Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:04 AM GMT

PDB ID	:	3GTM
Title	:	Co-complex of Backtracked RNA polymerase II with TFIIS
Authors	:	Wang, D.; Bushnell, D.A.; Huang, X.; Westover, K.D.; Levitt, M.; Kornberg, R.D.
Deposited on	:	2009-03-27
Resolution	:	3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

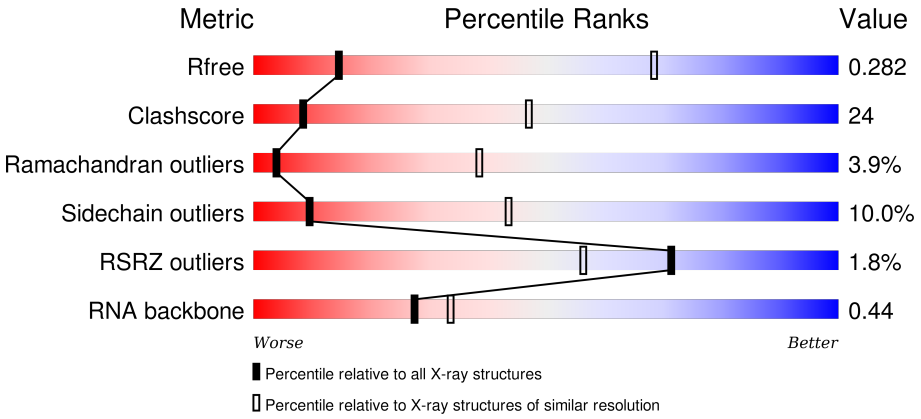
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)
RNA backbone	2183	1070 (4.76-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	1733	% 44% 32% 6% 18%
2	B	1224	46% 37% 6% 10%
3	C	318	51% 27% 5% • 16%
4	E	215	63% 32% •

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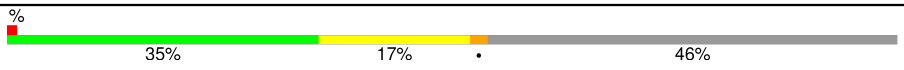
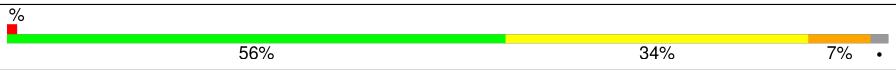
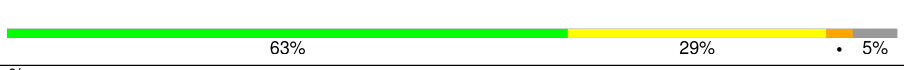
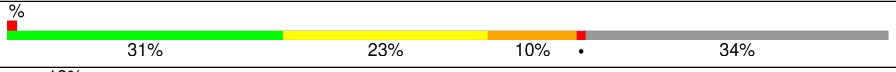
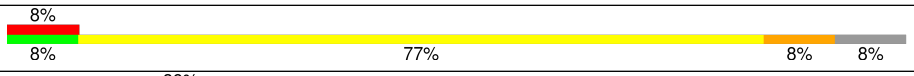
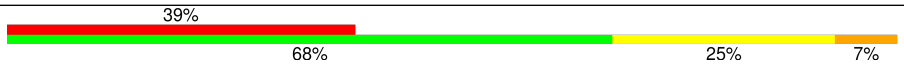
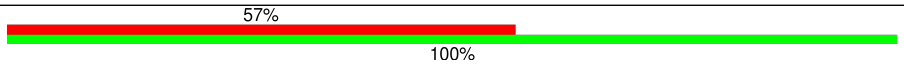
Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	S	173	
12	M	13	
13	N	28	
14	O	14	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 30560 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1426	Total	C	N	O	S	0	0	0
			11214	7069	1959	2124	62			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1104	Total	C	N	O	S	0	0	0
			8779	5560	1535	1630	54			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 11 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	S	163	Total	C	N	O	S	0	0	0
			1086	655	206	222	3			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	137	MET	-	EXPRESSION TAG	UNP P07273
S	138	ARG	-	EXPRESSION TAG	UNP P07273
S	139	GLY	-	EXPRESSION TAG	UNP P07273
S	140	SER	-	EXPRESSION TAG	UNP P07273
S	141	HIS	-	EXPRESSION TAG	UNP P07273
S	142	HIS	-	EXPRESSION TAG	UNP P07273
S	143	HIS	-	EXPRESSION TAG	UNP P07273
S	144	HIS	-	EXPRESSION TAG	UNP P07273
S	145	HIS	-	EXPRESSION TAG	UNP P07273
S	146	HIS	-	EXPRESSION TAG	UNP P07273
S	291	HIS	S	ENGINEERED	UNP P07273

- Molecule 12 is a RNA chain called RNA (5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*AP *UP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	12	Total	C	N	O	P	0	0	0
			241	107	47	76	11			

- Molecule 13 is a DNA chain called DNA (28-MER).

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

- Molecule 14 is a DNA chain called DNA (5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP *GP*TP*AP*G)-3').

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

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

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

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

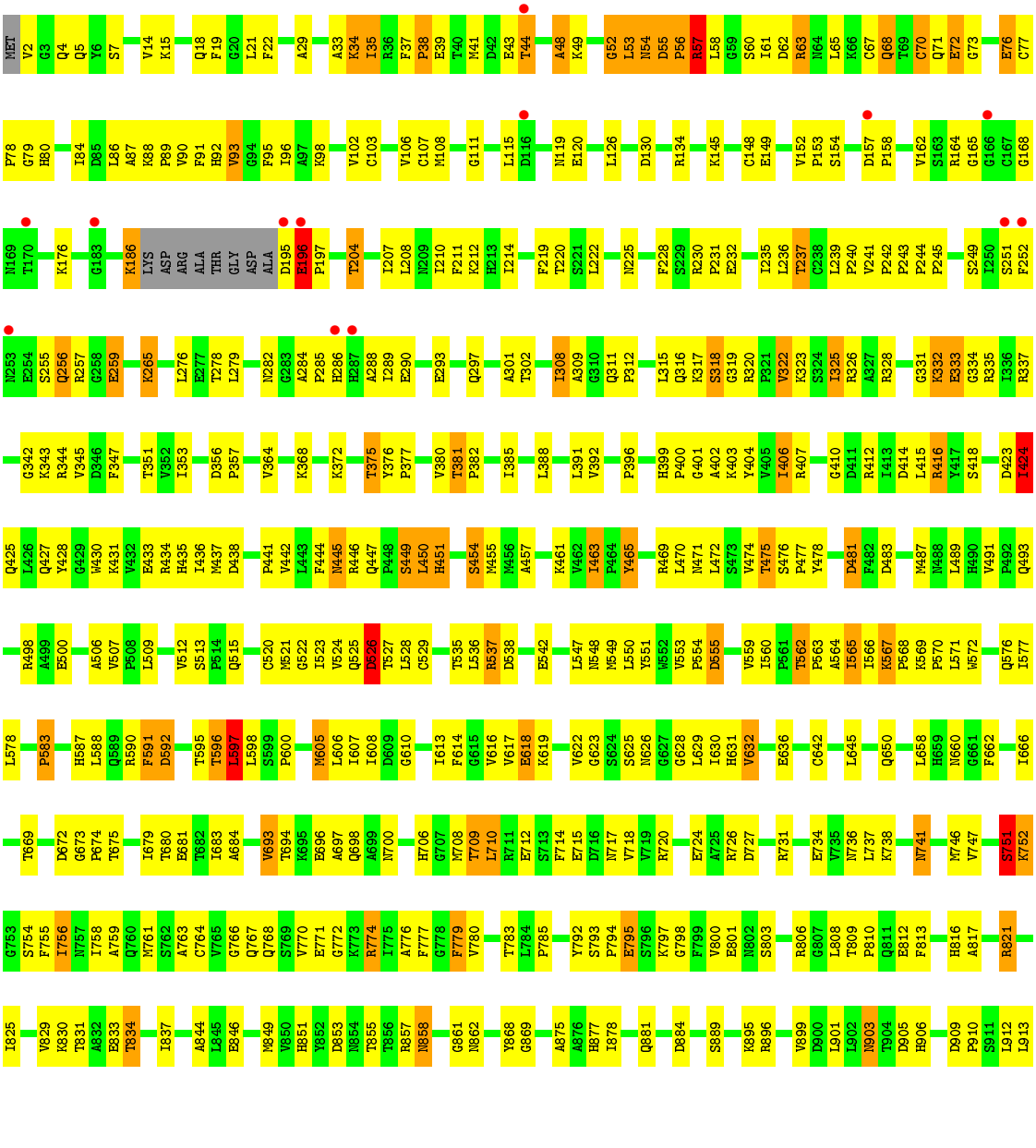
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	J	1	Total	Zn	0	0
			1	1		
16	B	1	Total	Zn	0	0
			1	1		
16	I	2	Total	Zn	0	0
			2	2		
16	C	1	Total	Zn	0	0
			1	1		
16	A	2	Total	Zn	0	0
			2	2		
16	L	1	Total	Zn	0	0
			1	1		
16	S	1	Total	Zn	0	0
			1	1		

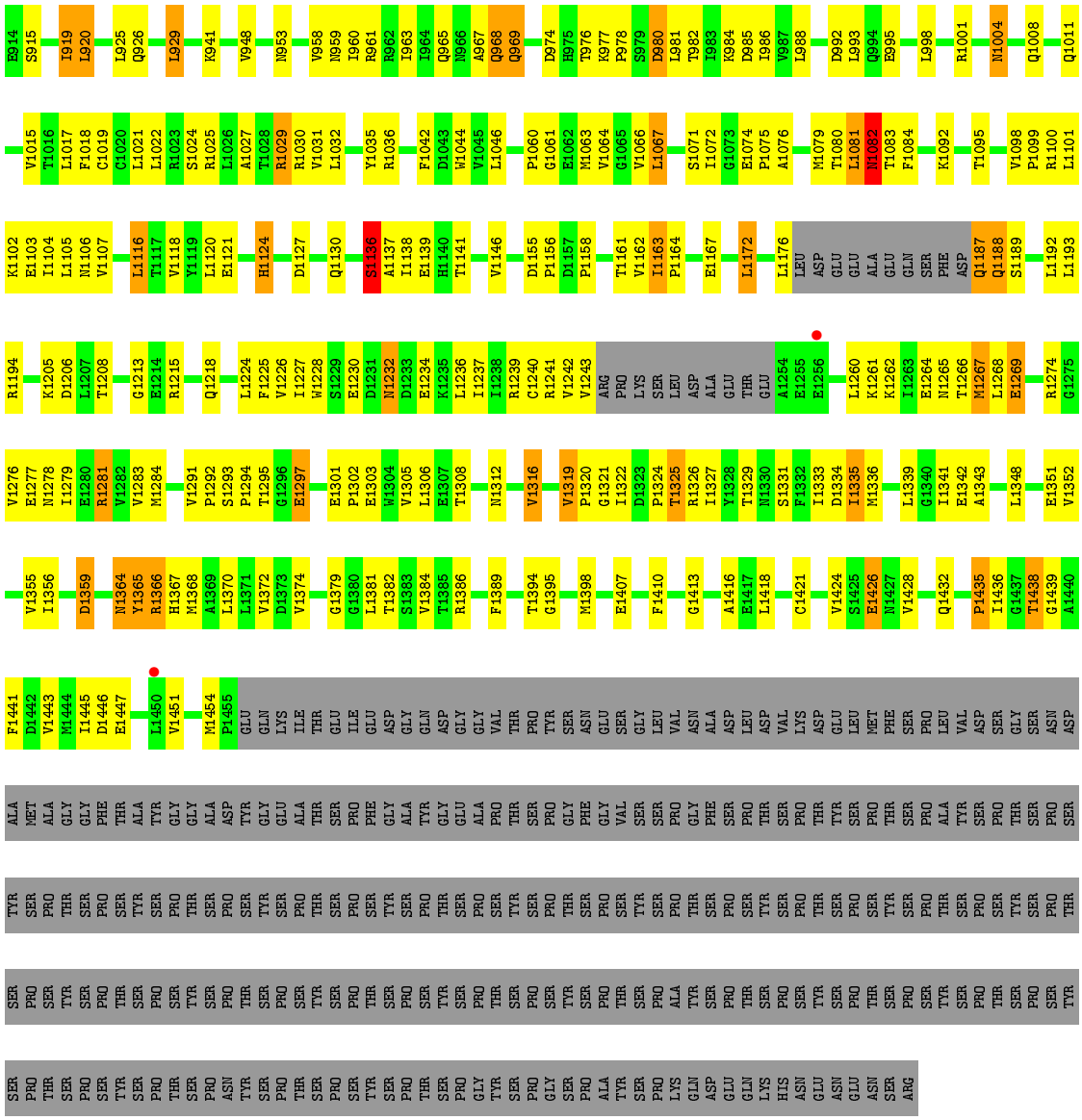
3 Residue-property plots (i)

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

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

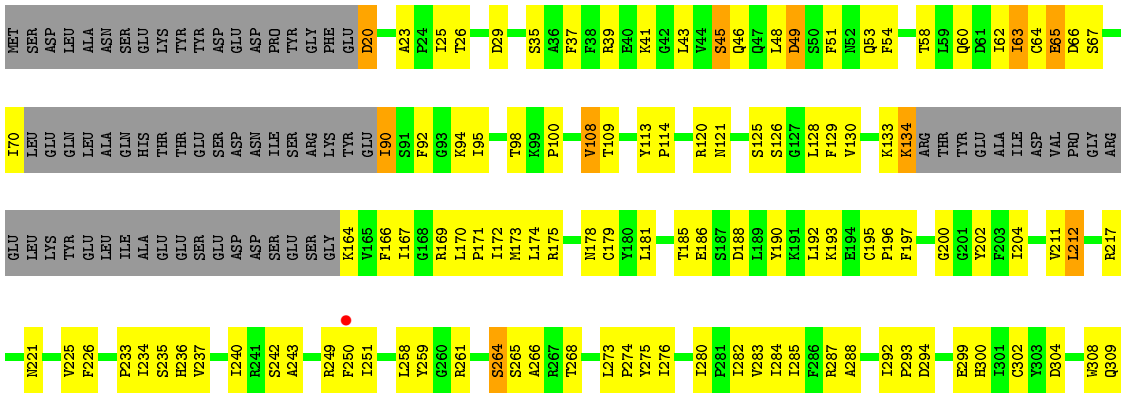
Chain A:

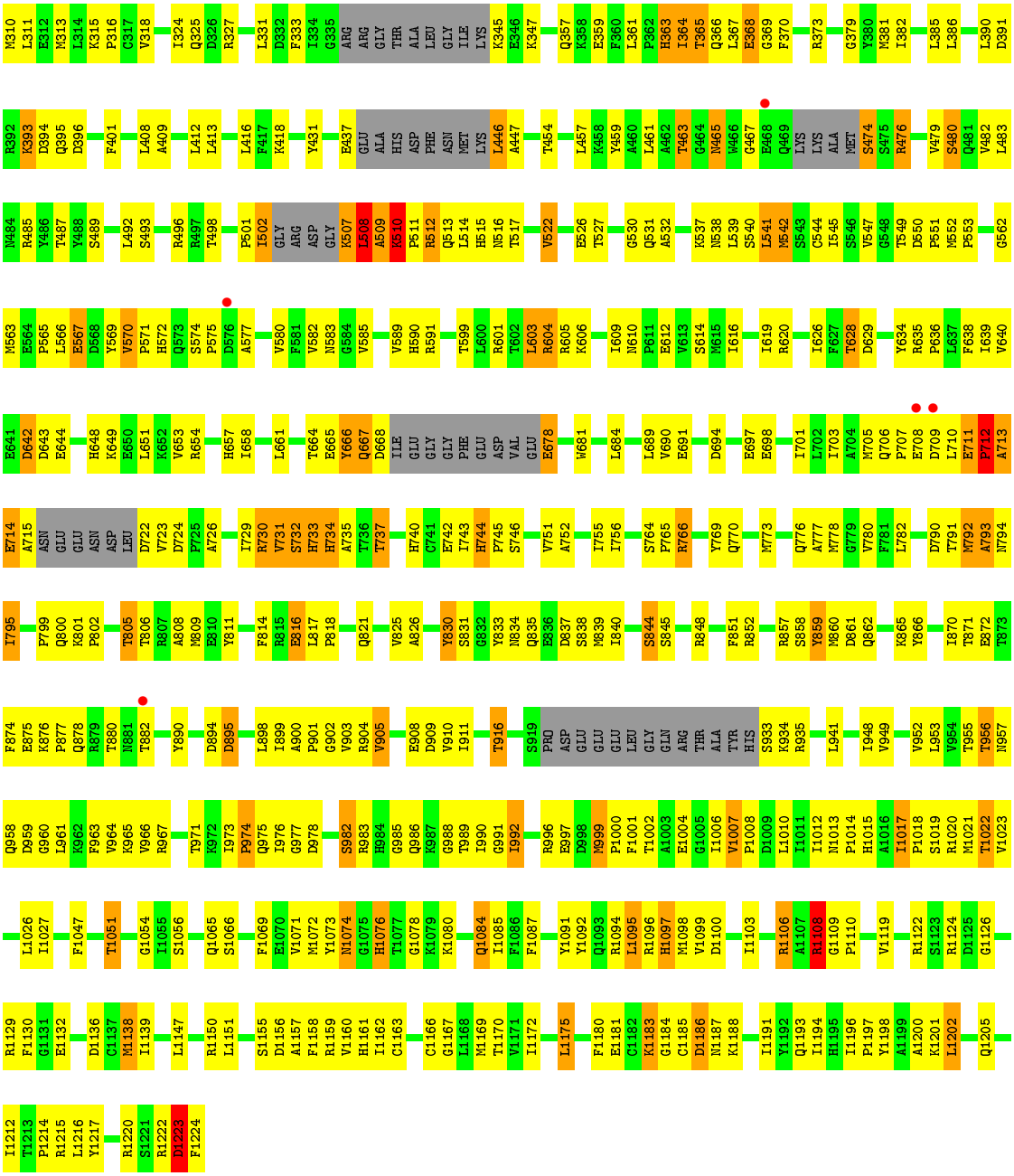




• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

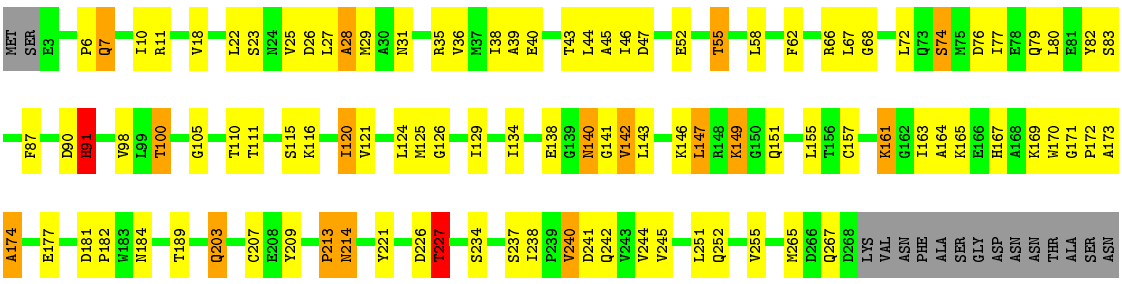
Chain B:





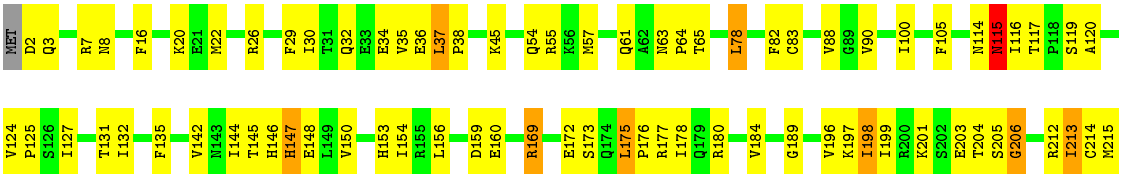
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



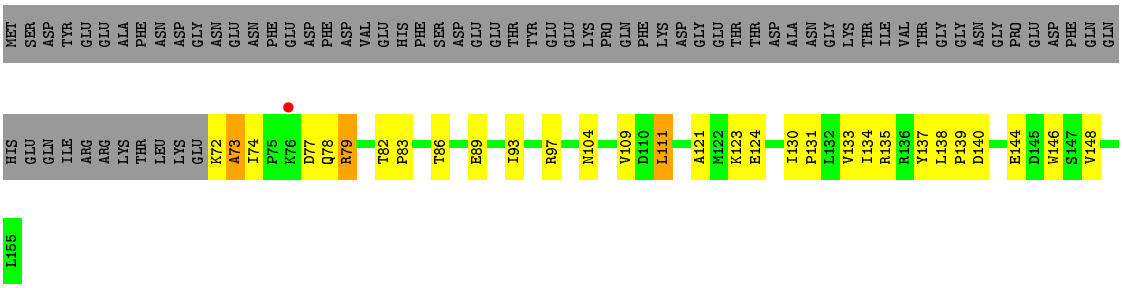
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



