



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:29 PM UTC

PDB ID : 1ARO / pdb_00001aro
Title : T7 RNA POLYMERASE COMPLEXED WITH T7 LYSOZYME
Authors : Steitz, T.; Jeruzalmi, D.
Deposited on : 1997-08-08
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

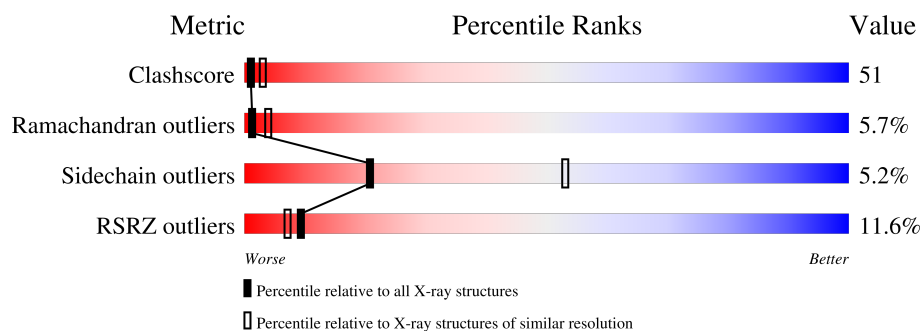
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7314 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 T7 RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	774	Total	C	N	O	S	161	0	0
			6124	3912	1065	1115	32			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	347	SER	CYS	conflict	UNP P00573
P	723	SER	CYS	engineered mutation	UNP P00573
P	839	SER	CYS	engineered mutation	UNP P00573

- Molecule 2 is a protein called T7 LYSOZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	149	Total	C	N	O	S	23	0	0
			1183	742	220	216	5			

- Molecule 3 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	6	Total	Hg	0	0
			6	6		
3	L	1	Total	Hg	0	0
			1	1		

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	273.38Å 95.61Å 63.58Å 90.00° 101.40° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.9 (30.00-2.80) 91.3 (30.00-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.54 (at 2.76Å)	Xtriage
Refinement program	CNS, X-PLOR	Depositor
R, R_{free}	0.262 , 0.309 0.274 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 77.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7314	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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.

4 Model quality

4.1 Standard geometry

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

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	P	0.93	19/6261 (0.3%)	1.50	118/8460 (1.4%)
2	L	0.67	0/1210	1.15	10/1630 (0.6%)
All	All	0.90	19/7471 (0.3%)	1.45	128/10090 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	10
2	L	0	1
All	All	0	11

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	559	VAL	C-N	-22.22	1.02	1.33
1	P	499	ASN	C-N	-17.02	1.09	1.33
1	P	74	ILE	N-CA	14.89	1.74	1.46
1	P	497	LEU	C-N	-14.72	1.13	1.33
1	P	58	GLN	C-O	13.39	1.39	1.23
1	P	9	ASN	C-N	-11.47	1.17	1.33
1	P	560	ASN	C-N	11.31	1.49	1.33
1	P	8	LYS	C-N	-10.02	1.19	1.33
1	P	58	GLN	CA-C	-9.96	1.36	1.52
1	P	58	GLN	CD-NE2	9.00	1.52	1.33
1	P	638	ALA	CA-C	7.96	1.56	1.52
1	P	74	ILE	CA-CB	7.89	1.75	1.54
1	P	74	ILE	CB-CG1	7.79	1.69	1.53
1	P	58	GLN	N-CA	-7.71	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	58	GLN	CG-CD	7.42	1.70	1.52
1	P	258	ALA	C-O	-6.60	1.15	1.23
1	P	550	LEU	C-N	6.13	1.42	1.33
1	P	132	THR	CA-CB	-5.80	1.48	1.53
1	P	635	MET	SD-CE	-5.48	1.65	1.79

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	559	VAL	O-C-N	-26.88	94.25	121.94
1	P	8	LYS	O-C-N	-20.31	90.50	123.00
1	P	559	VAL	CA-C-N	19.52	158.83	121.54
1	P	559	VAL	C-N-CA	19.52	158.83	121.54
1	P	8	LYS	CA-C-N	15.61	151.35	121.54
1	P	8	LYS	C-N-CA	15.61	151.35	121.54
1	P	497	LEU	O-C-N	-13.59	106.16	122.87
1	P	498	GLU	CB-CA-C	-13.38	83.79	110.42
1	P	499	ASN	CB-CA-C	12.53	136.76	110.32
1	P	497	LEU	CA-C-N	11.17	142.88	121.54
1	P	497	LEU	C-N-CA	11.17	142.88	121.54
1	P	767	SER	N-CA-C	10.86	125.21	110.55
1	P	74	ILE	CA-C-N	10.84	141.99	122.38
1	P	74	ILE	C-N-CA	10.84	141.99	122.38
1	P	751	PHE	N-CA-C	10.50	125.19	111.75
1	P	422	TRP	N-CA-C	-10.28	100.74	113.18
1	P	429	VAL	N-CA-C	10.13	121.00	110.36
1	P	30	GLU	N-CA-C	10.12	123.55	111.82
1	P	58	GLN	CB-CA-C	-9.98	89.02	111.77
1	P	256	THR	N-CA-C	9.55	122.67	111.02
1	P	162	PHE	N-CA-C	9.39	121.12	107.88
1	P	74	ILE	CA-CB-CG1	9.15	125.96	110.40
2	L	1071	GLY	N-CA-C	-8.90	102.88	115.43
1	P	713	LYS	N-CA-C	-8.78	101.54	113.30
1	P	499	ASN	O-C-N	-8.60	111.21	122.39
1	P	498	GLU	N-CA-CB	8.40	124.68	110.49
1	P	75	THR	N-CA-C	-8.29	102.88	113.16
1	P	499	ASN	CA-C-N	8.29	137.38	121.54
1	P	499	ASN	C-N-CA	8.29	137.38	121.54
1	P	107	GLN	N-CA-C	8.26	124.91	111.37
1	P	552	ASP	N-CA-CB	8.18	124.01	110.52
1	P	74	ILE	N-CA-CB	8.17	125.40	111.50
1	P	728	VAL	N-CA-C	8.14	119.57	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	640	GLY	N-CA-C	-8.10	99.69	111.03
2	L	1070	LYS	N-CA-C	8.09	122.63	109.76
1	P	257	ARG	N-CA-C	7.97	122.71	110.36
1	P	856	SER	N-CA-C	-7.90	105.62	114.62
1	P	9	ASN	CA-C-N	7.88	136.59	121.54
1	P	9	ASN	C-N-CA	7.88	136.59	121.54
1	P	402	LEU	N-CA-C	-7.81	103.56	113.72
1	P	281	ILE	N-CA-C	7.76	120.35	112.90
1	P	543	ILE	N-CA-C	-7.72	102.96	113.00
1	P	11	PHE	CB-CA-C	-7.69	95.87	109.71
1	P	74	ILE	N-CA-C	-7.58	89.79	111.00
1	P	388	ASP	N-CA-C	-7.52	104.61	114.31
1	P	690	VAL	N-CA-C	7.50	117.62	110.42
1	P	279	THR	N-CA-C	-7.38	97.30	108.52
1	P	259	GLY	CA-C-N	7.38	130.77	120.29
1	P	259	GLY	C-N-CA	7.38	130.77	120.29
1	P	560	ASN	CA-C-N	-7.29	111.20	122.49
1	P	560	ASN	C-N-CA	-7.29	111.20	122.49
1	P	74	ILE	CB-CA-C	-7.28	97.04	111.60
1	P	10	ASP	CB-CA-C	-7.27	95.95	110.42
1	P	97	GLY	N-CA-C	7.26	130.38	113.18
1	P	493	ALA	N-CA-C	-7.24	102.73	112.94
1	P	669	GLN	CA-C-N	7.24	128.89	119.84
1	P	669	GLN	C-N-CA	7.24	128.89	119.84
1	P	813	SER	N-CA-C	-7.21	96.42	108.75
1	P	733	PHE	CA-C-N	7.18	128.25	120.13
1	P	733	PHE	C-N-CA	7.18	128.25	120.13
1	P	614	LYS	N-CA-C	-7.06	105.09	113.21
1	P	465	ALA	N-CA-C	-7.03	103.23	111.03
1	P	10	ASP	N-CA-CB	-6.89	98.84	110.49
1	P	15	GLU	N-CA-C	-6.88	103.01	111.33
1	P	244	ILE	N-CA-C	6.88	121.94	113.00
1	P	332	LYS	N-CA-C	6.87	120.54	111.75
1	P	448	LYS	CA-C-N	-6.85	116.37	122.47
1	P	448	LYS	C-N-CA	-6.85	116.37	122.47
1	P	758	GLN	CA-C-N	6.83	126.79	120.03
1	P	758	GLN	C-N-CA	6.83	126.79	120.03
1	P	440	THR	N-CA-C	-6.81	103.94	111.36
1	P	311	VAL	N-CA-C	6.79	117.79	109.30
2	L	1039	GLN	N-CA-C	-6.68	105.12	113.20
1	P	702	ALA	N-CA-C	-6.58	104.51	112.54
1	P	269	GLN	CA-C-N	6.54	126.45	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	269	GLN	C-N-CA	6.54	126.45	119.85
1	P	313	MET	CA-C-N	6.42	125.65	118.97
1	P	313	MET	C-N-CA	6.42	125.65	118.97
1	P	9	ASN	CA-C-O	-6.41	111.35	120.51
1	P	129	ALA	N-CA-C	-6.35	105.59	113.15
1	P	74	ILE	CA-C-O	6.34	131.58	120.80
1	P	58	GLN	CA-C-O	-6.32	113.74	121.89
1	P	559	VAL	CB-CA-C	6.30	119.69	111.81
1	P	497	LEU	N-CA-C	-6.28	101.12	110.23
1	P	196	LEU	N-CA-C	6.21	119.37	108.56
1	P	548	ALA	N-CA-C	-6.15	104.20	111.03
1	P	449	GLY	N-CA-C	6.06	122.11	111.57
1	P	403	GLU	N-CA-C	-6.04	104.99	112.90
1	P	521	VAL	N-CA-C	-5.98	104.68	110.72
1	P	112	GLU	N-CA-C	-5.91	104.18	111.33
1	P	11	PHE	N-CA-CB	-5.88	101.80	110.85
1	P	860	LYS	N-CA-C	-5.83	102.96	111.30
1	P	260	ALA	N-CA-C	5.83	117.71	111.36
1	P	790	HIS	N-CA-C	-5.76	102.75	111.56
1	P	765	LYS	N-CA-C	5.75	119.59	112.58
1	P	658	ALA	N-CA-C	-5.74	106.41	113.41
2	L	1022	LYS	CA-C-N	5.74	125.44	119.82
2	L	1022	LYS	C-N-CA	5.74	125.44	119.82
1	P	755	PHE	N-CA-C	5.69	122.93	110.80
1	P	697	ASN	N-CA-C	-5.68	105.16	111.36
1	P	162	PHE	N-CA-CB	5.67	121.46	111.49
1	P	722	ARG	N-CA-C	-5.66	99.57	108.63
1	P	569	ASP	N-CA-C	5.60	118.57	110.28
1	P	9	ASN	O-C-N	-5.53	115.23	122.59
1	P	711	LYS	N-CA-C	5.53	119.03	112.72
1	P	551	ARG	CB-CA-C	5.52	121.41	110.42
1	P	875	ILE	N-CA-C	-5.50	104.86	112.50
1	P	92	VAL	N-CA-C	-5.49	105.15	110.42
1	P	103	PHE	N-CA-C	5.47	117.05	111.14
1	P	837	GLU	N-CA-C	-5.42	106.35	113.12
1	P	201	TRP	N-CA-C	5.39	119.02	109.96
1	P	784	HIS	N-CA-C	-5.35	105.45	111.28
2	L	1041	TRP	N-CA-C	5.33	118.08	109.40
1	P	259	GLY	O-C-N	-5.29	115.83	122.70
1	P	23	THR	N-CA-C	-5.21	106.61	113.12
1	P	27	HIS	N-CA-C	5.20	121.87	110.80
2	L	1037	LYS	N-CA-C	-5.18	104.89	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	542	GLY	N-CA-C	-5.17	100.92	113.18
1	P	524	HIS	N-CA-C	-5.14	106.93	114.39
2	L	1050	ILE	N-CA-C	5.12	114.95	107.37
2	L	1070	LYS	CA-CB-CG	-5.11	103.88	114.10
2	L	1064	ALA	N-CA-C	5.11	117.77	109.24
1	P	681	ILE	CB-CA-C	-5.06	105.49	111.97
1	P	244	ILE	CB-CA-C	-5.06	96.33	111.05
1	P	292	ARG	CA-C-N	5.02	125.29	119.92
1	P	292	ARG	C-N-CA	5.02	125.29	119.92
1	P	528	TYR	N-CA-C	5.02	117.71	110.28
1	P	700	LYS	N-CA-C	-5.02	106.26	112.38

