



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:32 AM UTC

PDB ID : 2NVX / pdb_00002nvx
Title : RNA polymerase II elongation complex in 5 mM Mg+2 with 2'-dUTP
Authors : Wang, D.; Bushnell, D.A.; Westover, K.D.; Kaplan, C.D.; Kornberg, R.D.
Deposited on : 2006-11-13
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

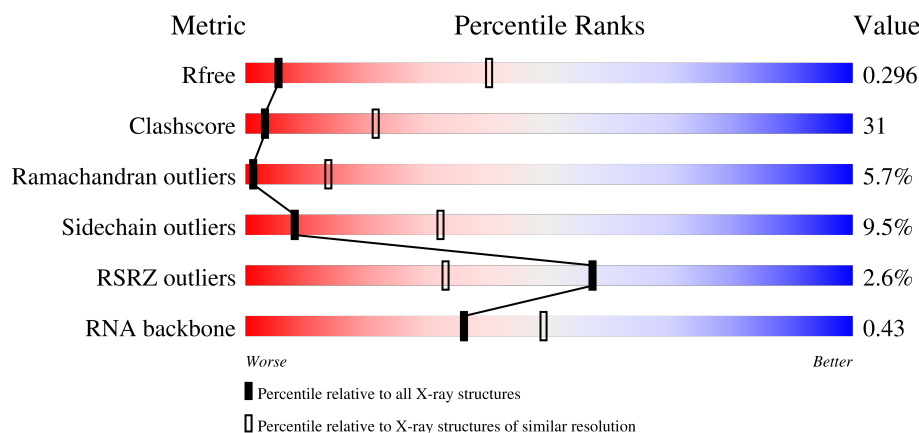
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

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

Mol	Chain	Length	Quality of chain
1	R	10	
2	N	14	
3	T	28	
4	A	1733	

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

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29436 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 5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3'.

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

- Molecule 3 is a DNA chain called 28-MER DNA template strand.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1402	Total	C	N	O	S	0	0	0
			11028	6950	1934	2083	61			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1114	Total	C	N	O	S	0	0	0
			8856	5605	1553	1644	54			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	88	Total	C	N	O	S	0	0	0
			712	455	120	134	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.

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

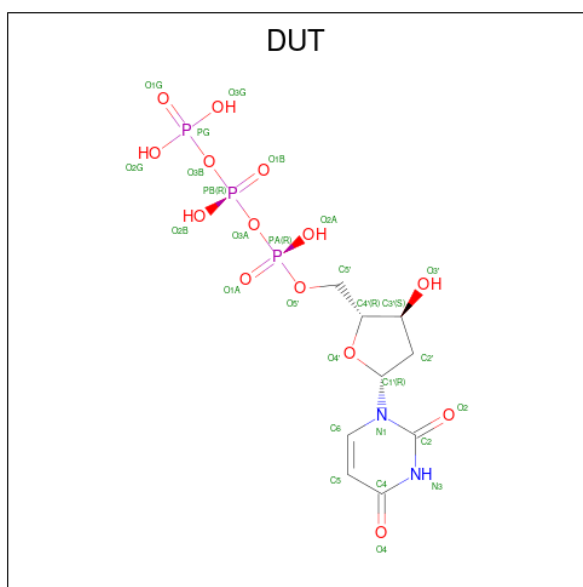
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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

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

- Molecule 16 is DEOXYURIDINE-5'-TRIPHOSPHATE (CCD ID: DUT) (formula: C₉H₁₅N₂O₁₄P₃).

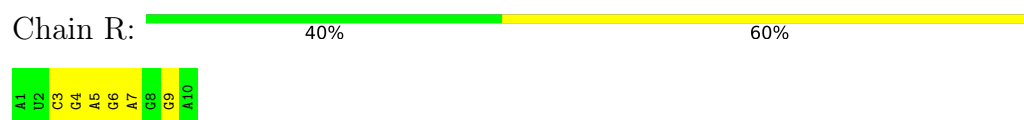


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	B	1	Total	C	N	O	P	0	1
			56	18	4	28	6		

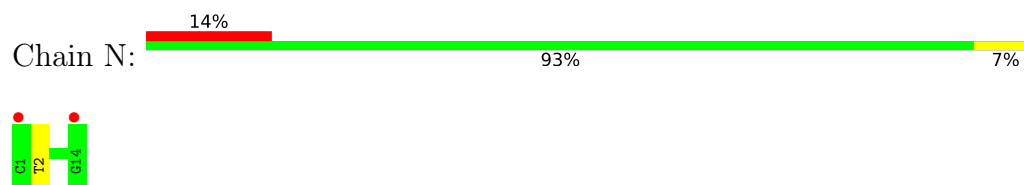
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

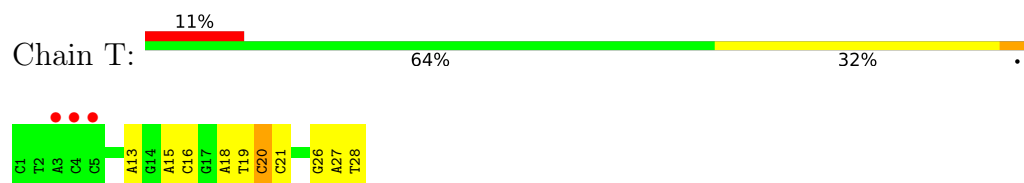
- Molecule 1: 5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3'



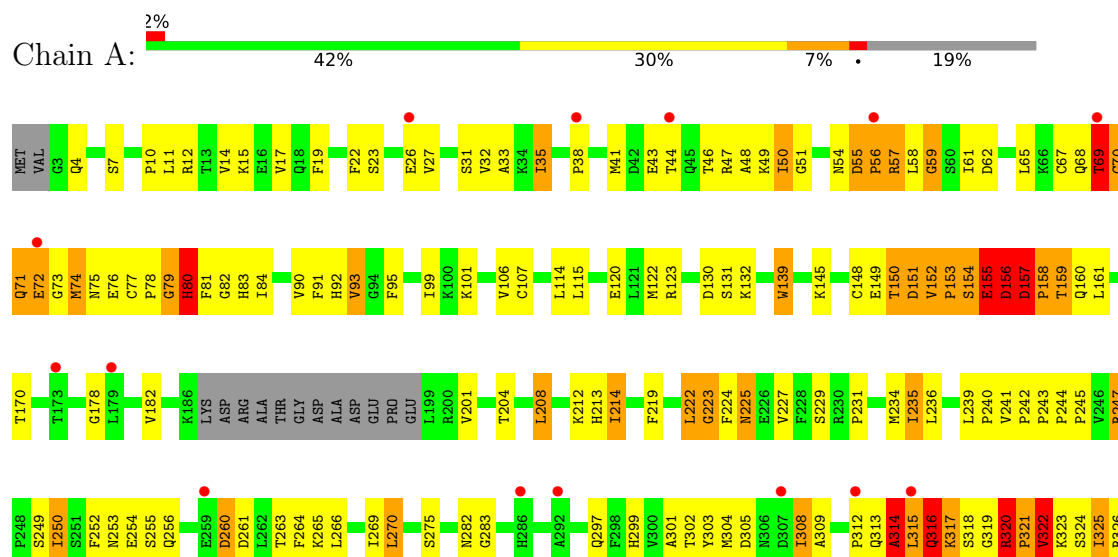
- Molecule 2: 5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3'



- Molecule 3: 28-MER DNA template strand



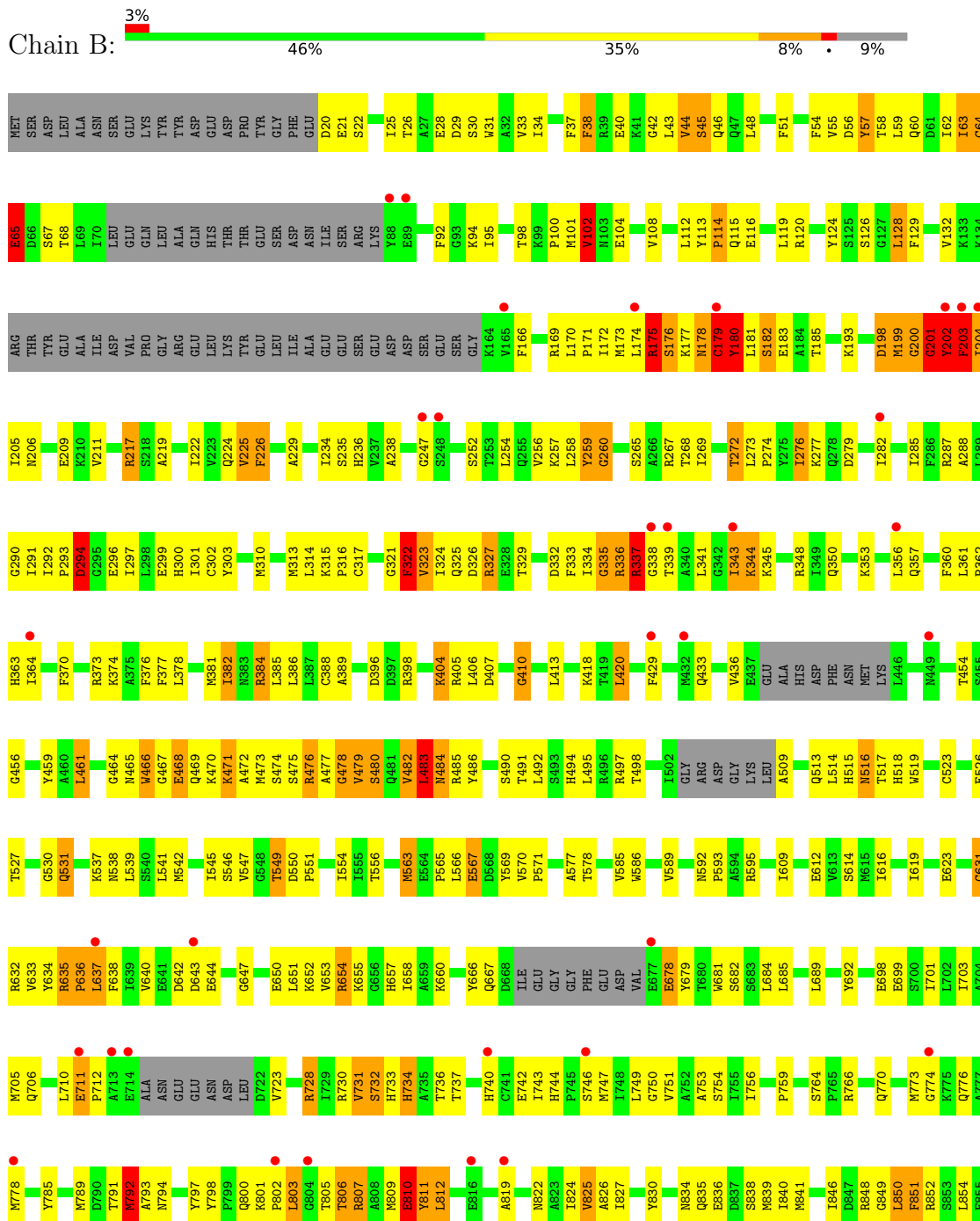
- Molecule 4: DNA-directed RNA polymerase II largest subunit

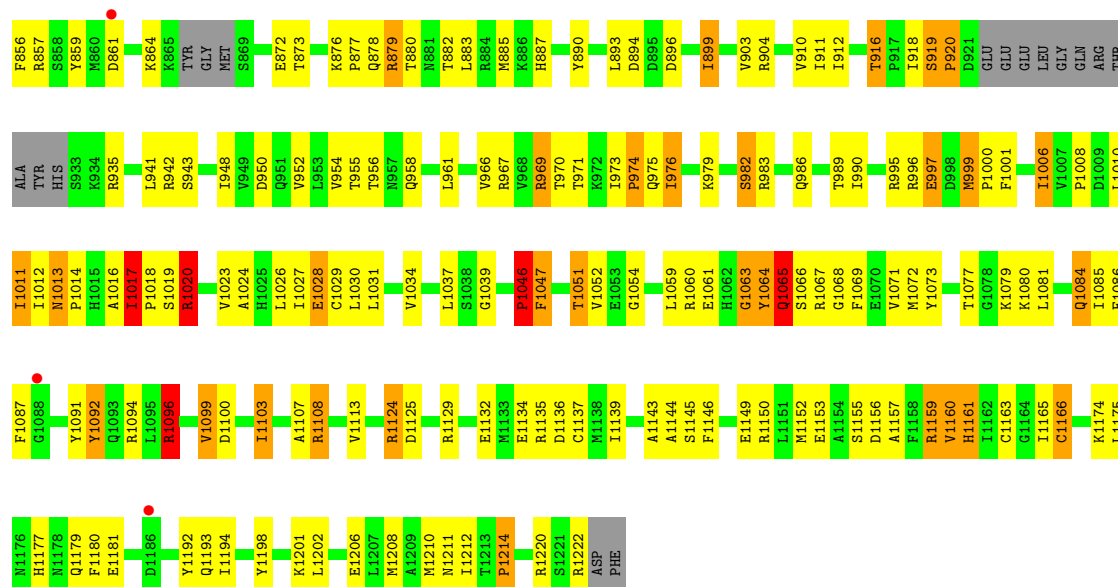




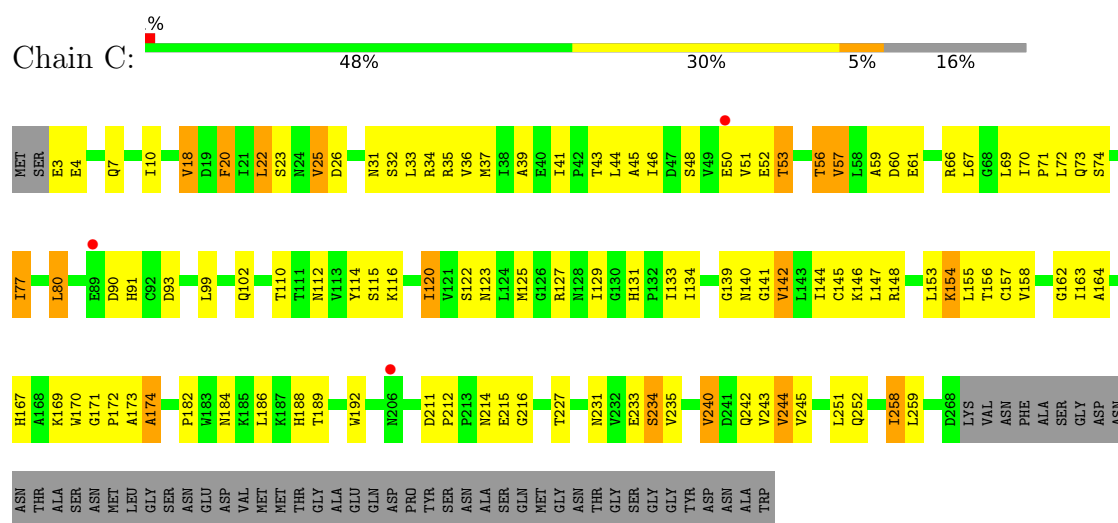
THR	PRO	PRO	SER	SER	TYR	SER	PRO	THR	THR	PRO	ASN	TYR	SER	SER	PRO	THR	SER	SER	SER	TYR	THR	THR	SER	PRO	PRO	PRO	GLY	TYR	SER	SER	PRO	GLY	GLY	SER	SER	PRO	PRO	ALA	ALA	TYR	SER	SER	PRO	PRO	LYS	GLN	ASN	GLP	GLN	GLU	GLN	LYS	HIS	ASN	ASN	GLU	GLU	ASN	ASN	SER	ARG
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- Molecule 5: DNA-directed RNA polymerase II 140 kDa polypeptide

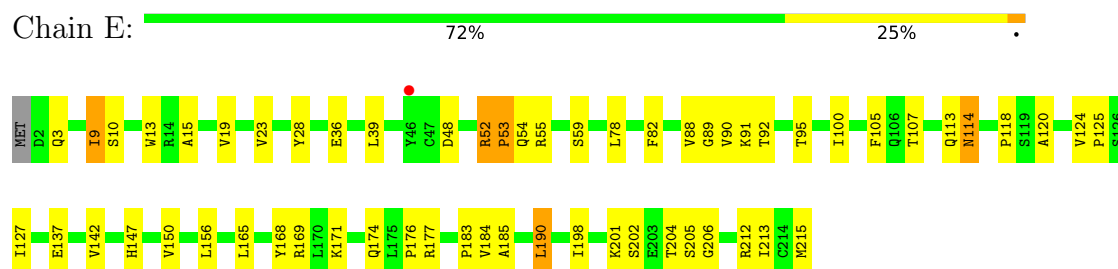




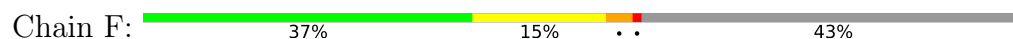
• Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide

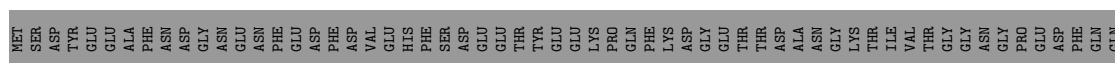


• Molecule 7: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

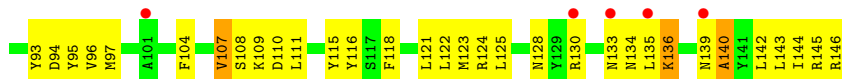


• Molecule 8: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

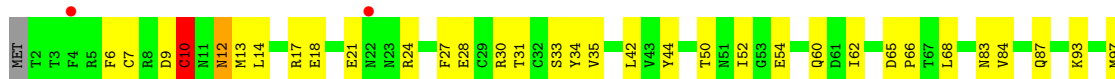




- Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



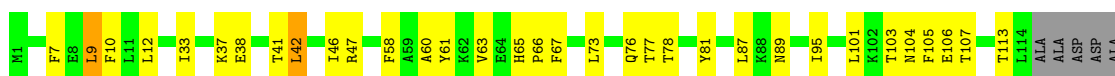
- Molecule 10: DNA-directed RNA polymerase II subunit 9



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

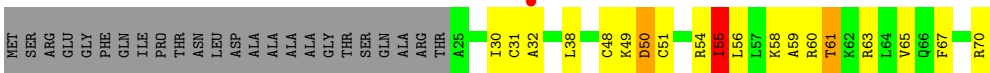


- Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide



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





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.72Å 222.41Å 193.07Å 90.00° 101.29° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 50.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	91.5 (50.00-3.60) 91.5 (50.00-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.285 , 0.304 0.282 , 0.296	Depositor DCC
R_{free} test set	3721 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	104.2	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 68.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	29436	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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, DUT, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	R	0.79	0/243	1.13	0/378
2	N	0.26	0/317	0.72	0/488
3	T	0.51	0/634	1.08	1/975 (0.1%)
4	A	0.80	3/11224 (0.0%)	0.96	21/15176 (0.1%)
5	B	0.92	9/9027 (0.1%)	0.97	8/12172 (0.1%)
6	C	0.80	0/2133	0.96	1/2891 (0.0%)
7	E	0.70	0/1788	0.87	0/2406
8	F	0.76	0/724	0.94	2/977 (0.2%)
9	H	0.72	0/1094	0.87	1/1480 (0.1%)
10	I	0.85	1/989 (0.1%)	0.95	0/1331
11	J	0.80	0/541	0.89	0/727
12	K	0.76	0/937	0.88	0/1265
13	L	0.86	0/366	1.02	1/485 (0.2%)
All	All	0.82	13/30017 (0.0%)	0.95	35/40751 (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	32
5	B	0	12
8	F	0	1
All	All	0	45

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	764	SER	CB-OG	9.06	1.60	1.42
5	B	490	SER	CB-OG	6.44	1.55	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1444	MET	SD-CE	6.42	1.95	1.79
5	B	114	PRO	N-CD	6.32	1.56	1.47
5	B	343	ILE	CA-CB	6.27	1.62	1.54
5	B	404	LYS	CE-NZ	6.18	1.67	1.49
5	B	1100	ASP	CG-OD1	6.13	1.37	1.25
10	I	52	ILE	CA-CB	5.70	1.60	1.53
5	B	1013	ASN	CG-OD1	5.63	1.34	1.23
5	B	789	MET	SD-CE	5.50	1.93	1.79
5	B	1100	ASP	CG-OD2	5.17	1.35	1.25
4	A	621	THR	CB-OG1	5.13	1.51	1.43
4	A	863	VAL	CA-CB	5.08	1.60	1.54

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	793	SER	CA-C-N	8.96	128.56	119.24
4	A	793	SER	C-N-CA	8.96	128.56	119.24
5	B	1071	VAL	CB-CA-C	-7.16	103.55	111.35
4	A	1343	ALA	N-CA-C	-6.94	103.81	112.90
4	A	927	VAL	N-CA-C	-6.34	107.32	113.53
4	A	878	ILE	N-CA-C	6.32	118.55	109.51
5	B	1017	ILE	CA-C-N	6.22	126.42	119.32
5	B	1017	ILE	C-N-CA	6.22	126.42	119.32
5	B	616	ILE	N-CA-C	6.13	115.44	106.55
4	A	977	LYS	CA-C-N	5.96	125.86	119.85
4	A	977	LYS	C-N-CA	5.96	125.86	119.85
5	B	479	VAL	N-CA-C	-5.90	101.93	109.30
4	A	452	LYS	N-CA-C	-5.85	104.83	111.14
4	A	59	GLY	N-CA-C	5.80	118.71	112.33
4	A	236	LEU	N-CA-C	5.76	117.68	108.41
5	B	296	GLU	N-CA-C	-5.70	105.04	112.23
4	A	886	ILE	N-CA-C	5.61	116.34	110.62
3	T	20	DC	O3'-P-O5'	-5.61	95.59	104.00
4	A	576	GLN	N-CA-C	5.60	117.07	111.07
4	A	247	ARG	CA-C-N	5.55	126.78	119.84
4	A	247	ARG	C-N-CA	5.55	126.78	119.84
4	A	1167	GLU	N-CA-C	-5.52	106.90	113.97
4	A	454	SER	N-CA-C	-5.45	106.50	112.72
4	A	1098	VAL	CB-CA-C	-5.27	108.76	114.35
4	A	1005	GLU	N-CA-C	5.22	116.97	111.28
8	F	74	ILE	CA-C-N	5.16	125.16	120.21
8	F	74	ILE	C-N-CA	5.16	125.16	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	59	ALA	CB-CA-C	-5.16	110.21	117.23
4	A	275	SER	N-CA-C	-5.13	106.95	114.39
6	C	20	PHE	N-CA-C	5.11	117.57	109.50
4	A	664	THR	CB-CA-C	-5.10	104.41	110.94
9	H	135	LEU	N-CA-C	5.10	116.69	110.41
4	A	229	SER	N-CA-C	5.08	116.69	108.26
5	B	102	VAL	N-CA-C	5.06	115.32	107.78
5	B	899	ILE	CB-CA-C	-5.01	104.72	111.63

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1020	CYS	Peptide
4	A	1022	LEU	Peptide
4	A	1023	ARG	Peptide
4	A	1024	SER	Peptide
4	A	1219	THR	Peptide
4	A	1220	PHE	Peptide
4	A	1230	GLU	Peptide
4	A	1231	ASP	Peptide
4	A	1232	ASN	Peptide
4	A	1233	ASP	Peptide
4	A	1236	LEU	Peptide
4	A	1263	ILE	Peptide
4	A	1264	GLU	Peptide
4	A	153	PRO	Peptide
4	A	154	SER	Peptide
4	A	155	GLU	Peptide
4	A	156	ASP	Peptide
4	A	249	SER	Peptide
4	A	314	ALA	Peptide
4	A	315	LEU	Peptide
4	A	316	GLN	Peptide
4	A	320	ARG	Peptide
4	A	416	ARG	Peptide
4	A	451	HIS	Peptide
4	A	70	CYS	Peptide
4	A	71	GLN	Peptide
4	A	778	GLY	Peptide
4	A	79	GLY	Peptide
4	A	80	HIS	Peptide

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Mol	Chain	Res	Type	Group
4	A	850	VAL	Peptide
4	A	851	HIS	Peptide
4	A	852	TYR	Peptide
5	B	1063	GLY	Peptide
5	B	1065	GLN	Peptide
5	B	176	SER	Peptide
5	B	178	ASN	Peptide
5	B	179	CYS	Peptide
5	B	180	TYR	Peptide
5	B	201	GLY	Peptide
5	B	202	TYR	Peptide
5	B	203	PHE	Peptide
5	B	678	GLU	Peptide
5	B	810	GLU	Peptide
5	B	919	SER	Peptide
8	F	69	LEU	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	7	0
2	N	284	0	161	1	0
3	T	566	0	316	11	0
4	A	11028	0	11120	939	0
5	B	8856	0	8897	750	0
6	C	2095	0	2051	80	0
7	E	1752	0	1776	35	0
8	F	712	0	738	48	0
9	H	1076	0	1052	40	0
10	I	971	0	930	23	0
11	J	532	0	542	43	0
12	K	919	0	929	20	0
13	L	364	0	387	19	0
14	A	2	0	0	1	0
14	B	1	0	0	1	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
16	B	56	0	22	1	0
All	All	29436	0	29030	1814	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 31.