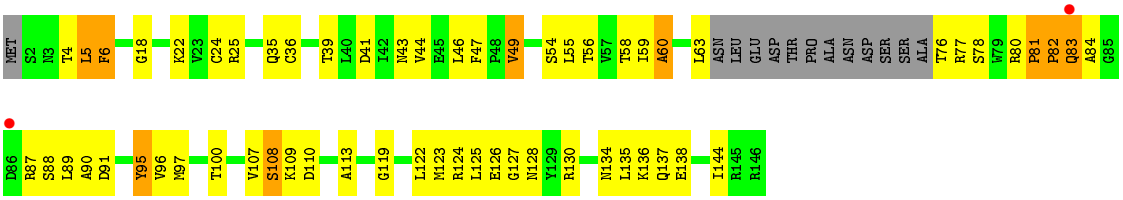
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



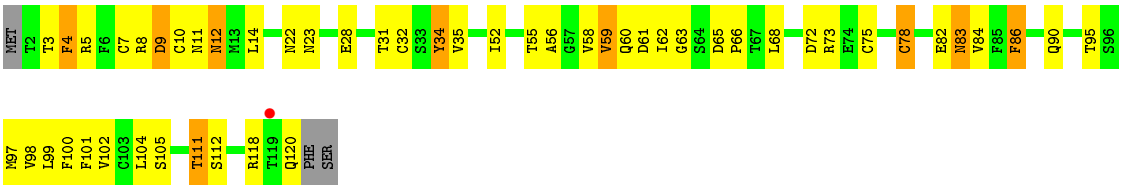
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



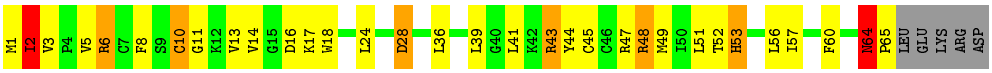
• Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I:

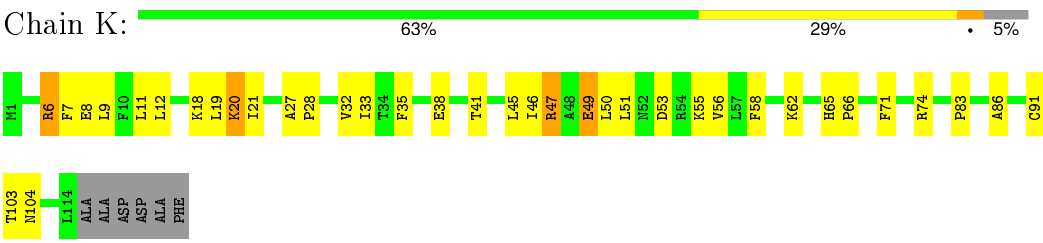


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

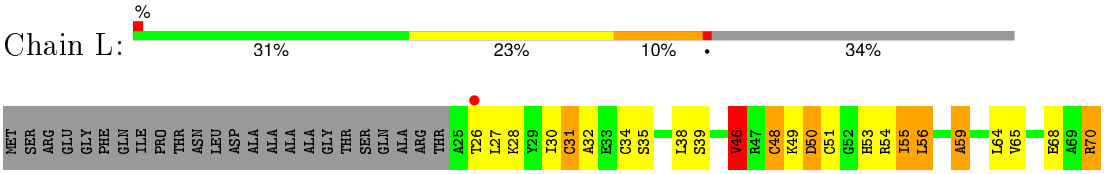
Chain J:



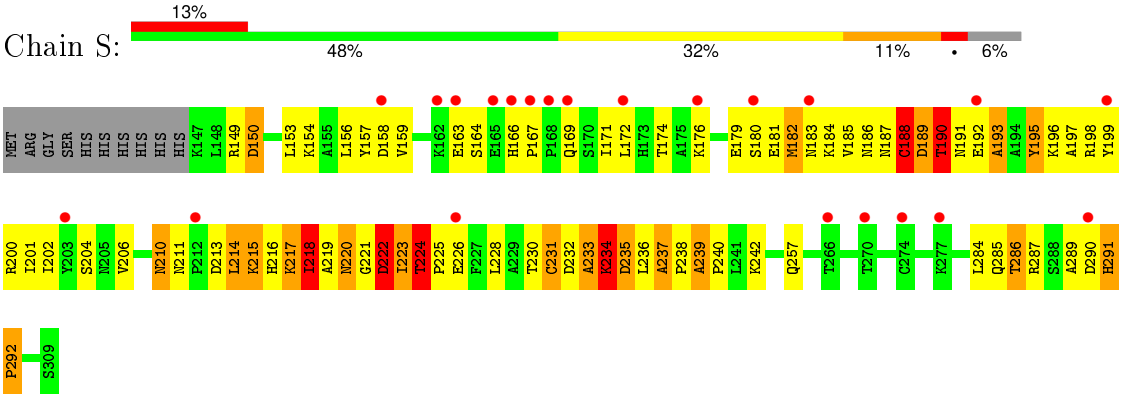
• Molecule 9: DNA-directed RNA polymerase II subunit RPB11



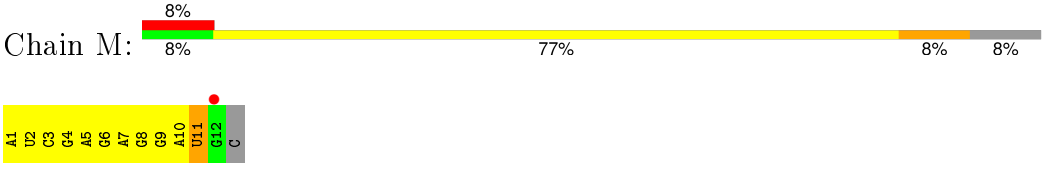
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



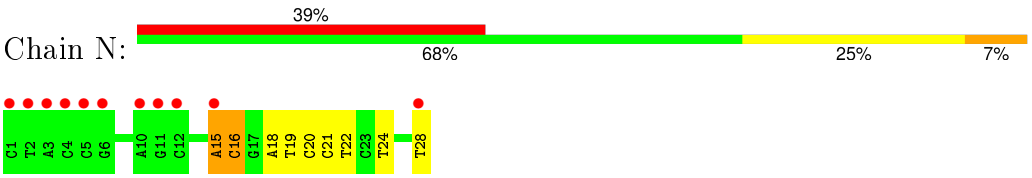
• Molecule 11: Transcription elongation factor S-II



• Molecule 12: RNA (5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*AP*UP*GP*C)-3')

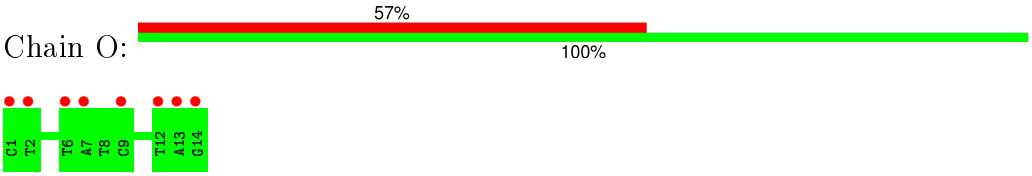


• Molecule 13: DNA (28-MER)



• Molecule 14: DNA (5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3')

Chain O:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	172.33Å 218.53Å 193.91Å 90.00° 100.32° 90.00°	Depositor
Resolution (Å)	40.00 – 3.80 39.89 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.80) 94.6 (39.89-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 3.76Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.234 , 0.289 0.225 , 0.282	Depositor DCC
R_{free} test set	3320 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	68.7	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 58.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 65630 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	30560	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.24	0/11417	0.52	12/15442 (0.1%)
2	B	0.27	0/8949	0.54	10/12066 (0.1%)
3	C	0.25	0/2133	0.49	0/2891
4	E	0.22	0/1788	0.45	1/2406 (0.0%)
5	F	0.24	0/691	0.47	0/933
6	H	0.31	1/1086 (0.1%)	0.54	2/1470 (0.1%)
7	I	0.24	0/989	0.48	0/1331
8	J	0.25	0/541	0.48	0/727
9	K	0.23	0/937	0.42	0/1265
10	L	0.24	0/366	0.65	2/485 (0.4%)
11	S	0.30	0/1100	0.64	1/1466 (0.1%)
12	M	0.42	0/270	0.89	0/421
13	N	0.51	0/634	1.18	5/975 (0.5%)
14	O	0.50	0/317	1.11	0/488
All	All	0.27	1/31218 (0.0%)	0.56	33/42366 (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
11	S	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	127	GLY	N-CA	5.03	1.53	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	597	LEU	N-CA-CB	-10.25	89.89	110.40
1	A	1189	SER	N-CA-CB	-9.86	95.72	110.50
1	A	596	THR	N-CA-C	-8.47	88.14	111.00
1	A	751	SER	CB-CA-C	-8.05	94.80	110.10
1	A	1188	GLN	N-CA-C	-7.44	90.90	111.00
1	A	1137	ALA	N-CA-CB	-7.44	99.68	110.10
2	B	474	SER	N-CA-C	-7.10	91.83	111.00
2	B	509	ALA	CB-CA-C	6.94	120.50	110.10
1	A	1036	ARG	N-CA-CB	6.87	122.97	110.60
1	A	1035	TYR	N-CA-C	6.79	129.33	111.00
1	A	1386	ARG	N-CA-CB	-6.74	98.48	110.60
10	L	35	SER	N-CA-CB	6.40	120.10	110.50
10	L	34	CYS	CB-CA-C	6.38	123.15	110.40
2	B	712	PRO	N-CA-C	6.24	128.32	112.10
2	B	510	LYS	N-CA-C	6.11	127.49	111.00
13	N	16	DC	O4'-C4'-C3'	-6.06	102.08	104.50
1	A	1262	LYS	CB-CA-C	6.04	122.48	110.40
2	B	642	ASP	CB-CA-C	-5.91	98.59	110.40
1	A	752	LYS	N-CA-CB	5.83	121.10	110.60
2	B	446	LEU	CB-CA-C	5.68	120.99	110.20
13	N	28	DT	O4'-C1'-N1	5.58	111.90	108.00
2	B	502	ILE	CB-CA-C	-5.51	100.57	111.60
2	B	45	SER	CB-CA-C	-5.43	99.77	110.10
6	H	6	PHE	N-CA-CB	-5.40	100.88	110.60
4	E	147	HIS	CB-CA-C	5.29	120.98	110.40
13	N	21	DC	O4'-C4'-C3'	-5.23	102.41	104.50
2	B	1175	LEU	N-CA-C	5.23	125.11	111.00
13	N	28	DT	C1'-O4'-C4'	-5.22	104.88	110.10
1	A	526	ASP	CB-CA-C	-5.21	99.99	110.40
11	S	222	ASP	CB-CA-C	-5.18	100.04	110.40
6	H	127	GLY	N-CA-C	-5.17	100.18	113.10
2	B	905	VAL	CB-CA-C	-5.10	101.72	111.40
13	N	15	DA	P-O3'-C3'	5.09	125.81	119.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	S	214	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11214	0	11286	566	0
2	B	8779	0	8806	502	0
3	C	2095	0	2051	78	0
4	E	1752	0	1776	59	0
5	F	679	0	701	22	0
6	H	1068	0	1040	63	0
7	I	971	0	927	44	0
8	J	532	0	543	34	0
9	K	919	0	929	32	0
10	L	364	0	387	20	0
11	S	1086	0	947	153	0
12	M	241	0	120	15	0
13	N	566	0	316	9	0
14	O	284	0	161	0	0
15	A	1	0	0	0	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
16	S	1	0	0	0	0
All	All	30560	0	29990	1450	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 24.

