



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:01 PM UTC

PDB ID : 1TWF / pdb_00001twf
Title : RNA polymerase II complexed with UTP at 2.3 Å resolution
Authors : Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.
Deposited on : 2004-06-30
Resolution : 2.30 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

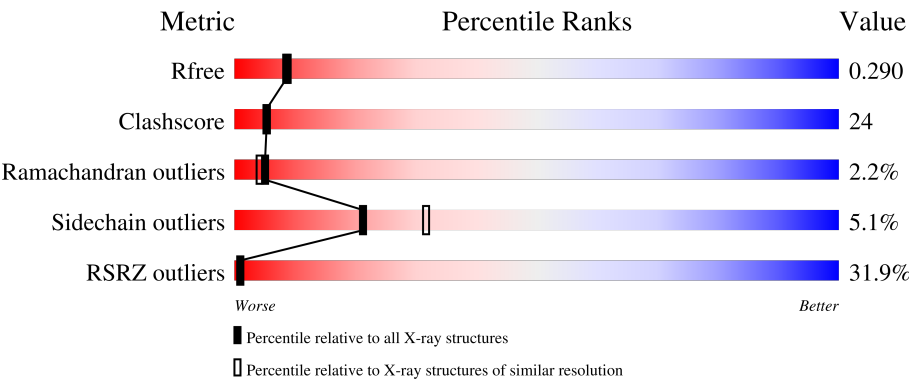
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	1733	24% 44% 33% 18%
2	B	1224	25% 48% 37% 11%
3	C	318	27% 42% 39% 16%
4	E	215	41% 64% 33%
5	F	155	9% 32% 21% 46%

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Mol	Chain	Length	Quality of chain
6	H	146	70% 42% 41% 8% 9%
7	I	122	32% 67% 30% • •
8	J	70	17% 44% 40% 9% 7%
9	K	120	23% 52% 39% • 5%
10	L	70	54% 31% 26% 9% 34%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 28318 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 largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1419	Total	C	N	O	S	0	0	0
			11154	7023	1952	2118	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1094	Total	C	N	O	S	0	0	0
			8711	5525	1519	1614	53			

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

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 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	215	Total	C	N	O	S	0	0	0
			1760	1116	310	322	12			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

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 14.5 kDa polypeptide.

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 14.2 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	122	Total	C	N	O	S	0	0	0
			997	613	182	191	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

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 13.6 kDa polypeptide.

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 7.7 kDa polypeptide.

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 ZINC ION (CCD ID: ZN) (formula: Zn).

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

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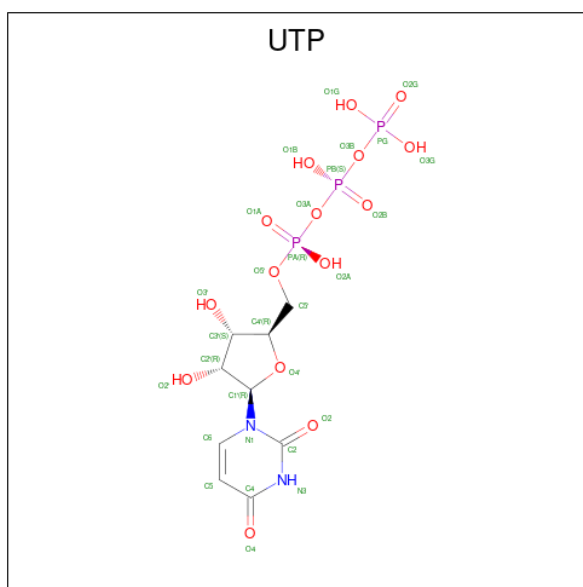
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	1	Total	Zn	0	0
			1	1		

- Molecule 12 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	2	Total	Mn	0	0
			2	2		

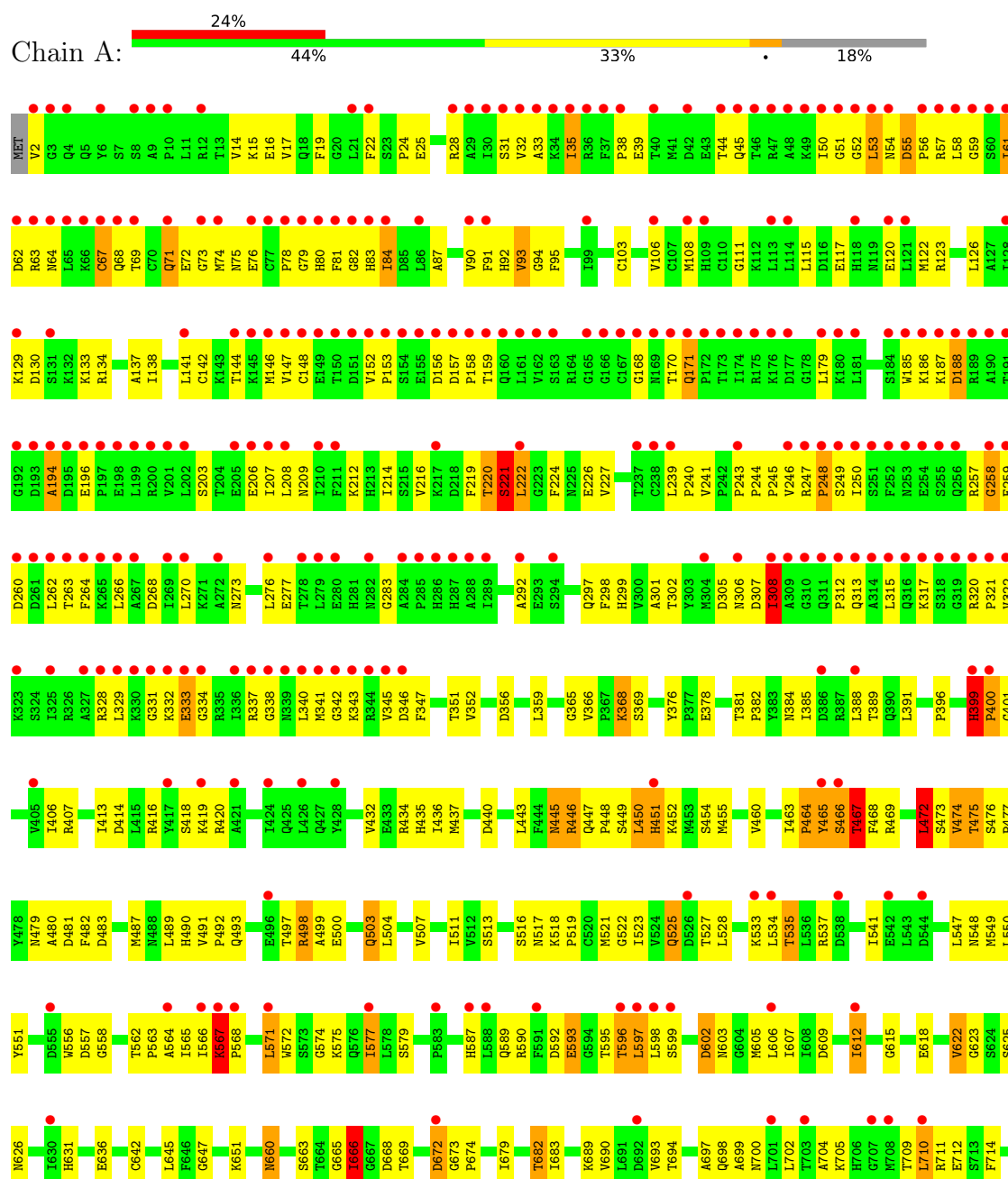
- Molecule 13 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$).

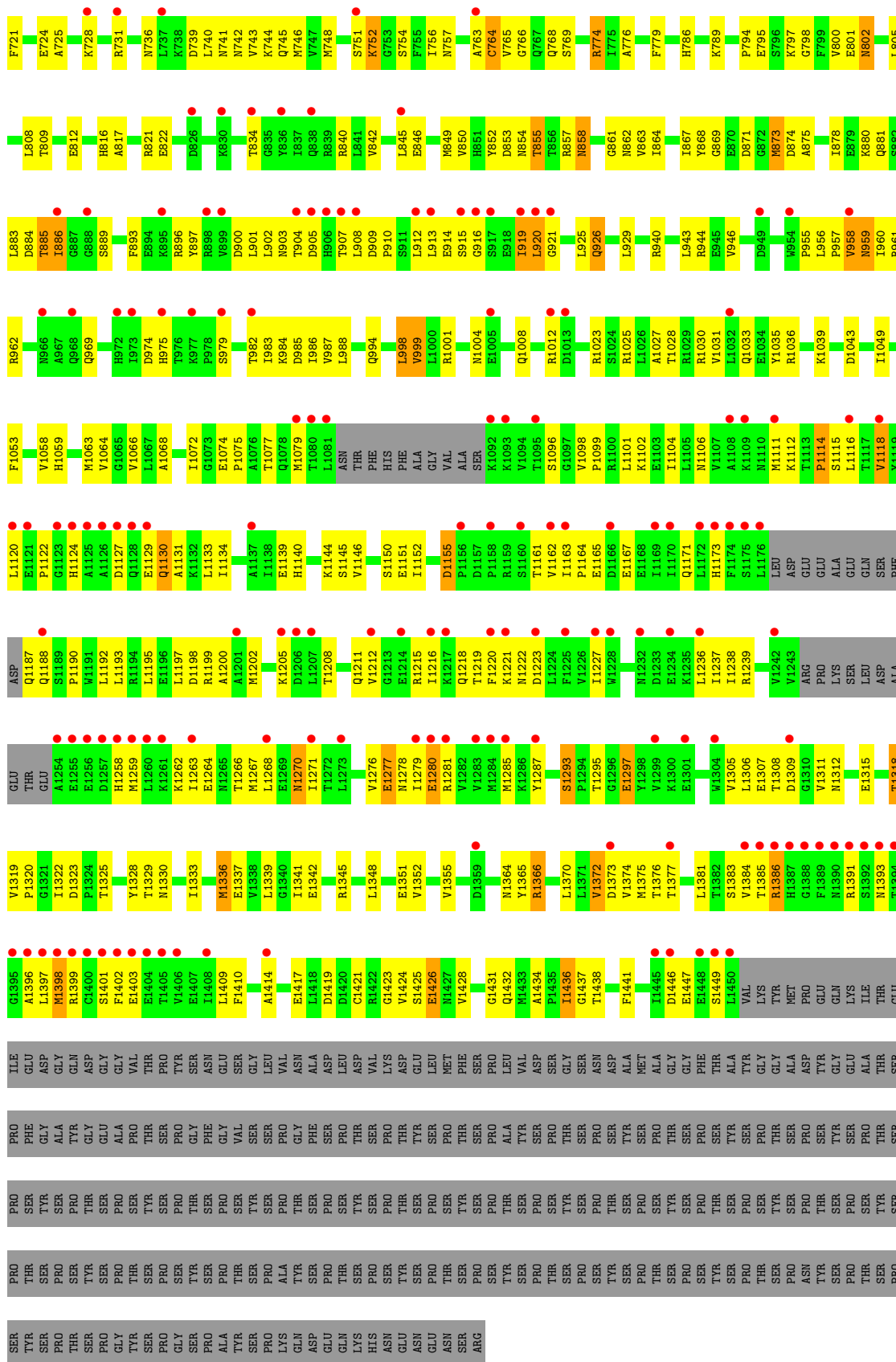


3 Residue-property plots

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

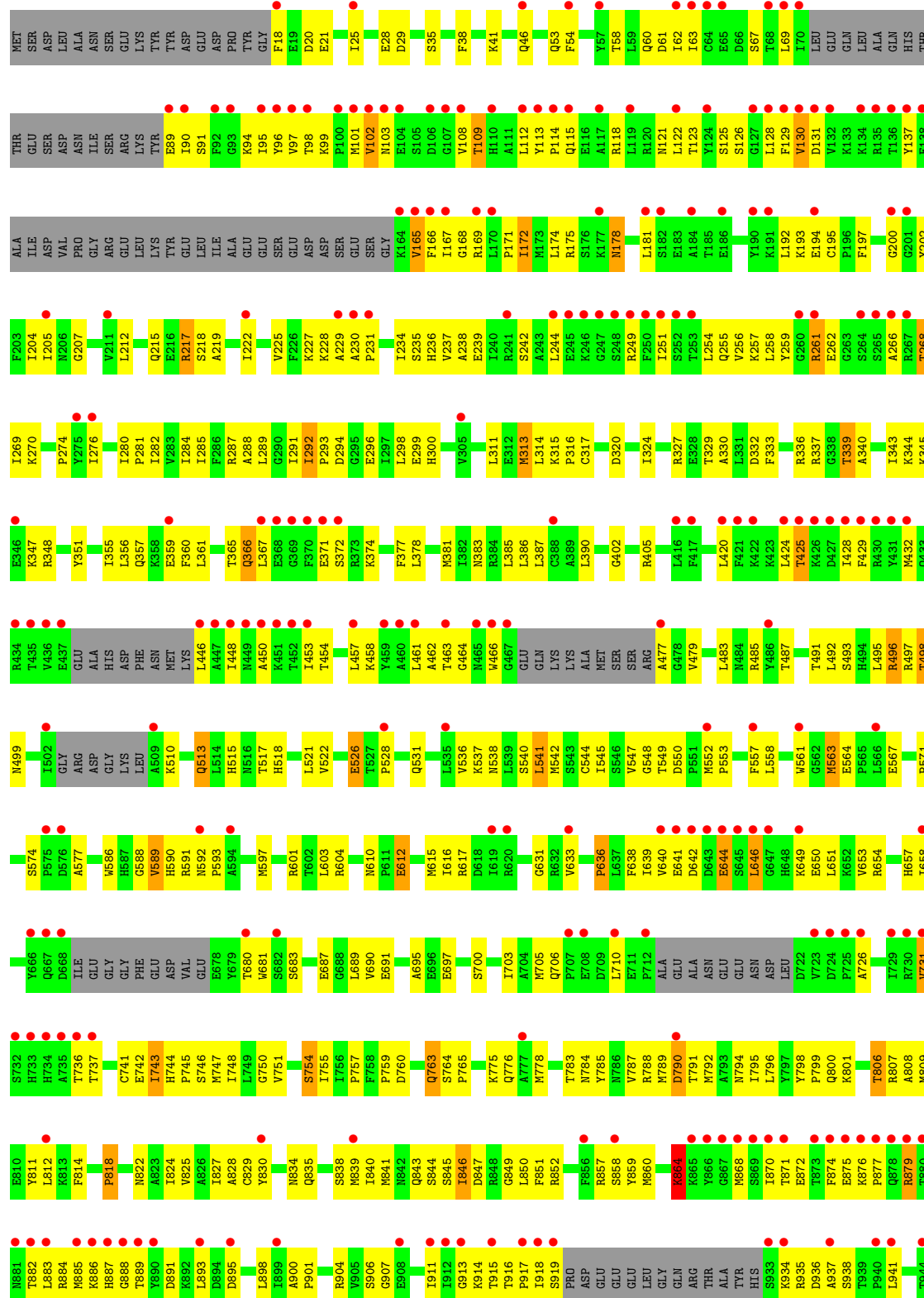
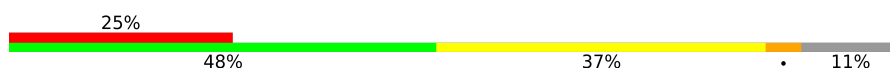
- Molecule 1: DNA-directed RNA polymerase II largest subunit

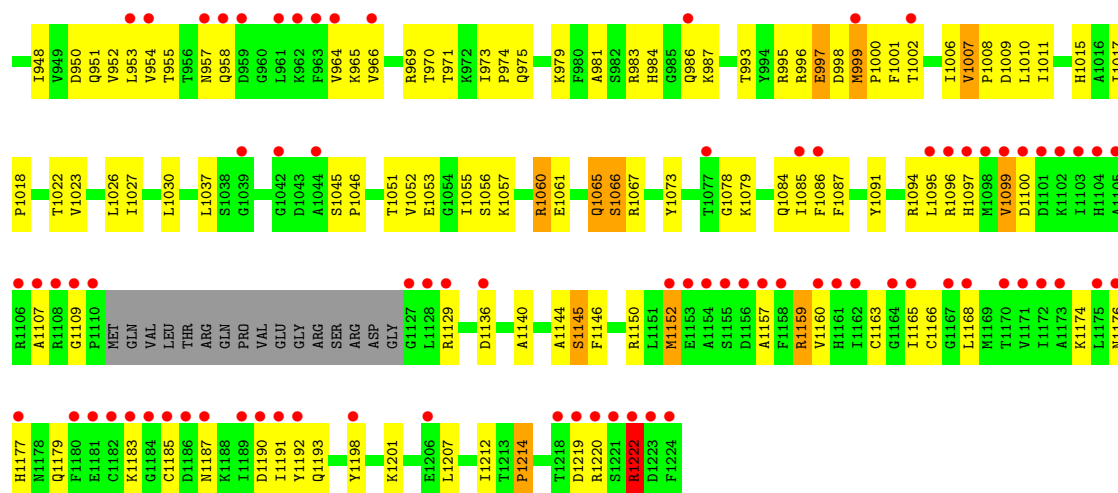




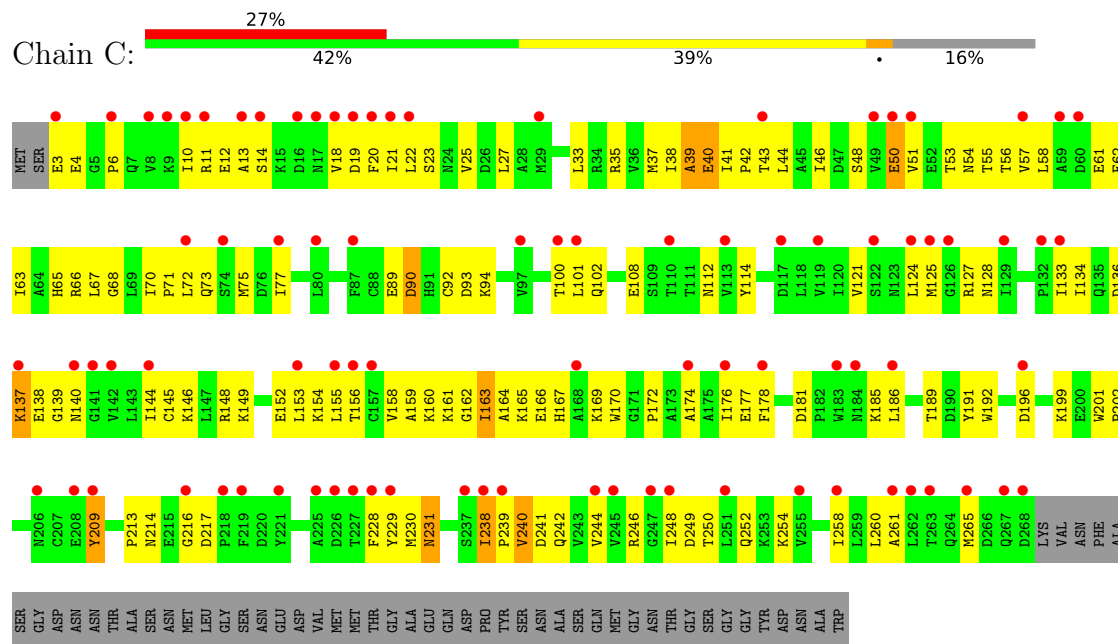
- Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide

Chain B:

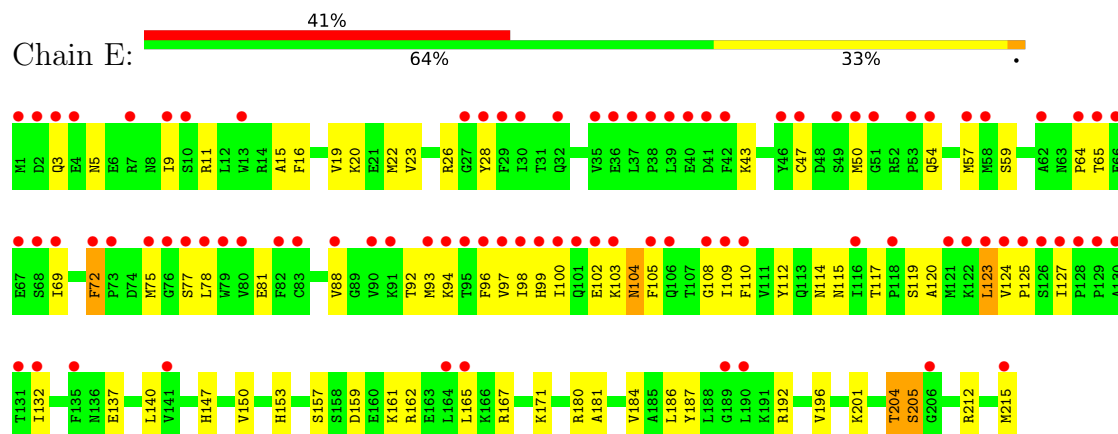




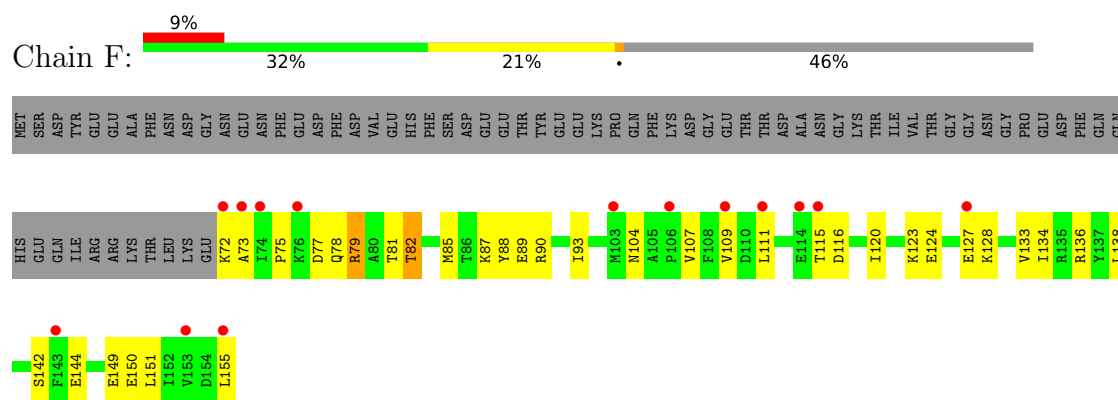
• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide



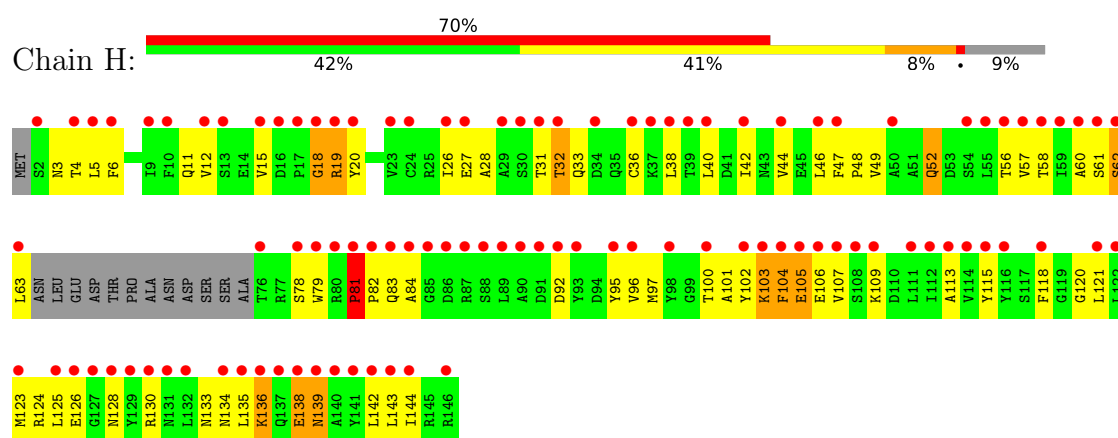
• Molecule 4: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide



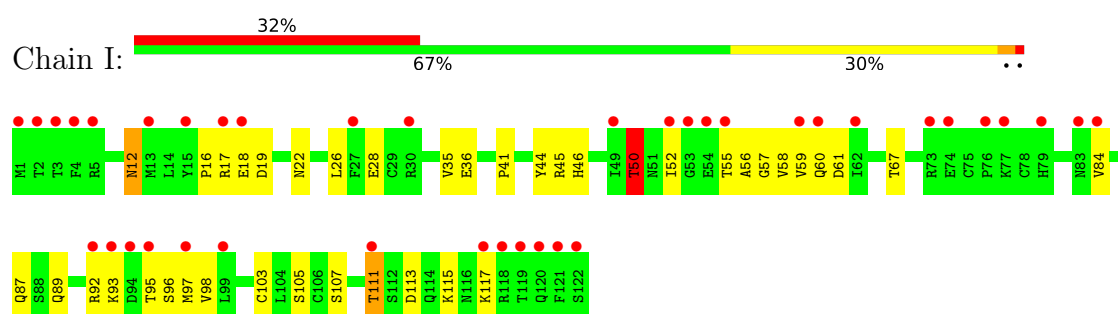
- Molecule 5: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