All (1814) 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:404:LYS:NZ	5:B:404:LYS:CE	1.67	1.52
4:A:1287:TYR:CD2	4:A:1305:VAL:HB	1.59	1.36
4:A:1229:SER:HB2	4:A:1236:LEU:CD1	1.59	1.33
4:A:1229:SER:CB	4:A:1236:LEU:HD12	1.64	1.27
5:B:203:PHE:CA	5:B:204:ILE:HD12	1.63	1.27
4:A:810:PRO:HA	5:B:1047:PHE:CE2	1.69	1.26
4:A:1287:TYR:CE2	4:A:1305:VAL:HB	1.72	1.25
4:A:1174:PHE:HA	4:A:1175:SER:CB	1.65	1.25
5:B:728:ARG:HD2	5:B:730:ARG:NH2	1.52	1.24
4:A:315:LEU:CA	4:A:320:ARG:HH12	1.51	1.23
4:A:1215:ARG:O	4:A:1219:THR:HG23	1.35	1.22
5:B:200:GLY:HA2	5:B:202:TYR:CE2	1.73	1.22
5:B:204:ILE:O	5:B:205:ILE:HD13	1.40	1.22
5:B:175:ARG:HH11	5:B:182:SER:CA	1.56	1.19
5:B:302:CYS:SG	5:B:310:MET:CE	2.31	1.18
5:B:302:CYS:CB	5:B:310:MET:HE3	1.73	1.17
8:F:71:GLU:HA	8:F:72:LYS:HB2	1.25	1.17
4:A:157:ASP:HB2	4:A:158:PRO:CD	1.71	1.16
4:A:810:PRO:CA	5:B:1047:PHE:HE2	1.57	1.16
4:A:1231:ASP:HA	4:A:1233:ASP:CG	1.70	1.15
5:B:302:CYS:HB2	5:B:310:MET:HE3	1.17	1.15
5:B:879:ARG:HH12	5:B:885:MET:HE1	1.09	1.14
4:A:1025:ARG:HG3	4:A:1025:ARG:HH11	1.02	1.14
5:B:175:ARG:NH1	5:B:182:SER:HA	1.62	1.14
4:A:1153:TYR:HE1	10:I:42:LEU:HD13	1.04	1.14
4:A:1231:ASP:HA	4:A:1233:ASP:OD1	1.45	1.14
4:A:78:PRO:HB3	5:B:1201:LYS:HE2	1.27	1.13
4:A:58:LEU:HD23	4:A:59:GLY:H	1.09	1.13
4:A:857:ARG:NH2	8:F:139:PRO:HG2	1.61	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:857:ARG:HG2	4:A:863:VAL:HA	1.23	1.13
4:A:1022:LEU:O	4:A:1023:ARG:HG3	1.48	1.13
4:A:320:ARG:N	4:A:320:ARG:HD2	1.56	1.13
5:B:1065:GLN:NE2	5:B:1067:ARG:H	1.47	1.12
4:A:567:LYS:HB2	4:A:568:PRO:HD2	1.12	1.12
4:A:1170:ILE:HB	4:A:1171:GLN:HA	1.13	1.12
4:A:857:ARG:HH21	8:F:139:PRO:HG2	1.05	1.12
4:A:316:GLN:HE21	4:A:317:LYS:CG	1.63	1.11
4:A:153:PRO:HA	4:A:154:SER:OG	1.50	1.11
5:B:1159:ARG:HB3	5:B:1159:ARG:HH11	1.11	1.11
4:A:315:LEU:HB2	4:A:320:ARG:HH22	1.09	1.11
4:A:1153:TYR:CE1	10:I:42:LEU:HD13	1.86	1.11
5:B:1065:GLN:NE2	5:B:1068:GLY:H	1.50	1.10
4:A:316:GLN:HA	4:A:318:SER:H	1.17	1.10
5:B:224:GLN:HB3	5:B:226:PHE:HE1	1.12	1.10
5:B:969:ARG:NH2	6:C:59:ALA:HB1	1.65	1.10
4:A:1244:ARG:HH11	4:A:1244:ARG:CB	1.65	1.09
5:B:174:LEU:C	5:B:179:CYS:SG	2.35	1.09
5:B:637:LEU:HD13	5:B:740:HIS:ND1	1.65	1.09
5:B:1124:ARG:H	5:B:1124:ARG:HD2	0.95	1.09
4:A:31:SER:HB2	4:A:82:GLY:HA2	1.29	1.09
7:E:53:PRO:CB	7:E:54:GLN:HA	1.83	1.08
4:A:58:LEU:CD2	4:A:59:GLY:H	1.66	1.08
4:A:1287:TYR:CD2	4:A:1305:VAL:CB	2.34	1.08
5:B:807:ARG:HG3	5:B:807:ARG:HH11	1.18	1.08
4:A:316:GLN:HE21	4:A:317:LYS:HG3	1.16	1.08
4:A:316:GLN:HG2	4:A:317:LYS:HA	1.22	1.08
4:A:316:GLN:HG2	4:A:317:LYS:CA	1.84	1.08
4:A:857:ARG:HH21	8:F:139:PRO:CG	1.67	1.07
4:A:1030:ARG:HD3	4:A:1035:TYR:CE1	1.89	1.07
4:A:1244:ARG:HB2	4:A:1244:ARG:NH1	1.69	1.07
4:A:1030:ARG:HH11	4:A:1030:ARG:HG3	1.11	1.07
4:A:302:THR:HG21	4:A:313:GLN:NE2	1.69	1.07
4:A:1025:ARG:HH11	4:A:1025:ARG:CG	1.67	1.07
7:E:53:PRO:HB2	7:E:54:GLN:CA	1.84	1.07
4:A:586:ILE:HD11	4:A:637:LYS:HD3	1.13	1.07
4:A:1024:SER:HB3	4:A:1025:ARG:O	1.54	1.07
5:B:1124:ARG:HD2	5:B:1124:ARG:N	1.66	1.07
5:B:919:SER:HB3	5:B:920:PRO:HA	1.09	1.06
4:A:1265:ASN:HD21	5:B:265:SER:HB3	1.20	1.06
5:B:879:ARG:O	5:B:882:THR:HG22	1.55	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1172:LEU:HB3	4:A:1173:HIS:HA	1.29	1.05
5:B:175:ARG:N	5:B:179:CYS:SG	2.30	1.05
5:B:969:ARG:HH21	6:C:59:ALA:HB1	0.97	1.05
5:B:1124:ARG:H	5:B:1124:ARG:CD	1.70	1.05
4:A:315:LEU:HA	4:A:320:ARG:HH12	1.15	1.04
4:A:1026:LEU:HD13	4:A:1026:LEU:N	1.69	1.04
5:B:982:SER:HA	5:B:1092:TYR:CD2	1.92	1.04
5:B:1016:ALA:O	5:B:1017:ILE:HG13	1.55	1.04
5:B:48:LEU:HD22	5:B:175:ARG:O	1.58	1.04
4:A:157:ASP:HB2	4:A:158:PRO:HD3	1.07	1.04
4:A:151:ASP:CA	4:A:152:VAL:HB	1.86	1.03
4:A:810:PRO:HA	5:B:1047:PHE:HE2	0.91	1.03
4:A:451:HIS:HB3	4:A:453:MET:H	1.19	1.02
4:A:567:LYS:CB	4:A:568:PRO:HD2	1.86	1.02
4:A:1174:PHE:CA	4:A:1175:SER:HB2	1.89	1.02
5:B:982:SER:HB3	5:B:1092:TYR:CE2	1.95	1.02
5:B:1124:ARG:HG2	5:B:1124:ARG:HH11	1.19	1.02
4:A:1244:ARG:HH11	4:A:1244:ARG:HB2	0.86	1.02
4:A:151:ASP:HA	4:A:152:VAL:CB	1.85	1.01
4:A:956:LEU:HD13	4:A:1021:LEU:HD22	1.41	1.01
4:A:1209:MET:HE2	4:A:1236:LEU:HD11	1.42	1.01
4:A:67:CYS:O	4:A:68:GLN:HG3	1.61	1.01
4:A:1021:LEU:H	4:A:1024:SER:CB	1.73	1.01
5:B:203:PHE:CE1	5:B:461:LEU:HD21	1.96	1.01
4:A:779:PHE:CE2	4:A:785:PRO:HG3	1.96	1.00
5:B:176:SER:N	5:B:179:CYS:SG	2.33	1.00
7:E:52:ARG:HB2	7:E:53:PRO:HD3	1.37	1.00
4:A:830:LYS:NZ	4:A:1080:THR:HA	1.77	1.00
4:A:1233:ASP:HB3	4:A:1235:LYS:O	1.61	1.00
5:B:203:PHE:HD1	5:B:204:ILE:N	1.59	1.00
5:B:302:CYS:CB	5:B:310:MET:CE	2.38	1.00
4:A:417:TYR:O	4:A:418:SER:HB3	1.59	1.00
5:B:224:GLN:HB3	5:B:226:PHE:CE1	1.97	0.99
4:A:1174:PHE:CA	4:A:1175:SER:CB	2.40	0.99
4:A:1167:GLU:O	4:A:1170:ILE:HG12	1.62	0.99
4:A:1174:PHE:HA	4:A:1175:SER:HB2	1.01	0.99
5:B:302:CYS:SG	5:B:310:MET:HE2	2.01	0.98
5:B:203:PHE:HA	5:B:204:ILE:HD12	1.01	0.98
5:B:299:GLU:HG2	5:B:571:PRO:HG2	1.46	0.98
4:A:666:ILE:CG2	5:B:1026:LEU:HB3	1.94	0.98
5:B:64:CYS:O	5:B:65:GLU:HG3	1.63	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1065:GLN:HE22	5:B:1067:ARG:N	1.61	0.97
5:B:174:LEU:HA	5:B:179:CYS:SG	2.04	0.97
4:A:542:GLU:HG3	4:A:544:ASP:OD1	1.65	0.97
4:A:666:ILE:HD12	5:B:1052:VAL:HG13	1.44	0.97
4:A:852:TYR:CD2	4:A:1060:PRO:HB3	1.99	0.97
8:F:72:LYS:HB3	8:F:73:ALA:HA	1.46	0.97
4:A:1021:LEU:H	4:A:1024:SER:HB2	1.28	0.96
5:B:273:LEU:O	5:B:276:ILE:HG22	1.66	0.96
4:A:1265:ASN:ND2	5:B:265:SER:HB3	1.80	0.96
4:A:541:ILE:HD12	4:A:546:VAL:HG22	1.47	0.96
4:A:302:THR:HG21	4:A:313:GLN:HE22	1.22	0.95
4:A:319:GLY:C	4:A:320:ARG:HD2	1.89	0.95
5:B:177:LYS:HE2	5:B:178:ASN:ND2	1.81	0.95
5:B:175:ARG:HH11	5:B:182:SER:HA	0.81	0.95
4:A:253:ASN:HD22	4:A:256:GLN:H	1.05	0.95
5:B:174:LEU:CA	5:B:179:CYS:SG	2.55	0.95
5:B:200:GLY:HA2	5:B:202:TYR:CD2	2.01	0.95
4:A:1021:LEU:N	4:A:1024:SER:HB2	1.82	0.95
5:B:879:ARG:NH2	5:B:885:MET:SD	2.38	0.95
4:A:315:LEU:HA	4:A:320:ARG:NH1	1.81	0.95
4:A:779:PHE:HE2	4:A:785:PRO:CD	1.80	0.95
4:A:315:LEU:HB2	4:A:320:ARG:NH2	1.80	0.94
5:B:711:GLU:H	5:B:712:PRO:CD	1.80	0.94
4:A:151:ASP:HA	4:A:152:VAL:HB	0.96	0.94
4:A:586:ILE:CD1	4:A:637:LYS:HD3	1.97	0.94
4:A:1025:ARG:HD3	4:A:1030:ARG:NH2	1.83	0.94
4:A:535:THR:HG21	4:A:617:VAL:H	1.32	0.94
4:A:1364:ASN:ND2	4:A:1366:ARG:HG2	1.81	0.94
5:B:203:PHE:HA	5:B:204:ILE:CD1	1.95	0.94
4:A:779:PHE:HE2	4:A:785:PRO:HD3	1.31	0.94
4:A:779:PHE:HE1	5:B:517:THR:HG22	1.31	0.94
9:H:38:LEU:HD11	9:H:123:MET:HE2	1.50	0.94
4:A:779:PHE:CE2	4:A:785:PRO:HD3	2.02	0.93
4:A:1287:TYR:CE2	4:A:1305:VAL:CB	2.51	0.93
4:A:451:HIS:HB3	4:A:453:MET:N	1.82	0.93
5:B:577:ALA:HB1	5:B:589:VAL:CG1	1.97	0.93
5:B:1084:GLN:HE22	6:C:192:TRP:H	1.10	0.93
5:B:1159:ARG:HB3	5:B:1159:ARG:NH1	1.82	0.93
4:A:1025:ARG:HG3	4:A:1025:ARG:NH1	1.70	0.93
9:H:81:PRO:CB	9:H:82:PRO:HD2	1.97	0.93
4:A:586:ILE:HD11	4:A:637:LYS:CD	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1172:LEU:CB	4:A:1173:HIS:HA	1.94	0.93
4:A:1026:LEU:N	4:A:1026:LEU:CD1	2.31	0.93
5:B:825:VAL:HG23	5:B:1010:LEU:HB3	1.50	0.92
4:A:633:VAL:O	4:A:637:LYS:HG2	1.69	0.92
8:F:69:LEU:HB2	8:F:70:LYS:HB2	1.50	0.92
5:B:200:GLY:HA2	5:B:202:TYR:HE2	1.30	0.92
4:A:779:PHE:HE2	4:A:785:PRO:CG	1.82	0.92
5:B:211:VAL:O	5:B:480:SER:HA	1.68	0.92
4:A:1364:ASN:HD21	4:A:1366:ARG:HH11	1.10	0.91
5:B:955:THR:HG22	5:B:956:THR:H	1.31	0.91
4:A:453:MET:HE3	4:A:520:CYS:SG	2.10	0.91
5:B:919:SER:CB	5:B:920:PRO:HA	1.98	0.91
4:A:1016:THR:O	4:A:1020:CYS:SG	2.27	0.91
4:A:500:GLU:OE1	5:B:1145:SER:HB2	1.70	0.91
4:A:852:TYR:CE2	4:A:1060:PRO:HB2	2.05	0.91
4:A:1153:TYR:HE1	10:I:42:LEU:CD1	1.82	0.91
4:A:1209:MET:SD	4:A:1236:LEU:HD21	2.09	0.91
5:B:792:MET:HE1	5:B:857:ARG:CZ	2.01	0.91
4:A:779:PHE:CE2	4:A:785:PRO:CG	2.54	0.91
4:A:1231:ASP:HA	4:A:1233:ASP:OD2	1.70	0.91
4:A:1287:TYR:HD2	4:A:1305:VAL:HB	1.25	0.90
4:A:636:GLU:HB3	4:A:637:LYS:HD2	1.52	0.90
4:A:250:ILE:HD11	4:A:254:GLU:OE2	1.71	0.90
4:A:666:ILE:HG22	5:B:1026:LEU:HB3	1.53	0.90
5:B:203:PHE:HE1	5:B:461:LEU:HD21	1.34	0.90
4:A:58:LEU:HD23	4:A:59:GLY:N	1.87	0.90
5:B:64:CYS:C	5:B:65:GLU:HG3	1.92	0.90
5:B:1065:GLN:HE22	5:B:1068:GLY:H	1.12	0.90
4:A:1170:ILE:CB	4:A:1171:GLN:HA	1.96	0.89
5:B:173:MET:O	5:B:179:CYS:SG	2.30	0.89
4:A:78:PRO:CB	5:B:1201:LYS:HE2	2.01	0.89
4:A:1234:GLU:C	4:A:1235:LYS:HD3	1.97	0.89
4:A:362:ASP:OD2	4:A:459:ARG:HD3	1.73	0.89
4:A:569:LYS:HD2	4:A:571:LEU:HD11	1.52	0.89
5:B:276:ILE:HG13	5:B:277:LYS:H	1.37	0.89
4:A:569:LYS:O	4:A:571:LEU:HD12	1.72	0.89
5:B:969:ARG:HH21	6:C:59:ALA:CB	1.85	0.89
4:A:852:TYR:CD2	4:A:1060:PRO:CB	2.56	0.89
5:B:1065:GLN:HE22	5:B:1067:ARG:H	0.91	0.89
4:A:33:ALA:HB3	4:A:82:GLY:HA3	1.53	0.88
4:A:264:PHE:HE1	4:A:317:LYS:HG3	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:336:ARG:HD2	5:B:336:ARG:O	1.74	0.88
11:J:45:CYS:SG	11:J:46:CYS:N	2.46	0.88
4:A:157:ASP:O	4:A:158:PRO:O	1.92	0.88
5:B:203:PHE:C	5:B:203:PHE:CD1	2.48	0.88
5:B:849:GLY:HA2	5:B:852:ARG:HD2	1.55	0.88
5:B:919:SER:HB3	5:B:920:PRO:CA	2.00	0.88
4:A:587:HIS:NE2	4:A:969:GLN:NE2	2.22	0.87
5:B:129:PHE:HE1	5:B:166:PHE:HD1	1.17	0.87
5:B:516:ASN:HD22	5:B:516:ASN:H	1.17	0.87
4:A:857:ARG:HH11	4:A:863:VAL:HG22	1.38	0.87
5:B:299:GLU:CG	5:B:571:PRO:HG2	2.05	0.87
4:A:777:PHE:CE1	4:A:782:ARG:HA	2.10	0.87
4:A:1030:ARG:HG3	4:A:1030:ARG:NH1	1.87	0.87
4:A:777:PHE:HB3	4:A:780:VAL:O	1.74	0.87
4:A:1030:ARG:HD3	4:A:1035:TYR:HE1	1.38	0.87
4:A:830:LYS:HZ3	4:A:1080:THR:HA	1.33	0.87
4:A:316:GLN:NE2	4:A:317:LYS:HG3	1.90	0.87
4:A:810:PRO:CA	5:B:1047:PHE:CE2	2.43	0.87
7:E:53:PRO:HB2	7:E:54:GLN:HA	0.92	0.86
4:A:416:ARG:NH2	4:A:417:TYR:CE2	2.43	0.86
4:A:541:ILE:HD11	4:A:577:ILE:HG12	1.57	0.86
4:A:1345:ARG:HG3	4:A:1346:ALA:N	1.89	0.86
5:B:48:LEU:CD2	5:B:175:ARG:O	2.24	0.86
5:B:173:MET:HA	5:B:203:PHE:HB3	1.56	0.86
4:A:315:LEU:CA	4:A:320:ARG:NH1	2.35	0.86
5:B:203:PHE:HE1	5:B:461:LEU:CD2	1.87	0.86
7:E:52:ARG:CB	7:E:53:PRO:HD3	2.05	0.86
4:A:1345:ARG:HG3	4:A:1346:ALA:H	1.40	0.86
4:A:149:GLU:HB3	4:A:152:VAL:HG21	1.58	0.86
4:A:153:PRO:HB2	4:A:154:SER:C	2.01	0.86
4:A:754:SER:H	4:A:757:ASN:HD22	1.22	0.86
4:A:809:THR:HB	4:A:810:PRO:HD2	1.55	0.85
4:A:1026:LEU:O	4:A:1030:ARG:CB	2.24	0.85
4:A:65:LEU:HD22	4:A:72:GLU:C	2.01	0.85
5:B:565:PRO:HB2	5:B:567:GLU:OE1	1.76	0.85
4:A:353:ILE:HD13	4:A:487:MET:HE3	1.58	0.85
4:A:320:ARG:N	4:A:320:ARG:CD	2.34	0.85
5:B:1016:ALA:O	5:B:1017:ILE:CG1	2.25	0.84
8:F:72:LYS:HB3	8:F:73:ALA:CA	2.06	0.84
4:A:1229:SER:HB2	4:A:1236:LEU:HD12	0.87	0.84
5:B:567:GLU:H	5:B:567:GLU:CD	1.84	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:81:PRO:HB3	9:H:82:PRO:HD2	1.59	0.84
4:A:1030:ARG:CD	4:A:1035:TYR:HE1	1.91	0.83
5:B:129:PHE:CE1	5:B:166:PHE:HD1	1.96	0.83
5:B:638:PHE:O	5:B:740:HIS:HB2	1.78	0.83
5:B:203:PHE:HD1	5:B:204:ILE:H	1.24	0.83
4:A:1030:ARG:CD	4:A:1035:TYR:CE1	2.60	0.83
11:J:10:CYS:SG	11:J:43:ARG:HD2	2.18	0.83
8:F:71:GLU:HA	8:F:72:LYS:CB	2.02	0.83
4:A:567:LYS:HB2	4:A:568:PRO:CD	2.03	0.83
5:B:225:VAL:C	5:B:226:PHE:HD1	1.86	0.83
4:A:58:LEU:CG	4:A:80:HIS:O	2.26	0.83
4:A:353:ILE:HD13	4:A:487:MET:CE	2.09	0.83
4:A:783:THR:HG21	4:A:815:PHE:HE1	1.44	0.82
4:A:1118:VAL:HG23	4:A:1306:LEU:HB2	1.61	0.82
5:B:174:LEU:H	5:B:203:PHE:H	1.26	0.82
5:B:203:PHE:CE1	5:B:461:LEU:CD2	2.61	0.82
5:B:1084:GLN:NE2	6:C:192:TRP:H	1.77	0.82
13:L:60:ARG:HG3	13:L:61:THR:H	1.43	0.82
4:A:1441:PHE:CE2	8:F:89:GLU:HG3	2.14	0.82
4:A:153:PRO:CA	4:A:154:SER:OG	2.28	0.82
4:A:1312:ASN:O	4:A:1316:VAL:HG23	1.79	0.82
5:B:982:SER:CB	5:B:1092:TYR:CE2	2.63	0.82
4:A:90:VAL:HG13	4:A:297:GLN:CD	2.04	0.82
5:B:269:ILE:HD11	5:B:386:LEU:HD21	1.60	0.82
5:B:982:SER:CA	5:B:1092:TYR:CE2	2.62	0.82
4:A:637:LYS:HB3	4:A:637:LYS:HZ3	1.45	0.82
5:B:1065:GLN:CD	5:B:1065:GLN:C	2.47	0.82
4:A:316:GLN:HA	4:A:318:SER:N	1.94	0.81
4:A:873:MET:HG2	4:A:957:PRO:HG3	1.62	0.81
5:B:203:PHE:CD1	5:B:204:ILE:N	2.47	0.81
5:B:202:TYR:O	5:B:202:TYR:CG	2.33	0.81
4:A:316:GLN:CA	4:A:318:SER:H	1.92	0.81
4:A:1209:MET:HE2	4:A:1236:LEU:CD1	2.10	0.81
5:B:1065:GLN:NE2	5:B:1065:GLN:C	2.38	0.81
4:A:450:LEU:O	4:A:451:HIS:CG	2.33	0.81
5:B:728:ARG:CD	5:B:730:ARG:NH2	2.39	0.81
4:A:544:ASP:CG	4:A:545:GLN:H	1.89	0.81
5:B:986:GLN:HE22	5:B:1020:ARG:HD2	1.46	0.81
4:A:1153:TYR:CE1	10:I:42:LEU:CD1	2.62	0.81
5:B:1124:ARG:HG2	5:B:1124:ARG:NH1	1.93	0.80
5:B:56:ASP:C	5:B:57:TYR:HD1	1.89	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:482:PHE:HD2	5:B:836:GLU:O	1.63	0.80
5:B:177:LYS:C	5:B:177:LYS:HD2	2.07	0.80
4:A:1170:ILE:HB	4:A:1171:GLN:CA	2.06	0.80
4:A:1287:TYR:CD2	4:A:1305:VAL:CG2	2.65	0.80
5:B:899:ILE:HD11	5:B:911:ILE:HG12	1.62	0.80
4:A:299:HIS:HA	4:A:302:THR:HG22	1.61	0.80
4:A:666:ILE:HG22	5:B:1026:LEU:CB	2.12	0.80
4:A:777:PHE:HD1	4:A:782:ARG:C	1.89	0.80
4:A:1206:ASP:HB2	4:A:1274:ARG:HH12	1.46	0.80
5:B:172:ILE:O	5:B:203:PHE:HB3	1.82	0.80
5:B:982:SER:CA	5:B:1092:TYR:CD2	2.65	0.80
4:A:868:TYR:CE1	4:A:1064:VAL:HG11	2.16	0.80
6:C:102:GLN:HG2	6:C:154:LYS:HD2	1.64	0.80
4:A:14:VAL:H	4:A:1432:GLN:HE22	1.30	0.79
8:F:71:GLU:CA	8:F:72:LYS:HB2	2.10	0.79
4:A:636:GLU:CB	4:A:637:LYS:HD2	2.12	0.79
4:A:1234:GLU:O	4:A:1235:LYS:HD3	1.81	0.79
4:A:541:ILE:CD1	4:A:577:ILE:HG12	2.11	0.79
4:A:1364:ASN:HD21	4:A:1366:ARG:NH1	1.80	0.79
5:B:202:TYR:O	5:B:204:ILE:HD11	1.82	0.79
4:A:67:CYS:O	4:A:68:GLN:CG	2.30	0.79
4:A:157:ASP:CB	4:A:158:PRO:HD3	2.02	0.79
5:B:1065:GLN:NE2	5:B:1068:GLY:N	2.30	0.79
4:A:777:PHE:CB	4:A:780:VAL:O	2.31	0.79
4:A:779:PHE:CE1	5:B:517:THR:HG22	2.17	0.79
4:A:1231:ASP:CA	4:A:1233:ASP:OD2	2.31	0.79
5:B:202:TYR:O	5:B:202:TYR:CD1	2.36	0.79
5:B:652:LYS:O	5:B:654:ARG:HD3	1.83	0.78
9:H:26:ILE:HG22	9:H:40:LEU:O	1.83	0.78
4:A:316:GLN:HE21	4:A:317:LYS:HG2	1.45	0.78
4:A:1234:GLU:HB3	4:A:1235:LYS:HD3	1.65	0.78
4:A:777:PHE:CD1	4:A:782:ARG:CA	2.67	0.78
6:C:99:LEU:HD23	6:C:120:ILE:HA	1.67	0.78
5:B:1065:GLN:CD	5:B:1066:SER:N	2.42	0.77
4:A:500:GLU:OE2	5:B:1143:ALA:CA	2.31	0.77
4:A:1025:ARG:HD3	4:A:1030:ARG:CZ	2.15	0.77
5:B:104:GLU:OE2	13:L:54:ARG:CZ	2.32	0.77
5:B:1160:VAL:HG12	5:B:1161:HIS:H	1.47	0.77
4:A:500:GLU:OE2	5:B:1143:ALA:HA	1.85	0.77
4:A:1345:ARG:CG	4:A:1346:ALA:N	2.47	0.77
5:B:56:ASP:C	5:B:57:TYR:CD1	2.61	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:299:GLU:HG2	5:B:571:PRO:CG	2.13	0.77
6:C:186:LEU:HB3	6:C:188:HIS:HD2	1.49	0.77
13:L:60:ARG:HG3	13:L:61:THR:N	1.98	0.77
4:A:325:ILE:HG21	5:B:1210:MET:SD	2.25	0.77
4:A:1220:PHE:O	4:A:1221:LYS:HB2	1.84	0.77
5:B:851:PHE:HB3	5:B:1094:ARG:HD2	1.65	0.77
4:A:1407:GLU:CD	4:A:1407:GLU:H	1.92	0.77
4:A:607:ILE:HG12	4:A:612:ILE:HG22	1.67	0.77
4:A:1021:LEU:N	4:A:1024:SER:CB	2.43	0.77
5:B:1063:GLY:C	5:B:1064:TYR:HD1	1.93	0.77
5:B:1065:GLN:CD	5:B:1067:ARG:H	1.91	0.77
4:A:315:LEU:N	4:A:320:ARG:HH12	1.82	0.77
4:A:381:THR:OG1	4:A:382:PRO:HD2	1.85	0.77
4:A:637:LYS:HB3	4:A:637:LYS:NZ	2.00	0.77
4:A:666:ILE:HD12	5:B:1052:VAL:CG1	2.14	0.77
4:A:1231:ASP:CA	4:A:1233:ASP:CG	2.55	0.76
4:A:1363:VAL:HB	4:A:1368:MET:HE3	1.64	0.76
5:B:807:ARG:HG3	5:B:807:ARG:NH1	1.98	0.76
4:A:645:LEU:HD11	4:A:649:ILE:HD11	1.68	0.76
4:A:154:SER:HA	4:A:155:GLU:O	1.85	0.76
4:A:329:LEU:HD13	4:A:336:ILE:HD11	1.65	0.76
4:A:775:ILE:HG13	4:A:798:GLY:HA3	1.65	0.76
5:B:879:ARG:HH12	5:B:885:MET:CE	1.96	0.76
4:A:91:PHE:HA	4:A:235:ILE:HG22	1.66	0.76
4:A:93:VAL:HG22	4:A:301:ALA:HA	1.68	0.76
5:B:797:TYR:HB3	5:B:798:TYR:CD1	2.21	0.76
5:B:879:ARG:NH1	5:B:885:MET:HE1	1.95	0.76
8:F:72:LYS:CB	8:F:73:ALA:HA	2.11	0.76
4:A:1026:LEU:O	4:A:1030:ARG:HB3	1.86	0.76
5:B:800:GLN:HB3	11:J:52:THR:CG2	2.15	0.76
4:A:1231:ASP:CA	4:A:1233:ASP:OD1	2.30	0.76
5:B:577:ALA:HB1	5:B:589:VAL:HG11	1.66	0.76
4:A:821:ARG:HH12	5:B:514:LEU:HD13	1.51	0.75
5:B:129:PHE:HE1	5:B:166:PHE:CD1	2.02	0.75
5:B:203:PHE:HD1	5:B:203:PHE:C	1.89	0.75
5:B:638:PHE:CE2	5:B:743:ILE:HD13	2.21	0.75
4:A:1234:GLU:HB3	4:A:1235:LYS:CD	2.16	0.75
4:A:590:ARG:HH22	4:A:592:ASP:CG	1.94	0.75
5:B:172:ILE:O	5:B:203:PHE:CB	2.34	0.75
4:A:65:LEU:HD22	4:A:72:GLU:CA	2.16	0.75
4:A:41:MET:C	4:A:50:ILE:HD11	2.12	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:79:GLY:O	4:A:243:PRO:HG3	1.87	0.75
5:B:637:LEU:CD1	5:B:740:HIS:ND1	2.48	0.75
4:A:590:ARG:NH2	4:A:592:ASP:CG	2.45	0.75
4:A:1025:ARG:C	4:A:1026:LEU:HD13	2.11	0.75
4:A:1233:ASP:CB	4:A:1235:LYS:O	2.35	0.75
5:B:728:ARG:HD2	5:B:730:ARG:CZ	2.16	0.75
4:A:416:ARG:NH2	4:A:417:TYR:HE2	1.84	0.75
5:B:654:ARG:H	5:B:657:HIS:HD2	1.35	0.75
3:T:28:DT:H1'	4:A:317:LYS:O	1.87	0.74
4:A:253:ASN:HD22	4:A:256:GLN:N	1.82	0.74
4:A:1155:ASP:OD2	4:A:1161:THR:HG23	1.87	0.74
4:A:417:TYR:O	4:A:418:SER:CB	2.35	0.74
5:B:204:ILE:O	5:B:205:ILE:CD1	2.30	0.74
5:B:225:VAL:C	5:B:226:PHE:CD1	2.65	0.74
5:B:807:ARG:HH11	5:B:807:ARG:CG	1.98	0.74
4:A:596:THR:C	4:A:598:LEU:H	1.96	0.74
4:A:1345:ARG:HD2	4:A:1346:ALA:HA	1.69	0.74
4:A:68:GLN:C	4:A:70:CYS:H	1.96	0.74
4:A:302:THR:CG2	4:A:313:GLN:HE22	2.00	0.74
4:A:58:LEU:HG	4:A:80:HIS:O	1.87	0.74
4:A:347:PHE:HE1	4:A:375:THR:HG22	1.52	0.74
4:A:157:ASP:CB	4:A:158:PRO:CD	2.57	0.74
5:B:177:LYS:HE2	5:B:178:ASN:HD21	1.53	0.74
5:B:577:ALA:HB1	5:B:589:VAL:HG13	1.70	0.74
5:B:999:MET:HE2	5:B:1011:ILE:HD13	1.69	0.74
4:A:156:ASP:CG	4:A:156:ASP:O	2.30	0.74
4:A:1174:PHE:HB3	4:A:1175:SER:HB3	1.68	0.74
5:B:1047:PHE:N	5:B:1047:PHE:CD1	2.53	0.74
4:A:316:GLN:HG2	4:A:317:LYS:N	2.02	0.73
4:A:361:LEU:HD13	4:A:646:PHE:CD2	2.23	0.73
4:A:446:ARG:HH12	4:A:448:PRO:HD2	1.54	0.73
5:B:57:TYR:HD1	5:B:57:TYR:N	1.85	0.73
5:B:302:CYS:HA	5:B:310:MET:HE1	1.70	0.73
4:A:1024:SER:CB	4:A:1025:ARG:O	2.34	0.73
4:A:857:ARG:HD3	4:A:863:VAL:HG22	1.71	0.73
4:A:779:PHE:CE2	4:A:785:PRO:CD	2.62	0.73
4:A:869:GLY:O	7:E:204:THR:HG21	1.89	0.73
4:A:31:SER:HB2	4:A:82:GLY:CA	2.16	0.72
4:A:316:GLN:CG	4:A:317:LYS:HA	2.11	0.72
4:A:852:TYR:HD2	4:A:1060:PRO:HB3	1.53	0.72
5:B:40:GLU:OE2	5:B:681:TRP:HB3	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:51:GLY:HA2	4:A:56:PRO:HG3	1.71	0.72
4:A:1101:LEU:HD13	4:A:1355:VAL:HG11	1.71	0.72
5:B:176:SER:OG	5:B:177:LYS:HB3	1.89	0.72
13:L:32:ALA:HB3	13:L:55:ILE:HD12	1.71	0.72
4:A:1323:ASP:OD1	4:A:1325:THR:HG22	1.88	0.72
5:B:290:GLY:CA	5:B:327:ARG:NH1	2.52	0.72
4:A:596:THR:O	4:A:598:LEU:N	2.21	0.72
4:A:1027:ALA:O	4:A:1030:ARG:N	2.22	0.72
4:A:49:LYS:HZ1	4:A:61:ILE:H	1.37	0.72
4:A:1209:MET:CG	4:A:1236:LEU:HD21	2.20	0.72
4:A:1287:TYR:HD2	4:A:1305:VAL:CB	1.87	0.72
4:A:1342:GLU:HG3	7:E:198:ILE:HD13	1.71	0.72
5:B:344:LYS:HD3	5:B:348:ARG:HB3	1.71	0.72
4:A:875:ALA:HB2	4:A:1366:ARG:HD2	1.72	0.72
5:B:179:CYS:O	5:B:181:LEU:HD12	1.90	0.72
4:A:69:THR:HG21	5:B:1174:LYS:HE3	1.72	0.71
4:A:222:LEU:O	4:A:224:PHE:CD2	2.42	0.71
5:B:60:GLN:HE22	5:B:94:LYS:HA	1.55	0.71
5:B:701:ILE:HD12	5:B:740:HIS:NE2	2.05	0.71
4:A:857:ARG:CG	4:A:863:VAL:HA	2.12	0.71
5:B:1166:CYS:SG	14:B:1307:ZN:ZN	1.78	0.71
5:B:57:TYR:CD1	5:B:57:TYR:N	2.56	0.71
5:B:64:CYS:C	5:B:65:GLU:CG	2.63	0.71
4:A:35:ILE:CG2	4:A:84:ILE:HD13	2.21	0.71
4:A:58:LEU:HD21	4:A:80:HIS:O	1.89	0.71
5:B:203:PHE:CA	5:B:204:ILE:CD1	2.57	0.71
4:A:250:ILE:CD1	4:A:254:GLU:OE2	2.38	0.71
4:A:855:THR:HG23	4:A:856:THR:N	2.04	0.71
5:B:711:GLU:H	5:B:712:PRO:HD2	1.53	0.71
4:A:857:ARG:HH21	8:F:139:PRO:CB	2.04	0.71
6:C:33:LEU:HG	6:C:37:MET:HE2	1.73	0.71
4:A:335:ARG:HD2	5:B:1202:LEU:HD22	1.72	0.71
8:F:69:LEU:CB	8:F:70:LYS:HB2	2.21	0.71
4:A:19:PHE:HD2	4:A:1412:ALA:HB1	1.54	0.71
5:B:40:GLU:CD	5:B:681:TRP:HB3	2.16	0.71
5:B:851:PHE:O	5:B:974:PRO:HD3	1.90	0.71
11:J:45:CYS:O	11:J:48:ARG:HG3	1.90	0.71
4:A:463:ILE:HD13	4:A:469:ARG:HG3	1.72	0.71
4:A:1173:HIS:O	4:A:1174:PHE:CG	2.44	0.71
5:B:336:ARG:HH11	5:B:336:ARG:H	1.36	0.71
5:B:770:GLN:OE1	5:B:983:ARG:HA	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:264:PHE:CE1	4:A:317:LYS:N	2.58	0.70
4:A:636:GLU:HB3	4:A:637:LYS:CD	2.22	0.70
4:A:1364:ASN:ND2	4:A:1366:ARG:HH11	1.87	0.70
5:B:55:VAL:HG11	5:B:177:LYS:NZ	2.06	0.70
4:A:319:GLY:C	4:A:320:ARG:HH11	1.98	0.70
4:A:852:TYR:CE2	4:A:1060:PRO:CB	2.73	0.70
4:A:41:MET:C	4:A:50:ILE:CD1	2.64	0.70
6:C:56:THR:HG21	6:C:145:CYS:SG	2.30	0.70
4:A:83:HIS:CA	4:A:241:VAL:HG23	2.21	0.70
4:A:637:LYS:HD2	4:A:637:LYS:N	2.06	0.70
4:A:857:ARG:HD3	4:A:863:VAL:CG2	2.22	0.70
4:A:1231:ASP:CG	4:A:1232:ASN:H	1.99	0.70
4:A:83:HIS:HA	4:A:241:VAL:HG23	1.71	0.70
5:B:104:GLU:OE1	5:B:120:ARG:NH2	2.20	0.70
5:B:322:PHE:C	5:B:322:PHE:CD2	2.70	0.70
6:C:186:LEU:HB3	6:C:188:HIS:CD2	2.26	0.70
4:A:55:ASP:O	4:A:58:LEU:N	2.25	0.70
4:A:795:GLU:OE2	5:B:731:VAL:HG11	1.91	0.70
4:A:1098:VAL:N	4:A:1099:PRO:HD2	2.06	0.70
4:A:1174:PHE:HA	4:A:1175:SER:HB3	1.70	0.70
5:B:806:THR:H	5:B:809:MET:HE3	1.56	0.70
4:A:795:GLU:OE2	5:B:731:VAL:CG1	2.40	0.70
5:B:703:ILE:HG12	5:B:740:HIS:CE1	2.26	0.70
4:A:1364:ASN:HD22	4:A:1366:ARG:HG2	1.56	0.69
5:B:653:VAL:HG22	5:B:689:LEU:HB3	1.74	0.69
4:A:1172:LEU:HA	4:A:1174:PHE:H	1.57	0.69
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.74	0.69
11:J:8:PHE:CD1	11:J:49:MET:HE1	2.27	0.69
4:A:90:VAL:HA	4:A:297:GLN:OE1	1.91	0.69
4:A:302:THR:CG2	4:A:313:GLN:NE2	2.53	0.69
4:A:567:LYS:CB	4:A:568:PRO:CD	2.65	0.69
5:B:299:GLU:OE2	5:B:571:PRO:HD2	1.92	0.69
5:B:1068:GLY:HA3	5:B:1086:PHE:CD1	2.28	0.69
8:F:93:ILE:HD11	8:F:134:ILE:HD11	1.73	0.69
4:A:90:VAL:HG13	4:A:297:GLN:OE1	1.92	0.69
5:B:1084:GLN:HE22	6:C:192:TRP:N	1.87	0.69
6:C:67:LEU:HA	6:C:70:ILE:HD12	1.72	0.69
5:B:637:LEU:CD1	5:B:740:HIS:CE1	2.75	0.69
6:C:142:VAL:H	11:J:16:ASP:HB3	1.55	0.69
4:A:672:ASP:H	4:A:736:ASN:HD21	1.41	0.69
4:A:809:THR:HB	4:A:810:PRO:CD	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1287:TYR:HE2	4:A:1305:VAL:HB	1.51	0.69
4:A:222:LEU:O	4:A:224:PHE:HD2	1.74	0.69
4:A:264:PHE:CE1	4:A:317:LYS:HG3	2.25	0.69
4:A:482:PHE:HE2	5:B:836:GLU:HB2	1.57	0.69
4:A:1172:LEU:HB3	4:A:1173:HIS:CA	2.15	0.69
4:A:1236:LEU:C	4:A:1237:ILE:HG13	2.18	0.69
5:B:290:GLY:HA2	5:B:327:ARG:HH11	1.57	0.69
4:A:777:PHE:CD1	4:A:782:ARG:HA	2.28	0.69
4:A:78:PRO:HB3	5:B:1201:LYS:CE	2.16	0.69
5:B:637:LEU:HD13	5:B:740:HIS:HD1	1.57	0.69
4:A:65:LEU:HD22	4:A:72:GLU:N	2.08	0.69
5:B:20:ASP:OD2	5:B:21:GLU:HG2	1.93	0.69
5:B:519:TRP:HZ2	5:B:705:MET:HE1	1.58	0.69
4:A:482:PHE:CE2	5:B:836:GLU:HB2	2.28	0.68
4:A:1026:LEU:O	4:A:1030:ARG:HB2	1.92	0.68
4:A:795:GLU:OE1	5:B:731:VAL:HG22	1.93	0.68
4:A:22:PHE:CD2	5:B:1211:ASN:HA	2.28	0.68
4:A:453:MET:CE	4:A:520:CYS:SG	2.81	0.68
5:B:541:LEU:HB2	5:B:747:MET:HE3	1.76	0.68
8:F:69:LEU:HB2	8:F:70:LYS:CB	2.24	0.68
4:A:58:LEU:CD2	4:A:80:HIS:O	2.42	0.68
4:A:58:LEU:CD2	4:A:59:GLY:N	2.50	0.68
4:A:793:SER:HB2	4:A:794:PRO:HD2	1.76	0.68
4:A:852:TYR:HE2	4:A:1060:PRO:HB2	1.56	0.68
4:A:888:GLY:O	4:A:940:ARG:NH2	2.27	0.68
4:A:1199:ARG:NH2	4:A:1232:ASN:OD1	2.27	0.68
4:A:67:CYS:HB3	4:A:70:CYS:HB3	1.76	0.68
4:A:765:VAL:HG22	4:A:800:VAL:HB	1.75	0.68
13:L:50:ASP:HA	13:L:51:CYS:C	2.19	0.68
9:H:81:PRO:CB	9:H:82:PRO:CD	2.71	0.67
5:B:40:GLU:OE2	5:B:682:SER:N	2.26	0.67
5:B:203:PHE:CZ	5:B:461:LEU:HD21	2.29	0.67
4:A:1287:TYR:HD2	4:A:1305:VAL:CG2	2.06	0.67
4:A:1356:ILE:HG13	4:A:1368:MET:HE2	1.75	0.67
5:B:258:LEU:HD13	5:B:269:ILE:HG12	1.75	0.67
5:B:177:LYS:CE	5:B:178:ASN:ND2	2.55	0.67
5:B:792:MET:HE1	5:B:857:ARG:NE	2.09	0.67
4:A:909:ASP:OD1	4:A:910:PRO:HD2	1.93	0.67
5:B:181:LEU:C	5:B:183:GLU:H	2.03	0.67
5:B:398:ARG:HD3	5:B:509:ALA:HB2	1.75	0.67
5:B:483:LEU:HD11	5:B:491:THR:HG23	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:569:TYR:CE1	5:B:589:VAL:HG21	2.29	0.67
5:B:476:ARG:O	5:B:478:GLY:N	2.27	0.67
9:H:84:ALA:HB1	9:H:89:LEU:HD11	1.76	0.67
4:A:1025:ARG:C	4:A:1026:LEU:CD1	2.67	0.67
5:B:217:ARG:NH1	5:B:407:ASP:OD1	2.27	0.67
5:B:516:ASN:H	5:B:516:ASN:ND2	1.93	0.67
5:B:1047:PHE:N	5:B:1047:PHE:HD1	1.90	0.67
6:C:22:LEU:HD22	6:C:25:VAL:HG21	1.77	0.66
4:A:148:CYS:SG	14:A:1734:ZN:ZN	1.84	0.66
4:A:852:TYR:HD2	4:A:1060:PRO:CB	2.07	0.66
5:B:655:LYS:HA	5:B:658:ILE:HD12	1.75	0.66
4:A:182:VAL:HG22	4:A:201:VAL:HG13	1.76	0.66
4:A:666:ILE:HG23	5:B:1026:LEU:HB3	1.74	0.66
5:B:711:GLU:H	5:B:712:PRO:HD3	1.61	0.66
5:B:793:ALA:HB3	5:B:856:PHE:HB2	1.77	0.66
5:B:1063:GLY:O	5:B:1064:TYR:CD1	2.49	0.66
4:A:92:HIS:NE2	4:A:304:MET:HE1	2.11	0.66
5:B:982:SER:N	5:B:1092:TYR:CE2	2.64	0.66
4:A:315:LEU:CB	4:A:320:ARG:HH12	2.07	0.66
4:A:535:THR:CG2	4:A:617:VAL:H	2.06	0.66
4:A:1199:ARG:CZ	4:A:1232:ASN:OD1	2.44	0.66
5:B:614:SER:H	5:B:632:ARG:HH12	1.42	0.66
4:A:1136:SER:O	4:A:1274:ARG:HD2	1.95	0.66
5:B:637:LEU:HD13	5:B:740:HIS:CE1	2.31	0.66
5:B:879:ARG:HB3	5:B:879:ARG:HH11	1.59	0.66
5:B:1065:GLN:HE22	5:B:1068:GLY:N	1.89	0.66
4:A:360:GLU:HB2	4:A:363:GLN:HG3	1.78	0.66
5:B:378:LEU:O	5:B:382:ILE:HG12	1.96	0.66
5:B:979:LYS:HA	5:B:989:THR:HG22	1.78	0.66
4:A:41:MET:CA	4:A:50:ILE:HD12	2.24	0.66
5:B:236:HIS:HD2	5:B:389:ALA:HB2	1.59	0.66
5:B:728:ARG:HD2	5:B:730:ARG:HH22	1.55	0.66
5:B:1016:ALA:O	5:B:1017:ILE:CB	2.42	0.66
6:C:7:GLN:HB2	6:C:23:SER:HB2	1.78	0.66
1:R:4:G:H2'	1:R:5:A:H8	1.61	0.65
4:A:1400:CYS:SG	4:A:1409:LEU:HG	2.35	0.65
5:B:177:LYS:HD2	5:B:177:LYS:O	1.96	0.65
5:B:360:PHE:CE2	5:B:361:LEU:HD13	2.31	0.65
9:H:81:PRO:HB2	9:H:82:PRO:HD2	1.77	0.65
4:A:1021:LEU:CA	4:A:1024:SER:HB2	2.26	0.65
4:A:153:PRO:HB2	4:A:154:SER:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:952:VAL:HG22	5:B:966:VAL:HG13	1.78	0.65
4:A:47:ARG:NH1	5:B:920:PRO:HB2	2.12	0.65
4:A:648:ASN:O	4:A:652:VAL:HG23	1.97	0.65
4:A:850:VAL:HG12	4:A:851:HIS:N	2.10	0.65
4:A:981:LEU:HD13	4:A:986:ILE:HD11	1.78	0.65
4:A:1287:TYR:CE2	4:A:1305:VAL:CG1	2.79	0.65
4:A:1441:PHE:CE2	8:F:89:GLU:CG	2.80	0.65
4:A:35:ILE:HG22	4:A:84:ILE:HD13	1.79	0.65
4:A:857:ARG:HD2	4:A:861:GLY:C	2.22	0.65
4:A:153:PRO:HA	4:A:154:SER:CB	2.26	0.65
4:A:754:SER:N	4:A:757:ASN:HD22	1.92	0.65
4:A:1134:ILE:O	4:A:1138:ILE:HG12	1.97	0.65
4:A:457:ALA:O	4:A:507:VAL:HG23	1.97	0.65
4:A:779:PHE:CD2	4:A:785:PRO:HG3	2.32	0.65
4:A:1206:ASP:HB2	4:A:1274:ARG:NH1	2.11	0.65
4:A:717:ASN:O	4:A:721:PHE:CD2	2.50	0.65
5:B:57:TYR:O	5:B:60:GLN:N	2.30	0.65
5:B:879:ARG:N	5:B:879:ARG:NE	2.45	0.65
4:A:68:GLN:O	4:A:70:CYS:N	2.30	0.64
5:B:30:SER:O	5:B:34:ILE:HD12	1.96	0.64
6:C:50:GLU:HB3	6:C:156:THR:HB	1.79	0.64
9:H:116:TYR:HB2	9:H:123:MET:HB3	1.78	0.64
11:J:48:ARG:HH21	11:J:49:MET:CE	2.10	0.64
4:A:337:ARG:HH21	4:A:839:ARG:HD2	1.63	0.64
4:A:717:ASN:O	4:A:721:PHE:HD2	1.80	0.64
5:B:969:ARG:NH2	6:C:59:ALA:CB	2.53	0.64
4:A:536:LEU:HB2	4:A:539:THR:HG22	1.79	0.64
5:B:376:PHE:HE2	5:B:569:TYR:HD2	1.45	0.64
5:B:982:SER:N	5:B:1092:TYR:HE2	1.96	0.64
5:B:1065:GLN:NE2	5:B:1065:GLN:O	2.30	0.64
5:B:176:SER:O	5:B:178:ASN:N	2.30	0.64
6:C:46:ILE:HD12	6:C:157:CYS:HB3	1.80	0.64
4:A:727:ASP:O	4:A:731:ARG:HG3	1.98	0.64
5:B:634:TYR:CD2	5:B:692:TYR:CD1	2.86	0.64
9:H:95:TYR:HE2	9:H:97:MET:CG	2.11	0.64
4:A:81:PHE:HE2	4:A:240:PRO:HB2	1.62	0.64
4:A:351:THR:HB	4:A:468:PHE:CD2	2.33	0.64
4:A:830:LYS:NZ	4:A:1080:THR:CA	2.57	0.64
4:A:664:THR:OG1	5:B:1014:PRO:HB3	1.97	0.64
5:B:175:ARG:NH1	5:B:181:LEU:O	2.31	0.64
5:B:1060:ARG:O	5:B:1063:GLY:N	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1021:LEU:CA	4:A:1024:SER:CB	2.77	0.63
4:A:58:LEU:HD11	4:A:80:HIS:O	1.97	0.63
