504:ARG:HD2	2.25	0.57
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.86	0.56
2:T:8:DT:H2"	2:T:9:DA:C8	2.39	0.56
4:A:253:ASN:ND2	4:A:253:ASN:O	2.38	0.56
5:B:90:ILE:O	5:B:90:ILE:HG22	2.04	0.56
5:B:881:ASN:HB2	5:B:933:SER:OG	2.05	0.56
5:B:69:LEU:HG	5:B:70:ILE:CB	2.25	0.56
7:E:42:PHE:HZ	7:E:58:MET:CE	2.18	0.56
4:A:265:LYS:HD3	4:A:313:GLN:HE22	1.69	0.56
5:B:1004:GLU:O	6:C:177:GLU:HG2	2.05	0.56
4:A:1161:THR:HG22	4:A:1163:ILE:N	2.20	0.56
5:B:502:ILE:HG22	5:B:503:GLY:H	1.70	0.56
2:T:23:DC:C4	2:T:24:DT:H73	2.40	0.56
5:B:837:ASP:HB3	5:B:1020:ARG:HH22	1.70	0.56
5:B:174:LEU:HD22	5:B:204:ILE:HD11	1.88	0.56
5:B:756:ILE:HG12	5:B:770:GLN:CG	2.35	0.56
4:A:1364:ASN:HD21	4:A:1366:ARG:HG2	1.64	0.56
4:A:335:ARG:HA	4:A:339:ASN:HB2	1.88	0.56
5:B:70:ILE:O	5:B:71:LEU:CG	2.53	0.56
4:A:357:PRO:HD2	5:B:833:TYR:CZ	2.41	0.56
5:B:975:GLN:HG2	5:B:976:ILE:N	2.20	0.56
11:J:7:CYS:HB2	11:J:49:MET:HG2	1.86	0.56
4:A:446:ARG:HB2	4:A:487:MET:CE	2.33	0.56
4:A:68:GLN:HG3	4:A:68:GLN:O	2.05	0.56
12:K:61:TYR:HA	12:K:72:LYS:O	2.05	0.56
4:A:380:VAL:HG23	4:A:430:TRP:O	2.06	0.56
5:B:798:TYR:HE2	11:J:2:ILE:CG2	2.15	0.56
5:B:805:THR:HG22	5:B:809:MET:SD	2.46	0.56
9:H:81:PRO:HB3	9:H:82:PRO:HD2	1.87	0.56
9:H:104:PHE:CE1	9:H:136:LYS:HG3	2.41	0.56
9:H:81:PRO:CB	9:H:82:PRO:CD	2.83	0.56
6:C:8:VAL:HG11	12:K:105:PHE:HD1	1.70	0.56
5:B:471:LYS:O	5:B:471:LYS:HD2	2.06	0.55
4:A:531:ILE:HG13	4:A:653:VAL:HG21	1.87	0.55
4:A:868:TYR:HE1	4:A:1064:VAL:CG1	2.13	0.55
5:B:142:VAL:HG21	5:B:145:ARG:CG	2.36	0.55
5:B:248:SER:H	5:B:418:LYS:HZ2	1.54	0.55
5:B:654:ARG:H	5:B:657:HIS:CD2	2.20	0.55
5:B:217:ARG:NH1	5:B:407:ASP:OD1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:482:VAL:O	5:B:483:LEU:C	2.43	0.55
2:T:1:DC:H2'	2:T:2:DT:C7	2.37	0.55
4:A:841:LEU:HD21	4:A:1105:LEU:HD21	1.88	0.55
5:B:269:ILE:HD11	5:B:386:LEU:HD21	1.89	0.55
4:A:1017:LEU:HB2	7:E:205:SER:HA	1.87	0.55
4:A:1053:PHE:O	4:A:1056:SER:N	2.36	0.55
5:B:408:LEU:HD22	5:B:545:ILE:HD13	1.88	0.55
5:B:71:LEU:N	5:B:71:LEU:HD12	2.21	0.55
6:C:7:GLN:HB2	6:C:23:SER:HB2	1.87	0.55
5:B:72:GLU:OE1	5:B:73:GLN:HG2	2.05	0.55
5:B:975:GLN:N	5:B:978:ASP:OD2	2.40	0.55
5:B:848:ARG:NH1	11:J:8:PHE:O	2.33	0.55
12:K:49:GLU:HG3	12:K:94:ILE:HG13	1.89	0.55
4:A:116:ASP:HB2	4:A:118:HIS:HD2	1.71	0.55
6:C:166:GLU:HG3	12:K:10:PHE:HZ	1.71	0.55
5:B:797:TYR:O	11:J:1:MET:HG2	2.06	0.55
12:K:58:PHE:HB3	12:K:76:GLN:HB3	1.87	0.55
2:T:16:DC:C2'	2:T:17:DG:C8	2.90	0.55
2:T:5:DC:H2''	2:T:6:DG:C8	2.42	0.55
4:A:775:ILE:HG13	4:A:798:GLY:HA3	1.89	0.55
10:I:17:ARG:HH12	10:I:28:GLU:CD	2.10	0.55
1:R:9:G:N2	2:T:20:DC:O2	2.40	0.55
5:B:944:THR:HG21	5:B:1122:ARG:HH12	1.71	0.55
5:B:801:LYS:O	11:J:52:THR:HG23	2.07	0.55
2:T:27:DA:C6	4:A:252:PHE:HE1	2.25	0.55
4:A:1364:ASN:ND2	4:A:1366:ARG:H	2.06	0.55
5:B:1017:ILE:HB	5:B:1018:PRO:HD3	1.88	0.55
5:B:119:LEU:HD22	5:B:953:LEU:HD11	1.88	0.55
2:T:5:DC:C2	2:T:6:DG:C5	2.95	0.55
4:A:249:SER:O	4:A:250:ILE:HG12	2.07	0.54
5:B:363:HIS:O	5:B:364:ILE:HB	2.07	0.54
5:B:978:ASP:HB2	5:B:980:PHE:HE1	1.72	0.54
4:A:828:ALA:HB1	5:B:530:GLY:HA2	1.88	0.54
6:C:66:ARG:NH2	11:J:3:VAL:O	2.39	0.54
9:H:2:SER:HB3	9:H:62:SER:OG	2.07	0.54
2:T:1:DC:H2''	2:T:2:DT:C6	2.42	0.54
5:B:504:ARG:C	5:B:504:ARG:CD	2.73	0.54
6:C:226:ASP:O	6:C:227:THR:HB	2.07	0.54
4:A:821:ARG:HB2	4:A:821:ARG:HH11	1.71	0.54
5:B:504:ARG:CD	5:B:505:ASP:N	2.69	0.54
7:E:205:SER:OG	7:E:205:SER:O	2.19	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1017:LEU:CD1	7:E:206:GLY:H	2.13	0.54
5:B:803:LEU:H	5:B:822:ASN:HD21	1.54	0.54
4:A:886:ILE:HD11	4:A:943:LEU:HB3	1.89	0.54
5:B:292:ILE:HD11	5:B:327:ARG:HG2	1.89	0.54
5:B:515:HIS:H	5:B:518:HIS:HD2	1.53	0.54
5:B:70:ILE:C	5:B:70:ILE:CD1	2.76	0.54
9:H:89:LEU:HB2	9:H:91:ASP:OD2	2.07	0.54
4:A:523:ILE:HG22	4:A:528:LEU:HD23	1.90	0.54
5:B:765:PRO:O	5:B:768:THR:HB	2.07	0.54
4:A:512:VAL:HA	4:A:519:PRO:HA	1.90	0.54
4:A:541:ILE:HD11	4:A:577:ILE:HG12	1.87	0.54
4:A:669:THR:O	4:A:762:SER:HB3	2.08	0.54
4:A:901:LEU:N	4:A:926:GLN:HE21	2.03	0.54
5:B:141:ASP:O	5:B:142:VAL:CB	2.49	0.54
4:A:778:GLY:HA3	5:B:516:ASN:ND2	2.23	0.54
6:C:252:GLN:HG3	12:K:95:ILE:HG23	1.88	0.54
4:A:440:ASP:O	4:A:460:VAL:HG23	2.08	0.54
4:A:559:VAL:HG12	4:A:559:VAL:O	2.07	0.54
7:E:153:HIS:O	7:E:154:ILE:HD13	2.08	0.54
5:B:119:LEU:HD22	5:B:953:LEU:CD1	2.37	0.53
6:C:22:LEU:HD22	6:C:25:VAL:HG21	1.90	0.53
1:R:9:G:C8	1:R:9:G:H5"	2.44	0.53
4:A:248:PRO:O	4:A:260:ASP:HB2	2.07	0.53
6:C:18:VAL:HG23	6:C:240:VAL:HB	1.90	0.53
1:R:10:A:H2	2:T:19:DT:O2	1.90	0.53
4:A:1363:VAL:HG12	4:A:1364:ASN:N	2.23	0.53
4:A:567:LYS:HG3	4:A:568:PRO:HD2	1.90	0.53
5:B:373:ARG:HA	5:B:566:LEU:HD23	1.91	0.53
3:N:9:DC:C4	3:N:10:DG:C6	2.97	0.53
4:A:836:TYR:CZ	4:A:840:ARG:HD2	2.42	0.53
5:B:142:VAL:CG2	5:B:145:ARG:HH11	2.22	0.53
4:A:1328:TYR:CZ	4:A:1350:LYS:HD3	2.44	0.53
4:A:668:ASP:HB3	4:A:743:VAL:HG23	1.91	0.53
5:B:370:PHE:CD2	5:B:373:ARG:HG3	2.44	0.53
4:A:849:MET:CE	4:A:1061:GLY:HA2	2.37	0.53
4:A:471:ASN:O	4:A:474:VAL:HG12	2.09	0.53
5:B:911:ILE:HG21	5:B:966:VAL:HG11	1.89	0.53
5:B:815:ARG:HB2	5:B:816:GLU:OE2	2.08	0.53
5:B:976:ILE:HG23	5:B:977:GLY:N	2.24	0.53
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.90	0.53
12:K:65:HIS:HD2	12:K:67:PHE:HB2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:582:ILE:HD12	4:A:629:LEU:HD11	1.90	0.53
5:B:142:VAL:CG2	5:B:145:ARG:HG2	2.38	0.53
5:B:825:VAL:HG22	5:B:1010:LEU:HB3	1.90	0.53
5:B:969:ARG:HH21	6:C:59:ALA:HB1	1.73	0.53
4:A:1156:PRO:O	4:A:1158:PRO:HD3	2.09	0.53
4:A:67:CYS:O	4:A:70:CYS:SG	2.67	0.53
5:B:692:TYR:N	5:B:692:TYR:HD2	2.06	0.53
6:C:73:GLN:NE2	6:C:75:MET:HB2	2.24	0.53
4:A:1149:ALA:HA	10:I:47:GLU:HA	1.91	0.53
4:A:1364:ASN:ND2	4:A:1366:ARG:HH11	2.06	0.53
7:E:72:PHE:H	7:E:73:PRO:CA	2.19	0.53
12:K:81:TYR:CE2	12:K:86:ALA:HB2	2.44	0.53
5:B:344:LYS:HA	5:B:345:LYS:CB	2.37	0.52
5:B:692:TYR:CD2	5:B:692:TYR:N	2.77	0.52
5:B:899:ILE:CG2	5:B:949:VAL:HG21	2.32	0.52
5:B:978:ASP:OD1	5:B:1098:MET:HB3	2.09	0.52
6:C:233:GLU:HG2	6:C:234:SER:H	1.74	0.52
5:B:521:LEU:CD2	5:B:635:ARG:HD3	2.39	0.52
9:H:95:TYR:HE2	9:H:97:MET:SD	2.32	0.52
2:T:8:DT:H2'	2:T:9:DA:C8	2.44	0.52
4:A:511:ILE:HG12	4:A:521:MET:HE3	1.90	0.52
5:B:69:LEU:CA	5:B:89:GLU:HG2	2.40	0.52
5:B:971:THR:OG1	6:C:61:GLU:HG3	2.09	0.52
6:C:229:TYR:CD1	6:C:229:TYR:N	2.77	0.52
8:F:101:ILE:HD13	8:F:120:ILE:HG22	1.91	0.52
4:A:1064:VAL:CG1	4:A:1370:LEU:HD22	2.39	0.52
5:B:345:LYS:N	5:B:348:ARG:H	2.07	0.52
4:A:901:LEU:HD12	4:A:926:GLN:HG2	1.92	0.52
5:B:1081:LEU:HD13	5:B:1085:ILE:HD11	1.90	0.52
5:B:344:LYS:HB3	5:B:345:LYS:C	2.29	0.52
5:B:70:ILE:HA	5:B:89:GLU:CD	2.29	0.52
5:B:760:ASP:OD1	5:B:760:ASP:N	2.43	0.52
2:T:6:DG:H1	3:N:9:DC:H42	1.56	0.52
1:R:10:A:C2	2:T:19:DT:O2	2.63	0.52
4:A:855:THR:HG23	4:A:857:ARG:HG3	1.91	0.52
5:B:333:PHE:H	5:B:334:ILE:HB	1.75	0.52
8:F:111:LEU:H	8:F:111:LEU:HD12	1.74	0.52
4:A:464:PRO:O	4:A:465:TYR:HB2	2.09	0.52
11:J:6:ARG:HA	11:J:12:LYS:O	2.09	0.52
4:A:1017:LEU:HD12	7:E:206:GLY:N	2.18	0.52
4:A:829:VAL:HG12	4:A:830:LYS:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1016:ALA:HB1	5:B:1020:ARG:HH21	1.74	0.52
5:B:238:ALA:HB3	5:B:256:VAL:HB	1.92	0.52
2:T:24:DT:OP1	5:B:857:ARG:NH2	2.43	0.52
2:T:18:DC:C4'	2:T:19:DT:OP1	2.57	0.52
4:A:499:ALA:C	4:A:501:LEU:H	2.12	0.51
6:C:40:GLU:HA	6:C:163:ILE:HG23	1.92	0.51
8:F:76:LYS:O	8:F:79:ARG:NE	2.42	0.51
9:H:5:LEU:HD22	9:H:133:ASN:O	2.10	0.51
4:A:567:LYS:HB3	9:H:96:VAL:H	1.76	0.51
4:A:567:LYS:HG3	4:A:568:PRO:CG	2.39	0.51
4:A:714:PHE:O	4:A:718:VAL:HG23	2.09	0.51
5:B:63:ILE:O	5:B:67:SER:HB2	2.10	0.51
4:A:1055:ARG:HD3	8:F:155:LEU:O	2.10	0.51
4:A:894:GLU:C	4:A:896:ARG:H	2.12	0.51
2:T:22:DT:OP2	5:B:1121:GLY:HA2	2.10	0.51
4:A:302:THR:OG1	4:A:306:ASN:HB3	2.11	0.51
4:A:853:ASP:C	4:A:855:THR:H	2.13	0.51
5:B:510:LYS:CD	5:B:511:PRO:HD2	2.41	0.51
4:A:1348:LEU:O	4:A:1352:VAL:HG23	2.11	0.51
4:A:344:ARG:HA	5:B:1129:ARG:HA	1.92	0.51
4:A:523:ILE:HG23	4:A:527:THR:HB	1.93	0.51
5:B:569:TYR:CE1	5:B:589:VAL:HG21	2.46	0.51
8:F:93:ILE:HD11	8:F:134:ILE:HD11	1.92	0.51
3:N:1:DC:O5'	3:N:1:DC:H6	1.93	0.51
2:T:19:DT:C2'	2:T:20:DC:C5'	2.81	0.51
4:A:330:LYS:HG2	4:A:331:GLY:N	2.26	0.51
4:A:728:LYS:O	4:A:732:LEU:HB2	2.11	0.51
5:B:526:GLU:HG3	5:B:771:SER:HB3	1.93	0.51
4:A:899:VAL:HB	4:A:929:LEU:HD12	1.91	0.51
5:B:788:ARG:NH1	5:B:790:ASP:OD2	2.44	0.51
2:T:5:DC:C2	2:T:6:DG:C6	2.98	0.51
4:A:642:CYS:O	4:A:645:LEU:HB3	2.10	0.51
5:B:115:GLN:HG3	5:B:119:LEU:HD12	1.93	0.51
5:B:143:PRO:CB	5:B:144:GLY:CA	2.73	0.51
5:B:89:GLU:OE1	5:B:89:GLU:O	2.29	0.51
6:C:33:LEU:O	6:C:37:MET:HE2	2.11	0.51
4:A:1116:LEU:HB2	4:A:1308:THR:OG1	2.10	0.50
4:A:445:ASN:CB	4:A:455:MET:HG2	2.38	0.50
4:A:567:LYS:CG	4:A:568:PRO:CD	2.88	0.50
5:B:1084:GLN:HE22	6:C:191:TYR:CA	2.16	0.50
5:B:476:ARG:O	5:B:478:GLY:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:828:ALA:CB	5:B:530:GLY:HA2	2.41	0.50
5:B:142:VAL:HG21	5:B:145:ARG:HH11	1.76	0.50
5:B:542:MET:HE3	5:B:636:PRO:HG3	1.93	0.50
4:A:645:LEU:CD1	4:A:649:ILE:HD11	2.41	0.50
5:B:20:ASP:OD2	5:B:21:GLU:N	2.44	0.50
5:B:37:PHE:O	5:B:38:PHE:HB2	2.12	0.50
5:B:41:LYS:O	5:B:45:SER:HB3	2.12	0.50
9:H:59:ILE:HG12	9:H:142:LEU:HD12	1.93	0.50
4:A:544:ASP:HB2	12:K:47:ARG:NH2	2.26	0.50
13:L:60:ARG:HG3	13:L:61:THR:N	2.23	0.50
4:A:1397:LEU:O	4:A:1400:CYS:HB2	2.11	0.50
4:A:93:VAL:HG22	4:A:301:ALA:HA	1.93	0.50
4:A:840:ARG:NH2	4:A:1106:ASN:OD1	2.45	0.50
5:B:488:TYR:HE2	5:B:813:LYS:HB2	1.76	0.50
10:I:68:LEU:HD13	10:I:84:VAL:HG11	1.94	0.50
4:A:23:SER:HB2	4:A:233:TRP:CE2	2.46	0.50
5:B:502:ILE:H	5:B:502:ILE:CD1	2.22	0.50
5:B:839:MET:HE2	5:B:980:PHE:HB2	1.94	0.50
4:A:316:GLN:H	4:A:317:LYS:HB3	1.76	0.50
4:A:407:ARG:HD3	4:A:413:ILE:HD11	1.93	0.50
4:A:606:LEU:HD11	4:A:608:ILE:HD11	1.93	0.50
6:C:41:ILE:HG13	6:C:172:PRO:HG2	1.93	0.50
4:A:353:ILE:HD13	4:A:487:MET:SD	2.52	0.50
5:B:1017:ILE:HB	5:B:1018:PRO:CD	2.42	0.50
4:A:472:LEU:HD11	5:B:835:GLN:HB3	1.94	0.50
8:F:127:GLU:O	8:F:129:LYS:N	2.45	0.50
2:T:19:DT:H3'	2:T:19:DT:H6	1.77	0.50
4:A:249:SER:O	4:A:250:ILE:O	2.30	0.50
5:B:1051:THR:HG22	5:B:1053:GLU:H	1.76	0.50
5:B:113:TYR:O	5:B:114:PRO:C	2.50	0.50
5:B:260:GLY:O	5:B:267:ARG:HD3	2.11	0.50
5:B:25:ILE:CG2	5:B:29:ASP:HB2	2.41	0.50
7:E:31:THR:OG1	7:E:34:GLU:HB2	2.12	0.50
9:H:139:ASN:O	9:H:140:ALA:CB	2.59	0.50
5:B:801:LYS:O	11:J:52:THR:CG2	2.60	0.50
2:T:22:DT:H72	2:T:23:DC:C5	2.47	0.50
4:A:256:GLN:HA	4:A:257:ARG:HG3	1.93	0.49
4:A:257:ARG:O	4:A:258:GLY:O	2.30	0.49
4:A:446:ARG:HD2	4:A:478:TYR:O	2.12	0.49
4:A:907:THR:HG22	4:A:908:LEU:H	1.76	0.49
5:B:998:ASP:HB3	5:B:1076:HIS:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:732:SER:HB2	5:B:734:HIS:HD2	1.77	0.49
8:F:97:ARG:HD2	8:F:101:ILE:CD1	2.36	0.49
4:A:546:VAL:HG13	4:A:577:ILE:HG21	1.94	0.49
6:C:241:ASP:HB3	12:K:109:TRP:CZ2	2.47	0.49
4:A:596:THR:C	4:A:598:LEU:H	2.16	0.49
6:C:67:LEU:HA	6:C:70:ILE:CD1	2.42	0.49
4:A:557:ASP:OD2	4:A:559:VAL:HB	2.12	0.49
5:B:338:GLY:HA2	5:B:340:ALA:N	2.20	0.49
5:B:365:THR:HG21	5:B:370:PHE:HB2	1.95	0.49
5:B:542:MET:HG3	5:B:747:MET:HE2	1.92	0.49
5:B:706:GLN:O	5:B:710:LEU:HB2	2.12	0.49
11:J:7:CYS:HA	11:J:49:MET:HG2	1.94	0.49
6:C:35:ARG:HB2	12:K:41:THR:HG23	1.93	0.49
5:B:145:ARG:N	5:B:146:GLU:HB2	2.28	0.49
7:E:23:VAL:O	7:E:28:TYR:HB2	2.12	0.49
12:K:49:GLU:HG3	12:K:94:ILE:CG1	2.43	0.49
4:A:58:LEU:HD23	4:A:80:HIS:O	2.13	0.49
2:T:11:DG:H2'	2:T:12:DC:OP2	2.13	0.49