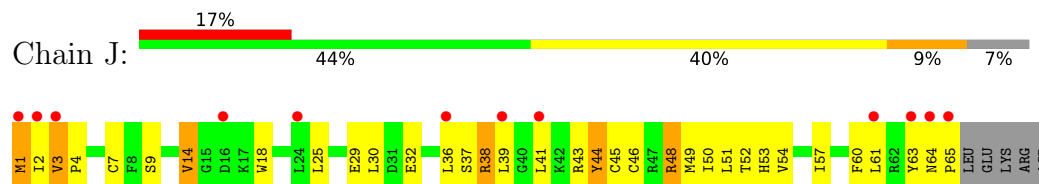
- Molecule 6: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



- Molecule 7: DNA-directed RNA polymerase II 14.2 kDa polypeptide

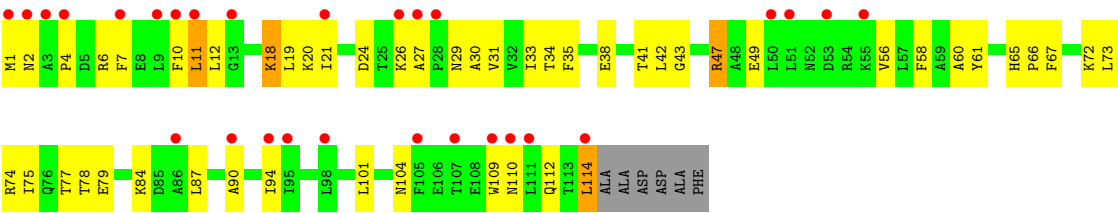


- Molecule 8: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide

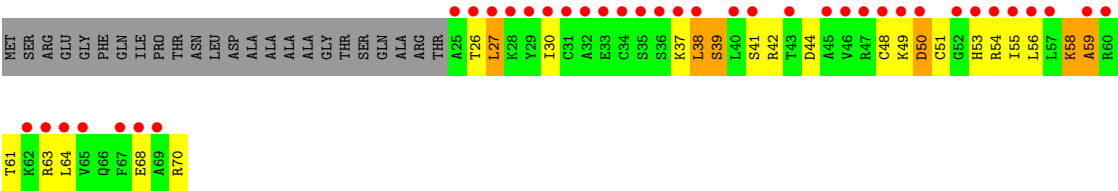
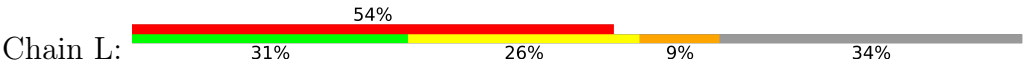


- Molecule 9: DNA-directed RNA polymerase II 13.6 kDa polypeptide





● Molecule 10: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.00Å 223.00Å 374.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.30 40.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.30) 92.0 (40.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.247 , 0.294 0.293 , 0.290	Depositor DCC
R_{free} test set	5166 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	28318	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.55	2/11352 (0.0%)	0.99	42/15352 (0.3%)
2	B	0.52	0/8882	0.96	27/11976 (0.2%)
3	C	0.48	0/2133	0.94	5/2891 (0.2%)
4	E	0.51	1/1796 (0.1%)	0.93	4/2416 (0.2%)
5	F	0.53	0/691	0.96	2/933 (0.2%)
6	H	0.35	0/1086	0.90	6/1470 (0.4%)
7	I	0.43	0/1016	0.90	1/1365 (0.1%)
8	J	0.53	0/541	0.88	1/727 (0.1%)
9	K	0.44	0/937	0.82	1/1265 (0.1%)
10	L	0.38	0/366	0.76	1/485 (0.2%)
All	All	0.52	3/28800 (0.0%)	0.96	90/38880 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	746	MET	SD-CE	-5.20	1.66	1.79
4	E	150	VAL	CA-CB	5.09	1.58	1.53
1	A	507	VAL	CA-CB	5.05	1.60	1.54

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	829	CYS	N-CA-C	-8.82	94.35	108.73
1	A	886	ILE	N-CA-C	8.40	119.21	110.72
1	A	779	PHE	N-CA-C	-8.39	97.50	110.17
1	A	999	VAL	N-CA-C	-8.35	105.10	112.12
1	A	333	GLU	N-CA-C	-8.09	103.13	113.16
1	A	491	VAL	N-CA-C	7.80	115.27	107.55
1	A	998	LEU	N-CA-C	7.63	122.13	109.46
6	H	102	TYR	N-CA-C	-7.60	104.06	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1155	ASP	CA-C-N	7.59	127.47	119.05
1	A	1155	ASP	C-N-CA	7.59	127.47	119.05
1	A	221	SER	N-CA-C	-7.31	103.30	111.71
1	A	846	GLU	N-CA-C	7.22	120.01	111.71
6	H	81	PRO	N-CA-C	7.09	119.35	110.70
3	C	10	ILE	N-CA-C	6.76	118.16	109.30
2	B	703	ILE	N-CA-C	6.62	117.83	108.36
1	A	798	GLY	N-CA-C	6.60	125.09	115.32
2	B	526	GLU	N-CA-C	6.55	119.49	108.23
2	B	828	ALA	N-CA-C	6.40	118.80	109.07
1	A	564	ALA	N-CA-C	-6.31	105.56	113.20
1	A	454	SER	N-CA-C	-6.31	105.62	113.38
1	A	474	VAL	N-CA-C	-6.26	106.89	112.90
1	A	660	ASN	N-CA-C	-6.23	105.70	113.55
9	K	27	ALA	N-CA-C	6.14	113.74	108.22
1	A	71	GLN	CB-CA-C	-6.12	109.54	116.63
1	A	445	ASN	N-CA-C	6.12	119.45	109.06
1	A	562	THR	CA-C-N	6.09	126.11	119.89
1	A	562	THR	C-N-CA	6.09	126.11	119.89
2	B	851	PHE	N-CA-C	6.08	120.49	113.38
1	A	802	ASN	N-CA-C	6.08	118.39	110.43
1	A	776	ALA	N-CA-C	6.04	119.43	110.48
2	B	610	ASN	CA-C-N	6.04	126.48	119.47
2	B	610	ASN	C-N-CA	6.04	126.48	119.47
8	J	9	SER	N-CA-C	6.04	117.66	111.14
3	C	39	ALA	N-CA-C	6.04	123.14	114.39
2	B	282	ILE	N-CA-C	6.03	117.50	110.62
6	H	3	ASN	N-CA-C	6.01	116.18	108.24
1	A	158	PRO	N-CA-C	-5.98	106.68	114.03
1	A	1270	ASN	N-CA-C	5.95	118.72	111.82
1	A	960	ILE	N-CA-C	5.93	116.67	110.62
1	A	399	HIS	CA-C-N	-5.92	112.44	119.84
1	A	399	HIS	C-N-CA	-5.92	112.44	119.84
10	L	58	LYS	N-CA-C	5.92	120.04	112.34
2	B	743	ILE	N-CA-C	-5.91	104.97	110.53
2	B	818	PRO	N-CA-C	5.90	120.27	111.41
2	B	288	ALA	N-CA-C	-5.84	106.00	113.01
4	E	171	LYS	N-CA-C	-5.84	101.88	110.52
4	E	72	PHE	CA-C-N	5.81	125.50	119.05
4	E	72	PHE	C-N-CA	5.81	125.50	119.05
6	H	92	ASP	N-CA-C	-5.78	106.85	112.97
1	A	987	VAL	N-CA-C	5.75	116.21	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	82	THR	N-CA-C	5.75	116.21	109.60
1	A	567	LYS	CA-C-N	-5.69	114.24	119.82
1	A	567	LYS	C-N-CA	-5.69	114.24	119.82
2	B	748	ILE	N-CA-C	-5.66	105.38	113.07
2	B	280	ILE	N-CA-C	5.60	114.05	107.77
2	B	510	LYS	CA-C-N	5.59	125.25	119.05
2	B	510	LYS	C-N-CA	5.59	125.25	119.05
6	H	136	LYS	N-CA-C	-5.59	104.70	112.30
2	B	736	THR	N-CA-C	-5.57	103.87	111.56
2	B	700	SER	N-CA-C	5.57	119.70	113.02
1	A	1118	VAL	N-CA-C	5.55	115.85	107.75
5	F	82	THR	CB-CA-C	-5.49	100.56	109.56
1	A	222	LEU	N-CA-C	-5.49	101.86	110.36
2	B	1085	ILE	N-CA-C	5.49	116.88	108.71
1	A	666	ILE	CB-CA-C	-5.48	104.74	112.14
3	C	216	GLY	N-CA-C	5.47	119.29	112.73
2	B	1078	GLY	N-CA-C	-5.46	108.58	115.08
3	C	40	GLU	N-CA-C	5.46	119.72	112.30
1	A	956	LEU	CA-C-N	-5.42	115.16	120.52
1	A	956	LEU	C-N-CA	-5.42	115.16	120.52
2	B	292	ILE	N-CA-C	5.40	120.55	108.88
2	B	1086	PHE	N-CA-C	-5.39	101.39	109.15
2	B	763	GLN	N-CA-C	-5.37	102.33	110.28
2	B	825	VAL	N-CA-C	5.37	115.69	108.17
1	A	472	LEU	CA-CB-CG	-5.36	97.54	116.30
1	A	220	THR	N-CA-C	-5.34	105.90	112.90
1	A	602	ASP	N-CA-C	-5.31	104.57	111.74
2	B	228	LYS	N-CA-C	5.29	116.32	108.86
2	B	541	LEU	N-CA-C	5.26	120.04	111.37
1	A	1221	LYS	CB-CA-C	-5.21	109.01	115.89
1	A	884	ASP	N-CA-C	5.18	117.33	111.11
2	B	1066	SER	N-CA-C	5.14	121.74	110.80
1	A	766	GLY	N-CA-C	5.13	118.01	111.85
2	B	172	ILE	N-CA-C	5.12	116.35	108.71
6	H	57	VAL	N-CA-C	5.11	115.33	108.17
3	C	191	TYR	N-CA-C	5.10	117.70	110.10
7	I	50	THR	N-CA-C	5.07	118.39	110.32
1	A	482	PHE	N-CA-C	5.03	121.52	110.80
1	A	852	TYR	N-CA-C	5.03	118.52	112.38
4	E	205	SER	N-CA-C	-5.01	101.83	109.65