4:A:361:LEU:HD13	4:A:646:PHE:HD2	1.60	0.63
5:B:169:ARG:HB2	5:B:454:THR:HG23	1.79	0.63
4:A:324:SER:O	4:A:326:ARG:N	2.31	0.63
4:A:821:ARG:O	4:A:825:ILE:HG12	1.98	0.63
5:B:203:PHE:N	5:B:204:ILE:HD12	2.13	0.63
5:B:986:GLN:HE22	5:B:1020:ARG:CD	2.10	0.63
5:B:1073:TYR:HE2	5:B:1080:LYS:HG3	1.63	0.63
4:A:68:GLN:CG	4:A:68:GLN:O	2.46	0.63
4:A:666:ILE:CD1	5:B:1052:VAL:HG13	2.24	0.63
4:A:830:LYS:HD3	4:A:1079:MET:O	1.98	0.63
4:A:779:PHE:HE1	5:B:517:THR:CG2	2.09	0.63
5:B:290:GLY:HA3	5:B:327:ARG:NH1	2.14	0.63
4:A:1021:LEU:N	4:A:1024:SER:OG	2.32	0.63
5:B:879:ARG:N	5:B:879:ARG:CZ	2.62	0.63
4:A:1441:PHE:CZ	8:F:89:GLU:HA	2.34	0.63
5:B:200:GLY:CA	5:B:202:TYR:HE2	2.09	0.63
5:B:903:VAL:HG12	5:B:904:ARG:H	1.64	0.63
6:C:46:ILE:O	6:C:169:LYS:HE3	1.99	0.63
6:C:56:THR:HG23	6:C:147:LEU:HD23	1.81	0.63
4:A:830:LYS:HZ2	4:A:1080:THR:HA	1.60	0.63
5:B:202:TYR:HD1	5:B:209:GLU:HB3	1.63	0.63
5:B:336:ARG:O	5:B:336:ARG:CD	2.47	0.63
5:B:1064:TYR:HD1	5:B:1064:TYR:N	1.96	0.63
5:B:1099:VAL:O	5:B:1103:ILE:HG12	1.98	0.63
4:A:41:MET:HA	4:A:50:ILE:HD12	1.81	0.63
4:A:351:THR:HG22	4:A:352:VAL:N	2.14	0.63
4:A:541:ILE:CD1	4:A:546:VAL:HG22	2.27	0.63
4:A:947:PHE:CE1	4:A:954:TRP:CE2	2.86	0.63
5:B:40:GLU:OE2	5:B:681:TRP:N	2.32	0.63
4:A:11:LEU:HA	5:B:1193:GLN:O	1.99	0.62
4:A:153:PRO:HA	4:A:154:SER:HG	1.59	0.62
5:B:982:SER:HA	5:B:1092:TYR:HD2	1.57	0.62
5:B:1063:GLY:C	5:B:1064:TYR:CD1	2.77	0.62
4:A:159:THR:CB	4:A:160:GLN:HA	2.30	0.62
4:A:853:ASP:O	4:A:855:THR:N	2.30	0.62
4:A:155:GLU:HG3	4:A:156:ASP:N	2.12	0.62
6:C:112:ASN:ND2	6:C:146:LYS:HG2	2.14	0.62
4:A:101:LYS:HG2	4:A:139:TRP:CZ3	2.35	0.62
4:A:628:GLY:O	4:A:632:VAL:HG23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1022:LEU:C	4:A:1023:ARG:HG3	2.22	0.62
5:B:706:GLN:H	5:B:710:LEU:HD12	1.64	0.62
5:B:200:GLY:CA	5:B:202:TYR:CE2	2.68	0.62
4:A:618:GLU:CD	4:A:619:LYS:N	2.58	0.62
4:A:795:GLU:OE1	5:B:731:VAL:HG13	2.00	0.62
4:A:963:ILE:HD13	4:A:1048:ASN:HB3	1.80	0.62
4:A:1026:LEU:O	4:A:1027:ALA:HB3	1.98	0.62
5:B:173:MET:HA	5:B:203:PHE:CD2	2.33	0.62
5:B:203:PHE:C	5:B:204:ILE:HD12	2.23	0.62
6:C:45:ALA:HA	6:C:72:LEU:HD12	1.82	0.62
11:J:41:LEU:HD22	11:J:46:CYS:O	2.00	0.62
4:A:500:GLU:OE2	5:B:1143:ALA:C	2.43	0.62
4:A:523:ILE:O	4:A:528:LEU:HB2	1.99	0.62
4:A:636:GLU:CG	4:A:637:LYS:HD2	2.30	0.62
10:I:6:PHE:O	10:I:14:LEU:HD13	2.00	0.62
5:B:345:LYS:HG3	5:B:348:ARG:HH21	1.64	0.62
5:B:370:PHE:HD1	5:B:373:ARG:HG3	1.65	0.62
5:B:404:LYS:NZ	5:B:404:LYS:CD	2.61	0.62
5:B:515:HIS:H	5:B:518:HIS:HD2	1.48	0.62
5:B:969:ARG:NH2	6:C:60:ASP:H	1.98	0.62
6:C:35:ARG:HB2	12:K:41:THR:HG23	1.80	0.62
4:A:49:LYS:HZ1	4:A:61:ILE:N	1.98	0.61
4:A:54:ASN:O	4:A:55:ASP:CB	2.48	0.61
4:A:446:ARG:NH1	4:A:448:PRO:HD2	2.14	0.61
4:A:590:ARG:HG3	4:A:605:MET:HB3	1.82	0.61
4:A:605:MET:SD	4:A:617:VAL:HG22	2.40	0.61
4:A:902:LEU:O	4:A:903:ASN:HB2	1.99	0.61
5:B:202:TYR:C	5:B:203:PHE:O	2.42	0.61
5:B:1017:ILE:HD13	5:B:1026:LEU:HD21	1.81	0.61
4:A:58:LEU:CD1	4:A:80:HIS:O	2.48	0.61
4:A:546:VAL:HG13	4:A:577:ILE:HG21	1.82	0.61
5:B:879:ARG:O	5:B:882:THR:CG2	2.40	0.61
5:B:1017:ILE:HB	5:B:1018:PRO:CD	2.30	0.61
8:F:136:ARG:O	8:F:143:PHE:HA	1.99	0.61
5:B:51:PHE:HD2	5:B:176:SER:HG	1.47	0.61
5:B:211:VAL:CG2	5:B:483:LEU:HD22	2.31	0.61
5:B:890:TYR:CD1	5:B:910:VAL:HG21	2.36	0.61
4:A:588:LEU:HD23	4:A:607:ILE:HD12	1.82	0.61
4:A:1063:MET:HG3	4:A:1436:ILE:HG23	1.83	0.61
5:B:710:LEU:O	5:B:711:GLU:HB3	2.00	0.61
5:B:1066:SER:C	5:B:1067:ARG:HG2	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:10:CYS:SG	11:J:43:ARG:CD	2.87	0.61
4:A:157:ASP:O	4:A:158:PRO:C	2.44	0.61
4:A:1172:LEU:CB	4:A:1173:HIS:CA	2.75	0.61
5:B:1019:SER:C	5:B:1020:ARG:HG2	2.26	0.61
9:H:44:VAL:HG13	9:H:48:PRO:HA	1.82	0.61
4:A:567:LYS:NZ	9:H:43:ASN:HB3	2.16	0.61
5:B:848:ARG:HA	6:C:69:LEU:HD21	1.81	0.61
12:K:47:ARG:HD2	12:K:60:ALA:HA	1.81	0.61
4:A:93:VAL:CG2	4:A:301:ALA:HA	2.31	0.61
4:A:1174:PHE:CB	4:A:1175:SER:HB3	2.30	0.61
5:B:180:TYR:O	5:B:182:SER:N	2.33	0.61
5:B:805:THR:HG22	5:B:809:MET:SD	2.41	0.61
11:J:48:ARG:HH21	11:J:49:MET:HE1	1.64	0.61
5:B:124:TYR:OH	5:B:179:CYS:C	2.44	0.61
5:B:217:ARG:NH1	5:B:407:ASP:CG	2.58	0.61
4:A:15:LYS:HE2	5:B:1220:ARG:HG2	1.83	0.60
4:A:668:ASP:HB3	4:A:743:VAL:HG23	1.82	0.60
1:R:3:C:H2'	1:R:4:G:C8	2.36	0.60
5:B:178:ASN:C	5:B:180:TYR:N	2.58	0.60
4:A:31:SER:OG	4:A:83:HIS:CD2	2.53	0.60
4:A:1024:SER:HB3	4:A:1025:ARG:C	2.25	0.60
5:B:173:MET:CA	5:B:203:PHE:HD2	2.15	0.60
5:B:176:SER:O	5:B:179:CYS:N	2.30	0.60
4:A:332:LYS:HG3	4:A:333:GLU:HG2	1.83	0.60
5:B:57:TYR:O	5:B:59:LEU:N	2.33	0.60
5:B:706:GLN:O	5:B:710:LEU:HB2	2.01	0.60
4:A:315:LEU:N	4:A:320:ARG:NH1	2.47	0.60
4:A:545:GLN:HB3	4:A:549:MET:HE3	1.84	0.60
4:A:1206:ASP:CB	4:A:1274:ARG:HH12	2.12	0.60
4:A:1231:ASP:CG	4:A:1232:ASN:N	2.55	0.60
4:A:131:SER:HB3	4:A:223:GLY:HA2	1.83	0.60
4:A:1234:GLU:C	4:A:1235:LYS:CD	2.72	0.60
5:B:1064:TYR:CD1	5:B:1064:TYR:N	2.67	0.60
3:T:15:DA:H2''	3:T:16:DC:O5'	2.02	0.60
4:A:456:MET:HB2	4:A:478:TYR:OH	2.02	0.60
4:A:669:THR:HG22	4:A:761:MET:HE3	1.83	0.60
5:B:918:ILE:HD12	5:B:935:ARG:HD2	1.84	0.60
5:B:1073:TYR:CE2	5:B:1080:LYS:HG3	2.37	0.60
4:A:765:VAL:HG13	4:A:802:ASN:O	2.02	0.60
4:A:1287:TYR:OH	4:A:1307:GLU:CD	2.45	0.60
4:A:544:ASP:CG	4:A:545:GLN:N	2.56	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:811:GLN:HB3	4:A:815:PHE:HE2	1.67	0.60
4:A:1027:ALA:O	4:A:1028:THR:C	2.44	0.60
4:A:1170:ILE:HD12	4:A:1171:GLN:HG3	1.83	0.60
4:A:1345:ARG:HD2	4:A:1346:ALA:CA	2.31	0.60
4:A:666:ILE:CG2	5:B:1026:LEU:CB	2.74	0.60
4:A:1020:CYS:N	4:A:1021:LEU:O	2.35	0.60
4:A:1295:THR:HB	4:A:1297:GLU:OE1	2.02	0.60
5:B:592:ASN:HD21	5:B:595:ARG:HD2	1.65	0.59
11:J:8:PHE:HD1	11:J:49:MET:HE1	1.65	0.59
4:A:35:ILE:HG13	4:A:241:VAL:HG21	1.84	0.59
4:A:115:LEU:HB2	4:A:122:MET:HE3	1.84	0.59
4:A:313:GLN:O	4:A:321:PRO:HA	2.02	0.59
4:A:855:THR:HG23	4:A:856:THR:H	1.68	0.59
5:B:684:LEU:HD23	5:B:689:LEU:HD12	1.83	0.59
5:B:835:GLN:HA	5:B:1013:ASN:HD22	1.66	0.59
4:A:676:MET:HA	4:A:679:ILE:HD12	1.84	0.59
4:A:1022:LEU:HA	4:A:1026:LEU:CD1	2.32	0.59
13:L:30:ILE:O	13:L:56:LEU:HA	2.02	0.59
4:A:587:HIS:NE2	4:A:969:GLN:CD	2.60	0.59
4:A:1390:ASN:O	4:A:1399:ARG:HD2	2.03	0.59
5:B:634:TYR:HD2	5:B:692:TYR:CD1	2.21	0.59
7:E:15:ALA:O	7:E:19:VAL:HG23	2.03	0.59
4:A:1023:ARG:N	4:A:1025:ARG:O	2.35	0.59
4:A:1352:VAL:O	4:A:1355:VAL:HG12	2.03	0.59
4:A:115:LEU:HD21	4:A:145:LYS:HD2	1.84	0.59
4:A:598:LEU:HD13	9:H:25:ARG:HH22	1.68	0.59
4:A:1150:SER:HA	4:A:1195:LEU:HD23	1.85	0.59
5:B:202:TYR:OH	5:B:485:ARG:NH2	2.36	0.59
5:B:807:ARG:NH1	5:B:807:ARG:CG	2.62	0.59
5:B:1160:VAL:HG12	5:B:1161:HIS:N	2.18	0.59
4:A:65:LEU:CD2	4:A:72:GLU:C	2.74	0.59
4:A:508:PRO:O	4:A:511:ILE:HG13	2.03	0.59
4:A:567:LYS:HZ1	9:H:43:ASN:HB3	1.68	0.59
4:A:814:PHE:CE1	5:B:514:LEU:HD21	2.38	0.59
5:B:857:ARG:NH2	5:B:942:ARG:NH1	2.50	0.59
3:T:20:DC:H2'	3:T:21:DC:O4'	2.03	0.59
4:A:1170:ILE:CD1	4:A:1171:GLN:HG3	2.32	0.59
4:A:1424:VAL:HG13	4:A:1436:ILE:HD11	1.85	0.59
5:B:800:GLN:HB3	11:J:52:THR:HG22	1.83	0.59
4:A:465:TYR:HB3	5:B:976:ILE:HG21	1.85	0.58
4:A:1174:PHE:CA	4:A:1175:SER:HB3	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:779:PHE:CE1	5:B:517:THR:HA	2.37	0.58
5:B:179:CYS:O	5:B:181:LEU:CG	2.51	0.58
8:F:69:LEU:H	8:F:70:LYS:HB2	1.68	0.58
9:H:84:ALA:HA	9:H:87:ARG:HB2	1.83	0.58
4:A:69:THR:HA	4:A:71:GLN:HG3	1.84	0.58
4:A:314:ALA:HA	4:A:320:ARG:HB3	1.85	0.58
4:A:1025:ARG:CD	4:A:1030:ARG:NH2	2.61	0.58
4:A:1244:ARG:HH11	4:A:1244:ARG:CG	2.16	0.58
4:A:54:ASN:O	4:A:55:ASP:HB2	2.02	0.58
4:A:153:PRO:CB	4:A:154:SER:C	2.76	0.58
5:B:982:SER:HB3	5:B:1092:TYR:CZ	2.36	0.58
8:F:69:LEU:N	8:F:70:LYS:HB2	2.18	0.58
4:A:463:ILE:CD1	4:A:469:ARG:HG3	2.33	0.58
4:A:472:LEU:HD13	5:B:835:GLN:OE1	2.04	0.58
4:A:1018:PHE:O	4:A:1021:LEU:HB3	2.03	0.58
5:B:276:ILE:HG13	5:B:277:LYS:N	2.13	0.58
6:C:66:ARG:NH2	11:J:3:VAL:O	2.36	0.58
4:A:92:HIS:ND1	4:A:95:PHE:HD2	2.02	0.58
4:A:396:PRO:HB3	4:A:403:LYS:HB3	1.84	0.58
4:A:810:PRO:N	5:B:1047:PHE:HE2	1.99	0.58
4:A:830:LYS:HZ2	4:A:1080:THR:CB	2.16	0.58
5:B:37:PHE:O	5:B:38:PHE:HB2	2.03	0.58
4:A:482:PHE:CD2	5:B:836:GLU:O	2.50	0.58
4:A:779:PHE:N	4:A:779:PHE:CD1	2.68	0.58
4:A:1019:CYS:C	4:A:1021:LEU:O	2.47	0.58
4:A:1392:SER:O	4:A:1394:THR:N	2.37	0.58
5:B:711:GLU:N	5:B:712:PRO:CD	2.56	0.58
5:B:839:MET:HE3	5:B:1010:LEU:HD11	1.86	0.58
5:B:1084:GLN:OE1	5:B:1084:GLN:N	2.36	0.58
7:E:177:ARG:HD3	7:E:215:MET:HE2	1.84	0.58
5:B:406:LEU:HD12	5:B:633:VAL:CG2	2.33	0.58
5:B:578:THR:OG1	5:B:593:PRO:HG3	2.03	0.58
12:K:33:ILE:HD13	12:K:87:LEU:HD22	1.86	0.58
4:A:316:GLN:CG	4:A:317:LYS:N	2.67	0.57
4:A:519:PRO:HB2	4:A:630:ILE:HD12	1.85	0.57
5:B:204:ILE:C	5:B:205:ILE:HD13	2.24	0.57
5:B:219:ALA:HB2	5:B:405:ARG:HG2	1.86	0.57
5:B:1001:PHE:CE1	6:C:34:ARG:CZ	2.87	0.57
8:F:73:ALA:O	8:F:74:ILE:HB	2.04	0.57
8:F:116:ASP:HB3	8:F:119:ARG:HB2	1.86	0.57
4:A:80:HIS:ND1	4:A:80:HIS:N	2.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:690:VAL:HG21	4:A:718:VAL:HG13	1.86	0.57
4:A:851:HIS:N	4:A:851:HIS:CD2	2.72	0.57
5:B:202:TYR:HE1	5:B:209:GLU:CD	2.13	0.57
5:B:302:CYS:SG	5:B:310:MET:HE1	2.35	0.57
5:B:1039:GLY:HA2	11:J:51:LEU:HD22	1.86	0.57
6:C:67:LEU:HD11	6:C:155:LEU:HD13	1.85	0.57
8:F:147:SER:O	8:F:151:LEU:HD12	2.04	0.57
11:J:3:VAL:HG21	11:J:18:TRP:CB	2.33	0.57
4:A:545:GLN:HB3	4:A:549:MET:CE	2.35	0.57
4:A:588:LEU:HD13	4:A:632:VAL:HG21	1.85	0.57
4:A:853:ASP:C	4:A:855:THR:H	2.12	0.57
5:B:173:MET:HA	5:B:203:PHE:HD2	1.69	0.57
4:A:22:PHE:CD1	4:A:26:GLU:OE2	2.57	0.57
4:A:159:THR:HB	4:A:160:GLN:HA	1.87	0.57
5:B:314:LEU:HD23	5:B:317:CYS:SG	2.44	0.57
4:A:1101:LEU:HB2	4:A:1355:VAL:HG21	1.85	0.57
5:B:175:ARG:HH11	5:B:182:SER:N	2.03	0.57
4:A:1345:ARG:HD2	4:A:1346:ALA:N	2.19	0.57
4:A:316:GLN:NE2	4:A:317:LYS:CG	2.48	0.57
5:B:292:ILE:H	5:B:293:PRO:HD2	1.70	0.57
5:B:731:VAL:HG12	5:B:732:SER:N	2.19	0.57
4:A:1161:THR:HG22	4:A:1162:VAL:N	2.20	0.57
5:B:1068:GLY:HA3	5:B:1086:PHE:CE1	2.39	0.57
10:I:7:CYS:SG	10:I:9:ASP:O	2.62	0.57
11:J:6:ARG:HA	11:J:12:LYS:O	2.04	0.57
5:B:685:LEU:HD11	5:B:692:TYR:CE2	2.39	0.57
5:B:698:GLU:HA	5:B:701:ILE:CD1	2.35	0.57
4:A:399:HIS:CE1	4:A:462:VAL:HG21	2.40	0.57
5:B:637:LEU:HD13	5:B:740:HIS:CG	2.37	0.57
5:B:800:GLN:HB3	11:J:52:THR:HG21	1.85	0.57
5:B:995:ARG:HH22	12:K:9:LEU:HD11	1.69	0.57
4:A:1344:GLY:O	4:A:1345:ARG:O	2.22	0.56
5:B:824:ILE:HG12	11:J:48:ARG:HH12	1.70	0.56
4:A:49:LYS:O	4:A:50:ILE:HB	2.04	0.56
5:B:361:LEU:HD21	5:B:377:PHE:HD2	1.71	0.56
5:B:744:HIS:CD2	5:B:746:SER:H	2.23	0.56
8:F:69:LEU:CA	8:F:70:LYS:HB2	2.35	0.56
4:A:10:PRO:O	5:B:1193:GLN:HB3	2.05	0.56
4:A:90:VAL:CA	4:A:297:GLN:OE1	2.52	0.56
4:A:354:SER:HA	4:A:482:PHE:HD1	1.71	0.56
4:A:779:PHE:O	4:A:780:VAL:C	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:845:LEU:O	4:A:846:GLU:C	2.47	0.56
4:A:939:ASP:CG	4:A:1023:ARG:HH11	2.12	0.56
4:A:939:ASP:OD1	4:A:1023:ARG:NH1	2.39	0.56
4:A:1017:LEU:HB2	7:E:205:SER:HA	1.85	0.56
5:B:785:TYR:CE1	11:J:60:PHE:CE1	2.94	0.56
5:B:803:LEU:HD12	5:B:822:ASN:CG	2.30	0.56
5:B:983:ARG:HD2	5:B:1091:TYR:HB3	1.88	0.56
7:E:202:SER:OG	7:E:204:THR:HG22	2.04	0.56
5:B:301:ILE:O	5:B:303:TYR:CE2	2.59	0.56
6:C:173:ALA:O	6:C:233:GLU:O	2.23	0.56
4:A:225:ASN:HD22	4:A:227:VAL:H	1.54	0.56
4:A:476:SER:N	4:A:477:PRO:HD2	2.20	0.56
4:A:524:VAL:HG12	4:A:525:GLN:N	2.20	0.56
5:B:226:PHE:HD2	5:B:398:ARG:NH2	2.03	0.56
11:J:64:ASN:HB3	11:J:65:PRO:HD3	1.87	0.56
4:A:11:LEU:HD12	5:B:1194:ILE:HA	1.87	0.56
4:A:447:GLN:HA	4:A:448:PRO:C	2.30	0.56
4:A:777:PHE:CD1	4:A:782:ARG:N	2.73	0.56
5:B:202:TYR:O	5:B:204:ILE:CD1	2.52	0.56
5:B:523:CYS:SG	5:B:750:GLY:N	2.78	0.56
5:B:1065:GLN:NE2	5:B:1067:ARG:N	2.30	0.56
5:B:1124:ARG:NH1	5:B:1124:ARG:CG	2.65	0.56
7:E:52:ARG:CB	7:E:53:PRO:CD	2.80	0.56
4:A:47:ARG:HH12	5:B:920:PRO:HB2	1.69	0.56
4:A:883:LEU:HD22	4:A:1020:CYS:O	2.06	0.56
4:A:1187:GLN:HE21	4:A:1187:GLN:N	2.03	0.56
5:B:302:CYS:CA	5:B:310:MET:HE1	2.34	0.56
5:B:341:LEU:HB2	5:B:344:LYS:HE3	1.88	0.56
4:A:956:LEU:HD11	4:A:1017:LEU:HD22	1.87	0.56
5:B:173:MET:CA	5:B:203:PHE:HB3	2.32	0.56
5:B:969:ARG:NE	6:C:61:GLU:OE1	2.39	0.56
5:B:797:TYR:HB3	5:B:798:TYR:CE1	2.39	0.56
4:A:81:PHE:O	4:A:241:VAL:O	2.23	0.56
4:A:351:THR:CG2	4:A:352:VAL:N	2.69	0.56
5:B:292:ILE:HD12	5:B:327:ARG:H	1.70	0.56
5:B:291:ILE:HG12	5:B:300:HIS:CE1	2.41	0.55
5:B:542:MET:HB3	5:B:636:PRO:HD3	1.87	0.55
5:B:851:PHE:CD1	5:B:1094:ARG:HB2	2.39	0.55
5:B:1160:VAL:O	5:B:1161:HIS:ND1	2.40	0.55
4:A:351:THR:HG21	4:A:466:SER:O	2.06	0.55
4:A:587:HIS:CE1	4:A:969:GLN:CD	2.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:177:LYS:C	5:B:177:LYS:CD	2.75	0.55
5:B:637:LEU:HD11	5:B:740:HIS:CE1	2.41	0.55
4:A:826:ASP:O	4:A:830:LYS:N	2.37	0.55
4:A:1162:VAL:C	4:A:1163:ILE:HG13	2.32	0.55
5:B:201:GLY:N	5:B:202:TYR:HD2	2.03	0.55
5:B:203:PHE:C	5:B:204:ILE:CG1	2.79	0.55
4:A:315:LEU:HG	4:A:316:GLN:HB2	1.89	0.55
5:B:179:CYS:O	5:B:181:LEU:CD1	2.54	0.55
9:H:82:PRO:O	9:H:83:GLN:HB2	2.06	0.55
4:A:1011:GLN:O	4:A:1015:VAL:HG23	2.05	0.55
4:A:1161:THR:HG21	4:A:1239:ARG:HH22	1.70	0.55
5:B:301:ILE:HG21	5:B:314:LEU:HD11	1.87	0.55
5:B:955:THR:HG22	5:B:956:THR:N	2.12	0.55
7:E:124:VAL:HB	7:E:125:PRO:HD3	1.88	0.55
10:I:7:CYS:SG	10:I:10:CYS:O	2.65	0.55
4:A:857:ARG:NH2	8:F:139:PRO:CG	2.42	0.55
5:B:234:ILE:HA	5:B:259:TYR:HA	1.89	0.55
5:B:879:ARG:NH1	5:B:879:ARG:HB3	2.21	0.55
5:B:104:GLU:OE2	13:L:54:ARG:NH1	2.39	0.55
11:J:3:VAL:HG21	11:J:18:TRP:CG	2.42	0.55
4:A:810:PRO:N	5:B:1047:PHE:CE2	2.74	0.55
5:B:172:ILE:O	5:B:203:PHE:HB2	2.04	0.55
5:B:996:ARG:NH2	6:C:174:ALA:O	2.40	0.55
5:B:1179:GLN:O	5:B:1180:PHE:CD1	2.60	0.55
4:A:1232:ASN:HA	4:A:1233:ASP:O	2.07	0.55
5:B:766:ARG:HH21	5:B:1020:ARG:HB3	1.72	0.55
5:B:824:ILE:HG12	11:J:48:ARG:NH1	2.22	0.55
9:H:95:TYR:HE2	9:H:97:MET:HG3	1.72	0.55
4:A:1234:GLU:O	4:A:1235:LYS:CD	2.54	0.55
5:B:173:MET:O	5:B:176:SER:HB3	2.07	0.55
5:B:879:ARG:NE	5:B:879:ARG:H	2.03	0.55
4:A:91:PHE:N	4:A:297:GLN:OE1	2.40	0.54
4:A:156:ASP:C	4:A:157:ASP:CG	2.74	0.54
4:A:1027:ALA:HB3	4:A:1030:ARG:HB2	1.88	0.54
5:B:290:GLY:CA	5:B:327:ARG:HH11	2.17	0.54
5:B:290:GLY:HA2	5:B:327:ARG:NH1	2.18	0.54
5:B:322:PHE:C	5:B:322:PHE:HD2	2.14	0.54
11:J:5:VAL:O	11:J:6:ARG:O	2.25	0.54
12:K:65:HIS:CD2	12:K:66:PRO:HD2	2.42	0.54
5:B:803:LEU:HD12	5:B:822:ASN:OD1	2.06	0.54
8:F:72:LYS:HB3	8:F:73:ALA:CB	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:253:ASN:ND2	4:A:256:GLN:H	1.89	0.54
4:A:590:ARG:O	4:A:591:PHE:HB2	2.07	0.54
5:B:33:VAL:HG21	5:B:638:PHE:CZ	2.43	0.54
5:B:890:TYR:CE1	5:B:910:VAL:HG21	2.42	0.54
6:C:99:LEU:CD2	6:C:120:ILE:HA	2.36	0.54
6:C:99:LEU:HB2	6:C:157:CYS:HB2	1.89	0.54
6:C:244:VAL:HG21	12:K:105:PHE:CZ	2.42	0.54
4:A:1171:GLN:OE1	4:A:1171:GLN:N	2.41	0.54
4:A:51:GLY:HA2	4:A:56:PRO:CG	2.37	0.54
5:B:363:HIS:HD2	5:B:585:VAL:HG22	1.71	0.54
5:B:1077:THR:HG23	5:B:1079:LYS:H	1.72	0.54
4:A:441:PRO:HD3	4:A:498:ARG:HH21	1.72	0.54
4:A:795:GLU:CD	5:B:731:VAL:HG13	2.33	0.54
4:A:841:LEU:HD23	4:A:1384:VAL:HG11	1.90	0.54
4:A:868:TYR:HE1	4:A:1064:VAL:HG11	1.71	0.54
5:B:798:TYR:CD2	11:J:4:PRO:HG3	2.43	0.54
13:L:38:LEU:HD21	13:L:49:LYS:HG2	1.89	0.54
4:A:14:VAL:H	4:A:1432:GLN:NE2	2.03	0.54
4:A:315:LEU:HB2	4:A:320:ARG:CZ	2.37	0.54
5:B:114:PRO:HG3	5:B:181:LEU:HD11	1.88	0.54
5:B:302:CYS:CA	5:B:310:MET:CE	2.85	0.54
8:F:69:LEU:H	8:F:70:LYS:CB	2.20	0.54
9:H:104:PHE:CZ	9:H:136:LYS:HA	2.43	0.54
4:A:642:CYS:O	4:A:645:LEU:HB3	2.07	0.54
4:A:690:VAL:CG2	4:A:718:VAL:HG13	2.37	0.54
5:B:181:LEU:C	5:B:183:GLU:N	2.62	0.54
5:B:290:GLY:HA3	5:B:327:ARG:HH12	1.71	0.54
4:A:1291:VAL:HG13	4:A:1292:PRO:HD2	1.90	0.54
4:A:777:PHE:CD1	4:A:782:ARG:C	2.77	0.53
4:A:1340:GLY:HA3	7:E:184:VAL:HG23	1.90	0.53
5:B:1023:VAL:O	5:B:1027:ILE:HG13	2.08	0.53
7:E:177:ARG:HG2	7:E:215:MET:HG3	1.90	0.53
4:A:17:VAL:HB	4:A:1419:ASP:HB3	1.90	0.53
4:A:1196:GLU:HG2	4:A:1197:LEU:N	2.23	0.53
5:B:698:GLU:HA	5:B:701:ILE:HD13	1.89	0.53
4:A:92:HIS:CD2	4:A:304:MET:HE1	2.43	0.53
4:A:635:ARG:HH21	4:A:877:HIS:HA	1.73	0.53
4:A:855:THR:OG1	4:A:865:GLN:O	2.24	0.53
5:B:29:ASP:HB3	5:B:658:ILE:HD13	1.89	0.53
4:A:1364:ASN:HD22	4:A:1366:ARG:CG	2.22	0.53
5:B:175:ARG:NH1	5:B:182:SER:CA	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:217:ARG:HH11	5:B:407:ASP:CG	2.16	0.53
6:C:214:ASN:O	6:C:216:GLY:N	2.41	0.53
7:E:171:LYS:HB2	7:E:174:GLN:HG3	1.90	0.53
4:A:795:GLU:CD	5:B:731:VAL:CG1	2.81	0.53
5:B:181:LEU:O	5:B:183:GLU:N	2.42	0.53
5:B:710:LEU:O	5:B:711:GLU:CB	2.56	0.53
5:B:302:CYS:SG	5:B:310:MET:HE3	2.22	0.53
5:B:809:MET:HE1	5:B:983:ARG:HH22	1.73	0.53
4:A:22:PHE:HD2	5:B:1211:ASN:HA	1.74	0.53
5:B:912:ILE:HD11	5:B:966:VAL:HG23	1.90	0.53
6:C:242:GLN:HA	6:C:245:VAL:HB	1.90	0.53
5:B:101:MET:HG3	5:B:169:ARG:HH12	1.74	0.53
5:B:238:ALA:HB3	5:B:256:VAL:HB	1.90	0.53
5:B:1163:CYS:SG	5:B:1166:CYS:SG	2.99	0.53
4:A:23:SER:O	4:A:27:VAL:HG23	2.07	0.53
4:A:449:SER:OG	5:B:1134:GLU:OE2	2.21	0.53
4:A:518:LYS:HB2	4:A:519:PRO:HD2	1.91	0.53
5:B:33:VAL:HG21	5:B:638:PHE:CE1	2.44	0.53
5:B:640:VAL:HG23	5:B:740:HIS:HA	1.91	0.53
4:A:354:SER:HA	4:A:482:PHE:CD1	2.45	0.53
4:A:370:ILE:HG22	4:A:374:LEU:HD12	1.90	0.53
4:A:403:LYS:HA	4:A:415:LEU:HB2	1.91	0.53
4:A:497:THR:HG21	5:B:1146:PHE:HD1	1.74	0.53
4:A:1023:ARG:O	4:A:1024:SER:HB2	2.09	0.53
5:B:67:SER:HB2	5:B:92:PHE:HB2	1.91	0.53
5:B:516:ASN:HD22	5:B:516:ASN:N	1.97	0.53
5:B:567:GLU:OE1	5:B:567:GLU:N	2.42	0.53
10:I:68:LEU:HB3	10:I:84:VAL:CG1	2.39	0.53
4:A:4:GLN:OE1	5:B:1159:ARG:NH1	2.42	0.52
4:A:22:PHE:HE2	5:B:1212:ILE:H	1.56	0.52
4:A:579:SER:HB3	4:A:611:GLN:HA	1.91	0.52
4:A:830:LYS:HZ3	4:A:1081:LEU:H	1.57	0.52
4:A:1021:LEU:HA	4:A:1024:SER:OG	2.10	0.52
4:A:1026:LEU:HD13	4:A:1026:LEU:H	1.65	0.52
5:B:51:PHE:HD2	5:B:176:SER:OG	1.92	0.52
5:B:315:LYS:N	5:B:316:PRO:HD2	2.23	0.52
5:B:986:GLN:NE2	5:B:1020:ARG:CD	2.72	0.52
1:R:9:G:C2	3:T:21:DC:O2	2.63	0.52
4:A:1207:LEU:HG	4:A:1274:ARG:NH2	2.25	0.52
4:A:1317:MET:HA	4:A:1322:ILE:HD11	1.91	0.52
5:B:55:VAL:HG11	5:B:177:LYS:HZ2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:778:MET:HE3	5:B:794:ASN:OD1	2.09	0.52
4:A:22:PHE:CE2	5:B:1212:ILE:N	2.78	0.52
4:A:777:PHE:HE1	4:A:782:ARG:HA	1.66	0.52
5:B:40:GLU:OE2	5:B:681:TRP:CB	2.58	0.52
5:B:57:TYR:O	5:B:58:THR:C	2.51	0.52
5:B:459:TYR:C	5:B:459:TYR:CD2	2.88	0.52
7:E:52:ARG:HB2	7:E:53:PRO:CD	2.26	0.52
11:J:48:ARG:HE	11:J:49:MET:HE2	1.74	0.52
5:B:175:ARG:NH1	5:B:181:LEU:C	2.67	0.52
5:B:619:ILE:HG13	10:I:65:ASP:HB2	1.92	0.52
5:B:986:GLN:NE2	5:B:1020:ARG:HD2	2.21	0.52
5:B:1065:GLN:NE2	5:B:1066:SER:N	2.57	0.52
9:H:93:TYR:HA	9:H:145:ARG:HB3	1.91	0.52
4:A:542:GLU:O	4:A:546:VAL:HG23	2.09	0.52
4:A:850:VAL:CG1	4:A:851:HIS:N	2.72	0.52
5:B:198:ASP:CG	5:B:202:TYR:HH	2.18	0.52
5:B:634:TYR:CE2	5:B:692:TYR:CD1	2.98	0.52
5:B:1034:VAL:HG22	5:B:1059:LEU:HD13	1.91	0.52
5:B:1073:TYR:HE2	5:B:1080:LYS:CG	2.22	0.52
5:B:1202:LEU:C	5:B:1202:LEU:HD23	2.34	0.52
4:A:68:GLN:HG3	4:A:68:GLN:O	2.08	0.52
4:A:153:PRO:CB	4:A:154:SER:O	2.58	0.52
4:A:1234:GLU:HB3	4:A:1235:LYS:CE	2.39	0.52
4:A:22:PHE:HE2	5:B:1212:ILE:N	2.08	0.52
4:A:58:LEU:HD22	4:A:59:GLY:H	1.68	0.52
4:A:1384:VAL:C	4:A:1389:PHE:HE1	2.17	0.52
5:B:302:CYS:HA	5:B:310:MET:CE	2.38	0.52
11:J:36:LEU:HD11	11:J:51:LEU:HB2	1.92	0.52
2:N:2:DT:H3	3:T:13:DA:H61	1.55	0.52
4:A:41:MET:C	4:A:50:ILE:HD12	2.33	0.52
4:A:472:LEU:O	4:A:475:THR:HB	2.10	0.52
4:A:666:ILE:HD11	5:B:1030:LEU:HD22	1.91	0.52
5:B:1047:PHE:HD1	5:B:1047:PHE:H	1.58	0.52
4:A:852:TYR:CE1	8:F:136:ARG:HG2	2.45	0.52
5:B:226:PHE:CD1	5:B:226:PHE:N	2.78	0.52
4:A:252:PHE:O	4:A:252:PHE:CD2	2.63	0.51
4:A:587:HIS:CD2	4:A:609:ASP:H	2.28	0.51
4:A:901:LEU:H	4:A:926:GLN:NE2	2.08	0.51
4:A:1035:TYR:CD2	4:A:1035:TYR:O	2.64	0.51
5:B:177:LYS:HE2	5:B:178:ASN:CG	2.34	0.51
5:B:642:ASP:O	5:B:644:GLU:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1001:PHE:CD1	6:C:34:ARG:NH2	2.78	0.51
8:F:93:ILE:CD1	8:F:134:ILE:HD11	2.40	0.51
4:A:68:GLN:C	4:A:70:CYS:N	2.61	0.51
4:A:707:GLY:HA3	4:A:1281:ARG:HG3	1.91	0.51
4:A:731:ARG:HG2	4:A:755:PHE:CZ	2.45	0.51
5:B:684:LEU:HD23	5:B:689:LEU:CD1	2.40	0.51
4:A:496:GLU:HG2	8:F:95:GLY:O	2.11	0.51
4:A:1266:THR:HG22	4:A:1266:THR:O	2.10	0.51
5:B:55:VAL:HG11	5:B:177:LYS:HZ3	1.75	0.51
4:A:544:ASP:OD2	4:A:545:GLN:HG3	2.10	0.51
4:A:618:GLU:CD	4:A:618:GLU:C	2.78	0.51
4:A:1229:SER:OG	4:A:1236:LEU:HD12	2.06	0.51
5:B:470:LYS:C	5:B:472:ALA:H	2.18	0.51
6:C:114:TYR:CD2	6:C:140:ASN:HB3	2.45	0.51
4:A:239:LEU:HD12	4:A:240:PRO:HD2	1.92	0.51
4:A:316:GLN:CA	4:A:318:SER:N	2.64	0.51
4:A:1170:ILE:CB	4:A:1171:GLN:CA	2.77	0.51
5:B:361:LEU:HD21	5:B:377:PHE:CD2	2.46	0.51
4:A:265:LYS:HD2	4:A:303:TYR:HA	1.92	0.51
4:A:795:GLU:OE1	5:B:731:VAL:CG2	2.58	0.51
4:A:1209:MET:HG3	4:A:1230:GLU:O	2.11	0.51
4:A:1344:GLY:O	4:A:1345:ARG:C	2.54	0.51
4:A:68:GLN:O	4:A:68:GLN:CD	2.54	0.51
4:A:845:LEU:HD12	4:A:1069:ALA:HB2	1.93	0.51
5:B:40:GLU:OE2	5:B:681:TRP:CA	2.58	0.51
6:C:77:ILE:O	6:C:77:ILE:HD13	2.10	0.51
4:A:406:ILE:HB	4:A:431:LYS:HB2	1.93	0.51
4:A:569:LYS:HD2	4:A:571:LEU:CD1	2.32	0.51
4:A:1434:ALA:O	4:A:1436:ILE:N	2.43	0.51
5:B:202:TYR:CZ	5:B:485:ARG:NH2	2.78	0.51
5:B:1175:LEU:C	5:B:1177:HIS:H	2.19	0.51
4:A:151:ASP:CA	4:A:152:VAL:CB	2.65	0.51
4:A:313:GLN:OE1	4:A:322:VAL:HG11	2.10	0.51
4:A:365:GLY:HA3	4:A:469:ARG:HB2	1.92	0.51
4:A:337:ARG:NH2	4:A:839:ARG:HD2	2.25	0.50
4:A:567:LYS:CG	4:A:568:PRO:HD2	2.40	0.50
4:A:1287:TYR:CD2	4:A:1305:VAL:HG21	2.42	0.50
4:A:1345:ARG:CD	4:A:1346:ALA:N	2.74	0.50
4:A:1364:ASN:ND2	4:A:1366:ARG:CG	2.66	0.50
6:C:167:HIS:CD2	13:L:70:ARG:HB3	2.45	0.50
4:A:821:ARG:NH1	5:B:514:LEU:HD13	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:852:TYR:CZ	8:F:136:ARG:HG2	2.46	0.50
4:A:457:ALA:HB3	4:A:506:ALA:HA	1.93	0.50
4:A:1193:LEU:O	4:A:1193:LEU:HG	2.10	0.50
5:B:120:ARG:HG2	5:B:955:THR:HG21	1.92	0.50
4:A:325:ILE:CG2	5:B:1210:MET:SD	2.99	0.50
5:B:1016:ALA:C	5:B:1017:ILE:HG13	2.33	0.50
8:F:82:THR:HG22	8:F:84:TYR:H	1.77	0.50
9:H:95:TYR:CE2	9:H:97:MET:HG3	2.46	0.50
4:A:355:GLY:N	4:A:482:PHE:CE1	2.79	0.50
4:A:496:GLU:HG2	8:F:95:GLY:C	2.35	0.50
5:B:373:ARG:HA	5:B:566:LEU:HD23	1.93	0.50
5:B:1017:ILE:HB	5:B:1018:PRO:HD2	1.94	0.50
6:C:31:ASN:O	6:C:35:ARG:HG3	2.12	0.50
9:H:82:PRO:C	9:H:84:ALA:H	2.18	0.50
1:R:4:G:H2'	1:R:5:A:C8	2.45	0.50
4:A:939:ASP:CG	4:A:1023:ARG:NH1	2.70	0.50
5:B:200:GLY:CA	5:B:202:TYR:CD2	2.85	0.50
5:B:950:ASP:OD2	5:B:967:ARG:NH2	2.29	0.50
6:C:93:ASP:OD1	6:C:122:SER:HB2	2.11	0.50
10:I:33:SER:O	10:I:34:TYR:C	2.55	0.50
10:I:33:SER:O	10:I:35:VAL:HG23	2.11	0.50
4:A:58:LEU:HG	4:A:80:HIS:C	2.36	0.50
5:B:809:MET:HE1	5:B:983:ARG:NH2	2.26	0.50
5:B:1027:ILE:O	5:B:1028:GLU:C	2.54	0.50
4:A:353:ILE:HD13	4:A:487:MET:HE1	1.90	0.50
4:A:468:PHE:CE1	4:A:489:LEU:HD13	2.47	0.50
4:A:631:HIS:CE1	4:A:879:GLU:HG2	2.47	0.50
5:B:63:ILE:HD11	5:B:95:ILE:HD12	1.92	0.50
5:B:785:TYR:CE1	11:J:60:PHE:HE1	2.30	0.50
7:E:113:GLN:HB3	7:E:137:GLU:OE1	2.12	0.50
4:A:899:VAL:HB	4:A:929:LEU:HD12	1.93	0.50
5:B:234:ILE:HD13	5:B:257:LYS:HD3	1.94	0.50
5:B:376:PHE:CE2	5:B:569:TYR:HD2	2.29	0.50
5:B:1017:ILE:CB	5:B:1018:PRO:CD	2.89	0.50
7:E:89:GLY:O	7:E:91:LYS:N	2.45	0.50
4:A:1363:VAL:HB	4:A:1368:MET:CE	2.37	0.49
5:B:48:LEU:HD22	5:B:175:ARG:C	2.35	0.49
10:I:27:PHE:O	10:I:35:VAL:HG13	2.12	0.49
4:A:497:THR:CG2	5:B:1146:PHE:HD1	2.25	0.49
4:A:646:PHE:O	4:A:647:GLY:C	2.55	0.49
5:B:1084:GLN:N	5:B:1084:GLN:CD	2.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:316:GLN:C	4:A:318:SER:N	2.70	0.49
4:A:1339:LEU:HD13	7:E:147:HIS:CD2	2.47	0.49
4:A:106:VAL:HG11	4:A:214:ILE:HD11	1.93	0.49
4:A:336:ILE:H	4:A:336:ILE:HD12	1.77	0.49
4:A:598:LEU:O	4:A:599:SER:C	2.56	0.49
4:A:612:ILE:O	4:A:612:ILE:HG13	2.11	0.49
4:A:1436:ILE:HD13	5:B:1139:ILE:HG23	1.93	0.49
5:B:515:HIS:H	5:B:518:HIS:CD2	2.29	0.49
4:A:1231:ASP:C	4:A:1233:ASP:N	2.71	0.49
5:B:334:ILE:O	5:B:336:ARG:HG3	2.13	0.49
5:B:797:TYR:HE1	5:B:854:LEU:HG	1.76	0.49
5:B:1028:GLU:O	5:B:1029:CYS:C	2.55	0.49
6:C:43:THR:OG1	6:C:44:LEU:N	2.45	0.49
7:E:89:GLY:HA2	7:E:120:ALA:HB2	1.95	0.49
4:A:381:THR:O	4:A:383:TYR:N	2.45	0.49
4:A:779:PHE:O	4:A:782:ARG:O	2.30	0.49
4:A:947:PHE:CD1	4:A:954:TRP:CE2	3.00	0.49
5:B:749:LEU:HD22	5:B:753:ALA:HB1	1.95	0.49
5:B:1124:ARG:O	5:B:1125:ASP:C	2.54	0.49
5:B:1155:SER:OG	5:B:1156:ASP:N	2.45	0.49
8:F:71:GLU:HB3	8:F:72:LYS:O	2.12	0.49
4:A:99:ILE:HG13	4:A:234:MET:SD	2.53	0.49
4:A:334:GLY:O	4:A:336:ILE:N	2.45	0.49
5:B:728:ARG:CD	5:B:730:ARG:HH22	2.17	0.49
4:A:830:LYS:HZ2	4:A:1080:THR:CA	2.21	0.49
5:B:179:CYS:O	5:B:181:LEU:HG	2.13	0.49
7:E:176:PRO:O	7:E:212:ARG:HA	2.13	0.49
4:A:22:PHE:HB2	5:B:1211:ASN:OD1	2.13	0.49
4:A:830:LYS:HZ3	4:A:1080:THR:CA	2.14	0.49
4:A:1206:ASP:C	4:A:1274:ARG:HH22	2.20	0.49
4:A:1436:ILE:O	4:A:1437:GLY:C	2.54	0.49
5:B:203:PHE:HE1	5:B:461:LEU:HD22	1.76	0.49
5:B:515:HIS:N	5:B:518:HIS:HD2	2.10	0.49
5:B:976:ILE:O	5:B:990:ILE:O	2.31	0.49
7:E:19:VAL:O	7:E:23:VAL:HG23	2.12	0.49
4:A:1030:ARG:NH1	4:A:1030:ARG:CG	2.65	0.49
5:B:226:PHE:HD1	5:B:226:PHE:N	2.08	0.49
5:B:226:PHE:CD2	5:B:398:ARG:NH2	2.81	0.49
6:C:184:ASN:HD21	6:C:189:THR:H	1.61	0.49
13:L:31:CYS:HB2	13:L:48:CYS:SG	2.53	0.49
4:A:73:GLY:C	4:A:75:ASN:N	2.70	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:266:LEU:HA	4:A:269:ILE:HD12	1.94	0.48
4:A:795:GLU:OE2	5:B:731:VAL:HG13	2.11	0.48
4:A:993:LEU:HD22	4:A:1046:LEU:HG	1.94	0.48
5:B:341:LEU:HD12	5:B:344:LYS:CE	2.42	0.48
5:B:824:ILE:HD12	11:J:44:TYR:HE1	1.78	0.48
5:B:1000:PRO:HB2	5:B:1072:MET:HE3	1.94	0.48
5:B:1064:TYR:O	5:B:1065:GLN:O	2.30	0.48
6:C:3:GLU:HB3	12:K:104:ASN:OD1	2.12	0.48
4:A:35:ILE:HG21	4:A:84:ILE:HD13	1.94	0.48
4:A:413:ILE:N	4:A:413:ILE:HD12	2.28	0.48
4:A:565:ILE:CG2	4:A:567:LYS:HG2	2.43	0.48
4:A:1022:LEU:HA	4:A:1026:LEU:HD11	1.95	0.48
4:A:1441:PHE:HE2	8:F:89:GLU:HG3	1.73	0.48
5:B:98:THR:OG1	5:B:126:SER:HB2	2.13	0.48
5:B:756:ILE:HG12	5:B:770:GLN:HG2	1.95	0.48
5:B:810:GLU:O	5:B:811:TYR:C	2.56	0.48
6:C:91:HIS:CE1	6:C:158:VAL:HG21	2.47	0.48
4:A:90:VAL:HG13	4:A:297:GLN:NE2	2.28	0.48
4:A:315:LEU:O	4:A:316:GLN:HB3	2.12	0.48
4:A:857:ARG:HG2	4:A:863:VAL:CA	2.16	0.48
4:A:918:GLU:OE2	4:A:918:GLU:C	2.57	0.48
5:B:25:ILE:HG22	5:B:26:THR:N	2.28	0.48
5:B:322:PHE:HE1	10:I:30:ARG:HD2	1.78	0.48
5:B:363:HIS:O	5:B:364:ILE:HB	2.13	0.48
5:B:732:SER:HB3	5:B:734:HIS:CD2	2.49	0.48
5:B:851:PHE:HD1	5:B:1094:ARG:HB2	1.78	0.48
4:A:92:HIS:HE2	4:A:304:MET:HE1	1.77	0.48
4:A:1244:ARG:CB	4:A:1244:ARG:NH1	2.50	0.48
5:B:955:THR:HG23	13:L:54:ARG:O	2.13	0.48
4:A:567:LYS:HB3	9:H:96:VAL:H	1.79	0.48
4:A:795:GLU:OE1	5:B:731:VAL:CG1	2.62	0.48
5:B:252:SER:HB3	5:B:362:PRO:HG2	1.95	0.48
5:B:294:ASP:HA	5:B:297:ILE:CG1	2.43	0.48
5:B:569:TYR:CZ	5:B:589:VAL:HG21	2.48	0.48
5:B:1028:GLU:O	5:B:1031:LEU:N	2.46	0.48
5:B:1212:ILE:O	5:B:1214:PRO:HD3	2.14	0.48
4:A:1026:LEU:O	4:A:1027:ALA:CB	2.61	0.48
5:B:44:VAL:CG1	5:B:495:LEU:HD13	2.42	0.48
5:B:515:HIS:HD2	5:B:517:THR:OG1	1.97	0.48
11:J:3:VAL:HG21	11:J:18:TRP:HB2	1.94	0.48