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	1046	TYR	Sidechain
1	P	162	PHE	Sidechain
1	P	497	LEU	Peptide,Mainchain
1	P	499	ASN	Peptide
1	P	559	VAL	Peptide,Mainchain
1	P	74	ILE	Mainchain
1	P	8	LYS	Peptide,Mainchain
1	P	9	ASN	Mainchain

4.2 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	P	6124	0	6086	618	1
2	L	1183	0	1156	97	0
3	L	1	0	0	0	0
3	P	6	0	0	2	0
All	All	7314	0	7242	709	1

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 51.

All (709) 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:P:74:ILE:CB	1:P:74:ILE:CA	1.75	1.55
1:P:73:LEU:C	1:P:74:ILE:HA	1.18	1.50
1:P:74:ILE:CA	1:P:74:ILE:N	1.74	1.45
1:P:74:ILE:N	1:P:75:THR:H	1.10	1.40
1:P:74:ILE:N	1:P:75:THR:N	1.82	1.25
1:P:28:TYR:CE1	1:P:183:MET:HB2	1.71	1.25
1:P:73:LEU:C	1:P:74:ILE:CA	2.10	1.23
1:P:58:GLN:C	1:P:59:LEU:N	2.01	1.19
1:P:162:PHE:CE2	1:P:163:LYS:HB2	1.79	1.17
1:P:230:HIS:CD2	1:P:245:GLU:HG3	1.81	1.16
1:P:162:PHE:CD2	1:P:163:LYS:N	2.17	1.13
2:L:1020:ALA:HB1	2:L:1085:ILE:HD12	1.31	1.11
1:P:871:ASN:HB2	1:P:875:ILE:HG21	1.30	1.08
1:P:499:ASN:O	1:P:501:TRP:N	1.90	1.02
1:P:186:VAL:HG21	1:P:325:ASN:HD21	1.20	1.01
1:P:473:VAL:CG2	1:P:474:PRO:HD2	1.92	0.99
1:P:452:ILE:HD12	1:P:452:ILE:H	1.28	0.98
1:P:324:GLN:NE2	1:P:418:TYR:H	1.61	0.97
1:P:162:PHE:CD2	1:P:163:LYS:HB2	2.00	0.96
1:P:550:LEU:HD12	1:P:691:ALA:HB1	1.45	0.95
1:P:269:GLN:HG2	1:P:404:GLN:HE22	1.31	0.95
1:P:473:VAL:HG22	1:P:474:PRO:HD2	1.48	0.95
1:P:186:VAL:HG21	1:P:325:ASN:ND2	1.81	0.95
1:P:132:THR:OG1	1:P:244:ILE:CG2	2.16	0.94
1:P:132:THR:CB	1:P:244:ILE:CG2	2.45	0.94
1:P:324:GLN:HE21	1:P:418:TYR:N	1.66	0.94
1:P:298:ARG:HH12	1:P:419:ASN:HB3	1.33	0.94
1:P:562:LEU:HG	1:P:876:LEU:HD11	1.49	0.93
1:P:530:CYS:HG	3:P:905:HG:HG	1.04	0.93
1:P:711:LYS:H	1:P:857:GLN:HE22	1.17	0.93
1:P:28:TYR:CE2	1:P:32:LEU:HD13	2.04	0.93
1:P:187:GLU:O	1:P:277:PRO:HG3	1.70	0.91
1:P:162:PHE:HE2	1:P:163:LYS:HB2	1.32	0.91
1:P:637:LEU:O	1:P:696:MET:HE2	1.69	0.91
1:P:826:LYS:HG2	1:P:829:ARG:HH22	1.33	0.91
1:P:278:TRP:H	1:P:321:ASN:HD21	1.17	0.91
1:P:74:ILE:N	1:P:74:ILE:C	2.29	0.91
1:P:266:PRO:HD2	1:P:404:GLN:NE2	1.86	0.90
1:P:162:PHE:HD2	1:P:163:LYS:H	1.15	0.90
1:P:728:VAL:H	1:P:848:GLN:HE22	1.18	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:74:ILE:CB	1:P:74:ILE:C	2.44	0.89
1:P:646:PHE:O	1:P:650:VAL:HG23	1.72	0.89
1:P:539:SER:O	1:P:540:CYS:SG	2.30	0.88
1:P:534:LEU:HD11	1:P:818:PRO:HG3	1.56	0.88
1:P:133:THR:HG22	1:P:135:GLN:H	1.38	0.88
1:P:648:GLN:O	1:P:652:GLU:HB2	1.73	0.87
1:P:28:TYR:CD2	1:P:32:LEU:HD13	2.09	0.87
1:P:132:THR:OG1	1:P:244:ILE:HG23	1.74	0.86
2:L:1137:ARG:HD3	2:L:1141:LYS:HD2	1.57	0.86
2:L:1052:ARG:HA	2:L:1099:GLN:OE1	1.75	0.86
1:P:36:GLN:HE21	1:P:273:VAL:HG22	1.38	0.86
1:P:115:ALA:O	1:P:119:ILE:HG13	1.75	0.86
1:P:87:ASP:O	1:P:91:GLU:HG3	1.75	0.86
1:P:642:LYS:HA	1:P:682:TRP:CZ3	2.11	0.85
1:P:298:ARG:NH1	1:P:419:ASN:HB3	1.92	0.84
1:P:306:MET:HE3	1:P:309:GLU:OE1	1.77	0.84
2:L:1091:PHE:HB2	2:L:1132:SER:HB2	1.60	0.84
1:P:19:ILE:HD12	1:P:19:ILE:H	1.41	0.84
1:P:28:TYR:HE1	1:P:183:MET:HB2	1.35	0.84
1:P:324:GLN:HE21	1:P:418:TYR:H	0.86	0.84
1:P:452:ILE:HG22	1:P:456:GLY:HA3	1.60	0.83
1:P:74:ILE:CA	1:P:74:ILE:HB	2.06	0.83
1:P:642:LYS:O	1:P:644:PHE:N	2.11	0.83
1:P:36:GLN:NE2	1:P:273:VAL:HG22	1.93	0.83
1:P:93:LYS:C	1:P:95:LYS:H	1.86	0.82
1:P:816:THR:HG22	1:P:817:ILE:H	1.43	0.82
1:P:551:ARG:NH2	1:P:836:TYR:O	2.13	0.82
1:P:763:THR:HG22	1:P:765:LYS:H	1.42	0.82
2:L:1002:ARG:HG2	2:L:1002:ARG:HH11	1.45	0.82
1:P:401:MET:CE	1:P:432:PHE:HA	2.11	0.81
1:P:28:TYR:CE2	1:P:183:MET:HE3	2.16	0.81
1:P:185:VAL:HB	1:P:274:PRO:HB2	1.62	0.81
1:P:399:GLU:O	1:P:403:GLU:HG2	1.81	0.81
1:P:233:ASN:C	1:P:756:ARG:O	2.25	0.80
1:P:93:LYS:O	1:P:95:LYS:N	2.14	0.80
1:P:750:MET:O	1:P:750:MET:HG2	1.83	0.79
1:P:132:THR:CB	1:P:244:ILE:HG23	2.12	0.79
1:P:401:MET:HE1	1:P:432:PHE:HA	1.65	0.79
1:P:636:THR:CG2	1:P:640:GLY:HA3	2.12	0.79
1:P:560:ASN:OD1	1:P:568:GLN:O	2.01	0.79
1:P:201:TRP:HE1	1:P:305:LEU:HD12	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:500:THR:HG22	1:P:500:THR:O	1.83	0.78
1:P:74:ILE:N	1:P:75:THR:HG23	1.98	0.78
1:P:186:VAL:HG23	1:P:325:ASN:OD1	1.84	0.78
1:P:232:GLN:O	1:P:233:ASN:OD1	2.02	0.78
1:P:147:ASP:OD1	1:P:292:ARG:HD2	1.84	0.77
1:P:473:VAL:HG22	1:P:474:PRO:CD	2.14	0.77
1:P:231:ARG:O	1:P:231:ARG:HG3	1.83	0.77
1:P:313:MET:SD	1:P:733:PHE:HA	2.24	0.77
1:P:162:PHE:CD2	1:P:163:LYS:CB	2.68	0.77
1:P:631:LYS:HA	1:P:634:VAL:HG12	1.67	0.77
1:P:871:ASN:HB2	1:P:875:ILE:CG2	2.13	0.77
1:P:797:TRP:CE2	1:P:801:LYS:HG3	2.19	0.77
1:P:185:VAL:H	1:P:274:PRO:HG2	1.50	0.77
2:L:1028:GLY:O	2:L:1032:ILE:HG12	1.85	0.77
1:P:534:LEU:CD1	1:P:818:PRO:HG3	2.15	0.76
1:P:215:ARG:HG3	1:P:219:MET:HE2	1.66	0.76
1:P:872:LEU:O	1:P:875:ILE:N	2.16	0.76
1:P:574:VAL:HG12	1:P:630:THR:HG21	1.68	0.76
1:P:422:TRP:CE2	1:P:423:ARG:HG3	2.21	0.76
1:P:643:GLU:HA	1:P:646:PHE:CD1	2.20	0.76
2:L:1060:ARG:NH1	2:L:1066:GLY:HA2	2.00	0.76
1:P:511:PHE:O	1:P:514:PHE:HB3	1.84	0.75
1:P:636:THR:HG21	1:P:640:GLY:HA3	1.67	0.75
1:P:452:ILE:HD12	1:P:452:ILE:N	2.00	0.75
2:L:1100:MET:HE3	2:L:1138:TRP:CE2	2.20	0.75
1:P:125:CYS:HG	3:P:904:HG:HG	1.28	0.75
1:P:185:VAL:HG12	1:P:185:VAL:O	1.84	0.75
1:P:579:ASN:OD1	1:P:625:VAL:HB	1.87	0.74
1:P:810:ILE:HG13	1:P:813:SER:OG	1.87	0.74
2:L:1028:GLY:H	2:L:1031:GLU:HG2	1.52	0.74
1:P:213:GLY:O	1:P:217:ILE:HG13	1.86	0.74
1:P:266:PRO:HD2	1:P:404:GLN:HE21	1.50	0.74
1:P:269:GLN:HG2	1:P:404:GLN:NE2	2.03	0.74
1:P:269:GLN:CG	1:P:404:GLN:HE22	2.00	0.74
1:P:613:THR:O	1:P:616:LEU:HG	1.88	0.73
1:P:74:ILE:CA	1:P:74:ILE:CG2	2.66	0.73
1:P:77:LEU:HD21	1:P:250:TYR:CE2	2.23	0.73
1:P:84:ARG:HG3	1:P:223:SER:HB3	1.68	0.73
1:P:616:LEU:C	1:P:618:GLY:H	1.96	0.73
1:P:186:VAL:CG2	1:P:325:ASN:OD1	2.36	0.73
1:P:433:ASN:C	1:P:433:ASN:HD22	1.93	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:586:ALA:HB3	1:P:617:ALA:HB2	1.68	0.72
1:P:129:ALA:HA	1:P:389:LYS:HE2	1.71	0.72
1:P:160:LYS:C	1:P:162:PHE:N	2.46	0.72
1:P:645:GLY:O	1:P:649:GLN:HG3	1.89	0.72
1:P:34:ARG:NH2	1:P:162:PHE:O	2.22	0.72
1:P:810:ILE:HG13	1:P:810:ILE:O	1.89	0.71
1:P:74:ILE:CG1	1:P:74:ILE:O	2.37	0.71
1:P:627:ARG:HH11	1:P:627:ARG:HG2	1.54	0.71
1:P:855:GLU:OE1	2:L:1030:ARG:HD2	1.90	0.71
1:P:562:LEU:CG	1:P:876:LEU:HD11	2.20	0.71