4:A:55:ASP:N	4:A:56:PRO:HD2	2.27	0.49
5:B:137:TYR:CE2	5:B:138:GLU:HG2	2.47	0.49
5:B:743:ILE:O	5:B:744:HIS:HB2	2.13	0.49
11:J:10:CYS:HB3	11:J:45:CYS:SG	2.52	0.49
4:A:562:THR:HG23	4:A:563:PRO:HD2	1.95	0.49
4:A:722:LEU:HD22	4:A:799:PHE:CG	2.48	0.49
2:T:15:DA:H4'	2:T:16:DC:OP1	2.13	0.49
2:T:23:DC:N4	2:T:24:DT:H73	2.28	0.49
4:A:754:SER:N	4:A:757:ASN:HD22	2.02	0.49
4:A:81:PHE:HE1	5:B:1209:ALA:HB2	1.77	0.49
5:B:636:PRO:CB	5:B:637:LEU:CA	2.76	0.49
1:R:2:U:H2'	1:R:3:C:H6	1.78	0.49
4:A:868:TYR:CE1	4:A:1064:VAL:HG21	2.48	0.49
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.46	0.49
3:N:7:DA:H2'	3:N:8:DT:C7	2.41	0.48
4:A:1105:LEU:HB3	4:A:1384:VAL:CG2	2.44	0.48
4:A:540:PHE:HB3	4:A:571:LEU:HD23	1.94	0.48
5:B:333:PHE:N	5:B:334:ILE:O	2.47	0.48
5:B:521:LEU:HD21	5:B:635:ARG:HD3	1.95	0.48
11:J:20:SER:HB3	11:J:39:LEU:HD21	1.95	0.48
4:A:1064:VAL:HG12	4:A:1370:LEU:CD2	2.42	0.48
4:A:323:LYS:O	4:A:324:SER:CB	2.61	0.48
4:A:450:LEU:H	4:A:450:LEU:CD1	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:666:ILE:HD11	5:B:1030:LEU:HD13	1.96	0.48
5:B:219:ALA:HB2	5:B:405:ARG:HG2	1.95	0.48
5:B:744:HIS:CD2	5:B:745:PRO:HD2	2.49	0.48
2:T:26:DG:N2	2:T:27:DA:H1'	2.28	0.48
4:A:1394:THR:HG22	4:A:1395:GLY:N	2.28	0.48
4:A:206:GLU:O	4:A:210:ILE:HG12	2.13	0.48
4:A:535:THR:HG23	4:A:575:LYS:HG2	1.94	0.48
4:A:894:GLU:O	4:A:896:ARG:N	2.45	0.48
7:E:64:PRO:O	7:E:65:THR:HG22	2.14	0.48
1:R:8:G:H1	2:T:21:DC:N4	2.11	0.48
4:A:548:ASN:HD21	12:K:47:ARG:CD	2.26	0.48
9:H:89:LEU:O	9:H:91:ASP:N	2.45	0.48
1:R:8:G:H1	2:T:21:DC:H42	1.61	0.48
4:A:508:PRO:O	4:A:511:ILE:HG13	2.14	0.48
4:A:901:LEU:HA	4:A:907:THR:HG23	1.94	0.48
5:B:527:THR:OG1	5:B:528:PRO:HD2	2.13	0.48
5:B:995:ARG:CZ	5:B:995:ARG:HB2	2.42	0.48
6:C:186:LEU:HB3	6:C:188:HIS:CD2	2.48	0.48
6:C:57:VAL:HG11	11:J:60:PHE:CB	2.28	0.48
9:H:94:ASP:N	9:H:94:ASP:OD1	2.47	0.48
3:N:5:DT:H2''	3:N:6:DT:OP2	2.14	0.48
5:B:214:ALA:O	5:B:498:THR:HA	2.14	0.48
5:B:843:GLN:HB2	5:B:993:THR:OG1	2.14	0.48
6:C:66:ARG:HE	11:J:2:ILE:CG1	2.25	0.48
10:I:68:LEU:HB3	10:I:84:VAL:CG1	2.41	0.48
4:A:1141:THR:CG2	4:A:1205:LYS:HD3	2.44	0.48
5:B:476:ARG:C	5:B:478:GLY:N	2.67	0.48
5:B:72:GLU:CD	5:B:73:GLN:CG	2.83	0.48
5:B:1023:VAL:HG12	5:B:1027:ILE:HD11	1.96	0.47
5:B:72:GLU:CG	5:B:73:GLN:H	2.27	0.47
6:C:239:PRO:HB2	6:C:241:ASP:OD1	2.14	0.47
1:R:5:A:H2'	1:R:6:G:C8	2.49	0.47
4:A:573:SER:H	4:A:576:GLN:HG3	1.78	0.47
4:A:661:GLY:O	4:A:662:PHE:HB2	2.15	0.47
5:B:756:ILE:O	5:B:759:PRO:HD3	2.14	0.47
12:K:63:VAL:HG23	12:K:63:VAL:O	2.14	0.47
2:T:18:DC:C3'	2:T:19:DT:H72	2.38	0.47
4:A:1027:ALA:O	4:A:1031:VAL:HG23	2.14	0.47
4:A:1120:LEU:HB3	4:A:1124:HIS:O	2.14	0.47
4:A:406:ILE:HB	4:A:431:LYS:HB2	1.95	0.47
4:A:438:ASP:HA	4:A:460:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:531:ILE:HD13	4:A:617:VAL:CG1	2.44	0.47
4:A:350:ARG:HB2	5:B:1128:LEU:HD11	1.97	0.47
5:B:642:ASP:O	5:B:644:GLU:N	2.32	0.47
5:B:71:LEU:HD13	5:B:72:GLU:HB2	1.96	0.47
4:A:159:THR:HA	4:A:160:GLN:HB2	1.96	0.47
5:B:1135:ARG:HG3	5:B:1147:LEU:HD21	1.97	0.47
5:B:256:VAL:HG12	5:B:385:LEU:HD22	1.96	0.47
4:A:158:PRO:HG2	4:A:160:GLN:NE2	2.30	0.47
4:A:847:ASP:N	4:A:847:ASP:OD1	2.34	0.47
8:F:152:ILE:N	8:F:152:ILE:HD12	2.30	0.47
2:T:12:DC:H2''	2:T:13:DA:C8	2.49	0.47
4:A:1436:ILE:O	4:A:1437:GLY:C	2.52	0.47
4:A:253:ASN:N	4:A:255:SER:HB2	2.26	0.47
4:A:947:PHE:CD2	4:A:954:TRP:CZ2	3.03	0.47
16:B:1308[A]:DGT:H5'	16:B:1308[A]:DGT:H8	1.97	0.47
4:A:618:GLU:O	4:A:622:VAL:HG12	2.15	0.47
5:B:142:VAL:HG21	5:B:145:ARG:HG2	1.97	0.47
7:E:42:PHE:HZ	7:E:58:MET:HE1	1.80	0.47
9:H:1:MET:CE	9:H:2:SER:OG	2.63	0.47
10:I:14:LEU:HB3	10:I:27:PHE:HB3	1.97	0.47
4:A:159:THR:CA	4:A:160:GLN:HB2	2.45	0.47
4:A:353:ILE:HG22	4:A:468:PHE:HB2	1.97	0.47
6:C:257:SER:HA	6:C:260:LEU:HG	1.96	0.47
7:E:67:GLU:CB	7:E:68:SER:CA	2.87	0.47
2:T:5:DC:H1'	2:T:6:DG:C8	2.50	0.47
4:A:1094:VAL:HA	4:A:1113:THR:HG21	1.96	0.47
4:A:1280:GLU:HB3	4:A:1281:ARG:H	1.59	0.47
4:A:1436:ILE:O	4:A:1438:THR:N	2.48	0.47
4:A:401:GLY:C	4:A:435:HIS:HD2	2.17	0.47
4:A:665:GLY:HA2	5:B:1086:PHE:CD1	2.50	0.47
5:B:501:PRO:CA	5:B:502:ILE:HD12	2.44	0.47
5:B:766:ARG:NH2	5:B:1020:ARG:HB3	2.30	0.47
6:C:99:LEU:N	6:C:157:CYS:O	2.39	0.47
5:B:69:LEU:CB	5:B:70:ILE:CB	2.83	0.47
9:H:2:SER:HB3	9:H:62:SER:CB	2.45	0.47
4:A:1397:LEU:HB2	4:A:1426:GLU:HG2	1.97	0.47
5:B:530:GLY:O	5:B:531:GLN:C	2.54	0.47
6:C:56:THR:HG21	6:C:145:CYS:SG	2.55	0.47
11:J:5:VAL:O	11:J:6:ARG:O	2.33	0.47
12:K:47:ARG:HD2	12:K:60:ALA:HA	1.97	0.47
4:A:672:ASP:HB3	4:A:675:THR:OG1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:484:ASN:HD22	5:B:484:ASN:C	2.19	0.46
4:A:1349:TYR:HB2	4:A:1372:VAL:HG21	1.98	0.46
4:A:567:LYS:O	4:A:569:LYS:N	2.48	0.46
4:A:690:VAL:CG2	4:A:718:VAL:HG13	2.45	0.46
5:B:378:LEU:O	5:B:382:ILE:HG12	2.16	0.46
5:B:698:GLU:HA	5:B:701:ILE:CD1	2.46	0.46
6:C:46:ILE:HG21	6:C:157:CYS:HB3	1.97	0.46
10:I:101:PHE:HE1	10:I:112:SER:HB3	1.79	0.46
4:A:1155:ASP:OD1	4:A:1162:VAL:HG23	2.15	0.46
4:A:215:SER:O	4:A:218:ASP:HB2	2.16	0.46
4:A:532:ARG:HH12	4:A:745:GLN:HE21	1.62	0.46
4:A:568:PRO:CB	6:C:221:TYR:CE1	2.98	0.46
5:B:283:VAL:HG21	5:B:321:GLY:HA3	1.96	0.46
5:B:291:ILE:N	5:B:291:ILE:HD12	2.31	0.46
4:A:947:PHE:HE2	7:E:203:GLU:HB2	1.80	0.46
4:A:568:PRO:HB3	6:C:221:TYR:CE1	2.50	0.46
4:A:587:HIS:NE2	4:A:969:GLN:HG2	2.31	0.46
5:B:1020:ARG:NH1	16:B:1308[A]:DGT:O1B	2.45	0.46
4:A:1352:VAL:O	4:A:1355:VAL:HG12	2.15	0.46
4:A:294:SER:O	4:A:298:PHE:HB2	2.16	0.46
5:B:315:LYS:N	5:B:316:PRO:HD2	2.31	0.46
5:B:493:SER:HB3	5:B:751:VAL:HB	1.96	0.46
5:B:864:LYS:HD3	5:B:870:ILE:O	2.16	0.46
7:E:61:GLN:HB3	7:E:79:TRP:HE3	1.81	0.46
4:A:109:HIS:CD2	4:A:169:ASN:HD21	2.33	0.46
4:A:253:ASN:ND2	4:A:253:ASN:C	2.68	0.46
4:A:821:ARG:HB2	4:A:821:ARG:NH1	2.30	0.46
5:B:984:HIS:HE1	5:B:1028:GLU:OE2	1.98	0.46
5:B:72:GLU:C	5:B:72:GLU:CD	2.73	0.46
4:A:26:GLU:O	4:A:27:VAL:C	2.53	0.46
4:A:424:ILE:HD12	4:A:424:ILE:O	2.15	0.46
5:B:258:LEU:HB2	5:B:385:LEU:HD21	1.97	0.46
5:B:615:MET:HG2	5:B:626:ILE:HG23	1.98	0.46
5:B:634:TYR:CE1	5:B:692:TYR:HD1	2.31	0.46
4:A:567:LYS:NZ	9:H:95:TYR:CZ	2.70	0.46
12:K:92:ASN:HA	12:K:95:ILE:HD12	1.97	0.46
5:B:102:VAL:HG23	5:B:112:LEU:HD22	1.97	0.46
5:B:145:ARG:CA	5:B:146:GLU:HB2	2.45	0.46
2:T:13:DA:C2	3:N:2:DT:O2	2.69	0.46
2:T:22:DT:H3'	2:T:22:DT:H6	1.80	0.46
4:A:1155:ASP:OD2	4:A:1161:THR:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:855:THR:HG21	4:A:857:ARG:HE	1.81	0.46
5:B:142:VAL:HG11	5:B:144:GLY:C	2.36	0.46
5:B:544:CYS:HB2	5:B:634:TYR:CZ	2.51	0.46
4:A:1111:MET:HG3	4:A:1114:PRO:HG3	1.96	0.45
4:A:296:LEU:O	4:A:296:LEU:HG	2.16	0.45
4:A:800:VAL:HA	4:A:812:GLU:HG2	1.98	0.45
5:B:1157:ALA:H	5:B:1197:PRO:HA	1.82	0.45
5:B:142:VAL:HG11	5:B:144:GLY:CA	2.34	0.45
2:T:6:DG:N2	2:T:7:DA:C2	2.84	0.45
5:B:108:VAL:HG12	5:B:109:THR:H	1.81	0.45
5:B:841:MET:HG2	5:B:846:ILE:HD11	1.96	0.45
8:F:93:ILE:CD1	8:F:134:ILE:HD11	2.46	0.45
9:H:104:PHE:CZ	9:H:136:LYS:HA	2.52	0.45
9:H:84:ALA:HA	9:H:87:ARG:HB2	1.98	0.45
1:R:6:G:H2'	1:R:7:A:C8	2.52	0.45
4:A:365:GLY:O	4:A:468:PHE:HA	2.15	0.45
4:A:662:PHE:O	5:B:828:ALA:HA	2.16	0.45
5:B:176:SER:O	5:B:182:SER:CB	2.63	0.45
5:B:783:THR:CG2	5:B:783:THR:O	2.62	0.45
6:C:148:ARG:H	6:C:151:GLN:HG3	1.81	0.45
4:A:361:LEU:HD22	4:A:646:PHE:CD1	2.51	0.45
5:B:72:GLU:OE1	5:B:73:GLN:CG	2.64	0.45
5:B:741:CYS:SG	5:B:742:GLU:N	2.89	0.45
4:A:662:PHE:HD2	5:B:829:CYS:SG	2.39	0.45
6:C:31:ASN:O	6:C:34:ARG:HB3	2.16	0.45
12:K:65:HIS:CD2	12:K:67:PHE:H	2.29	0.45
4:A:1194:ARG:HH21	4:A:1237:ILE:HD13	1.80	0.45
4:A:455:MET:CE	5:B:1134:GLU:HB3	2.46	0.45
5:B:1119:VAL:O	5:B:1126:GLY:HA3	2.16	0.45
5:B:212:LEU:HD21	5:B:461:LEU:HD11	1.99	0.45
5:B:361:LEU:N	5:B:362:PRO:HD3	2.32	0.45
11:J:32:GLU:O	11:J:36:LEU:CD2	2.64	0.45
2:T:16:DC:H2''	2:T:17:DG:C8	2.51	0.45
2:T:19:DT:C6	2:T:20:DC:C5	3.04	0.45
4:A:672:ASP:H	4:A:736:ASN:ND2	2.11	0.45
5:B:100:PRO:HA	5:B:126:SER:HB3	1.99	0.45
7:E:68:SER:HA	7:E:69:ILE:HA	1.65	0.45
12:K:57:LEU:HB2	12:K:76:GLN:HG2	1.98	0.45
4:A:1239:ARG:HH12	4:A:1241:ARG:HH12	1.64	0.45
4:A:765:VAL:HG22	4:A:800:VAL:HB	1.98	0.45
4:A:897:TYR:CD2	4:A:936:LEU:HD13	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1072:MET:HB2	5:B:1085:ILE:HD12	1.99	0.45
7:E:75:MET:CB	7:E:76:GLY:CA	2.94	0.45
9:H:80:ARG:HA	9:H:81:PRO:HD3	1.66	0.45
4:A:1127:ASP:HB3	4:A:1130:GLN:HB3	1.99	0.45
4:A:691:LEU:HD11	4:A:695:LYS:HZ1	1.81	0.45
5:B:1134:GLU:CD	5:B:1134:GLU:N	2.70	0.45
5:B:326:ASP:OD1	5:B:329:THR:OG1	2.33	0.45
4:A:1154:TYR:CE1	10:I:18:GLU:HG3	2.52	0.45
4:A:241:VAL:HA	4:A:242:PRO:HD2	1.86	0.45
4:A:873:MET:HG2	4:A:957:PRO:HG3	1.98	0.45
5:B:1013:ASN:OD1	5:B:1014:PRO:HD2	2.17	0.45
5:B:193:LYS:HB3	5:B:787:VAL:HG11	1.99	0.45
5:B:292:ILE:H	5:B:293:PRO:HD3	1.82	0.45
8:F:99:LEU:O	8:F:99:LEU:HD13	2.17	0.45
4:A:40:THR:HG22	4:A:41:MET:HG3	1.99	0.45
4:A:901:LEU:HB2	4:A:926:GLN:HG2	1.98	0.45
4:A:981:LEU:HD13	4:A:986:ILE:HD11	1.98	0.45
5:B:826:ALA:O	5:B:1011:ILE:HA	2.17	0.45
5:B:1074:ASN:OD1	5:B:1076:HIS:HB2	2.17	0.45
5:B:373:ARG:HD3	5:B:567:GLU:OE2	2.16	0.45
5:B:898:LEU:HD11	5:B:964:VAL:HG21	1.98	0.45
12:K:77:THR:HG21	12:K:81:TYR:HD2	1.82	0.45
4:A:1392:SER:O	4:A:1394:THR:N	2.49	0.44
4:A:457:ALA:O	4:A:507:VAL:HG23	2.17	0.44
5:B:338:GLY:CA	5:B:340:ALA:H	2.23	0.44
5:B:476:ARG:C	5:B:478:GLY:H	2.20	0.44
5:B:510:LYS:HA	5:B:510:LYS:HD3	1.66	0.44
4:A:915:SER:O	4:A:919:ILE:CG1	2.64	0.44
5:B:145:ARG:CB	5:B:146:GLU:CB	2.77	0.44
5:B:836:GLU:O	5:B:837:ASP:OD2	2.35	0.44
4:A:1364:ASN:HD22	4:A:1366:ARG:H	1.64	0.44
4:A:1448:GLU:HA	4:A:1449:SER:HA	1.49	0.44
4:A:447:GLN:HG2	5:B:1134:GLU:OE2	2.17	0.44
5:B:472:ALA:HB3	5:B:473:MET:CE	2.47	0.44
5:B:830:TYR:CE2	5:B:1000:PRO:HD3	2.52	0.44
6:C:46:ILE:O	6:C:169:LYS:HE3	2.17	0.44
7:E:179:GLN:OE1	7:E:179:GLN:HA	2.18	0.44
11:J:2:ILE:HA	11:J:2:ILE:HD12	1.68	0.44
3:N:8:DT:C2'	3:N:9:DC:O5'	2.56	0.44
2:T:20:DC:H4'	4:A:447:GLN:OE1	2.17	0.44
4:A:35:ILE:HG13	4:A:241:VAL:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1073:TYR:N	5:B:1073:TYR:HD1	2.16	0.44
4:A:265:LYS:NZ	4:A:322:VAL:HB	2.31	0.44
4:A:360:GLU:HB2	4:A:363:GLN:OE1	2.18	0.44
4:A:391:LEU:O	4:A:394:ASN:N	2.51	0.44
4:A:65:LEU:O	4:A:71:GLN:HA	2.18	0.44
5:B:286:PHE:HB3	5:B:297:ILE:CD1	2.44	0.44
7:E:69:ILE:O	7:E:70:SER:HB2	2.18	0.44
4:A:322:VAL:HB	4:A:323:LYS:H	1.56	0.44
5:B:473:MET:C	5:B:475:SER:H	2.21	0.44
5:B:71:LEU:O	5:B:71:LEU:HD12	2.15	0.44
5:B:850:LEU:HB2	11:J:8:PHE:CG	2.53	0.44
4:A:443:LEU:HD11	4:A:455:MET:HB3	2.00	0.44
5:B:333:PHE:O	5:B:333:PHE:CD1	2.70	0.44
5:B:428:ILE:HD11	5:B:448:ILE:HA	2.00	0.44
5:B:800:GLN:HB3	11:J:52:THR:HG22	1.99	0.44
6:C:46:ILE:H	6:C:46:ILE:HG12	1.57	0.44
4:A:1151:GLU:HG2	10:I:45:ARG:HG3	2.00	0.44
4:A:548:ASN:HD21	12:K:47:ARG:NE	2.16	0.44
4:A:1399:ARG:NH1	4:A:1408:ILE:HD12	2.33	0.44
4:A:107:CYS:CA	4:A:171:GLN:HE21	2.19	0.44
5:B:114:PRO:HB2	5:B:118:ARG:NH2	2.32	0.44
5:B:323:VAL:C	5:B:324:ILE:HG13	2.38	0.44
5:B:802:PRO:HB3	5:B:1091:TYR:CG	2.53	0.44
8:F:97:ARG:NH1	8:F:100:GLN:OE1	2.51	0.44
11:J:1:MET:N	11:J:56:LEU:H	2.16	0.44
12:K:20:LYS:HB2	12:K:20:LYS:NZ	2.33	0.44
2:T:15:DA:H1'	2:T:16:DC:O5'	2.17	0.44
4:A:255:SER:HB2	4:A:256:GLN:C	2.38	0.44
4:A:313:GLN:HG2	4:A:314:ALA:H	1.83	0.44
5:B:287:ARG:HA	5:B:291:ILE:O	2.17	0.44
5:B:333:PHE:N	5:B:334:ILE:HB	2.31	0.44
7:E:205:SER:O	7:E:207:ARG:N	2.50	0.44
4:A:11:LEU:HD13	5:B:1195:HIS:HD2	1.81	0.43
4:A:456:MET:HB2	4:A:478:TYR:OH	2.18	0.43