4:A:605:MET:HA	4:A:605:MET:HE3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:199:MET:N	5:B:199:MET:SD	2.83	0.48
5:B:357:GLN:HA	5:B:374:LYS:NZ	2.28	0.48
4:A:308:ILE:CG1	4:A:309:ALA:H	2.27	0.48
4:A:633:VAL:HG13	4:A:637:LYS:HG3	1.96	0.48
4:A:842:VAL:HG11	5:B:1136:ASP:OD2	2.14	0.48
4:A:1116:LEU:CD2	4:A:1311:VAL:HA	2.44	0.48
5:B:199:MET:SD	5:B:200:GLY:N	2.86	0.48
6:C:148:ARG:NH1	11:J:64:ASN:HA	2.29	0.48
7:E:185:ALA:HA	7:E:190:LEU:HD23	1.95	0.48
4:A:598:LEU:HB3	9:H:25:ARG:HH22	1.78	0.48
4:A:790:ASP:HB3	10:I:87:GLN:HG3	1.96	0.48
4:A:1064:VAL:O	4:A:1065:GLY:C	2.56	0.48
4:A:1151:GLU:O	4:A:1193:LEU:HD12	2.13	0.48
4:A:1271:ILE:O	4:A:1271:ILE:HG22	2.13	0.47
5:B:326:ASP:O	5:B:327:ARG:C	2.56	0.47
5:B:703:ILE:HA	5:B:740:HIS:O	2.14	0.47
6:C:71:PRO:HB2	6:C:133:ILE:HD13	1.96	0.47
4:A:76:GLU:OE2	5:B:1159:ARG:NH1	2.45	0.47
4:A:326:ARG:HG2	4:A:1406:VAL:HG21	1.96	0.47
5:B:259:TYR:OH	5:B:279:ASP:OD2	2.32	0.47
5:B:542:MET:HG2	5:B:747:MET:HB3	1.96	0.47
4:A:150:THR:O	4:A:151:ASP:CG	2.57	0.47
4:A:1144:LYS:HD2	4:A:1269:GLU:OE2	2.14	0.47
5:B:174:LEU:C	5:B:176:SER:H	2.23	0.47
5:B:203:PHE:C	5:B:204:ILE:HG13	2.38	0.47
5:B:492:LEU:HB2	5:B:751:VAL:HG11	1.96	0.47
7:E:205:SER:O	7:E:206:GLY:C	2.56	0.47
9:H:93:TYR:CD1	9:H:143:LEU:HD22	2.49	0.47
9:H:110:ASP:OD2	9:H:110:ASP:N	2.48	0.47
10:I:54:GLU:OE2	10:I:118:ARG:NH1	2.47	0.47
4:A:563:PRO:HB3	4:A:572:TRP:CE2	2.48	0.47
4:A:577:ILE:H	4:A:577:ILE:HG13	1.60	0.47
5:B:660:LYS:HE3	5:B:679:TYR:CD1	2.50	0.47
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.49	0.47
5:B:879:ARG:CZ	5:B:879:ARG:CA	2.92	0.47
5:B:1159:ARG:HD3	5:B:1193:GLN:HG3	1.96	0.47
5:B:1202:LEU:HD21	5:B:1206:GLU:OE2	2.15	0.47
4:A:474:VAL:HG12	4:A:478:TYR:CE2	2.48	0.47
4:A:637:LYS:CD	4:A:637:LYS:N	2.72	0.47
4:A:856:THR:HB	4:A:865:GLN:HB2	1.96	0.47
5:B:40:GLU:CD	5:B:682:SER:H	2.19	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:999:MET:HG2	5:B:1008:PRO:HD2	1.97	0.47
5:B:1065:GLN:OE1	5:B:1067:ARG:N	2.47	0.47
1:R:9:G:N2	3:T:21:DC:H1'	2.29	0.47
4:A:404:TYR:HA	4:A:413:ILE:O	2.14	0.47
4:A:807:GLY:HA3	5:B:728:ARG:HH12	1.77	0.47
4:A:1345:ARG:O	4:A:1346:ALA:C	2.54	0.47
4:A:1428:VAL:HG21	5:B:1135:ARG:HD2	1.97	0.47
5:B:483:LEU:O	5:B:484:ASN:CB	2.62	0.47
5:B:778:MET:HE3	5:B:794:ASN:HB3	1.95	0.47
6:C:52:GLU:HB3	6:C:154:LYS:HB3	1.95	0.47
4:A:569:LYS:O	4:A:571:LEU:CD1	2.54	0.47
4:A:588:LEU:HB3	4:A:607:ILE:HB	1.96	0.47
4:A:1244:ARG:NH1	4:A:1244:ARG:CG	2.76	0.47
5:B:292:ILE:N	5:B:293:PRO:HD2	2.29	0.47
5:B:337:ARG:HD3	5:B:337:ARG:HA	1.55	0.47
5:B:350:GLN:HE22	5:B:353:LYS:HD3	1.79	0.47
5:B:364:ILE:HD13	5:B:585:VAL:HG13	1.96	0.47
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.96	0.47
5:B:1024:ALA:HA	5:B:1027:ILE:HD12	1.97	0.47
5:B:1060:ARG:O	5:B:1061:GLU:C	2.57	0.47
5:B:1073:TYR:CE2	5:B:1080:LYS:CG	2.98	0.47
4:A:526:ASP:HB2	5:B:835:GLN:NE2	2.30	0.47
4:A:675:THR:HG22	4:A:679:ILE:HD11	1.96	0.47
4:A:1418:LEU:HD13	5:B:1222:ARG:HD2	1.97	0.47
5:B:839:MET:HB3	5:B:1012:ILE:HG22	1.96	0.47
7:E:114:ASN:HD22	7:E:114:ASN:HA	1.54	0.47
4:A:43:GLU:HG3	4:A:43:GLU:O	2.15	0.47
5:B:203:PHE:CE1	5:B:461:LEU:HD22	2.46	0.47
5:B:323:VAL:HG12	5:B:324:ILE:HG12	1.96	0.47
5:B:546:SER:OG	5:B:631:GLY:N	2.42	0.47
5:B:857:ARG:NH2	5:B:942:ARG:HH12	2.11	0.47
6:C:162:GLY:HA3	6:C:170:TRP:CD2	2.50	0.47
4:A:78:PRO:HA	5:B:1201:LYS:HE3	1.96	0.47
4:A:451:HIS:NE2	4:A:1074:GLU:HG3	2.29	0.47
4:A:741:ASN:C	4:A:741:ASN:ND2	2.73	0.47
4:A:1234:GLU:CB	4:A:1235:LYS:HD3	2.40	0.47
5:B:44:VAL:O	5:B:45:SER:C	2.58	0.47
5:B:294:ASP:HA	5:B:297:ILE:HG13	1.97	0.47
4:A:476:SER:N	4:A:477:PRO:CD	2.77	0.46
4:A:490:HIS:HB3	5:B:1150:ARG:NH2	2.31	0.46
4:A:857:ARG:NH2	8:F:139:PRO:CB	2.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:203:PHE:C	5:B:204:ILE:CD1	2.87	0.46
5:B:337:ARG:O	5:B:339:THR:N	2.48	0.46
10:I:65:ASP:HA	10:I:66:PRO:HD3	1.67	0.46
4:A:482:PHE:C	4:A:484:GLY:H	2.24	0.46
4:A:1364:ASN:HD21	4:A:1366:ARG:HG2	1.74	0.46
5:B:236:HIS:CD2	5:B:389:ALA:HB2	2.44	0.46
5:B:321:GLY:O	5:B:323:VAL:N	2.48	0.46
11:J:8:PHE:H	11:J:49:MET:HE3	1.80	0.46
4:A:483:ASP:OD1	4:A:485:ASP:OD1	2.33	0.46
4:A:589:GLN:HB3	4:A:961:ARG:NH2	2.30	0.46
4:A:810:PRO:HG3	5:B:1047:PHE:CD2	2.51	0.46
5:B:547:VAL:HG12	5:B:612:GLU:OE2	2.15	0.46
5:B:635:ARG:HB2	5:B:636:PRO:CD	2.45	0.46
6:C:73:GLN:O	6:C:129:ILE:HD12	2.15	0.46
8:F:81:THR:HG21	8:F:136:ARG:HD3	1.98	0.46
8:F:135:ARG:HG2	8:F:145:ASP:OD1	2.15	0.46
12:K:12:LEU:H	12:K:12:LEU:HD12	1.80	0.46
4:A:347:PHE:CE1	4:A:375:THR:HG22	2.43	0.46
4:A:523:ILE:HG23	4:A:527:THR:HB	1.97	0.46
4:A:547:LEU:HD22	12:K:58:PHE:HD1	1.80	0.46
4:A:1021:LEU:CA	4:A:1024:SER:OG	2.63	0.46
5:B:202:TYR:HA	5:B:203:PHE:O	2.15	0.46
5:B:376:PHE:HB3	5:B:586:TRP:CZ3	2.50	0.46
5:B:973:ILE:HG23	5:B:974:PRO:HD2	1.97	0.46
4:A:73:GLY:O	4:A:76:GLU:N	2.48	0.46
4:A:519:PRO:HG3	4:A:630:ILE:HG13	1.97	0.46
4:A:575:LYS:HB3	4:A:612:ILE:HD11	1.98	0.46
4:A:1284:MET:HG2	4:A:1306:LEU:CD2	2.46	0.46
5:B:224:GLN:HA	5:B:396:ASP:OD2	2.16	0.46
5:B:1149:GLU:HG3	5:B:1153:GLU:OE1	2.14	0.46
8:F:107:VAL:HG12	8:F:109:VAL:H	1.80	0.46
13:L:48:CYS:SG	13:L:51:CYS:SG	3.14	0.46
4:A:530:GLY:O	4:A:534:LEU:N	2.46	0.46
4:A:624:SER:HA	4:A:630:ILE:HD11	1.97	0.46
5:B:650:GLU:HG3	5:B:651:LEU:N	2.31	0.46
5:B:878:GLN:HA	5:B:879:ARG:HH21	1.79	0.46
1:R:3:C:H4'	4:A:323:LYS:NZ	2.30	0.46
4:A:67:CYS:CB	4:A:70:CYS:HB3	2.44	0.46
4:A:156:ASP:O	4:A:157:ASP:CG	2.58	0.46
4:A:907:THR:HG22	4:A:908:LEU:N	2.30	0.46
5:B:325:GLN:HE22	10:I:12:ASN:HD21	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:518:HIS:CE1	5:B:537:LYS:HE2	2.50	0.46
5:B:526:GLU:HG2	5:B:538:ASN:ND2	2.31	0.46
5:B:1179:GLN:O	5:B:1180:PHE:HD1	1.98	0.46
12:K:37:LYS:O	12:K:38:GLU:HG2	2.15	0.46
4:A:1173:HIS:O	4:A:1174:PHE:CD1	2.68	0.46
5:B:911:ILE:HG22	5:B:912:ILE:HG13	1.98	0.46
4:A:495:GLU:O	4:A:498:ARG:HB2	2.16	0.46
4:A:587:HIS:CE1	4:A:969:GLN:NE2	2.82	0.46
4:A:649:ILE:O	4:A:653:VAL:HG23	2.16	0.46
4:A:846:GLU:C	4:A:848:ILE:H	2.24	0.46
4:A:1243:VAL:HG12	4:A:1244:ARG:H	1.81	0.46
4:A:1327:ILE:O	4:A:1327:ILE:HG23	2.16	0.46
5:B:37:PHE:O	5:B:38:PHE:CB	2.64	0.46
5:B:299:GLU:CD	5:B:571:PRO:HG2	2.41	0.46
5:B:1017:ILE:N	5:B:1018:PRO:HD2	2.30	0.46
5:B:1202:LEU:HD23	5:B:1202:LEU:O	2.16	0.46
6:C:115:SER:OG	6:C:141:GLY:O	2.21	0.46
4:A:315:LEU:O	4:A:316:GLN:CB	2.64	0.46
4:A:470:LEU:C	4:A:470:LEU:HD12	2.41	0.46
4:A:886:ILE:HD11	4:A:943:LEU:HB3	1.97	0.46
5:B:115:GLN:HG2	5:B:193:LYS:HB2	1.98	0.46
8:F:103:MET:O	8:F:104:ASN:C	2.59	0.46
13:L:48:CYS:SG	13:L:49:LYS:N	2.88	0.46
4:A:855:THR:CG2	4:A:856:THR:N	2.72	0.45
4:A:1116:LEU:HD22	4:A:1311:VAL:HA	1.97	0.45
4:A:1279:ILE:HA	4:A:1310:GLY:HA3	1.97	0.45
5:B:102:VAL:O	5:B:102:VAL:HG12	2.16	0.45
5:B:785:TYR:HE1	11:J:60:PHE:CZ	2.34	0.45
5:B:1016:ALA:O	5:B:1017:ILE:HB	2.16	0.45
6:C:134:ILE:HD13	6:C:139:GLY:O	2.16	0.45
9:H:38:LEU:CD1	9:H:123:MET:HE2	2.35	0.45
3:T:27:DA:H2'	3:T:27:DA:N3	2.32	0.45
4:A:741:ASN:C	4:A:741:ASN:HD22	2.24	0.45
4:A:830:LYS:NZ	4:A:1080:THR:HG23	2.32	0.45
4:A:851:HIS:O	4:A:853:ASP:OD1	2.34	0.45
4:A:1022:LEU:O	4:A:1022:LEU:HD23	2.16	0.45
5:B:483:LEU:CD1	5:B:491:THR:HG23	2.46	0.45
5:B:486:TYR:OH	5:B:1096:ARG:HB3	2.16	0.45
5:B:1051:THR:O	5:B:1054:GLY:N	2.49	0.45
9:H:5:LEU:HD22	9:H:133:ASN:O	2.17	0.45
5:B:113:TYR:HB3	5:B:114:PRO:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:177:LYS:HG3	5:B:178:ASN:N	2.31	0.45
5:B:329:THR:O	5:B:332:ASP:HB3	2.17	0.45
5:B:744:HIS:HD2	5:B:746:SER:CB	2.29	0.45
6:C:80:LEU:HD12	6:C:127:ARG:NH2	2.32	0.45
10:I:68:LEU:HB3	10:I:84:VAL:HG13	1.99	0.45
12:K:58:PHE:HB3	12:K:76:GLN:HB3	1.97	0.45
4:A:1345:ARG:O	4:A:1347:ALA:N	2.49	0.45
5:B:175:ARG:CA	5:B:179:CYS:SG	3.04	0.45
5:B:955:THR:CG2	5:B:956:THR:H	2.10	0.45
4:A:590:ARG:NH2	4:A:592:ASP:OD2	2.30	0.45
4:A:608:ILE:HG12	4:A:613:ILE:HG13	1.98	0.45
4:A:666:ILE:HG22	5:B:1026:LEU:HB2	1.96	0.45
4:A:775:ILE:O	4:A:797:LYS:HE2	2.16	0.45
4:A:784:LEU:HB3	4:A:786:HIS:HD2	1.82	0.45
4:A:909:ASP:C	4:A:911:SER:H	2.24	0.45
4:A:1209:MET:SD	4:A:1236:LEU:CD2	2.94	0.45
4:A:1216:ILE:O	4:A:1219:THR:OG1	2.33	0.45
4:A:1236:LEU:O	4:A:1237:ILE:HG13	2.16	0.45
5:B:405:ARG:CZ	5:B:632:ARG:HG2	2.47	0.45
5:B:903:VAL:HG12	5:B:904:ARG:N	2.29	0.45
5:B:1065:GLN:HG2	5:B:1069:PHE:HB2	1.98	0.45
5:B:1160:VAL:CG1	5:B:1161:HIS:H	2.22	0.45
6:C:51:VAL:HG22	6:C:155:LEU:CD2	2.47	0.45
4:A:208:LEU:HD22	4:A:212:LYS:HG3	1.99	0.45
4:A:447:GLN:H	4:A:447:GLN:HG2	1.67	0.45
4:A:596:THR:C	4:A:598:LEU:N	2.64	0.45
4:A:857:ARG:HH11	4:A:863:VAL:CG2	2.19	0.45
4:A:1288:ASP:OD1	4:A:1300:LYS:NZ	2.49	0.45
5:B:299:GLU:OE2	5:B:571:PRO:HG2	2.17	0.45
5:B:827:ILE:HG23	5:B:1012:ILE:HD12	1.98	0.45
5:B:956:THR:HA	5:B:961:LEU:O	2.17	0.45
5:B:1037:LEU:O	11:J:47:ARG:NH1	2.50	0.45
9:H:139:ASN:O	9:H:140:ALA:HB2	2.17	0.45
13:L:32:ALA:HB3	13:L:55:ILE:CD1	2.44	0.45
4:A:308:ILE:HG13	4:A:309:ALA:H	1.81	0.45
5:B:343:ILE:O	5:B:344:LYS:HG3	2.16	0.45
5:B:635:ARG:HH22	5:B:742:GLU:CD	2.24	0.45
5:B:1107:ALA:O	5:B:1108:ARG:HB3	2.17	0.45
8:F:82:THR:HG22	8:F:84:TYR:HB2	1.99	0.45
4:A:73:GLY:O	4:A:74:MET:C	2.60	0.45
4:A:341:MET:HE3	5:B:1132:GLU:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:456:MET:HE3	4:A:478:TYR:CE2	2.52	0.45
4:A:809:THR:H	4:A:812:GLU:HB2	1.82	0.45
4:A:1100:ARG:HH21	4:A:1351:GLU:HG2	1.81	0.45
4:A:1169:ILE:HG22	4:A:1169:ILE:O	2.17	0.45
4:A:1233:ASP:C	4:A:1235:LYS:N	2.75	0.45
6:C:18:VAL:CG2	6:C:240:VAL:HB	2.47	0.45
9:H:30:SER:HB2	9:H:36:CYS:SG	2.57	0.45
4:A:19:PHE:CD2	4:A:1412:ALA:HB1	2.43	0.45
4:A:451:HIS:CE1	4:A:1074:GLU:HG3	2.52	0.45
4:A:463:ILE:HD13	4:A:469:ARG:CG	2.46	0.45
4:A:946:VAL:HG22	7:E:201:LYS:HB3	1.99	0.45
5:B:115:GLN:HE21	5:B:119:LEU:HD11	1.82	0.45
5:B:174:LEU:C	5:B:176:SER:N	2.73	0.45
5:B:464:GLY:HA2	5:B:479:VAL:O	2.18	0.45
5:B:1068:GLY:HA3	5:B:1086:PHE:HD1	1.79	0.45
4:A:31:SER:CB	4:A:82:GLY:HA2	2.21	0.44
4:A:120:GLU:HG3	4:A:123:ARG:HD3	1.99	0.44
4:A:605:MET:HE3	4:A:614:PHE:O	2.17	0.44
4:A:1031:VAL:HG13	4:A:1037:LEU:HD12	1.98	0.44
6:C:235:VAL:HG21	11:J:6:ARG:HH21	1.81	0.44
4:A:325:ILE:HG22	4:A:326:ARG:N	2.31	0.44
5:B:494:HIS:HD2	5:B:497:ARG:NH1	2.15	0.44
5:B:1087:PHE:CE2	11:J:44:TYR:OH	2.70	0.44
4:A:325:ILE:O	4:A:328:ARG:N	2.33	0.44
4:A:586:ILE:HD11	4:A:637:LYS:CE	2.47	0.44
4:A:810:PRO:HD3	5:B:1047:PHE:HD2	1.82	0.44
4:A:1063:MET:CG	4:A:1436:ILE:HG23	2.46	0.44
5:B:31:TRP:HA	5:B:34:ILE:HD13	1.99	0.44
5:B:48:LEU:CD2	5:B:175:ARG:C	2.88	0.44
5:B:201:GLY:HA3	5:B:495:LEU:HD22	1.99	0.44
4:A:33:ALA:O	4:A:83:HIS:CD2	2.70	0.44
4:A:38:PRO:HA	4:A:270:LEU:HD13	2.00	0.44
4:A:72:GLU:CD	4:A:76:GLU:HG2	2.43	0.44
4:A:666:ILE:HA	5:B:1026:LEU:HD13	1.99	0.44
5:B:202:TYR:CD1	5:B:209:GLU:HB3	2.48	0.44
12:K:65:HIS:CG	12:K:66:PRO:HD2	2.53	0.44
4:A:22:PHE:HZ	5:B:1208:MET:HG2	1.82	0.44
4:A:260:ASP:OD1	4:A:261:ASP:N	2.50	0.44
4:A:533:LYS:HB2	4:A:533:LYS:HE2	1.65	0.44
4:A:566:ILE:HG22	4:A:566:ILE:O	2.18	0.44
4:A:855:THR:OG1	4:A:866:PHE:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1234:GLU:C	4:A:1235:LYS:CG	2.90	0.44
3:T:20:DC:H5"	5:B:1129:ARG:HD3	1.98	0.44
4:A:452:LYS:NZ	4:A:1067:LEU:HD22	2.32	0.44
4:A:553:VAL:HG13	4:A:648:ASN:HB3	1.98	0.44
4:A:779:PHE:N	4:A:779:PHE:HD1	2.13	0.44
4:A:810:PRO:CD	5:B:1047:PHE:HD2	2.31	0.44
4:A:1154:TYR:CE1	10:I:18:GLU:HG3	2.52	0.44
4:A:1400:CYS:O	4:A:1402:PHE:N	2.42	0.44
5:B:834:ASN:O	5:B:1013:ASN:HB2	2.17	0.44
9:H:145:ARG:HD2	9:H:146:ARG:HD2	1.99	0.44
5:B:341:LEU:HD12	5:B:344:LYS:HE3	2.00	0.44
5:B:550:ASP:OD1	5:B:551:PRO:HD2	2.18	0.44
4:A:264:PHE:HE1	4:A:317:LYS:H	1.54	0.44
4:A:316:GLN:NE2	4:A:317:LYS:HG2	2.23	0.44
4:A:455:MET:HG3	5:B:1137:CYS:CB	2.48	0.44
4:A:1424:VAL:HG11	5:B:1139:ILE:HD13	2.00	0.44
5:B:34:ILE:HD11	5:B:743:ILE:HG22	1.98	0.44
5:B:224:GLN:O	5:B:238:ALA:HA	2.18	0.44
5:B:258:LEU:HB2	5:B:385:LEU:HD21	1.99	0.44
5:B:468:GLU:HB3	5:B:469:GLN:H	1.53	0.44
5:B:1060:ARG:HA	5:B:1060:ARG:HD2	1.71	0.44
6:C:73:GLN:HE21	6:C:74:SER:H	1.65	0.44
12:K:65:HIS:HD2	12:K:67:PHE:H	1.65	0.44
4:A:244:PRO:HD2	4:A:245:PRO:HD3	1.99	0.44
4:A:320:ARG:CD	4:A:320:ARG:H	2.23	0.44
4:A:516:SER:O	4:A:517:ASN:C	2.60	0.44
4:A:588:LEU:CB	4:A:607:ILE:HB	2.48	0.44
4:A:618:GLU:O	4:A:622:VAL:HG12	2.17	0.44
4:A:857:ARG:CD	4:A:863:VAL:HG22	2.44	0.44
5:B:744:HIS:CD2	5:B:746:SER:HB3	2.52	0.44
5:B:997:GLU:CD	5:B:997:GLU:H	2.26	0.44
5:B:1084:GLN:CD	5:B:1084:GLN:H	2.26	0.44
6:C:184:ASN:ND2	6:C:189:THR:O	2.51	0.44
9:H:115:TYR:CE2	9:H:124:ARG:HG3	2.52	0.44
9:H:118:PHE:HB2	9:H:121:LEU:HB2	2.00	0.44
4:A:56:PRO:O	4:A:57:ARG:HB2	2.17	0.43
4:A:107:CYS:HB3	4:A:114:LEU:HD21	1.99	0.43
4:A:777:PHE:HB2	4:A:780:VAL:O	2.16	0.43
4:A:1170:ILE:C	4:A:1172:LEU:H	2.26	0.43
5:B:254:LEU:HD12	5:B:272:THR:O	2.18	0.43
5:B:754:SER:O	5:B:806:THR:OG1	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:872:GLU:HG2	5:B:916:THR:HB	2.00	0.43
5:B:1013:ASN:OD1	5:B:1014:PRO:HD2	2.18	0.43
5:B:1156:ASP:OD2	5:B:1198:TYR:N	2.50	0.43
7:E:100:ILE:HG23	7:E:105:PHE:HB2	2.00	0.43
10:I:87:GLN:HE22	10:I:97:MET:HG3	1.83	0.43
4:A:41:MET:HA	4:A:50:ILE:CD1	2.46	0.43
4:A:783:THR:HG21	4:A:815:PHE:CE1	2.36	0.43
4:A:837:ILE:HD13	4:A:840:ARG:HH12	1.83	0.43
5:B:547:VAL:HG12	5:B:612:GLU:CD	2.42	0.43
5:B:1006:ILE:CD1	11:J:43:ARG:HB2	2.48	0.43
4:A:93:VAL:HG21	4:A:304:MET:HB2	2.00	0.43
4:A:304:MET:HE3	5:B:1210:MET:HA	1.99	0.43
4:A:315:LEU:HB2	4:A:320:ARG:NH1	2.33	0.43
4:A:355:GLY:CA	4:A:482:PHE:CE1	3.02	0.43
4:A:807:GLY:HA3	5:B:728:ARG:NH1	2.33	0.43
4:A:1097:GLY:C	4:A:1099:PRO:HD2	2.43	0.43
4:A:1153:TYR:HD2	4:A:1163:ILE:HD11	1.84	0.43
5:B:45:SER:OG	5:B:46:GLN:N	2.49	0.43
5:B:482:VAL:O	5:B:483:LEU:C	2.61	0.43
8:F:72:LYS:CE	8:F:72:LYS:HA	2.48	0.43
4:A:159:THR:HB	4:A:160:GLN:HG3	2.00	0.43
4:A:456:MET:HE1	4:A:521:MET:HE2	2.00	0.43
4:A:1021:LEU:HA	4:A:1024:SER:CB	2.46	0.43
4:A:1209:MET:HE3	4:A:1228:TRP:HB2	2.00	0.43
5:B:350:GLN:NE2	5:B:353:LYS:HD3	2.34	0.43
5:B:766:ARG:HD3	5:B:766:ARG:HA	1.80	0.43
5:B:899:ILE:HD11	5:B:911:ILE:CG1	2.42	0.43
6:C:53:THR:O	6:C:153:LEU:HA	2.18	0.43
9:H:56:THR:O	9:H:144:ILE:HA	2.19	0.43
4:A:1017:LEU:O	4:A:1017:LEU:HD23	2.18	0.43
4:A:1215:ARG:C	4:A:1219:THR:HG23	2.30	0.43
4:A:1230:GLU:HB3	4:A:1231:ASP:H	1.68	0.43
5:B:202:TYR:CA	5:B:203:PHE:O	2.66	0.43
5:B:429:PHE:O	5:B:433:GLN:HG3	2.19	0.43
5:B:890:TYR:HB3	5:B:893:LEU:HD12	2.01	0.43
5:B:1064:TYR:C	5:B:1065:GLN:O	2.60	0.43
5:B:1081:LEU:HD13	5:B:1085:ILE:HD11	2.00	0.43
6:C:60:ASP:HB3	13:L:67:PHE:CE1	2.54	0.43
7:E:9:ILE:O	7:E:13:TRP:N	2.43	0.43
4:A:709:THR:HG21	10:I:93:LYS:O	2.18	0.43
4:A:840:ARG:O	4:A:841:LEU:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:875:ALA:HA	4:A:878:ILE:HD12	1.99	0.43
4:A:1161:THR:CG2	4:A:1162:VAL:N	2.82	0.43
5:B:28:GLU:O	5:B:30:SER:N	2.51	0.43
5:B:800:GLN:CB	11:J:52:THR:HG22	2.48	0.43
5:B:1136:ASP:HA	5:B:1139:ILE:HD12	2.00	0.43
4:A:7:SER:HB2	5:B:1193:GLN:OE1	2.19	0.43
4:A:157:ASP:C	4:A:158:PRO:O	2.60	0.43
4:A:873:MET:HB3	4:A:878:ILE:HD11	2.00	0.43
4:A:1098:VAL:N	4:A:1099:PRO:CD	2.77	0.43
5:B:54:PHE:HA	5:B:58:THR:HB	1.99	0.43
5:B:285:ILE:O	5:B:288:ALA:HB3	2.18	0.43
5:B:335:GLY:HA3	5:B:336:ARG:HA	1.71	0.43
5:B:801:LYS:O	11:J:52:THR:HG23	2.18	0.43
5:B:835:GLN:HA	5:B:1013:ASN:ND2	2.34	0.43
4:A:153:PRO:CB	4:A:154:SER:OG	2.67	0.43
4:A:575:LYS:NZ	4:A:602:ASP:OD2	2.52	0.43
4:A:779:PHE:HB2	4:A:782:ARG:O	2.18	0.43
4:A:873:MET:HG2	4:A:957:PRO:CG	2.39	0.43
4:A:894:GLU:O	4:A:895:LYS:C	2.62	0.43
4:A:915:SER:O	4:A:918:GLU:HG3	2.18	0.43
5:B:48:LEU:HD23	5:B:173:MET:SD	2.59	0.43
5:B:67:SER:HB2	5:B:92:PHE:HD2	1.84	0.43
5:B:876:LYS:HA	5:B:877:PRO:HD3	1.78	0.43
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.51	0.43
4:A:12:ARG:NH1	5:B:1192:TYR:CE1	2.87	0.43
4:A:694:THR:HA	4:A:714:PHE:HE1	1.83	0.43
4:A:779:PHE:HA	5:B:699:GLU:OE1	2.18	0.43
4:A:1392:SER:C	4:A:1394:THR:H	2.27	0.43
5:B:287:ARG:HA	5:B:291:ILE:O	2.19	0.43
5:B:954:VAL:O	13:L:55:ILE:O	2.37	0.43
5:B:1027:ILE:HG13	5:B:1027:ILE:H	1.71	0.43
9:H:38:LEU:HD13	9:H:125:LEU:HD13	2.01	0.43
4:A:264:PHE:CE1	4:A:317:LYS:CG	3.01	0.43
4:A:775:ILE:H	4:A:775:ILE:HG12	1.53	0.43
4:A:1025:ARG:C	4:A:1026:LEU:HD12	2.41	0.43
5:B:128:LEU:O	5:B:129:PHE:CD1	2.72	0.43
5:B:530:GLY:O	5:B:531:GLN:C	2.62	0.43
5:B:1065:GLN:CD	5:B:1067:ARG:N	2.71	0.43
5:B:1152:MET:O	5:B:1157:ALA:HB2	2.19	0.43
9:H:41:ASP:OD2	9:H:122:LEU:N	2.49	0.43
4:A:308:ILE:HG13	4:A:309:ALA:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:850:LEU:O	5:B:851:PHE:C	2.62	0.42
12:K:61:TYR:HB3	12:K:73:LEU:HD12	2.01	0.42
3:T:28:DT:C1'	4:A:317:LYS:O	2.62	0.42
4:A:399:HIS:O	4:A:401:GLY:N	2.44	0.42
4:A:542:GLU:C	4:A:544:ASP:OD1	2.62	0.42
4:A:841:LEU:HD21	4:A:1105:LEU:HD22	2.00	0.42
4:A:983:ILE:HD13	4:A:983:ILE:HA	1.81	0.42
4:A:1173:HIS:C	4:A:1174:PHE:CG	2.94	0.42
4:A:1220:PHE:HD1	4:A:1220:PHE:HA	1.72	0.42
5:B:112:LEU:HD12	5:B:116:GLU:HB3	2.00	0.42
5:B:1010:LEU:HD12	5:B:1010:LEU:HA	1.81	0.42
6:C:57:VAL:HG11	11:J:60:PHE:HB3	2.00	0.42
9:H:125:LEU:HG	9:H:130:ARG:NH1	2.35	0.42
4:A:26:GLU:O	4:A:27:VAL:C	2.61	0.42
4:A:73:GLY:O	4:A:75:ASN:N	2.52	0.42
4:A:78:PRO:HA	5:B:1201:LYS:CE	2.49	0.42
4:A:618:GLU:OE1	4:A:619:LYS:N	2.52	0.42
4:A:635:ARG:HD3	4:A:635:ARG:HA	1.76	0.42
4:A:1279:ILE:HG13	4:A:1308:THR:HG21	2.00	0.42
5:B:301:ILE:HG22	5:B:302:CYS:N	2.33	0.42
5:B:759:PRO:CG	5:B:1046:PRO:HG3	2.49	0.42
4:A:65:LEU:HB3	4:A:72:GLU:H	1.85	0.42
4:A:155:GLU:HG3	4:A:156:ASP:HB3	2.02	0.42
5:B:209:GLU:OE1	5:B:485:ARG:NE	2.45	0.42
5:B:378:LEU:HA	5:B:381:MET:HE3	2.00	0.42
5:B:1008:PRO:HG2	5:B:1011:ILE:HD11	2.00	0.42
5:B:1159:ARG:HH11	5:B:1159:ARG:CB	2.03	0.42
6:C:36:VAL:HG21	6:C:251:LEU:HD13	2.01	0.42
6:C:41:ILE:HD11	6:C:243:VAL:HG13	2.01	0.42
4:A:376:TYR:HA	4:A:377:PRO:HD2	1.95	0.42
6:C:123:ASN:HD22	6:C:125:MET:HG2	1.84	0.42
6:C:252:GLN:HG3	12:K:95:ILE:HG23	2.02	0.42
4:A:91:PHE:H	4:A:297:GLN:CD	2.26	0.42
4:A:335:ARG:H	4:A:335:ARG:HE	1.67	0.42
4:A:417:TYR:OH	5:B:887:HIS:NE2	2.31	0.42
4:A:774:ARG:O	4:A:775:ILE:C	2.63	0.42
4:A:1345:ARG:C	4:A:1345:ARG:CD	2.92	0.42
5:B:260:GLY:O	5:B:267:ARG:HD3	2.20	0.42
5:B:830:TYR:CE2	5:B:1000:PRO:HD3	2.54	0.42
4:A:534:LEU:O	4:A:574:GLY:HA3	2.20	0.42
4:A:567:LYS:HB2	9:H:95:TYR:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:741:ASN:HD22	4:A:744:LYS:H	1.68	0.42
4:A:898:ARG:HB2	4:A:933:TYR:CE1	2.54	0.42
4:A:947:PHE:CD1	4:A:954:TRP:CZ2	3.07	0.42
4:A:1022:LEU:HA	4:A:1026:LEU:HD13	2.01	0.42
5:B:62:ILE:HD12	5:B:418:LYS:HE2	2.01	0.42
5:B:179:CYS:O	5:B:181:LEU:HB2	2.19	0.42
5:B:198:ASP:OD1	5:B:485:ARG:NH2	2.52	0.42
5:B:841:MET:SD	5:B:990:ILE:HD11	2.59	0.42
6:C:18:VAL:HG22	6:C:240:VAL:HB	2.01	0.42
4:A:80:HIS:O	4:A:243:PRO:HB3	2.19	0.42
4:A:399:HIS:NE2	4:A:462:VAL:HG21	2.34	0.42
4:A:412:ARG:NH2	4:A:433:GLU:OE2	2.52	0.42
4:A:547:LEU:HB3	12:K:58:PHE:CE1	2.55	0.42
9:H:109:LYS:HD2	9:H:111:LEU:HD12	2.02	0.42
3:T:18:DA:H2'	3:T:19:DT:C6	2.55	0.42
4:A:69:THR:CA	4:A:71:GLN:HG3	2.47	0.42
4:A:242:PRO:O	4:A:247:ARG:NH2	2.52	0.42
4:A:541:ILE:HD13	4:A:577:ILE:HG12	1.99	0.42
4:A:1187:GLN:N	4:A:1187:GLN:NE2	2.67	0.42
4:A:1274:ARG:HE	4:A:1274:ARG:HB2	1.69	0.42
5:B:710:LEU:HD23	5:B:733:HIS:HA	2.01	0.42
5:B:840:ILE:HB	5:B:1011:ILE:HB	2.00	0.42
4:A:523:ILE:O	4:A:523:ILE:HG22	2.19	0.42
4:A:679:ILE:O	4:A:682:THR:HB	2.19	0.42
5:B:1037:LEU:CD2	11:J:44:TYR:HB3	2.49	0.42
13:L:55:ILE:O	13:L:56:LEU:HB2	2.19	0.42
4:A:78:PRO:CA	5:B:1201:LYS:HE2	2.50	0.41
4:A:853:ASP:C	4:A:855:THR:N	2.77	0.41
4:A:1441:PHE:HE1	8:F:92:ARG:HD3	1.85	0.41
5:B:225:VAL:HG13	5:B:385:LEU:HD12	2.01	0.41
5:B:299:GLU:OE2	5:B:571:PRO:CD	2.64	0.41
6:C:10:ILE:HD13	6:C:20:PHE:HB3	2.02	0.41
7:E:28:TYR:HE1	7:E:78:LEU:HD13	1.84	0.41
8:F:72:LYS:HB3	8:F:73:ALA:HB2	2.02	0.41
4:A:55:ASP:O	4:A:56:PRO:C	2.62	0.41
4:A:529:CYS:O	4:A:533:LYS:HG2	2.20	0.41
4:A:853:ASP:O	4:A:853:ASP:CG	2.64	0.41
4:A:1231:ASP:C	4:A:1233:ASP:CG	2.88	0.41
4:A:618:GLU:CD	4:A:620:LYS:H	2.28	0.41
4:A:1441:PHE:HZ	8:F:89:GLU:HA	1.79	0.41
5:B:28:GLU:C	5:B:30:SER:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:200:GLY:C	5:B:202:TYR:HD2	2.29	0.41
5:B:797:TYR:C	5:B:798:TYR:CD1	2.99	0.41
5:B:812:LEU:HD22	5:B:812:LEU:HA	1.84	0.41
5:B:896:ASP:OD2	13:L:58:LYS:HE2	2.19	0.41
6:C:171:GLY:HA2	6:C:172:PRO:HD3	1.82	0.41
8:F:81:THR:HG22	8:F:82:THR:N	2.34	0.41
8:F:147:SER:C	8:F:149:GLU:H	2.28	0.41
11:J:8:PHE:CD1	11:J:49:MET:CE	3.01	0.41
1:R:6:G:H2'	1:R:7:A:H8	1.85	0.41
4:A:69:THR:CG2	5:B:1174:LYS:HE3	2.47	0.41
4:A:452:LYS:O	4:A:455:MET:HB2	2.20	0.41
4:A:474:VAL:HG12	4:A:474:VAL:O	2.19	0.41
4:A:500:GLU:OE2	5:B:1143:ALA:CB	2.68	0.41
4:A:779:PHE:CE1	5:B:517:THR:CG2	2.95	0.41
4:A:1100:ARG:C	4:A:1102:LYS:N	2.78	0.41
4:A:1170:ILE:HG13	4:A:1171:GLN:HG3	2.02	0.41
5:B:345:LYS:CG	5:B:348:ARG:HH21	2.33	0.41
5:B:420:LEU:HD21	5:B:456:GLY:HA3	2.02	0.41
5:B:918:ILE:HG22	5:B:920:PRO:HD3	2.02	0.41
6:C:32:SER:O	6:C:36:VAL:HG23	2.20	0.41
4:A:451:HIS:CB	4:A:453:MET:N	2.70	0.41
4:A:525:GLN:HG3	5:B:836:GLU:HG2	2.02	0.41
4:A:897:TYR:HE1	4:A:1024:SER:O	2.04	0.41
5:B:63:ILE:O	5:B:67:SER:HB3	2.21	0.41
5:B:287:ARG:HG2	5:B:292:ILE:HA	2.01	0.41
5:B:356:LEU:HA	5:B:360:PHE:HB3	2.03	0.41
5:B:899:ILE:HD11	5:B:911:ILE:HA	2.02	0.41
5:B:955:THR:CG2	5:B:956:THR:N	2.78	0.41
5:B:983:ARG:HD2	5:B:1091:TYR:HD2	1.85	0.41
6:C:48:SER:HB3	6:C:158:VAL:HB	2.01	0.41
7:E:55:ARG:HB3	7:E:82:PHE:HB3	2.02	0.41
4:A:77:CYS:HA	4:A:78:PRO:HD3	1.85	0.41
4:A:474:VAL:CG1	4:A:478:TYR:HE2	2.34	0.41
4:A:500:GLU:OE2	5:B:1144:ALA:N	2.53	0.41
4:A:567:LYS:O	4:A:569:LYS:N	2.53	0.41
4:A:779:PHE:HE1	5:B:517:THR:HA	1.85	0.41
4:A:853:ASP:O	4:A:853:ASP:OD1	2.39	0.41
4:A:1024:SER:HB3	4:A:1025:ARG:CA	2.50	0.41
4:A:1173:HIS:O	4:A:1174:PHE:CB	2.67	0.41
5:B:38:PHE:O	5:B:42:GLY:N	2.52	0.41
5:B:526:GLU:HG2	5:B:538:ASN:HD22	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:636:PRO:O	5:B:637:LEU:HG	2.21	0.41
5:B:711:GLU:N	5:B:712:PRO:HD2	2.28	0.41
5:B:785:TYR:CE1	11:J:60:PHE:CZ	3.08	0.41
5:B:841:MET:SD	5:B:846:ILE:HD11	2.61	0.41
9:H:130:ARG:HB3	9:H:134:ASN:HB2	2.03	0.41
4:A:91:PHE:HD2	4:A:297:GLN:CD	2.28	0.41
4:A:132:LYS:NZ	4:A:1399:ARG:HH12	2.19	0.41
4:A:598:LEU:HA	9:H:122:LEU:HD13	2.03	0.41
4:A:715:GLU:OE2	4:A:774:ARG:HD3	2.21	0.41
4:A:840:ARG:HE	4:A:1385:THR:HG22	1.86	0.41
4:A:1234:GLU:HB3	4:A:1235:LYS:HE2	2.03	0.41
4:A:1316:VAL:O	4:A:1322:ILE:HD11	2.21	0.41
4:A:1407:GLU:CD	4:A:1407:GLU:N	2.71	0.41
5:B:483:LEU:HB3	5:B:484:ASN:H	1.63	0.41
5:B:554:ILE:HD11	5:B:609:ILE:HG23	2.01	0.41
5:B:879:ARG:O	5:B:880:THR:OG1	2.34	0.41
7:E:23:VAL:HG12	7:E:28:TYR:HB2	2.02	0.41
3:T:26:DG:C2	3:T:27:DA:C8	3.09	0.41
4:A:1170:ILE:CG1	4:A:1171:GLN:HG3	2.51	0.41
4:A:1340:GLY:H	7:E:183:PRO:HG2	1.86	0.41
5:B:315:LYS:N	5:B:316:PRO:CD	2.83	0.41
5:B:315:LYS:HG3	10:I:13:MET:HE1	2.03	0.41
5:B:549:THR:HG22	5:B:550:ASP:H	1.85	0.41
5:B:773:MET:O	5:B:776:GLN:N	2.47	0.41
6:C:114:TYR:CG	6:C:140:ASN:HB3	2.56	0.41
8:F:70:LYS:HD3	8:F:70:LYS:HA	1.84	0.41
12:K:7:PHE:HA	12:K:10:PHE:CE2	2.56	0.41
4:A:69:THR:C	4:A:71:GLN:HG3	2.46	0.41
4:A:414:ASP:O	4:A:417:TYR:O	2.39	0.41
4:A:586:ILE:CD1	4:A:637:LYS:HE3	2.50	0.41
4:A:846:GLU:O	4:A:848:ILE:N	2.53	0.41
4:A:1022:LEU:CA	4:A:1025:ARG:O	2.69	0.41
4:A:1195:LEU:HD11	4:A:1267:MET:HE3	2.03	0.41
4:A:1271:ILE:HG22	4:A:1273:LEU:HD12	2.03	0.41
4:A:1277:GLU:O	4:A:1278:ASN:HB2	2.21	0.41
4:A:1293:SER:HB2	4:A:1299:VAL:HG23	2.03	0.41
4:A:1410:PHE:HD2	5:B:1212:ILE:HD11	1.86	0.41
5:B:170:LEU:HA	5:B:171:PRO:HD2	1.84	0.41
5:B:310:MET:O	5:B:313:MET:HB2	2.20	0.41
5:B:324:ILE:O	5:B:324:ILE:HG22	2.20	0.41
5:B:333:PHE:O	5:B:333:PHE:CG	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:879:ARG:NH1	5:B:879:ARG:CB	2.83	0.41
5:B:970:THR:HG22	5:B:971:THR:O	2.21	0.41
5:B:1161:HIS:CE1	5:B:1193:GLN:HB2	2.55	0.41
6:C:73:GLN:HB3	6:C:131:HIS:H	1.86	0.41
13:L:48:CYS:CB	13:L:51:CYS:SG	3.08	0.41
4:A:250:ILE:CD1	4:A:254:GLU:CD	2.94	0.41
4:A:380:VAL:HG22	4:A:388:LEU:HD13	2.02	0.41
5:B:292:ILE:N	5:B:293:PRO:CD	2.84	0.41
5:B:1019:SER:OG	16:B:1308[A]:DUT:H2'1	2.20	0.41
5:B:1065:GLN:CD	5:B:1066:SER:H	2.27	0.41
4:A:315:LEU:HD12	4:A:316:GLN:HA	2.03	0.40
4:A:381:THR:C	4:A:383:TYR:N	2.75	0.40
4:A:1231:ASP:O	4:A:1233:ASP:N	2.53	0.40
5:B:173:MET:HG2	5:B:174:LEU:O	2.21	0.40
5:B:410:GLY:O	5:B:413:LEU:N	2.54	0.40
5:B:479:VAL:O	5:B:480:SER:HB3	2.21	0.40
5:B:819:ALA:O	5:B:1091:TYR:OH	2.38	0.40
5:B:1016:ALA:C	5:B:1018:PRO:HD2	2.46	0.40
9:H:24:CYS:HB2	9:H:44:VAL:CG2	2.50	0.40
10:I:44:TYR:CD2	10:I:44:TYR:C	3.00	0.40
4:A:41:MET:CA	4:A:50:ILE:CD1	2.93	0.40
4:A:302:THR:HA	4:A:305:ASP:O	2.20	0.40
4:A:315:LEU:HB2	4:A:320:ARG:HH12	1.83	0.40
4:A:367:PRO:HB3	4:A:465:TYR:O	2.20	0.40
4:A:453:MET:HE3	4:A:520:CYS:HG	1.81	0.40
4:A:1345:ARG:O	4:A:1348:LEU:N	2.54	0.40
5:B:473:MET:C	5:B:475:SER:H	2.29	0.40
5:B:475:SER:O	5:B:476:ARG:C	2.64	0.40
11:J:32:GLU:CD	11:J:32:GLU:H	2.29	0.40
12:K:77:THR:HB	12:K:81:TYR:HB3	2.03	0.40
4:A:91:PHE:N	4:A:297:GLN:HE22	2.19	0.40
4:A:91:PHE:C	4:A:297:GLN:HE22	2.29	0.40
4:A:219:PHE:HE1	4:A:231:PRO:HD2	1.86	0.40
4:A:244:PRO:HB2	4:A:245:PRO:HD3	2.03	0.40
4:A:351:THR:HB	4:A:468:PHE:HD2	1.83	0.40
4:A:365:GLY:N	4:A:469:ARG:O	2.47	0.40
4:A:463:ILE:CD1	4:A:469:ARG:CG	2.99	0.40
4:A:1021:LEU:C	4:A:1024:SER:HB2	2.46	0.40
5:B:113:TYR:O	5:B:114:PRO:C	2.62	0.40
6:C:234:SER:HB3	6:C:240:VAL:HG13	2.02	0.40
4:A:58:LEU:HD22	4:A:244:PRO:CD	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:282:ASN:HB3	4:A:283:GLY:H	1.74	0.40
4:A:344:ARG:HA	5:B:1129:ARG:HA	2.03	0.40
4:A:414:ASP:OD1	4:A:416:ARG:HD3	2.20	0.40
4:A:443:LEU:HD12	5:B:1146:PHE:CE2	2.56	0.40
4:A:685:GLU:O	4:A:689:LYS:HB2	2.21	0.40
4:A:737:LEU:HD11	4:A:758:ILE:CG2	2.50	0.40
4:A:1063:MET:HE3	4:A:1063:MET:HB3	1.90	0.40
5:B:37:PHE:HD1	5:B:681:TRP:CE2	2.40	0.40
5:B:202:TYR:CE1	5:B:209:GLU:CD	2.96	0.40
5:B:314:LEU:C	5:B:316:PRO:HD2	2.46	0.40
5:B:384:ARG:NH2	5:B:623:GLU:OE1	2.53	0.40
6:C:116:LYS:HG2	6:C:116:LYS:O	2.21	0.40
4:A:59:GLY:HA2	4:A:67:CYS:SG	2.61	0.40
4:A:79:GLY:O	4:A:243:PRO:CG	2.64	0.40
4:A:757:ASN:O	4:A:761:MET:HG3	2.21	0.40
5:B:744:HIS:HD2	5:B:746:SER:H	1.64	0.40
5:B:826:ALA:HB3	5:B:1011:ILE:HG13	2.03	0.40
5:B:859:TYR:OH	5:B:941:LEU:HD22	2.22	0.40
6:C:211:ASP:HA	6:C:212:PRO:HD3	1.91	0.40
6:C:258:ILE:HD13	12:K:42:LEU:HD21	2.02	0.40
7:E:78:LEU:HD12	7:E:107:THR:HB	2.02	0.40
7:E:168:TYR:C	7:E:169:ARG:HG2	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	1392/1733 (80%)	1118 (80%)	182 (13%)	92 (7%)	1	12
5	B	1096/1224 (90%)	897 (82%)	124 (11%)	75 (7%)	1	11
6	C	264/318 (83%)	229 (87%)	28 (11%)	7 (3%)	4	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	E	212/215 (99%)	190 (90%)	15 (7%)	7 (3%)	3	24
8	F	86/155 (56%)	75 (87%)	6 (7%)	5 (6%)	1	13
9	H	130/146 (89%)	105 (81%)	18 (14%)	7 (5%)	1	14
10	I	117/122 (96%)	96 (82%)	18 (15%)	3 (3%)	4	27
11	J	63/70 (90%)	53 (84%)	8 (13%)	2 (3%)	3	24
12	K	112/120 (93%)	107 (96%)	5 (4%)	0	100	100
13	L	44/70 (63%)	29 (66%)	13 (30%)	2 (4%)	2	17
All	All	3516/4173 (84%)	2899 (82%)	417 (12%)	200 (6%)	1	13