All (1450) 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)
2:B:507:LYS:C	2:B:508:LEU:HD23	1.55	1.26
1:A:49:LYS:HD2	1:A:55:ASP:CG	1.63	1.18
11:S:183:ASN:HA	11:S:186:ASN:ND2	1.58	1.17
1:A:829:VAL:HG13	2:B:508:LEU:HD12	1.23	1.16
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.22	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:64:ASN:HB3	8:J:65:PRO:HD3	1.27	1.11
6:H:81:PRO:HB2	6:H:82:PRO:HD3	1.18	1.10
1:A:49:LYS:HD2	1:A:55:ASP:OD2	1.50	1.09
2:B:508:LEU:HD23	2:B:508:LEU:N	1.69	1.07
11:S:190:THR:HG22	11:S:191:ASN:N	1.63	1.06
2:B:667:GLN:HA	2:B:668:ASP:C	1.69	1.04
6:H:81:PRO:HB2	6:H:82:PRO:CD	1.88	1.03
1:A:56:PRO:O	1:A:57:ARG:HB2	1.54	1.03
1:A:567:LYS:HB3	6:H:96:VAL:H	1.20	1.03
1:A:567:LYS:HB2	1:A:568:PRO:CD	1.86	1.03
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.37	1.01
1:A:829:VAL:HG22	2:B:508:LEU:HD13	1.43	1.00
11:S:188:CYS:O	11:S:189:ASP:HB2	1.58	1.00
11:S:190:THR:HG22	11:S:191:ASN:H	1.24	0.98
2:B:39:ARG:NH2	2:B:665:GLU:HG3	1.77	0.98
1:A:33:ALA:HB1	1:A:56:PRO:HB2	1.44	0.98
1:A:54:ASN:H	1:A:54:ASN:HD22	1.01	0.97
10:L:28:LYS:HB2	10:L:39:SER:HA	1.43	0.97
2:B:711:GLU:H	2:B:712:PRO:HD3	1.29	0.96
11:S:211:ASN:HA	11:S:214:LEU:HB2	1.46	0.95
11:S:187:ASN:HB3	11:S:190:THR:HB	1.49	0.94
3:C:142:VAL:H	8:J:16:ASP:HB3	1.29	0.94
1:A:1017:LEU:HB2	4:E:206:GLY:H	1.31	0.94
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.47	0.94
1:A:54:ASN:O	1:A:55:ASP:HB2	1.64	0.93
2:B:667:GLN:CA	2:B:668:ASP:C	2.37	0.93
2:B:1156:ASP:HB3	2:B:1198:TYR:H	1.34	0.93
1:A:55:ASP:N	1:A:56:PRO:CD	2.33	0.92
1:A:965:GLN:HA	1:A:968:GLN:HG3	1.52	0.92
2:B:134:LYS:HD3	2:B:134:LYS:N	1.84	0.91
2:B:508:LEU:HB3	2:B:509:ALA:HB2	1.51	0.91
11:S:223:ILE:C	11:S:225:PRO:HD3	1.90	0.91
2:B:933:SER:CB	2:B:935:ARG:HH21	1.84	0.91
2:B:508:LEU:N	2:B:508:LEU:CD2	2.34	0.91
2:B:903:VAL:HG12	2:B:904:ARG:H	1.35	0.90
3:C:105:GLY:HA3	3:C:149:LYS:O	1.72	0.90
8:J:48:ARG:HE	8:J:49:MET:HE2	1.37	0.90
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.53	0.89
1:A:829:VAL:HG21	2:B:509:ALA:CB	2.02	0.89
1:A:54:ASN:H	1:A:54:ASN:ND2	1.69	0.88
1:A:53:LEU:O	1:A:56:PRO:HG2	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LYS:HA	1:A:186:LYS:HE3	1.51	0.88
12:M:5:A:H2'	12:M:6:G:H8	1.38	0.88
2:B:507:LYS:C	2:B:508:LEU:CD2	2.41	0.88
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.54	0.88
11:S:180:SER:O	11:S:184:LYS:HG3	1.74	0.88
11:S:216:HIS:HA	11:S:219:ALA:H	1.38	0.88
11:S:183:ASN:CA	11:S:186:ASN:ND2	2.37	0.87
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.03	0.87
11:S:164:SER:HB2	11:S:166:HIS:HD2	1.37	0.87
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.56	0.86
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.10	0.86
1:A:1136:SER:HB3	1:A:1205:LYS:HA	1.58	0.86
8:J:52:THR:HG22	8:J:53:HIS:H	1.40	0.86
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.56	0.86
11:S:221:GLY:C	11:S:223:ILE:H	1.79	0.85
3:C:167:HIS:HD2	3:C:169:LYS:H	1.20	0.85
2:B:1160:VAL:HG11	2:B:1169:MET:SD	2.17	0.85
1:A:550:LEU:HD13	1:A:560:ILE:HG22	1.59	0.85
8:J:64:ASN:HB3	8:J:65:PRO:CD	2.07	0.84
1:A:39:GLU:O	1:A:53:LEU:HD13	1.78	0.84
1:A:54:ASN:C	1:A:56:PRO:HD3	1.98	0.84
2:B:862:GLN:HG2	2:B:963:PHE:HD1	1.42	0.83
11:S:190:THR:CG2	11:S:191:ASN:N	2.36	0.83
12:M:5:A:H2'	12:M:6:G:C8	2.13	0.83
2:B:431:TYR:CD1	2:B:447:ALA:HB1	2.14	0.83
11:S:231:CYS:HB3	11:S:233:ALA:H	1.44	0.82
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.60	0.82
4:E:175:LEU:HD23	4:E:176:PRO:HD2	1.61	0.82
6:H:47:PHE:HB3	6:H:95:TYR:HD1	1.45	0.81
2:B:35:SER:HA	2:B:811:TYR:HE2	1.45	0.81
6:H:5:LEU:HB2	6:H:60:ALA:H	1.44	0.81
11:S:183:ASN:HA	11:S:186:ASN:HD22	1.43	0.81
11:S:223:ILE:C	11:S:225:PRO:CD	2.49	0.81
10:L:32:ALA:HB3	10:L:55:ILE:HD12	1.63	0.80
2:B:1084:GLN:HE21	2:B:1084:GLN:N	1.78	0.80
3:C:22:LEU:HD23	3:C:25:VAL:HG21	1.61	0.80
2:B:1051:THR:HB	2:B:1054:GLY:H	1.46	0.80
2:B:1065:GLN:HG2	2:B:1069:PHE:HB2	1.64	0.79
2:B:1183:LYS:HE3	2:B:1183:LYS:H	1.47	0.79
1:A:33:ALA:CB	1:A:56:PRO:HB2	2.12	0.79
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:VAL:HG21	1:A:758:ILE:HD11	1.65	0.79
11:S:181:GLU:O	11:S:185:VAL:HG23	1.83	0.79
2:B:431:TYR:CE1	2:B:447:ALA:HB1	2.18	0.79
1:A:53:LEU:O	1:A:56:PRO:CG	2.30	0.78
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.66	0.78
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.63	0.78
2:B:599:THR:O	2:B:603:LEU:HB2	1.84	0.78
2:B:509:ALA:C	2:B:511:PRO:HD2	2.03	0.78
11:S:222:ASP:O	11:S:225:PRO:HD3	1.83	0.78
2:B:542:MET:HE1	2:B:636:PRO:HG2	1.66	0.78
11:S:188:CYS:O	11:S:189:ASP:CB	2.32	0.78
2:B:830:TYR:CZ	2:B:1000:PRO:HG3	2.19	0.77
1:A:70:CYS:O	1:A:72:GLU:HG2	1.83	0.77
2:B:667:GLN:HG3	2:B:667:GLN:O	1.83	0.77
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.67	0.77
8:J:5:VAL:HG12	8:J:6:ARG:HG3	1.65	0.77
11:S:216:HIS:H	11:S:218:ILE:H	1.33	0.77
2:B:723:VAL:HG22	2:B:724:ASP:H	1.50	0.77
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.64	0.76
1:A:54:ASN:N	1:A:54:ASN:HD22	1.81	0.76
1:A:58:LEU:O	1:A:67:CYS:SG	2.43	0.76
2:B:212:LEU:HD12	2:B:409:ALA:HA	1.67	0.76
1:A:49:LYS:HB2	1:A:55:ASP:OD2	1.85	0.76
1:A:567:LYS:HZ2	6:H:46:LEU:HB2	1.50	0.76
2:B:501:PRO:O	2:B:502:ILE:HG13	1.86	0.76
2:B:35:SER:HA	2:B:811:TYR:CE2	2.21	0.76
2:B:542:MET:CE	2:B:636:PRO:HG2	2.16	0.76
1:A:583:PRO:O	1:A:610:GLY:HA3	1.85	0.76
1:A:1329:THR:HG22	1:A:1331:SER:H	1.49	0.76
1:A:382:PRO:HD3	1:A:428:TYR:HD2	1.50	0.76
1:A:567:LYS:HB3	6:H:96:VAL:N	1.99	0.76
2:B:848:ARG:HH22	2:B:996:ARG:HD3	1.49	0.76
4:E:29:PHE:O	4:E:30:ILE:HG13	1.86	0.75
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.21	0.75
1:A:881:GLN:HA	1:A:961:ARG:HH21	1.51	0.75
1:A:829:VAL:HG13	2:B:508:LEU:CD1	2.12	0.75
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.68	0.75
2:B:654:ARG:H	2:B:657:HIS:HD2	1.34	0.75
11:S:164:SER:HB2	11:S:166:HIS:CD2	2.20	0.75
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.86	0.74
11:S:225:PRO:HA	11:S:228:LEU:HB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:CYS:HB3	1:A:168:GLY:HA2	1.69	0.74
1:A:388:LEU:HD23	1:A:391:LEU:HD12	1.70	0.74
2:B:933:SER:HB3	2:B:935:ARG:HH21	1.51	0.74
3:C:62:PHE:CE2	3:C:66:ARG:HD2	2.23	0.74
1:A:381:THR:HG22	1:A:382:PRO:HD2	1.70	0.74
1:A:54:ASN:O	1:A:55:ASP:CB	2.34	0.74
2:B:956:THR:HG23	2:B:960:GLY:HA2	1.67	0.73
1:A:710:LEU:H	1:A:710:LEU:HD12	1.53	0.73
1:A:1341:ILE:HD12	1:A:1379:GLY:O	1.88	0.73
1:A:858:ASN:HD21	1:A:862:ASN:H	1.36	0.73
11:S:192:GLU:O	11:S:193:ALA:HB2	1.86	0.73
1:A:62:ASP:O	1:A:63:ARG:HB2	1.86	0.73
8:J:52:THR:HG22	8:J:53:HIS:N	2.03	0.73
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.71	0.73
6:H:81:PRO:CB	6:H:82:PRO:HD3	2.10	0.73
1:A:1136:SER:CB	1:A:1205:LYS:HA	2.17	0.73
11:S:157:TYR:OH	11:S:176:LYS:HG3	1.89	0.73
2:B:666:TYR:O	2:B:666:TYR:CD2	2.42	0.73
1:A:1342:GLU:HG3	4:E:198:ILE:HG21	1.71	0.72
2:B:1084:GLN:HE21	2:B:1084:GLN:H	1.37	0.72
11:S:180:SER:HA	11:S:183:ASN:HB2	1.70	0.72
9:K:32:VAL:HG22	9:K:74:ARG:HG3	1.70	0.72
2:B:508:LEU:CB	2:B:509:ALA:HB2	2.19	0.72
11:S:192:GLU:O	11:S:193:ALA:CB	2.38	0.72
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.71	0.72
3:C:203:GLN:HG2	3:C:207:CYS:SG	2.29	0.72
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.70	0.72
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.71	0.72
8:J:64:ASN:CB	8:J:65:PRO:HD3	2.14	0.72
2:B:509:ALA:O	2:B:512:ARG:HG3	1.89	0.72
6:H:58:THR:HG22	6:H:59:ILE:H	1.53	0.72
1:A:49:LYS:CD	1:A:55:ASP:OD2	2.33	0.72
12:M:6:G:H2'	12:M:7:A:H8	1.55	0.72
1:A:567:LYS:NZ	6:H:43:ASN:HB3	2.05	0.72
2:B:800:GLN:HB3	8:J:52:THR:HG21	1.69	0.72
1:A:225:ASN:HD22	1:A:228:PHE:H	1.38	0.72
1:A:500:GLU:OE2	1:A:1438:THR:HG21	1.89	0.71
2:B:100:PRO:HG3	2:B:172:ILE:HD12	1.72	0.71
11:S:235:ASP:O	11:S:242:LYS:HE3	1.90	0.71
11:S:191:ASN:HD22	11:S:195:TYR:N	1.88	0.71
6:H:49:VAL:HG11	6:H:55:LEU:HD11	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:68:LEU:HB3	7:I:84:VAL:HG23	1.73	0.70
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.73	0.70
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.74	0.70
2:B:733:HIS:O	2:B:734:HIS:HB2	1.90	0.70
8:J:3:VAL:HG21	8:J:18:TRP:CG	2.27	0.70
1:A:196:GLU:HG2	1:A:197:PRO:HD2	1.72	0.70
1:A:588:LEU:HD23	1:A:605:MET:HG2	1.74	0.69
2:B:723:VAL:HG22	2:B:724:ASP:N	2.06	0.69
1:A:1230:GLU:HG2	11:S:201:ILE:HG23	1.72	0.69
1:A:961:ARG:HG2	1:A:1025:ARG:HH12	1.57	0.69
1:A:164:ARG:HG3	1:A:165:GLY:H	1.57	0.69
2:B:806:THR:HG22	2:B:808:ALA:H	1.58	0.69
11:S:215:LYS:C	11:S:217:LYS:HG2	2.13	0.69
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.74	0.69
1:A:608:ILE:HB	1:A:613:ILE:HD11	1.75	0.69
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.72	0.69
1:A:829:VAL:CG1	2:B:508:LEU:HD12	2.13	0.69
2:B:821:GLN:HE22	2:B:851:PHE:H	1.41	0.69
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.26	0.69
1:A:1176:LEU:HD13	11:S:200:ARG:HG2	1.75	0.69
1:A:265:LYS:HE3	1:A:265:LYS:HA	1.75	0.69
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.75	0.69
1:A:829:VAL:HG22	2:B:508:LEU:CD1	2.23	0.68
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.58	0.68
1:A:96:ILE:HD13	1:A:176:LYS:HE3	1.74	0.68
1:A:606:LEU:HG	1:A:613:ILE:HD12	1.74	0.68
2:B:211:VAL:O	2:B:480:SER:HA	1.93	0.68
2:B:664:THR:HG1	2:B:678:GLU:N	1.92	0.68
9:K:53:ASP:HB3	9:K:56:VAL:HG23	1.75	0.68
2:B:731:VAL:HG12	2:B:732:SER:H	1.55	0.68
2:B:1222:ARG:O	2:B:1223:ASP:HB2	1.92	0.68
2:B:507:LYS:CA	2:B:508:LEU:HD23	2.24	0.68
11:S:187:ASN:CB	11:S:190:THR:HB	2.23	0.68
4:E:114:ASN:O	4:E:115:ASN:HB3	1.92	0.68
2:B:549:THR:HG22	2:B:550:ASP:H	1.57	0.68
1:A:693:VAL:HG12	1:A:693:VAL:O	1.92	0.68
4:E:16:PHE:CE2	4:E:20:LYS:HE2	2.29	0.68
1:A:548:ASN:HD21	9:K:47:ARG:HH21	1.42	0.68
4:E:124:VAL:HG13	4:E:132:ILE:HB	1.75	0.68
2:B:1156:ASP:HB3	2:B:1198:TYR:N	2.06	0.68
2:B:799:PRO:HB2	2:B:818:PRO:HG2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:S:217:LYS:N	11:S:217:LYS:HD3	2.08	0.67
1:A:149:GLU:HB2	1:A:164:ARG:HH21	1.59	0.67
1:A:1446:ASP:HB2	5:F:133:VAL:HG23	1.76	0.67
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.75	0.67
2:B:872:GLU:HG2	2:B:916:THR:HG23	1.76	0.67
2:B:39:ARG:HH21	2:B:665:GLU:HG3	1.59	0.67
11:S:223:ILE:O	11:S:225:PRO:CD	2.43	0.67
11:S:182:MET:HB3	11:S:199:TYR:CE2	2.29	0.67
11:S:216:HIS:HA	11:S:218:ILE:N	2.09	0.67
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.41	0.67
8:J:10:CYS:SG	8:J:11:GLY:N	2.67	0.67
2:B:953:LEU:HD21	2:B:965:LYS:HB2	1.77	0.67
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.76	0.67
2:B:1187:ASN:O	2:B:1188:LYS:HB2	1.93	0.67
2:B:825:VAL:HG22	2:B:1010:LEU:HB3	1.76	0.67
11:S:230:THR:C	11:S:232:ASP:HA	2.15	0.67
1:A:535:THR:HG21	1:A:616:VAL:HA	1.75	0.67
1:A:57:ARG:HG2	1:A:68:GLN:HG2	1.77	0.67
1:A:565:ILE:HG12	1:A:567:LYS:HE2	1.76	0.67
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.76	0.67
2:B:125:SER:HB3	2:B:171:PRO:HA	1.77	0.67
7:I:4:PHE:H	7:I:4:PHE:HD2	1.42	0.67
1:A:444:PHE:HE2	1:A:470:LEU:HD23	1.60	0.66
11:S:231:CYS:HB3	11:S:233:ALA:N	2.10	0.66
1:A:899:VAL:HG22	1:A:1029:ARG:CG	2.25	0.66
1:A:279:LEU:O	1:A:284:ALA:HB2	1.94	0.66
1:A:751:SER:O	1:A:752:LYS:HG2	1.94	0.66
6:H:82:PRO:C	6:H:84:ALA:H	1.99	0.66
1:A:1081:LEU:HD13	1:A:1099:PRO:HD3	1.76	0.66
11:S:221:GLY:C	11:S:223:ILE:N	2.45	0.66
1:A:285:PRO:HB2	1:A:288:ALA:HB3	1.77	0.66
1:A:434:ARG:HE	1:A:437:MET:HG3	1.60	0.66
2:B:508:LEU:HD22	2:B:512:ARG:NH2	2.10	0.66
11:S:189:ASP:O	11:S:190:THR:C	2.34	0.66
2:B:794:ASN:O	2:B:795:ILE:HD12	1.95	0.66
11:S:285:GLN:O	11:S:286:THR:C	2.33	0.66
2:B:1002:THR:HG23	2:B:1004:GLU:HB2	1.77	0.66
1:A:55:ASP:N	1:A:56:PRO:HD2	2.09	0.66
11:S:206:VAL:HA	11:S:214:LEU:HD22	1.78	0.66
2:B:882:THR:OG1	2:B:933:SER:HB3	1.96	0.66
6:H:5:LEU:HB3	6:H:59:ILE:HB	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:142:VAL:H	8:J:16:ASP:CB	2.07	0.66
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.76	0.66
2:B:1159:ARG:HD3	2:B:1193:GLN:HG2	1.78	0.66
2:B:714:GLU:O	2:B:715:ALA:C	2.32	0.66
2:B:882:THR:OG1	2:B:933:SER:CB	2.44	0.66
11:S:216:HIS:CE1	11:S:220:ASN:HB3	2.31	0.65
2:B:955:THR:HG22	2:B:956:THR:N	2.11	0.65
2:B:1106:ARG:HD3	2:B:1126:GLY:C	2.17	0.65
1:A:249:SER:HB3	1:A:259:GLU:HG3	1.79	0.65
8:J:43:ARG:HG3	8:J:45:CYS:SG	2.36	0.65
2:B:408:LEU:HD11	2:B:545:ILE:HD13	1.79	0.65
7:I:58:VAL:HG12	7:I:60:GLN:H	1.61	0.65
3:C:7:GLN:HG3	9:K:104:ASN:ND2	2.11	0.65
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.36	0.65
2:B:108:VAL:HG12	2:B:109:THR:H	1.61	0.65
1:A:53:LEU:O	1:A:56:PRO:CD	2.44	0.64
1:A:55:ASP:C	1:A:57:ARG:H	1.98	0.64
2:B:955:THR:HG23	10:L:54:ARG:O	1.96	0.64
2:B:126:SER:OG	2:B:172:ILE:HD11	1.97	0.64
2:B:1159:ARG:HD3	2:B:1193:GLN:CG	2.27	0.64
1:A:55:ASP:O	1:A:57:ARG:N	2.30	0.64
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.30	0.64
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.79	0.64
2:B:733:HIS:O	2:B:733:HIS:ND1	2.30	0.64
1:A:1343:ALA:HB2	4:E:150:VAL:HG22	1.78	0.64
4:E:90:VAL:HA	4:E:120:ALA:HB2	1.80	0.64
11:S:239:ALA:CB	11:S:240:PRO:CD	2.75	0.64
4:E:32:GLN:HE21	4:E:36:GLU:HG3	1.62	0.64
2:B:60:GLN:HE22	2:B:94:LYS:HA	1.63	0.64
10:L:28:LYS:HB2	10:L:39:SER:CA	2.24	0.64
2:B:325:GLN:HG2	7:I:31:THR:HG21	1.79	0.64
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.79	0.64
1:A:56:PRO:O	1:A:57:ARG:CB	2.36	0.64
1:A:1072:ILE:O	1:A:1075:PRO:HD2	1.98	0.64
4:E:169:ARG:HH12	5:F:74:ILE:HD11	1.62	0.64
2:B:711:GLU:H	2:B:712:PRO:CD	2.07	0.64
7:I:68:LEU:HB3	7:I:84:VAL:CG2	2.27	0.64
1:A:34:LYS:HD2	1:A:34:LYS:N	2.13	0.64
2:B:363:HIS:O	2:B:364:ILE:HB	1.97	0.64
11:S:187:ASN:O	11:S:188:CYS:C	2.36	0.64
11:S:216:HIS:HA	11:S:219:ALA:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:S:216:HIS:N	11:S:218:ILE:H	1.96	0.64
1:A:752:LYS:HD2	2:B:1019:SER:HB2	1.80	0.64
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.62	0.64
11:S:195:TYR:O	11:S:199:TYR:HD1	1.81	0.64
11:S:220:ASN:HD22	11:S:220:ASN:H	1.44	0.64
3:C:43:THR:HG22	3:C:44:LEU:N	2.13	0.63
1:A:1410:PHE:CD2	2:B:1212:ILE:HD11	2.34	0.63
1:A:877:HIS:O	1:A:878:ILE:HG13	1.97	0.63
6:H:5:LEU:HB2	6:H:60:ALA:N	2.13	0.63
2:B:830:TYR:CE1	2:B:1000:PRO:HG3	2.32	0.63
2:B:953:LEU:CD2	2:B:965:LYS:HB2	2.27	0.63
1:A:284:ALA:HB1	1:A:289:ILE:HD11	1.79	0.63
2:B:508:LEU:CA	2:B:509:ALA:HB2	2.29	0.63
1:A:515:GLN:HA	1:A:1367:HIS:NE2	2.13	0.63
1:A:39:GLU:O	1:A:53:LEU:CD1	2.47	0.63
1:A:72:GLU:HB3	1:A:76:GLU:HG3	1.80	0.63
2:B:733:HIS:O	2:B:735:ALA:N	2.27	0.63
10:L:46:VAL:HG12	10:L:56:LEU:HD12	1.80	0.63
1:A:618:GLU:O	1:A:622:VAL:HG12	1.98	0.63
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.64	0.63
6:H:58:THR:HG22	6:H:59:ILE:N	2.13	0.63
1:A:1277:GLU:O	1:A:1278:ASN:HB2	1.99	0.63
2:B:730:ARG:HH22	2:B:1047:PHE:HB3	1.63	0.62
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.79	0.62
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	1.81	0.62
1:A:483:ASP:HA	2:B:988:GLY:HA2	1.81	0.62
2:B:837:ASP:OD1	2:B:1020:ARG:NH2	2.29	0.62
11:S:231:CYS:N	11:S:232:ASP:HA	2.12	0.62
6:H:95:TYR:HE2	6:H:97:MET:CG	2.13	0.62
1:A:442:VAL:HB	1:A:489:LEU:HD11	1.80	0.62
1:A:858:ASN:ND2	1:A:862:ASN:H	1.96	0.62
2:B:737:THR:HG21	7:I:66:PRO:HA	1.81	0.62
2:B:510:LYS:N	2:B:511:PRO:HD2	2.13	0.62
6:H:5:LEU:HD13	6:H:59:ILE:HG22	1.80	0.62
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	2.00	0.62
8:J:48:ARG:HE	8:J:49:MET:CE	2.13	0.62
2:B:801:LYS:O	8:J:52:THR:HG23	1.99	0.62
2:B:852:ARG:CZ	2:B:973:ILE:HD11	2.29	0.62
1:A:672:ASP:HB2	1:A:675:THR:HB	1.82	0.62
2:B:1099:VAL:HG13	2:B:1100:ASP:N	2.14	0.62
6:H:84:ALA:HA	6:H:87:ARG:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:130:ILE:HB	5:F:148:VAL:HG21	1.80	0.62
4:E:127:ILE:HD11	4:E:132:ILE:HD11	1.81	0.62
2:B:902:GLY:O	10:L:65:VAL:HG11	2.00	0.62
1:A:1384:VAL:HG12	1:A:1384:VAL:O	1.99	0.62
2:B:619:ILE:HD13	7:I:65:ASP:HB2	1.82	0.62
3:C:167:HIS:CD2	3:C:169:LYS:H	2.10	0.62
2:B:373:ARG:HG3	2:B:566:LEU:HD23	1.82	0.62
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.82	0.61
1:A:901:LEU:HD12	1:A:926:GLN:HG2	1.82	0.61
1:A:55:ASP:N	1:A:56:PRO:HD3	2.09	0.61
1:A:875:ALA:HB2	1:A:1366:ARG:CD	2.31	0.61
11:S:224:THR:N	11:S:225:PRO:HD3	2.16	0.61
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.36	0.61
2:B:1183:LYS:HE3	2:B:1183:LYS:N	2.14	0.61
1:A:58:LEU:HD22	1:A:80:HIS:O	1.99	0.61
4:E:22:MET:O	4:E:26:ARG:HG3	2.00	0.61
11:S:206:VAL:HG13	11:S:217:LYS:HE3	1.81	0.61
12:M:6:G:H2'	12:M:7:A:C8	2.35	0.61
11:S:239:ALA:HB1	11:S:240:PRO:CD	2.31	0.61
1:A:53:LEU:HB3	1:A:54:ASN:HD22	1.64	0.61
2:B:903:VAL:HG12	2:B:904:ARG:N	2.12	0.61
2:B:90:ILE:O	2:B:90:ILE:HG22	2.01	0.61
2:B:507:LYS:O	2:B:508:LEU:CG	2.49	0.61
2:B:565:PRO:HB2	2:B:567:GLU:HG2	1.82	0.61
1:A:1364:ASN:HD22	1:A:1365:TYR:N	1.99	0.60
11:S:187:ASN:O	11:S:189:ASP:N	2.34	0.60
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.58	0.60
2:B:743:ILE:O	2:B:744:HIS:HB2	2.00	0.60
1:A:881:GLN:OE1	1:A:959:ASN:HA	2.02	0.60
2:B:393:LYS:HE3	2:B:394:ASP:H	1.65	0.60
4:E:20:LYS:HB3	4:E:35:VAL:HG22	1.82	0.60
1:A:1261:LYS:HA	1:A:1264:GLU:HB3	1.81	0.60
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.84	0.60
10:L:28:LYS:CB	10:L:39:SER:HA	2.25	0.60
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.17	0.60
6:H:76:THR:HG22	6:H:77:ARG:HG3	1.83	0.60
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.02	0.60
1:A:278:THR:O	1:A:282:ASN:HB2	2.01	0.60
11:S:237:ALA:N	11:S:238:PRO:CD	2.65	0.60
1:A:538:ASP:OD2	6:H:22:LYS:HB2	2.01	0.60
1:A:559:VAL:HG22	6:H:78:SER:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:S:223:ILE:O	11:S:225:PRO:HD2	2.02	0.60
2:B:667:GLN:CG	2:B:667:GLN:O	2.50	0.60
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.84	0.60
2:B:770:GLN:HE21	2:B:985:GLY:H	1.48	0.60
2:B:991:GLY:O	2:B:992:ILE:HB	2.02	0.60
1:A:1445:ILE:H	1:A:1445:ILE:HD12	1.65	0.60
2:B:865:LYS:HG2	2:B:866:TYR:H	1.67	0.60
2:B:1212:ILE:O	2:B:1214:PRO:HD3	2.01	0.60
2:B:465:ASN:HD22	2:B:465:ASN:N	1.99	0.60
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.84	0.59
1:A:471:ASN:O	1:A:474:VAL:HG12	2.02	0.59
11:S:192:GLU:HA	11:S:192:GLU:OE2	2.02	0.59
11:S:228:LEU:HD23	11:S:233:ALA:HB3	1.84	0.59
11:S:233:ALA:O	11:S:235:ASP:N	2.35	0.59
2:B:986:GLN:HE22	2:B:1020:ARG:HE	1.51	0.59
2:B:667:GLN:HA	2:B:668:ASP:O	2.01	0.59
11:S:172:LEU:O	11:S:176:LYS:HD2	2.03	0.59
2:B:530:GLY:O	2:B:532:ALA:N	2.35	0.59
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.15	0.59
2:B:522:VAL:HG21	2:B:537:LYS:HD2	1.84	0.59
7:I:55:THR:HG22	7:I:56:ALA:H	1.67	0.59
1:A:356:ASP:HB2	1:A:469:ARG:HH11	1.68	0.59
7:I:59:VAL:C	7:I:61:ASP:H	2.05	0.59
1:A:1079:MET:HA	1:A:1359:ASP:OD1	2.02	0.59
3:C:234:SER:HB2	3:C:240:VAL:HG13	1.84	0.59
1:A:666:ILE:HG23	2:B:1026:LEU:HB3	1.83	0.59
11:S:225:PRO:HA	11:S:228:LEU:HD12	1.84	0.59
3:C:167:HIS:HD2	3:C:169:LYS:N	1.96	0.59
1:A:535:THR:CG2	1:A:616:VAL:HA	2.33	0.59
3:C:7:GLN:HG3	9:K:104:ASN:HD22	1.67	0.59
11:S:224:THR:O	11:S:228:LEU:HG	2.03	0.59
11:S:157:TYR:HE2	11:S:172:LEU:HD23	1.68	0.58
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.33	0.58
1:A:1017:LEU:HB2	4:E:206:GLY:N	2.12	0.58
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.38	0.58
1:A:1139:GLU:OE2	1:A:1205:LYS:HE2	2.03	0.58
11:S:185:VAL:O	11:S:187:ASN:ND2	2.35	0.58
2:B:114:PRO:HG3	2:B:181:LEU:CD1	2.24	0.58
2:B:324:ILE:HD11	2:B:333:PHE:HB2	1.85	0.58
1:A:565:ILE:HG22	1:A:571:LEU:H	1.69	0.58
2:B:733:HIS:CE1	2:B:735:ALA:HB3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:TYR:HB2	1:A:433:GLU:HB2	1.84	0.58
1:A:896:ARG:HH22	1:A:1030:ARG:NH2	2.01	0.58
1:A:598:LEU:HD12	6:H:124:ARG:HB2	1.84	0.58
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.86	0.58
1:A:829:VAL:HG21	2:B:509:ALA:HB2	1.83	0.58
12:M:4:G:H2'	12:M:5:A:C8	2.38	0.58
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.86	0.58
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.86	0.58
2:B:386:LEU:O	2:B:390:LEU:HG	2.03	0.58
3:C:134:ILE:HG23	3:C:141:GLY:H	1.68	0.58
1:A:19:PHE:HB3	1:A:1413:GLY:HA2	1.85	0.58
8:J:6:ARG:HG2	8:J:13:VAL:HA	1.84	0.58
1:A:463:ILE:HD13	1:A:469:ARG:HD2	1.85	0.58
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.84	0.58
6:H:113:ALA:HB2	6:H:126:GLU:HG3	1.86	0.58
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.86	0.57
3:C:173:ALA:O	3:C:174:ALA:HB3	2.03	0.57
2:B:242:SER:HB2	2:B:363:HIS:HB3	1.86	0.57
1:A:666:ILE:HG23	2:B:1026:LEU:CB	2.34	0.57
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.86	0.57
1:A:974:ASP:HB2	6:H:136:LYS:NZ	2.19	0.57
1:A:447:GLN:NE2	13:N:20:DC:H4'	2.19	0.57
11:S:289:ALA:N	11:S:292:PRO:O	2.38	0.57
11:S:180:SER:HB2	11:S:184:LYS:HE3	1.86	0.57
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.32	0.57
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.85	0.57
1:A:598:LEU:CD1	6:H:124:ARG:HB2	2.34	0.57
1:A:406:ILE:HG13	1:A:431:LYS:HB2	1.86	0.57
2:B:860:MET:HG3	2:B:965:LYS:HE2	1.86	0.57
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.85	0.57
1:A:1164:PRO:HA	1:A:1167:GLU:HG3	1.86	0.57
1:A:332:LYS:C	1:A:334:GLY:H	2.07	0.57
2:B:1138:MET:HA	2:B:1138:MET:CE	2.35	0.57
3:C:39:ALA:O	3:C:40:GLU:HG2	2.05	0.57
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.86	0.57
10:L:30:ILE:O	10:L:56:LEU:HA	2.05	0.57
2:B:865:LYS:HG2	2:B:866:TYR:N	2.20	0.57
1:A:628:GLY:O	1:A:632:VAL:HG23	2.05	0.57
2:B:274:PRO:O	2:B:275:TYR:HB2	2.04	0.57
2:B:54:PHE:HA	2:B:58:THR:HB	1.86	0.57
2:B:708:GLU:HG3	2:B:709:ASP:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:S:156:LEU:N	11:S:156:LEU:HD23	2.20	0.57
3:C:22:LEU:CD2	3:C:25:VAL:HG21	2.32	0.57
1:A:1072:ILE:HD11	1:A:1368:MET:HA	1.87	0.57
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.87	0.57
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.34	0.57
1:A:899:VAL:HG22	1:A:1029:ARG:HG3	1.84	0.57
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.86	0.57
2:B:516:ASN:ND2	2:B:516:ASN:H	2.03	0.57
11:S:198:ARG:HG2	11:S:232:ASP:OD2	2.05	0.56
1:A:980:ASP:N	1:A:980:ASP:OD1	2.38	0.56
2:B:510:LYS:O	2:B:513:GLN:HB2	2.05	0.56
11:S:230:THR:O	11:S:231:CYS:CB	2.53	0.56
2:B:1087:PHE:HD1	8:J:44:TYR:HH	1.52	0.56
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.35	0.56
2:B:62:ILE:HG23	2:B:418:LYS:HG2	1.88	0.56
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.87	0.56
1:A:49:LYS:CD	1:A:55:ASP:CG	2.56	0.56
11:S:217:LYS:H	11:S:217:LYS:HD3	1.69	0.56