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11154	0	11224	602	0
2	B	8711	0	8738	449	0
3	C	2095	0	2051	142	0
4	E	1760	0	1788	58	0
5	F	679	0	701	36	0
6	H	1068	0	1040	63	0
7	I	997	0	953	43	0
8	J	532	0	542	55	0
9	K	919	0	929	63	0
10	L	364	0	389	32	0
11	A	2	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	I	2	0	0	0	0
11	J	1	0	0	0	0
11	L	1	0	0	0	0
12	A	2	0	0	0	0
13	B	29	0	11	1	0
All	All	28318	0	28366	1376	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 (1376) 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)
1:A:855:THR:HG21	1:A:857:ARG:HE	1.09	1.14
6:H:130:ARG:HA	6:H:133:ASN:HD22	1.11	1.11
1:A:1364:ASN:ND2	1:A:1366:ARG:HH11	1.53	1.05
1:A:351:THR:HG22	1:A:352:VAL:H	1.20	1.05
1:A:1364:ASN:HD21	1:A:1366:ARG:NH1	1.58	0.99
1:A:901:LEU:H	1:A:926:GLN:NE2	1.60	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:680:THR:HG22	2:B:681:TRP:H	1.28	0.98
1:A:725:ALA:HA	1:A:728:LYS:HE3	1.48	0.95
9:K:65:HIS:HD2	9:K:67:PHE:H	1.01	0.94
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.32	0.93
2:B:118:ARG:NH1	2:B:204:ILE:HD11	1.83	0.93
1:A:1162:VAL:HG11	7:I:41:PRO:HG3	1.51	0.92
3:C:137:LYS:H	3:C:137:LYS:HD2	1.35	0.91
1:A:849:MET:HE1	1:A:1436:ILE:HA	1.49	0.91
1:A:337:ARG:HG2	1:A:341:MET:HE2	1.51	0.91
8:J:48:ARG:HH11	8:J:48:ARG:HG2	1.34	0.91
1:A:901:LEU:H	1:A:926:GLN:HE21	1.19	0.90
1:A:849:MET:HE3	1:A:1063:MET:SD	2.10	0.90
1:A:187:LYS:HB2	1:A:194:ALA:HB1	1.53	0.90
1:A:1376:THR:HG22	4:E:212:ARG:HH22	1.37	0.89
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.55	0.89
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.52	0.88
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.03	0.88
1:A:446:ARG:HD3	1:A:480:ALA:HB2	1.52	0.88
5:F:81:THR:CG2	5:F:136:ARG:HH11	1.87	0.88
2:B:63:ILE:HB	2:B:95:ILE:HD11	1.55	0.87
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.09	0.87
3:C:242:GLN:HE21	3:C:246:ARG:HH21	1.23	0.87
1:A:1116:LEU:HD12	1:A:1329:THR:HB	1.57	0.86
1:A:55:ASP:H	1:A:56:PRO:HD2	1.40	0.86
1:A:313:GLN:HE21	1:A:322:VAL:HG12	1.40	0.86
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.57	0.86
1:A:351:THR:HG22	1:A:352:VAL:N	1.90	0.86
3:C:33:LEU:HG	3:C:37:MET:HE2	1.57	0.86
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.56	0.85
1:A:1376:THR:HG22	4:E:212:ARG:NH2	1.91	0.85
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.58	0.85
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	0.86	0.85
1:A:246:VAL:HG12	1:A:328:ARG:HH12	1.39	0.85
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.57	0.85
5:F:90:ARG:HD3	5:F:155:LEU:HD12	1.58	0.85
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.58	0.85
1:A:317:LYS:HD2	1:A:321:PRO:HG2	1.57	0.85
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.76	0.85
1:A:1208:THR:HB	1:A:1211:GLN:HG3	1.59	0.85
3:C:167:HIS:HD2	3:C:169:LYS:H	1.21	0.85
9:K:65:HIS:CD2	9:K:67:PHE:H	1.93	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:73:GLN:HE21	3:C:75:MET:H	1.25	0.84
6:H:101:ALA:HB1	6:H:103:LYS:HG3	1.58	0.84
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.58	0.84
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.58	0.84
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.60	0.83
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.43	0.83
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.59	0.83
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.08	0.83
2:B:526:GLU:HG2	2:B:538:ASN:ND2	1.93	0.83
3:C:56:THR:HG23	3:C:58:LEU:H	1.42	0.83
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.60	0.83
2:B:864:LYS:HB3	2:B:871:THR:HA	1.58	0.83
4:E:124:VAL:HG13	4:E:132:ILE:HB	1.59	0.83
5:F:81:THR:HG22	5:F:136:ARG:NH1	1.93	0.82
1:A:605:MET:HE3	1:A:606:LEU:H	1.44	0.82
3:C:258:ILE:HD11	9:K:42:LEU:HD21	1.61	0.82
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.44	0.82
1:A:873:MET:HE3	1:A:957:PRO:HG3	1.60	0.82
2:B:25:ILE:HD12	2:B:653:VAL:HG23	1.62	0.82
3:C:54:ASN:OD1	3:C:56:THR:HG22	1.80	0.82
1:A:356:ASP:HB3	1:A:359:LEU:HD12	1.62	0.81
1:A:869:GLY:O	4:E:204:THR:HG21	1.80	0.81
3:C:22:LEU:HD12	3:C:230:MET:HE1	1.62	0.81
1:A:1398:MET:HG3	1:A:1426:GLU:HG2	1.62	0.81
7:I:98:VAL:HG21	7:I:113:ASP:HB2	1.63	0.81
1:A:666:ILE:HD12	2:B:1030:LEU:HD22	1.64	0.80
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.63	0.80
1:A:982:THR:O	1:A:985:ASP:HB2	1.82	0.80
1:A:855:THR:CG2	1:A:857:ARG:HE	1.91	0.80
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.64	0.79
2:B:871:THR:HG22	2:B:872:GLU:H	1.44	0.79
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.29	0.79
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.13	0.79
1:A:1266:THR:HG23	1:A:1270:ASN:HD22	1.48	0.79
3:C:258:ILE:HD13	9:K:35:PHE:HE2	1.48	0.78
1:A:741:ASN:HD22	1:A:744:LYS:H	1.31	0.78
5:F:81:THR:HG22	5:F:136:ARG:HH11	1.49	0.78
1:A:1446:ASP:HB2	5:F:133:VAL:HG23	1.63	0.78
2:B:882:THR:HG21	2:B:935:ARG:HG2	1.67	0.77
1:A:1398:MET:HG2	1:A:1425:SER:HB2	1.65	0.77
2:B:193:LYS:HE2	8:J:65:PRO:HG3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:265:MET:HE1	9:K:19:LEU:HB2	1.67	0.77
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.30	0.77
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.66	0.77
2:B:1006:ILE:HD11	8:J:43:ARG:HB2	1.67	0.77
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.49	0.77
2:B:313:MET:HE2	2:B:390:LEU:HG	1.65	0.77
3:C:73:GLN:NE2	3:C:75:MET:HB2	2.00	0.77
6:H:26:ILE:HD12	6:H:42:ILE:HD12	1.65	0.76
1:A:472:LEU:HD13	2:B:835:GLN:NE2	1.98	0.76
1:A:672:ASP:H	1:A:736:ASN:ND2	1.84	0.76
1:A:709:THR:HB	1:A:712:GLU:HG3	1.66	0.76
2:B:801:LYS:O	8:J:52:THR:HG23	1.86	0.76
1:A:399:HIS:O	1:A:401:GLY:N	2.18	0.76
1:A:855:THR:HG21	1:A:857:ARG:NE	1.94	0.76
1:A:108:MET:H	1:A:171:GLN:NE2	1.83	0.75
1:A:840:ARG:HH11	1:A:1386:ARG:HB3	1.51	0.75
2:B:515:HIS:HD2	2:B:517:THR:H	1.33	0.75
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.52	0.74
2:B:901:PRO:HD3	10:L:58:LYS:HB3	1.69	0.74
2:B:918:ILE:HD12	2:B:935:ARG:HD2	1.68	0.74
3:C:124:LEU:O	3:C:127:ARG:HG2	1.87	0.74
1:A:55:ASP:N	1:A:56:PRO:HD2	2.02	0.74
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.69	0.74
2:B:809:MET:HG2	2:B:814:PHE:HB3	1.70	0.74
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.69	0.74
2:B:680:THR:HG22	2:B:681:TRP:N	2.02	0.74
1:A:179:LEU:HG	1:A:308:ILE:HG21	1.67	0.74
5:F:81:THR:CG2	5:F:136:ARG:NH1	2.50	0.74
1:A:946:VAL:HG22	4:E:201:LYS:HD2	1.69	0.74
1:A:1215:ARG:HA	1:A:1218:GLN:HE21	1.53	0.74
1:A:450:LEU:HD12	1:A:450:LEU:H	1.50	0.73
1:A:666:ILE:HD11	2:B:1030:LEU:HB2	1.69	0.73
2:B:324:ILE:HG12	2:B:329:THR:HG22	1.70	0.73
10:L:38:LEU:HG	10:L:39:SER:H	1.53	0.73
2:B:953:LEU:HD21	2:B:955:THR:HG23	1.68	0.73
2:B:914:LYS:HB3	2:B:937:ALA:O	1.87	0.73
1:A:446:ARG:HB2	1:A:487:MET:HE2	1.69	0.73
3:C:51:VAL:HG22	3:C:155:LEU:HD22	1.71	0.73
1:A:907:THR:HG22	1:A:908:LEU:H	1.53	0.73
1:A:79:GLY:HA3	1:A:245:PRO:HG3	1.71	0.73
1:A:605:MET:HE1	1:A:612:ILE:HG13	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:PRO:HB3	3:C:161:LYS:HE3	1.69	0.72
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.24	0.72
1:A:1151:GLU:HG2	7:I:45:ARG:HD2	1.71	0.72
2:B:46:GLN:HE22	2:B:496:ARG:HB3	1.54	0.72
1:A:567:LYS:HB3	6:H:96:VAL:N	2.05	0.72
3:C:57:VAL:HG11	8:J:60:PHE:HB3	1.72	0.72
1:A:571:LEU:HD22	6:H:46:LEU:HD11	1.71	0.72
9:K:43:GLY:O	9:K:47:ARG:HB2	1.89	0.72
1:A:1342:GLU:OE2	4:E:212:ARG:NH1	2.23	0.72
2:B:294:ASP:H	7:I:12:ASN:ND2	1.87	0.72
3:C:214:ASN:HB2	3:C:217:ASP:OD2	1.90	0.71
2:B:281:PRO:HG2	2:B:284:ILE:HD12	1.71	0.71
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.54	0.71
1:A:103:CYS:SG	1:A:207:ILE:HD12	2.31	0.71
1:A:208:LEU:HD21	1:A:212:LYS:HE3	1.72	0.71
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.73	0.71
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.04	0.71
1:A:875:ALA:HB2	1:A:1366:ARG:CD	2.19	0.71
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.73	0.71
2:B:1222:ARG:H	2:B:1222:ARG:HD2	1.55	0.71
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.72	0.71
5:F:72:LYS:N	5:F:142:SER:HA	2.06	0.71
1:A:55:ASP:H	1:A:56:PRO:CD	2.04	0.71
1:A:567:LYS:HB3	6:H:96:VAL:H	1.55	0.71
1:A:1192:LEU:HD11	1:A:1239:ARG:HB2	1.73	0.70
1:A:1438:THR:HG22	2:B:1144:ALA:H	1.56	0.70
2:B:644:GLU:HB2	2:B:654:ARG:HH22	1.55	0.70
1:A:587:HIS:HA	1:A:607:ILE:O	1.91	0.70
2:B:806:THR:HG22	2:B:809:MET:H	1.57	0.70
1:A:567:LYS:HE2	6:H:95:TYR:CZ	2.27	0.70
1:A:246:VAL:HG12	1:A:328:ARG:NH1	2.06	0.70
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.72	0.70
2:B:705:MET:CE	2:B:745:PRO:HB3	2.21	0.70
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.72	0.70
1:A:754:SER:H	1:A:757:ASN:HD22	1.38	0.70
1:A:1364:ASN:ND2	1:A:1366:ARG:H	1.89	0.70
1:A:340:LEU:HD13	1:A:1399:ARG:HG2	1.74	0.70
1:A:574:GLY:O	1:A:577:ILE:HG13	1.92	0.70
2:B:864:LYS:HG2	2:B:871:THR:HG23	1.73	0.70
1:A:1059:HIS:HE1	5:F:155:LEU:HD22	1.56	0.70
1:A:1276:VAL:HB	1:A:1279:ILE:HD13	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:824:ILE:HD11	8:J:48:ARG:NH1	2.07	0.70
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.27	0.69
2:B:324:ILE:HD13	2:B:330:ALA:HA	1.73	0.69
1:A:134:ARG:HD2	1:A:221:SER:O	1.91	0.69
2:B:542:MET:HG3	2:B:747:MET:HE3	1.72	0.69
6:H:81:PRO:HB2	6:H:82:PRO:HD3	1.75	0.69
2:B:824:ILE:HD11	8:J:48:ARG:HH12	1.57	0.69
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.73	0.69
1:A:264:PHE:HD1	1:A:315:LEU:HB3	1.58	0.69
2:B:542:MET:HE1	2:B:743:ILE:HD12	1.75	0.69
3:C:20:PHE:HE1	3:C:22:LEU:HG	1.58	0.69
2:B:755:ILE:HG22	2:B:755:ILE:O	1.91	0.69
2:B:957:ASN:ND2	2:B:958:GLN:H	1.91	0.69
3:C:56:THR:HG21	3:C:63:ILE:HD11	1.73	0.68
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.76	0.68
1:A:683:ILE:HD11	1:A:764:CYS:HB2	1.74	0.68
1:A:381:THR:HG22	5:F:104:ASN:OD1	1.93	0.68
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.75	0.68
2:B:955:THR:HG22	10:L:55:ILE:HA	1.73	0.68
2:B:955:THR:HG22	10:L:54:ARG:O	1.94	0.68
1:A:533:LYS:NZ	1:A:660:ASN:HD21	1.92	0.68
2:B:67:SER:O	2:B:91:SER:HA	1.93	0.68
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.75	0.68
1:A:351:THR:CG2	1:A:352:VAL:H	2.01	0.68
1:A:914:GLU:HG3	1:A:979:SER:O	1.94	0.68
2:B:69:LEU:HD21	2:B:425:THR:HG23	1.73	0.68
1:A:567:LYS:HE2	6:H:95:TYR:CE1	2.29	0.68
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.29	0.68
1:A:53:LEU:HD23	1:A:54:ASN:H	1.58	0.67
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.76	0.67
1:A:598:LEU:HG	6:H:115:TYR:HE2	1.60	0.67
1:A:1277:GLU:O	1:A:1278:ASN:HB2	1.92	0.67
1:A:786:HIS:HE1	2:B:742:GLU:OE2	1.76	0.67
1:A:853:ASP:OD1	1:A:855:THR:HB	1.95	0.67
1:A:82:GLY:HA3	1:A:241:VAL:HB	1.76	0.67
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.77	0.67
2:B:879:ARG:HB3	2:B:883:LEU:HD23	1.77	0.67
3:C:73:GLN:HE21	3:C:75:MET:N	1.92	0.67
1:A:665:GLY:C	2:B:1026:LEU:HD13	2.20	0.67
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.76	0.67
2:B:268:THR:HG21	2:B:270:LYS:HE3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.77	0.67
5:F:79:ARG:HH22	5:F:150:GLU:CD	2.03	0.67
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.25	0.67
1:A:907:THR:HG22	1:A:908:LEU:N	2.09	0.67
6:H:40:LEU:HD13	6:H:123:MET:HB2	1.76	0.66
1:A:1066:VAL:HG12	2:B:1140:ALA:HB2	1.77	0.66
2:B:950:ASP:HB2	2:B:969:ARG:HB2	1.77	0.66
5:F:109:VAL:HG11	5:F:123:LYS:HG2	1.77	0.66
6:H:79:TRP:CZ3	6:H:81:PRO:HG3	2.30	0.66
2:B:324:ILE:HD11	2:B:333:PHE:HB2	1.76	0.66
3:C:35:ARG:NH1	9:K:41:THR:N	2.43	0.66
1:A:203:SER:OG	1:A:206:GLU:HG3	1.95	0.66
2:B:876:LYS:HE3	2:B:893:LEU:O	1.96	0.66
3:C:166:GLU:HG2	10:L:70:ARG:NH1	2.09	0.66
1:A:472:LEU:O	1:A:475:THR:HB	1.96	0.66
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.77	0.66
6:H:103:LYS:HB3	6:H:105:GLU:OE2	1.96	0.66
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.76	0.66
6:H:130:ARG:HA	6:H:133:ASN:ND2	1.97	0.66
1:A:31:SER:HB2	1:A:83:HIS:HB2	1.78	0.65
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.77	0.65
1:A:1124:HIS:HB3	1:A:1130:GLN:HG3	1.77	0.65
1:A:1145:SER:HB2	1:A:1205:LYS:NZ	2.10	0.65
2:B:175:ARG:HH11	2:B:175:ARG:HB3	1.61	0.65
1:A:694:THR:O	1:A:698:GLN:HG3	1.96	0.65
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.12	0.65
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.93	0.65
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.78	0.65
2:B:1174:LYS:HD2	2:B:1179:GLN:HB2	1.77	0.65
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.77	0.65
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.78	0.65
1:A:605:MET:HE2	1:A:607:ILE:HG13	1.79	0.65
1:A:834:THR:HG21	1:A:1077:THR:HA	1.79	0.65
8:J:48:ARG:NH2	8:J:49:MET:HE1	2.12	0.65
2:B:864:LYS:CG	2:B:871:THR:HG23	2.27	0.65
3:C:57:VAL:HG11	8:J:60:PHE:CB	2.26	0.65
1:A:567:LYS:CB	1:A:568:PRO:CD	2.75	0.65
2:B:89:GLU:HB2	2:B:137:TYR:HB2	1.79	0.65
2:B:531:GLN:CD	2:B:531:GLN:H	2.05	0.65
1:A:867:ILE:HD11	1:A:999:VAL:HG11	1.79	0.65
1:A:1279:ILE:HD11	1:A:1312:ASN:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:998:LEU:HD12	1:A:1001:ARG:NH1	2.10	0.64
1:A:1068:ALA:O	1:A:1072:ILE:HG13	1.97	0.64
5:F:87:LYS:HA	5:F:155:LEU:HD13	1.78	0.64
1:A:1263:ILE:O	1:A:1267:MET:HG3	1.96	0.64
2:B:276:ILE:HG23	2:B:337:ARG:HB2	1.80	0.64
8:J:36:LEU:HD11	8:J:51:LEU:HB2	1.80	0.64
1:A:347:PHE:H	2:B:1107:ALA:HA	1.63	0.64
1:A:673:GLY:N	1:A:674:PRO:HD2	2.12	0.64
5:F:81:THR:HG21	5:F:136:ARG:HH11	1.59	0.64
2:B:872:GLU:HB3	2:B:914:LYS:HD3	1.78	0.64
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.78	0.64
1:A:1449:SER:HB3	5:F:149:GLU:OE2	1.97	0.64
3:C:196:ASP:HB3	3:C:199:LYS:HB2	1.78	0.64
1:A:903:ASN:ND2	1:A:905:ASP:H	1.95	0.64
2:B:125:SER:HA	2:B:171:PRO:HA	1.80	0.64
2:B:25:ILE:HD13	2:B:658:ILE:HD11	1.80	0.63
2:B:577:ALA:HB1	2:B:589:VAL:HG22	1.80	0.63
1:A:1258:HIS:O	1:A:1262:LYS:HG3	1.98	0.63
2:B:205:ILE:HD11	2:B:461:LEU:HD23	1.80	0.63
3:C:248:ILE:HD13	9:K:101:LEU:HD13	1.80	0.63
1:A:754:SER:N	1:A:757:ASN:HD22	1.95	0.63
1:A:789:LYS:HE3	7:I:67:THR:OG1	1.98	0.63
1:A:903:ASN:C	1:A:903:ASN:HD22	2.06	0.63
1:A:986:ILE:HG21	1:A:1028:THR:HA	1.81	0.63
2:B:464:GLY:O	2:B:477:ALA:HB3	1.98	0.63
6:H:4:THR:HA	6:H:60:ALA:HA	1.79	0.63
1:A:864:ILE:HD13	1:A:1374:VAL:HG22	1.80	0.63
1:A:1151:GLU:CG	7:I:45:ARG:HD2	2.28	0.63
2:B:550:ASP:OD1	2:B:552:MET:HG3	1.98	0.63
2:B:195:CYS:SG	2:B:783:THR:HG23	2.38	0.63
2:B:239:GLU:CD	2:B:255:GLN:HE21	2.07	0.63
2:B:839:MET:CE	2:B:1010:LEU:HG	2.28	0.63
1:A:443:LEU:HB3	1:A:490:HIS:HB2	1.80	0.63
1:A:567:LYS:HD3	6:H:96:VAL:H	1.64	0.63
1:A:672:ASP:H	1:A:736:ASN:HD21	1.47	0.63
1:A:858:ASN:C	1:A:858:ASN:HD22	2.06	0.63
1:A:1398:MET:HE2	1:A:1423:GLY:HA3	1.79	0.63
2:B:130:VAL:HG12	2:B:131:ASP:H	1.63	0.63
2:B:879:ARG:HG3	2:B:885:MET:HE2	1.80	0.63
4:E:43:LYS:O	4:E:47:CYS:HB2	1.98	0.63
4:E:64:PRO:HG2	4:E:75:MET:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:242:GLN:NE2	3:C:246:ARG:HH21	1.94	0.62
10:L:27:LEU:HD13	10:L:37:LYS:HE2	1.81	0.62
1:A:728:LYS:HA	1:A:731:ARG:HD2	1.80	0.62
2:B:58:THR:O	2:B:62:ILE:HG13	1.98	0.62
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.34	0.62
1:A:914:GLU:C	1:A:916:GLY:H	2.06	0.62
7:I:59:VAL:HG12	7:I:60:GLN:H	1.65	0.62
1:A:329:LEU:O	1:A:333:GLU:HG2	2.00	0.62
1:A:31:SER:CB	1:A:83:HIS:HB2	2.30	0.62
1:A:525:GLN:HB2	2:B:835:GLN:OE1	2.00	0.62
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.35	0.62
3:C:92:CYS:SG	3:C:94:LYS:HB2	2.40	0.62
1:A:901:LEU:N	1:A:926:GLN:NE2	2.43	0.62
1:A:1318:THR:HG21	4:E:11:ARG:HH12	1.65	0.62
1:A:714:PHE:HB2	7:I:97:MET:HE1	1.82	0.62
1:A:1025:ARG:HD3	1:A:1030:ARG:HH21	1.64	0.62
2:B:477:ALA:HB1	2:B:479:VAL:HG23	1.82	0.62
1:A:867:ILE:HD11	1:A:999:VAL:CG1	2.30	0.61
1:A:1164:PRO:O	1:A:1167:GLU:HG3	1.99	0.61
7:I:50:THR:HG22	7:I:52:ILE:HG22	1.81	0.61
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.81	0.61
1:A:873:MET:CE	1:A:957:PRO:HG3	2.30	0.61
3:C:148:ARG:NH1	8:J:64:ASN:HA	2.15	0.61
1:A:32:VAL:HG11	1:A:68:GLN:HE22	1.65	0.61
1:A:137:ALA:O	1:A:141:LEU:HD13	2.00	0.61
1:A:902:LEU:HD23	1:A:921:GLY:HA2	1.82	0.61
2:B:638:PHE:CE1	2:B:743:ILE:HA	2.36	0.61
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.41	0.61
1:A:579:SER:OG	1:A:612:ILE:HG22	2.01	0.61
1:A:243:PRO:C	1:A:245:PRO:HD2	2.26	0.61
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.30	0.61
1:A:1318:THR:CG2	4:E:11:ARG:HH12	2.13	0.61
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.81	0.61
1:A:857:ARG:HG2	1:A:863:VAL:HA	1.81	0.61
3:C:58:LEU:HD11	8:J:2:ILE:CD1	2.31	0.61
9:K:47:ARG:HH11	9:K:47:ARG:HB3	1.66	0.60
10:L:26:THR:HG22	10:L:27:LEU:H	1.65	0.60
1:A:489:LEU:C	1:A:489:LEU:HD23	2.26	0.60
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.82	0.60
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.66	0.60
7:I:59:VAL:HG12	7:I:60:GLN:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LYS:HB2	1:A:194:ALA:CB	2.31	0.60
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.31	0.60
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.65	0.60
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.82	0.60
3:C:22:LEU:HD12	3:C:230:MET:CE	2.29	0.60
1:A:345:VAL:HG11	2:B:1129:ARG:HA	1.84	0.60
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.82	0.60
7:I:56:ALA:O	7:I:89:GLN:HG3	2.02	0.60
1:A:535:THR:CG2	1:A:575:LYS:HG2	2.31	0.60
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.82	0.60
1:A:1219:THR:HG21	1:A:1271:ILE:HG12	1.82	0.60
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.67	0.60
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.65	0.60
7:I:45:ARG:HG2	7:I:45:ARG:HH11	1.65	0.60
1:A:535:THR:O	1:A:575:LYS:HE2	2.02	0.60
1:A:1333:ILE:O	1:A:1337:GLU:HG3	2.02	0.60
2:B:515:HIS:H	2:B:518:HIS:CD2	2.19	0.60
3:C:166:GLU:HG2	10:L:70:ARG:HH12	1.67	0.60
2:B:60:GLN:HA	2:B:95:ILE:HD12	1.84	0.60
2:B:841:MET:HE2	2:B:1010:LEU:HD11	1.84	0.60
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.31	0.59
2:B:193:LYS:HD3	2:B:787:VAL:HG11	1.83	0.59
2:B:365:THR:HG22	2:B:367:LEU:H	1.65	0.59
1:A:1323:ASP:OD1	1:A:1325:THR:HB	2.03	0.59
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.84	0.59
3:C:258:ILE:CD1	9:K:42:LEU:HD21	2.31	0.59
1:A:35:ILE:HD12	1:A:35:ILE:N	2.18	0.59
2:B:25:ILE:HD12	2:B:653:VAL:CG2	2.32	0.59
4:E:117:THR:HG22	4:E:119:SER:H	1.67	0.59
8:J:48:ARG:HG2	8:J:48:ARG:NH1	2.11	0.59
1:A:61:ILE:HG22	1:A:62:ASP:H	1.67	0.59
1:A:388:LEU:HD22	1:A:432:VAL:HB	1.85	0.59
1:A:903:ASN:HD22	1:A:904:THR:N	2.00	0.59
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.84	0.59
2:B:377:PHE:CD2	2:B:381:MET:HE2	2.37	0.59
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.84	0.59
9:K:29:ASN:HD21	9:K:79:GLU:HA	1.67	0.59
1:A:80:HIS:O	1:A:243:PRO:HB3	2.02	0.59
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.83	0.59
2:B:1008:PRO:HB3	2:B:1087:PHE:CE1	2.32	0.59
2:B:885:MET:HA	2:B:936:ASP:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:27:LEU:HB3	10:L:37:LYS:HD3	1.84	0.59
1:A:313:GLN:HB3	1:A:320:ARG:C	2.27	0.59
1:A:523:ILE:HD12	1:A:523:ILE:N	2.17	0.59
2:B:755:ILE:O	2:B:755:ILE:CG2	2.50	0.59
1:A:883:LEU:O	1:A:886:ILE:HG22	2.03	0.58
3:C:71:PRO:O	3:C:72:LEU:HD23	2.03	0.58
6:H:6:PHE:O	6:H:58:THR:HG23	2.03	0.58
2:B:651:LEU:CD2	2:B:710:LEU:HD11	2.33	0.58
2:B:874:PHE:O	2:B:875:GLU:HG3	2.04	0.58
1:A:587:HIS:CE1	1:A:609:ASP:H	2.21	0.58
1:A:1096:SER:O	1:A:1099:PRO:HG2	2.03	0.58
2:B:130:VAL:HG21	2:B:167:ILE:HD12	1.85	0.58
2:B:792:MET:SD	2:B:857:ARG:NH2	2.76	0.58
1:A:264:PHE:HB3	1:A:315:LEU:HD22	1.85	0.58
1:A:537:ARG:NH1	6:H:120:GLY:O	2.36	0.58
1:A:598:LEU:HG	6:H:115:TYR:CE2	2.38	0.58
2:B:644:GLU:CD	2:B:646:LEU:HB2	2.29	0.58
2:B:953:LEU:HD21	2:B:955:THR:CG2	2.33	0.58
3:C:62:PHE:O	3:C:66:ARG:HG3	2.03	0.58
1:A:1064:VAL:HG12	1:A:1370:LEU:CD2	2.34	0.58
2:B:791:THR:HG22	2:B:792:MET:HG3	1.85	0.58
3:C:39:ALA:O	3:C:163:ILE:HG23	2.04	0.58
1:A:739:ASP:OD2	6:H:19:ARG:HD2	2.03	0.58
1:A:523:ILE:HB	1:A:622:VAL:CG1	2.33	0.58
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.85	0.58
1:A:317:LYS:CD	1:A:321:PRO:HG2	2.31	0.58
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.38	0.58
2:B:839:MET:HE1	2:B:1010:LEU:HG	1.86	0.58
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.02	0.58
4:E:180:ARG:HH21	4:E:192:ARG:HB2	1.69	0.57
1:A:451:HIS:CG	1:A:1074:GLU:HG3	2.40	0.57
1:A:986:ILE:HD12	1:A:1028:THR:HG23	1.86	0.57
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.39	0.57
7:I:17:ARG:HG3	7:I:28:GLU:HG2	1.86	0.57
1:A:208:LEU:C	1:A:208:LEU:HD23	2.28	0.57
1:A:913:LEU:HD12	1:A:914:GLU:N	2.19	0.57
1:A:1066:VAL:CG1	2:B:1140:ALA:HB2	2.34	0.57
4:E:15:ALA:O	4:E:19:VAL:HG23	2.03	0.57
9:K:20:LYS:HB2	9:K:34:THR:HB	1.86	0.57
1:A:878:ILE:CG2	1:A:955:PRO:HB2	2.34	0.57
8:J:2:ILE:HG22	8:J:3:VAL:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.70	0.57
1:A:1220:PHE:O	1:A:1223:ASP:HB2	2.05	0.57
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	2.20	0.57
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.52	0.57
1:A:129:LYS:HE3	4:E:215:MET:HE1	1.87	0.57
1:A:329:LEU:HB3	1:A:333:GLU:HB3	1.86	0.57
1:A:550:LEU:HD22	1:A:556:TRP:NE1	2.19	0.57
1:A:244:PRO:N	1:A:245:PRO:HD2	2.20	0.57
2:B:522:VAL:HG11	2:B:537:LYS:HD2	1.85	0.57
2:B:754:SER:HB3	2:B:812:LEU:HD11	1.87	0.57
2:B:785:TYR:CD2	2:B:795:ILE:HG12	2.40	0.57
2:B:824:ILE:CD1	8:J:48:ARG:HH12	2.18	0.57
2:B:834:ASN:HA	2:B:838:SER:OG	2.05	0.57
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.40	0.57
2:B:230:ALA:N	2:B:231:PRO:HD2	2.20	0.56
7:I:103:CYS:O	7:I:107:SER:HA	2.05	0.56
2:B:172:ILE:HD11	2:B:178:ASN:HD22	1.70	0.56
1:A:605:MET:HE1	1:A:612:ILE:CG1	2.33	0.56
1:A:886:ILE:HD12	1:A:943:LEU:HB3	1.87	0.56
1:A:913:LEU:HD12	1:A:914:GLU:H	1.68	0.56
1:A:1364:ASN:HD22	1:A:1366:ARG:H	1.53	0.56
1:A:1366:ARG:HB3	1:A:1366:ARG:CZ	2.36	0.56
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.88	0.56
2:B:879:ARG:HD3	2:B:883:LEU:HD22	1.88	0.56
2:B:1065:GLN:O	2:B:1065:GLN:HG3	2.05	0.56
1:A:14:VAL:N	1:A:1432:GLN:HE22	2.00	0.56
1:A:679:ILE:HD13	1:A:763:ALA:HB2	1.88	0.56
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.86	0.56
1:A:858:ASN:ND2	1:A:862:ASN:H	2.03	0.56
2:B:175:ARG:HB3	2:B:175:ARG:NH1	2.21	0.56
2:B:215:GLN:HE22	2:B:499:ASN:ND2	2.03	0.56
1:A:1127:ASP:HB2	1:A:1130:GLN:HB2	1.87	0.56
2:B:1159:ARG:HH11	2:B:1159:ARG:HB3	1.71	0.56
4:E:19:VAL:HG22	4:E:140:LEU:HD13	1.87	0.56
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.40	0.56
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.36	0.56
3:C:6:PRO:HG2	9:K:101:LEU:HB2	1.87	0.56
1:A:587:HIS:NE2	1:A:969:GLN:HG2	2.21	0.56
2:B:809:MET:HG2	2:B:814:PHE:CB	2.36	0.56
2:B:751:VAL:HG13	2:B:812:LEU:HD22	1.87	0.55
3:C:125:MET:HE3	3:C:127:ARG:NH2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1025:ARG:HD3	1:A:1030:ARG:NH2	2.20	0.55
2:B:871:THR:HG22	2:B:872:GLU:N	2.17	0.55
10:L:38:LEU:HG	10:L:39:SER:N	2.21	0.55
1:A:106:VAL:HG21	1:A:214:ILE:HG12	1.88	0.55
2:B:800:GLN:HB3	8:J:52:THR:HG21	1.88	0.55
3:C:56:THR:HG23	3:C:58:LEU:N	2.18	0.55
6:H:118:PHE:HB2	6:H:121:LEU:HB2	1.88	0.55
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.87	0.55
2:B:680:THR:O	2:B:683:SER:HB2	2.07	0.55
2:B:822:ASN:ND2	8:J:52:THR:HG21	2.21	0.55
2:B:871:THR:O	2:B:917:PRO:HD2	2.07	0.55
3:C:22:LEU:HD21	9:K:101:LEU:HD21	1.89	0.55
9:K:24:ASP:HB3	9:K:30:ALA:HB3	1.89	0.55
1:A:503:GLN:HE21	5:F:90:ARG:HH21	1.55	0.55
2:B:193:LYS:CE	8:J:65:PRO:HG3	2.35	0.55
2:B:680:THR:CG2	2:B:681:TRP:H	2.09	0.55
2:B:800:GLN:CB	8:J:52:THR:HG22	2.37	0.55
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.39	0.55
3:C:248:ILE:HD13	9:K:101:LEU:CD1	2.37	0.55
5:F:93:ILE:CD1	5:F:134:ILE:HD11	2.35	0.55
6:H:113:ALA:HB1	6:H:124:ARG:HE	1.72	0.55
1:A:901:LEU:O	1:A:920:LEU:HD23	2.07	0.54
2:B:542:MET:CG	2:B:747:MET:HE3	2.37	0.54
1:A:15:LYS:O	1:A:1421:CYS:HB2	2.07	0.54
1:A:273:ASN:O	1:A:277:GLU:HG3	2.07	0.54
2:B:841:MET:HG3	2:B:1010:LEU:HD12	1.90	0.54
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.08	0.54
3:C:258:ILE:HD13	9:K:35:PHE:CE2	2.37	0.54
6:H:12:VAL:HA	6:H:28:ALA:HB2	1.88	0.54
7:I:55:THR:O	7:I:58:VAL:HG23	2.07	0.54
7:I:115:LYS:O	7:I:117:LYS:HG3	2.06	0.54
1:A:709:THR:HG22	1:A:710:LEU:N	2.22	0.54
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.89	0.54
2:B:971:THR:OG1	3:C:61:GLU:HG3	2.07	0.54
3:C:11:ARG:HD2	3:C:21:ILE:HD11	1.89	0.54
4:E:5:ASN:O	4:E:9:ILE:HG13	2.07	0.54
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.90	0.54
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.73	0.54
1:A:885:THR:HG22	1:A:893:PHE:HE1	1.73	0.54
2:B:1051:THR:O	2:B:1055:ILE:HG13	2.07	0.54
1:A:519:PRO:HD3	1:A:631:HIS:ND1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.89	0.54
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.37	0.54
2:B:172:ILE:CD1	2:B:178:ASN:HD22	2.20	0.54
3:C:43:THR:HG22	3:C:44:LEU:N	2.23	0.54
4:E:26:ARG:O	4:E:75:MET:HE1	2.08	0.54
8:J:48:ARG:NH1	8:J:48:ARG:CG	2.71	0.54
2:B:757:PRO:HD3	2:B:983:ARG:NH2	2.23	0.54
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.88	0.54
1:A:697:ALA:HB2	1:A:702:LEU:HD23	1.89	0.54
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.43	0.54
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.43	0.54
1:A:1336:MET:HE3	1:A:1381:LEU:HG	1.89	0.54
1:A:464:PRO:O	1:A:465:TYR:O	2.25	0.54
7:I:57:GLY:O	7:I:59:VAL:HG23	2.08	0.54
10:L:26:THR:HG22	10:L:27:LEU:N	2.23	0.54
1:A:689:LYS:O	1:A:693:VAL:HG23	2.08	0.54
1:A:929:LEU:HD11	1:A:983:ILE:HD13	1.90	0.54
2:B:41:LYS:HE2	2:B:544:CYS:SG	2.48	0.54
2:B:205:ILE:HG21	2:B:462:ALA:HB2	1.89	0.54
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.90	0.54
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.90	0.54
4:E:96:PHE:CE2	4:E:110:PHE:HB2	2.43	0.54
9:K:56:VAL:HA	9:K:77:THR:HG22	1.89	0.54
2:B:204:ILE:C	2:B:205:ILE:HD12	2.32	0.53
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.08	0.53
1:A:666:ILE:CD1	2:B:1030:LEU:HD22	2.36	0.53
1:A:1102:LYS:HD3	1:A:1106:ASN:HD21	1.73	0.53
2:B:339:THR:HG23	2:B:343:ILE:HD12	1.89	0.53
5:F:77:ASP:O	5:F:78:GLN:HB2	2.07	0.53
1:A:69:THR:O	2:B:1174:LYS:HG2	2.08	0.53
1:A:500:GLU:OE2	2:B:1145:SER:HB2	2.09	0.53
2:B:281:PRO:HG2	2:B:284:ILE:CD1	2.38	0.53
6:H:97:MET:HE3	6:H:142:LEU:HD23	1.90	0.53
7:I:50:THR:HB	7:I:92:ARG:HH22	1.73	0.53
1:A:523:ILE:HG23	1:A:527:THR:HB	1.90	0.53
2:B:1023:VAL:HG12	2:B:1027:ILE:HD11	1.90	0.53
3:C:25:VAL:HG23	3:C:228:PHE:HE1	1.73	0.53
5:F:107:VAL:HG11	5:F:111:LEU:HD11	1.90	0.53
8:J:48:ARG:HH11	8:J:48:ARG:CG	2.10	0.53
9:K:47:ARG:C	9:K:47:ARG:HD2	2.32	0.53
1:A:320:ARG:N	1:A:321:PRO:HD3	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:THR:HG22	1:A:711:ARG:H	1.74	0.53
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.71	0.53
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.91	0.53
4:E:114:ASN:OD1	4:E:115:ASN:N	2.42	0.53
1:A:434:ARG:HH21	1:A:437:MET:HG3	1.74	0.53
1:A:1111:MET:CE	1:A:1114:PRO:HA	2.38	0.53
2:B:515:HIS:H	2:B:518:HIS:HD2	1.56	0.53
2:B:845:SER:HB3	2:B:850:LEU:HD22	1.91	0.53
2:B:868:MET:O	2:B:870:ILE:HG13	2.08	0.53
2:B:954:VAL:O	10:L:55:ILE:O	2.26	0.53
8:J:48:ARG:HH21	8:J:49:MET:HE1	1.73	0.53
10:L:42:ARG:C	10:L:44:ASP:H	2.17	0.53
1:A:1199:ARG:HA	1:A:1202:MET:HB2	1.91	0.53
3:C:258:ILE:HD11	9:K:42:LEU:CD2	2.38	0.53
4:E:161:LYS:HE2	4:E:165:LEU:HD11	1.91	0.53
8:J:25:LEU:O	8:J:29:GLU:HA	2.09	0.53
1:A:858:ASN:HD21	1:A:862:ASN:H	1.56	0.53
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.44	0.53
4:E:127:ILE:HD11	4:E:132:ILE:HD11	1.91	0.53
1:A:366:VAL:HG11	1:A:436:ILE:HD11	1.90	0.53
1:A:499:ALA:O	1:A:503:GLN:HB2	2.08	0.53
2:B:344:LYS:H	2:B:347:LYS:HE3	1.74	0.53
2:B:429:PHE:HA	2:B:432:MET:CE	2.39	0.53
3:C:58:LEU:HD11	8:J:2:ILE:HD12	1.91	0.53
6:H:125:LEU:C	6:H:130:ARG:HH12	2.17	0.53
1:A:55:ASP:N	1:A:56:PRO:CD	2.69	0.52
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.91	0.52
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.44	0.52
2:B:953:LEU:C	2:B:953:LEU:HD23	2.34	0.52
5:F:128:LYS:HD2	5:F:149:GLU:HA	1.91	0.52
1:A:122:MET:HE1	1:A:138:ILE:HG23	1.90	0.52
1:A:1264:GLU:OE1	7:I:44:TYR:HE2	1.93	0.52
1:A:1279:ILE:N	1:A:1279:ILE:HD12	2.24	0.52
2:B:636:PRO:HA	2:B:691:GLU:O	2.08	0.52
3:C:21:ILE:HG12	3:C:229:TYR:HD2	1.74	0.52
4:E:181:ALA:HA	4:E:186:LEU:HD21	1.91	0.52
5:F:107:VAL:HG12	5:F:109:VAL:H	1.74	0.52
7:I:50:THR:CB	7:I:92:ARG:HH22	2.22	0.52
1:A:528:LEU:HD23	1:A:751:SER:HB3	1.91	0.52
1:A:473:SER:OG	1:A:522:GLY:O	2.23	0.52
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:SER:O	1:A:518:LYS:HG2	2.10	0.52
1:A:533:LYS:NZ	1:A:660:ASN:ND2	2.56	0.52
1:A:901:LEU:HD23	1:A:907:THR:HG23	1.92	0.52
2:B:249:ARG:O	2:B:251:ILE:HG13	2.10	0.52
2:B:296:GLU:O	2:B:300:HIS:HD2	1.93	0.52
2:B:898:LEU:HD21	2:B:964:VAL:HG11	1.92	0.52
4:E:124:VAL:HB	4:E:125:PRO:HD3	1.90	0.52
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.38	0.52
9:K:1:MET:HG3	9:K:2:ASN:N	2.25	0.52
2:B:759:PRO:HG2	2:B:1046:PRO:HB3	1.91	0.52
3:C:242:GLN:OE1	3:C:242:GLN:HA	2.10	0.52
6:H:40:LEU:HD11	6:H:97:MET:HE1	1.90	0.52
1:A:341:MET:HE3	1:A:343:LYS:HE3	1.91	0.52
1:A:817:ALA:HA	2:B:764:SER:OG	2.09	0.52
2:B:1002:THR:HG22	2:B:1006:ILE:N	2.24	0.52
4:E:124:VAL:HB	4:E:125:PRO:CD	2.40	0.52
1:A:492:PRO:CB	1:A:497:THR:HG22	2.40	0.52
1:A:868:TYR:HE1	1:A:1064:VAL:CG1	2.23	0.52
2:B:313:MET:HE3	2:B:386:LEU:CD2	2.37	0.52
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.43	0.52
1:A:1162:VAL:CG1	7:I:41:PRO:HG3	2.34	0.52
2:B:552:MET:N	2:B:553:PRO:HD2	2.25	0.52
2:B:864:LYS:HB2	2:B:864:LYS:NZ	2.25	0.52
3:C:6:PRO:HB2	9:K:101:LEU:HD23	1.92	0.52
1:A:795:GLU:HG2	2:B:731:VAL:CG2	2.40	0.52
1:A:842:VAL:HG11	2:B:1136:ASP:CG	2.35	0.52
1:A:873:MET:HE3	1:A:957:PRO:CG	2.36	0.52
2:B:528:PRO:HG3	2:B:536:VAL:HB	1.92	0.52
2:B:846:ILE:HG12	2:B:974:PRO:HB2	1.92	0.52
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.92	0.52
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.92	0.52
1:A:575:LYS:HD3	1:A:612:ILE:CD1	2.40	0.51
2:B:292:ILE:N	2:B:293:PRO:HD2	2.26	0.51
5:F:109:VAL:HG21	5:F:124:GLU:HA	1.92	0.51
1:A:24:PRO:HG2	1:A:25:GLU:OE2	2.10	0.51
1:A:516:SER:O	1:A:517:ASN:C	2.52	0.51
2:B:314:LEU:O	2:B:317:CYS:HB2	2.11	0.51
2:B:377:PHE:HD2	2:B:381:MET:HE2	1.75	0.51
2:B:885:MET:HA	2:B:936:ASP:CB	2.40	0.51
3:C:145:CYS:SG	3:C:146:LYS:N	2.83	0.51
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:LEU:HB3	2:B:167:ILE:O	2.11	0.51
2:B:852:ARG:NH2	10:L:70:ARG:O	2.38	0.51
3:C:53:THR:O	3:C:153:LEU:HA	2.10	0.51
1:A:384:ASN:OD1	1:A:388:LEU:HD12	2.10	0.51
1:A:465:TYR:CE2	9:K:4:PRO:HD2	2.45	0.51
1:A:673:GLY:N	1:A:674:PRO:CD	2.73	0.51
1:A:1376:THR:HG22	1:A:1376:THR:O	2.09	0.51
1:A:1187:GLN:HG3	1:A:1188:GLN:H	1.75	0.51
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.93	0.51
1:A:418:SER:C	1:A:420:ARG:H	2.17	0.51
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.25	0.51
2:B:574:SER:HB3	2:B:591:ARG:NH2	2.26	0.51
2:B:859:TYR:O	2:B:965:LYS:HA	2.11	0.51
2:B:1037:LEU:HD21	8:J:44:TYR:HD2	1.75	0.51
4:E:93:MET:O	4:E:97:VAL:HG23	2.10	0.51
1:A:32:VAL:HG23	1:A:33:ALA:N	2.24	0.51
1:A:523:ILE:CG2	1:A:527:THR:HB	2.41	0.51
1:A:705:LYS:H	1:A:705:LYS:HD2	1.75	0.51
1:A:840:ARG:NH1	1:A:1386:ARG:HB3	2.23	0.51
2:B:577:ALA:HB1	2:B:589:VAL:CG2	2.39	0.51
2:B:653:VAL:HG13	2:B:689:LEU:HB3	1.92	0.51
2:B:1198:TYR:CE1	2:B:1201:LYS:HD2	2.46	0.51
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.39	0.51
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.26	0.51
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.44	0.51
1:A:2:VAL:HG21	2:B:1157:ALA:O	2.11	0.51
1:A:216:VAL:HA	1:A:219:PHE:CZ	2.46	0.51
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.11	0.51
1:A:903:ASN:HD22	1:A:905:ASP:H	1.58	0.51
1:A:1348:LEU:HD21	1:A:1375:MET:CE	2.40	0.51
2:B:847:ASP:O	3:C:65:HIS:HE1	1.94	0.51
3:C:58:LEU:HD11	8:J:2:ILE:HD11	1.92	0.51
5:F:81:THR:HB	5:F:144:GLU:OE1	2.11	0.51
7:I:98:VAL:CG2	7:I:113:ASP:HB2	2.39	0.51
8:J:57:ILE:O	8:J:61:LEU:HG	2.10	0.51
1:A:95:PHE:CE2	1:A:1414:ALA:HB2	2.46	0.51
1:A:313:GLN:HB2	1:A:320:ARG:HB3	1.93	0.51
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.93	0.51
2:B:913:GLY:HA2	2:B:938:SER:CB	2.41	0.50
3:C:14:SER:HA	9:K:114:LEU:O	2.10	0.50
6:H:104:PHE:O	6:H:106:GLU:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:49:GLU:HG3	9:K:94:ILE:CG1	2.41	0.50
1:A:497:THR:HG23	2:B:1146:PHE:HD1	1.76	0.50
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.93	0.50
1:A:208:LEU:CD2	1:A:212:LYS:HE3	2.41	0.50
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.59	0.50