2:L:1096:THR:HG22	2:L:1098:ALA:H	1.55	0.71
1:P:473:VAL:HG23	1:P:474:PRO:HD2	1.72	0.71
2:L:1028:GLY:H	2:L:1031:GLU:CG	2.04	0.71
1:P:230:HIS:CD2	1:P:245:GLU:CG	2.69	0.71
1:P:433:ASN:ND2	1:P:435:GLN:H	1.88	0.70
1:P:631:LYS:HA	1:P:634:VAL:CG1	2.21	0.70
1:P:871:ASN:CB	1:P:875:ILE:HG12	2.21	0.70
2:L:1121:ALA:O	2:L:1124:GLU:HB3	1.89	0.70
1:P:28:TYR:CD1	1:P:183:MET:HB2	2.27	0.70
1:P:84:ARG:CG	1:P:223:SER:HB3	2.20	0.70
1:P:298:ARG:HG3	1:P:298:ARG:HH11	1.57	0.70
1:P:132:THR:HB	1:P:244:ILE:CG2	2.20	0.69
1:P:249:GLU:HG3	1:P:250:TYR:CD1	2.27	0.69
2:L:1020:ALA:CB	2:L:1085:ILE:HD12	2.18	0.69
1:P:132:THR:CB	1:P:244:ILE:HG22	2.23	0.68
2:L:1017:HIS:CE1	2:L:1122:HIS:CD2	2.81	0.68
1:P:577:LYS:NZ	1:P:581:ILE:HD11	2.08	0.68
1:P:636:THR:O	1:P:640:GLY:O	2.11	0.68
1:P:741:LYS:O	1:P:767:SER:HB3	1.92	0.68
1:P:571:TYR:HD1	1:P:634:VAL:HG11	1.58	0.68
1:P:630:THR:HG23	1:P:681:ILE:HD12	1.76	0.68
2:L:1017:HIS:HE1	2:L:1122:HIS:CD2	2.11	0.68
1:P:229:LEU:HD23	1:P:230:HIS:N	2.09	0.68
1:P:89:PHE:O	1:P:103:PHE:HZ	1.75	0.68
1:P:630:THR:HG22	1:P:630:THR:O	1.94	0.68
1:P:690:VAL:O	1:P:693:VAL:HG12	1.94	0.67
1:P:664:GLY:HA2	1:P:666:MET:SD	2.34	0.67
1:P:81:MET:HE2	1:P:220:LEU:HA	1.74	0.67
1:P:391:ARG:HH11	1:P:391:ARG:HB3	1.60	0.67
1:P:160:LYS:O	1:P:161:HIS:C	2.38	0.67
1:P:108:GLU:HG2	1:P:108:GLU:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:186:VAL:HG21	1:P:325:ASN:CG	2.20	0.67
1:P:201:TRP:NE1	1:P:305:LEU:HD12	2.08	0.67
1:P:81:MET:HB3	1:P:115:ALA:HB1	1.76	0.66
1:P:636:THR:O	1:P:636:THR:HG22	1.93	0.66
1:P:15:GLU:O	1:P:19:ILE:CD1	2.42	0.66
1:P:227:VAL:HG12	1:P:246:LEU:HD23	1.78	0.66
1:P:458:TYR:CD1	1:P:479:ILE:HD11	2.31	0.66
1:P:401:MET:HE1	1:P:431:MET:O	1.96	0.65
1:P:441:LYS:HE2	1:P:810:ILE:HD12	1.77	0.65
1:P:42:GLU:HG2	1:P:50:ARG:NH1	2.12	0.65
1:P:230:HIS:O	1:P:231:ARG:HB3	1.95	0.65
1:P:77:LEU:HA	1:P:224:THR:HG21	1.77	0.65
1:P:421:ASP:HB3	1:P:423:ARG:H	1.61	0.65
1:P:19:ILE:HG21	1:P:192:SER:HB3	1.78	0.65
1:P:58:GLN:O	1:P:59:LEU:N	2.28	0.65
1:P:763:THR:HG22	1:P:764:ASN:N	2.12	0.65
1:P:132:THR:HG21	1:P:244:ILE:HG22	1.77	0.65
1:P:24:LEU:HD21	1:P:287:TRP:CD2	2.32	0.65
1:P:586:ALA:CB	1:P:617:ALA:HB2	2.27	0.64
1:P:722:ARG:HE	1:P:771:ALA:HB2	1.62	0.64
1:P:76:THR:O	1:P:79:PRO:HD2	1.95	0.64
1:P:148:GLU:O	1:P:152:GLY:N	2.30	0.64
1:P:740:LYS:HB3	1:P:767:SER:HB2	1.79	0.64
1:P:544:GLN:HE22	1:P:561:LEU:HD12	1.61	0.64
2:L:1029:VAL:N	2:L:1049:ILE:HD11	2.12	0.64
2:L:1034:GLN:HE21	2:L:1034:GLN:C	2.05	0.64
1:P:15:GLU:O	1:P:19:ILE:HD12	1.97	0.64
1:P:278:TRP:H	1:P:321:ASN:ND2	1.92	0.64
1:P:796:VAL:O	1:P:800:GLU:HG3	1.98	0.63
1:P:316:VAL:HG22	1:P:731:ASP:OD2	1.98	0.63
1:P:660:ASP:OD1	1:P:661:SER:N	2.31	0.63
1:P:721:LYS:HB3	2:L:1038:GLU:OE2	1.98	0.63
1:P:752:LEU:O	1:P:752:LEU:HG	1.97	0.63
1:P:211:HIS:HA	1:P:214:VAL:HG12	1.81	0.62
1:P:28:TYR:HE2	1:P:32:LEU:HD13	1.58	0.62
1:P:132:THR:OG1	1:P:244:ILE:HG21	1.97	0.62
1:P:206:LYS:HB2	1:P:206:LYS:NZ	2.14	0.62
2:L:1046:TYR:CZ	2:L:1080:CYS:SG	2.92	0.62
1:P:613:THR:C	1:P:615:ALA:H	2.04	0.62
1:P:42:GLU:O	1:P:120:LYS:HE3	1.98	0.62
1:P:829:ARG:HD2	1:P:877:GLU:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:450:LYS:HB2	1:P:819:ALA:CB	2.30	0.62
2:L:1060:ARG:NH1	2:L:1065:VAL:O	2.32	0.62
1:P:160:LYS:O	1:P:162:PHE:N	2.33	0.62
1:P:74:ILE:O	1:P:74:ILE:HG13	1.99	0.62
2:L:1125:VAL:HG12	2:L:1125:VAL:O	1.98	0.62
2:L:1137:ARG:HH11	2:L:1141:LYS:HE3	1.64	0.62
1:P:132:THR:HB	1:P:244:ILE:HG23	1.81	0.61
1:P:185:VAL:O	1:P:187:GLU:OE2	2.18	0.61
1:P:211:HIS:O	1:P:214:VAL:HG12	1.99	0.61
1:P:28:TYR:CZ	1:P:183:MET:HE3	2.36	0.61
1:P:335:LEU:HD11	1:P:406:ASN:HD21	1.65	0.61
1:P:711:LYS:H	1:P:857:GLN:NE2	1.94	0.61
1:P:458:TYR:CE1	1:P:479:ILE:HD11	2.36	0.60
1:P:162:PHE:HD2	1:P:163:LYS:CB	2.14	0.60
1:P:9:ASN:O	1:P:11:PHE:N	2.35	0.60
1:P:81:MET:HE2	1:P:220:LEU:CA	2.31	0.60
1:P:118:THR:HG23	1:P:141:ILE:HD13	1.84	0.60
1:P:220:LEU:HD21	1:P:226:MET:HE2	1.82	0.60
1:P:631:LYS:CA	1:P:634:VAL:HG12	2.31	0.60
1:P:636:THR:HG22	1:P:640:GLY:CA	2.31	0.60
1:P:457:TYR:CD1	1:P:521:VAL:HG11	2.36	0.60
2:L:1134:ASP:OD1	2:L:1137:ARG:HB2	2.01	0.60
1:P:872:LEU:O	1:P:874:ASP:N	2.35	0.60
2:L:1141:LYS:C	2:L:1143:GLU:H	2.09	0.60
1:P:132:THR:CG2	1:P:244:ILE:HG22	2.32	0.59
1:P:534:LEU:O	1:P:815:GLY:HA3	2.01	0.59
1:P:825:PHE:HD1	1:P:825:PHE:H	1.50	0.59
1:P:636:THR:HG22	1:P:640:GLY:HA3	1.84	0.59
1:P:36:GLN:HE22	1:P:271:CYS:HB3	1.67	0.59
1:P:249:GLU:HG3	1:P:250:TYR:H	1.67	0.59
1:P:298:ARG:HH12	1:P:419:ASN:CB	2.12	0.59
1:P:737:GLN:NE2	1:P:781:ASN:OD1	2.35	0.59
1:P:797:TRP:NE1	1:P:801:LYS:HG3	2.18	0.59
1:P:28:TYR:CD2	1:P:183:MET:HE3	2.38	0.59
1:P:446:LEU:HB2	1:P:531:SER:O	2.02	0.59
1:P:550:LEU:CD1	1:P:691:ALA:HB1	2.25	0.59
1:P:133:THR:HG22	1:P:135:GLN:N	2.12	0.59
1:P:633:SER:HB2	1:P:646:PHE:CD2	2.37	0.59
1:P:843:ALA:O	1:P:846:TYR:HB3	2.03	0.59
1:P:489:ILE:HG23	1:P:515:CYS:SG	2.43	0.59
1:P:616:LEU:C	1:P:618:GLY:N	2.61	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:28:TYR:HD1	1:P:185:VAL:CG2	2.15	0.58
1:P:433:ASN:C	1:P:433:ASN:ND2	2.57	0.58
1:P:550:LEU:HD12	1:P:691:ALA:CB	2.29	0.58
1:P:185:VAL:O	1:P:185:VAL:CG1	2.51	0.58
1:P:580:GLU:O	1:P:584:ALA:HB2	2.04	0.58
1:P:500:THR:O	1:P:500:THR:CG2	2.51	0.58
1:P:93:LYS:C	1:P:95:LYS:N	2.51	0.58
1:P:288:ALA:O	1:P:291:ARG:HG2	2.03	0.58
1:P:455:GLU:O	1:P:456:GLY:C	2.45	0.58
1:P:689:VAL:HG23	1:P:689:VAL:O	2.04	0.58
1:P:814:PHE:HE2	1:P:824:LEU:HD22	1.69	0.58
1:P:769:ILE:CG2	1:P:770:ASP:N	2.67	0.57
1:P:19:ILE:H	1:P:19:ILE:CD1	2.15	0.57
1:P:104:GLN:O	1:P:104:GLN:HG2	2.04	0.57
1:P:631:LYS:O	1:P:634:VAL:HG12	2.05	0.57
2:L:1122:HIS:C	2:L:1124:GLU:H	2.12	0.57
1:P:28:TYR:HD2	1:P:32:LEU:HD13	1.68	0.57
1:P:120:LYS:NZ	1:P:267:MET:HA	2.19	0.57
1:P:335:LEU:HD21	1:P:406:ASN:HD22	1.69	0.57
1:P:574:VAL:HG12	1:P:630:THR:CG2	2.34	0.57
1:P:577:LYS:HZ3	1:P:581:ILE:HD11	1.68	0.57
1:P:720:ARG:HD3	2:L:1034:GLN:OE1	2.04	0.57
1:P:480:LYS:O	1:P:481:PHE:C	2.47	0.57
1:P:846:TYR:HB2	1:P:864:LEU:HD21	1.87	0.57
2:L:1029:VAL:HG13	2:L:1030:ARG:N	2.19	0.57
1:P:763:THR:CG2	1:P:764:ASN:N	2.68	0.56
1:P:856:SER:HA	1:P:859:ASP:CG	2.30	0.56
1:P:111:PRO:HA	1:P:114:VAL:HB	1.86	0.56
1:P:230:HIS:HD2	1:P:245:GLU:HG3	1.57	0.56
1:P:543:ILE:HG22	1:P:559:VAL:HG21	1.87	0.56
1:P:740:LYS:HB3	1:P:767:SER:CB	2.35	0.56