4:A:524:VAL:HG12	4:A:525:GLN:HG3	2.00	0.43
4:A:577:ILE:H	4:A:577:ILE:HG13	1.57	0.43
5:B:291:ILE:HG22	5:B:297:ILE:HD13	2.00	0.43
5:B:377:PHE:C	5:B:379:GLY:H	2.20	0.43
5:B:507:LYS:O	5:B:507:LYS:HG3	2.18	0.43
5:B:800:GLN:O	5:B:1091:TYR:HE1	2.00	0.43
7:E:81:GLU:HB3	7:E:96:PHE:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1345:ARG:HG3	4:A:1376:THR:HG21	1.99	0.43
4:A:247:ARG:N	4:A:248:PRO:HD3	2.33	0.43
4:A:754:SER:O	4:A:757:ASN:HB2	2.18	0.43
4:A:908:LEU:O	4:A:909:ASP:C	2.56	0.43
4:A:983:ILE:HG22	4:A:983:ILE:O	2.17	0.43
5:B:1013:ASN:HD21	5:B:1015:HIS:HD2	1.66	0.43
5:B:240:ILE:HG23	5:B:240:ILE:O	2.18	0.43
4:A:1064:VAL:HG12	4:A:1064:VAL:O	2.18	0.43
4:A:51:GLY:CA	4:A:56:PRO:HG3	2.39	0.43
5:B:570:VAL:HA	5:B:571:PRO:HD3	1.77	0.43
5:B:70:ILE:C	5:B:70:ILE:HD12	2.39	0.43
4:A:93:VAL:CG2	4:A:301:ALA:HA	2.49	0.43
4:A:618:GLU:HG3	4:A:619:LYS:N	2.33	0.43
4:A:11:LEU:HA	5:B:1193:GLN:O	2.18	0.43
5:B:213:ILE:O	5:B:215:GLN:HG2	2.18	0.43
5:B:504:ARG:CD	5:B:505:ASP:H	2.28	0.43
5:B:526:GLU:HG2	5:B:538:ASN:ND2	2.33	0.43
5:B:519:TRP:CZ2	5:B:705:MET:HE1	2.45	0.43
5:B:913:GLY:HA2	5:B:938:SER:OG	2.18	0.43
2:T:19:DT:H2"	2:T:20:DC:C4'	2.47	0.43
4:A:244:PRO:HB2	4:A:245:PRO:CD	2.48	0.43
4:A:401:GLY:O	4:A:435:HIS:HD2	1.96	0.43
5:B:142:VAL:CG2	5:B:143:PRO:CD	2.67	0.43
5:B:475:SER:O	5:B:477:ALA:N	2.51	0.43
5:B:72:GLU:CG	5:B:73:GLN:N	2.78	0.43
8:F:83:PRO:HB2	8:F:152:ILE:HD13	1.98	0.43
4:A:1369:ALA:O	4:A:1373:ASP:HB2	2.18	0.43
4:A:407:ARG:HG2	4:A:430:TRP:CZ2	2.53	0.43
5:B:412:LEU:HA	5:B:412:LEU:HD23	1.58	0.43
2:T:21:DC:H2"	2:T:22:DT:OP2	2.19	0.43
5:B:142:VAL:CG1	5:B:144:GLY:C	2.86	0.43
2:T:9:DA:N1	3:N:7:DA:C2	2.87	0.43
4:A:9:ALA:HA	4:A:10:PRO:HD3	1.89	0.43
4:A:1267:MET:HA	4:A:1271:ILE:HG12	2.01	0.43
4:A:1093:LYS:HD2	4:A:1281:ARG:NH2	2.34	0.43
4:A:1390:ASN:O	4:A:1399:ARG:HD2	2.19	0.43
4:A:315:LEU:HA	4:A:316:GLN:HA	1.81	0.43
4:A:840:ARG:HE	4:A:1385:THR:HG23	1.84	0.43
6:C:66:ARG:CZ	11:J:2:ILE:HG23	2.38	0.43
4:A:1117:THR:N	4:A:1328:TYR:O	2.47	0.43
4:A:253:ASN:HA	4:A:254:GLU:HA	1.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:316:GLN:N	4:A:317:LYS:HB3	2.34	0.43
4:A:323:LYS:O	4:A:324:SER:HB3	2.19	0.43
5:B:100:PRO:N	5:B:126:SER:HB3	2.34	0.43
4:A:1410:PHE:HD1	5:B:1212:ILE:HD11	1.84	0.43
4:A:444:PHE:HE2	4:A:470:LEU:CD2	2.32	0.43
4:A:586:ILE:HD13	4:A:586:ILE:HA	1.86	0.43
5:B:1134:GLU:CD	5:B:1134:GLU:H	2.21	0.43
5:B:416:LEU:HD11	5:B:460:ALA:HB3	2.01	0.43
5:B:882:THR:HB	5:B:934:LYS:O	2.19	0.43
5:B:944:THR:HG21	5:B:1122:ARG:NH1	2.33	0.43
5:B:839:MET:HE1	5:B:980:PHE:HB2	2.00	0.43
11:J:6:ARG:H	11:J:14:VAL:H	1.66	0.43
4:A:321:PRO:O	4:A:322:VAL:HG13	2.19	0.42
5:B:142:VAL:CG2	5:B:145:ARG:CG	2.97	0.42
5:B:185:THR:OG1	5:B:188:ASP:OD2	2.37	0.42
5:B:416:LEU:HD13	5:B:457:LEU:HD23	2.00	0.42
5:B:506:GLY:O	5:B:507:LYS:HB3	2.19	0.42
5:B:642:ASP:HB3	5:B:649:LYS:HG3	2.01	0.42
5:B:654:ARG:HA	5:B:654:ARG:HD3	1.84	0.42
5:B:998:ASP:HB3	5:B:1076:HIS:HE1	1.84	0.42
7:E:94:LYS:HE2	7:E:94:LYS:HA	2.01	0.42
4:A:1394:THR:HG22	4:A:1395:GLY:H	1.84	0.42
4:A:99:ILE:HG13	4:A:234:MET:SD	2.59	0.42
5:B:334:ILE:HD13	5:B:335:GLY:O	2.19	0.42
5:B:428:ILE:HD13	5:B:428:ILE:HA	1.86	0.42
5:B:510:LYS:HD2	5:B:511:PRO:HD2	2.01	0.42
6:C:8:VAL:HG11	12:K:105:PHE:CD1	2.53	0.42
4:A:1101:LEU:HG	4:A:1105:LEU:CD1	2.49	0.42
4:A:982:THR:C	4:A:984:LYS:N	2.73	0.42
5:B:1212:ILE:O	5:B:1214:PRO:HD3	2.18	0.42
5:B:137:TYR:CG	5:B:138:GLU:N	2.87	0.42
5:B:344:LYS:O	5:B:347:LYS:HB2	2.18	0.42
5:B:377:PHE:O	5:B:380:TYR:N	2.51	0.42
5:B:450:ALA:O	5:B:452:THR:N	2.51	0.42
5:B:809:MET:HA	5:B:812:LEU:HB2	2.01	0.42
5:B:488:TYR:CE2	5:B:813:LYS:HB2	2.53	0.42
5:B:850:LEU:HB2	11:J:8:PHE:CD1	2.54	0.42
4:A:482:PHE:O	5:B:989:THR:HG23	2.19	0.42
1:R:8:G:N2	2:T:22:DT:C4	2.86	0.42
2:T:12:DC:C2'	2:T:13:DA:C8	3.02	0.42
4:A:156:ASP:HA	4:A:157:ASP:HA	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:599:SER:OG	4:A:614:PHE:CD2	2.67	0.42
4:A:760:GLN:HG2	4:A:765:VAL:HA	2.02	0.42
5:B:189:LEU:HA	5:B:189:LEU:HD23	1.81	0.42
5:B:291:ILE:HG12	5:B:300:HIS:CD2	2.54	0.42
5:B:333:PHE:H	5:B:334:ILE:CA	2.32	0.42
5:B:89:GLU:N	5:B:89:GLU:OE2	2.35	0.42
6:C:100:THR:CG2	6:C:102:GLN:HE21	2.32	0.42
8:F:93:ILE:HD11	8:F:134:ILE:CD1	2.49	0.42
2:T:18:DC:H2'	2:T:19:DT:C5	2.55	0.42
5:B:144:GLY:HA2	5:B:145:ARG:HA	1.49	0.42
5:B:48:LEU:HD23	5:B:48:LEU:HA	1.78	0.42
5:B:834:ASN:HB2	5:B:839:MET:HA	2.02	0.42
5:B:848:ARG:HH22	5:B:996:ARG:HH12	1.63	0.42
9:H:44:VAL:O	9:H:44:VAL:HG12	2.20	0.42
6:C:66:ARG:CZ	11:J:2:ILE:HG13	2.39	0.42
12:K:36:GLU:O	12:K:37:LYS:C	2.57	0.42
12:K:77:THR:CG2	12:K:81:TYR:HD2	2.32	0.42
4:A:367:PRO:HG2	4:A:370:ILE:HD12	2.00	0.42
4:A:405:VAL:HG23	4:A:415:LEU:HD11	2.02	0.42
4:A:535:THR:HG21	4:A:617:VAL:H	1.84	0.42
5:B:386:LEU:O	5:B:390:LEU:HD12	2.19	0.42
5:B:507:LYS:O	5:B:508:LEU:CB	2.68	0.42
2:T:20:DC:H2'	2:T:21:DC:H5''	1.63	0.42
4:A:253:ASN:CA	4:A:255:SER:CB	2.74	0.42
5:B:600:LEU:HD23	5:B:600:LEU:HA	1.71	0.42
6:C:262:LEU:HD11	12:K:87:LEU:HD23	2.01	0.42
4:A:1174:PHE:HA	4:A:1175:SER:HA	1.62	0.42
4:A:335:ARG:HE	4:A:335:ARG:HB2	1.63	0.42
4:A:518:LYS:HB2	4:A:519:PRO:CD	2.48	0.42
4:A:544:ASP:HB2	12:K:47:ARG:HH21	1.85	0.42
5:B:164:LYS:NZ	5:B:443:ASN:HB3	2.35	0.42
5:B:603:LEU:HB3	5:B:609:ILE:HG12	2.01	0.42
5:B:610:ASN:OD1	5:B:612:GLU:HB3	2.20	0.42
5:B:71:LEU:HD22	5:B:72:GLU:HG2	2.02	0.42
9:H:44:VAL:HG13	9:H:48:PRO:HA	2.01	0.42
9:H:91:ASP:HA	9:H:93:TYR:HD1	1.85	0.42
4:A:1029:ARG:HG3	4:A:1029:ARG:HH11	1.85	0.42
4:A:351:THR:CG2	4:A:352:VAL:N	2.71	0.42
5:B:142:VAL:HG13	5:B:143:PRO:N	2.33	0.42
6:C:246:ARG:O	6:C:250:THR:OG1	2.33	0.42
7:E:71:LYS:HB3	7:E:75:MET:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1060:PRO:HD2	8:F:86:THR:HG21	2.02	0.42
4:A:152:VAL:HA	4:A:153:PRO:HA	1.77	0.42
4:A:15:LYS:HD3	4:A:15:LYS:HA	1.84	0.42
5:B:482:VAL:C	5:B:483:LEU:O	2.58	0.42
4:A:153:PRO:O	4:A:161:LEU:HA	2.21	0.41
4:A:414:ASP:OD1	4:A:416:ARG:HG2	2.19	0.41
4:A:512:VAL:HG12	4:A:512:VAL:O	2.18	0.41
4:A:455:MET:HE1	5:B:1134:GLU:HB3	2.02	0.41
5:B:560:GLU:O	5:B:561:TRP:CD1	2.72	0.41
2:T:5:DC:H2''	2:T:6:DG:N7	2.35	0.41
4:A:1015:VAL:O	4:A:1016:THR:C	2.58	0.41
4:A:316:GLN:HB3	4:A:317:LYS:HB3	2.00	0.41
4:A:366:VAL:HA	4:A:367:PRO:HD2	1.83	0.41
4:A:853:ASP:O	4:A:855:THR:N	2.53	0.41
5:B:552:MET:N	5:B:553:PRO:CD	2.83	0.41
5:B:744:HIS:HA	5:B:745:PRO:HD3	1.84	0.41
6:C:163:ILE:HD13	12:K:10:PHE:CE1	2.55	0.41
10:I:71:SER:HB3	10:I:85:PHE:CD2	2.55	0.41
4:A:1048:ASN:H	4:A:1048:ASN:HD22	1.69	0.41
4:A:86:LEU:HA	4:A:273:ASN:HD21	1.85	0.41
5:B:377:PHE:C	5:B:379:GLY:N	2.74	0.41
5:B:737:THR:HB	10:I:66:PRO:HB3	2.02	0.41
2:T:1:DC:H2'	2:T:2:DT:H71	2.02	0.41
4:A:1066:VAL:HG21	5:B:1139:ILE:HG21	2.02	0.41
4:A:1198:ASP:O	4:A:1202:MET:HG2	2.20	0.41
4:A:722:LEU:HD22	4:A:799:PHE:CD1	2.56	0.41
4:A:886:ILE:HG23	4:A:944:ARG:HG2	2.02	0.41
5:B:487:THR:HG22	5:B:488:TYR:H	1.86	0.41
5:B:804:GLY:O	5:B:983:ARG:NH2	2.53	0.41
7:E:56:LYS:HG3	7:E:84:ASP:OD1	2.20	0.41
9:H:93:TYR:CD2	9:H:145:ARG:HB3	2.56	0.41
4:A:313:GLN:HG2	4:A:314:ALA:N	2.36	0.41
4:A:924:LYS:HE3	4:A:924:LYS:HB2	1.86	0.41
5:B:510:LYS:HD3	5:B:511:PRO:HD2	2.03	0.41
4:A:871:ASP:HB3	7:E:204:THR:OG1	2.20	0.41
4:A:185:TRP:CZ3	4:A:200:ARG:HB3	2.55	0.41
4:A:825:ILE:HA	4:A:825:ILE:HD13	1.91	0.41
5:B:860:MET:SD	5:B:861:ASP:N	2.94	0.41
6:C:39:ALA:HA	6:C:164:ALA:HB3	2.02	0.41
6:C:44:LEU:HD12	6:C:160:LYS:O	2.21	0.41
7:E:190:LEU:HB3	7:E:214:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:822:ASN:HD22	11:J:52:THR:HG21	1.85	0.41
13:L:46:VAL:HB	13:L:47:ARG:H	1.64	0.41
2:T:23:DC:C4	2:T:24:DT:C7	3.03	0.41
5:B:1132:GLU:HG3	5:B:1132:GLU:H	1.66	0.41
8:F:96:THR:O	8:F:96:THR:HG22	2.21	0.41
9:H:102:TYR:OH	9:H:122:LEU:HD22	2.20	0.41
10:I:56:ALA:HB3	10:I:89:GLN:HG3	2.01	0.41
4:A:1363:VAL:HB	4:A:1368:MET:HE3	2.01	0.41
4:A:596:THR:C	4:A:598:LEU:N	2.74	0.41
4:A:929:LEU:HD21	4:A:983:ILE:CG2	2.51	0.41
4:A:1287:TYR:CD2	4:A:1305:VAL:HB	2.56	0.41
4:A:399:HIS:CB	4:A:400:PRO:HD3	2.49	0.41
4:A:531:ILE:HD13	4:A:617:VAL:HG11	2.01	0.41
5:B:142:VAL:HG13	5:B:144:GLY:N	2.26	0.41
4:A:711:ARG:HH12	10:I:95:THR:HB	1.86	0.41
5:B:345:LYS:H	5:B:348:ARG:N	2.13	0.41
5:B:500:THR:HA	5:B:501:PRO:HD3	1.85	0.41
5:B:523:CYS:SG	5:B:750:GLY:N	2.92	0.41
6:C:112:ASN:HD22	6:C:146:LYS:HG2	1.84	0.41
4:A:568:PRO:HB2	6:C:221:TYR:CE1	2.56	0.41
12:K:43:GLY:HA2	12:K:71:PHE:CE1	2.55	0.41
2:T:21:DC:C2	2:T:22:DT:C4	3.09	0.41
2:T:23:DC:H2'	2:T:23:DC:O2	2.21	0.41
4:A:407:ARG:HH11	4:A:413:ILE:HD11	1.86	0.41
5:B:623:GLU:OE1	5:B:625:LYS:HE2	2.21	0.41
5:B:519:TRP:CZ2	5:B:705:MET:CE	2.96	0.41
5:B:845:SER:HB3	5:B:850:LEU:HD22	2.03	0.41
5:B:975:GLN:CG	5:B:976:ILE:H	2.29	0.41
6:C:52:GLU:OE2	6:C:154:LYS:HG2	2.21	0.41
6:C:54:ASN:OD1	6:C:56:THR:OG1	2.39	0.41
12:K:57:LEU:HD21	12:K:78:THR:HG23	2.02	0.41
4:A:15:LYS:O	5:B:1220:ARG:NH1	2.54	0.40
4:A:382:PRO:CA	4:A:428:TYR:HE1	2.34	0.40
5:B:724:ASP:HA	5:B:725:PRO:HD3	1.96	0.40
5:B:973:ILE:HG22	5:B:974:PRO:HD2	2.02	0.40
6:C:226:ASP:O	6:C:227:THR:CB	2.69	0.40
13:L:55:ILE:O	13:L:56:LEU:HB2	2.21	0.40
4:A:249:SER:C	4:A:250:ILE:O	2.59	0.40
4:A:362:ASP:OD2	4:A:459:ARG:HD3	2.21	0.40
4:A:586:ILE:HG13	4:A:633:VAL:HG22	2.03	0.40
4:A:858:ASN:ND2	4:A:858:ASN:C	2.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:885:THR:HG22	4:A:940:ARG:HB2	2.03	0.40
5:B:321:GLY:C	5:B:323:VAL:H	2.24	0.40
5:B:778:MET:HE2	5:B:1094:ARG:CG	2.48	0.40
5:B:982:SER:HB3	5:B:1092:TYR:CE1	2.56	0.40
6:C:56:THR:CG2	6:C:147:LEU:HD23	2.51	0.40
6:C:162:GLY:HA3	6:C:170:TRP:CE2	2.57	0.40
7:E:164:LEU:HD13	7:E:211:TYR:CE2	2.56	0.40
10:I:68:LEU:HD23	10:I:68:LEU:HA	1.77	0.40
11:J:1:MET:O	11:J:2:ILE:O	2.39	0.40
2:T:5:DC:N3	2:T:6:DG:C6	2.89	0.40
5:B:128:LEU:HB2	5:B:167:ILE:O	2.21	0.40
5:B:174:LEU:HD12	5:B:174:LEU:HA	1.68	0.40
5:B:69:LEU:CB	5:B:70:ILE:CG2	2.98	0.40
5:B:842:ASN:O	5:B:846:ILE:HG13	2.22	0.40
6:C:97:VAL:HG21	6:C:129:ILE:HG23	2.03	0.40
10:I:65:ASP:HA	10:I:66:PRO:HD3	1.92	0.40
1:R:7:A:H5"	1:R:8:G:OP2	2.21	0.40
2:T:21:DC:H2"	2:T:22:DT:H71	2.02	0.40
4:A:1141:THR:HG21	4:A:1205:LYS:HD3	2.04	0.40
4:A:533:LYS:HE3	4:A:745:GLN:NE2	2.32	0.40
4:A:900:ASP:HA	4:A:926:GLN:NE2	2.37	0.40
5:B:1069:PHE:HA	5:B:1085:ILE:O	2.22	0.40
4:A:1428:VAL:HG22	5:B:1147:LEU:HD11	2.02	0.40
5:B:879:ARG:HB3	5:B:880:THR:H	1.39	0.40
5:B:884:ARG:O	5:B:936:ASP:HB3	2.21	0.40
7:E:204:THR:HG23	7:E:205:SER:N	2.36	0.40
8:F:124:GLU:O	8:F:130:ILE:HG13	2.21	0.40
4:A:1060:PRO:HD2	8:F:86:THR:CG2	2.51	0.40
12:K:40:HIS:O	12:K:41:THR:C	2.60	0.40
4:A:1366:ARG:H	4:A:1366:ARG:HG2	1.68	0.40
4:A:535:THR:HG21	4:A:617:VAL:HG23	2.03	0.40
5:B:1010:LEU:HA	5:B:1010:LEU:HD12	1.61	0.40
5:B:457:LEU:HA	5:B:457:LEU:HD23	1.97	0.40
7:E:190:LEU:HA	7:E:190:LEU:HD13	1.95	0.40
9:H:82:PRO:O	9:H:83:GLN:CB	2.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	1401/1733 (81%)	1186 (85%)	160 (11%)	55 (4%)	3	23
5	B	1129/1224 (92%)	938 (83%)	133 (12%)	58 (5%)	2	17
6	C	264/318 (83%)	226 (86%)	33 (12%)	5 (2%)	8	37
7	E	211/215 (98%)	176 (83%)	29 (14%)	6 (3%)	5	30
8	F	84/155 (54%)	74 (88%)	7 (8%)	3 (4%)	3	25
9	H	130/146 (89%)	104 (80%)	21 (16%)	5 (4%)	3	23
10	I	117/122 (96%)	95 (81%)	19 (16%)	3 (3%)	5	31
11	J	63/70 (90%)	55 (87%)	4 (6%)	4 (6%)	1	12
12	K	112/120 (93%)	102 (91%)	8 (7%)	2 (2%)	8	38
13	L	44/70 (63%)	30 (68%)	7 (16%)	7 (16%)	0	2
All	All	3555/4173 (85%)	2986 (84%)	421 (12%)	148 (4%)	3	22