All (200) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	55	ASP
4	A	56	PRO
4	A	74	MET
4	A	157	ASP
4	A	158	PRO
4	A	308	ILE
4	A	316	GLN
4	A	317	LYS
4	A	321	PRO
4	A	335	ARG
4	A	418	SER
4	A	544	ASP
4	A	597	LEU
4	A	1022	LEU
4	A	1023	ARG
4	A	1024	SER
4	A	1175	SER
4	A	1221	LYS
4	A	1232	ASN
4	A	1393	ASN
5	B	45	SER
5	B	64	CYS
5	B	179	CYS
5	B	202	TYR
5	B	203	PHE
5	B	274	PRO
5	B	338	GLY
5	B	477	ALA

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Mol	Chain	Res	Type
5	B	484	ASN
5	B	531	GLN
5	B	636	PRO
5	B	643	ASP
5	B	711	GLU
5	B	728	ARG
5	B	810	GLU
5	B	811	TYR
5	B	883	LEU
5	B	1017	ILE
5	B	1065	GLN
6	C	215	GLU
7	E	52	ARG
7	E	59	SER
7	E	90	VAL
8	F	104	ASN
9	H	81	PRO
9	H	82	PRO
11	J	2	ILE
11	J	6	ARG
4	A	50	ILE
4	A	69	THR
4	A	80	HIS
4	A	178	GLY
4	A	223	GLY
4	A	255	SER
4	A	260	ASP
4	A	623	GLY
4	A	647	GLY
4	A	779	PHE
4	A	780	VAL
4	A	851	HIS
4	A	852	TYR
4	A	903	ASN
4	A	1027	ALA
4	A	1220	PHE
4	A	1233	ASP
4	A	1345	ARG
4	A	1388	GLY
4	A	1401	SER
4	A	1437	GLY
5	B	175	ARG