2:L:1132:SER:O	2:L:1147:SER:O	2.23	0.56
1:P:497:LEU:O	1:P:499:ASN:N	2.33	0.56
1:P:28:TYR:CD2	1:P:32:LEU:CD1	2.86	0.56
1:P:133:THR:O	1:P:134:VAL:C	2.49	0.56
2:L:1072:TYR:CE2	2:L:1125:VAL:HG11	2.40	0.56
1:P:24:LEU:HD21	1:P:287:TRP:CE2	2.41	0.56
2:L:1036:HIS:CD2	2:L:1045:GLY:H	2.24	0.56
2:L:1092:ASP:O	2:L:1094:ASN:N	2.39	0.56
1:P:14:ILE:O	1:P:15:GLU:C	2.49	0.56
1:P:871:ASN:HB2	1:P:875:ILE:HG12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1133:PHE:HE1	2:L:1135:LEU:HD12	1.71	0.56
1:P:77:LEU:HD21	1:P:250:TYR:CZ	2.40	0.56
1:P:550:LEU:O	1:P:551:ARG:HB2	2.06	0.56
1:P:793:LYS:HB3	1:P:793:LYS:NZ	2.21	0.56
1:P:19:ILE:CG2	1:P:192:SER:HB3	2.35	0.56
2:L:1022:LYS:H	2:L:1025:GLN:HE21	1.54	0.56
1:P:452:ILE:HD11	1:P:528:TYR:O	2.05	0.55
2:L:1002:ARG:HH11	2:L:1002:ARG:CG	2.16	0.55
1:P:856:SER:O	1:P:859:ASP:N	2.37	0.55
2:L:1035:TRP:O	2:L:1038:GLU:HB2	2.07	0.55
1:P:390:ALA:O	1:P:394:ARG:HG3	2.06	0.55
1:P:571:TYR:CD1	1:P:631:LYS:HB2	2.41	0.55
1:P:682:TRP:HA	1:P:685:VAL:HG22	1.88	0.55
1:P:249:GLU:HG3	1:P:250:TYR:HD1	1.70	0.55
1:P:452:ILE:H	1:P:452:ILE:CD1	1.98	0.55
1:P:574:VAL:O	1:P:578:VAL:HG23	2.07	0.55
1:P:182:PHE:HE2	1:P:413:ALA:HB2	1.71	0.55
1:P:532:LEU:C	1:P:532:LEU:HD23	2.31	0.55
1:P:870:LEU:O	1:P:871:ASN:C	2.49	0.55
2:L:1135:LEU:N	2:L:1150:GLY:O	2.34	0.55
1:P:690:VAL:HG13	1:P:691:ALA:N	2.22	0.55
1:P:754:GLN:HG3	1:P:755:PHE:CE2	2.41	0.55
2:L:1107:LEU:HD22	2:L:1119:LEU:HD13	1.89	0.55
1:P:685:VAL:C	1:P:687:VAL:H	2.14	0.55
1:P:232:GLN:CD	1:P:755:PHE:CE1	2.85	0.54
1:P:452:ILE:HG23	1:P:818:PRO:HB2	1.88	0.54
1:P:517:GLU:O	1:P:521:VAL:HG23	2.07	0.54
1:P:85:ILE:HD12	1:P:115:ALA:HB2	1.89	0.54
1:P:162:PHE:CD2	1:P:163:LYS:CA	2.89	0.54
1:P:838:SER:O	1:P:839:SER:HB3	2.07	0.54
2:L:1019:SER:HB2	2:L:1021:THR:HG23	1.89	0.54
1:P:74:ILE:N	1:P:75:THR:HG1	2.06	0.54
1:P:631:LYS:C	1:P:634:VAL:HG12	2.32	0.54
2:L:1017:HIS:CE1	2:L:1130:CYS:SG	3.00	0.54
2:L:1136:LYS:O	2:L:1140:GLU:HG3	2.08	0.54
1:P:101:THR:HG22	1:P:101:THR:O	2.06	0.54
1:P:552:ASP:OD2	1:P:690:VAL:HG12	2.08	0.54
1:P:664:GLY:O	1:P:666:MET:N	2.41	0.54
1:P:335:LEU:HD11	1:P:406:ASN:ND2	2.23	0.54
1:P:395:ARG:HG2	1:P:395:ARG:HH11	1.72	0.54
1:P:452:ILE:CD1	1:P:528:TYR:O	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:814:PHE:CE2	1:P:824:LEU:HD22	2.42	0.53
1:P:878:SER:O	1:P:879:ASP:HB2	2.08	0.53
2:L:1008:ARG:HD2	2:L:1075:ASN:HA	1.88	0.53
1:P:182:PHE:CE2	1:P:413:ALA:HB2	2.43	0.53
1:P:229:LEU:HD23	1:P:230:HIS:H	1.73	0.53
1:P:873:ARG:O	1:P:876:LEU:HB2	2.08	0.53
1:P:45:GLU:HB3	1:P:155:ARG:HH21	1.73	0.53
1:P:129:ALA:HB2	1:P:393:SER:OG	2.09	0.53
1:P:160:LYS:O	1:P:162:PHE:HA	2.09	0.53
1:P:331:ASN:OD1	1:P:334:VAL:HG23	2.08	0.53
1:P:570:ILE:HG23	1:P:571:TYR:N	2.24	0.53
1:P:747:LEU:HD21	1:P:761:ILE:HD11	1.90	0.53
1:P:480:LYS:O	1:P:482:ILE:N	2.42	0.53
1:P:744:GLN:HA	1:P:764:ASN:ND2	2.23	0.53
1:P:872:LEU:O	1:P:873:ARG:C	2.51	0.53
1:P:856:SER:O	1:P:857:GLN:C	2.50	0.53
2:L:1086:ASP:O	2:L:1088:LYS:N	2.42	0.53
1:P:690:VAL:O	1:P:694:GLU:HG3	2.09	0.52
1:P:810:ILE:O	1:P:813:SER:OG	2.20	0.52
1:P:35:GLU:OE2	1:P:411:HIS:HE1	1.91	0.52
1:P:710:VAL:HG13	1:P:857:GLN:OE1	2.09	0.52
1:P:728:VAL:H	1:P:848:GLN:NE2	1.98	0.52
1:P:808:ALA:O	1:P:814:PHE:HA	2.09	0.52
2:L:1072:TYR:HE2	2:L:1125:VAL:HG11	1.73	0.52
1:P:425:ARG:HB2	1:P:427:TYR:HE1	1.75	0.52
2:L:1060:ARG:HH11	2:L:1066:GLY:HA2	1.73	0.52
1:P:855:GLU:HA	2:L:1030:ARG:CD	2.40	0.52
1:P:871:ASN:O	1:P:872:LEU:C	2.51	0.52
2:L:1020:ALA:HB1	2:L:1085:ILE:CD1	2.22	0.52
1:P:132:THR:CG2	1:P:244:ILE:CG2	2.88	0.52
1:P:553:GLU:O	1:P:556:GLY:N	2.42	0.52
2:L:1068:HIS:CG	2:L:1069:ALA:N	2.77	0.52
1:P:132:THR:HG21	1:P:244:ILE:CG2	2.39	0.52
1:P:877:GLU:C	1:P:879:ASP:N	2.66	0.52
1:P:509:PHE:C	1:P:511:PHE:H	2.18	0.52
1:P:525:GLY:C	1:P:527:SER:H	2.17	0.52
2:L:1070:LYS:HG2	2:L:1073:ASN:HD21	1.75	0.52
1:P:458:TYR:O	1:P:461:LYS:HB2	2.10	0.52
1:P:571:TYR:HD1	1:P:634:VAL:CG1	2.23	0.51
1:P:797:TRP:CD1	1:P:801:LYS:HG3	2.46	0.51
1:P:77:LEU:O	1:P:81:MET:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:313:MET:HE1	1:P:733:PHE:CD1	2.45	0.51
1:P:782:PHE:O	1:P:785:SER:HB3	2.10	0.51
1:P:83:ALA:O	1:P:86:ASN:N	2.30	0.51
1:P:92:VAL:O	1:P:94:ALA:N	2.43	0.51
1:P:511:PHE:O	1:P:514:PHE:N	2.43	0.51
1:P:399:GLU:O	1:P:403:GLU:CG	2.56	0.51
1:P:473:VAL:CG2	1:P:474:PRO:CD	2.76	0.51
1:P:646:PHE:CE1	1:P:682:TRP:HE3	2.29	0.51
1:P:18:ALA:HB1	1:P:22:ASN:ND2	2.26	0.51
1:P:43:SER:HA	1:P:120:LYS:NZ	2.26	0.51
1:P:232:GLN:NE2	1:P:755:PHE:CE1	2.79	0.51
1:P:260:ALA:C	1:P:262:ALA:H	2.19	0.51
1:P:678:ALA:O	1:P:679:LYS:C	2.54	0.51
2:L:1095:PHE:HE2	2:L:1133:PHE:HD2	1.59	0.51
2:L:1029:VAL:N	2:L:1049:ILE:CD1	2.74	0.51
1:P:109:ILE:HD13	1:P:145:ILE:HG23	1.93	0.50
1:P:294:LEU:CD2	1:P:429:VAL:HG21	2.40	0.50
1:P:655:ILE:HG22	1:P:656:GLN:N	2.26	0.50
1:P:122:THR:O	1:P:126:LEU:HD13	2.10	0.50
1:P:537:ASP:OD1	1:P:813:SER:HB3	2.12	0.50
1:P:553:GLU:HG3	1:P:870:LEU:HD12	1.92	0.50
1:P:586:ALA:HB3	1:P:617:ALA:CB	2.38	0.50
1:P:616:LEU:HD12	1:P:676:TYR:HB2	1.93	0.50
1:P:620:TRP:CZ2	1:P:655:ILE:HD11	2.47	0.50
1:P:826:LYS:HA	1:P:829:ARG:NH1	2.27	0.50
1:P:148:GLU:OE1	1:P:148:GLU:HA	2.10	0.50
1:P:636:THR:CG2	1:P:640:GLY:CA	2.85	0.50
1:P:150:ARG:O	1:P:150:ARG:HG3	2.10	0.50
1:P:791:LEU:O	1:P:792:ARG:C	2.51	0.50
1:P:294:LEU:HD21	1:P:429:VAL:HG21	1.93	0.50
1:P:721:LYS:HG2	1:P:722:ARG:N	2.27	0.50
2:L:1002:ARG:CG	2:L:1002:ARG:NH1	2.73	0.50
2:L:1043:ASP:OD1	2:L:1044:VAL:N	2.44	0.50
2:L:1044:VAL:HG22	2:L:1046:TYR:H	1.76	0.50
1:P:627:ARG:HG2	1:P:627:ARG:NH1	2.26	0.50
1:P:634:VAL:HG22	1:P:634:VAL:O	2.11	0.50
1:P:747:LEU:HG	1:P:761:ILE:HG13	1.94	0.50
1:P:89:PHE:O	1:P:103:PHE:CZ	2.61	0.50
1:P:572:GLY:HA2	1:P:627:ARG:HB3	1.94	0.50
1:P:855:GLU:HA	2:L:1030:ARG:HD2	1.94	0.50
2:L:1146:THR:O	2:L:1147:SER:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:74:ILE:O	1:P:74:ILE:HD12	2.11	0.49
1:P:76:THR:C	1:P:79:PRO:HD2	2.37	0.49
1:P:92:VAL:C	1:P:94:ALA:H	2.20	0.49
1:P:106:LEU:O	1:P:109:ILE:HB	2.12	0.49
1:P:452:ILE:HG22	1:P:456:GLY:CA	2.36	0.49
1:P:582:LEU:O	1:P:586:ALA:HB3	2.11	0.49
1:P:818:PRO:O	1:P:819:ALA:C	2.55	0.49
1:P:295:ALA:O	1:P:419:ASN:ND2	2.45	0.49
1:P:709:GLU:HB2	1:P:722:ARG:HH11	1.77	0.49
1:P:48:GLU:O	1:P:52:ARG:HG3	2.12	0.49
1:P:110:LYS:HB3	1:P:112:GLU:HG2	1.93	0.49