All (148) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	50	ILE
4	A	55	ASP
4	A	56	PRO
4	A	250	ILE
4	A	312	PRO
4	A	321	PRO
4	A	322	VAL
4	A	335	ARG
4	A	399	HIS
4	A	424	ILE
4	A	609	ASP
4	A	854	ASN
4	A	1393	ASN
4	A	1446	ASP

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Mol	Chain	Res	Type
5	B	70	ILE
5	B	71	LEU
5	B	72	GLU
5	B	249	ARG
5	B	451	LYS
5	B	469	GLN
5	B	476	ARG
5	B	636	PRO
5	B	643	ASP
5	B	677	GLU
5	B	712	PRO
5	B	731	VAL
5	B	813	LYS
5	B	883	LEU
5	B	1156	ASP
5	B	1181	GLU
7	E	70	SER
7	E	72	PHE
7	E	206	GLY
10	I	3	THR
13	L	53	HIS
4	A	155	GLU
4	A	214	ILE
4	A	253	ASN
4	A	256	GLN
4	A	258	GLY
4	A	332	LYS
4	A	404	TYR
4	A	517	ASN
4	A	895	LYS
4	A	998	LEU
4	A	1403	GLU
4	A	1437	GLY
5	B	138	GLU
5	B	143	PRO
5	B	446	LEU
5	B	477	ALA
5	B	483	LEU
5	B	484	ASN
5	B	531	GLN
5	B	1096	ARG
8	F	128	LYS