2:B:914:LYS:HD2	2:B:937:ALA:HB3	1.92	0.50
10:L:30:ILE:HG13	10:L:59:ALA:HB2	1.93	0.50
1:A:38:PRO:HB3	1:A:270:LEU:HB3	1.92	0.50
1:A:1004:ASN:ND2	4:E:167:ARG:HD2	2.26	0.50
2:B:558:LEU:O	2:B:563:MET:HB2	2.12	0.50
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.92	0.50
1:A:1391:ARG:NH2	1:A:1417:GLU:OE2	2.44	0.50
4:E:65:THR:O	4:E:69:ILE:HG13	2.12	0.50
8:J:64:ASN:N	8:J:65:PRO:HD2	2.26	0.50
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	2.12	0.50
1:A:1376:THR:O	1:A:1376:THR:CG2	2.59	0.50
3:C:73:GLN:NE2	3:C:75:MET:CB	2.74	0.50
1:A:714:PHE:CB	7:I:97:MET:HE1	2.42	0.50
2:B:38:PHE:HZ	2:B:541:LEU:HB3	1.77	0.50
2:B:168:GLY:H	2:B:450:ALA:HB1	1.77	0.50
1:A:1195:LEU:HD11	1:A:1267:MET:HE3	1.94	0.50
1:A:53:LEU:CD2	1:A:54:ASN:H	2.23	0.50
1:A:147:VAL:HG22	1:A:170:THR:HG22	1.93	0.50
2:B:63:ILE:CB	2:B:95:ILE:HD11	2.34	0.50
2:B:169:ARG:O	2:B:457:LEU:HD12	2.11	0.50
2:B:378:LEU:HA	2:B:381:MET:HE3	1.93	0.50
1:A:1399:ARG:HH11	1:A:1401:SER:HA	1.75	0.49
2:B:314:LEU:HD21	2:B:386:LEU:HD11	1.92	0.49
2:B:1177:HIS:CB	2:B:1179:GLN:HE21	2.23	0.49
8:J:1:MET:N	8:J:1:MET:HE3	2.27	0.49
10:L:38:LEU:HD13	10:L:48:CYS:HA	1.94	0.49
1:A:338:GLY:HA2	1:A:343:LYS:HD2	1.94	0.49
1:A:1120:LEU:HG	1:A:1134:ILE:HD12	1.94	0.49
4:E:100:ILE:HD13	4:E:108:GLY:HA3	1.94	0.49
4:E:112:TYR:O	4:E:137:GLU:HG3	2.12	0.49
1:A:1336:MET:HE3	1:A:1381:LEU:CG	2.42	0.49
2:B:901:PRO:CD	10:L:58:LYS:HB3	2.40	0.49
3:C:50:GLU:HB2	3:C:156:THR:HB	1.93	0.49
1:A:219:PHE:O	1:A:224:PHE:HB2	2.13	0.49
1:A:786:HIS:CE1	2:B:742:GLU:OE2	2.62	0.49
2:B:492:LEU:O	2:B:496:ARG:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PHE:HZ	1:A:1397:LEU:HG	1.78	0.49
2:B:870:ILE:HG23	2:B:917:PRO:O	2.13	0.49
3:C:46:ILE:HB	3:C:68:GLY:HA2	1.93	0.49
3:C:71:PRO:C	3:C:72:LEU:HD23	2.38	0.49
6:H:11:GLN:HE21	6:H:52:GLN:HA	1.77	0.49
10:L:68:GLU:C	10:L:70:ARG:H	2.21	0.49
1:A:463:ILE:HD11	1:A:469:ARG:HG3	1.94	0.49
1:A:873:MET:HE1	1:A:1053:PHE:CZ	2.47	0.49
1:A:1285:MET:HG3	1:A:1307:GLU:OE1	2.13	0.49
1:A:17:VAL:HB	1:A:1419:ASP:HB2	1.94	0.49
1:A:71:GLN:HG2	2:B:1176:ASN:ND2	2.27	0.49
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.45	0.49
1:A:724:GLU:O	1:A:728:LYS:HG2	2.13	0.49
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.95	0.49
1:A:58:LEU:HD22	1:A:80:HIS:O	2.12	0.49
1:A:75:ASN:HB2	1:A:76:GLU:OE2	2.13	0.49
1:A:1139:GLU:HG3	1:A:1280:GLU:O	2.13	0.49
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.12	0.49
2:B:332:ASP:O	2:B:336:ARG:HG3	2.13	0.49
2:B:806:THR:CG2	2:B:808:ALA:H	2.26	0.49
3:C:73:GLN:NE2	3:C:75:MET:N	2.60	0.49
1:A:376:TYR:CZ	1:A:498:ARG:HD2	2.48	0.49
1:A:1438:THR:HG23	2:B:1144:ALA:HB3	1.95	0.49
2:B:219:ALA:HB3	2:B:222:ILE:HD12	1.94	0.49
2:B:650:GLU:HG3	2:B:651:LEU:N	2.28	0.49
3:C:137:LYS:H	3:C:137:LYS:CD	2.10	0.49
1:A:148:CYS:O	1:A:168:GLY:HA2	2.13	0.49
2:B:54:PHE:HA	2:B:58:THR:HB	1.95	0.49
2:B:234:ILE:HD13	2:B:257:LYS:HD3	1.95	0.49
2:B:913:GLY:HA2	2:B:938:SER:HB3	1.94	0.49
2:B:918:ILE:CD1	2:B:935:ARG:HD2	2.41	0.49
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.48	0.49
3:C:12:GLU:HB2	3:C:19:ASP:HB3	1.94	0.49
1:A:984:LYS:HB3	1:A:988:LEU:HD12	1.94	0.48
1:A:1215:ARG:HA	1:A:1218:GLN:HG2	1.95	0.48
1:A:1410:PHE:CD2	2:B:1212:ILE:HD11	2.39	0.48
2:B:1022:THR:HG23	2:B:1022:THR:O	2.13	0.48
2:B:1051:THR:HG22	2:B:1052:VAL:N	2.28	0.48
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.48	0.48
1:A:1146:VAL:HG12	1:A:1197:LEU:HD22	1.95	0.48
2:B:101:MET:HE3	2:B:109:THR:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.95	0.48
2:B:843:GLN:HB2	2:B:993:THR:HB	1.94	0.48
1:A:1116:LEU:HD13	1:A:1311:VAL:HG13	1.94	0.48
1:A:1341:ILE:HD11	1:A:1376:THR:HG23	1.94	0.48
2:B:25:ILE:HG23	2:B:29:ASP:CB	2.43	0.48
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.95	0.48
2:B:545:ILE:HG12	2:B:633:VAL:HG22	1.94	0.48
3:C:163:ILE:HG23	3:C:165:LYS:H	1.78	0.48
6:H:95:TYR:CE2	6:H:97:MET:HG3	2.49	0.48
9:K:12:LEU:HD12	9:K:12:LEU:N	2.28	0.48
9:K:20:LYS:O	9:K:33:ILE:HA	2.13	0.48
1:A:597:LEU:HD12	1:A:597:LEU:H	1.78	0.48
1:A:1193:LEU:HD21	1:A:1267:MET:HE2	1.95	0.48
2:B:1065:GLN:HE21	2:B:1067:ARG:N	2.11	0.48
3:C:40:GLU:OE2	3:C:254:LYS:NZ	2.44	0.48
1:A:38:PRO:HB3	1:A:270:LEU:HD23	1.95	0.48
1:A:338:GLY:CA	1:A:343:LYS:HD2	2.44	0.48
1:A:534:LEU:O	1:A:574:GLY:HA3	2.14	0.48
1:A:845:LEU:HD22	1:A:1374:VAL:HG21	1.94	0.48
2:B:122:LEU:CD2	2:B:958:GLN:HG2	2.43	0.48
2:B:591:ARG:O	2:B:592:ASN:HB2	2.13	0.48
10:L:48:CYS:SG	10:L:49:LYS:N	2.87	0.48
1:A:765:VAL:HG23	1:A:802:ASN:O	2.14	0.48
1:A:1198:ASP:OD1	1:A:1200:ALA:HB3	2.13	0.48
2:B:298:LEU:HD22	2:B:314:LEU:HD13	1.93	0.48
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.13	0.48
2:B:979:LYS:CE	2:B:987:LYS:HD2	2.44	0.48
2:B:979:LYS:HE3	2:B:987:LYS:HD2	1.95	0.48
3:C:136:ASP:C	3:C:138:GLU:H	2.21	0.48
6:H:26:ILE:HD13	6:H:49:VAL:HG11	1.95	0.48
9:K:61:TYR:HA	9:K:72:LYS:O	2.12	0.48
1:A:472:LEU:HD21	2:B:835:GLN:HB2	1.96	0.48
1:A:517:ASN:HB2	1:A:878:ILE:O	2.13	0.48
1:A:547:LEU:HD22	9:K:58:PHE:CD1	2.48	0.48
1:A:1102:LYS:HD3	1:A:1106:ASN:ND2	2.28	0.48
2:B:315:LYS:N	2:B:316:PRO:HD2	2.27	0.48
2:B:497:ARG:HH22	2:B:775:LYS:HE3	1.78	0.48
2:B:806:THR:HG23	2:B:808:ALA:H	1.79	0.48
1:A:605:MET:HE2	1:A:607:ILE:CG1	2.42	0.48
1:A:1434:ALA:O	1:A:1436:ILE:N	2.41	0.48
1:A:1447:GLU:OE1	1:A:1447:GLU:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:324:ILE:HD11	2:B:333:PHE:CB	2.43	0.48
3:C:134:ILE:HG21	3:C:139:GLY:HA2	1.96	0.48
6:H:62:SER:O	6:H:63:LEU:C	2.56	0.48
9:K:30:ALA:HA	9:K:75:ILE:O	2.14	0.48
1:A:249:SER:HB2	1:A:258:GLY:O	2.13	0.48
1:A:881:GLN:CD	1:A:959:ASN:HA	2.39	0.48
2:B:98:THR:HG22	2:B:99:LYS:N	2.28	0.48
8:J:1:MET:HG3	8:J:60:PHE:HE2	1.78	0.48
1:A:38:PRO:C	1:A:39:GLU:HG3	2.38	0.48
1:A:51:GLY:O	1:A:56:PRO:HB3	2.13	0.48
1:A:682:THR:HG21	1:A:728:LYS:HG3	1.96	0.48
1:A:857:ARG:HD3	1:A:861:GLY:O	2.14	0.48
2:B:564:GLU:HB2	2:B:589:VAL:HG12	1.96	0.48
3:C:209:TYR:CD1	3:C:209:TYR:N	2.82	0.48
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.96	0.48
1:A:740:LEU:HD12	1:A:740:LEU:N	2.29	0.47
2:B:294:ASP:H	7:I:12:ASN:HD22	1.57	0.47
2:B:776:GLN:HA	2:B:1096:ARG:NH1	2.29	0.47
3:C:108:GLU:OE1	3:C:149:LYS:HD3	2.14	0.47
3:C:121:VAL:HG12	3:C:121:VAL:O	2.14	0.47
7:I:50:THR:CB	7:I:92:ARG:HH12	2.27	0.47
2:B:285:ILE:O	2:B:289:LEU:HG	2.13	0.47
3:C:166:GLU:CG	10:L:70:ARG:HH12	2.27	0.47
4:E:99:HIS:O	4:E:103:LYS:HG2	2.15	0.47
1:A:602:ASP:O	1:A:615:GLY:HA2	2.14	0.47
1:A:1118:VAL:CG2	1:A:1306:LEU:HD12	2.44	0.47
1:A:1431:GLY:HA2	2:B:1152:MET:HE2	1.96	0.47
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.44	0.47
3:C:73:GLN:NE2	3:C:75:MET:H	2.05	0.47
1:A:73:GLY:C	1:A:75:ASN:H	2.22	0.47
1:A:144:THR:O	1:A:146:MET:HG3	2.14	0.47
1:A:329:LEU:C	1:A:331:GLY:H	2.21	0.47
1:A:483:ASP:OD1	13:B:3571:UTP:O1B	2.32	0.47
1:A:605:MET:HE1	1:A:612:ILE:CD1	2.43	0.47
1:A:1279:ILE:HD11	1:A:1312:ASN:CB	2.43	0.47
1:A:1281:ARG:HB2	1:A:1309:ASP:HB2	1.97	0.47
2:B:108:VAL:HG12	2:B:109:THR:N	2.29	0.47
2:B:202:TYR:CD2	2:B:202:TYR:N	2.83	0.47
2:B:528:PRO:CG	2:B:536:VAL:HB	2.44	0.47
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.79	0.47
3:C:244:VAL:O	3:C:248:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:58:LYS:O	10:L:59:ALA:HB3	2.14	0.47
1:A:346:ASP:O	1:A:347:PHE:HB2	2.15	0.47
1:A:663:SER:OG	2:B:827:ILE:O	2.29	0.47
1:A:914:GLU:C	1:A:916:GLY:N	2.72	0.47
9:K:49:GLU:HG3	9:K:94:ILE:HG12	1.95	0.47
1:A:984:LYS:O	1:A:988:LEU:HB2	2.14	0.47
2:B:914:LYS:HG2	2:B:915:THR:N	2.28	0.47
2:B:955:THR:CG2	10:L:55:ILE:HA	2.43	0.47
2:B:1165:ILE:HG13	2:B:1187:ASN:ND2	2.29	0.47
7:I:50:THR:CG2	7:I:52:ILE:HG22	2.45	0.47
7:I:95:THR:HG22	7:I:96:SER:O	2.14	0.47
1:A:44:THR:O	1:A:45:GLN:HB2	2.14	0.47
1:A:440:ASP:O	1:A:460:VAL:HG23	2.15	0.47
1:A:598:LEU:HD11	6:H:124:ARG:CB	2.44	0.47
1:A:1167:GLU:O	1:A:1171:GLN:HG3	2.14	0.47
1:A:1431:GLY:HA2	2:B:1152:MET:CE	2.45	0.47
1:A:1436:ILE:O	1:A:1437:GLY:C	2.58	0.47
2:B:794:ASN:C	2:B:795:ILE:HD12	2.39	0.47
3:C:167:HIS:CD2	3:C:169:LYS:H	2.13	0.47
5:F:81:THR:HG21	5:F:136:ARG:HD3	1.96	0.47
5:F:109:VAL:HG13	5:F:127:GLU:OE1	2.15	0.47
6:H:40:LEU:CD1	6:H:123:MET:HB2	2.42	0.47
6:H:100:THR:HG23	6:H:138:GLU:HG3	1.96	0.47
7:I:98:VAL:HG22	7:I:111:THR:HG22	1.97	0.47
8:J:2:ILE:HD11	8:J:57:ILE:CD1	2.45	0.47
2:B:1060:ARG:NH2	3:C:202:PRO:HG3	2.30	0.47
5:F:134:ILE:HD12	5:F:151:LEU:CD1	2.45	0.47
8:J:2:ILE:HD11	8:J:57:ILE:HD12	1.96	0.47
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.96	0.47
1:A:381:THR:HB	1:A:382:PRO:HD2	1.97	0.47
1:A:880:LYS:HA	1:A:955:PRO:HA	1.95	0.47
2:B:429:PHE:HA	2:B:432:MET:HE3	1.96	0.47
2:B:461:LEU:HD12	2:B:466:TRP:HH2	1.80	0.47
2:B:558:LEU:HD13	2:B:563:MET:HE2	1.96	0.47
8:J:32:GLU:CD	8:J:32:GLU:H	2.23	0.47
1:A:365:GLY:O	1:A:468:PHE:HA	2.14	0.47
1:A:1146:VAL:HG11	1:A:1202:MET:SD	2.55	0.47
1:A:1351:GLU:O	1:A:1355:VAL:HG23	2.14	0.47
3:C:55:THR:HB	3:C:152:GLU:H	1.80	0.47
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.40	0.47
4:E:120:ALA:O	4:E:123:LEU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:HA	1:A:74:MET:HE2	1.96	0.46
1:A:268:ASP:HB3	1:A:299:HIS:CD2	2.51	0.46
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.51	0.46
1:A:1064:VAL:HG12	1:A:1370:LEU:HD22	1.97	0.46
1:A:1124:HIS:CB	1:A:1130:GLN:HG3	2.45	0.46
2:B:683:SER:O	2:B:687:GLU:HG3	2.14	0.46
3:C:35:ARG:NH1	9:K:41:THR:H	2.12	0.46
6:H:96:VAL:HG13	6:H:143:LEU:CD2	2.45	0.46
6:H:125:LEU:HB3	6:H:130:ARG:NH1	2.31	0.46
10:L:51:CYS:HB3	10:L:53:HIS:CD2	2.50	0.46
1:A:115:LEU:CD1	1:A:141:LEU:HB3	2.44	0.46
1:A:1277:GLU:O	1:A:1278:ASN:CB	2.61	0.46
2:B:287:ARG:NH1	2:B:324:ILE:O	2.48	0.46
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.97	0.46
2:B:889:THR:HG22	2:B:891:ASP:H	1.80	0.46
7:I:95:THR:HG22	7:I:96:SER:N	2.31	0.46
1:A:565:ILE:HG23	1:A:567:LYS:CG	2.44	0.46
1:A:907:THR:CG2	1:A:908:LEU:H	2.26	0.46
1:A:1129:GLU:O	1:A:1133:LEU:HG	2.15	0.46
2:B:60:GLN:O	2:B:63:ILE:HG22	2.16	0.46
2:B:97:VAL:HG12	2:B:178:ASN:HD21	1.80	0.46
2:B:98:THR:O	2:B:126:SER:HB3	2.15	0.46
2:B:420:LEU:HD13	2:B:453:ILE:HA	1.97	0.46
2:B:778:MET:SD	2:B:1094:ARG:HD3	2.56	0.46
3:C:44:LEU:HG	3:C:159:ALA:HB1	1.97	0.46
3:C:93:ASP:HB3	3:C:125:MET:HE2	1.98	0.46
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.51	0.46
1:A:1293:SER:HB3	1:A:1297:GLU:O	2.15	0.46
2:B:642:ASP:HB3	2:B:649:LYS:HG2	1.98	0.46
2:B:651:LEU:HD23	2:B:710:LEU:HD11	1.96	0.46
1:A:345:VAL:CG1	2:B:1129:ARG:HA	2.46	0.46
1:A:401:GLY:H	1:A:435:HIS:HD1	1.64	0.46
1:A:704:ALA:HB2	1:A:710:LEU:HD12	1.98	0.46
8:J:30:LEU:HD11	8:J:38:ARG:NH2	2.31	0.46
1:A:106:VAL:CG2	1:A:111:GLY:C	2.89	0.46
1:A:1079:MET:HE3	1:A:1098:VAL:HG22	1.96	0.46
2:B:103:ASN:HB2	2:B:169:ARG:NH1	2.31	0.46
2:B:859:TYR:CD1	2:B:859:TYR:N	2.83	0.46
2:B:884:ARG:O	2:B:936:ASP:HB2	2.16	0.46
6:H:12:VAL:HG13	6:H:26:ILE:HG23	1.98	0.46
6:H:130:ARG:HD3	6:H:134:ASN:HD21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:MET:CE	1:A:1436:ILE:HA	2.35	0.46
1:A:912:LEU:HD22	1:A:1033:GLN:HA	1.97	0.46
1:A:1039:LYS:O	1:A:1043:ASP:OD1	2.34	0.46
3:C:11:ARG:HD2	3:C:21:ILE:CD1	2.46	0.46
1:A:226:GLU:HG3	1:A:227:VAL:HG23	1.98	0.46
1:A:1339:LEU:HD13	4:E:147:HIS:CD2	2.51	0.46
1:A:1348:LEU:HD21	1:A:1375:MET:HE2	1.98	0.46
1:A:1396:ALA:HB2	1:A:1417:GLU:OE1	2.16	0.46
2:B:25:ILE:HG13	2:B:654:ARG:HA	1.97	0.46
2:B:174:LEU:O	2:B:200:GLY:O	2.33	0.46
2:B:616:ILE:HG13	2:B:697:GLU:HA	1.98	0.46
3:C:102:GLN:OE1	3:C:154:LYS:HE2	2.16	0.46
3:C:242:GLN:HE21	3:C:246:ARG:NH2	2.03	0.46
2:B:886:LYS:C	2:B:888:GLY:H	2.24	0.46
2:B:1183:LYS:C	2:B:1185:CYS:H	2.24	0.46
3:C:89:GLU:O	3:C:90:ASP:HB3	2.16	0.46
3:C:249:ASP:O	3:C:252:GLN:HB3	2.16	0.46
6:H:12:VAL:HA	6:H:28:ALA:CB	2.46	0.46
1:A:666:ILE:HG12	2:B:1026:LEU:HB3	1.98	0.46
1:A:1152:ILE:HB	7:I:44:TYR:HB3	1.97	0.46
1:A:1212:VAL:O	1:A:1216:ILE:HG13	2.16	0.46
2:B:493:SER:OG	2:B:497:ARG:NH2	2.49	0.46
4:E:16:PHE:CZ	4:E:20:LYS:HE2	2.50	0.46
10:L:26:THR:C	10:L:27:LEU:HD23	2.41	0.46
1:A:35:ILE:HD13	1:A:83:HIS:H	1.81	0.45
1:A:752:LYS:HG2	2:B:1015:HIS:O	2.17	0.45
1:A:795:GLU:HG2	2:B:731:VAL:HG22	1.98	0.45
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.30	0.45
2:B:705:MET:HB3	2:B:706:GLN:NE2	2.31	0.45
2:B:227:LYS:NZ	2:B:236:HIS:HE1	2.15	0.45
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.97	0.45
2:B:1191:ILE:HG22	2:B:1192:TYR:N	2.30	0.45
3:C:42:PRO:HG3	3:C:163:ILE:HD11	1.97	0.45
3:C:55:THR:HG22	3:C:55:THR:O	2.16	0.45
4:E:180:ARG:HB2	4:E:215:MET:OXT	2.16	0.45
10:L:49:LYS:O	10:L:50:ASP:HB2	2.16	0.45
1:A:62:ASP:HB2	1:A:64:ASN:ND2	2.31	0.45
1:A:239:LEU:HD23	1:A:240:PRO:N	2.31	0.45
1:A:1259:MET:O	1:A:1263:ILE:HG13	2.15	0.45
2:B:118:ARG:HG3	2:B:204:ILE:HD13	1.97	0.45
2:B:864:LYS:HB2	2:B:864:LYS:HZ3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:906:SER:O	2:B:907:GLY:C	2.58	0.45
2:B:1051:THR:HG22	2:B:1053:GLU:N	2.23	0.45
3:C:6:PRO:CB	9:K:101:LEU:HD23	2.46	0.45
6:H:105:GLU:O	6:H:107:VAL:HG23	2.15	0.45
1:A:489:LEU:HD23	1:A:490:HIS:N	2.31	0.45
1:A:565:ILE:HG23	1:A:567:LYS:HE3	1.98	0.45
1:A:853:ASP:O	1:A:854:ASN:HB2	2.17	0.45
6:H:31:THR:HG22	6:H:32:THR:N	2.31	0.45
1:A:1295:THR:HB	1:A:1297:GLU:OE1	2.17	0.45
1:A:1386:ARG:O	1:A:1386:ARG:HG3	2.16	0.45
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.51	0.45
2:B:904:ARG:HH21	2:B:948:ILE:HD11	1.81	0.45
2:B:999:MET:HE3	2:B:999:MET:HA	1.98	0.45
3:C:6:PRO:HA	3:C:25:VAL:HG13	1.98	0.45
3:C:57:VAL:HG12	3:C:57:VAL:O	2.17	0.45
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.98	0.45
6:H:56:THR:O	6:H:144:ILE:HA	2.17	0.45
9:K:33:ILE:HD13	9:K:87:LEU:HD22	1.97	0.45
10:L:41:SER:HB2	10:L:42:ARG:HH21	1.82	0.45
1:A:71:GLN:HG2	2:B:1176:ASN:HD22	1.82	0.45
1:A:84:ILE:HG23	1:A:84:ILE:O	2.17	0.45
1:A:464:PRO:HB2	9:K:4:PRO:HD3	1.98	0.45
1:A:765:VAL:HB	1:A:800:VAL:CG1	2.47	0.45
1:A:822:GLU:HG3	2:B:513:GLN:HE22	1.81	0.45
2:B:276:ILE:CD1	2:B:355:ILE:HD13	2.47	0.45
2:B:830:TYR:CE1	2:B:1000:PRO:HB3	2.51	0.45
10:L:38:LEU:O	10:L:39:SER:HB2	2.17	0.45
1:A:697:ALA:HB1	7:I:97:MET:HE3	1.98	0.45
1:A:1364:ASN:ND2	1:A:1366:ARG:CG	2.79	0.45
1:A:1365:TYR:CD2	1:A:1365:TYR:C	2.94	0.45
2:B:1084:GLN:NE2	3:C:192:TRP:N	2.65	0.45
3:C:25:VAL:HG23	3:C:228:PHE:CE1	2.49	0.45
9:K:12:LEU:HD12	9:K:12:LEU:H	1.82	0.45
1:A:368:LYS:NZ	1:A:368:LYS:HB2	2.32	0.45
1:A:511:ILE:HA	1:A:521:MET:HE3	1.98	0.45
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.98	0.45
2:B:276:ILE:HD11	2:B:355:ILE:HD13	1.98	0.45
2:B:638:PHE:HB2	2:B:741:CYS:O	2.17	0.45
3:C:48:SER:HB3	3:C:158:VAL:HB	1.99	0.45
1:A:329:LEU:HA	1:A:332:LYS:HB2	1.99	0.45
1:A:805:LEU:CD1	2:B:1052:VAL:HG21	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:GLU:OE1	2:B:807:ARG:NH2	2.50	0.45
2:B:1023:VAL:O	2:B:1027:ILE:HG13	2.17	0.45
2:B:1079:LYS:HB2	3:C:27:LEU:HD21	1.97	0.45
4:E:88:VAL:HG13	4:E:92:THR:HB	1.99	0.45
6:H:31:THR:HG22	6:H:32:THR:H	1.81	0.45
8:J:14:VAL:HG23	8:J:41:LEU:HD21	1.99	0.45
8:J:36:LEU:HD21	8:J:50:ILE:HB	1.99	0.45
1:A:388:LEU:HD22	1:A:432:VAL:CB	2.46	0.45
1:A:744:LYS:HG2	1:A:748:MET:HE2	1.99	0.45
2:B:98:THR:HG22	2:B:99:LYS:H	1.82	0.45
2:B:345:LYS:HA	2:B:348:ARG:NH1	2.32	0.45
2:B:402:GLY:HA2	2:B:695:ALA:HB3	1.99	0.45
9:K:21:ILE:HG12	9:K:33:ILE:HG12	1.97	0.45
1:A:55:ASP:O	1:A:56:PRO:C	2.59	0.44
1:A:92:HIS:C	1:A:92:HIS:CD2	2.95	0.44
1:A:682:THR:HG23	1:A:728:LYS:NZ	2.32	0.44
1:A:709:THR:HG21	7:I:93:LYS:O	2.17	0.44
2:B:757:PRO:HD3	2:B:983:ARG:CZ	2.47	0.44
3:C:100:THR:HG22	3:C:101:LEU:N	2.32	0.44
3:C:261:ALA:O	3:C:265:MET:HB2	2.17	0.44
5:F:85:MET:O	5:F:155:LEU:HD21	2.17	0.44
1:A:849:MET:CE	1:A:1437:GLY:H	2.31	0.44
1:A:1025:ARG:O	1:A:1035:TYR:HE1	2.00	0.44
2:B:872:GLU:HG2	2:B:916:THR:OG1	2.17	0.44
3:C:35:ARG:HH12	9:K:41:THR:H	1.64	0.44
3:C:239:PRO:O	3:C:242:GLN:HB2	2.16	0.44
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.98	0.44
1:A:35:ILE:HA	1:A:52:GLY:O	2.17	0.44
1:A:208:LEU:HD23	1:A:208:LEU:O	2.17	0.44
1:A:589:GLN:HB2	1:A:961:ARG:NH2	2.32	0.44
1:A:704:ALA:HB2	1:A:710:LEU:HA	1.99	0.44
1:A:1150:SER:HB3	1:A:1195:LEU:HD22	2.00	0.44
1:A:1190:PRO:HG3	7:I:18:GLU:OE2	2.18	0.44
1:A:1236:LEU:C	1:A:1237:ILE:HD12	2.42	0.44
1:A:54:ASN:HD21	1:A:259:GLU:HG2	1.83	0.44
1:A:472:LEU:HD13	2:B:835:GLN:HE21	1.82	0.44
1:A:854:ASN:O	1:A:867:ILE:HA	2.17	0.44
1:A:1144:LYS:HB2	1:A:1268:LEU:O	2.18	0.44
2:B:405:ARG:HA	2:B:631:GLY:O	2.17	0.44
4:E:159:ASP:HA	4:E:162:ARG:NH1	2.32	0.44
1:A:592:ASP:O	1:A:593:GLU:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:940:ARG:O	1:A:944:ARG:HG3	2.18	0.44
1:A:1220:PHE:HE1	1:A:1267:MET:HG2	1.83	0.44
2:B:654:ARG:N	2:B:657:HIS:HD2	2.16	0.44
2:B:744:HIS:HD2	2:B:746:SER:H	1.66	0.44
2:B:1159:ARG:CG	2:B:1193:GLN:HE21	2.31	0.44
6:H:42:ILE:HG23	6:H:95:TYR:CE1	2.53	0.44
8:J:45:CYS:O	8:J:48:ARG:HG3	2.18	0.44
1:A:247:ARG:HD3	1:A:263:THR:OG1	2.17	0.44
2:B:53:GLN:HB2	2:B:547:VAL:CG2	2.48	0.44
2:B:238:ALA:HB3	2:B:256:VAL:HB	2.00	0.44
2:B:849:GLY:HA2	2:B:852:ARG:HG3	1.99	0.44
2:B:1177:HIS:HB2	2:B:1179:GLN:HE21	1.81	0.44
3:C:66:ARG:NH2	8:J:3:VAL:O	2.51	0.44
1:A:16:GLU:HG3	2:B:1220:ARG:HA	1.99	0.44
1:A:57:ARG:O	1:A:68:GLN:HG3	2.16	0.44
1:A:117:GLU:CD	1:A:117:GLU:H	2.26	0.44
1:A:248:PRO:O	1:A:260:ASP:HB2	2.17	0.44
1:A:464:PRO:O	1:A:465:TYR:C	2.61	0.44
1:A:672:ASP:HB2	1:A:736:ASN:OD1	2.17	0.44
1:A:1295:THR:HG22	1:A:1295:THR:O	2.18	0.44
1:A:1315:GLU:O	1:A:1318:THR:HG22	2.17	0.44
1:A:1424:VAL:O	1:A:1428:VAL:HG23	2.17	0.44
2:B:46:GLN:HE21	2:B:496:ARG:HH11	1.66	0.44
2:B:1009:ASP:O	2:B:1010:LEU:HD12	2.18	0.44
5:F:138:LEU:HD12	5:F:142:SER:OG	2.18	0.44
10:L:61:THR:HB	10:L:63:ARG:HG2	1.99	0.44
1:A:185:TRP:O	1:A:186:LYS:HB2	2.18	0.44
1:A:302:THR:HG21	1:A:312:PRO:CG	2.48	0.44
2:B:299:GLU:HG2	2:B:571:PRO:HG2	1.98	0.44
2:B:791:THR:O	2:B:857:ARG:HA	2.18	0.44
6:H:81:PRO:HD2	6:H:82:PRO:HD2	1.99	0.44
1:A:445:ASN:ND2	1:A:446:ARG:N	2.65	0.44
1:A:541:ILE:HG12	1:A:549:MET:HE1	2.00	0.44
1:A:598:LEU:O	1:A:599:SER:C	2.60	0.44
1:A:668:ASP:CG	1:A:742:ASN:HD22	2.25	0.44
5:F:81:THR:HG21	5:F:136:ARG:CD	2.48	0.44
7:I:50:THR:HB	7:I:92:ARG:HH12	1.82	0.44
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.43	0.43
1:A:647:GLY:O	1:A:651:LYS:HG3	2.18	0.43
1:A:768:GLN:HG3	1:A:816:HIS:HA	2.00	0.43
1:A:1364:ASN:HD22	1:A:1366:ARG:N	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:491:THR:O	2:B:495:LEU:HD12	2.18	0.43
2:B:979:LYS:NZ	2:B:987:LYS:HD2	2.33	0.43
8:J:64:ASN:N	8:J:65:PRO:CD	2.81	0.43
1:A:50:ILE:C	1:A:52:GLY:H	2.26	0.43
1:A:523:ILE:HD13	1:A:622:VAL:HG13	2.00	0.43
1:A:1112:LYS:C	1:A:1114:PRO:HD3	2.44	0.43
1:A:1322:ILE:HG13	1:A:1323:ASP:N	2.31	0.43
2:B:235:SER:OG	2:B:236:HIS:HD2	2.01	0.43
2:B:900:ALA:HB2	10:L:58:LYS:HD2	2.00	0.43
3:C:62:PHE:CD2	3:C:66:ARG:HD2	2.53	0.43
6:H:11:GLN:C	6:H:28:ALA:HB1	2.43	0.43
8:J:64:ASN:H	8:J:65:PRO:HD2	1.81	0.43
9:K:110:ASN:C	9:K:112:GLN:H	2.26	0.43
1:A:481:ASP:C	1:A:481:ASP:OD1	2.62	0.43
1:A:533:LYS:HE3	1:A:745:GLN:HE22	1.83	0.43
1:A:642:CYS:O	1:A:645:LEU:HB3	2.19	0.43
1:A:800:VAL:HG22	1:A:812:GLU:HB3	2.00	0.43
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.99	0.43
1:A:1152:ILE:HA	1:A:1192:LEU:O	2.18	0.43
1:A:1328:TYR:CG	1:A:1329:THR:N	2.86	0.43
2:B:548:GLY:N	2:B:612:GLU:OE2	2.51	0.43
3:C:148:ARG:HD2	8:J:61:LEU:O	2.19	0.43
4:E:93:MET:HG3	4:E:97:VAL:HG23	2.00	0.43
7:I:45:ARG:HG2	7:I:45:ARG:NH1	2.28	0.43
1:A:276:LEU:HD13	1:A:292:ALA:HB3	2.01	0.43
1:A:466:SER:C	1:A:467:THR:HG23	2.43	0.43
1:A:596:THR:C	1:A:598:LEU:N	2.77	0.43
1:A:958:VAL:HG11	1:A:1049:ILE:HG23	2.00	0.43
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.33	0.43
1:A:1341:ILE:CG1	1:A:1376:THR:HG23	2.48	0.43
1:A:1438:THR:CG2	2:B:1144:ALA:H	2.29	0.43
2:B:785:TYR:CE2	2:B:795:ILE:HG12	2.53	0.43
2:B:798:TYR:CD2	8:J:4:PRO:HG3	2.54	0.43
2:B:973:ILE:O	2:B:975:GLN:HG3	2.18	0.43
3:C:38:ILE:CG1	3:C:176:ILE:HD12	2.48	0.43
5:F:116:ASP:O	5:F:120:ILE:HG13	2.18	0.43
1:A:79:GLY:HA3	1:A:245:PRO:CG	2.45	0.43
1:A:313:GLN:HG2	1:A:322:VAL:HB	2.00	0.43
1:A:774:ARG:HB2	1:A:797:LYS:HB3	2.00	0.43
1:A:1104:ILE:HD13	1:A:1351:GLU:HB3	2.01	0.43
1:A:1111:MET:HE1	1:A:1330:ASN:ND2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:GLN:HE21	2:B:496:ARG:NH1	2.16	0.43
2:B:446:LEU:O	2:B:448:ILE:HG13	2.18	0.43
2:B:979:LYS:HE2	2:B:1095:LEU:HD12	2.00	0.43
3:C:185:LYS:HG2	3:C:213:PRO:HB3	2.00	0.43
4:E:204:THR:CG2	4:E:205:SER:N	2.81	0.43
5:F:109:VAL:HG23	5:F:124:GLU:HG2	2.00	0.43
2:B:274:PRO:HG3	2:B:359:GLU:HB3	2.00	0.43
2:B:327:ARG:NH2	2:B:371:GLU:HG2	2.34	0.43
2:B:800:GLN:O	2:B:818:PRO:HB2	2.18	0.43
3:C:242:GLN:NE2	3:C:246:ARG:HE	2.16	0.43
1:A:479:ASN:O	1:A:479:ASN:CG	2.62	0.43
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.59	0.43
2:B:212:LEU:HD11	2:B:461:LEU:HD11	2.00	0.43
2:B:860:MET:HA	2:B:964:VAL:O	2.18	0.43
2:B:877:PRO:HB3	2:B:915:THR:CG2	2.48	0.43
3:C:169:LYS:NZ	10:L:70:ARG:HG2	2.34	0.43
4:E:28:TYR:CE1	4:E:75:MET:HE2	2.53	0.43
6:H:138:GLU:O	6:H:139:ASN:C	2.62	0.43
1:A:440:ASP:OD1	1:A:498:ARG:NH2	2.52	0.43
1:A:1287:TYR:CD1	1:A:1305:VAL:HG21	2.54	0.43
2:B:557:PHE:CZ	2:B:603:LEU:HD11	2.54	0.43
2:B:561:TRP:O	2:B:590:HIS:HE1	2.02	0.43
2:B:1222:ARG:H	2:B:1222:ARG:CD	2.21	0.43
3:C:260:LEU:HD12	3:C:260:LEU:O	2.18	0.43
4:E:22:MET:HA	4:E:187:TYR:CZ	2.54	0.43
1:A:262:LEU:O	1:A:266:LEU:HG	2.19	0.43
1:A:566:ILE:O	1:A:567:LYS:O	2.37	0.43
1:A:1118:VAL:O	1:A:1118:VAL:HG23	2.18	0.43
2:B:281:PRO:CG	2:B:284:ILE:HD12	2.46	0.43
2:B:681:TRP:CH2	2:B:690:VAL:HG11	2.54	0.43
2:B:796:LEU:O	2:B:799:PRO:HD3	2.18	0.43
2:B:1212:ILE:O	2:B:1214:PRO:HD3	2.19	0.43
3:C:58:LEU:HD22	3:C:62:PHE:CE2	2.53	0.43
6:H:18:GLY:O	6:H:20:TYR:N	2.52	0.43
7:I:19:ASP:OD1	7:I:22:ASN:HB2	2.19	0.43
1:A:187:LYS:O	1:A:188:ASP:HB2	2.18	0.43
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.47	0.43
2:B:839:MET:HE3	2:B:1010:LEU:HG	2.00	0.43
2:B:986:GLN:NE2	2:B:987:LYS:O	2.48	0.43
3:C:43:THR:O	3:C:161:LYS:HA	2.19	0.43
4:E:153:HIS:CG	4:E:184:VAL:HG11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:50:THR:HB	7:I:92:ARG:NH2	2.33	0.43
1:A:903:ASN:ND2	1:A:903:ASN:C	2.76	0.42
2:B:789:MET:HE3	2:B:965:LYS:HB3	2.01	0.42
3:C:63:ILE:O	3:C:67:LEU:HG	2.19	0.42
8:J:48:ARG:CZ	8:J:49:MET:HE1	2.49	0.42
1:A:550:LEU:HD13	1:A:556:TRP:CZ2	2.54	0.42
1:A:909:ASP:CG	1:A:910:PRO:HD2	2.44	0.42
2:B:38:PHE:HE1	2:B:747:MET:HE1	1.84	0.42
2:B:497:ARG:HG3	2:B:498:THR:H	1.84	0.42
3:C:13:ALA:O	9:K:114:LEU:HB3	2.18	0.42
1:A:914:GLU:O	1:A:916:GLY:N	2.52	0.42
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.83	0.42
2:B:268:THR:CG2	2:B:270:LYS:HE3	2.46	0.42
2:B:281:PRO:HB3	2:B:320:ASP:OD2	2.19	0.42
2:B:1166:CYS:C	2:B:1168:LEU:H	2.27	0.42
3:C:44:LEU:HD12	3:C:160:LYS:C	2.44	0.42
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.34	0.42
4:E:77:SER:HG	4:E:105:PHE:HD2	1.64	0.42
1:A:623:GLY:C	1:A:625:SER:H	2.27	0.42
1:A:1173:HIS:NE2	1:A:1227:ILE:HG23	2.35	0.42
2:B:225:VAL:HA	2:B:237:VAL:O	2.20	0.42
2:B:424:LEU:O	2:B:428:ILE:HG13	2.19	0.42
2:B:604:ARG:CZ	2:B:615:MET:HE2	2.49	0.42
2:B:750:GLY:O	2:B:754:SER:HB2	2.19	0.42
9:K:78:THR:HG22	9:K:79:GLU:N	2.35	0.42
1:A:557:ASP:HA	9:K:26:LYS:HD2	2.02	0.42
1:A:741:ASN:ND2	1:A:743:VAL:HB	2.34	0.42
1:A:974:ASP:HA	6:H:136:LYS:HE2	2.01	0.42
2:B:784:ASN:HB3	8:J:63:TYR:OH	2.19	0.42
2:B:875:GLU:HG2	2:B:895:ASP:O	2.20	0.42
2:B:953:LEU:CD2	2:B:955:THR:HG23	2.43	0.42
2:B:983:ARG:HH11	2:B:1091:TYR:CB	2.32	0.42
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.84	0.42
9:K:58:PHE:HE2	9:K:74:ARG:HB3	1.84	0.42
1:A:450:LEU:HD12	1:A:450:LEU:N	2.25	0.42
1:A:636:GLU:OE2	1:A:962:ARG:HD3	2.19	0.42
1:A:699:ALA:O	1:A:700:ASN:HB3	2.20	0.42
1:A:853:ASP:OD1	1:A:855:THR:CB	2.66	0.42
1:A:858:ASN:C	1:A:858:ASN:ND2	2.73	0.42
1:A:1008:GLN:O	1:A:1012:ARG:HG3	2.18	0.42
2:B:46:GLN:NE2	2:B:496:ARG:HB3	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:LEU:HD11	2:B:366:GLN:HE22	1.85	0.42
2:B:1023:VAL:HG12	2:B:1027:ILE:CD1	2.49	0.42
4:E:16:PHE:CE2	4:E:20:LYS:HE2	2.54	0.42
1:A:342:GLY:O	1:A:345:VAL:HG13	2.20	0.42
1:A:418:SER:C	1:A:420:ARG:N	2.78	0.42
1:A:808:LEU:HD12	1:A:808:LEU:N	2.34	0.42
2:B:315:LYS:HE3	2:B:315:LYS:HB2	1.80	0.42
2:B:586:TRP:NE1	2:B:588:GLY:O	2.52	0.42
2:B:957:ASN:ND2	2:B:958:GLN:N	2.65	0.42
3:C:57:VAL:O	3:C:57:VAL:CG1	2.67	0.42
4:E:102:GLU:C	4:E:104:ASN:H	2.28	0.42
7:I:17:ARG:CG	7:I:28:GLU:HG2	2.48	0.42
9:K:90:ALA:O	9:K:94:ILE:HG13	2.19	0.42
1:A:78:PRO:O	1:A:79:GLY:C	2.61	0.42
1:A:447:GLN:HA	1:A:448:PRO:C	2.45	0.42
1:A:551:TYR:CE1	9:K:74:ARG:HD3	2.55	0.42
2:B:653:VAL:HG12	2:B:689:LEU:HD13	2.02	0.42
2:B:654:ARG:H	2:B:657:HIS:HD2	1.67	0.42
2:B:950:ASP:O	2:B:951:GLN:HB2	2.20	0.42
5:F:75:PRO:C	5:F:77:ASP:N	2.77	0.42
9:K:21:ILE:HG23	9:K:31:VAL:CG1	2.50	0.42
1:A:92:HIS:CD2	1:A:94:GLY:H	2.38	0.42
1:A:219:PHE:CD1	1:A:219:PHE:C	2.98	0.42
1:A:329:LEU:HD23	1:A:332:LYS:HB2	2.00	0.42
1:A:1385:THR:O	1:A:1386:ARG:C	2.62	0.42
2:B:102:VAL:HG11	2:B:122:LEU:HD13	2.01	0.42
2:B:174:LEU:HD12	2:B:174:LEU:N	2.35	0.42
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	2.01	0.42
4:E:78:LEU:HD11	4:E:109:ILE:HG13	2.02	0.42
1:A:2:VAL:O	1:A:2:VAL:HG13	2.20	0.42
1:A:337:ARG:HH12	1:A:1403:GLU:HA	1.85	0.42
1:A:596:THR:C	1:A:598:LEU:H	2.27	0.42
2:B:383:ASN:O	2:B:387:LEU:HB2	2.20	0.42
3:C:58:LEU:HD12	3:C:145:CYS:SG	2.60	0.42
7:I:35:VAL:HG22	7:I:36:GLU:N	2.35	0.42
1:A:122:MET:HE3	1:A:126:LEU:HD21	2.01	0.41
1:A:834:THR:HG21	1:A:1077:THR:CA	2.47	0.41
2:B:35:SER:HA	2:B:811:TYR:CE2	2.55	0.41
2:B:844:SER:OG	2:B:996:ARG:N	2.43	0.41
2:B:1002:THR:HG21	2:B:1006:ILE:HB	2.02	0.41
3:C:42:PRO:HA	3:C:163:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:THR:CG2	3:C:44:LEU:N	2.83	0.41
1:A:855:THR:CG2	1:A:857:ARG:HG3	2.43	0.41
1:A:1115:SER:HA	1:A:1308:THR:O	2.21	0.41
2:B:94:LYS:HD3	2:B:96:TYR:CZ	2.55	0.41
2:B:858:SER:HA	2:B:966:VAL:O	2.20	0.41
4:E:204:THR:HG22	4:E:205:SER:N	2.36	0.41
6:H:18:GLY:C	6:H:20:TYR:H	2.28	0.41
9:K:18:LYS:HE3	9:K:38:GLU:HG2	2.02	0.41
1:A:391:LEU:HD23	1:A:400:PRO:O	2.20	0.41
1:A:443:LEU:CD2	1:A:455:MET:HE2	2.50	0.41
1:A:925:LEU:HD13	1:A:983:ILE:HD12	2.02	0.41
1:A:975:HIS:ND1	1:A:1036:ARG:HG3	2.35	0.41
1:A:1319:VAL:HG13	1:A:1320:PRO:HD2	2.03	0.41
2:B:1163:CYS:SG	2:B:1165:ILE:HB	2.61	0.41
3:C:166:GLU:HA	9:K:6:ARG:HB3	2.01	0.41
4:E:59:SER:OG	4:E:81:GLU:HA	2.21	0.41
4:E:88:VAL:HG21	4:E:110:PHE:CE2	2.55	0.41
6:H:125:LEU:HB3	6:H:130:ARG:CZ	2.50	0.41
8:J:52:THR:HG22	8:J:52:THR:O	2.19	0.41
9:K:21:ILE:HD13	9:K:84:LYS:HE2	2.01	0.41
1:A:103:CYS:SG	1:A:207:ILE:HG23	2.60	0.41
1:A:369:SER:CB	9:K:2:ASN:HD21	2.33	0.41
2:B:229:ALA:C	2:B:231:PRO:HD2	2.46	0.41
2:B:339:THR:CG2	2:B:343:ILE:HB	2.50	0.41
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.49	0.41
2:B:640:VAL:HG22	2:B:651:LEU:CD2	2.50	0.41
3:C:35:ARG:HH11	9:K:41:THR:N	2.18	0.41
4:E:94:LYS:O	4:E:98:ILE:HG13	2.20	0.41
6:H:82:PRO:O	6:H:84:ALA:N	2.52	0.41
1:A:246:VAL:O	1:A:328:ARG:NH2	2.54	0.41
1:A:356:ASP:OD2	9:K:65:HIS:HE1	2.04	0.41
1:A:396:PRO:HG3	1:A:416:ARG:HB3	2.02	0.41
1:A:672:ASP:C	1:A:674:PRO:HD2	2.45	0.41
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.85	0.41
2:B:121:ASN:HA	2:B:207:GLY:CA	2.51	0.41
2:B:235:SER:HA	2:B:261:ARG:NH2	2.35	0.41
2:B:361:LEU:O	2:B:374:LYS:HE2	2.21	0.41
2:B:875:GLU:O	2:B:877:PRO:HD3	2.21	0.41
2:B:995:ARG:HD2	2:B:997:GLU:OE2	2.20	0.41
3:C:22:LEU:CD2	9:K:101:LEU:HD21	2.50	0.41
4:E:54:GLN:HB3	4:E:57:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:57:ILE:HA	8:J:60:PHE:CD2	2.55	0.41
1:A:476:SER:N	1:A:477:PRO:HD2	2.36	0.41
1:A:556:TRP:CH2	1:A:558:GLY:HA2	2.56	0.41
2:B:242:SER:O	2:B:251:ILE:HA	2.19	0.41
2:B:324:ILE:HD11	2:B:333:PHE:CG	2.56	0.41
2:B:515:HIS:CD2	2:B:517:THR:H	2.23	0.41
2:B:1159:ARG:HG3	2:B:1193:GLN:HE21	1.85	0.41
7:I:16:PRO:HA	7:I:26:LEU:O	2.21	0.41
9:K:65:HIS:CD2	9:K:66:PRO:HD2	2.55	0.41
1:A:32:VAL:HG23	1:A:33:ALA:H	1.85	0.41
1:A:406:ILE:HD12	1:A:406:ILE:N	2.36	0.41
1:A:874:ASP:OD1	1:A:874:ASP:C	2.63	0.41
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.21	0.41
2:B:123:THR:OG1	2:B:458:LYS:HE3	2.21	0.41
2:B:757:PRO:HD3	2:B:983:ARG:HH21	1.86	0.41
3:C:258:ILE:HG23	9:K:19:LEU:HD11	2.02	0.41
6:H:5:LEU:HD11	6:H:135:LEU:HG	2.03	0.41
1:A:81:PHE:HA	1:A:243:PRO:HD3	2.03	0.41
1:A:157:ASP:C	1:A:159:THR:N	2.78	0.41
1:A:186:LYS:HG2	1:A:187:LYS:H	1.86	0.41
1:A:378:GLU:OE1	1:A:434:ARG:HD3	2.21	0.41
2:B:115:GLN:HG2	2:B:193:LYS:CB	2.50	0.41
2:B:339:THR:HG22	2:B:340:ALA:O	2.20	0.41
2:B:870:ILE:HD11	2:B:919:SER:OG	2.21	0.41
6:H:12:VAL:HG13	6:H:26:ILE:CG2	2.51	0.41
6:H:113:ALA:HA	6:H:125:LEU:O	2.21	0.41
7:I:98:VAL:CG2	7:I:111:THR:HG22	2.50	0.41
7:I:103:CYS:SG	7:I:105:SER:HB2	2.60	0.41
1:A:91:PHE:HZ	1:A:207:ILE:HG13	1.86	0.41
1:A:220:THR:O	1:A:222:LEU:O	2.39	0.41
1:A:313:GLN:CB	1:A:320:ARG:HB3	2.51	0.41
1:A:590:ARG:HH11	1:A:590:ARG:HG2	1.86	0.41
1:A:850:VAL:HG21	1:A:1058:VAL:HG21	2.03	0.41
1:A:1027:ALA:O	1:A:1031:VAL:HG23	2.21	0.41
1:A:1104:ILE:CD1	1:A:1351:GLU:HB3	2.51	0.41
2:B:97:VAL:HG12	2:B:178:ASN:ND2	2.35	0.41
2:B:129:PHE:CZ	2:B:166:PHE:HB2	2.56	0.41
2:B:165:VAL:HG12	2:B:167:ILE:HG13	2.03	0.41
2:B:351:TYR:CE2	2:B:355:ILE:HD11	2.55	0.41
2:B:1006:ILE:HD11	8:J:43:ARG:CB	2.46	0.41
3:C:62:PHE:CE2	3:C:66:ARG:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:163:ILE:CG2	3:C:165:LYS:H	2.33	0.41
4:E:72:PHE:HE2	4:E:157:SER:HA	1.85	0.41
6:H:15:VAL:HG22	6:H:26:ILE:HG12	2.03	0.41
6:H:36:CYS:HA	6:H:126:GLU:O	2.21	0.41
6:H:97:MET:CE	6:H:142:LEU:HD23	2.50	0.41
8:J:39:LEU:HD23	8:J:39:LEU:HA	1.92	0.41
8:J:41:LEU:HD22	8:J:46:CYS:HB3	2.02	0.41
1:A:120:GLU:HG3	1:A:123:ARG:NH2	2.36	0.41
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.36	0.41
1:A:901:LEU:HA	1:A:907:THR:HG23	2.03	0.41
1:A:946:VAL:CG2	4:E:201:LYS:HD2	2.45	0.41
1:A:1059:HIS:CE1	5:F:155:LEU:HD22	2.45	0.41
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.51	0.41
2:B:760:ASP:OD1	2:B:760:ASP:N	2.53	0.41
2:B:795:ILE:HD12	2:B:795:ILE:N	2.36	0.41
9:K:21:ILE:HG21	9:K:84:LYS:HE2	2.03	0.41
1:A:24:PRO:O	1:A:28:ARG:HG3	2.21	0.40
1:A:334:GLY:HA2	1:A:337:ARG:HB3	2.02	0.40
1:A:443:LEU:HD21	1:A:455:MET:HE2	2.02	0.40
1:A:463:ILE:HB	1:A:464:PRO:HD2	2.03	0.40
1:A:548:ASN:HA	9:K:60:ALA:HB1	2.02	0.40
2:B:324:ILE:HG12	2:B:329:THR:CG2	2.45	0.40
6:H:27:GLU:HA	6:H:38:LEU:O	2.20	0.40
9:K:29:ASN:ND2	9:K:79:GLU:HA	2.35	0.40
1:A:1120:LEU:HD21	1:A:1131:ALA:HA	2.02	0.40
1:A:1150:SER:OG	7:I:46:HIS:HB3	2.21	0.40
5:F:88:TYR:O	5:F:89:GLU:C	2.65	0.40
1:A:115:LEU:HD12	1:A:142:CYS:SG	2.61	0.40
1:A:302:THR:HG23	1:A:306:ASN:ND2	2.36	0.40
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.21	0.40
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.21	0.40
1:A:1345:ARG:NH1	1:A:1373:ASP:OD1	2.54	0.40
2:B:217:ARG:HG2	2:B:218:SER:O	2.21	0.40
4:E:201:LYS:HD3	4:E:201:LYS:HA	1.92	0.40
9:K:18:LYS:HE3	9:K:38:GLU:CG	2.52	0.40
1:A:305:ASP:O	1:A:308:ILE:HD11	2.21	0.40
1:A:690:VAL:HG11	1:A:794:PRO:HD3	2.03	0.40
1:A:1376:THR:CG2	4:E:212:ARG:NH2	2.76	0.40
2:B:344:LYS:HB2	2:B:347:LYS:HE2	2.02	0.40
2:B:483:LEU:HD11	2:B:491:THR:HG23	2.04	0.40
2:B:597:MET:HE2	2:B:601:ARG:NE	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:882:THR:HB	2:B:934:LYS:O	2.22	0.40
2:B:1057:LYS:O	2:B:1061:GLU:HG3	2.21	0.40
3:C:73:GLN:HA	3:C:133:ILE:HD11	2.02	0.40
5:F:107:VAL:HG13	5:F:124:GLU:OE2	2.22	0.40
1:A:298:PHE:CZ	1:A:312:PRO:HD3	2.57	0.40
1:A:333:GLU:O	1:A:337:ARG:HB2	2.22	0.40
1:A:901:LEU:CD2	1:A:907:THR:HG23	2.51	0.40
1:A:1195:LEU:HD11	1:A:1267:MET:HE1	2.04	0.40
2:B:259:TYR:HB2	2:B:268:THR:HG22	2.04	0.40
2:B:311:LEU:HA	2:B:314:LEU:HD12	2.04	0.40
2:B:840:ILE:HB	2:B:1011:ILE:HB	2.04	0.40
2:B:996:ARG:NH2	3:C:174:ALA:O	2.54	0.40
3:C:3:GLU:HB2	9:K:104:ASN:OD1	2.21	0.40
3:C:250:THR:O	3:C:254:LYS:HG3	2.22	0.40
6:H:32:THR:HB	6:H:33:GLN:H	1.54	0.40
6:H:95:TYR:HE2	6:H:97:MET:HE2	1.86	0.40
8:J:53:HIS:CG	8:J:54:VAL:N	2.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1411/1733 (81%)	1250 (89%)	123 (9%)	38 (3%)	4	3
2	B	1074/1224 (88%)	950 (88%)	110 (10%)	14 (1%)	9	10
3	C	264/318 (83%)	236 (89%)	24 (9%)	4 (2%)	8	8
4	E	213/215 (99%)	189 (89%)	22 (10%)	2 (1%)	14	17
5	F	82/155 (53%)	76 (93%)	5 (6%)	1 (1%)	10	12
6	H	129/146 (88%)	93 (72%)	21 (16%)	15 (12%)	0	0
7	I	120/122 (98%)	103 (86%)	17 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	J	63/70 (90%)	59 (94%)	3 (5%)	1 (2%)	7	7
9	K	112/120 (93%)	106 (95%)	6 (5%)	0	100	100
10	L	44/70 (63%)	25 (57%)	16 (36%)	3 (7%)	1	0
All	All	3512/4173 (84%)	3087 (88%)	347 (10%)	78 (2%)	5	4