1:P:246:LEU:O	1:P:247:ALA:C	2.53	0.49
1:P:769:ILE:HG22	1:P:770:ASP:N	2.27	0.49
1:P:878:SER:O	1:P:879:ASP:CB	2.61	0.49
1:P:118:THR:HG21	1:P:216:CYS:HB3	1.95	0.49
1:P:124:ALA:O	1:P:127:THR:HB	2.12	0.49
1:P:425:ARG:HB2	1:P:427:TYR:CE1	2.48	0.49
1:P:569:ASP:O	1:P:573:ILE:HG13	2.12	0.49
1:P:806:SER:O	1:P:816:THR:HG23	2.12	0.49
1:P:706:LEU:HD11	1:P:849:PHE:CG	2.48	0.49
1:P:761:ILE:O	1:P:762:ASN:C	2.55	0.49
2:L:1002:ARG:HG2	2:L:1002:ARG:NH1	2.20	0.49
1:P:90:GLU:HA	1:P:93:LYS:HB2	1.94	0.49
1:P:232:GLN:CD	1:P:755:PHE:CD1	2.91	0.49
1:P:786:GLN:O	1:P:787:ASP:C	2.56	0.49
1:P:398:LEU:HD11	1:P:439:MET:HE1	1.95	0.49
1:P:422:TRP:CD2	1:P:423:ARG:HG3	2.48	0.49
1:P:450:LYS:O	1:P:529:ASN:HA	2.12	0.49
1:P:231:ARG:O	1:P:231:ARG:CG	2.57	0.49
1:P:250:TYR:O	1:P:253:ALA:HB3	2.12	0.49
1:P:507:SER:HB2	1:P:510:CYS:HB2	1.94	0.49
1:P:133:THR:HA	1:P:241:SER:O	2.13	0.48
1:P:693:VAL:HG13	1:P:694:GLU:N	2.27	0.48
1:P:877:GLU:C	1:P:879:ASP:H	2.21	0.48
1:P:58:GLN:O	1:P:58:GLN:HG2	2.08	0.48
1:P:73:LEU:HB2	1:P:260:ALA:HB1	1.95	0.48
1:P:249:GLU:HG3	1:P:250:TYR:N	2.27	0.48
1:P:643:GLU:CA	1:P:646:PHE:CD1	2.94	0.48
1:P:399:GLU:O	1:P:403:GLU:OE2	2.30	0.48
1:P:463:HIS:CG	1:P:534:LEU:HD22	2.49	0.48
1:P:571:TYR:CD1	1:P:634:VAL:CG1	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1074:HIS:CE1	2:L:1075:ASN:OD1	2.66	0.48
1:P:206:LYS:HB2	1:P:206:LYS:HZ3	1.79	0.48
2:L:1083:GLY:O	2:L:1095:PHE:HE1	1.97	0.48
2:L:1093:ALA:HB1	2:L:1144:LEU:HD11	1.94	0.48
1:P:232:GLN:NE2	1:P:755:PHE:HE1	2.11	0.48
1:P:797:TRP:CD2	1:P:801:LYS:HG3	2.49	0.48
1:P:75:THR:O	1:P:79:PRO:HG2	2.13	0.48
1:P:207:GLU:O	1:P:210:ILE:HB	2.14	0.48
2:L:1034:GLN:O	2:L:1035:TRP:C	2.56	0.48
1:P:313:MET:SD	1:P:734:PRO:HD3	2.54	0.48
1:P:577:LYS:HZ2	1:P:581:ILE:HD11	1.78	0.48
1:P:769:ILE:H	1:P:769:ILE:HD12	1.79	0.48
1:P:243:THR:HG22	1:P:243:THR:O	2.14	0.47
1:P:685:VAL:C	1:P:687:VAL:N	2.72	0.47
1:P:109:ILE:CD1	1:P:145:ILE:CG2	2.92	0.47
1:P:132:THR:HB	1:P:244:ILE:HG22	1.87	0.47
1:P:418:TYR:CE2	1:P:428:ALA:HB2	2.50	0.47
1:P:433:ASN:HB2	1:P:434:PRO:HD2	1.96	0.47
1:P:522:GLN:O	1:P:523:HIS:ND1	2.47	0.47
1:P:613:THR:C	1:P:615:ALA:N	2.72	0.47
1:P:44:TYR:N	1:P:44:TYR:CD1	2.82	0.47
1:P:190:MET:O	1:P:190:MET:HG2	2.14	0.47
1:P:391:ARG:HD2	1:P:391:ARG:C	2.40	0.47
1:P:552:ASP:C	1:P:552:ASP:OD1	2.56	0.47
1:P:685:VAL:HG23	1:P:686:SER:N	2.30	0.47
1:P:790:HIS:CE1	1:P:832:MET:HE2	2.49	0.47
1:P:266:PRO:CD	1:P:404:GLN:HE21	2.25	0.47
1:P:854:HIS:O	1:P:855:GLU:C	2.57	0.47
1:P:23:THR:O	1:P:27:HIS:HB2	2.14	0.47
1:P:28:TYR:HD1	1:P:185:VAL:HG23	1.79	0.47
1:P:648:GLN:O	1:P:652:GLU:CB	2.55	0.47
1:P:871:ASN:HB3	1:P:875:ILE:HG12	1.94	0.47
2:L:1018:CYS:O	2:L:1019:SER:C	2.57	0.47
2:L:1046:TYR:CE2	2:L:1080:CYS:SG	3.08	0.47
1:P:871:ASN:CB	1:P:875:ILE:HG21	2.21	0.47
1:P:73:LEU:CB	1:P:260:ALA:HB1	2.45	0.47
1:P:744:GLN:NE2	1:P:762:ASN:O	2.48	0.47
1:P:19:ILE:O	1:P:20:PRO:C	2.56	0.47
1:P:41:HIS:CD2	1:P:155:ARG:HG3	2.50	0.47
1:P:199:GLU:OE2	1:P:302:LYS:HD2	2.16	0.47
2:L:1123:HIS:C	2:L:1123:HIS:HD1	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:74:ILE:O	1:P:74:ILE:CD1	2.63	0.46
1:P:553:GLU:O	1:P:555:GLY:N	2.48	0.46
1:P:401:MET:SD	1:P:432:PHE:HA	2.55	0.46
1:P:553:GLU:CG	1:P:870:LEU:HD12	2.44	0.46
1:P:633:SER:HB2	1:P:646:PHE:CE2	2.51	0.46
1:P:763:THR:CG2	1:P:764:ASN:H	2.28	0.46
1:P:642:LYS:C	1:P:644:PHE:N	2.73	0.46
1:P:643:GLU:CA	1:P:646:PHE:HD1	2.28	0.46
1:P:722:ARG:HE	1:P:771:ALA:CB	2.26	0.46
1:P:113:ALA:O	1:P:114:VAL:C	2.57	0.46
1:P:537:ASP:OD1	1:P:813:SER:CB	2.64	0.46
2:L:1113:LYS:O	2:L:1113:LYS:CG	2.63	0.46
1:P:413:ALA:O	1:P:414:ILE:HG23	2.15	0.46
2:L:1027:VAL:HA	2:L:1031:GLU:HG3	1.96	0.46
1:P:15:GLU:O	1:P:19:ILE:HD13	2.15	0.46
1:P:78:LEU:O	1:P:82:ILE:HG13	2.14	0.46
1:P:297:VAL:HG13	1:P:421:ASP:O	2.16	0.46
1:P:761:ILE:O	1:P:763:THR:N	2.49	0.46
1:P:244:ILE:HD13	1:P:389:LYS:CE	2.46	0.46
2:L:1068:HIS:CG	2:L:1069:ALA:H	2.34	0.46
2:L:1081:LEU:HD22	2:L:1099:GLN:HE21	1.81	0.46
1:P:230:HIS:CG	1:P:245:GLU:HG3	2.42	0.45
1:P:395:ARG:HG2	1:P:395:ARG:NH1	2.31	0.45
1:P:416:PHE:CE2	1:P:433:ASN:HA	2.51	0.45
1:P:419:ASN:HD22	1:P:419:ASN:HA	1.54	0.45
1:P:420:MET:HA	1:P:425:ARG:O	2.16	0.45
2:L:1126:ALA:C	2:L:1128:LYS:H	2.24	0.45
2:L:1141:LYS:C	2:L:1143:GLU:N	2.73	0.45
2:L:1129:ALA:HA	2:L:1148:ASP:OD1	2.16	0.45
1:P:28:TYR:CD1	1:P:185:VAL:CG2	2.99	0.45
1:P:46:MET:HE3	1:P:116:TYR:CE1	2.51	0.45
1:P:85:ILE:HD13	1:P:114:VAL:CG1	2.46	0.45
1:P:201:TRP:CD1	1:P:305:LEU:HD12	2.51	0.45
1:P:211:HIS:CA	1:P:214:VAL:HG12	2.44	0.45
1:P:749:LEU:HD23	1:P:751:PHE:HE1	1.81	0.45
1:P:800:GLU:O	1:P:801:LYS:C	2.58	0.45
2:L:1113:LYS:O	2:L:1113:LYS:HG2	2.17	0.45
1:P:83:ALA:O	1:P:84:ARG:C	2.59	0.45
1:P:514:PHE:O	1:P:515:CYS:C	2.60	0.45
1:P:543:ILE:HG22	1:P:543:ILE:O	2.17	0.45
1:P:73:LEU:N	1:P:74:ILE:N	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:489:ILE:O	1:P:492:CYS:HB2	2.17	0.45
1:P:643:GLU:HA	1:P:646:PHE:HD1	1.74	0.45
1:P:731:ASP:CG	1:P:792:ARG:HH21	2.24	0.45
2:L:1017:HIS:ND1	2:L:1130:CYS:CB	2.80	0.45
1:P:480:LYS:C	1:P:482:ILE:N	2.72	0.45
1:P:642:LYS:O	1:P:643:GLU:C	2.59	0.45
1:P:824:LEU:O	1:P:827:ALA:HB3	2.16	0.45
1:P:26:ASP:OD1	1:P:26:ASP:O	2.35	0.45
1:P:74:ILE:HG21	1:P:263:GLY:H	1.82	0.45
1:P:109:ILE:HG22	1:P:114:VAL:HG23	1.98	0.45
1:P:552:ASP:OD1	1:P:552:ASP:O	2.35	0.45
1:P:824:LEU:O	1:P:827:ALA:N	2.49	0.45
1:P:873:ARG:C	1:P:875:ILE:H	2.22	0.45
2:L:1134:ASP:HA	2:L:1149:ARG:O	2.16	0.45
1:P:185:VAL:O	1:P:187:GLU:CD	2.60	0.45
1:P:313:MET:HE1	1:P:733:PHE:HD1	1.82	0.45
1:P:20:PRO:HG3	1:P:289:ASN:HB2	1.99	0.45
1:P:185:VAL:HB	1:P:274:PRO:CB	2.41	0.45
1:P:509:PHE:C	1:P:511:PHE:N	2.74	0.45
1:P:814:PHE:HE2	1:P:824:LEU:CD2	2.29	0.45
1:P:128:SER:C	1:P:130:ASP:H	2.24	0.45
1:P:425:ARG:HD2	1:P:427:TYR:OH	2.17	0.45
1:P:728:VAL:N	1:P:848:GLN:HE22	2.01	0.45
1:P:823:ASN:O	1:P:824:LEU:C	2.57	0.45
1:P:77:LEU:CD2	1:P:224:THR:HB	2.47	0.44
1:P:185:VAL:N	1:P:274:PRO:HG2	2.26	0.44
1:P:496:PRO:HG2	1:P:497:LEU:H	1.80	0.44
2:L:1137:ARG:CD	2:L:1141:LYS:HD2	2.39	0.44
1:P:133:THR:O	1:P:136:ALA:N	2.51	0.44
1:P:249:GLU:CG	1:P:250:TYR:H	2.30	0.44
1:P:562:LEU:O	1:P:876:LEU:HG	2.16	0.44
1:P:616:LEU:HD12	1:P:676:TYR:CG	2.51	0.44
1:P:642:LYS:HA	1:P:682:TRP:CE3	2.51	0.44
1:P:433:ASN:ND2	1:P:435:GLN:N	2.63	0.44