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Mol	Chain	Res	Type
11	J	2	ILE
11	J	6	ARG
13	L	45	ALA
13	L	46	VAL
13	L	55	ILE
4	A	27	VAL
4	A	76	GLU
4	A	248	PRO
4	A	251	SER
4	A	324	SER
4	A	568	PRO
4	A	1173	HIS
4	A	1388	GLY
5	B	68	THR
5	B	69	LEU
5	B	142	VAL
5	B	146	GLU
5	B	277	LYS
5	B	322	PHE
5	B	338	GLY
5	B	367	LEU
5	B	468	GLU
5	B	474	SER
5	B	792	MET
5	B	1021	MET
5	B	1046	PRO
5	B	1165	ILE
6	C	214	ASN
6	C	215	GLU
7	E	64	PRO
9	H	81	PRO
9	H	82	PRO
9	H	128	ASN
9	H	140	ALA
10	I	47	GLU
12	K	37	LYS
12	K	50	LEU
13	L	50	ASP
4	A	152	VAL
4	A	178	GLY
4	A	245	PRO
4	A	926	GLN

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Mol	Chain	Res	Type
4	A	1448	GLU
5	B	65	GLU
5	B	540	SER
5	B	648	HIS
5	B	981	ALA
5	B	1017	ILE
5	B	1222	ARG
6	C	142	VAL
8	F	74	ILE
8	F	104	ASN
10	I	90	GLN
13	L	47	ARG
4	A	68	GLN
4	A	149	GLU
4	A	597	LEU
4	A	827	THR
4	A	846	GLU
4	A	958	VAL
4	A	1255	GLU
5	B	90	ILE
5	B	214	ALA
5	B	334	ILE
5	B	410	GLY
5	B	508	LEU
5	B	519	TRP
5	B	1171	VAL
6	C	90	ASP
6	C	227	THR
7	E	124	VAL
9	H	90	ALA
11	J	4	PRO
4	A	44	THR
4	A	51	GLY
4	A	1424	VAL
5	B	266	ALA
5	B	467	GLY
5	B	974	PRO
5	B	1097	HIS
11	J	5	VAL
13	L	56	LEU
4	A	153	PRO
7	E	51	GLY