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Mol	Chain	Res	Type
5	B	182	SER
5	B	229	ALA
5	B	260	GLY
5	B	294	ASP
5	B	322	PHE
5	B	327	ARG
5	B	410	GLY
5	B	471	LYS
5	B	563	MET
5	B	731	VAL
5	B	734	HIS
5	B	774	GLY
5	B	943	SER
5	B	958	GLN
5	B	982	SER
5	B	1181	GLU
6	C	90	ASP
6	C	142	VAL
7	E	3	GLN
8	F	70	LYS
9	H	108	SER
9	H	140	ALA
13	L	55	ILE
4	A	214	ILE
4	A	314	ALA
4	A	404	TYR
4	A	451	HIS
4	A	483	ASP
4	A	568	PRO
4	A	846	GLU
4	A	854	ASN
4	A	855	THR
4	A	922	ASP
4	A	958	VAL
4	A	1021	LEU
4	A	1170	ILE
4	A	1234	GLU
5	B	180	TYR
5	B	337	ARG
5	B	344	LYS
5	B	476	ARG
5	B	478	GLY

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Mol	Chain	Res	Type
5	B	483	LEU
5	B	894	ASP
5	B	1020	ARG
6	C	110	THR
6	C	174	ALA
7	E	53	PRO
8	F	74	ILE
10	I	10	CYS
10	I	60	GLN
4	A	46	THR
4	A	48	ALA
4	A	57	ARG
4	A	62	ASP
4	A	150	THR
4	A	152	VAL
4	A	312	PRO
4	A	333	GLU
4	A	423	ASP
4	A	424	ILE
4	A	517	ASN
4	A	543	LEU
4	A	567	LYS
4	A	895	LYS
4	A	1025	ARG
4	A	1028	THR
4	A	1065	GLY
4	A	1229	SER
5	B	38	PHE
5	B	467	GLY
5	B	468	GLU
5	B	637	LEU
5	B	647	GLY
5	B	792	MET
5	B	864	LYS
5	B	1096	ARG
9	H	128	ASN
4	A	130	ASP
4	A	151	ASP
4	A	213	HIS
4	A	325	ILE
4	A	591	PHE
4	A	972	HIS