1:P:453:GLY:HA2	1:P:526:LEU:HB3	1.98	0.44
1:P:638:ALA:HA	1:P:696:MET:CE	2.48	0.44
1:P:15:GLU:O	1:P:18:ALA:HB3	2.18	0.44
1:P:56:GLU:O	1:P:59:LEU:N	2.50	0.44
1:P:577:LYS:O	1:P:581:ILE:HG13	2.18	0.44
1:P:583:GLN:O	1:P:584:ALA:C	2.60	0.44
1:P:617:ALA:O	1:P:621:LEU:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:723:SER:OG	1:P:724:ALA:N	2.51	0.44
1:P:770:ASP:OD1	1:P:770:ASP:C	2.60	0.44
2:L:1038:GLU:C	2:L:1040:GLY:H	2.26	0.44
2:L:1089:GLY:O	2:L:1090:LYS:HD3	2.17	0.44
1:P:45:GLU:HB3	1:P:155:ARG:NH2	2.32	0.44
1:P:298:ARG:NH1	1:P:298:ARG:HG3	2.28	0.44
1:P:470:VAL:HG12	1:P:470:VAL:O	2.17	0.44
1:P:697:ASN:N	1:P:697:ASN:HD22	2.16	0.44
2:L:1029:VAL:CG1	2:L:1030:ARG:N	2.80	0.44
2:L:1064:ALA:O	2:L:1065:VAL:C	2.60	0.44
1:P:118:THR:CG2	1:P:216:CYS:HB3	2.47	0.44
1:P:463:HIS:CD2	1:P:467:CYS:SG	3.10	0.44
1:P:582:LEU:O	1:P:583:GLN:C	2.61	0.44
1:P:664:GLY:O	1:P:665:LEU:C	2.61	0.44
1:P:770:ASP:OD1	1:P:770:ASP:O	2.35	0.44
1:P:515:CYS:O	1:P:516:PHE:C	2.60	0.44
1:P:677:MET:O	1:P:678:ALA:C	2.61	0.44
1:P:770:ASP:O	1:P:772:HIS:N	2.51	0.44
1:P:637:LEU:HD12	1:P:637:LEU:HA	1.61	0.44
1:P:682:TRP:O	1:P:685:VAL:HG22	2.18	0.44
1:P:792:ARG:O	1:P:796:VAL:HG23	2.18	0.44
1:P:869:ASN:O	1:P:869:ASN:OD1	2.36	0.44
1:P:36:GLN:O	1:P:39:LEU:HB3	2.17	0.43
1:P:108:GLU:O	1:P:108:GLU:CG	2.65	0.43
1:P:855:GLU:OE1	2:L:1031:GLU:OE2	2.36	0.43
2:L:1022:LYS:H	2:L:1025:GLN:NE2	2.14	0.43
1:P:211:HIS:C	1:P:214:VAL:HG12	2.43	0.43
1:P:571:TYR:CE1	1:P:634:VAL:HG13	2.53	0.43
1:P:616:LEU:HD12	1:P:676:TYR:CB	2.48	0.43
1:P:709:GLU:O	1:P:710:VAL:C	2.61	0.43
1:P:616:LEU:O	1:P:618:GLY:N	2.51	0.43
2:L:1092:ASP:O	2:L:1094:ASN:ND2	2.51	0.43
1:P:19:ILE:HD12	1:P:19:ILE:N	2.21	0.43
1:P:422:TRP:CZ2	1:P:423:ARG:HG3	2.54	0.43
1:P:455:GLU:O	1:P:458:TYR:HB3	2.17	0.43
1:P:579:ASN:OD1	1:P:625:VAL:CB	2.63	0.43
1:P:192:SER:C	1:P:194:GLY:H	2.27	0.43
1:P:438:ASP:HA	1:P:441:LYS:HB2	2.00	0.43
1:P:710:VAL:HG12	1:P:712:ASP:H	1.84	0.43
1:P:146:GLU:O	1:P:149:ALA:HB3	2.18	0.43
1:P:162:PHE:CG	1:P:163:LYS:N	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:232:GLN:OE1	1:P:755:PHE:CE1	2.72	0.43
1:P:441:LYS:CE	1:P:810:ILE:HD12	2.47	0.43
1:P:490:MET:O	1:P:493:ALA:HB2	2.19	0.43
1:P:873:ARG:C	1:P:875:ILE:N	2.76	0.43
1:P:37:LEU:O	1:P:38:ALA:C	2.62	0.43
1:P:265:SER:HB3	1:P:269:GLN:OE1	2.19	0.43
1:P:496:PRO:HG2	1:P:497:LEU:N	2.34	0.43
1:P:28:TYR:HD2	1:P:32:LEU:CD1	2.28	0.43
1:P:873:ARG:O	1:P:876:LEU:CB	2.67	0.43
1:P:123:LEU:HD12	1:P:264:ILE:HG21	2.01	0.43
1:P:141:ILE:O	1:P:145:ILE:HG12	2.18	0.43
1:P:85:ILE:HD13	1:P:114:VAL:HG12	2.00	0.42
1:P:774:GLN:OE1	1:P:774:GLN:HA	2.19	0.42
1:P:836:TYR:HE1	1:P:841:VAL:HG21	1.82	0.42
1:P:120:LYS:HZ1	1:P:267:MET:HA	1.83	0.42
1:P:298:ARG:NH1	1:P:419:ASN:CB	2.73	0.42
1:P:460:LEU:O	1:P:463:HIS:HB3	2.18	0.42
2:L:1123:HIS:C	2:L:1123:HIS:ND1	2.77	0.42
1:P:36:GLN:HA	1:P:36:GLN:OE1	2.20	0.42
1:P:313:MET:SD	1:P:316:VAL:HG21	2.59	0.42
1:P:74:ILE:N	1:P:75:THR:CG2	2.78	0.42
1:P:109:ILE:HD13	1:P:145:ILE:CG2	2.50	0.42
1:P:244:ILE:CD1	1:P:389:LYS:HE3	2.49	0.42
1:P:633:SER:CB	1:P:646:PHE:CD2	3.03	0.42
2:L:1009:GLU:O	2:L:1010:SER:HB3	2.20	0.42
2:L:1051:LYS:C	2:L:1053:ASP:N	2.76	0.42
1:P:58:GLN:CA	1:P:59:LEU:N	2.75	0.42
1:P:534:LEU:HD11	1:P:818:PRO:CG	2.37	0.42
1:P:619:GLN:O	1:P:666:MET:HG3	2.19	0.42
1:P:782:PHE:HE1	1:P:845:PHE:CE1	2.37	0.42
2:L:1034:GLN:HE22	2:L:1038:GLU:HG3	1.85	0.42
1:P:80:LYS:O	1:P:83:ALA:HB3	2.19	0.42
1:P:877:GLU:H	1:P:877:GLU:HG2	1.63	0.42
2:L:1114:TYR:O	2:L:1115:GLU:C	2.62	0.42
2:L:1136:LYS:HE2	2:L:1140:GLU:OE2	2.19	0.42
1:P:92:VAL:C	1:P:94:ALA:N	2.76	0.42
1:P:278:TRP:HE1	1:P:324:GLN:HE22	1.66	0.42
1:P:342:THR:HB	1:P:398:LEU:HD21	2.02	0.42
1:P:820:ASP:O	1:P:821:ALA:C	2.61	0.42
1:P:159:ALA:O	1:P:162:PHE:O	2.38	0.42
1:P:553:GLU:O	1:P:554:VAL:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:664:GLY:C	1:P:666:MET:N	2.76	0.42
1:P:669:GLN:HA	1:P:670:PRO:HD2	1.77	0.42
1:P:150:ARG:O	1:P:150:ARG:CG	2.68	0.42
1:P:211:HIS:HA	1:P:214:VAL:CG1	2.49	0.42
1:P:657:PRO:O	1:P:660:ASP:OD1	2.38	0.42
2:L:1120:ARG:HH21	2:L:1125:VAL:HG21	1.84	0.42
1:P:12:SER:C	1:P:14:ILE:H	2.28	0.42
1:P:74:ILE:C	1:P:74:ILE:CG1	2.93	0.42
1:P:802:TYR:HD2	1:P:823:ASN:HD22	1.66	0.42
2:L:1051:LYS:HA	2:L:1082:VAL:HG21	2.01	0.42
1:P:21:PHE:CD2	1:P:21:PHE:C	2.98	0.41
1:P:39:LEU:CD1	1:P:269:GLN:NE2	2.83	0.41
1:P:39:LEU:HD11	1:P:269:GLN:NE2	2.35	0.41
1:P:186:VAL:HG21	1:P:325:ASN:OD1	2.10	0.41
1:P:211:HIS:O	1:P:214:VAL:CG1	2.68	0.41
1:P:275:PRO:HG2	1:P:324:GLN:HG2	2.02	0.41
1:P:426:VAL:O	1:P:426:VAL:HG23	2.20	0.41
1:P:638:ALA:HA	1:P:696:MET:HE2	2.02	0.41
2:L:1063:MET:HE3	2:L:1063:MET:HB3	1.93	0.41
1:P:491:ALA:C	1:P:493:ALA:H	2.27	0.41
1:P:576:LYS:CG	1:P:577:LYS:N	2.83	0.41
1:P:685:VAL:O	1:P:687:VAL:N	2.53	0.41
2:L:1086:ASP:OD1	2:L:1087:ASP:N	2.53	0.41
1:P:77:LEU:HD21	1:P:250:TYR:OH	2.20	0.41
1:P:495:SER:OG	1:P:496:PRO:HD3	2.20	0.41
1:P:816:THR:HG22	1:P:817:ILE:N	2.23	0.41
1:P:873:ARG:HA	1:P:873:ARG:HD3	1.90	0.41
1:P:273:VAL:O	1:P:274:PRO:C	2.62	0.41
1:P:335:LEU:HD21	1:P:406:ASN:ND2	2.35	0.41
1:P:505:GLN:HG3	1:P:511:PHE:CD2	2.56	0.41
1:P:826:LYS:HG2	1:P:829:ARG:NH2	2.16	0.41
1:P:422:TRP:CZ2	1:P:423:ARG:HD3	2.55	0.41
1:P:511:PHE:O	1:P:512:LEU:C	2.62	0.41
1:P:550:LEU:HD23	1:P:550:LEU:HA	1.75	0.41
2:L:1122:HIS:C	2:L:1124:GLU:N	2.78	0.41
1:P:185:VAL:H	1:P:274:PRO:CG	2.28	0.41
1:P:699:LEU:C	1:P:701:SER:N	2.75	0.41
1:P:543:ILE:HG22	1:P:559:VAL:CG2	2.51	0.41
1:P:571:TYR:CG	1:P:631:LYS:HB2	2.55	0.41
1:P:779:ALA:N	1:P:780:PRO:HD2	2.36	0.41
1:P:791:LEU:HD11	1:P:809:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:42:GLU:CG	1:P:50:ARG:NH1	2.83	0.41
1:P:490:MET:C	1:P:492:CYS:N	2.77	0.41
1:P:829:ARG:HH11	1:P:829:ARG:HB2	1.85	0.41
1:P:109:ILE:CD1	1:P:145:ILE:HG22	2.51	0.40
2:L:1050:ILE:HG22	2:L:1099:GLN:HG3	2.02	0.40
1:P:116:TYR:C	1:P:118:THR:N	2.79	0.40
1:P:733:PHE:HA	1:P:734:PRO:HD3	1.69	0.40
2:L:1037:LYS:HB3	2:L:1037:LYS:HE2	1.85	0.40
2:L:1090:LYS:HD3	2:L:1090:LYS:HA	1.87	0.40
1:P:45:GLU:CB	1:P:155:ARG:NH2	2.85	0.40
1:P:80:LYS:HD2	1:P:224:THR:HG22	2.02	0.40
1:P:464:GLY:HA2	1:P:467:CYS:SG	2.62	0.40
2:L:1036:HIS:O	2:L:1037:LYS:C	2.65	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:233:ASN:OD1	1:P:838:SER:O[1_554]	1.63	0.57