3:C:11:ARG:HD3	3:C:209:TYR:CE2	2.40	0.56
9:K:46:ILE:O	9:K:50:LEU:HB2	2.06	0.56
2:B:261:ARG:NH1	2:B:261:ARG:HB3	2.20	0.56
2:B:507:LYS:O	2:B:508:LEU:CB	2.54	0.56
1:A:54:ASN:C	1:A:56:PRO:CD	2.67	0.56
11:S:191:ASN:HD22	11:S:195:TYR:CA	2.17	0.56
1:A:567:LYS:CB	6:H:96:VAL:H	2.06	0.56
2:B:733:HIS:NE2	2:B:735:ALA:HB3	2.20	0.56
11:S:206:VAL:C	11:S:214:LEU:HD13	2.25	0.56
2:B:1099:VAL:HG13	2:B:1100:ASP:H	1.71	0.56
2:B:764:SER:HB3	2:B:765:PRO:HD3	1.88	0.56
1:A:406:ILE:HG22	1:A:412:ARG:HA	1.88	0.56
9:K:7:PHE:C	9:K:9:LEU:H	2.08	0.56
2:B:63:ILE:O	2:B:67:SER:HB3	2.06	0.56
1:A:53:LEU:HD22	1:A:54:ASN:ND2	2.20	0.56
1:A:858:ASN:HD22	1:A:858:ASN:C	2.08	0.56
1:A:709:THR:HB	1:A:712:GLU:HB2	1.88	0.56
1:A:1172:LEU:HD22	11:S:204:SER:HB3	1.88	0.56
2:B:1072:MET:HE2	2:B:1085:ILE:HG12	1.88	0.56
11:S:185:VAL:O	11:S:187:ASN:CG	2.44	0.56
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.87	0.55
1:A:569:LYS:HD2	3:C:221:TYR:O	2.05	0.55
2:B:64:CYS:O	2:B:65:GLU:HB3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:121:ALA:HA	5:F:124:GLU:HB2	1.87	0.55
11:S:191:ASN:O	11:S:192:GLU:CB	2.54	0.55
2:B:273:LEU:HD12	2:B:276:ILE:CD1	2.37	0.55
2:B:666:TYR:O	2:B:666:TYR:CG	2.59	0.55
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.35	0.55
2:B:1215:ARG:HB3	2:B:1217:TYR:HE1	1.72	0.55
5:F:79:ARG:HA	5:F:144:GLU:OE1	2.06	0.55
1:A:477:PRO:HG3	1:A:521:MET:HG2	1.87	0.55
4:E:153:HIS:HB3	4:E:196:VAL:HG11	1.87	0.55
2:B:1087:PHE:HD1	8:J:44:TYR:OH	1.90	0.55
2:B:957:ASN:O	2:B:959:ASP:N	2.40	0.55
1:A:727:ASP:HB3	1:A:731:ARG:HH21	1.72	0.55
1:A:108:MET:SD	1:A:210:ILE:HD13	2.47	0.55
1:A:33:ALA:HB1	1:A:56:PRO:CB	2.30	0.55
9:K:12:LEU:H	9:K:12:LEU:HD12	1.71	0.55
1:A:72:GLU:HB3	1:A:76:GLU:CG	2.37	0.55
4:E:169:ARG:NH1	5:F:74:ILE:HD11	2.22	0.55
1:A:364:VAL:HG13	1:A:364:VAL:O	2.06	0.55
2:B:640:VAL:HG22	2:B:651:LEU:HD22	1.87	0.55
1:A:810:PRO:HD3	2:B:730:ARG:NH2	2.22	0.55
2:B:98:THR:OG1	2:B:126:SER:HB2	2.07	0.55
10:L:32:ALA:HB3	10:L:55:ILE:CD1	2.36	0.55
1:A:396:PRO:HG3	1:A:403:LYS:HA	1.89	0.54
11:S:216:HIS:CA	11:S:218:ILE:N	2.70	0.54
2:B:778:MET:SD	2:B:794:ASN:HB3	2.47	0.54
2:B:619:ILE:CD1	7:I:65:ASP:HB2	2.38	0.54
11:S:290:ASP:CA	11:S:291:HIS:O	2.54	0.54
2:B:516:ASN:HD22	2:B:516:ASN:H	1.53	0.54
8:J:24:LEU:HA	8:J:28:ASP:HB2	1.88	0.54
2:B:190:TYR:CZ	2:B:196:PRO:HG3	2.43	0.54
3:C:11:ARG:HD3	3:C:209:TYR:CZ	2.43	0.54
2:B:526:GLU:OE1	2:B:752:ALA:HB3	2.07	0.54
1:A:1121:GLU:HB2	1:A:1321:GLY:O	2.08	0.54
1:A:673:GLY:N	1:A:674:PRO:HD2	2.23	0.54
2:B:574:SER:HB3	2:B:577:ALA:HB2	1.90	0.54
11:S:239:ALA:HB1	11:S:240:PRO:HD3	1.88	0.54
2:B:507:LYS:O	2:B:508:LEU:HG	2.08	0.54
6:H:5:LEU:HD13	6:H:59:ILE:CG2	2.37	0.54
2:B:235:SER:OG	2:B:236:HIS:HD2	1.90	0.54
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.38	0.54
1:A:591:PHE:HA	1:A:595:THR:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:THR:O	1:A:834:THR:HG22	2.08	0.54
11:S:221:GLY:O	11:S:223:ILE:N	2.41	0.54
2:B:903:VAL:CG1	2:B:904:ARG:H	2.16	0.54
1:A:795:GLU:CD	1:A:795:GLU:H	2.10	0.54
11:S:198:ARG:O	11:S:202:ILE:HG13	2.08	0.54
11:S:237:ALA:H	11:S:238:PRO:CD	2.19	0.54
1:A:770:VAL:HG12	1:A:771:GLU:HG3	1.88	0.54
1:A:1276:VAL:HB	1:A:1279:ILE:HD12	1.90	0.54
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.42	0.54
2:B:43:LEU:HD11	2:B:811:TYR:O	2.08	0.54
1:A:347:PHE:HE2	1:A:375:THR:HG23	1.72	0.54
1:A:720:ARG:O	1:A:724:GLU:HB2	2.08	0.54
1:A:103:CYS:HG	1:A:211:PHE:HE1	1.54	0.54
2:B:363:HIS:O	2:B:364:ILE:CB	2.55	0.54
1:A:1324:PRO:HB2	4:E:142:VAL:HG11	1.89	0.54
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	1.89	0.54
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.08	0.54
5:F:93:ILE:HD13	5:F:148:VAL:HG12	1.91	0.53
1:A:284:ALA:CB	1:A:289:ILE:HD11	2.38	0.53
2:B:1215:ARG:HB3	2:B:1217:TYR:CE1	2.42	0.53
1:A:476:SER:N	1:A:477:PRO:CD	2.71	0.53
9:K:65:HIS:CD2	9:K:66:PRO:HD2	2.44	0.53
2:B:563:MET:CE	2:B:580:VAL:HB	2.37	0.53
1:A:1072:ILE:HG23	1:A:1356:ILE:HD11	1.89	0.53
2:B:1124:ARG:HH11	12:M:1:A:H5"	1.73	0.53
11:S:149:ARG:NH1	11:S:183:ASN:CG	2.61	0.53
2:B:501:PRO:C	2:B:502:ILE:HG13	2.29	0.53
10:L:38:LEU:HD13	10:L:48:CYS:SG	2.49	0.53
1:A:18:GLN:HG2	1:A:1418:LEU:HD13	1.89	0.53
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.91	0.53
2:B:45:SER:O	2:B:49:ASP:HB2	2.08	0.53
1:A:829:VAL:HG21	2:B:509:ALA:HB1	1.88	0.53
11:S:220:ASN:HD22	11:S:220:ASN:N	2.07	0.53
2:B:134:LYS:N	2:B:134:LYS:CD	2.66	0.53
2:B:25:ILE:HG22	2:B:26:THR:N	2.24	0.53
4:E:55:ARG:HB3	4:E:82:PHE:HB3	1.91	0.53
2:B:48:LEU:HD23	2:B:173:MET:SD	2.48	0.53
1:A:727:ASP:HB3	1:A:731:ARG:NH2	2.23	0.53
1:A:55:ASP:C	1:A:57:ARG:N	2.62	0.53
1:A:1081:LEU:CD1	1:A:1099:PRO:HD3	2.37	0.53
1:A:1138:ILE:HG22	1:A:1279:ILE:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:CYS:O	1:A:645:LEU:HB3	2.08	0.53
1:A:1394:THR:HG21	1:A:1398:MET:CE	2.39	0.53
4:E:124:VAL:HB	4:E:125:PRO:HD3	1.90	0.53
2:B:681:TRP:CH2	2:B:690:VAL:HG11	2.43	0.53
1:A:481:ASP:OD1	1:A:481:ASP:N	2.42	0.53
3:C:164:ALA:HB2	3:C:171:GLY:HA3	1.90	0.53
10:L:38:LEU:HD22	10:L:56:LEU:HD21	1.91	0.53
1:A:351:THR:HB	2:B:1103:ILE:HD12	1.91	0.53
1:A:982:THR:O	1:A:985:ASP:HB2	2.07	0.53
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	1.89	0.53
1:A:351:THR:HG21	2:B:1103:ILE:HG13	1.91	0.53
1:A:1325:THR:O	4:E:148:GLU:HB2	2.09	0.53
2:B:1069:PHE:HA	2:B:1085:ILE:O	2.09	0.53
11:S:180:SER:O	11:S:184:LYS:CG	2.53	0.52
2:B:665:GLU:O	2:B:665:GLU:CG	2.57	0.52
2:B:882:THR:HB	2:B:934:LYS:H	1.74	0.52
1:A:457:ALA:O	1:A:507:VAL:HG23	2.09	0.52
2:B:487:THR:HG22	2:B:489:SER:H	1.74	0.52
4:E:177:ARG:HD3	4:E:215:MET:SD	2.49	0.52
1:A:49:LYS:HD2	1:A:55:ASP:CB	2.37	0.52
1:A:49:LYS:CB	1:A:55:ASP:OD2	2.57	0.52
1:A:523:ILE:O	1:A:528:LEU:HD13	2.09	0.52
2:B:769:TYR:HE2	11:S:290:ASP:O	1.92	0.52
1:A:207:ILE:HG22	1:A:235:ILE:HD11	1.90	0.52
2:B:508:LEU:HA	2:B:509:ALA:HB2	1.91	0.52
1:A:1232:ASN:HD21	11:S:238:PRO:HG3	1.75	0.52
1:A:320:ARG:O	1:A:322:VAL:HG23	2.10	0.52
3:C:46:ILE:HB	3:C:68:GLY:HA2	1.92	0.52
1:A:1260:LEU:O	1:A:1260:LEU:HG	2.10	0.52
5:F:111:LEU:H	5:F:111:LEU:HD12	1.75	0.52
1:A:186:LYS:CE	1:A:186:LYS:HA	2.31	0.52
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.90	0.52
2:B:933:SER:O	2:B:934:LYS:HG3	2.09	0.52
1:A:381:THR:CG2	1:A:382:PRO:HD2	2.39	0.52
1:A:551:TYR:CE1	9:K:74:ARG:HD3	2.45	0.52
1:A:537:ARG:HH22	6:H:122:LEU:HD12	1.74	0.52
2:B:1000:PRO:HB2	2:B:1072:MET:HE3	1.91	0.52
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.56	0.52
2:B:121:ASN:HD21	2:B:965:LYS:NZ	2.08	0.52
1:A:559:VAL:HG13	6:H:78:SER:HA	1.92	0.52
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:ASN:HD22	1:A:905:ASP:H	1.56	0.52
1:A:29:ALA:HB1	2:B:1184:GLY:HA2	1.92	0.52
11:S:182:MET:O	11:S:186:ASN:N	2.42	0.52
1:A:793:SER:CB	1:A:794:PRO:HD2	2.39	0.52
1:A:444:PHE:CE2	1:A:470:LEU:HD23	2.43	0.52
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.10	0.52
6:H:100:THR:HG23	6:H:138:GLU:HA	1.91	0.52
2:B:616:ILE:HG13	2:B:697:GLU:HA	1.91	0.52
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	2.45	0.52
12:M:11:U:H5"	12:M:11:U:H6	1.75	0.52
2:B:792:MET:O	2:B:793:ALA:HB2	2.10	0.52
3:C:35:ARG:HD3	9:K:41:THR:HA	1.92	0.52
1:A:513:SER:HB2	1:A:520:CYS:HB3	1.92	0.52
7:I:28:GLU:HB2	7:I:35:VAL:HG22	1.92	0.52
11:S:230:THR:O	11:S:231:CYS:HB3	2.10	0.51
2:B:933:SER:CB	2:B:935:ARG:NH2	2.64	0.51
2:B:999:MET:HB3	2:B:1007:VAL:CG2	2.39	0.51
2:B:769:TYR:CE2	11:S:290:ASP:O	2.63	0.51
9:K:21:ILE:HG12	9:K:33:ILE:HG12	1.92	0.51
2:B:174:LEU:HD11	2:B:204:ILE:HG13	1.91	0.51
6:H:110:ASP:O	6:H:128:ASN:HB2	2.10	0.51
1:A:1291:VAL:HG13	1:A:1292:PRO:HD2	1.92	0.51
2:B:628:THR:CG2	2:B:628:THR:O	2.57	0.51
1:A:335:ARG:NH1	2:B:1202:LEU:HD22	2.26	0.51
3:C:184:ASN:HD21	3:C:189:THR:H	1.58	0.51
1:A:851:HIS:ND1	5:F:139:PRO:HG3	2.25	0.51
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.10	0.51
11:S:183:ASN:O	11:S:186:ASN:OD1	2.27	0.51
13:N:15:DA:H1'	13:N:16:DC:O5'	2.11	0.51
1:A:1064:VAL:HG12	1:A:1370:LEU:HD22	1.90	0.51
1:A:356:ASP:OD2	1:A:469:ARG:HD3	2.10	0.51
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.45	0.51
1:A:19:PHE:O	1:A:1416:ALA:HA	2.10	0.51
11:S:290:ASP:CA	11:S:291:HIS:C	2.78	0.51
2:B:857:ARG:NH2	13:N:24:DT:OP1	2.43	0.51
1:A:71:GLN:HG3	1:A:72:GLU:N	2.26	0.51
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.38	0.51
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.92	0.51
3:C:124:LEU:O	3:C:125:MET:HB2	2.10	0.51
1:A:761:MET:O	1:A:803:SER:HB2	2.11	0.51
2:B:1099:VAL:O	2:B:1103:ILE:HD13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:CYS:SG	2:B:304:ASP:O	2.69	0.51
2:B:292:ILE:N	2:B:293:PRO:HD3	2.25	0.51
1:A:776:ALA:O	1:A:783:THR:HG22	2.10	0.51
2:B:133:LYS:O	2:B:134:LYS:HB3	2.11	0.51
2:B:563:MET:HE3	2:B:580:VAL:HB	1.92	0.51
10:L:49:LYS:O	10:L:50:ASP:CB	2.59	0.51
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.41	0.51
2:B:512:ARG:O	2:B:513:GLN:C	2.49	0.51
11:S:183:ASN:O	11:S:186:ASN:ND2	2.43	0.51
2:B:95:ILE:HD11	2:B:128:LEU:HG	1.91	0.51
2:B:859:TYR:CD1	2:B:859:TYR:N	2.79	0.51
2:B:261:ARG:HH11	2:B:261:ARG:HB3	1.75	0.51
1:A:1116:LEU:O	1:A:1116:LEU:HG	2.11	0.51
3:C:36:VAL:HG23	9:K:41:THR:HG21	1.93	0.51
9:K:19:LEU:HD21	9:K:35:PHE:CD2	2.45	0.51
3:C:66:ARG:NH2	8:J:3:VAL:O	2.43	0.51
1:A:208:LEU:HD21	1:A:212:LYS:HE3	1.93	0.50
2:B:113:TYR:HB3	2:B:114:PRO:HD2	1.93	0.50
3:C:29:MET:HA	9:K:45:LEU:HD13	1.93	0.50
2:B:283:VAL:HG21	2:B:318:VAL:HA	1.93	0.50
2:B:240:ILE:HG21	2:B:381:MET:HE1	1.94	0.50
2:B:1065:GLN:HB3	2:B:1069:PHE:O	2.11	0.50
1:A:71:GLN:HG3	1:A:72:GLU:H	1.75	0.50
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.93	0.50
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.93	0.50
7:I:5:ARG:O	7:I:14:LEU:HD12	2.12	0.50
1:A:380:VAL:HG11	1:A:427:GLN:O	2.11	0.50
3:C:28:ALA:HB1	9:K:45:LEU:HA	1.93	0.50
1:A:465:TYR:HB3	2:B:976:ILE:HG21	1.92	0.50
1:A:1187:GLN:HG2	1:A:1188:GLN:HG3	1.92	0.50
1:A:553:VAL:HG12	1:A:555:ASP:H	1.76	0.50
2:B:365:THR:HG23	2:B:367:LEU:H	1.75	0.50
8:J:36:LEU:HD11	8:J:51:LEU:HB2	1.92	0.50
2:B:507:LYS:C	2:B:508:LEU:CG	2.78	0.50
2:B:509:ALA:O	2:B:511:PRO:HD2	2.12	0.50
2:B:1084:GLN:NE2	2:B:1084:GLN:H	2.08	0.50
1:A:806:ARG:NH1	2:B:729:ILE:HD11	2.26	0.50
3:C:164:ALA:HA	3:C:167:HIS:O	2.11	0.50
2:B:408:LEU:CD1	2:B:545:ILE:HD13	2.41	0.50
1:A:1063:MET:HG3	1:A:1436:ILE:HG23	1.94	0.50
1:A:451:HIS:HB2	1:A:454:SER:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:S:180:SER:O	11:S:184:LYS:N	2.38	0.50
2:B:665:GLU:HG2	2:B:665:GLU:O	2.11	0.50
2:B:361:LEU:HG	2:B:364:ILE:HD12	1.94	0.50
1:A:675:THR:O	1:A:679:ILE:HG13	2.12	0.50
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.12	0.50
2:B:92:PHE:HD2	2:B:130:VAL:HG11	1.77	0.50
2:B:698:GLU:O	2:B:701:ILE:HG12	2.12	0.50
11:S:232:ASP:O	11:S:234:LYS:N	2.45	0.50
1:A:830:LYS:HA	1:A:1081:LEU:HD23	1.93	0.50
6:H:44:VAL:O	6:H:44:VAL:CG1	2.60	0.50
8:J:8:PHE:CD1	8:J:49:MET:SD	3.05	0.50
7:I:4:PHE:N	7:I:4:PHE:CD2	2.77	0.50
2:B:975:GLN:HG2	2:B:976:ILE:H	1.76	0.50
3:C:116:LYS:HD3	3:C:140:ASN:HB3	1.94	0.50
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.12	0.50
2:B:192:LEU:O	2:B:193:LYS:HB2	2.12	0.50
11:S:182:MET:HB3	11:S:199:TYR:CD2	2.47	0.49
1:A:567:LYS:HZ1	6:H:43:ASN:HB3	1.72	0.49
2:B:431:TYR:CE1	2:B:447:ALA:CB	2.91	0.49
3:C:6:PRO:HB3	3:C:25:VAL:CG1	2.42	0.49
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.93	0.49
1:A:535:THR:HB	1:A:616:VAL:HG13	1.93	0.49
1:A:1224:LEU:O	1:A:1226:VAL:HG23	2.12	0.49
11:S:202:ILE:HD13	11:S:228:LEU:HD13	1.93	0.49
10:L:27:LEU:N	10:L:27:LEU:HD23	2.27	0.49
1:A:326:ARG:HH21	1:A:1407:GLU:HG3	1.77	0.49
1:A:1141:THR:OG1	1:A:1205:LYS:HD3	2.12	0.49
4:E:144:ILE:HG13	4:E:145:THR:N	2.26	0.49
2:B:898:LEU:HD13	2:B:952:VAL:HG11	1.93	0.49
2:B:861:ASP:OD1	2:B:862:GLN:N	2.46	0.49
2:B:45:SER:O	2:B:49:ASP:CB	2.61	0.49
2:B:874:PHE:O	2:B:875:GLU:HB3	2.12	0.49
1:A:134:ARG:NH1	1:A:220:THR:O	2.43	0.49
1:A:1042:PHE:CE2	1:A:1046:LEU:HD11	2.47	0.49
11:S:215:LYS:O	11:S:217:LYS:HG2	2.11	0.49
2:B:955:THR:HG22	2:B:956:THR:H	1.76	0.49
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.95	0.49
1:A:251:SER:HB3	1:A:257:ARG:NH1	2.27	0.49
1:A:915:SER:O	1:A:919:ILE:HD12	2.13	0.49
11:S:183:ASN:O	11:S:186:ASN:CG	2.50	0.49
11:S:191:ASN:O	11:S:192:GLU:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:4:THR:HG22	6:H:5:LEU:H	1.76	0.49
1:A:71:GLN:O	1:A:73:GLY:N	2.46	0.49
1:A:693:VAL:HG11	1:A:717:ASN:HD22	1.78	0.49
1:A:851:HIS:HB2	1:A:855:THR:HG22	1.94	0.49
2:B:315:LYS:HB3	2:B:316:PRO:HD3	1.95	0.49
1:A:672:ASP:CG	1:A:736:ASN:HD21	2.15	0.49
2:B:393:LYS:HA	2:B:393:LYS:CE	2.43	0.49
12:M:8:G:C2	13:N:22:DT:N3	2.81	0.49
1:A:449:SER:HA	1:A:454:SER:OG	2.13	0.49
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.32	0.49
4:E:88:VAL:HB	4:E:116:ILE:HG12	1.94	0.49
4:E:176:PRO:O	4:E:212:ARG:HA	2.12	0.49
2:B:999:MET:HG3	2:B:1000:PRO:CD	2.43	0.49
1:A:447:GLN:HE22	13:N:20:DC:H4'	1.77	0.49
1:A:15:LYS:HB3	2:B:1220:ARG:HE	1.78	0.49
2:B:288:ALA:HA	2:B:331:LEU:HD12	1.95	0.49
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.33	0.49
1:A:1421:CYS:HA	1:A:1426:GLU:HG3	1.95	0.49
3:C:44:LEU:HD13	3:C:129:ILE:HD11	1.95	0.48
1:A:525:GLN:O	1:A:528:LEU:N	2.46	0.48
6:H:89:LEU:C	6:H:91:ASP:H	2.16	0.48
1:A:1066:VAL:HG11	2:B:1136:ASP:O	2.13	0.48
1:A:1206:ASP:HB2	1:A:1274:ARG:HH22	1.78	0.48
2:B:1006:ILE:HG22	2:B:1007:VAL:N	2.28	0.48
2:B:273:LEU:HD12	2:B:276:ILE:HD13	1.95	0.48
2:B:766:ARG:NH2	2:B:1020:ARG:HB3	2.28	0.48
1:A:857:ARG:NH1	5:F:139:PRO:HB2	2.28	0.48
1:A:1334:ASP:C	1:A:1336:MET:H	2.16	0.48
2:B:666:TYR:C	2:B:666:TYR:CD2	2.87	0.48
2:B:1020:ARG:O	2:B:1021:MET:HB2	2.14	0.48
1:A:714:PHE:O	1:A:718:VAL:HG23	2.12	0.48
11:S:150:ASP:N	11:S:150:ASP:OD1	2.45	0.48
1:A:1230:GLU:OE1	11:S:204:SER:HB2	2.13	0.48
11:S:216:HIS:N	11:S:218:ILE:N	2.61	0.48
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	2.29	0.48
3:C:147:LEU:CD2	3:C:147:LEU:N	2.76	0.48
8:J:57:ILE:HA	8:J:60:PHE:HD2	1.77	0.48
2:B:703:ILE:HG21	2:B:742:GLU:OE1	2.13	0.48
4:E:124:VAL:HA	4:E:132:ILE:HD12	1.94	0.48
1:A:777:PHE:HE1	1:A:792:TYR:CZ	2.31	0.48
7:I:22:ASN:O	7:I:23:ASN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:244:VAL:HG12	3:C:244:VAL:O	2.12	0.48
1:A:317:LYS:O	1:A:318:SER:CB	2.62	0.48
2:B:905:VAL:HB	2:B:941:LEU:HD22	1.96	0.48
1:A:577:ILE:HG13	1:A:578:LEU:N	2.28	0.48
2:B:70:ILE:O	2:B:70:ILE:HG22	2.13	0.48
11:S:217:LYS:C	11:S:219:ALA:N	2.66	0.48
2:B:948:ILE:HG22	2:B:949:VAL:O	2.11	0.48
13:N:18:DA:H2'	13:N:19:DT:C6	2.49	0.48
1:A:357:PRO:HD2	2:B:833:TYR:CE2	2.48	0.48
1:A:977:LYS:HA	1:A:978:PRO:HD3	1.75	0.48
7:I:73:ARG:HH12	7:I:112:SER:HA	1.78	0.48
1:A:1092:LYS:HD2	1:A:1092:LYS:HA	1.66	0.48
1:A:332:LYS:NZ	13:N:19:DT:P	2.87	0.48
2:B:274:PRO:HB2	2:B:359:GLU:HB3	1.95	0.48
1:A:1303:GLU:HG3	1:A:1305:VAL:HG23	1.95	0.48
4:E:153:HIS:HB3	4:E:196:VAL:CG1	2.44	0.48
3:C:213:PRO:O	3:C:214:ASN:HB3	2.14	0.48
1:A:800:VAL:HA	1:A:812:GLU:HG2	1.96	0.48
1:A:1004:ASN:H	1:A:1004:ASN:HD22	1.62	0.48
11:S:149:ARG:O	11:S:153:LEU:N	2.32	0.48
2:B:999:MET:HB3	2:B:1007:VAL:HG21	1.96	0.48
2:B:1017:ILE:HB	2:B:1018:PRO:CD	2.40	0.48
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.49	0.48
5:F:77:ASP:O	5:F:78:GLN:HB2	2.14	0.48
1:A:1243:VAL:HG13	1:A:1243:VAL:O	2.14	0.48
2:B:459:TYR:CD2	2:B:459:TYR:C	2.87	0.48
2:B:549:THR:HG22	2:B:550:ASP:N	2.28	0.48
2:B:327:ARG:O	2:B:331:LEU:HD13	2.14	0.48
1:A:662:PHE:HZ	1:A:746:MET:HG3	1.79	0.48
11:S:186:ASN:OD1	11:S:187:ASN:N	2.47	0.47
2:B:866:TYR:CD1	2:B:870:ILE:O	2.67	0.47
1:A:600:PRO:HA	6:H:25:ARG:NH1	2.28	0.47
1:A:290:GLU:HA	1:A:293:GLU:CB	2.44	0.47
1:A:115:LEU:HD22	1:A:119:ASN:HD22	1.79	0.47
2:B:604:ARG:HG2	2:B:604:ARG:O	2.13	0.47
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.72	0.47
1:A:49:LYS:NZ	1:A:61:ILE:HG13	2.29	0.47
1:A:986:ILE:CD1	1:A:1032:LEU:HD11	2.44	0.47
4:E:61:GLN:HE21	4:E:105:PHE:HE2	1.63	0.47
2:B:393:LYS:HA	2:B:393:LYS:HE3	1.96	0.47
1:A:130:ASP:O	1:A:134:ARG:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:PHE:HB2	1:A:256:GLN:HB3	1.96	0.47
1:A:86:LEU:HB2	1:A:237:THR:O	2.14	0.47
1:A:444:PHE:HE2	1:A:470:LEU:CD2	2.27	0.47
1:A:351:THR:HB	2:B:1103:ILE:CD1	2.45	0.47
1:A:332:LYS:C	1:A:333:GLU:HG2	2.34	0.47
4:E:154:ILE:O	4:E:196:VAL:HA	2.15	0.47
2:B:582:VAL:O	2:B:583:ASN:HB2	2.14	0.47
11:S:186:ASN:O	11:S:187:ASN:CB	2.62	0.47
11:S:225:PRO:O	11:S:228:LEU:HB2	2.15	0.47
7:I:58:VAL:HA	7:I:62:ILE:HD11	1.96	0.47
1:A:35:ILE:HD12	1:A:241:VAL:HG21	1.96	0.47
1:A:896:ARG:NH2	1:A:1030:ARG:NH2	2.62	0.47
11:S:287:ARG:O	11:S:292:PRO:O	2.31	0.47
1:A:913:LEU:HD11	1:A:981:LEU:O	2.14	0.47
6:H:63:LEU:HB3	6:H:90:ALA:HB2	1.96	0.47
2:B:496:ARG:NH1	2:B:539:LEU:HB2	2.29	0.47
2:B:544:CYS:HB2	2:B:634:TYR:CZ	2.49	0.47
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.80	0.47
2:B:368:GLU:O	2:B:370:PHE:N	2.48	0.47
1:A:974:ASP:HB2	6:H:136:LYS:HZ2	1.79	0.47
2:B:235:SER:OG	2:B:236:HIS:CD2	2.67	0.47
2:B:703:ILE:HA	2:B:740:HIS:O	2.14	0.47
1:A:1155:ASP:HA	1:A:1156:PRO:HD3	1.71	0.47
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.96	0.47
1:A:353:ILE:HD13	1:A:487:MET:CE	2.45	0.47
2:B:816:GLU:O	2:B:817:LEU:HD23	2.14	0.47
1:A:1454:MET:O	1:A:1454:MET:HG3	2.12	0.47
9:K:27:ALA:HB1	9:K:28:PRO:HD2	1.97	0.47
2:B:840:ILE:HG21	2:B:999:MET:HE1	1.97	0.47
2:B:1119:VAL:O	2:B:1126:GLY:HA3	2.15	0.47
2:B:776:GLN:HE22	12:M:9:G:H5"	1.79	0.47
2:B:640:VAL:O	2:B:640:VAL:HG12	2.13	0.47
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.97	0.47
1:A:903:ASN:HB3	1:A:906:HIS:HB2	1.96	0.47
1:A:342:GLY:O	2:B:1129:ARG:NH1	2.47	0.47
1:A:472:LEU:O	1:A:475:THR:HB	2.15	0.47
9:K:62:LYS:O	9:K:62:LYS:HG3	2.15	0.47
1:A:1447:GLU:O	1:A:1451:VAL:HG23	2.14	0.47
1:A:1193:LEU:HD21	1:A:1267:MET:CE	2.44	0.47
1:A:759:ALA:O	1:A:763:ALA:HB3	2.15	0.47
1:A:91:PHE:HB2	1:A:297:GLN:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HE3	6:H:46:LEU:HD12	1.97	0.47
1:A:399:HIS:O	1:A:435:HIS:CD2	2.67	0.47
2:B:1185:CYS:O	2:B:1186:ASP:C	2.54	0.47
1:A:1027:ALA:O	1:A:1031:VAL:HG23	2.14	0.47
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.97	0.47
1:A:774:ARG:NH2	1:A:797:LYS:HB2	2.30	0.47
1:A:998:LEU:HD22	1:A:1001:ARG:NH1	2.30	0.47
1:A:658:LEU:HD13	2:B:831:SER:HA	1.96	0.47
1:A:57:ARG:O	1:A:68:GLN:NE2	2.35	0.47
11:S:204:SER:C	11:S:206:VAL:H	2.18	0.47
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.95	0.47
2:B:983:ARG:HD2	2:B:1091:TYR:CD2	2.46	0.47
2:B:737:THR:CG2	7:I:66:PRO:HA	2.44	0.47
6:H:113:ALA:HA	6:H:125:LEU:O	2.15	0.47
1:A:855:THR:HG21	1:A:857:ARG:HE	1.80	0.47
2:B:635:ARG:HH22	2:B:742:GLU:CD	2.18	0.47
2:B:265:SER:O	2:B:266:ALA:HB3	2.15	0.47
6:H:56:THR:O	6:H:144:ILE:HA	2.15	0.47
1:A:1063:MET:SD	1:A:1436:ILE:HG23	2.55	0.46
11:S:228:LEU:C	11:S:232:ASP:HB3	2.34	0.46
2:B:39:ARG:NH2	2:B:665:GLU:CG	2.65	0.46
2:B:862:GLN:HG2	2:B:963:PHE:CD1	2.34	0.46
2:B:121:ASN:HD21	2:B:965:LYS:HZ3	1.63	0.46
1:A:523:ILE:HD12	1:A:622:VAL:HG21	1.97	0.46
1:A:869:GLY:O	4:E:204:THR:HG21	2.14	0.46
1:A:837:ILE:HG23	1:A:1105:LEU:HD12	1.96	0.46
1:A:756:ILE:H	1:A:756:ILE:HG13	1.47	0.46
1:A:1225:PHE:O	1:A:1240:CYS:HA	2.16	0.46
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.50	0.46
2:B:705:MET:H	2:B:710:LEU:HD12	1.79	0.46
2:B:706:GLN:H	2:B:710:LEU:HD12	1.79	0.46
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.97	0.46
1:A:401:GLY:C	1:A:435:HIS:CD2	2.89	0.46
1:A:1336:MET:HG2	1:A:1341:ILE:HA	1.98	0.46
3:C:43:THR:CG2	3:C:44:LEU:N	2.78	0.46
1:A:1279:ILE:HD11	1:A:1316:VAL:HG22	1.98	0.46
1:A:325:ILE:O	1:A:328:ARG:HB2	2.15	0.46
2:B:310:MET:O	2:B:313:MET:HB2	2.15	0.46
9:K:20:LYS:HE3	9:K:20:LYS:HB2	1.70	0.46
11:S:189:ASP:O	11:S:192:GLU:N	2.49	0.46
11:S:225:PRO:HA	11:S:228:LEU:CB	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:ASN:C	1:A:1364:ASN:HD22	2.18	0.46
2:B:733:HIS:O	2:B:734:HIS:CB	2.56	0.46
1:A:901:LEU:O	1:A:920:LEU:HD23	2.15	0.46
2:B:562:GLY:HA3	2:B:590:HIS:HE1	1.80	0.46
1:A:49:LYS:HD3	1:A:55:ASP:HB2	1.98	0.46
2:B:712:PRO:O	2:B:713:ALA:HB2	2.15	0.46
11:S:210:ASN:O	11:S:214:LEU:HG	2.16	0.46
4:E:205:SER:O	4:E:206:GLY:C	2.53	0.46
2:B:1002:THR:CG2	2:B:1004:GLU:HB2	2.45	0.46
2:B:345:LYS:C	2:B:347:LYS:H	2.19	0.46
2:B:1108:ARG:HG2	2:B:1109:GLY:N	2.31	0.46
1:A:1100:ARG:O	1:A:1104:ILE:HG13	2.16	0.46
1:A:982:THR:H	1:A:985:ASP:CG	2.18	0.46
1:A:853:ASP:HB3	5:F:138:LEU:HD22	1.98	0.46
1:A:697:ALA:HB1	7:I:97:MET:HE1	1.96	0.46
1:A:629:LEU:HD23	1:A:629:LEU:O	2.16	0.46
11:S:216:HIS:N	11:S:217:LYS:HB2	2.31	0.46
1:A:84:ILE:HG22	1:A:239:LEU:O	2.16	0.46
2:B:569:TYR:CD1	2:B:589:VAL:HG21	2.51	0.46
12:M:8:G:O2'	12:M:9:G:H5'	2.16	0.46
7:I:55:THR:HG23	7:I:100:PHE:CD2	2.50	0.46
1:A:1394:THR:HG21	1:A:1398:MET:HE2	1.98	0.46
3:C:82:TYR:CG	3:C:161:LYS:HD3	2.51	0.46
1:A:1327:ILE:HG22	4:E:147:HIS:CE1	2.51	0.46
1:A:1060:PRO:HD2	5:F:86:THR:HG21	1.97	0.46
1:A:567:LYS:HB3	6:H:95:TYR:HA	1.97	0.46
1:A:34:LYS:HD2	1:A:34:LYS:H	1.80	0.46
1:A:1394:THR:HG22	1:A:1395:GLY:N	2.31	0.46
2:B:791:THR:O	2:B:792:MET:HB2	2.16	0.46
3:C:184:ASN:ND2	3:C:189:THR:O	2.48	0.46
1:A:98:LYS:O	1:A:102:VAL:HG23	2.16	0.46
2:B:610:ASN:OD1	2:B:612:GLU:HB2	2.15	0.46
9:K:83:PRO:O	9:K:86:ALA:HB3	2.16	0.46
11:S:199:TYR:HA	11:S:202:ILE:HD12	1.97	0.46
1:A:71:GLN:CG	1:A:72:GLU:H	2.25	0.46
2:B:1162:ILE:HD13	2:B:1216:LEU:HB3	1.98	0.46
2:B:870:ILE:O	2:B:870:ILE:HG22	2.16	0.46
2:B:616:ILE:N	2:B:616:ILE:HD12	2.31	0.46
7:I:73:ARG:N	7:I:83:ASN:HD21	2.14	0.46
2:B:1076:HIS:ND1	2:B:1076:HIS:N	2.64	0.46
2:B:648:HIS:N	2:B:648:HIS:ND1	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:933:SER:OG	2:B:935:ARG:NH2	2.49	0.45
2:B:835:GLN:HA	2:B:1013:ASN:HD22	1.80	0.45
2:B:1181:GLU:H	2:B:1188:LYS:HA	1.81	0.45
1:A:434:ARG:NE	1:A:437:MET:HG3	2.28	0.45
2:B:770:GLN:NE2	2:B:985:GLY:H	2.13	0.45
2:B:463:THR:HB	2:B:465:ASN:H	1.80	0.45
2:B:365:THR:HG23	2:B:366:GLN:N	2.31	0.45
6:H:44:VAL:O	6:H:44:VAL:HG12	2.15	0.45
2:B:510:LYS:HA	2:B:510:LYS:HD3	1.63	0.45
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.15	0.45
3:C:43:THR:HG22	3:C:44:LEU:H	1.78	0.45
1:A:1327:ILE:HG22	4:E:147:HIS:HE1	1.82	0.45
1:A:564:ALA:N	1:A:576:GLN:HE22	2.14	0.45
11:S:149:ARG:CZ	11:S:183:ASN:OD1	2.64	0.45
3:C:226:ASP:O	3:C:227:THR:C	2.55	0.45
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.98	0.45
2:B:755:ILE:O	2:B:809:MET:HE1	2.17	0.45