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	464	PRO
1	A	465	TYR
1	A	466	SER
1	A	567	LYS
1	A	593	GLU
1	A	1393	ASN
2	B	1222	ARG
6	H	128	ASN
1	A	35	ILE
1	A	307	ASP
1	A	467	THR
1	A	525	GLN
1	A	1398	MET
2	B	646	LEU
2	B	879	ARG
2	B	887	HIS
3	C	4	GLU
3	C	231	ASN
4	E	3	GLN
4	E	50	MET
6	H	18	GLY
6	H	19	ARG
6	H	61	SER
6	H	78	SER
6	H	105	GLU
6	H	138	GLU
1	A	67	CYS
1	A	156	ASP
1	A	258	GLY
1	A	283	GLY
1	A	626	ASN
1	A	915	SER

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Mol	Chain	Res	Type
1	A	958	VAL
1	A	1386	ARG
2	B	165	VAL
2	B	262	GLU
2	B	266	ALA
2	B	1190	ASP
3	C	90	ASP
3	C	137	LYS
5	F	73	ALA
6	H	52	GLN
6	H	81	PRO
6	H	103	LYS
8	J	44	TYR
10	L	39	SER
1	A	72	GLU
1	A	188	ASP
1	A	194	ALA
1	A	196	GLU
1	A	248	PRO
1	A	752	LYS
1	A	764	CYS
2	B	864	LYS
2	B	1100	ASP
6	H	62	SER
10	L	56	LEU
10	L	59	ALA
1	A	257	ARG
1	A	308	ILE
1	A	419	LYS
1	A	959	ASN
1	A	1402	PHE
2	B	90	ILE
2	B	1099	VAL
6	H	83	GLN
6	H	109	LYS
6	H	139	ASN
1	A	250	ILE
6	H	47	PHE
1	A	84	ILE
1	A	399	HIS
2	B	1214	PRO
1	A	61	ILE