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	760/828 (92%)	591 (78%)	120 (16%)	49 (6%)	1	3
2	L	-	110 (75%)	34 (23%)	3 (2%)	6	21
All	All	907/828 (110%)	701 (77%)	154 (17%)	52 (6%)	1	4

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	94	ALA
1	P	197	GLY
1	P	498	GLU
1	P	554	VAL
1	P	584	ALA
1	P	643	GLU
1	P	670	PRO
1	P	762	ASN
1	P	769	ILE
1	P	855	GLU
1	P	873	ARG
2	L	1093	ALA
1	P	93	LYS
1	P	97	GLY
1	P	500	THR
1	P	642	LYS
1	P	665	LEU
1	P	755	PHE
1	P	771	ALA
2	L	1087	ASP
1	P	10	ASP
1	P	57	ARG
1	P	253	ALA
1	P	481	PHE
1	P	560	ASN
1	P	567	VAL
1	P	582	LEU
1	P	617	ALA
1	P	872	LEU
1	P	193	LYS
1	P	526	LEU
1	P	540	CYS
1	P	551	ARG
1	P	637	LEU
1	P	686	SER
1	P	9	ASN
1	P	46	MET
1	P	83	ALA
1	P	204	TRP
1	P	251	ALA
1	P	261	LEU
1	P	425	ARG
1	P	454	LYS