4:E:213:ILE:HG12	4:E:214:CYS:N	2.30	0.45
1:A:89:PRO:HB2	1:A:204:THR:HB	1.98	0.45
1:A:565:ILE:CG2	1:A:567:LYS:HE3	2.47	0.45
1:A:567:LYS:HZ3	6:H:43:ASN:HB3	1.78	0.45
8:J:52:THR:CG2	8:J:53:HIS:H	2.10	0.45
2:B:357:GLN:NE2	2:B:368:GLU:HA	2.31	0.45
2:B:412:LEU:HA	2:B:412:LEU:HD23	1.79	0.45
11:S:222:ASP:O	11:S:225:PRO:CD	2.59	0.45
3:C:115:SER:HB3	3:C:142:VAL:HB	1.98	0.45
1:A:1176:LEU:HD13	11:S:200:ARG:CG	2.44	0.45
2:B:1004:GLU:O	3:C:177:GLU:HG2	2.17	0.45
2:B:1158:PHE:CG	2:B:1159:ARG:N	2.83	0.45
1:A:1424:VAL:HG13	1:A:1436:ILE:HD11	1.99	0.45
3:C:238:ILE:HG22	3:C:242:GLN:HB2	1.98	0.45
11:S:154:LYS:O	11:S:158:ASP:CB	2.65	0.45
1:A:1266:THR:C	1:A:1268:LEU:H	2.18	0.45
2:B:20:ASP:HB2	2:B:23:ALA:HB2	1.97	0.45
1:A:376:TYR:HA	1:A:377:PRO:HD3	1.68	0.45
11:S:182:MET:CB	11:S:199:TYR:CE2	2.98	0.45
1:A:587:HIS:HD2	1:A:969:GLN:HG2	1.82	0.45
1:A:925:LEU:O	1:A:929:LEU:HB2	2.17	0.45
1:A:960:ILE:O	1:A:963:ILE:HG22	2.17	0.45
8:J:14:VAL:HG22	8:J:41:LEU:HD21	1.98	0.45
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:MET:HG3	1:A:606:LEU:N	2.31	0.45
2:B:1006:ILE:HG22	2:B:1007:VAL:H	1.82	0.45
11:S:289:ALA:O	11:S:290:ASP:C	2.55	0.45
2:B:684:LEU:HD23	2:B:689:LEU:HD12	1.98	0.45
1:A:21:LEU:HD21	1:A:95:PHE:CZ	2.52	0.45
1:A:424:ILE:HG22	1:A:424:ILE:O	2.16	0.45
11:S:225:PRO:C	11:S:228:LEU:H	2.21	0.45
11:S:214:LEU:HD23	11:S:214:LEU:HA	1.76	0.45
2:B:540:SER:O	2:B:542:MET:N	2.50	0.45
2:B:620:ARG:HH21	7:I:56:ALA:HB2	1.81	0.45
4:E:153:HIS:CE1	4:E:184:VAL:HG11	2.52	0.45
1:A:770:VAL:C	1:A:772:GLY:H	2.20	0.45
1:A:37:PHE:HA	1:A:38:PRO:HD3	1.63	0.45
3:C:100:THR:OG1	3:C:121:VAL:HG21	2.16	0.45
3:C:47:ASP:HA	3:C:169:LYS:NZ	2.32	0.45
3:C:36:VAL:HG23	9:K:41:THR:CG2	2.47	0.45
1:A:1301:GLU:HA	1:A:1302:PRO:HD3	1.72	0.45
2:B:570:VAL:HA	2:B:571:PRO:HD2	1.85	0.45
5:F:82:THR:HA	5:F:83:PRO:HD3	1.77	0.45
2:B:744:HIS:CD2	2:B:746:SER:OG	2.70	0.44
1:A:315:LEU:HD13	1:A:319:GLY:HA2	1.99	0.44
2:B:1013:ASN:HA	2:B:1014:PRO:HD3	1.91	0.44
2:B:1162:ILE:HD13	2:B:1216:LEU:CB	2.47	0.44
7:I:59:VAL:O	7:I:60:GLN:HB2	2.18	0.44
2:B:590:HIS:CD2	2:B:591:ARG:N	2.85	0.44
1:A:821:ARG:HH22	2:B:514:LEU:HD13	1.81	0.44
6:H:82:PRO:HB2	6:H:83:GLN:H	1.56	0.44
2:B:723:VAL:CG2	2:B:724:ASP:H	2.27	0.44
1:A:1076:ALA:HA	1:A:1079:MET:HG3	1.99	0.44
2:B:51:PHE:O	2:B:54:PHE:HB3	2.17	0.44
2:B:236:HIS:N	2:B:236:HIS:CD2	2.85	0.44
3:C:252:GLN:HG3	9:K:95:ILE:HG23	1.99	0.44
2:B:413:LEU:HD21	2:B:461:LEU:HD11	1.99	0.44
1:A:106:VAL:HG12	1:A:107:CYS:N	2.32	0.44
11:S:191:ASN:HD22	11:S:195:TYR:CB	2.29	0.44
11:S:215:LYS:HE2	11:S:215:LYS:HB3	1.75	0.44
1:A:207:ILE:O	1:A:211:PHE:HD1	2.00	0.44
2:B:638:PHE:CD2	2:B:653:VAL:HG21	2.52	0.44
2:B:976:ILE:O	2:B:990:ILE:O	2.35	0.44
6:H:135:LEU:HB3	6:H:137:GLN:HG3	1.99	0.44
7:I:118:ARG:HB3	7:I:120:GLN:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:802:PRO:HG3	2:B:814:PHE:CE2	2.53	0.44
2:B:1196:ILE:HB	2:B:1197:PRO:HD2	2.00	0.44
5:F:135:ARG:HG2	5:F:137:TYR:CE1	2.52	0.44
2:B:508:LEU:HD22	2:B:512:ARG:HH21	1.80	0.44
1:A:41:MET:CB	1:A:49:LYS:HA	2.48	0.44
11:S:195:TYR:HD2	11:S:199:TYR:CE1	2.35	0.44
2:B:900:ALA:O	2:B:903:VAL:HG23	2.17	0.44
1:A:65:LEU:HD22	1:A:71:GLN:HB2	1.99	0.44
2:B:952:VAL:HG22	2:B:966:VAL:HG13	2.00	0.44
2:B:282:ILE:CD1	2:B:382:ILE:HD13	2.48	0.44
1:A:953:ASN:N	1:A:953:ASN:HD22	2.16	0.44
2:B:508:LEU:HA	2:B:509:ALA:CB	2.44	0.44
1:A:565:ILE:O	1:A:570:PRO:HA	2.17	0.44
2:B:120:ARG:CG	2:B:955:THR:HG21	2.37	0.44
1:A:380:VAL:HG12	1:A:428:TYR:HA	1.99	0.44
7:I:84:VAL:HG13	7:I:102:VAL:HB	2.00	0.44
1:A:706:HIS:ND1	11:S:257:GLN:HB2	2.32	0.44
1:A:1067:LEU:HD12	1:A:1067:LEU:O	2.17	0.44
1:A:49:LYS:CD	1:A:55:ASP:HB2	2.47	0.44
2:B:955:THR:CG2	2:B:956:THR:N	2.79	0.44
1:A:1329:THR:CG2	1:A:1331:SER:HB3	2.47	0.44
11:S:239:ALA:HB3	11:S:240:PRO:HD2	2.00	0.44
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	2.00	0.44
1:A:614:PHE:HB3	6:H:122:LEU:HD21	1.98	0.44
1:A:549:MET:SD	1:A:577:ILE:HD11	2.57	0.44
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.83	0.44
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.16	0.44
11:S:190:THR:O	11:S:191:ASN:C	2.56	0.44
2:B:479:VAL:HG12	2:B:480:SER:N	2.32	0.44
1:A:596:THR:O	1:A:598:LEU:N	2.51	0.44
1:A:18:GLN:O	2:B:1215:ARG:HG2	2.17	0.44
7:I:73:ARG:H	7:I:83:ASN:HD21	1.65	0.44
3:C:165:LYS:O	9:K:6:ARG:NH1	2.45	0.44
11:S:179:GLU:O	11:S:183:ASN:N	2.46	0.44
6:H:82:PRO:C	6:H:84:ALA:N	2.67	0.44
1:A:858:ASN:ND2	1:A:861:GLY:H	2.16	0.44
1:A:751:SER:HB2	2:B:1015:HIS:CE1	2.53	0.44
1:A:515:GLN:HB2	1:A:1071:SER:HB3	2.00	0.44
2:B:1099:VAL:CG1	2:B:1100:ASP:N	2.79	0.44
11:S:289:ALA:O	11:S:292:PRO:O	2.34	0.44
2:B:1073:TYR:CD1	2:B:1073:TYR:N	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:31:ASN:O	3:C:35:ARG:HG3	2.18	0.44
3:C:23:SER:HB3	3:C:227:THR:HA	1.98	0.44
1:A:230:ARG:HB3	1:A:232:GLU:HG2	2.00	0.44
5:F:109:VAL:HG11	5:F:123:LYS:HG2	1.99	0.44
2:B:53:GLN:HG3	2:B:53:GLN:O	2.17	0.44
2:B:711:GLU:N	2:B:712:PRO:CD	2.75	0.43
11:S:157:TYR:CE2	11:S:172:LEU:HD23	2.51	0.43
11:S:285:GLN:O	11:S:286:THR:O	2.36	0.43
11:S:159:VAL:O	11:S:163:GLU:HG3	2.18	0.43
1:A:1106:ASN:O	1:A:1107:VAL:C	2.56	0.43
2:B:956:THR:CG2	2:B:960:GLY:HA2	2.43	0.43
4:E:198:ILE:HG13	4:E:198:ILE:H	1.40	0.43
2:B:542:MET:HE2	2:B:743:ILE:HG13	2.00	0.43
2:B:826:ALA:HB2	2:B:1087:PHE:CE2	2.53	0.43
3:C:62:PHE:HE2	3:C:66:ARG:HD2	1.79	0.43
1:A:562:THR:HA	1:A:563:PRO:HD3	1.81	0.43
1:A:1081:LEU:O	1:A:1082:ASN:C	2.57	0.43
1:A:1118:VAL:O	1:A:1305:VAL:HG13	2.18	0.43
4:E:153:HIS:ND1	4:E:184:VAL:HG11	2.33	0.43
2:B:705:MET:HE2	2:B:745:PRO:HG3	2.01	0.43
1:A:414:ASP:OD1	1:A:416:ARG:HG2	2.17	0.43
1:A:1120:LEU:HD23	1:A:1124:HIS:O	2.17	0.43
1:A:623:GLY:C	1:A:625:SER:H	2.21	0.43
5:F:97:ARG:HA	5:F:97:ARG:HD2	1.73	0.43
8:J:2:ILE:HA	8:J:2:ILE:HD13	1.87	0.43
1:A:41:MET:HE3	1:A:48:ALA:H	1.83	0.43
3:C:164:ALA:HB2	3:C:171:GLY:CA	2.48	0.43
4:E:178:ILE:HB	4:E:212:ARG:HD3	1.99	0.43
2:B:1017:ILE:CB	2:B:1018:PRO:HD3	2.41	0.43
8:J:1:MET:HG3	8:J:60:PHE:HE2	1.82	0.43
7:I:111:THR:HG22	7:I:112:SER:H	1.82	0.43
1:A:219:PHE:CE2	1:A:231:PRO:HD2	2.53	0.43
3:C:251:LEU:O	3:C:255:VAL:HG23	2.18	0.43
6:H:87:ARG:HG2	6:H:88:SER:H	1.82	0.43
1:A:1172:LEU:HG	1:A:1172:LEU:H	1.63	0.43
1:A:529:CYS:HB2	1:A:751:SER:HB3	1.99	0.43
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.19	0.43
2:B:852:ARG:NH2	2:B:973:ILE:HD11	2.33	0.43
1:A:884:ASP:HB3	1:A:896:ARG:HH12	1.83	0.43
1:A:19:PHE:HB3	1:A:1413:GLY:CA	2.49	0.43
1:A:1215:ARG:HD2	1:A:1215:ARG:HA	1.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ARG:HD3	1:A:592:ASP:OD1	2.19	0.43
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.46	0.43
2:B:284:ILE:HD13	2:B:324:ILE:HD12	2.00	0.43
1:A:1107:VAL:HG21	1:A:1381:LEU:O	2.18	0.43
1:A:90:VAL:HB	1:A:236:LEU:HB2	2.00	0.43
2:B:1023:VAL:O	2:B:1027:ILE:HG13	2.18	0.43
10:L:70:ARG:HG2	10:L:70:ARG:HH11	1.84	0.43
1:A:587:HIS:CE1	1:A:965:GLN:HB3	2.54	0.43
1:A:401:GLY:N	1:A:435:HIS:HD2	2.16	0.43
7:I:55:THR:HG22	7:I:56:ALA:N	2.34	0.43
6:H:36:CYS:HA	6:H:126:GLU:O	2.19	0.43
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.19	0.43
2:B:661:LEU:HD11	2:B:684:LEU:HD11	2.00	0.43
12:M:11:U:H6	12:M:11:U:C5'	2.31	0.43
1:A:1194:ARG:HH21	1:A:1237:ILE:CD1	2.31	0.43
1:A:821:ARG:O	1:A:825:ILE:HG13	2.17	0.43
1:A:993:LEU:C	1:A:995:GLU:H	2.22	0.43
1:A:49:LYS:CG	1:A:55:ASP:OD2	2.67	0.43
11:S:195:TYR:CG	11:S:196:LYS:N	2.85	0.43
1:A:568:PRO:HB2	3:C:221:TYR:CE1	2.54	0.43
2:B:844:SER:HB3	2:B:848:ARG:NH1	2.34	0.43
4:E:29:PHE:HB2	4:E:65:THR:HG22	2.00	0.43
3:C:55:THR:HB	3:C:151:GLN:HA	2.00	0.43
2:B:550:ASP:HA	2:B:551:PRO:HD3	1.79	0.43
1:A:960:ILE:HA	1:A:963:ILE:HG22	2.01	0.43
9:K:49:GLU:C	9:K:51:LEU:H	2.22	0.43
8:J:17:LYS:HG3	8:J:39:LEU:HD22	1.99	0.43
2:B:1160:VAL:CG1	2:B:1161:HIS:N	2.81	0.43
1:A:93:VAL:HG13	1:A:301:ALA:HB1	2.00	0.43
2:B:1223:ASP:HB3	2:B:1224:PHE:H	1.46	0.43
2:B:871:THR:HG22	2:B:872:GLU:N	2.34	0.43
10:L:30:ILE:HD11	10:L:59:ALA:HB2	1.99	0.43
1:A:403:LYS:O	1:A:404:TYR:CG	2.72	0.43
2:B:651:LEU:HD11	2:B:707:PRO:HB3	2.00	0.43
1:A:92:HIS:HD2	1:A:236:LEU:HD11	1.84	0.43
1:A:547:LEU:HD13	9:K:58:PHE:CD1	2.54	0.43
2:B:894:ASP:O	2:B:895:ASP:HB2	2.19	0.43
3:C:74:SER:OG	3:C:237:SER:HB2	2.18	0.43
1:A:1319:VAL:HA	1:A:1320:PRO:HD3	1.81	0.43
1:A:1213:GLY:HA3	1:A:1228:TRP:CE3	2.53	0.43
11:S:225:PRO:HD2	11:S:226:GLU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:711:GLU:N	2:B:712:PRO:HD3	2.07	0.43
1:A:587:HIS:CD2	1:A:969:GLN:HG2	2.53	0.43
2:B:801:LYS:HG3	8:J:52:THR:HG23	1.99	0.43
2:B:542:MET:CE	2:B:636:PRO:CG	2.93	0.43
3:C:173:ALA:O	3:C:174:ALA:CB	2.67	0.43
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.19	0.43
2:B:390:LEU:O	2:B:391:ASP:HB2	2.19	0.43
1:A:553:VAL:HA	1:A:554:PRO:HD3	1.74	0.43
6:H:135:LEU:HD13	6:H:137:GLN:CD	2.39	0.43
2:B:308:TRP:CZ2	2:B:309:GLN:HG3	2.53	0.43
1:A:1269:GLU:OE2	2:B:264:SER:HB3	2.19	0.43
1:A:737:LEU:HD22	1:A:741:ASN:OD1	2.18	0.43
1:A:1335:ILE:O	1:A:1335:ILE:HG22	2.19	0.43
1:A:1339:LEU:HD23	4:E:144:ILE:HB	2.00	0.43
1:A:1008:GLN:HA	1:A:1011:GLN:HB3	2.01	0.43
2:B:25:ILE:CG2	2:B:26:THR:N	2.82	0.43
1:A:855:THR:HG23	1:A:857:ARG:HG3	2.00	0.43
2:B:898:LEU:HD22	2:B:964:VAL:HG11	2.01	0.43
2:B:858:SER:HA	2:B:966:VAL:O	2.19	0.43
1:A:343:LYS:HZ1	2:B:1197:PRO:HB3	1.84	0.43
1:A:308:ILE:HG22	1:A:309:ALA:H	1.84	0.43
2:B:1074:ASN:O	2:B:1078:GLY:HA2	2.19	0.43
2:B:1198:TYR:O	2:B:1201:LYS:HB3	2.19	0.42
6:H:6:PHE:O	6:H:58:THR:HG23	2.19	0.42
1:A:67:CYS:O	1:A:70:CYS:HB3	2.18	0.42
2:B:733:HIS:C	2:B:735:ALA:H	2.19	0.42
1:A:1074:GLU:N	1:A:1075:PRO:CD	2.82	0.42
1:A:18:GLN:O	2:B:1215:ARG:CG	2.67	0.42
1:A:565:ILE:HG21	1:A:567:LYS:HE3	2.01	0.42
2:B:733:HIS:C	2:B:735:ALA:N	2.73	0.42
2:B:550:ASP:O	2:B:553:PRO:HD2	2.19	0.42
7:I:86:PHE:CE1	7:I:100:PHE:HB2	2.54	0.42
2:B:526:GLU:HG2	2:B:538:ASN:ND2	2.34	0.42
1:A:537:ARG:HG3	1:A:537:ARG:H	1.59	0.42
7:I:8:ARG:HE	7:I:34:TYR:HE1	1.66	0.42
1:A:1156:PRO:O	1:A:1158:PRO:HD3	2.18	0.42
2:B:1197:PRO:HG2	2:B:1200:ALA:HB2	2.02	0.42
1:A:145:LYS:HA	1:A:145:LYS:HD3	1.72	0.42
11:S:153:LEU:HA	11:S:179:GLU:OE2	2.19	0.42
11:S:197:ALA:O	11:S:201:ILE:HB	2.19	0.42
11:S:216:HIS:O	11:S:216:HIS:CD2	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:901:PRO:O	2:B:949:VAL:O	2.37	0.42
2:B:603:LEU:HB3	2:B:609:ILE:HD11	2.01	0.42
1:A:535:THR:O	1:A:536:LEU:C	2.57	0.42
10:L:31:CYS:HB2	10:L:48:CYS:SG	2.59	0.42
1:A:345:VAL:CG1	2:B:1130:PHE:HB2	2.49	0.42
2:B:243:ALA:HB2	2:B:251:ILE:HG12	2.01	0.42
11:S:206:VAL:O	11:S:206:VAL:HG12	2.19	0.42
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.95	0.42
9:K:46:ILE:HG22	9:K:50:LEU:HD12	2.02	0.42
3:C:116:LYS:CD	3:C:140:ASN:HB3	2.49	0.42
1:A:345:VAL:HG11	2:B:1130:PHE:HB2	2.00	0.42
1:A:323:LYS:HZ1	12:M:3:C:H4'	1.83	0.42
1:A:323:LYS:HZ3	12:M:3:C:H5'	1.84	0.42
1:A:157:ASP:HA	1:A:158:PRO:HD3	1.83	0.42
1:A:683:ILE:HG21	1:A:801:GLU:HG3	2.00	0.42
2:B:37:PHE:O	2:B:41:LYS:HG3	2.19	0.42
3:C:52:GLU:HA	10:L:64:LEU:HD22	1.99	0.42
3:C:171:GLY:HA2	3:C:172:PRO:HD3	1.72	0.42
4:E:172:GLU:O	4:E:175:LEU:HB2	2.20	0.42
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.35	0.42
1:A:899:VAL:HG22	1:A:1029:ARG:HG2	2.01	0.42
1:A:364:VAL:HA	1:A:469:ARG:O	2.19	0.42
1:A:666:ILE:H	1:A:666:ILE:HG13	1.63	0.42
2:B:982:SER:HB3	2:B:1092:TYR:CZ	2.54	0.42
2:B:1094:ARG:HH21	2:B:1098:MET:HG2	1.84	0.42
4:E:63:ASN:HA	4:E:64:PRO:HD3	1.88	0.42
1:A:808:LEU:HD23	1:A:813:PHE:HA	2.01	0.42
2:B:258:LEU:HB2	2:B:385:LEU:HD21	2.01	0.42
3:C:265:MET:C	3:C:267:GLN:H	2.23	0.42
2:B:294:ASP:H	7:I:12:ASN:ND2	2.17	0.42
11:S:217:LYS:CD	11:S:217:LYS:N	2.78	0.42
2:B:933:SER:HB3	2:B:935:ARG:NH2	2.27	0.42
7:I:34:TYR:CD2	7:I:35:VAL:N	2.87	0.42
2:B:292:ILE:N	2:B:293:PRO:CD	2.83	0.42
9:K:91:CYS:HA	9:K:94:ILE:HD12	2.01	0.42
1:A:392:VAL:HG13	1:A:415:LEU:HD11	2.01	0.42
1:A:767:GLN:HE22	1:A:798:GLY:C	2.23	0.42
1:A:967:ALA:HB2	1:A:1044:TRP:CZ3	2.54	0.42
1:A:53:LEU:HB3	1:A:54:ASN:ND2	2.32	0.42
1:A:618:GLU:HB2	1:A:619:LYS:H	1.73	0.42
9:K:7:PHE:C	9:K:9:LEU:N	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:83:PRO:HA	5:F:146:TRP:CZ3	2.55	0.42
1:A:527:THR:HG21	1:A:650:GLN:HG3	2.02	0.42
1:A:407:ARG:HA	1:A:430:TRP:CD1	2.55	0.42
11:S:187:ASN:HB3	11:S:190:THR:CB	2.35	0.42
2:B:667:GLN:N	2:B:668:ASP:C	2.73	0.42
6:H:5:LEU:CB	6:H:60:ALA:H	2.25	0.42
1:A:34:LYS:O	1:A:35:ILE:O	2.38	0.42
7:I:65:ASP:HA	7:I:66:PRO:HD3	1.86	0.42
2:B:1217:TYR:N	2:B:1217:TYR:CD1	2.88	0.42
1:A:855:THR:CG2	1:A:857:ARG:HG3	2.49	0.42
4:E:88:VAL:HB	4:E:116:ILE:HG23	2.02	0.42
2:B:614:SER:HB2	2:B:694:ASP:OD1	2.20	0.42
7:I:72:ASP:N	7:I:72:ASP:OD1	2.52	0.42
4:E:54:GLN:HE21	4:E:54:GLN:HA	1.85	0.42
2:B:300:HIS:O	2:B:379:GLY:HA3	2.20	0.42
2:B:508:LEU:HA	2:B:509:ALA:HA	1.80	0.42
5:F:89:GLU:O	5:F:93:ILE:HG13	2.19	0.42
1:A:535:THR:HG21	1:A:617:VAL:H	1.84	0.42
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.35	0.42
4:E:32:GLN:HE21	4:E:36:GLU:CG	2.32	0.42
2:B:1109:GLY:HA3	2:B:1110:PRO:HD2	1.89	0.42
1:A:587:HIS:HA	1:A:607:ILE:O	2.19	0.42
1:A:62:ASP:O	1:A:63:ARG:CB	2.60	0.42
1:A:402:ALA:CB	1:A:434:ARG:HA	2.50	0.42
2:B:363:HIS:CD2	2:B:585:VAL:HG22	2.54	0.42
1:A:1424:VAL:HG13	1:A:1436:ILE:CD1	2.50	0.42
1:A:332:LYS:C	1:A:334:GLY:N	2.72	0.42
12:M:1:A:H2'	12:M:2:U:C6	2.54	0.42
3:C:82:TYR:CD2	3:C:161:LYS:HD3	2.55	0.42
2:B:978:ASP:OD2	2:B:1094:ARG:NH2	2.53	0.42
4:E:7:ARG:HG3	4:E:8:ASN:N	2.35	0.42
4:E:156:LEU:HD22	4:E:160:GLU:HB3	2.02	0.42
2:B:476:ARG:HB2	2:B:476:ARG:HH11	1.85	0.42
1:A:567:LYS:CB	6:H:95:TYR:HA	2.50	0.41
11:S:201:ILE:HA	11:S:204:SER:OG	2.20	0.41
1:A:1017:LEU:CB	4:E:205:SER:HA	2.50	0.41
3:C:38:ILE:HG22	3:C:39:ALA:HB2	2.02	0.41
10:L:53:HIS:HB3	10:L:55:ILE:CD1	2.50	0.41
1:A:1334:ASP:C	1:A:1336:MET:N	2.73	0.41
1:A:242:PRO:HA	1:A:243:PRO:HD2	1.81	0.41
2:B:1162:ILE:HD11	2:B:1194:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:S:239:ALA:CB	11:S:240:PRO:HD2	2.49	0.41
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.38	0.41
2:B:226:PHE:HA	2:B:395:GLN:HG3	2.02	0.41
2:B:225:VAL:HA	2:B:237:VAL:O	2.20	0.41
2:B:601:ARG:O	2:B:605:ARG:HG3	2.20	0.41
1:A:698:GLN:CD	7:I:99:LEU:HD11	2.40	0.41
11:S:186:ASN:O	11:S:187:ASN:HB2	2.20	0.41
2:B:996:ARG:HH22	3:C:173:ALA:HB1	1.83	0.41
1:A:1116:LEU:O	1:A:1308:THR:HG22	2.19	0.41
2:B:130:VAL:HG21	2:B:167:ILE:HD12	2.01	0.41
4:E:37:LEU:HA	4:E:38:PRO:HD3	1.72	0.41
2:B:890:TYR:CD2	2:B:910:VAL:HG21	2.55	0.41
1:A:441:PRO:HG2	1:A:498:ARG:HB2	2.01	0.41
1:A:41:MET:HA	1:A:49:LYS:HA	2.03	0.41
11:S:232:ASP:N	11:S:234:LYS:HB2	2.35	0.41
2:B:756:ILE:HG12	2:B:770:GLN:HG2	2.01	0.41
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.56	0.41
2:B:705:MET:CE	2:B:705:MET:HA	2.51	0.41
7:I:97:MET:HE3	7:I:97:MET:HB2	1.90	0.41
2:B:178:ASN:O	2:B:179:CYS:C	2.59	0.41
5:F:72:LYS:O	5:F:73:ALA:HB3	2.21	0.41
7:I:101:PHE:N	7:I:101:PHE:CD1	2.87	0.41
2:B:903:VAL:O	2:B:948:ILE:HG23	2.20	0.41
2:B:211:VAL:HG21	2:B:483:LEU:HD13	2.02	0.41
4:E:16:PHE:CZ	4:E:20:LYS:HE2	2.56	0.41
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.85	0.41
1:A:737:LEU:HA	1:A:737:LEU:HD23	1.84	0.41
4:E:197:LYS:O	4:E:199:ILE:HG13	2.20	0.41
6:H:39:THR:O	6:H:123:MET:HA	2.20	0.41
6:H:80:ARG:HA	6:H:81:PRO:HD3	1.73	0.41
6:H:82:PRO:O	6:H:84:ALA:N	2.51	0.41
10:L:53:HIS:HB3	10:L:55:ILE:HD11	2.03	0.41
2:B:273:LEU:HD11	2:B:285:ILE:HD13	2.01	0.41
2:B:1099:VAL:CG1	2:B:1100:ASP:H	2.33	0.41
1:A:1104:ILE:HD11	1:A:1355:VAL:HG21	2.01	0.41
1:A:1322:ILE:O	1:A:1324:PRO:HD3	2.20	0.41
6:H:24:CYS:SG	6:H:44:VAL:HG21	2.60	0.41
1:A:694:THR:HA	1:A:714:PHE:HE1	1.85	0.41
1:A:290:GLU:HA	1:A:293:GLU:HB3	2.03	0.41
1:A:889:SER:HB3	1:A:1297:GLU:HG3	2.02	0.41
2:B:876:LYS:HA	2:B:877:PRO:HD3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:ASN:OD1	1:A:631:HIS:CD2	2.74	0.41
1:A:910:PRO:C	1:A:912:LEU:H	2.24	0.41
1:A:436:ILE:CD1	1:A:491:VAL:HG11	2.51	0.41
7:I:78:CYS:SG	7:I:105:SER:HB2	2.60	0.41
1:A:53:LEU:HD22	1:A:54:ASN:HD22	1.85	0.41
2:B:746:SER:HA	2:B:1047:PHE:HE1	1.85	0.41
2:B:744:HIS:HD2	2:B:746:SER:OG	2.02	0.41
2:B:973:ILE:HG23	2:B:974:PRO:HD2	2.01	0.41
1:A:1232:ASN:HD22	1:A:1232:ASN:HA	1.58	0.41
1:A:1104:ILE:H	1:A:1104:ILE:HG13	1.70	0.41
7:I:28:GLU:CB	7:I:35:VAL:HG22	2.51	0.41
11:S:171:ILE:H	11:S:171:ILE:HG13	1.72	0.41
1:A:53:LEU:HB3	1:A:54:ASN:H	1.58	0.41
1:A:49:LYS:NZ	1:A:60:SER:HA	2.36	0.41
1:A:1172:LEU:HD13	11:S:204:SER:CB	2.50	0.41
1:A:1136:SER:HB2	1:A:1205:LYS:HA	2.00	0.41
2:B:603:LEU:HD22	2:B:603:LEU:HA	1.83	0.41
9:K:53:ASP:C	9:K:55:LYS:H	2.24	0.41
2:B:792:MET:HE1	13:N:24:DT:OP1	2.21	0.41
7:I:7:CYS:HB2	7:I:34:TYR:CD1	2.55	0.41
2:B:302:CYS:SG	2:B:311:LEU:HD21	2.60	0.41
1:A:344:ARG:HA	2:B:1129:ARG:HA	2.03	0.41
1:A:1215:ARG:HD2	1:A:1218:GLN:HE21	1.86	0.41
2:B:780:VAL:HG21	8:J:56:LEU:HD11	2.03	0.41
3:C:76:ASP:O	3:C:79:GLN:HG2	2.21	0.41
3:C:181:ASP:N	3:C:182:PRO:HD3	2.35	0.41
4:E:201:LYS:HA	4:E:201:LYS:HD3	1.91	0.41
2:B:1172:ILE:HG13	2:B:1183:LYS:HE2	2.02	0.41
1:A:858:ASN:ND2	1:A:858:ASN:C	2.73	0.41
1:A:1075:PRO:O	1:A:1079:MET:HG3	2.20	0.41
4:E:83:CYS:SG	4:E:88:VAL:HG22	2.61	0.41
1:A:1193:LEU:HD21	1:A:1267:MET:HE1	2.02	0.41
3:C:161:LYS:O	3:C:170:TRP:NE1	2.53	0.41
2:B:129:PHE:HE2	2:B:166:PHE:HD1	1.68	0.41
1:A:984:LYS:O	1:A:988:LEU:HB2	2.19	0.41
1:A:522:GLY:HA2	1:A:630:ILE:CD1	2.51	0.41
1:A:2:VAL:HG11	2:B:1157:ALA:HB1	2.03	0.41
1:A:1021:LEU:O	1:A:1024:SER:HB3	2.20	0.41
1:A:450:LEU:H	1:A:450:LEU:HD12	1.86	0.41
1:A:49:LYS:CD	1:A:55:ASP:CB	2.97	0.41
11:S:234:LYS:C	11:S:236:LEU:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:S:210:ASN:HB2	11:S:214:LEU:HG	2.03	0.41
1:A:588:LEU:HB3	1:A:607:ILE:HB	2.02	0.41
6:H:58:THR:CG2	6:H:59:ILE:N	2.83	0.41
1:A:809:THR:HB	1:A:810:PRO:HD2	2.03	0.41
1:A:72:GLU:HB2	1:A:73:GLY:H	1.74	0.41
2:B:722:ASP:HB3	2:B:723:VAL:H	1.56	0.41
2:B:60:GLN:HG3	2:B:60:GLN:O	2.21	0.41
1:A:1163:ILE:HG13	1:A:1163:ILE:H	1.64	0.41
1:A:817:ALA:HA	2:B:764:SER:OG	2.21	0.41
11:S:237:ALA:H	11:S:238:PRO:HD2	1.86	0.41
1:A:332:LYS:HZ1	13:N:19:DT:P	2.43	0.41
1:A:210:ILE:O	1:A:214:ILE:HG13	2.21	0.41
2:B:640:VAL:HG13	2:B:651:LEU:HD23	2.02	0.41
6:H:25:ARG:HB2	6:H:41:ASP:OD1	2.21	0.41
2:B:838:SER:HA	2:B:989:THR:O	2.21	0.41
2:B:294:ASP:HB2	7:I:12:ASN:HA	2.03	0.41
3:C:120:ILE:H	3:C:120:ILE:HG13	1.32	0.41
9:K:18:LYS:NZ	9:K:38:GLU:HG2	2.36	0.41
2:B:299:GLU:OE1	2:B:572:HIS:HB3	2.21	0.41
2:B:170:LEU:HD12	2:B:457:LEU:HD13	2.03	0.41
1:A:43:GLU:O	1:A:44:THR:HB	2.21	0.41
7:I:63:GLY:HA3	7:I:104:LEU:HD22	2.02	0.41
1:A:566:ILE:O	1:A:567:LYS:C	2.59	0.41
2:B:431:TYR:CD1	2:B:447:ALA:CB	2.97	0.41
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.86	0.41
4:E:173:SER:HB2	4:E:177:ARG:HH21	1.86	0.41
2:B:628:THR:O	2:B:628:THR:HG23	2.20	0.41
6:H:63:LEU:HA	6:H:63:LEU:HD23	1.64	0.41
1:A:88:LYS:HA	1:A:89:PRO:HD3	1.90	0.41
2:B:978:ASP:O	2:B:989:THR:HB	2.21	0.41
2:B:129:PHE:HE2	2:B:166:PHE:CD1	2.39	0.41
1:A:1018:PHE:O	1:A:1021:LEU:HB3	2.20	0.41
1:A:681:GLU:O	1:A:684:ALA:HB3	2.21	0.41
1:A:895:LYS:O	1:A:895:LYS:HG2	2.20	0.41
12:M:6:G:N3	12:M:7:A:C8	2.89	0.40
4:E:30:ILE:HG23	4:E:34:GLU:HB3	2.03	0.40
2:B:121:ASN:ND2	2:B:965:LYS:NZ	2.70	0.40
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.36	0.40
2:B:221:ASN:OD1	2:B:242:SER:HA	2.22	0.40
1:A:777:PHE:C	1:A:779:PHE:H	2.24	0.40
2:B:620:ARG:HH21	7:I:56:ALA:CB	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:CYS:HA	2:B:196:PRO:HD2	1.80	0.40
9:K:19:LEU:HD23	9:K:35:PHE:HA	2.03	0.40
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	2.20	0.40
1:A:1105:LEU:HA	1:A:1105:LEU:HD23	1.77	0.40
2:B:805:THR:HA	2:B:809:MET:HE3	2.02	0.40
9:K:38:GLU:HB3	9:K:71:PHE:HE2	1.86	0.40
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.56	0.40
1:A:311:GLN:N	1:A:312:PRO:CD	2.85	0.40
11:S:195:TYR:O	11:S:199:TYR:CD1	2.69	0.40
2:B:844:SER:HB3	2:B:848:ARG:HH12	1.86	0.40
2:B:1187:ASN:HB3	2:B:1188:LYS:H	1.61	0.40
2:B:60:GLN:OE1	2:B:95:ILE:HG22	2.21	0.40
2:B:766:ARG:HD2	2:B:1022:THR:HB	2.02	0.40
1:A:1284:MET:HG2	1:A:1306:LEU:HD22	2.03	0.40
7:I:34:TYR:C	7:I:34:TYR:CD2	2.95	0.40
1:A:316:GLN:O	1:A:317:LYS:C	2.60	0.40
1:A:219:PHE:O	1:A:222:LEU:N	2.53	0.40
10:L:70:ARG:HG2	10:L:70:ARG:NH1	2.36	0.40
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.54	0.40
1:A:152:VAL:HG13	1:A:153:PRO:HD2	2.02	0.40
1:A:833:GLU:OE1	1:A:1102:LYS:HD2	2.21	0.40
4:E:78:LEU:C	4:E:78:LEU:HD23	2.41	0.40
2:B:860:MET:CG	2:B:965:LYS:HG2	2.51	0.40
2:B:60:GLN:NE2	2:B:94:LYS:HA	2.32	0.40
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	2.02	0.40
1:A:596:THR:C	1:A:598:LEU:N	2.73	0.40
2:B:195:CYS:SG	2:B:782:LEU:HD22	2.61	0.40
1:A:1279:ILE:HG23	1:A:1308:THR:OG1	2.21	0.40
2:B:515:HIS:HD2	2:B:517:THR:H	1.69	0.40
3:C:241:ASP:O	3:C:245:VAL:HG23	2.22	0.40
2:B:511:PRO:HG2	2:B:512:ARG:H	1.86	0.40
1:A:567:LYS:HD2	1:A:568:PRO:HD2	2.02	0.40
2:B:370:PHE:HE2	2:B:373:ARG:HH11	1.68	0.40
2:B:773:MET:O	2:B:776:GLN:N	2.50	0.40
6:H:63:LEU:HB3	6:H:90:ALA:CB	2.52	0.40
1:A:1225:PHE:CE2	1:A:1227:ILE:HD11	2.57	0.40
1:A:697:ALA:HB1	7:I:97:MET:CE	2.51	0.40
2:B:282:ILE:HD13	2:B:382:ILE:HD13	2.04	0.40
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	2.02	0.40
2:B:186:GLU:C	2:B:188:ASP:H	2.24	0.40
1:A:446:ARG:HD3	1:A:478:TYR:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:198:ILE:HD11	4:E:212:ARG:CG	2.52	0.40
4:E:198:ILE:HD11	4:E:212:ARG:HG3	2.04	0.40
8:J:5:VAL:O	8:J:6:ARG:O	2.40	0.40
1:A:1284:MET:O	11:S:257:GLN:HA	2.22	0.40
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.62	0.40
2:B:684:LEU:HB3	2:B:690:VAL:HG23	2.03	0.40
2:B:582:VAL:HG22	2:B:626:ILE:HB	2.03	0.40
3:C:98:VAL:HA	3:C:157:CYS:O	2.21	0.40
1:A:844:ALA:HA	1:A:1389:PHE:CE1	2.56	0.40
3:C:91:HIS:O	3:C:91:HIS:CG	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1418/1733 (82%)	1160 (82%)	210 (15%)	48 (3%)	5 43
2	B	1084/1224 (89%)	882 (81%)	167 (15%)	35 (3%)	5 44
3	C	264/318 (83%)	213 (81%)	37 (14%)	14 (5%)	2 30
4	E	212/215 (99%)	187 (88%)	20 (9%)	5 (2%)	7 50
5	F	82/155 (53%)	70 (85%)	11 (13%)	1 (1%)	16 63
6	H	129/146 (88%)	103 (80%)	17 (13%)	9 (7%)	1 23
7	I	117/122 (96%)	91 (78%)	24 (20%)	2 (2%)	11 56
8	J	63/70 (90%)	50 (79%)	9 (14%)	4 (6%)	2 26
9	K	112/120 (93%)	102 (91%)	9 (8%)	1 (1%)	21 68
10	L	44/70 (63%)	28 (64%)	11 (25%)	5 (11%)	0 9
11	S	161/173 (93%)	107 (66%)	35 (22%)	19 (12%)	0 9
All	All	3686/4346 (85%)	2993 (81%)	550 (15%)	143 (4%)	4 38