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Mol	Chain	Res	Type
4	A	1243	VAL
4	A	1424	VAL
4	A	1433	MET
5	B	65	GLU
5	B	204	ILE
5	B	247	GLY
5	B	474	SER
5	B	480	SER
5	B	974	PRO
5	B	1028	GLU
5	B	1046	PRO
5	B	1108	ARG
7	E	36	GLU
8	F	148	VAL
9	H	77	ARG
10	I	12	ASN
13	L	50	ASP
4	A	35	ILE
4	A	72	GLU
4	A	250	ILE
4	A	1270	ASN
5	B	201	GLY
5	B	259	TYR
5	B	466	TRP
5	B	631	GLY
5	B	851	PHE
6	C	227	THR
4	A	910	PRO
5	B	802	PRO
5	B	920	PRO
5	B	1214	PRO
9	H	107	VAL
5	B	100	PRO
5	B	276	ILE
5	B	335	GLY
5	B	1165	ILE
4	A	1384	VAL
4	A	322	VAL
4	A	599	SER
4	A	837	ILE
4	A	1435	PRO
5	B	200	GLY

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Mol	Chain	Res	Type
8	F	139	PRO
5	B	1103	ILE
6	C	182	PRO
7	E	118	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	1225/1520 (81%)	1108 (90%)	117 (10%)	8	32
5	B	967/1061 (91%)	869 (90%)	98 (10%)	7	30
6	C	234/274 (85%)	214 (92%)	20 (8%)	10	35
7	E	196/197 (100%)	181 (92%)	15 (8%)	12	38
8	F	78/137 (57%)	73 (94%)	5 (6%)	16	43
9	H	118/128 (92%)	108 (92%)	10 (8%)	10	35
10	I	113/116 (97%)	104 (92%)	9 (8%)	11	37
11	J	60/65 (92%)	52 (87%)	8 (13%)	4	21
12	K	99/102 (97%)	88 (89%)	11 (11%)	6	27
13	L	40/57 (70%)	36 (90%)	4 (10%)	7	30
All	All	3130/3657 (86%)	2833 (90%)	297 (10%)	8	32