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Mol	Chain	Res	Type
4	A	35	ILE
4	A	567	LYS
5	B	114	PRO
4	A	983	ILE
5	B	901	PRO
4	A	484	GLY
5	B	482	VAL
4	A	158	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	1233/1520 (81%)	1121 (91%)	112 (9%)	9	35
5	B	991/1061 (93%)	871 (88%)	120 (12%)	5	23
6	C	234/274 (85%)	214 (92%)	20 (8%)	10	38
7	E	195/197 (99%)	185 (95%)	10 (5%)	24	57
8	F	76/137 (56%)	70 (92%)	6 (8%)	12	41
9	H	118/128 (92%)	105 (89%)	13 (11%)	6	27
10	I	113/116 (97%)	101 (89%)	12 (11%)	6	29
11	J	60/65 (92%)	53 (88%)	7 (12%)	5	24
12	K	99/102 (97%)	86 (87%)	13 (13%)	4	20
13	L	40/57 (70%)	32 (80%)	8 (20%)	1	5
All	All	3159/3657 (86%)	2838 (90%)	321 (10%)	7	30

All (321) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	13	THR
4	A	22	PHE
4	A	23	SER
4	A	31	SER
4	A	32	VAL

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Mol	Chain	Res	Type
4	A	60	SER
4	A	69	THR
4	A	80	HIS
4	A	86	LEU
4	A	93	VAL
4	A	105	CYS
4	A	146	MET
4	A	147	VAL
4	A	222	LEU
4	A	237	THR
4	A	251	SER
4	A	252	PHE
4	A	253	ASN
4	A	259	GLU
4	A	265	LYS
4	A	266	LEU
4	A	270	LEU
4	A	322	VAL
4	A	332	LYS
4	A	335	ARG
4	A	359	LEU
4	A	375	THR
4	A	387	ARG
4	A	409	SER
4	A	434	ARG
4	A	437	MET
4	A	449	SER
4	A	450	LEU
4	A	454	SER
4	A	463	ILE
4	A	472	LEU
4	A	475	THR
4	A	501	LEU
4	A	509	LEU
4	A	513	SER
4	A	518	LYS
4	A	527	THR
4	A	531	ILE
4	A	550	LEU
4	A	566	ILE
4	A	573	SER
4	A	577	ILE

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Mol	Chain	Res	Type
4	A	595	THR
4	A	598	LEU
4	A	616	VAL
4	A	660	ASN
4	A	666	ILE
4	A	675	THR
4	A	702	LEU
4	A	709	THR
4	A	732	LEU
4	A	740	LEU
4	A	756	ILE
4	A	762	SER
4	A	773	LYS
4	A	774	ARG
4	A	775	ILE
4	A	783	THR
4	A	803	SER
4	A	805	LEU
4	A	809	THR
4	A	821	ARG
4	A	826	ASP
4	A	829	VAL
4	A	855	THR
4	A	858	ASN
4	A	871	ASP
4	A	880	LYS
4	A	884	ASP
4	A	896	ARG
4	A	902	LEU
4	A	913	LEU
4	A	922	ASP
4	A	929	LEU
4	A	948	VAL
4	A	982	THR
4	A	990	VAL
4	A	996	ASN
4	A	1001	ARG
4	A	1017	LEU
4	A	1025	ARG
4	A	1029	ARG
4	A	1047	SER
4	A	1067	LEU

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Mol	Chain	Res	Type
4	A	1077	THR
4	A	1113	THR
4	A	1118	VAL
4	A	1142	THR
4	A	1172	LEU
4	A	1215	ARG
4	A	1259	MET
4	A	1272	THR
4	A	1274	ARG
4	A	1280	GLU
4	A	1285	MET
4	A	1308	THR
4	A	1329	THR
4	A	1333	ILE
4	A	1335	ILE
4	A	1336	MET
4	A	1359	ASP
4	A	1366	ARG
4	A	1376	THR
4	A	1382	THR
4	A	1385	THR
4	A	1403	GLU
4	A	1449	SER
5	B	21	GLU
5	B	28	GLU
5	B	40	GLU
5	B	58	THR
5	B	63	ILE
5	B	70	ILE
5	B	71	LEU
5	B	72	GLU
5	B	73	GLN
5	B	89	GLU
5	B	90	ILE
5	B	94	LYS
5	B	98	THR
5	B	109	THR
5	B	110	HIS
5	B	120	ARG
5	B	134	LYS
5	B	141	ASP
5	B	142	VAL

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Mol	Chain	Res	Type
5	B	194	GLU
5	B	199	MET
5	B	217	ARG
5	B	225	VAL
5	B	234	ILE
5	B	239	GLU
5	B	250	PHE
5	B	264	SER
5	B	287	ARG
5	B	322	PHE
5	B	337	ARG
5	B	339	THR
5	B	343	ILE
5	B	365	THR
5	B	384	ARG
5	B	387	LEU
5	B	393	LYS
5	B	408	LEU
5	B	412	LEU
5	B	416	LEU
5	B	423	LYS
5	B	424	LEU
5	B	425	THR
5	B	452	THR
5	B	463	THR
5	B	469	GLN
5	B	471	LYS
5	B	473	MET
5	B	474	SER
5	B	479	VAL
5	B	482	VAL
5	B	483	LEU
5	B	484	ASN
5	B	485	ARG
5	B	487	THR
5	B	500	THR
5	B	502	ILE
5	B	504	ARG
5	B	505	ASP
5	B	510	LYS
5	B	513	GLN
5	B	537	LYS

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Mol	Chain	Res	Type
5	B	539	LEU
5	B	570	VAL
5	B	574	SER
5	B	591	ARG
5	B	628	THR
5	B	637	LEU
5	B	658	ILE
5	B	694	ASP
5	B	701	ILE
5	B	755	ILE
5	B	764	SER
5	B	791	THR
5	B	796	LEU
5	B	799	PRO
5	B	805	THR
5	B	812	LEU
5	B	827	ILE
5	B	831	SER
5	B	850	LEU
5	B	878	GLN
5	B	879	ARG
5	B	880	THR
5	B	883	LEU
5	B	886	LYS
5	B	889	THR
5	B	905	VAL
5	B	906	SER
5	B	916	THR
5	B	936	ASP
5	B	963	PHE
5	B	964	VAL
5	B	967	ARG
5	B	973	ILE
5	B	986	GLN
5	B	992	ILE
5	B	993	THR
5	B	999	MET
5	B	1007	VAL
5	B	1022	THR
5	B	1065	GLN
5	B	1073	TYR
5	B	1076	HIS