All (143) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	55	ASP
1	A	57	ARG
1	A	567	LYS
1	A	709	THR
2	B	65	GLU
2	B	364	ILE
2	B	369	GLY
2	B	541	LEU
2	B	711	GLU
2	B	992	ILE
2	B	1097	HIS
3	C	91	HIS
3	C	110	THR
3	C	149	LYS
4	E	206	GLY
6	H	81	PRO
6	H	82	PRO
6	H	108	SER
8	J	53	HIS
10	L	50	ASP
11	S	188	CYS
11	S	189	ASP
11	S	190	THR
11	S	193	ALA
11	S	231	CYS
11	S	234	LYS
11	S	237	ALA
11	S	239	ALA
11	S	284	LEU
11	S	286	THR
11	S	292	PRO
1	A	72	GLU
1	A	76	GLU
1	A	78	PRO
1	A	286	HIS
1	A	423	ASP
1	A	465	TYR
1	A	708	MET
1	A	751	SER
1	A	1136	SER
1	A	1281	ARG

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Mol	Chain	Res	Type
2	B	368	GLU
2	B	480	SER
2	B	793	ALA
2	B	895	ASP
2	B	974	PRO
2	B	982	SER
2	B	1017	ILE
2	B	1108	ARG
2	B	1155	SER
2	B	1167	GLY
2	B	1175	LEU
2	B	1186	ASP
2	B	1223	ASP
3	C	28	ALA
3	C	161	LYS
3	C	227	THR
4	E	45	LYS
4	E	115	ASN
6	H	119	GLY
7	I	9	ASP
7	I	11	ASN
8	J	2	ILE
8	J	6	ARG
8	J	64	ASN
1	A	4	GLN
1	A	5	GLN
1	A	48	ALA
1	A	56	PRO
1	A	322	VAL
1	A	331	GLY
1	A	424	ILE
1	A	583	PRO
1	A	1082	ASN
2	B	108	VAL
2	B	249	ARG
2	B	531	GLN
2	B	643	ASP
2	B	712	PRO
2	B	880	THR
2	B	958	GLN
3	C	90	ASP
4	E	189	GLY