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Mol	Chain	Res	Type
2	B	1109	GLY
1	A	1114	PRO
1	A	400	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1239/1520 (82%)	1175 (95%)	64 (5%)	21	31
2	B	950/1061 (90%)	895 (94%)	55 (6%)	18	26
3	C	234/274 (85%)	226 (97%)	8 (3%)	32	49
4	E	197/197 (100%)	193 (98%)	4 (2%)	48	67
5	F	74/137 (54%)	71 (96%)	3 (4%)	27	41
6	H	117/128 (91%)	115 (98%)	2 (2%)	53	72
7	I	116/116 (100%)	110 (95%)	6 (5%)	21	31
8	J	60/65 (92%)	53 (88%)	7 (12%)	5	6
9	K	99/102 (97%)	94 (95%)	5 (5%)	21	32
10	L	40/57 (70%)	36 (90%)	4 (10%)	7	9
All	All	3126/3657 (86%)	2968 (95%)	158 (5%)	21	32

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
1	A	53	LEU
1	A	93	VAL
1	A	171	GLN
1	A	209	ASN
1	A	221	SER
1	A	308	ILE
1	A	368	LYS
1	A	385	ILE
1	A	389	THR

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Mol	Chain	Res	Type
1	A	446	ARG
1	A	449	SER
1	A	450	LEU
1	A	451	HIS
1	A	452	LYS
1	A	467	THR
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	493	GLN
1	A	498	ARG
1	A	503	GLN
1	A	504	LEU
1	A	513	SER
1	A	535	THR
1	A	571	LEU
1	A	577	ILE
1	A	596	THR
1	A	597	LEU
1	A	612	ILE
1	A	618	GLU
1	A	622	VAL
1	A	666	ILE
1	A	669	THR
1	A	672	ASP
1	A	682	THR
1	A	710	LEU
1	A	756	ILE
1	A	769	SER
1	A	774	ARG
1	A	821	ARG
1	A	855	THR
1	A	858	ASN
1	A	873	MET
1	A	885	THR
1	A	919	ILE
1	A	920	LEU
1	A	926	GLN
1	A	1122	PRO
1	A	1130	GLN
1	A	1222	ASN
1	A	1277	GLU

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Mol	Chain	Res	Type
1	A	1280	GLU
1	A	1293	SER
1	A	1297	GLU
1	A	1318	THR
1	A	1336	MET
1	A	1366	ARG
1	A	1372	VAL
1	A	1377	THR
1	A	1383	SER
1	A	1384	VAL
1	A	1426	GLU
1	A	1436	ILE
2	B	18	PHE
2	B	20	ASP
2	B	21	GLU
2	B	61	ASP
2	B	102	VAL
2	B	109	THR
2	B	130	VAL
2	B	178	ASN
2	B	194	GLU
2	B	217	ARG
2	B	261	ARG
2	B	268	THR
2	B	313	MET
2	B	339	THR
2	B	357	GLN
2	B	366	GLN
2	B	372	SER
2	B	425	THR
2	B	463	THR
2	B	485	ARG
2	B	487	THR
2	B	496	ARG
2	B	498	THR
2	B	513	GLN
2	B	540	SER
2	B	549	THR
2	B	563	MET
2	B	567	GLU
2	B	589	VAL
2	B	612	GLU

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Mol	Chain	Res	Type
2	B	636	PRO
2	B	641	GLU
2	B	644	GLU
2	B	731	VAL
2	B	737	THR
2	B	754	SER
2	B	790	ASP
2	B	806	THR
2	B	846	ILE
2	B	864	LYS
2	B	970	THR
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1060	ARG
2	B	1065	GLN
2	B	1097	HIS
2	B	1099	VAL
2	B	1145	SER
2	B	1150	ARG
2	B	1152	MET
2	B	1159	ARG
2	B	1160	VAL
2	B	1219	ASP
2	B	1222	ARG
3	C	23	SER
3	C	50	GLU
3	C	77	ILE
3	C	163	ILE
3	C	189	THR
3	C	209	TYR
3	C	238	ILE
3	C	240	VAL
4	E	104	ASN
4	E	123	LEU
4	E	196	VAL
4	E	204	THR
5	F	79	ARG
5	F	82	THR
5	F	115	THR
6	H	32	THR
6	H	104	PHE

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Mol	Chain	Res	Type
7	I	12	ASN
7	I	50	THR
7	I	61	ASP
7	I	84	VAL
7	I	87	GLN
7	I	111	THR
8	J	1	MET
8	J	3	VAL
8	J	7	CYS
8	J	14	VAL
8	J	37	SER
8	J	38	ARG
8	J	48	ARG
9	K	11	LEU
9	K	18	LYS
9	K	47	ARG
9	K	73	LEU
9	K	114	LEU
10	L	27	LEU
10	L	38	LEU
10	L	50	ASP
10	L	64	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	68	GLN
1	A	80	HIS
1	A	92	HIS
1	A	171	GLN
1	A	299	HIS
1	A	313	GLN
1	A	390	GLN
1	A	394	ASN
1	A	397	ASN
1	A	427	GLN
1	A	445	ASN
1	A	479	ASN
1	A	503	GLN
1	A	510	GLN
1	A	659	HIS

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Mol	Chain	Res	Type
1	A	660	ASN
1	A	736	ASN
1	A	741	ASN
1	A	742	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	858	ASN
1	A	903	ASN
1	A	906	HIS
1	A	926	GLN
1	A	994	GLN
1	A	1128	GLN
1	A	1218	GLN
1	A	1270	ASN
1	A	1364	ASN
1	A	1387	HIS
1	A	1393	ASN
1	A	1432	GLN
2	B	46	GLN
2	B	178	ASN
2	B	215	GLN
2	B	236	HIS
2	B	255	GLN
2	B	325	GLN
2	B	363	HIS
2	B	366	GLN
2	B	465	ASN
2	B	484	ASN
2	B	513	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	587	HIS
2	B	590	HIS
2	B	657	HIS
2	B	706	GLN
2	B	734	HIS
2	B	744	HIS
2	B	767	ASN
2	B	770	GLN

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Mol	Chain	Res	Type
2	B	786	ASN
2	B	957	ASN
2	B	1015	HIS
2	B	1062	HIS
2	B	1065	GLN
2	B	1084	GLN
2	B	1093	GLN
2	B	1161	HIS
2	B	1176	ASN
2	B	1179	GLN
2	B	1187	ASN
2	B	1193	GLN
2	B	1205	GLN
3	C	65	HIS
3	C	73	GLN
3	C	112	ASN
3	C	131	HIS
3	C	151	GLN
3	C	167	HIS
3	C	242	GLN
4	E	101	GLN
4	E	104	ASN
4	E	113	GLN
4	E	147	HIS
6	H	11	GLN
6	H	128	ASN
6	H	131	ASN
6	H	133	ASN
6	H	134	ASN
7	I	12	ASN
7	I	60	GLN
7	I	79	HIS
7	I	108	HIS
8	J	26	GLN
8	J	53	HIS
9	K	29	ASN
9	K	65	HIS
9	K	76	GLN
9	K	110	ASN
10	L	53	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
13	UTP	B	3571	12	29,30,30	1.38	4 (13%)	43,47,47	1.10	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	UTP	B	3571	12	-	5/22/38/38	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	3571	UTP	PA-O3A	4.21	1.64	1.59
13	B	3571	UTP	C2-N1	3.59	1.44	1.38
13	B	3571	UTP	C1'-N1	2.29	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	3571	UTP	PB-O1B	-2.12	1.45	1.55

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	3571	UTP	O1B-PB-O3A	3.20	115.93	107.27
13	B	3571	UTP	O4'-C1'-C2'	-2.76	100.70	106.62
13	B	3571	UTP	O3A-PB-O2B	-2.49	103.21	110.70

There are no chirality outliers.