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Mol	Chain	Res	Type
5	B	1082	MET
5	B	1090	THR
5	B	1095	LEU
5	B	1097	HIS
5	B	1113	VAL
5	B	1115	THR
5	B	1124	ARG
5	B	1133	MET
5	B	1159	ARG
5	B	1165	ILE
5	B	1166	CYS
5	B	1191	ILE
5	B	1194	ILE
5	B	1196	ILE
5	B	1202	LEU
5	B	1218	THR
5	B	1220	ARG
6	C	22	LEU
6	C	25	VAL
6	C	26	ASP
6	C	33	LEU
6	C	40	GLU
6	C	41	ILE
6	C	66	ARG
6	C	77	ILE
6	C	99	LEU
6	C	137	LYS
6	C	140	ASN
6	C	143	LEU
6	C	157	CYS
6	C	186	LEU
6	C	189	THR
6	C	190	ASP
6	C	215	GLU
6	C	240	VAL
6	C	244	VAL
6	C	250	THR
7	E	9	ILE
7	E	65	THR
7	E	74	ASP
7	E	84	ASP
7	E	104	ASN

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Mol	Chain	Res	Type
7	E	127	ILE
7	E	156	LEU
7	E	159	ASP
7	E	165	LEU
7	E	169	ARG
8	F	97	ARG
8	F	104	ASN
8	F	120	ILE
8	F	123	LYS
8	F	125	LEU
8	F	133	VAL
9	H	2	SER
9	H	27	GLU
9	H	31	THR
9	H	32	THR
9	H	34	ASP
9	H	62	SER
9	H	78	SER
9	H	88	SER
9	H	89	LEU
9	H	91	ASP
9	H	94	ASP
9	H	111	LEU
9	H	136	LYS
10	I	5	ARG
10	I	10	CYS
10	I	11	ASN
10	I	12	ASN
10	I	24	ARG
10	I	30	ARG
10	I	59	VAL
10	I	62	ILE
10	I	81	ARG
10	I	83	ASN
10	I	88	SER
10	I	107	SER
11	J	2	ILE
11	J	7	CYS
11	J	14	VAL
11	J	20	SER
11	J	46	CYS
11	J	48	ARG

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Mol	Chain	Res	Type
11	J	64	ASN
12	K	1	MET
12	K	5	ASP
12	K	6	ARG
12	K	32	VAL
12	K	33	ILE
12	K	41	THR
12	K	42	LEU
12	K	47	ARG
12	K	56	VAL
12	K	89	ASN
12	K	93	SER
12	K	101	LEU
12	K	113	THR
13	L	27	LEU
13	L	42	ARG
13	L	46	VAL
13	L	48	CYS
13	L	51	CYS
13	L	61	THR
13	L	62	LYS
13	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	80	HIS
4	A	83	HIS
4	A	109	HIS
4	A	118	HIS
4	A	160	GLN
4	A	171	GLN
4	A	297	GLN
4	A	313	GLN
4	A	435	HIS
4	A	503	GLN
4	A	517	ASN
4	A	548	ASN
4	A	660	ASN
4	A	736	ASN
4	A	741	ASN
4	A	745	GLN

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Mol	Chain	Res	Type
4	A	757	ASN
4	A	786	HIS
4	A	858	ASN
4	A	926	GLN
4	A	965	GLN
4	A	996	ASN
4	A	1048	ASN
4	A	1265	ASN
4	A	1270	ASN
4	A	1278	ASN
4	A	1364	ASN
4	A	1432	GLN
5	B	73	GLN
5	B	121	ASN
5	B	325	GLN
5	B	366	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	686	ASN
5	B	734	HIS
5	B	744	HIS
5	B	794	ASN
5	B	822	ASN
5	B	878	GLN
5	B	975	GLN
5	B	984	HIS
5	B	986	GLN
5	B	1013	ASN
5	B	1015	HIS
5	B	1062	HIS
5	B	1076	HIS
5	B	1097	HIS
5	B	1161	HIS
5	B	1195	HIS
6	C	73	GLN
6	C	102	GLN
6	C	112	ASN

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Mol	Chain	Res	Type
6	C	242	GLN
7	E	61	GLN
7	E	147	HIS
9	H	131	ASN
9	H	137	GLN
9	H	139	ASN
10	I	12	ASN
10	I	83	ASN
12	K	65	HIS
12	K	89	ASN
12	K	110	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	9/10 (90%)	5 (55%)	1 (11%)

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	U
1	R	3	C
1	R	7	A
1	R	8	G
1	R	9	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	1	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 9 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
16	DGT	B	1308[A]	-	26,33,33	1.16	2 (7%)	32,52,52	1.97	9 (28%)
16	DGT	B	1308[B]	-	26,33,33	1.08	2 (7%)	32,52,52	1.92	6 (18%)

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
16	DGT	B	1308[A]	-	-	5/18/34/34	0/3/3/3
16	DGT	B	1308[B]	-	-	6/18/34/34	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	1308[A]	DGT	C6-C5	4.33	1.48	1.41
16	B	1308[B]	DGT	C6-C5	4.10	1.48	1.41
16	B	1308[A]	DGT	C5-C4	2.57	1.47	1.40
16	B	1308[B]	DGT	C5-C4	2.50	1.47	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	1308[B]	DGT	C6-C5-C4	-4.99	116.03	120.80
16	B	1308[A]	DGT	C6-C5-C4	-4.81	116.20	120.80
16	B	1308[B]	DGT	C2-N3-C4	4.28	120.24	115.36
16	B	1308[A]	DGT	C2-N3-C4	4.26	120.23	115.36
16	B	1308[A]	DGT	C6-N1-C2	4.24	122.66	115.93
16	B	1308[B]	DGT	C6-N1-C2	4.21	122.61	115.93
16	B	1308[B]	DGT	C5-C6-N1	-3.82	118.21	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	1308[A]	DGT	C5-C6-N1	-3.77	118.28	123.43
16	B	1308[A]	DGT	N3-C2-N1	-3.58	122.45	127.22
16	B	1308[B]	DGT	N3-C2-N1	-3.30	122.82	127.22
16	B	1308[A]	DGT	C2'-C1'-N9	-2.48	108.56	114.27
16	B	1308[A]	DGT	C2'-C3'-C4'	2.43	107.83	102.76
16	B	1308[B]	DGT	C4-C5-N7	-2.25	107.05	109.40
16	B	1308[A]	DGT	O5'-C5'-C4'	2.18	116.50	108.99
16	B	1308[A]	DGT	O4'-C1'-C2'	2.01	110.04	106.25

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	B	1308[B]	DGT	C5'-O5'-PA-O3A
16	B	1308[B]	DGT	C3'-C4'-C5'-O5'
16	B	1308[A]	DGT	C5'-O5'-PA-O2A
16	B	1308[A]	DGT	C4'-C5'-O5'-PA
16	B	1308[B]	DGT	O4'-C4'-C5'-O5'
16	B	1308[A]	DGT	O4'-C4'-C5'-O5'
16	B	1308[A]	DGT	C5'-O5'-PA-O3A
16	B	1308[B]	DGT	C4'-C5'-O5'-PA
16	B	1308[B]	DGT	C5'-O5'-PA-O1A
16	B	1308[B]	DGT	C5'-O5'-PA-O2A
16	B	1308[A]	DGT	C5'-O5'-PA-O1A

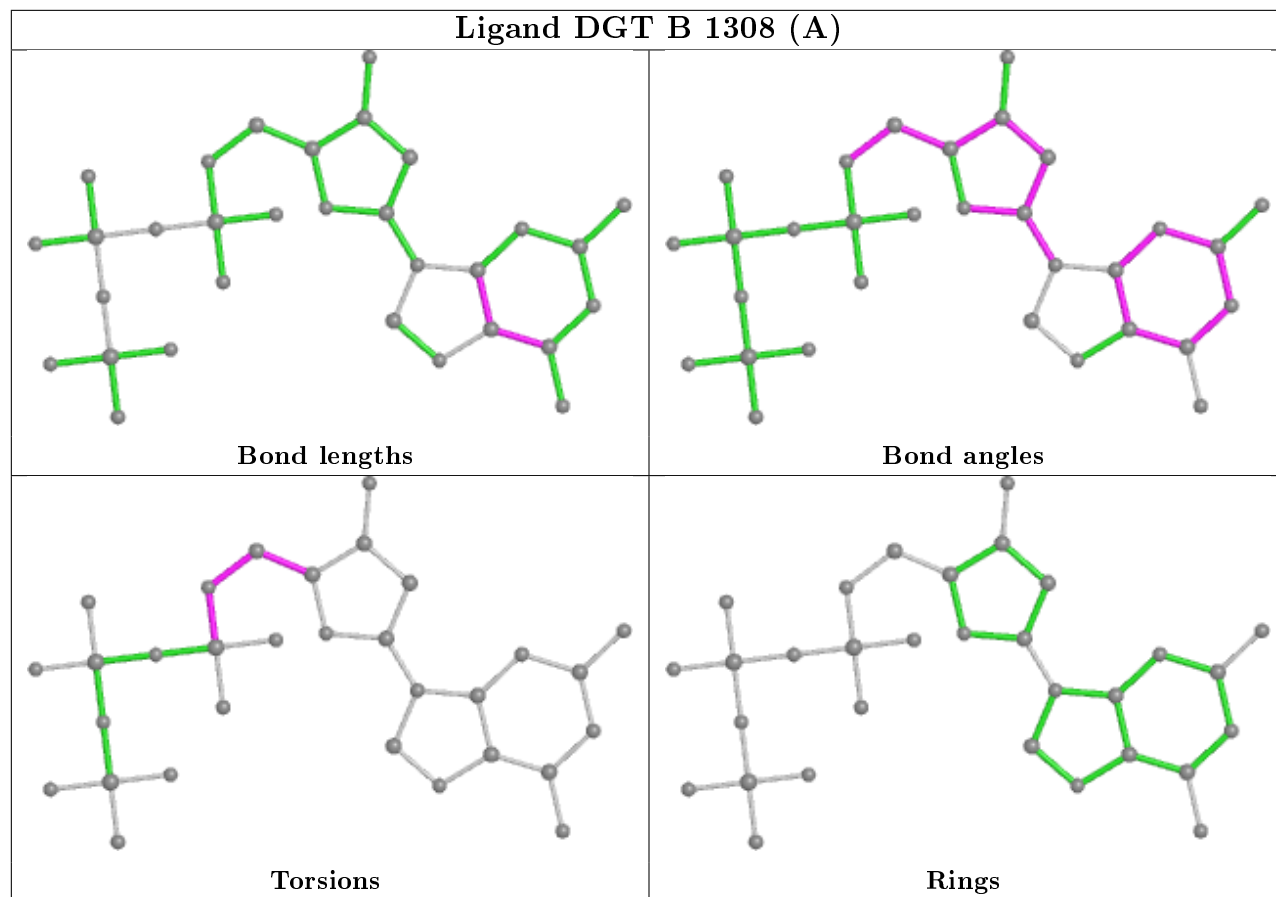
There are no ring outliers.

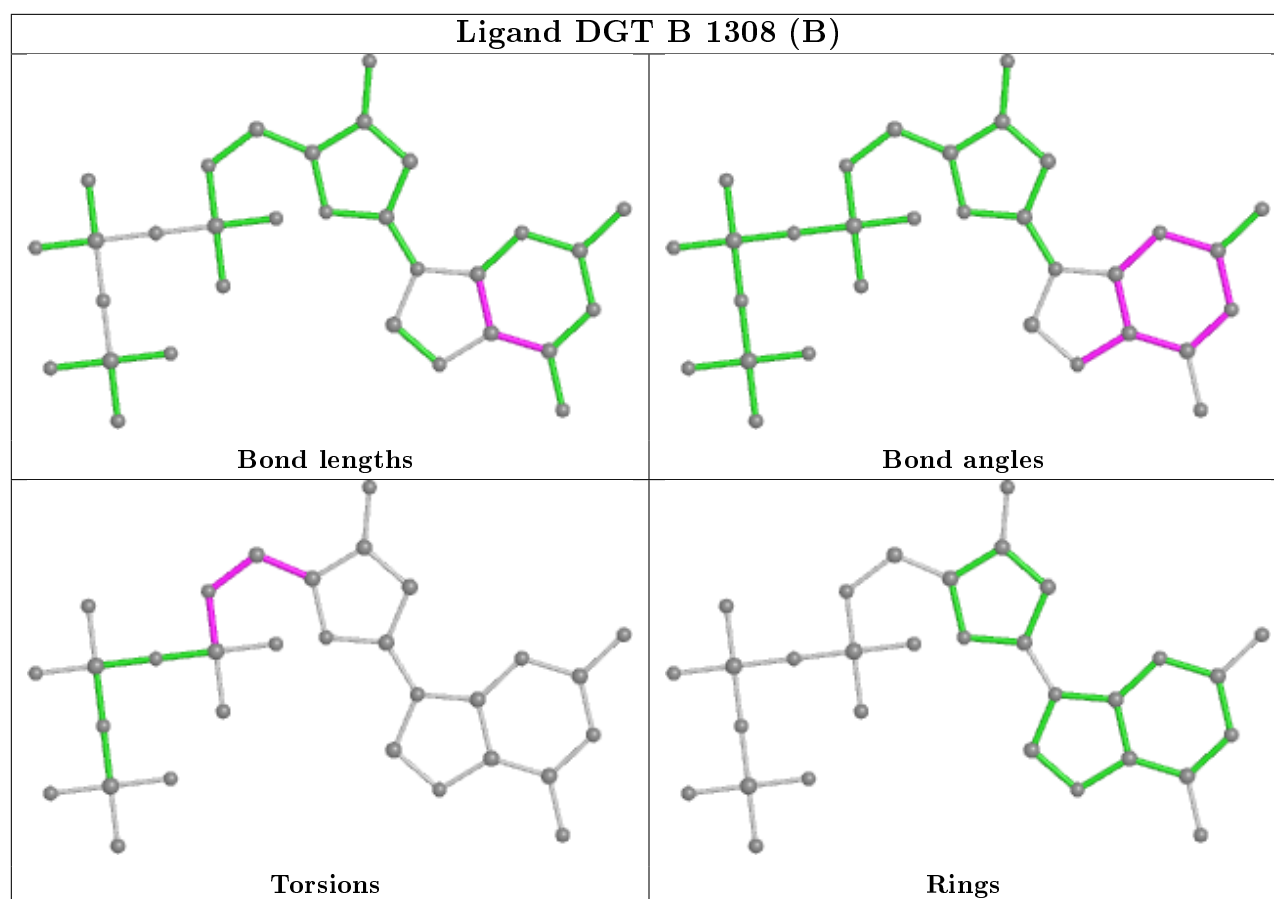
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1308[A]	DGT	2	0