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Mol	Chain	Res	Type
5	F	73	ALA
6	H	60	ALA
11	S	169	GLN
11	S	217	LYS
11	S	222	ASP
11	S	233	ALA
11	S	291	HIS
1	A	196	GLU
1	A	318	SER
1	A	332	LYS
1	A	418	SER
1	A	526	ASP
1	A	592	ASP
1	A	597	LEU
1	A	1435	PRO
2	B	713	ALA
3	C	87	PHE
3	C	142	VAL
3	C	213	PRO
4	E	3	GLN
9	K	8	GLU
10	L	59	ALA
11	S	167	PRO
1	A	44	THR
1	A	63	ARG
1	A	693	VAL
1	A	780	VAL
1	A	846	GLU
1	A	1084	PHE
2	B	49	ASP
2	B	508	LEU
2	B	744	HIS
3	C	126	GLY
3	C	174	ALA
3	C	214	ASN
6	H	83	GLN
6	H	109	LYS
10	L	26	THR
1	A	111	GLY
1	A	591	PHE
1	A	958	VAL
1	A	1267	MET

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Mol	Chain	Res	Type
1	A	1365	TYR
2	B	575	PRO
3	C	10	ILE
10	L	56	LEU
11	S	224	THR
1	A	325	ILE
2	B	731	VAL
1	A	52	GLY
1	A	1335	ILE
2	B	467	GLY
2	B	751	VAL
11	S	218	ILE
1	A	410	GLY
1	A	632	VAL
6	H	107	VAL
6	H	18	GLY
10	L	46	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1246/1520 (82%)	1123 (90%)	123 (10%)	10 44
2	B	959/1061 (90%)	860 (90%)	99 (10%)	9 42
3	C	234/274 (85%)	213 (91%)	21 (9%)	12 49
4	E	196/197 (100%)	179 (91%)	17 (9%)	13 50
5	F	74/137 (54%)	69 (93%)	5 (7%)	20 61
6	H	117/128 (91%)	109 (93%)	8 (7%)	20 61
7	I	113/116 (97%)	95 (84%)	18 (16%)	3 23
8	J	60/65 (92%)	54 (90%)	6 (10%)	9 43
9	K	99/102 (97%)	93 (94%)	6 (6%)	23 65
10	L	40/57 (70%)	33 (82%)	7 (18%)	2 17
11	S	96/151 (64%)	81 (84%)	15 (16%)	3 24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3234/3808 (85%)	2909 (90%)	325 (10%)	9 43