All (297) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	32	VAL
4	A	44	THR
4	A	69	THR
4	A	80	HIS
4	A	93	VAL
4	A	139	TRP
4	A	155	GLU
4	A	156	ASP
4	A	157	ASP

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Mol	Chain	Res	Type
4	A	159	THR
4	A	161	LEU
4	A	170	THR
4	A	204	THR
4	A	208	LEU
4	A	222	LEU
4	A	225	ASN
4	A	235	ILE
4	A	263	THR
4	A	270	LEU
4	A	320	ARG
4	A	322	VAL
4	A	329	LEU
4	A	333	GLU
4	A	335	ARG
4	A	388	LEU
4	A	391	LEU
4	A	409	SER
4	A	416	ARG
4	A	443	LEU
4	A	447	GLN
4	A	470	LEU
4	A	475	THR
4	A	504	LEU
4	A	535	THR
4	A	539	THR
4	A	550	LEU
4	A	569	LYS
4	A	577	ILE
4	A	582	ILE
4	A	590	ARG
4	A	592	ASP
4	A	596	THR
4	A	602	ASP
4	A	605	MET
4	A	618	GLU
4	A	637	LYS
4	A	703	THR
4	A	709	THR
4	A	735	VAL
4	A	740	LEU
4	A	741	ASN

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Mol	Chain	Res	Type
4	A	743	VAL
4	A	765	VAL
4	A	770	VAL
4	A	775	ILE
4	A	779	PHE
4	A	805	LEU
4	A	851	HIS
4	A	852	TYR
4	A	854	ASN
4	A	859	SER
4	A	867	ILE
4	A	871	ASP
4	A	885	THR
4	A	889	SER
4	A	902	LEU
4	A	913	LEU
4	A	915	SER
4	A	918	GLU
4	A	920	LEU
4	A	937	VAL
4	A	953	ASN
4	A	961	ARG
4	A	982	THR
4	A	983	ILE
4	A	993	LEU
4	A	1015	VAL
4	A	1017	LEU
4	A	1020	CYS
4	A	1021	LEU
4	A	1025	ARG
4	A	1026	LEU
4	A	1030	ARG
4	A	1048	ASN
4	A	1054	LEU
4	A	1058	VAL
4	A	1064	VAL
4	A	1081	LEU
4	A	1094	VAL
4	A	1116	LEU
4	A	1118	VAL
4	A	1128	GLN
4	A	1132	LYS

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Mol	Chain	Res	Type
4	A	1162	VAL
4	A	1174	PHE
4	A	1187	GLN
4	A	1220	PHE
4	A	1227	ILE
4	A	1229	SER
4	A	1231	ASP
4	A	1232	ASN
4	A	1233	ASP
4	A	1234	GLU
4	A	1235	LYS
4	A	1244	ARG
4	A	1258	HIS
4	A	1263	ILE
4	A	1265	ASN
4	A	1308	THR
4	A	1314	SER
4	A	1319	VAL
4	A	1336	MET
4	A	1345	ARG
4	A	1391	ARG
4	A	1394	THR
4	A	1406	VAL
4	A	1407	GLU
5	B	22	SER
5	B	43	LEU
5	B	44	VAL
5	B	57	TYR
5	B	63	ILE
5	B	65	GLU
5	B	68	THR
5	B	102	VAL
5	B	108	VAL
5	B	128	LEU
5	B	132	VAL
5	B	175	ARG
5	B	185	THR
5	B	198	ASP
5	B	199	MET
5	B	203	PHE
5	B	206	ASN
5	B	217	ARG

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Mol	Chain	Res	Type
5	B	222	ILE
5	B	225	VAL
5	B	226	PHE
5	B	235	SER
5	B	268	THR
5	B	272	THR
5	B	282	ILE
5	B	294	ASP
5	B	322	PHE
5	B	323	VAL
5	B	336	ARG
5	B	337	ARG
5	B	382	ILE
5	B	384	ARG
5	B	388	CYS
5	B	420	LEU
5	B	436	VAL
5	B	461	LEU
5	B	465	ASN
5	B	466	TRP
5	B	471	LYS
5	B	482	VAL
5	B	483	LEU
5	B	498	THR
5	B	513	GLN
5	B	516	ASN
5	B	527	THR
5	B	539	LEU
5	B	545	ILE
5	B	549	THR
5	B	556	THR
5	B	563	MET
5	B	567	GLU
5	B	570	VAL
5	B	635	ARG
5	B	654	ARG
5	B	666	TYR
5	B	667	GLN
5	B	678	GLU
5	B	723	VAL
5	B	732	SER
5	B	736	THR

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Mol	Chain	Res	Type
5	B	737	THR
5	B	791	THR
5	B	792	MET
5	B	803	LEU
5	B	806	THR
5	B	807	ARG
5	B	812	LEU
5	B	825	VAL
5	B	838	SER
5	B	850	LEU
5	B	861	ASP
5	B	873	THR
5	B	879	ARG
5	B	916	THR
5	B	948	ILE
5	B	969	ARG
5	B	975	GLN
5	B	976	ILE
5	B	997	GLU
5	B	999	MET
5	B	1006	ILE
5	B	1011	ILE
5	B	1020	ARG
5	B	1046	PRO
5	B	1047	PHE
5	B	1051	THR
5	B	1064	TYR
5	B	1065	GLN
5	B	1084	GLN
5	B	1092	TYR
5	B	1096	ARG
5	B	1099	VAL
5	B	1113	VAL
5	B	1124	ARG
5	B	1159	ARG
5	B	1160	VAL
5	B	1161	HIS
5	B	1166	CYS
6	C	4	GLU
6	C	18	VAL
6	C	22	LEU
6	C	25	VAL

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Mol	Chain	Res	Type
6	C	26	ASP
6	C	53	THR
6	C	56	THR
6	C	57	VAL
6	C	77	ILE
6	C	80	LEU
6	C	120	ILE
6	C	144	ILE
6	C	154	LYS
6	C	163	ILE
6	C	231	ASN
6	C	234	SER
6	C	240	VAL
6	C	244	VAL
6	C	258	ILE
6	C	259	LEU
7	E	9	ILE
7	E	10	SER
7	E	39	LEU
7	E	48	ASP
7	E	88	VAL
7	E	92	THR
7	E	95	THR
7	E	114	ASN
7	E	127	ILE
7	E	142	VAL
7	E	150	VAL
7	E	156	LEU
7	E	165	LEU
7	E	190	LEU
7	E	213	ILE
8	F	72	LYS
8	F	93	ILE
8	F	120	ILE
8	F	123	LYS
8	F	139	PRO
9	H	31	THR
9	H	32	THR
9	H	41	ASP
9	H	42	ILE
9	H	46	LEU
9	H	86	ASP

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Mol	Chain	Res	Type
9	H	94	ASP
9	H	107	VAL
9	H	136	LYS
9	H	142	LEU
10	I	10	CYS
10	I	17	ARG
10	I	21	GLU
10	I	24	ARG
10	I	28	GLU
10	I	31	THR
10	I	50	THR
10	I	62	ILE
10	I	83	ASN
11	J	2	ILE
11	J	5	VAL
11	J	7	CYS
11	J	13	VAL
11	J	14	VAL
11	J	20	SER
11	J	45	CYS
11	J	48	ARG
12	K	9	LEU
12	K	42	LEU
12	K	46	ILE
12	K	63	VAL
12	K	78	THR
12	K	89	ASN
12	K	101	LEU
12	K	103	THR
12	K	106	GLU
12	K	107	THR
12	K	113	THR
13	L	55	ILE
13	L	61	THR
13	L	63	ARG
13	L	65	VAL

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

Mol	Chain	Res	Type
4	A	64	ASN
4	A	80	HIS

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Mol	Chain	Res	Type
4	A	83	HIS
4	A	171	GLN
4	A	225	ASN
4	A	253	ASN
4	A	287	HIS
4	A	316	GLN
4	A	363	GLN
4	A	390	GLN
4	A	394	ASN
4	A	435	HIS
4	A	503	GLN
4	A	548	ASN
4	A	741	ASN
4	A	742	ASN
4	A	757	ASN
4	A	768	GLN
4	A	851	HIS
4	A	926	GLN
4	A	953	ASN
4	A	969	GLN
4	A	1011	GLN
4	A	1048	ASN
4	A	1078	GLN
4	A	1106	ASN
4	A	1218	GLN
4	A	1265	ASN
4	A	1270	ASN
4	A	1364	ASN
4	A	1390	ASN
4	A	1432	GLN
5	B	121	ASN
5	B	178	ASN
5	B	215	GLN
5	B	255	GLN
5	B	300	HIS
5	B	325	GLN
5	B	350	GLN
5	B	363	HIS
5	B	366	GLN
5	B	383	ASN
5	B	395	GLN
5	B	400	HIS

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Mol	Chain	Res	Type
5	B	415	GLN
5	B	484	ASN
5	B	494	HIS
5	B	513	GLN
5	B	515	HIS
5	B	516	ASN
5	B	518	HIS
5	B	592	ASN
5	B	657	HIS
5	B	686	ASN
5	B	734	HIS
5	B	744	HIS
5	B	822	ASN
5	B	957	ASN
5	B	975	GLN
5	B	984	HIS
5	B	986	GLN
5	B	1015	HIS
5	B	1065	GLN
5	B	1084	GLN
5	B	1195	HIS
6	C	65	HIS
6	C	73	GLN
6	C	91	HIS
6	C	102	GLN
6	C	112	ASN
6	C	123	ASN
6	C	135	GLN
6	C	151	GLN
6	C	188	HIS
6	C	203	GLN
6	C	231	ASN
6	C	242	GLN
7	E	61	GLN
7	E	101	GLN
7	E	104	ASN
7	E	106	GLN
7	E	114	ASN
7	E	146	HIS
9	H	33	GLN
9	H	83	GLN
9	H	137	GLN

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Mol	Chain	Res	Type
10	I	83	ASN
10	I	108	HIS
10	I	116	ASN
12	K	40	HIS
12	K	65	HIS

5.3.3 RNA ⓘ

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

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	DUT	B	1308[B]	15	28,29,29	1.31	5 (17%)	41,45,45	1.63	7 (17%)
16	DUT	B	1308[A]	-	28,29,29	1.90	6 (21%)	41,45,45	1.54	6 (14%)

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	DUT	B	1308[B]	15	-	4/22/34/34	0/2/2/2
16	DUT	B	1308[A]	-	-	5/22/34/34	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	1308[A]	DUT	PB-O3A	6.17	1.66	1.59
16	B	1308[A]	DUT	PA-O3A	5.37	1.65	1.59
16	B	1308[A]	DUT	PB-O3B	3.45	1.63	1.59
16	B	1308[B]	DUT	PB-O3A	2.81	1.62	1.59
16	B	1308[B]	DUT	PA-O3A	2.47	1.62	1.59
16	B	1308[B]	DUT	C2-N1	-2.26	1.34	1.38
16	B	1308[A]	DUT	C6-C5	2.23	1.40	1.35
16	B	1308[B]	DUT	PB-O3B	2.20	1.61	1.59
16	B	1308[B]	DUT	C4-N3	-2.16	1.34	1.38
16	B	1308[A]	DUT	O2-C2	2.05	1.26	1.23
16	B	1308[A]	DUT	C5-C4	-2.03	1.39	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	1308[B]	DUT	N3-C2-N1	4.66	120.95	114.89
16	B	1308[B]	DUT	C4-N3-C2	-4.56	120.95	126.61
16	B	1308[A]	DUT	N3-C2-N1	4.22	120.39	114.89
16	B	1308[A]	DUT	C4-N3-C2	-4.17	121.44	126.61
16	B	1308[A]	DUT	O4-C4-C5	-3.53	119.07	125.16
16	B	1308[B]	DUT	C5-C4-N3	3.34	119.48	114.80
16	B	1308[A]	DUT	C5-C4-N3	2.99	118.98	114.80
16	B	1308[B]	DUT	O4'-C1'-N1	2.84	112.90	107.86
16	B	1308[A]	DUT	O2-C2-N1	-2.23	119.89	122.80
16	B	1308[A]	DUT	O3G-PG-O2G	2.13	115.81	107.80
16	B	1308[B]	DUT	O4-C4-C5	-2.13	121.48	125.16
16	B	1308[B]	DUT	O2A-PA-O1A	2.03	121.90	112.44
16	B	1308[B]	DUT	C2'-C1'-N1	-2.02	108.75	113.81

There are no chirality outliers.

All (9) torsion outliers are listed below:

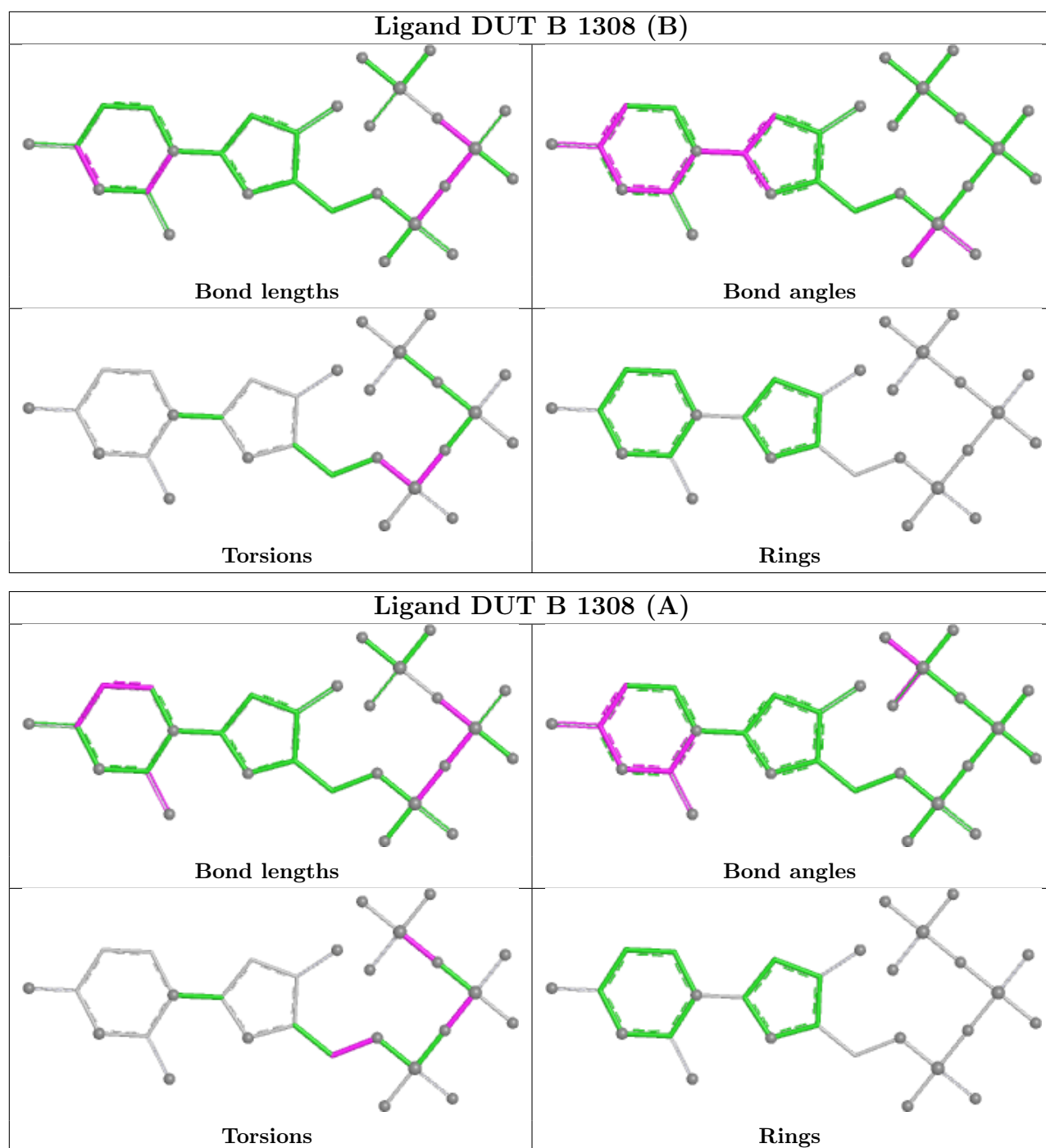
Mol	Chain	Res	Type	Atoms
16	B	1308[B]	DUT	C5'-O5'-PA-O1A
16	B	1308[B]	DUT	C5'-O5'-PA-O2A
16	B	1308[B]	DUT	C5'-O5'-PA-O3A
16	B	1308[A]	DUT	PB-O3B-PG-O1G
16	B	1308[A]	DUT	C4'-C5'-O5'-PA
16	B	1308[A]	DUT	PB-O3B-PG-O2G
16	B	1308[A]	DUT	PB-O3B-PG-O3G
16	B	1308[A]	DUT	PA-O3A-PB-O2B
16	B	1308[B]	DUT	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1308[A]	DUT	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	R	10/10 (100%)	0.31	0 100 100	85, 109, 154, 170	0
2	N	14/14 (100%)	1.52	2 (14%) 6 6	178, 182, 198, 202	0
3	T	28/28 (100%)	1.04	3 (10%) 11 9	93, 173, 189, 192	0
4	A	1402/1733 (80%)	0.32	34 (2%) 59 34	75, 103, 150, 163	0
5	B	1114/1224 (91%)	0.38	36 (3%) 50 29	26, 102, 133, 143	0
6	C	266/318 (83%)	0.18	3 (1%) 78 52	81, 100, 128, 144	0
7	E	214/215 (99%)	0.27	1 (0%) 87 66	91, 131, 165, 167	0
8	F	88/155 (56%)	0.05	0 100 100	84, 104, 130, 137	0
9	H	134/146 (91%)	0.62	11 (8%) 17 12	100, 119, 152, 155	0
10	I	119/122 (97%)	0.37	2 (1%) 69 41	87, 104, 122, 138	0
11	J	65/70 (92%)	0.36	1 (1%) 72 44	92, 102, 122, 125	0
12	K	114/120 (95%)	0.00	0 100 100	82, 105, 119, 120	0
13	L	46/70 (65%)	0.74	1 (2%) 62 36	108, 145, 156, 157	0
All	All	3614/4225 (85%)	0.34	94 (2%) 57 33	26, 104, 150, 202	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	816	GLU	5.2
5	B	89	GLU	4.7
4	A	69	THR	4.5
4	A	72	GLU	3.9
5	B	248	SER	3.8
9	H	130	ARG	3.6
4	A	1378	GLN	3.6
4	A	1234	GLU	3.6
5	B	203	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
5	B	179	CYS	3.4
4	A	496	GLU	3.3
5	B	1186	ASP	3.1
9	H	139	ASN	3.1
5	B	429	PHE	3.1
9	H	90	ALA	3.1
5	B	338	GLY	3.0
6	C	89	GLU	2.9
5	B	774	GLY	2.9
4	A	1022	LEU	2.9
5	B	740	HIS	2.9
4	A	462	VAL	2.8
5	B	643	ASP	2.8
4	A	1267	MET	2.8
5	B	356	LEU	2.8
5	B	802	PRO	2.8
4	A	259	GLU	2.8
4	A	544	ASP	2.7
5	B	204	ILE	2.7
11	J	55	ASP	2.7
5	B	677	GLU	2.7
5	B	713	ALA	2.7
9	H	7	ASP	2.7
4	A	38	PRO	2.7
9	H	60	ALA	2.6
5	B	174	LEU	2.6
5	B	804	GLY	2.6
4	A	1020	CYS	2.5
9	H	135	LEU	2.5
9	H	32	THR	2.5
5	B	165	VAL	2.5
4	A	855	THR	2.5
5	B	88	TYR	2.5
6	C	50	GLU	2.4
4	A	312	PRO	2.4
5	B	247	GLY	2.4
4	A	1132	LYS	2.4
7	E	46	TYR	2.4
5	B	861	ASP	2.4
4	A	286	HIS	2.4
2	N	1	DC	2.4
5	B	282	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
4	A	315	LEU	2.3
4	A	44	THR	2.3
13	L	32	ALA	2.3
4	A	780	VAL	2.3
2	N	14	DG	2.3
5	B	778	MET	2.3
5	B	637	LEU	2.3
3	T	5	DC	2.3
4	A	292	ALA	2.2
5	B	819	ALA	2.2
9	H	51	ALA	2.2
9	H	101	ALA	2.2
5	B	339	THR	2.2
4	A	56	PRO	2.2
9	H	133	ASN	2.2
6	C	206	ASN	2.2
10	I	22	ASN	2.2
4	A	1237	ILE	2.2
5	B	343	ILE	2.2
4	A	701	LEU	2.1
4	A	307	ASP	2.1
4	A	665	GLY	2.1
5	B	1088	GLY	2.1
5	B	711	GLU	2.1
4	A	1080	THR	2.1
3	T	3	DA	2.1
4	A	588	LEU	2.1
4	A	179	LEU	2.1
4	A	486	GLU	2.1
3	T	4	DC	2.1
5	B	202	TYR	2.1
5	B	746	SER	2.1
4	A	686	ALA	2.1
10	I	4	PHE	2.1
4	A	590	ARG	2.0
5	B	714	GLU	2.0
9	H	84	ALA	2.0
5	B	449	ASN	2.0
5	B	432	MET	2.0
4	A	26	GLU	2.0
5	B	364	ILE	2.0
4	A	173	THR	2.0

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Mol	Chain	Res	Type	RSRZ
4	A	1081	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

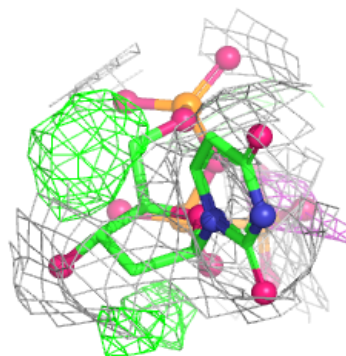
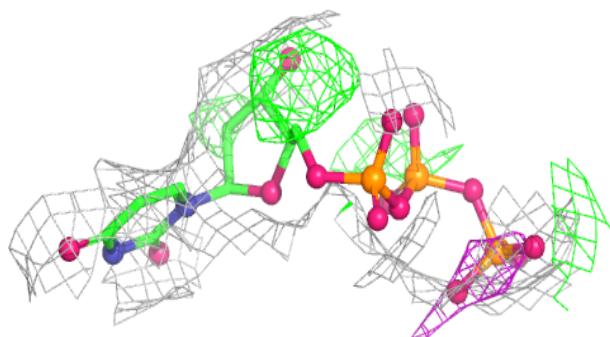
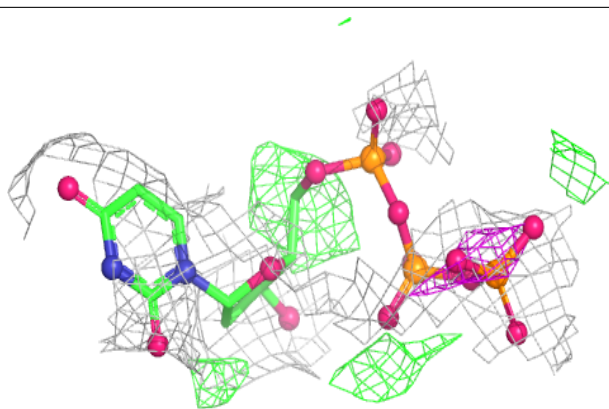
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	DUT	B	1308[A]	28/28	0.67	0.15	131,133,149,150	28
16	DUT	B	1308[B]	28/28	0.67	0.15	57,59,61,62	28
14	ZN	J	101	1/1	0.89	0.10	149,149,149,149	0
14	ZN	L	105	1/1	0.91	0.07	181,181,181,181	0
15	MG	A	2000	1/1	0.95	0.13	74,74,74,74	0
14	ZN	A	1735	1/1	0.97	0.03	142,142,142,142	0
14	ZN	B	1307	1/1	0.97	0.06	126,126,126,126	0
14	ZN	I	203	1/1	0.97	0.04	97,97,97,97	0
14	ZN	A	1734	1/1	0.97	0.04	159,159,159,159	0
14	ZN	I	204	1/1	0.98	0.04	107,107,107,107	0
14	ZN	C	319	1/1	1.00	0.02	104,104,104,104	0

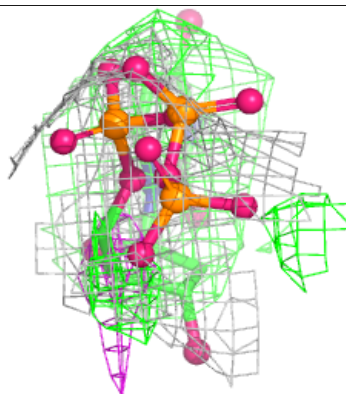
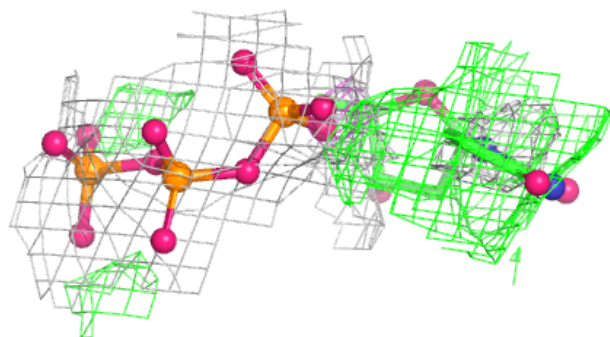
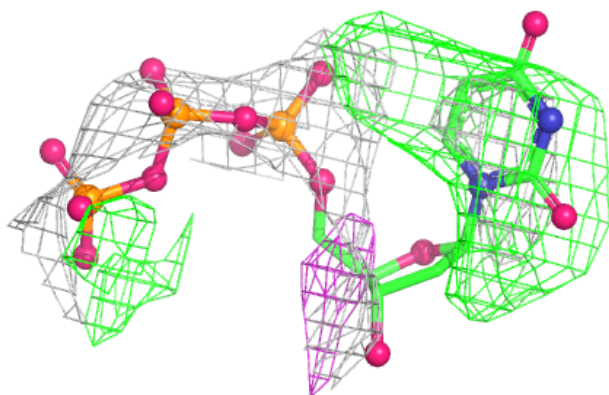
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DUT 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)

**Electron density around DUT 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.