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

equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	R	10/10 (100%)	0.03	1 (10%) 7 9	72, 93, 202, 234	0
2	T	28/28 (100%)	0.43	1 (3%) 42 42	118, 195, 427, 447	0
3	N	14/14 (100%)	0.44	1 (7%) 16 19	270, 338, 424, 426	0
4	A	1411/1733 (81%)	0.26	71 (5%) 28 29	56, 105, 206, 247	0
5	B	1143/1224 (93%)	0.14	39 (3%) 45 44	27, 88, 156, 185	0
6	C	266/318 (83%)	-0.12	0 100 100	59, 91, 135, 151	0
7	E	213/215 (99%)	0.35	14 (6%) 18 20	96, 142, 228, 233	0
8	F	86/155 (55%)	-0.01	1 (1%) 79 77	83, 117, 137, 141	0
9	H	134/146 (91%)	0.67	12 (8%) 9 12	35, 140, 171, 175	0
10	I	119/122 (97%)	0.04	0 100 100	85, 121, 156, 165	0
11	J	65/70 (92%)	-0.19	0 100 100	60, 82, 110, 117	0
12	K	114/120 (95%)	0.01	0 100 100	77, 102, 119, 122	0
13	L	46/70 (65%)	1.00	6 (13%) 3 5	87, 165, 176, 179	0
All	All	3649/4225 (86%)	0.20	146 (4%) 38 38	27, 103, 198, 447	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	L	26	THR	9.2
4	A	69	THR	8.0
4	A	152	VAL	7.6
4	A	144	THR	7.0
4	A	150	THR	6.3
4	A	72	GLU	6.1
13	L	27	LEU	5.8
4	A	1126	ALA	5.3
5	B	866	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
5	B	865	LYS	5.2
4	A	320	ARG	5.1
5	B	1224	PHE	5.1
4	A	151	ASP	4.8
5	B	474	SER	4.8
5	B	869	SER	4.7
4	A	105	CYS	4.6
4	A	311	GLN	4.6
7	E	121	MET	4.3
5	B	433	GLN	4.2
13	L	50	ASP	4.1
4	A	199	LEU	4.1
4	A	149	GLU	4.0
4	A	104	GLU	4.0
7	E	81	GLU	4.0
4	A	175	ARG	3.7
5	B	883	LEU	3.7
4	A	44	THR	3.7
5	B	1173	ALA	3.6
9	H	86	ASP	3.6
5	B	643	ASP	3.5
13	L	25	ALA	3.5
5	B	340	ALA	3.5
4	A	143	LYS	3.4
5	B	1223	ASP	3.4
4	A	91	PHE	3.4
4	A	66	LYS	3.4
4	A	182	VAL	3.4
4	A	286	HIS	3.3
4	A	161	LEU	3.3
4	A	165	GLY	3.3
9	H	137	GLN	3.3
4	A	145	LYS	3.3
4	A	114	LEU	3.3
4	A	115	LEU	3.2
5	B	429	PHE	3.2
5	B	341	LEU	3.2
4	A	317	LYS	3.1
4	A	315	LEU	3.1
4	A	139	TRP	3.0
4	A	312	PRO	3.0
7	E	82	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
9	H	83	GLN	3.0
4	A	1232	ASN	3.0
4	A	186	LYS	3.0
4	A	191	THR	3.0
4	A	106	VAL	3.0
5	B	1184	GLY	2.9
4	A	171	GLN	2.9
5	B	432	MET	2.9
5	B	666	TYR	2.9
5	B	92	PHE	2.9
4	A	42	ASP	2.9
5	B	646	LEU	2.9
9	H	112	ILE	2.9
4	A	103	CYS	2.9
4	A	1169	ILE	2.8
5	B	250	PHE	2.8
5	B	645	SER	2.8
9	H	139	ASN	2.8
4	A	1267	MET	2.8
7	E	69	ILE	2.7
5	B	339	THR	2.7
5	B	1221	SER	2.7
3	N	8	DT	2.7
4	A	45	GLN	2.7
5	B	73	GLN	2.7
5	B	356	LEU	2.7
1	R	1	A	2.7
7	E	83	CYS	2.7
4	A	426	LEU	2.7
7	E	102	GLU	2.6
4	A	50	ILE	2.6
9	H	140	ALA	2.6
9	H	51	ALA	2.6
5	B	1172	ILE	2.6
5	B	337	ARG	2.5
5	B	167	ILE	2.5
9	H	132	LEU	2.5
4	A	158	PRO	2.5
5	B	867	GLY	2.5
4	A	176	LYS	2.5
4	A	154	SER	2.5
4	A	53	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
4	A	179	LEU	2.5
4	A	1124	HIS	2.5
9	H	130	ARG	2.4
9	H	133	ASN	2.4
4	A	108	MET	2.4
9	H	82	PRO	2.4
4	A	1092	LYS	2.4
4	A	48	ALA	2.4
5	B	91	SER	2.4
9	H	114	VAL	2.3
4	A	146	MET	2.3
13	L	43	THR	2.3
5	B	71	LEU	2.3
5	B	708	GLU	2.3
4	A	153	PRO	2.3
4	A	1256	GLU	2.3
7	E	7	ARG	2.3
7	E	70	SER	2.3
4	A	141	LEU	2.3
5	B	509	ALA	2.3
4	A	1446	ASP	2.3
13	L	45	ALA	2.3
4	A	1447	GLU	2.2
7	E	109	ILE	2.2
4	A	322	VAL	2.2
2	T	3	DA	2.2
4	A	96	ILE	2.2
8	F	120	ILE	2.2
4	A	174	ILE	2.2
4	A	265	LYS	2.2
5	B	132	VAL	2.2
7	E	20	LYS	2.2
4	A	113	LEU	2.2
5	B	832	GLY	2.2
5	B	128	LEU	2.1
4	A	323	LYS	2.1
5	B	72	GLU	2.1
5	B	1175	LEU	2.1
4	A	190	ALA	2.1
5	B	868	MET	2.1
4	A	140	THR	2.1
5	B	89	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
7	E	132	ILE	2.1
4	A	1028	THR	2.1
4	A	164	ARG	2.1
4	A	928	LEU	2.0
4	A	112	LYS	2.0
4	A	57	ARG	2.0
4	A	314	ALA	2.0
4	A	157	ASP	2.0
7	E	43	LYS	2.0
7	E	96	PHE	2.0
7	E	110	PHE	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 carbohydrates in this entry.

6.4 Ligands [i](#)

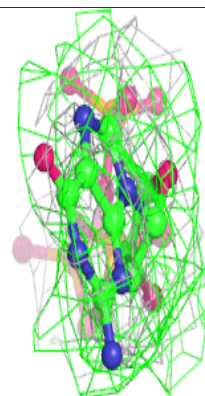
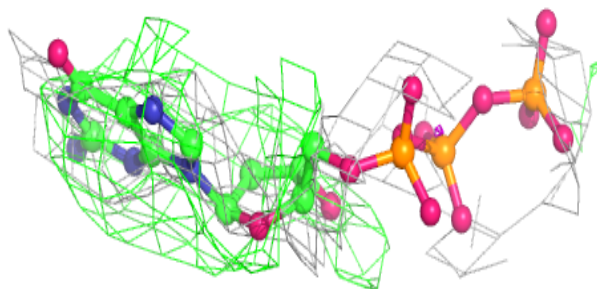
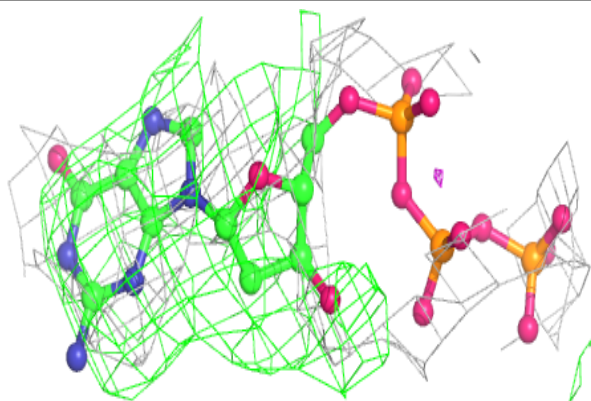
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	DGT	B	1308[B]	31/31	0.87	0.41	80,86,113,113	31
16	DGT	B	1308[A]	31/31	0.87	0.41	126,132,152,153	31
14	ZN	A	1735	1/1	0.94	0.10	139,139,139,139	0
14	ZN	A	1734	1/1	0.94	0.05	226,226,226,226	0
14	ZN	B	1307	1/1	0.97	0.13	143,143,143,143	0
14	ZN	I	203	1/1	0.97	0.15	131,131,131,131	0
15	MG	A	2001	1/1	0.98	0.38	116,116,116,116	0
14	ZN	L	105	1/1	0.98	0.07	190,190,190,190	0
14	ZN	C	319	1/1	0.99	0.10	95,95,95,95	0
14	ZN	J	101	1/1	0.99	0.13	105,105,105,105	0
14	ZN	I	204	1/1	0.99	0.12	106,106,106,106	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.

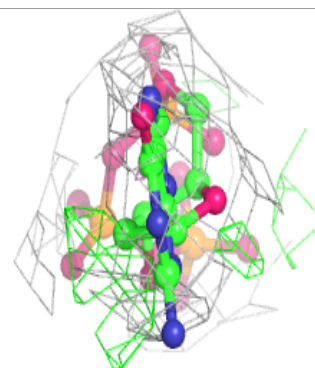
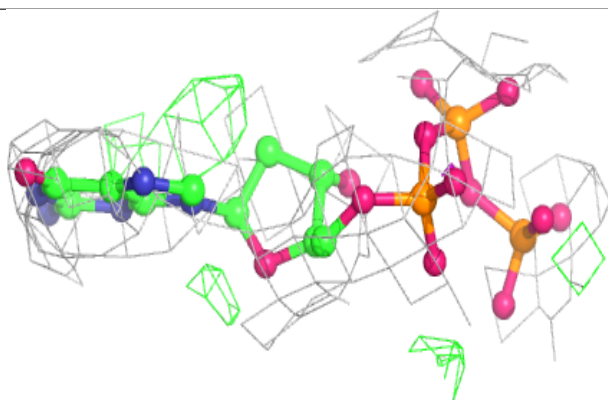
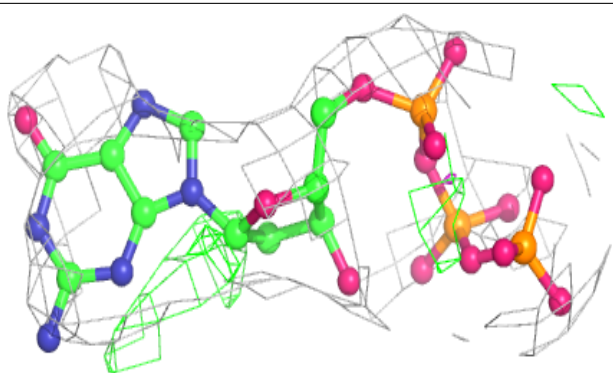
Electron density around DGT B 1308 (B):

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



Electron density around DGT B 1308 (A):

$2mF_o-DF_c$ (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.