All (325) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	22	PHE
1	A	34	LYS
1	A	38	PRO
1	A	53	LEU
1	A	54	ASN
1	A	57	ARG
1	A	68	GLN
1	A	70	CYS
1	A	77	CYS
1	A	93	VAL
1	A	120	GLU
1	A	126	LEU
1	A	186	LYS
1	A	195	ASP
1	A	196	GLU
1	A	204	THR
1	A	237	THR
1	A	255	SER
1	A	256	GLN
1	A	259	GLU
1	A	265	LYS
1	A	302	THR
1	A	308	ILE
1	A	333	GLU
1	A	375	THR
1	A	381	THR
1	A	385	ILE
1	A	406	ILE
1	A	416	ARG
1	A	424	ILE
1	A	425	GLN
1	A	438	ASP
1	A	445	ASN
1	A	449	SER
1	A	450	LEU
1	A	451	HIS

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Mol	Chain	Res	Type
1	A	454	SER
1	A	461	LYS
1	A	463	ILE
1	A	475	THR
1	A	481	ASP
1	A	493	GLN
1	A	509	LEU
1	A	512	VAL
1	A	524	VAL
1	A	537	ARG
1	A	542	GLU
1	A	555	ASP
1	A	562	THR
1	A	565	ILE
1	A	597	LEU
1	A	605	MET
1	A	618	GLU
1	A	636	GLU
1	A	660	ASN
1	A	669	THR
1	A	680	THR
1	A	696	GLU
1	A	700	ASN
1	A	710	LEU
1	A	734	GLU
1	A	738	LYS
1	A	741	ASN
1	A	754	SER
1	A	755	PHE
1	A	756	ILE
1	A	764	CYS
1	A	774	ARG
1	A	779	PHE
1	A	795	GLU
1	A	821	ARG
1	A	834	THR
1	A	858	ASN
1	A	903	ASN
1	A	909	ASP
1	A	919	ILE
1	A	920	LEU
1	A	929	LEU

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Mol	Chain	Res	Type
1	A	941	LYS
1	A	948	VAL
1	A	968	GLN
1	A	969	GLN
1	A	976	THR
1	A	980	ASP
1	A	992	ASP
1	A	1004	ASN
1	A	1029	ARG
1	A	1067	LEU
1	A	1080	THR
1	A	1081	LEU
1	A	1082	ASN
1	A	1083	THR
1	A	1095	THR
1	A	1103	GLU
1	A	1116	LEU
1	A	1124	HIS
1	A	1136	SER
1	A	1146	VAL
1	A	1163	ILE
1	A	1172	LEU
1	A	1187	GLN
1	A	1208	THR
1	A	1232	ASN
1	A	1234	GLU
1	A	1242	VAL
1	A	1265	ASN
1	A	1269	GLU
1	A	1281	ARG
1	A	1283	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1316	VAL
1	A	1319	VAL
1	A	1325	THR
1	A	1333	ILE
1	A	1359	ASP
1	A	1364	ASN
1	A	1366	ARG
1	A	1382	THR
1	A	1426	GLU

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Mol	Chain	Res	Type
1	A	1438	THR
1	A	1443	VAL
2	B	20	ASP
2	B	46	GLN
2	B	63	ILE
2	B	66	ASP
2	B	90	ILE
2	B	134	LYS
2	B	164	LYS
2	B	175	ARG
2	B	185	THR
2	B	212	LEU
2	B	217	ARG
2	B	250	PHE
2	B	264	SER
2	B	280	ILE
2	B	363	HIS
2	B	365	THR
2	B	393	LYS
2	B	396	ASP
2	B	401	PHE
2	B	416	LEU
2	B	437	GLU
2	B	446	LEU
2	B	463	THR
2	B	465	ASN
2	B	474	SER
2	B	476	ARG
2	B	482	VAL
2	B	485	ARG
2	B	492	LEU
2	B	493	SER
2	B	498	THR
2	B	507	LYS
2	B	508	LEU
2	B	510	LYS
2	B	512	ARG
2	B	522	VAL
2	B	527	THR
2	B	541	LEU
2	B	542	MET
2	B	547	VAL

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Mol	Chain	Res	Type
2	B	552	MET
2	B	567	GLU
2	B	570	VAL
2	B	603	LEU
2	B	604	ARG
2	B	606	LYS
2	B	628	THR
2	B	629	ASP
2	B	644	GLU
2	B	666	TYR
2	B	667	GLN
2	B	678	GLU
2	B	714	GLU
2	B	730	ARG
2	B	732	SER
2	B	733	HIS
2	B	734	HIS
2	B	737	THR
2	B	766	ARG
2	B	790	ASP
2	B	792	MET
2	B	795	ILE
2	B	805	THR
2	B	816	GLU
2	B	830	TYR
2	B	839	MET
2	B	844	SER
2	B	845	SER
2	B	859	TYR
2	B	878	GLN
2	B	908	GLU
2	B	909	ASP
2	B	916	THR
2	B	956	THR
2	B	961	LEU
2	B	967	ARG
2	B	971	THR
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1012	ILE
2	B	1022	THR

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Mol	Chain	Res	Type
2	B	1051	THR
2	B	1071	VAL
2	B	1074	ASN
2	B	1076	HIS
2	B	1084	GLN
2	B	1095	LEU
2	B	1106	ARG
2	B	1108	ARG
2	B	1122	ARG
2	B	1138	MET
2	B	1147	LEU
2	B	1150	ARG
2	B	1163	CYS
2	B	1170	THR
2	B	1183	LYS
2	B	1202	LEU
2	B	1223	ASP
3	C	7	GLN
3	C	18	VAL
3	C	26	ASP
3	C	27	LEU
3	C	55	THR
3	C	58	LEU
3	C	74	SER
3	C	77	ILE
3	C	80	LEU
3	C	83	SER
3	C	91	HIS
3	C	100	THR
3	C	111	THR
3	C	120	ILE
3	C	138	GLU
3	C	140	ASN
3	C	147	LEU
3	C	163	ILE
3	C	203	GLN
3	C	227	THR
3	C	240	VAL
4	E	2	ASP
4	E	37	LEU
4	E	57	MET
4	E	78	LEU

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Mol	Chain	Res	Type
4	E	115	ASN
4	E	117	THR
4	E	119	SER
4	E	131	THR
4	E	135	PHE
4	E	146	HIS
4	E	159	ASP
4	E	169	ARG
4	E	175	LEU
4	E	180	ARG
4	E	198	ILE
4	E	203	GLU
4	E	213	ILE
5	F	79	ARG
5	F	104	ASN
5	F	111	LEU
5	F	131	PRO
5	F	140	ASP
6	H	5	LEU
6	H	35	GLN
6	H	49	VAL
6	H	54	SER
6	H	95	TYR
6	H	108	SER
6	H	130	ARG
6	H	134	ASN
7	I	3	THR
7	I	4	PHE
7	I	9	ASP
7	I	10	CYS
7	I	12	ASN
7	I	32	CYS
7	I	34	TYR
7	I	52	ILE
7	I	59	VAL
7	I	75	CYS
7	I	78	CYS
7	I	82	GLU
7	I	83	ASN
7	I	86	PHE
7	I	90	GLN
7	I	95	THR

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Mol	Chain	Res	Type
7	I	98	VAL
7	I	111	THR
8	J	2	ILE
8	J	10	CYS
8	J	28	ASP
8	J	43	ARG
8	J	48	ARG
8	J	64	ASN
9	K	6	ARG
9	K	11	LEU
9	K	20	LYS
9	K	47	ARG
9	K	49	GLU
9	K	103	THR
10	L	31	CYS
10	L	46	VAL
10	L	48	CYS
10	L	51	CYS
10	L	55	ILE
10	L	68	GLU
10	L	70	ARG
11	S	150	ASP
11	S	174	THR
11	S	182	MET
11	S	188	CYS
11	S	190	THR
11	S	195	TYR
11	S	210	ASN
11	S	213	ASP
11	S	215	LYS
11	S	218	ILE
11	S	220	ASN
11	S	223	ILE
11	S	224	THR
11	S	234	LYS
11	S	235	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	71	GLN

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Mol	Chain	Res	Type
1	A	83	HIS
1	A	225	ASN
1	A	435	HIS
1	A	493	GLN
1	A	517	ASN
1	A	548	ASN
1	A	587	HIS
1	A	603	ASN
1	A	631	HIS
1	A	660	ASN
1	A	717	ASN
1	A	736	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	767	GLN
1	A	786	HIS
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	935	GLN
1	A	953	ASN
1	A	969	GLN
1	A	1009	ASN
1	A	1048	ASN
1	A	1232	ASN
1	A	1364	ASN
1	A	1432	GLN
2	B	121	ASN
2	B	215	GLN
2	B	236	HIS
2	B	357	GLN
2	B	465	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	531	GLN
2	B	538	ASN
2	B	587	HIS
2	B	590	HIS
2	B	592	ASN
2	B	657	HIS

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Mol	Chain	Res	Type
2	B	744	HIS
2	B	770	GLN
2	B	776	GLN
2	B	821	GLN
2	B	1015	HIS
2	B	1176	ASN
2	B	1193	GLN
3	C	112	ASN
3	C	167	HIS
3	C	242	GLN
4	E	32	GLN
4	E	54	GLN
4	E	61	GLN
4	E	114	ASN
4	E	147	HIS
6	H	52	GLN
6	H	128	ASN
6	H	133	ASN
7	I	12	ASN
7	I	22	ASN
7	I	83	ASN
8	J	53	HIS
9	K	65	HIS
9	K	76	GLN
9	K	112	GLN
11	S	166	HIS
11	S	191	ASN
11	S	220	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	M	10/13 (76%)	2 (20%)	1 (10%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	M	10	A
12	M	11	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	M	11	U

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1426/1733 (82%)	-0.36	15 (1%) 82 69	26, 75, 156, 230	0
2	B	1104/1224 (90%)	-0.44	6 (0%) 91 85	24, 63, 135, 230	0
3	C	266/318 (83%)	-0.50	0 100 100	30, 61, 101, 141	0
4	E	214/215 (99%)	-0.26	0 100 100	45, 111, 169, 197	0
5	F	84/155 (54%)	-0.24	1 (1%) 81 67	46, 80, 123, 140	0
6	H	133/146 (91%)	-0.23	2 (1%) 76 62	52, 97, 163, 186	0
7	I	119/122 (97%)	-0.18	1 (0%) 87 77	36, 86, 147, 190	0
8	J	65/70 (92%)	-0.51	0 100 100	33, 53, 92, 105	0
9	K	114/120 (95%)	-0.42	0 100 100	38, 69, 104, 150	0
10	L	46/70 (65%)	-0.05	1 (2%) 65 50	34, 99, 161, 185	0
11	S	163/173 (94%)	0.62	22 (13%) 4 4	109, 159, 211, 255	0
12	M	12/13 (92%)	0.24	1 (8%) 14 9	65, 90, 194, 223	0
13	N	28/28 (100%)	1.30	11 (39%) 0 1	66, 232, 305, 320	0
14	O	14/14 (100%)	2.70	8 (57%) 0 1	260, 286, 320, 326	0
All	All	3788/4401 (86%)	-0.31	68 (1%) 71 56	24, 74, 165, 326	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	O	1	DC	5.7
14	O	14	DG	5.6
1	A	253	ASN	5.0
13	N	5	DC	5.0
11	S	176	LYS	5.0
14	O	7	DA	4.7
13	N	4	DC	4.4
2	B	882	THR	4.3

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Mol	Chain	Res	Type	RSRZ
11	S	165	GLU	4.3
13	N	2	DT	4.2
1	A	195	ASP	3.8
7	I	119	THR	3.7
12	M	12	G	3.6
13	N	1	DC	3.6
14	O	12	DT	3.5
13	N	3	DA	3.4
14	O	9	DC	3.4
1	A	286	HIS	3.3
2	B	709	ASP	3.3
11	S	169	GLN	3.3
11	S	163	GLU	3.3
11	S	172	LEU	3.2
1	A	196	GLU	3.2
14	O	2	DT	3.1
11	S	158	ASP	3.0
11	S	166	HIS	3.0
11	S	212	PRO	3.0
1	A	251	SER	3.0
11	S	203	TYR	2.9
14	O	13	DA	2.8
11	S	192	GLU	2.8
6	H	86	ASP	2.8
11	S	266	THR	2.7
11	S	183	ASN	2.7
13	N	15	DA	2.7
1	A	44	THR	2.6
13	N	12	DC	2.6
11	S	274	CYS	2.6
10	L	26	THR	2.6
11	S	226	GLU	2.5
13	N	6	DG	2.5
11	S	167	PRO	2.5
13	N	28	DT	2.4
11	S	270	THR	2.4
2	B	576	ASP	2.4
11	S	199	TYR	2.4
13	N	11	DG	2.4
1	A	287	HIS	2.3
1	A	166	GLY	2.3
11	S	290	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1256	GLU	2.3
2	B	468	GLU	2.3
2	B	250	PHE	2.3
1	A	183	GLY	2.3
2	B	708	GLU	2.3
1	A	116	ASP	2.2
13	N	10	DA	2.2
14	O	6	DT	2.2
1	A	252	PHE	2.2
1	A	1450	LEU	2.1
11	S	162	LYS	2.1
6	H	83	GLN	2.1
5	F	76	LYS	2.1
11	S	180	SER	2.1
1	A	157	ASP	2.0
11	S	168	PRO	2.0
1	A	170	THR	2.0
11	S	277	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
16	ZN	S	310	1/1	0.83	0.29	-0.38	228,228,228,228	0
16	ZN	A	1736	1/1	0.98	0.09	-1.54	73,73,73,73	0
16	ZN	C	319	1/1	0.98	0.08	-1.93	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
16	ZN	I	203	1/1	0.98	0.07	-2.03	73,73,73,73	0
16	ZN	J	101	1/1	0.99	0.11	-2.13	35,35,35,35	0
16	ZN	L	105	1/1	0.97	0.10	-2.19	124,124,124,124	0
16	ZN	I	204	1/1	1.00	0.07	-2.29	37,37,37,37	0
16	ZN	A	1735	1/1	0.96	0.06	-3.02	128,128,128,128	0
15	MG	A	1734	1/1	0.96	0.15	-	48,48,48,48	0
16	ZN	B	1307	1/1	0.99	0.06	-	82,82,82,82	0

6.5 Other polymers

There are no such residues in this entry.