All (5) torsion outliers are listed below:

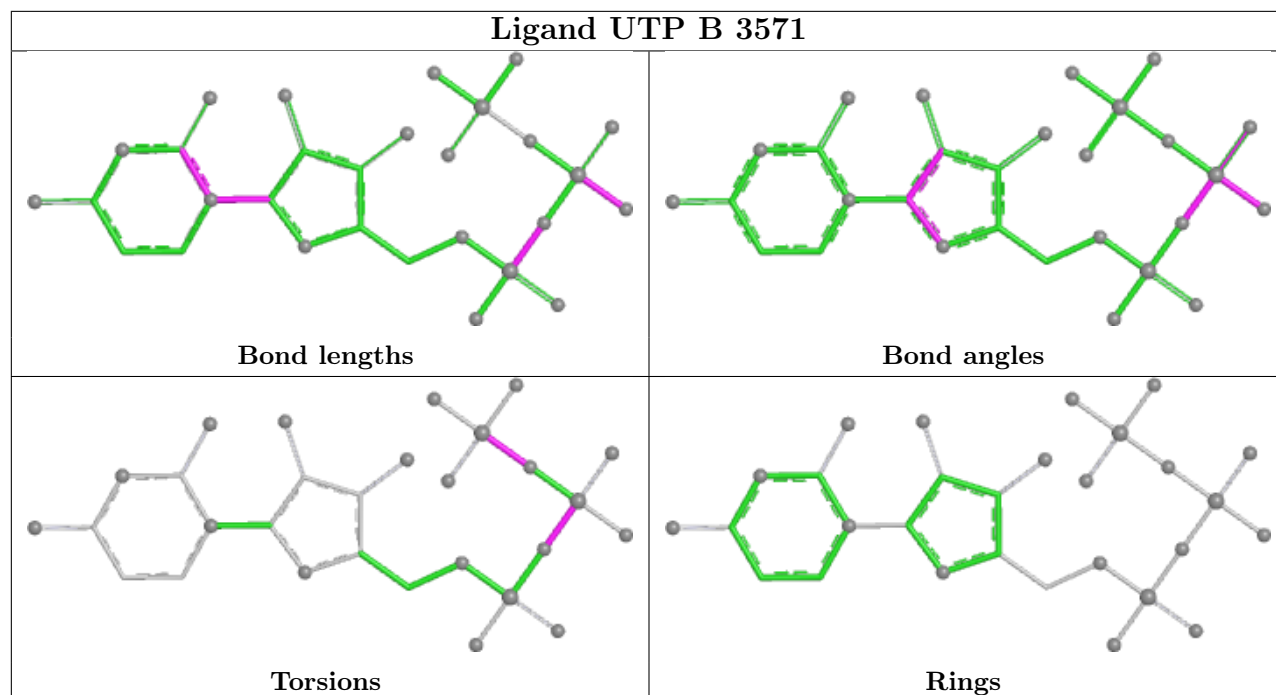
Mol	Chain	Res	Type	Atoms
13	B	3571	UTP	PA-O3A-PB-O2B
13	B	3571	UTP	PB-O3B-PG-O2G
13	B	3571	UTP	PA-O3A-PB-O1B
13	B	3571	UTP	PB-O3B-PG-O1G
13	B	3571	UTP	PB-O3B-PG-O3G

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	3571	UTP	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1419/1733 (81%)	1.54	417 (29%) 1 1	15, 54, 147, 169	0
2	B	1094/1224 (89%)	1.49	311 (28%) 1 1	16, 50, 129, 158	0
3	C	266/318 (83%)	1.70	87 (32%) 1 1	27, 58, 95, 144	0
4	E	215/215 (100%)	1.79	88 (40%) 0 0	23, 67, 113, 149	0
5	F	84/155 (54%)	1.25	14 (16%) 4 5	20, 49, 77, 98	0
6	H	133/146 (91%)	3.08	102 (76%) 0 0	63, 99, 141, 150	0
7	I	122/122 (100%)	1.72	39 (31%) 1 1	41, 64, 108, 130	0
8	J	65/70 (92%)	1.33	12 (18%) 3 4	29, 49, 80, 94	0
9	K	114/120 (95%)	1.61	28 (24%) 2 2	31, 67, 86, 97	0
10	L	46/70 (65%)	3.07	38 (82%) 0 0	52, 105, 132, 137	0
All	All	3558/4173 (85%)	1.63	1136 (31%) 1 1	15, 56, 135, 169	0

All (1136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	340	LEU	10.9
1	A	1176	LEU	10.5
6	H	104	PHE	10.2
1	A	1175	SER	9.9
10	L	27	LEU	9.0
2	B	1105	ALA	8.9
1	A	250	ILE	7.6
2	B	1184	GLY	7.3
6	H	132	LEU	7.3
6	H	107	VAL	7.2
6	H	63	LEU	7.2
1	A	1397	LEU	7.1
1	A	1396	ALA	7.1

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Mol	Chain	Res	Type	RSRZ
2	B	1128	LEU	7.0
2	B	1224	PHE	6.8
2	B	1103	ILE	6.7
6	H	90	ALA	6.7
6	H	112	ILE	6.6
1	A	336	ILE	6.6
1	A	309	ALA	6.4
1	A	65	LEU	6.4
2	B	436	VAL	6.3
2	B	883	LEU	6.3
1	A	329	LEU	6.2
2	B	643	ASP	6.1
2	B	1107	ALA	6.0
9	K	114	LEU	5.9
1	A	249	SER	5.9
2	B	732	SER	5.9
2	B	1100	ASP	5.9
2	B	1155	SER	5.8
7	I	122	SER	5.8
1	A	345	VAL	5.7
6	H	85	GLY	5.7
2	B	866	TYR	5.7
1	A	252	PHE	5.6
2	B	250	PHE	5.6
1	A	1389	PHE	5.4
2	B	1110	PRO	5.4
7	I	1	MET	5.3
6	H	134	ASN	5.3
7	I	53	GLY	5.3
2	B	367	LEU	5.3
2	B	733	HIS	5.3
2	B	869	SER	5.3
1	A	187	LYS	5.3
1	A	190	ALA	5.3
1	A	1254	ALA	5.3
6	H	84	ALA	5.3
1	A	199	LEU	5.3
2	B	18	PHE	5.2
1	A	2	VAL	5.2
2	B	723	VAL	5.2
1	A	251	SER	5.2
10	L	55	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
2	B	106	ASP	5.2
2	B	108	VAL	5.2
2	B	870	ILE	5.2
6	H	136	LYS	5.1
1	A	1392	SER	5.1
1	A	342	GLY	5.1
2	B	247	GLY	5.1
6	H	127	GLY	5.1
2	B	1102	LYS	5.1
5	F	155	LEU	5.0
2	B	1099	VAL	5.0
7	I	121	PHE	5.0
1	A	58	LEU	5.0
1	A	912	LEU	5.0
2	B	919	SER	5.0
2	B	137	TYR	4.9
2	B	1189	ILE	4.9
1	A	191	THR	4.9
1	A	1126	ALA	4.9
1	A	270	LEU	4.9
1	A	61	ILE	4.9
2	B	918	ILE	4.9
1	A	248	PRO	4.9
1	A	1287	TYR	4.9
6	H	126	GLU	4.8
2	B	132	VAL	4.8
1	A	315	LEU	4.8
2	B	1156	ASP	4.8
1	A	246	VAL	4.8
1	A	341	MET	4.8
1	A	259	GLU	4.8
1	A	1450	LEU	4.8
2	B	646	LEU	4.8
6	H	103	LYS	4.8
2	B	70	ILE	4.7
9	K	111	LEU	4.7
1	A	266	LEU	4.7
1	A	1081	LEU	4.7
2	B	128	LEU	4.7
7	I	93	LYS	4.7
1	A	1402	PHE	4.7
2	B	963	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
4	E	108	GLY	4.7
1	A	147	VAL	4.6
6	H	79	TRP	4.6
1	A	339	ASN	4.6
2	B	882	THR	4.6
2	B	1098	MET	4.6
1	A	1400	CYS	4.6
1	A	69	THR	4.6
6	H	135	LEU	4.6
6	H	130	ARG	4.6
6	H	129	TYR	4.5
2	B	868	MET	4.5
2	B	69	LEU	4.5
2	B	130	VAL	4.5
10	L	56	LEU	4.5
1	A	312	PRO	4.5
10	L	38	LEU	4.5
3	C	8	VAL	4.5
1	A	184	SER	4.5
2	B	1180	PHE	4.5
1	A	194	ALA	4.5
2	B	644	GLU	4.5
2	B	1157	ALA	4.5
6	H	59	ILE	4.4
1	A	344	ARG	4.4
2	B	129	PHE	4.4
6	H	139	ASN	4.4
6	H	141	TYR	4.4
1	A	1384	VAL	4.4
1	A	51	GLY	4.4
1	A	253	ASN	4.4
1	A	68	GLN	4.4
7	I	74	GLU	4.4
1	A	1390	ASN	4.4
2	B	1101	ASP	4.4
1	A	343	LYS	4.3
2	B	165	VAL	4.3
4	E	132	ILE	4.3
10	L	25	ALA	4.3
2	B	446	LEU	4.3
2	B	1191	ILE	4.3
2	B	731	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
7	I	83	ASN	4.3
1	A	321	PRO	4.3
1	A	188	ASP	4.3
2	B	1223	ASP	4.3
10	L	45	ALA	4.3
1	A	78	PRO	4.3
2	B	136	THR	4.3
10	L	40	LEU	4.3
1	A	1125	ALA	4.2
2	B	184	ALA	4.2
1	A	308	ILE	4.2
1	A	973	ILE	4.2
5	F	74	ILE	4.2
1	A	318	SER	4.2
2	B	877	PRO	4.2
1	A	258	GLY	4.2
10	L	30	ILE	4.2
1	A	1385	THR	4.2
2	B	265	SER	4.2
4	E	1	MET	4.2
1	A	314	ALA	4.2
1	A	37	PHE	4.2
1	A	262	LEU	4.2
3	C	255	VAL	4.1
6	H	60	ALA	4.1
2	B	961	LEU	4.1
2	B	369	GLY	4.1
1	A	66	LYS	4.1
1	A	38	PRO	4.1
1	A	53	LEU	4.1
7	I	2	THR	4.1
1	A	751	SER	4.1
2	B	190	TYR	4.1
2	B	874	PHE	4.1
6	H	6	PHE	4.1
2	B	467	GLY	4.1
1	A	1359	ASP	4.1
1	A	1256	GLU	4.1
2	B	65	GLU	4.1
2	B	92	PHE	4.0
10	L	65	VAL	4.0
1	A	56	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
6	H	111	LEU	4.0
1	A	1123	GLY	4.0
1	A	146	MET	4.0
6	H	57	VAL	4.0
1	A	48	ALA	4.0
1	A	79	GLY	4.0
1	A	921	GLY	4.0
6	H	26	ILE	4.0
1	A	175	ARG	4.0
1	A	247	ARG	4.0
1	A	1220	PHE	4.0
2	B	264	SER	4.0
2	B	1104	HIS	3.9
6	H	46	LEU	3.9
1	A	949	ASP	3.9
3	C	221	TYR	3.9
6	H	95	TYR	3.9
6	H	102	TYR	3.9
6	H	144	ILE	3.9
1	A	10	PRO	3.9
1	A	1391	ARG	3.9
6	H	114	VAL	3.9
1	A	162	VAL	3.9
2	B	102	VAL	3.9
6	H	18	GLY	3.9
2	B	477	ALA	3.9
1	A	322	VAL	3.9
4	E	35	VAL	3.9
1	A	1080	THR	3.9
4	E	49	SER	3.8
2	B	167	ILE	3.8
6	H	115	TYR	3.8
5	F	72	LYS	3.8
3	C	80	LEU	3.8
7	I	4	PHE	3.8
1	A	1284	MET	3.8
1	A	597	LEU	3.8
5	F	111	LEU	3.8
2	B	1154	ALA	3.8
1	A	1403	GLU	3.8
1	A	84	ILE	3.8
2	B	1172	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	1032	LEU	3.8
2	B	1109	GLY	3.8
10	L	28	LYS	3.8
1	A	1271	ILE	3.8
2	B	734	HIS	3.8
2	B	710	LEU	3.8
10	L	57	LEU	3.8
2	B	865	LYS	3.7
4	E	67	GLU	3.7
1	A	1281	ARG	3.7
6	H	142	LEU	3.7
1	A	555	ASP	3.7
3	C	17	ASN	3.7
10	L	26	THR	3.7
2	B	127	GLY	3.7
1	A	1405	THR	3.7
2	B	25	ILE	3.7
2	B	101	MET	3.7
1	A	6	TYR	3.7
2	B	726	ALA	3.7
6	H	54	SER	3.7
2	B	246	LYS	3.7
1	A	325	ILE	3.6
1	A	33	ALA	3.6
1	A	1173	HIS	3.6
4	E	126	SER	3.6
6	H	62	SER	3.6
2	B	708	GLU	3.6
1	A	1225	PHE	3.6
4	E	42	PHE	3.6
1	A	57	ARG	3.6
1	A	1207	LEU	3.6
2	B	640	VAL	3.6
7	I	111	THR	3.6
6	H	83	GLN	3.6
7	I	92	ARG	3.6
1	A	166	GLY	3.6
2	B	1127	GLY	3.6
2	B	447	ALA	3.6
3	C	3	GLU	3.6
3	C	209	TYR	3.6
2	B	1106	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
7	I	118	ARG	3.6
2	B	448	ILE	3.6
1	A	331	GLY	3.6
4	E	96	PHE	3.6
6	H	38	LEU	3.6
2	B	1186	ASP	3.6
4	E	53	PRO	3.6
4	E	77	SER	3.5
6	H	143	LEU	3.5
1	A	1393	ASN	3.5
4	E	128	PRO	3.5
6	H	105	GLU	3.5
2	B	1221	SER	3.5
1	A	128	ILE	3.5
1	A	81	PHE	3.5
2	B	244	LEU	3.5
2	B	370	PHE	3.5
9	K	98	LEU	3.5
1	A	54	ASN	3.5
1	A	975	HIS	3.5
6	H	31	THR	3.5
2	B	712	PRO	3.5
2	B	115	GLN	3.5
10	L	46	VAL	3.5
1	A	74	MET	3.5
1	A	1093	LYS	3.5
4	E	69	ILE	3.5
1	A	1386	ARG	3.5
4	E	3	GLN	3.5
7	I	119	THR	3.5
6	H	15	VAL	3.5
1	A	323	LYS	3.5
1	A	338	GLY	3.5
3	C	10	ILE	3.5
3	C	129	ILE	3.5
3	C	258	ILE	3.5
2	B	1222	ARG	3.5
2	B	958	GLN	3.5
1	A	44	THR	3.4
2	B	880	THR	3.4
2	B	1152	MET	3.4
1	A	288	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
10	L	32	ALA	3.4
1	A	3	GLY	3.4
2	B	1190	ASP	3.4
6	H	146	ARG	3.4
2	B	431	TYR	3.4
1	A	1174	PHE	3.4
3	C	110	THR	3.4
4	E	125	PRO	3.4
3	C	18	VAL	3.4
2	B	1182	CYS	3.4
2	B	1161	HIS	3.4
10	L	53	HIS	3.4
2	B	908	GLU	3.4
1	A	50	ILE	3.4
1	A	1170	ILE	3.4
2	B	164	LYS	3.4
6	H	116	TYR	3.4
2	B	166	PHE	3.4
1	A	197	PRO	3.4
4	E	75	MET	3.4
1	A	263	THR	3.4
1	A	1406	VAL	3.4
4	E	90	VAL	3.4
4	E	83	CYS	3.4
10	L	48	CYS	3.4
1	A	210	ILE	3.4
1	A	612	ILE	3.4
1	A	1172	LEU	3.4
2	B	729	ILE	3.4
4	E	116	ILE	3.4
1	A	591	PHE	3.4
1	A	1394	THR	3.4
2	B	435	THR	3.4
2	B	138	GLU	3.4
2	B	1097	HIS	3.4
1	A	52	GLY	3.4
1	A	73	GLY	3.4
1	A	174	ILE	3.3
6	H	10	PHE	3.3
6	H	80	ARG	3.3
6	H	137	GLN	3.3
2	B	888	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
9	K	11	LEU	3.3
2	B	428	ILE	3.3
1	A	1449	SER	3.3
1	A	193	ASP	3.3
1	A	826	ASP	3.3
9	K	2	ASN	3.3
2	B	1185	CYS	3.3
10	L	54	ARG	3.3
1	A	159	THR	3.3
1	A	763	ALA	3.3
4	E	97	VAL	3.3
6	H	23	VAL	3.3
6	H	91	ASP	3.3
6	H	128	ASN	3.3
6	H	89	LEU	3.3
1	A	1445	ILE	3.3
2	B	90	ILE	3.3
4	E	100	ILE	3.3
8	J	65	PRO	3.3
6	H	58	THR	3.3
10	L	43	THR	3.3
2	B	830	TYR	3.3
2	B	509	ALA	3.2
5	F	73	ALA	3.2
1	A	319	GLY	3.2
2	B	200	GLY	3.2
4	E	51	GLY	3.2
2	B	434	ARG	3.2
1	A	567	LYS	3.2
2	B	707	PRO	3.2
2	B	1165	ILE	3.2
3	C	6	PRO	3.2
1	A	171	GLN	3.2
7	I	3	THR	3.2
1	A	154	SER	3.2
1	A	108	MET	3.2
3	C	265	MET	3.2
2	B	1108	ARG	3.2
3	C	216	GLY	3.2
3	C	184	ASN	3.2
1	A	30	ILE	3.2
1	A	60	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1285	MET	3.2
1	A	49	LYS	3.2
1	A	905	ASP	3.2
2	B	466	TRP	3.2
2	B	1206	GLU	3.2
4	E	66	GLU	3.2
6	H	131	ASN	3.2
10	L	62	LYS	3.2
1	A	400	PRO	3.2
4	E	105	PHE	3.2
1	A	165	GLY	3.2
1	A	205	GLU	3.2
1	A	1388	GLY	3.2
2	B	245	GLU	3.2
3	C	245	VAL	3.2
3	C	261	ALA	3.2
1	A	109	HIS	3.2
1	A	121	LEU	3.2
1	A	913	LEU	3.2
6	H	125	LEU	3.2
1	A	834	THR	3.2
1	A	1398	MET	3.2
1	A	120	GLU	3.1
2	B	465	ASN	3.1
1	A	153	PRO	3.1
4	E	7	ARG	3.1
4	E	121	MET	3.1
1	A	46	THR	3.1
1	A	278	THR	3.1
9	K	55	LYS	3.1
1	A	67	CYS	3.1
7	I	54	GLU	3.1
6	H	88	SER	3.1
9	K	10	PHE	3.1
1	A	239	LEU	3.1
1	A	1260	LEU	3.1
6	H	93	TYR	3.1
2	B	658	ILE	3.1
2	B	899	ILE	3.1
4	E	9	ILE	3.1
1	A	904	THR	3.1
6	H	24	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	192	GLY	3.1
1	A	195	ASP	3.1
9	K	3	ALA	3.1
2	B	1129	ARG	3.1
4	E	78	LEU	3.1
6	H	55	LEU	3.1
1	A	35	ILE	3.1
1	A	1227	ILE	3.1
2	B	895	ASP	3.1
3	C	126	GLY	3.1
3	C	219	PHE	3.1
1	A	544	ASP	3.1
6	H	140	ALA	3.1
1	A	285	PRO	3.1
1	A	317	LYS	3.1
6	H	82	PRO	3.1
1	A	1120	LEU	3.1
3	C	22	LEU	3.1
3	C	153	LEU	3.1
3	C	155	LEU	3.1
1	A	333	GLU	3.0
1	A	1234	GLU	3.0
1	A	170	THR	3.0
2	B	886	LYS	3.0
2	B	725	PRO	3.0
2	B	112	LEU	3.0
1	A	198	GLU	3.0
2	B	1181	GLU	3.0
10	L	33	GLU	3.0
1	A	919	ILE	3.0
2	B	1085	ILE	3.0
1	A	917	SER	3.0
1	A	59	GLY	3.0
1	A	62	ASP	3.0
1	A	1166	ASP	3.0
2	B	54	PHE	3.0
4	E	47	CYS	3.0
4	E	64	PRO	3.0
2	B	461	LEU	3.0
2	B	1162	ILE	3.0
1	A	12	ARG	3.0
1	A	189	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	332	LYS	3.0
2	B	260	GLY	3.0
4	E	206	GLY	3.0
1	A	264	PHE	3.0
3	C	20	PHE	3.0
2	B	117	ALA	3.0
2	B	450	ALA	3.0
2	B	735	ALA	3.0
3	C	174	ALA	3.0
1	A	179	LEU	3.0
1	A	238	CYS	3.0
1	A	701	LEU	3.0
3	C	186	LEU	3.0
1	A	145	LYS	3.0
1	A	176	LYS	3.0
4	E	54	GLN	3.0
1	A	1095	THR	3.0
1	A	346	ASP	3.0
1	A	1446	ASP	3.0
6	H	106	GLU	3.0
4	E	82	PHE	2.9
1	A	899	VAL	2.9
1	A	1212	VAL	2.9
6	H	12	VAL	2.9
2	B	249	ARG	2.9
6	H	78	SER	2.9
6	H	108	SER	2.9
10	L	68	GLU	2.9
2	B	575	PRO	2.9
2	B	417	PHE	2.9
6	H	47	PHE	2.9
1	A	287	HIS	2.9
1	A	1387	HIS	2.9
3	C	101	LEU	2.9
2	B	1220	ARG	2.9
1	A	316	GLN	2.9
3	C	21	ILE	2.9
1	A	173	THR	2.9
1	A	1214	GLU	2.9
1	A	1280	GLU	2.9
2	B	89	GLU	2.9
2	B	96	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	64	ASN	2.9
2	B	248	SER	2.9
2	B	933	SER	2.9
1	A	158	PRO	2.9
1	A	564	ALA	2.9
3	C	183	TRP	2.9
6	H	87	ARG	2.9
2	B	964	VAL	2.9
4	E	124	VAL	2.9
10	L	34	CYS	2.9
1	A	237	THR	2.9
9	K	1	MET	2.9
1	A	599	SER	2.9
3	C	14	SER	2.9
2	B	93	GLY	2.9
2	B	647	GLY	2.9
10	L	29	TYR	2.9
10	L	49	LYS	2.9
4	E	88	VAL	2.9
1	A	148	CYS	2.9
2	B	641	GLU	2.9
1	A	708	MET	2.9
2	B	944	THR	2.9
4	E	50	MET	2.9
7	I	55	THR	2.9
2	B	1219	ASP	2.9
1	A	1258	HIS	2.8
10	L	60	ARG	2.8
2	B	46	GLN	2.8
1	A	1236	LEU	2.8
4	E	29	PHE	2.8
9	K	7	PHE	2.8
5	F	153	VAL	2.8
2	B	873	THR	2.8
2	B	889	THR	2.8
3	C	238	ILE	2.8
4	E	109	ILE	2.8
1	A	186	LYS	2.8
3	C	137	LYS	2.8
2	B	449	ASN	2.8
1	A	200	ARG	2.8
1	A	1395	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	645	SER	2.8
3	C	237	SER	2.8
1	A	1156	PRO	2.8
2	B	114	PRO	2.8
6	H	17	PRO	2.8
7	I	76	PRO	2.8
1	A	327	ALA	2.8
2	B	875	GLU	2.8
4	E	40	GLU	2.8
4	E	215	MET	2.8
8	J	1	MET	2.8
1	A	728	LYS	2.8
1	A	47	ARG	2.8
1	A	269	ILE	2.8
1	A	289	ILE	2.8
2	B	68	THR	2.8
1	A	260	ASP	2.8
2	B	103	ASN	2.8
2	B	592	ASN	2.8
10	L	50	ASP	2.8
1	A	82	GLY	2.8
6	H	2	SER	2.8
6	H	61	SER	2.8
1	A	21	LEU	2.8
2	B	181	LEU	2.8
2	B	893	LEU	2.8
6	H	27	GLU	2.8
1	A	421	ALA	2.8
2	B	432	MET	2.8
3	C	142	VAL	2.8
2	B	452	THR	2.8
1	A	282	ASN	2.8
1	A	1257	ASP	2.8
2	B	182	SER	2.8
1	A	172	PRO	2.8
9	K	4	PRO	2.8
1	A	276	LEU	2.8
2	B	1175	LEU	2.8
6	H	5	LEU	2.8
6	H	40	LEU	2.8
1	A	330	LYS	2.8
4	E	103	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
6	H	123	MET	2.8
7	I	117	LYS	2.8
9	K	26	LYS	2.8
8	J	3	VAL	2.8
7	I	79	HIS	2.7
2	B	502	ILE	2.7
2	B	871	THR	2.7
7	I	94	ASP	2.7
1	A	888	GLY	2.7
1	A	1401	SER	2.7
1	A	196	GLU	2.7
1	A	1092	LYS	2.7
1	A	304	MET	2.7
9	K	50	LEU	2.7
3	C	13	ALA	2.7
7	I	84	VAL	2.7
1	A	150	THR	2.7
2	B	913	GLY	2.7
1	A	1005	GLU	2.7
1	A	265	LYS	2.7
2	B	1183	LYS	2.7
1	A	113	LEU	2.7
1	A	571	LEU	2.7
2	B	879	ARG	2.7
1	A	152	VAL	2.7
1	A	311	GLN	2.7
4	E	106	GLN	2.7
7	I	120	GLN	2.7
2	B	1176	ASN	2.7
3	C	16	ASP	2.7
1	A	424	ILE	2.7
1	A	542	GLU	2.7
1	A	568	PRO	2.7
1	A	915	SER	2.7
2	B	528	PRO	2.7
2	B	876	LYS	2.7
2	B	934	LYS	2.7
1	A	320	ARG	2.7
2	B	135	ARG	2.7
2	B	561	TRP	2.7
2	B	1096	ARG	2.7
1	A	1268	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	424	LEU	2.7
2	B	887	HIS	2.7
10	L	59	ALA	2.7
1	A	836	TYR	2.7
1	A	201	VAL	2.7
2	B	957	ASN	2.7
1	A	155	GLU	2.7
3	C	9	LYS	2.7
4	E	131	THR	2.7
1	A	1158	PRO	2.7
3	C	74	SER	2.7
6	H	13	SER	2.7
9	K	28	PRO	2.7
10	L	36	SER	2.7
1	A	328	ARG	2.7
4	E	57	MET	2.7
7	I	13	MET	2.7
1	A	920	LEU	2.7
1	A	1414	ALA	2.6
1	A	217	LYS	2.6
4	E	135	PHE	2.6
2	B	642	ASP	2.6
2	B	1153	GLU	2.6
1	A	40	THR	2.6
1	A	596	THR	2.6
1	A	886	ILE	2.6
1	A	916	GLY	2.6
2	B	453	ILE	2.6
4	E	98	ILE	2.6
2	B	64	CYS	2.6
8	J	39	LEU	2.6
1	A	1228	TRP	2.6
10	L	69	ALA	2.6
1	A	1232	ASN	2.6
2	B	1158	PHE	2.6
4	E	2	ASP	2.6
6	H	98	TYR	2.6
10	L	47	ARG	2.6
2	B	211	VAL	2.6
6	H	96	VAL	2.6
1	A	1279	ILE	2.6
2	B	885	MET	2.6

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Mol	Chain	Res	Type	RSRZ
7	I	49	ILE	2.6
10	L	35	SER	2.6
1	A	181	LEU	2.6
4	E	123	LEU	2.6
2	B	962	LYS	2.6
1	A	1448	GLU	2.6
6	H	29	ALA	2.6
3	C	19	ASP	2.6
1	A	144	THR	2.6
1	A	1162	VAL	2.6
2	B	966	VAL	2.6
6	H	4	THR	2.6
4	E	129	PRO	2.6
6	H	44	VAL	2.6
6	H	100	THR	2.6
2	B	100	PRO	2.6
3	C	239	PRO	2.6
4	E	127	ILE	2.6
9	K	94	ILE	2.6
2	B	420	LEU	2.6
7	I	99	LEU	2.6
2	B	186	GLU	2.6
1	A	267	ALA	2.6
2	B	266	ALA	2.6
3	C	225	ALA	2.6
1	A	185	TRP	2.6
1	A	954	TRP	2.6
1	A	1304	TRP	2.6
1	A	1309	ASP	2.6
1	A	1259	MET	2.6
3	C	125	MET	2.6
3	C	87	PHE	2.6
4	E	27	GLY	2.6
6	H	32	THR	2.6
6	H	76	THR	2.6
6	H	81	PRO	2.6
2	B	251	ILE	2.6
3	C	122	SER	2.6
1	A	838	GLN	2.5
1	A	908	LEU	2.5
2	B	371	GLU	2.5
1	A	29	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	77	CYS	2.5
2	B	881	ASN	2.5
4	E	38	PRO	2.5
9	K	13	GLY	2.5
1	A	958	VAL	2.5
2	B	451	LYS	2.5
3	C	51	VAL	2.5
3	C	113	VAL	2.5
3	C	77	ILE	2.5
4	E	32	GLN	2.5
4	E	46	TYR	2.5
8	J	63	TYR	2.5
2	B	620	ARG	2.5
2	B	552	MET	2.5
1	A	157	ASP	2.5
1	A	1201	ALA	2.5
3	C	157	CYS	2.5
4	E	62	ALA	2.5
4	E	130	ALA	2.5
6	H	86	ASP	2.5
1	A	1109	LYS	2.5
2	B	191	LYS	2.5
4	E	76	GLY	2.5
4	E	189	GLY	2.5
6	H	39	THR	2.5
1	A	1299	VAL	2.5
2	B	633	VAL	2.5
3	C	244	VAL	2.5
1	A	1404	GLU	2.5
2	B	437	GLU	2.5
1	A	1399	ARG	2.5
2	B	169	ARG	2.5
1	A	710	LEU	2.5
6	H	122	LEU	2.5
9	K	9	LEU	2.5
1	A	129	LYS	2.5
1	A	1137	ALA	2.5
2	B	427	ASP	2.5
9	K	53	ASP	2.5
1	A	286	HIS	2.5
1	A	451	HIS	2.5
1	A	707	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1124	HIS	2.5
10	L	52	GLY	2.5
7	I	60	GLN	2.5
1	A	91	PHE	2.5
2	B	104	GLU	2.5
4	E	10	SER	2.5
4	E	36	GLU	2.5
6	H	30	SER	2.5
2	B	95	ILE	2.5
4	E	30	ILE	2.5
7	I	52	ILE	2.5
1	A	428	TYR	2.5
2	B	275	TYR	2.5
8	J	24	LEU	2.5
4	E	93	MET	2.5
2	B	134	LYS	2.5
1	A	118	HIS	2.5
2	B	1167	GLY	2.5
3	C	132	PRO	2.5
1	A	1129	GLU	2.4
2	B	425	THR	2.4
2	B	1218	THR	2.4
3	C	156	THR	2.4
1	A	8	SER	2.4
2	B	63	ILE	2.4
3	C	133	ILE	2.4
9	K	21	ILE	2.4
2	B	459	TYR	2.4
1	A	1205	LYS	2.4
4	E	122	LYS	2.4
1	A	538	ASP	2.4
1	A	4	GLN	2.4
1	A	1188	GLN	2.4
1	A	334	GLY	2.4
1	A	898	ARG	2.4
1	A	1108	ALA	2.4
2	B	430	ARG	2.4
2	B	867	GLY	2.4
3	C	247	GLY	2.4
7	I	5	ARG	2.4
1	A	907	THR	2.4
2	B	915	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	466	SER	2.4
1	A	207	ILE	2.4
1	A	1242	VAL	2.4
2	B	1160	VAL	2.4
3	C	176	ILE	2.4
7	I	59	VAL	2.4
10	L	67	PHE	2.4
2	B	457	LEU	2.4
4	E	28	TYR	2.4
6	H	20	TYR	2.4
1	A	80	HIS	2.4
1	A	399	HIS	2.4
1	A	63	ARG	2.4
2	B	576	ASP	2.4
2	B	878	GLN	2.4
3	C	268	ASP	2.4
7	I	30	ARG	2.4
1	A	254	GLU	2.4
2	B	229	ALA	2.4
3	C	141	GLY	2.4
2	B	372	SER	2.4
1	A	180	LYS	2.4
1	A	419	LYS	2.4
2	B	97	VAL	2.4
2	B	205	ILE	2.4
2	B	421	PHE	2.4
2	B	649	LYS	2.4
7	I	77	LYS	2.4
10	L	31	CYS	2.4
2	B	1171	VAL	2.4
6	H	9	ILE	2.4
1	A	598	LEU	2.4
2	B	416	LEU	2.4
2	B	812	LEU	2.4
4	E	164	LEU	2.4
1	A	45	GLN	2.4
1	A	206	GLU	2.4
1	A	1127	ASP	2.4
3	C	218	PRO	2.4
4	E	73	PRO	2.4
1	A	310	GLY	2.4
2	B	426	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	294	SER	2.4
2	B	62	ILE	2.4
2	B	1086	PHE	2.4
3	C	97	VAL	2.4
4	E	72	PHE	2.4
7	I	97	MET	2.4
1	A	426	LEU	2.4
1	A	1273	LEU	2.4
2	B	110	HIS	2.4
2	B	1177	HIS	2.4
1	A	968	GLN	2.4
3	C	267	GLN	2.4
4	E	4	GLU	2.4
1	A	417	TYR	2.3
1	A	672	ASP	2.3
8	J	64	ASN	2.3
2	B	231	PRO	2.3
1	A	1221	LYS	2.3
2	B	460	ALA	2.3
3	C	100	THR	2.3
4	E	95	THR	2.3
2	B	252	SER	2.3
4	E	68	SER	2.3
1	A	32	VAL	2.3
2	B	911	ILE	2.3
6	H	42	ILE	2.3
1	A	906	HIS	2.3
8	J	36	LEU	2.3
4	E	102	GLU	2.3
2	B	668	ASP	2.3
2	B	486	TYR	2.3
4	E	79	TRP	2.3
7	I	15	TYR	2.3
9	K	109	TRP	2.3
1	A	9	ALA	2.3
2	B	230	ALA	2.3
7	I	95	THR	2.3
7	I	73	ARG	2.3
1	A	71	GLN	2.3
1	A	106	VAL	2.3
1	A	405	VAL	2.3
1	A	972	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
7	I	62	ILE	2.3
1	A	1121	GLU	2.3
2	B	368	GLU	2.3
5	F	143	PHE	2.3
2	B	170	LEU	2.3
2	B	388	CYS	2.3
8	J	41	LEU	2.3
1	A	151	ASP	2.3
2	B	1136	ASP	2.3
3	C	60	ASP	2.3
3	C	226	ASP	2.3
5	F	106	PRO	2.3
2	B	201	GLY	2.3
1	A	292	ALA	2.3
5	F	115	THR	2.3
1	A	163	SER	2.3
2	B	267	ARG	2.3
6	H	19	ARG	2.3
1	A	313	GLN	2.3
1	A	1128	GLN	2.3
5	F	127	GLU	2.3
1	A	1263	ILE	2.3
2	B	276	ILE	2.3
3	C	248	ILE	2.3
2	B	305	VAL	2.3
3	C	49	VAL	2.3
6	H	118	PHE	2.3
3	C	72	LEU	2.3
1	A	692	ASP	2.3
6	H	34	ASP	2.3
2	B	124	TYR	2.3
3	C	229	TYR	2.3
1	A	982	THR	2.3
2	B	253	THR	2.3
9	K	107	THR	2.3
2	B	858	SER	2.3
1	A	566	ILE	2.3
1	A	577	ILE	2.3
1	A	1216	ILE	2.3
1	A	114	LEU	2.2
1	A	208	LEU	2.2
1	A	737	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	535	LEU	2.2
3	C	124	LEU	2.2
1	A	1206	ASP	2.2
1	A	1223	ASP	2.2
2	B	959	ASP	2.2
4	E	41	ASP	2.2
2	B	917	PRO	2.2
1	A	28	ARG	2.2
1	A	1079	MET	2.2
2	B	107	GLY	2.2
2	B	261	ARG	2.2
2	B	999	MET	2.2
2	B	937	ALA	2.2
2	B	1044	ALA	2.2
6	H	50	ALA	2.2
2	B	736	THR	2.2
7	I	18	GLU	2.2
1	A	1217	LYS	2.2
1	A	161	LEU	2.2
1	A	222	LEU	2.2
2	B	954	VAL	2.2
3	C	251	LEU	2.2
2	B	557	PHE	2.2
4	E	110	PHE	2.2
1	A	1013	ASP	2.2
2	B	131	ASP	2.2
2	B	790	ASP	2.2
8	J	16	ASP	2.2
9	K	110	ASN	2.2
2	B	940	PRO	2.2
2	B	1039	GLY	2.2
1	A	149	GLU	2.2
2	B	194	GLU	2.2
2	B	346	GLU	2.2
3	C	208	GLU	2.2
1	A	34	LYS	2.2
1	A	1377	THR	2.2
2	B	1077	THR	2.2
9	K	90	ALA	2.2
1	A	465	TYR	2.2
1	A	979	SER	2.2
2	B	666	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
4	E	13	TRP	2.2
3	C	144	ILE	2.2
1	A	388	LEU	2.2
1	A	588	LEU	2.2
4	E	37	LEU	2.2
10	L	64	LEU	2.2
4	E	141	VAL	2.2
1	A	22	PHE	2.2
3	C	178	PHE	2.2
1	A	583	PRO	2.2
1	A	168	GLY	2.2
1	A	160	GLN	2.2
1	A	1261	LYS	2.2
2	B	177	LYS	2.2
6	H	37	LYS	2.2
2	B	98	THR	2.2
2	B	594	ALA	2.2
2	B	680	THR	2.2
4	E	65	THR	2.2
2	B	890	TYR	2.2
2	B	1198	TYR	2.2
1	A	202	LEU	2.2
1	A	279	LEU	2.2
1	A	845	LEU	2.2
2	B	1095	LEU	2.2
3	C	11	ARG	2.2
6	H	121	LEU	2.2
10	L	63	ARG	2.2
1	A	177	ASP	2.2
1	A	211	PHE	2.2
2	B	429	PHE	2.2
1	A	243	PRO	2.2
1	A	76	GLU	2.2
5	F	114	GLU	2.2
6	H	36	CYS	2.2
1	A	284	ALA	2.2
2	B	777	ALA	2.2
2	B	1002	THR	2.2
3	C	227	THR	2.2
3	C	263	THR	2.2
6	H	56	THR	2.2
9	K	86	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	36	ARG	2.1
2	B	1192	TYR	2.1
7	I	17	ARG	2.1
1	A	99	ILE	2.1
2	B	222	ILE	2.1
2	B	1168	LEU	2.1
1	A	90	VAL	2.1
1	A	966	ASN	2.1
1	A	1283	VAL	2.1
3	C	119	VAL	2.1
3	C	196	ASP	2.1
1	A	895	LYS	2.1
1	A	977	LYS	2.1
2	B	856	PHE	2.1
3	C	228	PHE	2.1
4	E	118	PRO	2.1
1	A	256	GLN	2.1
1	A	587	HIS	2.1
2	B	1042	GLY	2.1
1	A	255	SER	2.1
2	B	463	THR	2.1
3	C	43	THR	2.1
3	C	168	ALA	2.1
2	B	730	ARG	2.1
1	A	141	LEU	2.1
3	C	29	MET	2.1
6	H	109	LYS	2.1
8	J	2	ILE	2.1
8	J	61	LEU	2.1
9	K	51	LEU	2.1
1	A	386	ASP	2.1
1	A	526	ASP	2.1
2	B	359	GLU	2.1
3	C	206	ASN	2.1
9	K	105	PHE	2.1
1	A	703	THR	2.1
1	A	1160	SER	2.1
1	A	830	LYS	2.1
2	B	839	MET	2.1
1	A	86	LEU	2.1
1	A	280	GLU	2.1
1	A	1116	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1301	GLU	2.1
1	A	42	ASP	2.1
1	A	156	ASP	2.1
1	A	1169	ILE	2.1
1	A	1408	ILE	2.1
2	B	912	ILE	2.1
2	B	953	LEU	2.1
4	E	190	LEU	2.1
2	B	113	TYR	2.1
2	B	986	GLN	2.1
4	E	101	GLN	2.1
1	A	731	ARG	2.1
1	A	31	SER	2.1
2	B	737	THR	2.1
1	A	533	LYS	2.1
2	B	422	LYS	2.1
1	A	1111	MET	2.1
6	H	138	GLU	2.1
1	A	534	LEU	2.1
1	A	606	LEU	2.1
2	B	122	LEU	2.1
1	A	169	ASN	2.1
3	C	117	ASP	2.1
4	E	99	HIS	2.1
2	B	619	ILE	2.1
1	A	1118	VAL	2.1
5	F	109	VAL	2.1
2	B	1164	GLY	2.1
7	I	27	PHE	2.1
4	E	94	LYS	2.0
5	F	76	LYS	2.0
10	L	37	LYS	2.0
1	A	131	SER	2.0
2	B	1170	THR	2.0
1	A	167	CYS	2.0
6	H	113	ALA	2.0
9	K	27	ALA	2.0
1	A	261	ASP	2.0
1	A	306	ASN	2.0
1	A	1373	ASP	2.0
2	B	119	LEU	2.0
2	B	566	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	724	ASP	2.0
2	B	1187	ASN	2.0
3	C	140	ASN	2.0
1	A	1163	ILE	2.0
9	K	95	ILE	2.0
2	B	57	TYR	2.0
3	C	57	VAL	2.0
4	E	80	VAL	2.0
1	A	496	GLU	2.0
1	A	1255	GLU	2.0
2	B	682	SER	2.0
3	C	50	GLU	2.0
4	E	58	MET	2.0
5	F	103	MET	2.0
10	L	41	SER	2.0
1	A	272	ALA	2.0
2	B	1173	ALA	2.0
3	C	59	ALA	2.0
1	A	83	HIS	2.0
2	B	667	GLN	2.0
2	B	941	LEU	2.0
3	C	262	LEU	2.0
4	E	39	LEU	2.0
4	E	165	LEU	2.0
6	H	16	ASP	2.0
6	H	92	ASP	2.0
1	A	337	ARG	2.0
1	A	630	ILE	2.0
1	A	1012	ARG	2.0
2	B	241	ARG	2.0
4	E	91	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 oligosaccharides in this entry.

6.4 Ligands

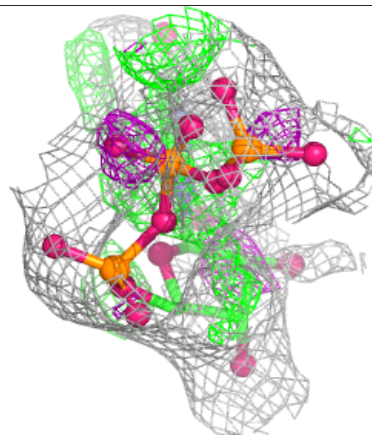
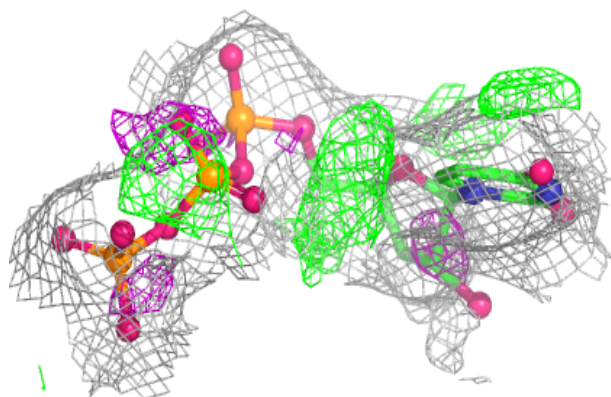
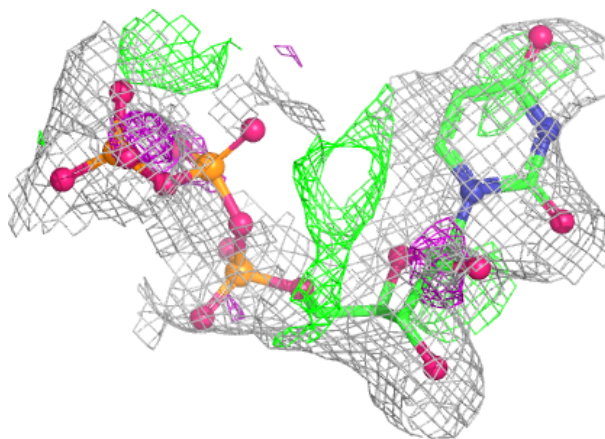
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	UTP	B	3571	29/29	0.79	0.14	53,61,64,65	0
11	ZN	A	3006	1/1	0.90	0.08	53,53,53,53	0
11	ZN	I	3003	1/1	0.93	0.05	58,58,58,58	0
11	ZN	A	3008	1/1	0.94	0.08	97,97,97,97	0
11	ZN	B	3007	1/1	0.94	0.06	55,55,55,55	0
11	ZN	J	3001	1/1	0.95	0.05	45,45,45,45	0
11	ZN	L	3005	1/1	0.95	0.06	89,89,89,89	0
11	ZN	C	3002	1/1	0.95	0.05	48,48,48,48	0
12	MN	A	3010	1/1	0.96	0.04	40,40,40,40	0
11	ZN	I	3004	1/1	0.96	0.06	74,74,74,74	0
12	MN	A	3009	1/1	0.97	0.12	44,44,44,44	0

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

Electron density around UTP B 3571:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.