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Mol	Chain	Res	Type
1	P	470	VAL
2	L	1125	VAL
1	P	275	PRO
1	P	114	VAL
1	P	283	GLY
1	P	495	SER
1	P	710	VAL
1	P	563	PRO
1	P	761	ILE

4.3.2 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	P	642/680 (94%)	609 (95%)	33 (5%)	21	54
2	L	-	117 (94%)	7 (6%)	19	50
All	All	766/680 (113%)	726 (95%)	40 (5%)	21	53

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	73	LEU
1	P	74	ILE
1	P	81	MET
1	P	89	PHE
1	P	125	CYS
1	P	161	HIS
1	P	206	LYS
1	P	229	LEU
1	P	273	VAL
1	P	289	ASN
1	P	296	LEU
1	P	305	LEU
1	P	333	LYS
1	P	391	ARG

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Mol	Chain	Res	Type
1	P	395	ARG
1	P	403	GLU
1	P	419	ASN
1	P	433	ASN
1	P	452	ILE
1	P	471	ASP
1	P	510	CYS
1	P	532	LEU
1	P	544	GLN
1	P	553	GLU
1	P	562	LEU
1	P	626	THR
1	P	627	ARG
1	P	637	LEU
1	P	720	ARG
1	P	728	VAL
1	P	743	ILE
1	P	754	GLN
1	P	851	ASP
2	L	1003	VAL
2	L	1031	GLU
2	L	1034	GLN
2	L	1035	TRP
2	L	1049	ILE
2	L	1085	ILE
2	L	1128	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	27	HIS
1	P	41	HIS
1	P	86	ASN
1	P	135	GLN
1	P	161	HIS
1	P	230	HIS
1	P	269	GLN
1	P	289	ASN
1	P	321	ASN
1	P	324	GLN
1	P	339	ASN
1	P	404	GLN

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Mol	Chain	Res	Type
1	P	406	ASN
1	P	411	HIS
1	P	419	ASN
1	P	433	ASN
1	P	463	HIS
1	P	544	GLN
1	P	545	HIS
1	P	560	ASN
1	P	648	GLN
1	P	671	ASN
1	P	697	ASN
1	P	737	GLN
1	P	744	GLN
1	P	758	GLN
1	P	764	ASN
1	P	784	HIS
1	P	790	HIS
1	P	811	HIS
1	P	848	GLN
1	P	854	HIS
1	P	857	GLN
1	P	869	ASN
2	L	1007	GLN
2	L	1025	GLN
2	L	1034	GLN
2	L	1036	HIS
2	L	1039	GLN
2	L	1068	HIS
2	L	1074	HIS
2	L	1099	GLN
2	L	1101	GLN
2	L	1122	HIS

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	P	7

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	73:LEU	C	74:ILE	N	3.03
1	P	58:GLN	C	59:LEU	N	2.01
1	P	8:LYS	C	9:ASN	N	1.19
1	P	9:ASN	C	10:ASP	N	1.17
1	P	497:LEU	C	498:GLU	N	1.13
1	P	499:ASN	C	500:THR	N	1.09
1	P	559:VAL	C	560:ASN	N	1.02

5 Fit of model and data ⓘ

5.1 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	P	723/828 (87%)	0.74	87 (12%) 9 6	19, 74, 110, 123	39 (5%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	538	GLY	16.7
1	P	539	SER	7.1
1	P	233	ASN	6.0
1	P	712	ASP	5.3
1	P	241	SER	4.9
1	P	589	GLY	4.8
1	P	558	ALA	4.6
1	P	752	LEU	4.3
1	P	478	ARG	4.3
1	P	638	ALA	4.1
1	P	76	THR	3.9
1	P	137	VAL	3.9
1	P	183	MET	3.8
1	P	28	TYR	3.8
1	P	185	VAL	3.6
1	P	559	VAL	3.5
1	P	563	PRO	3.5
1	P	633	SER	3.5
1	P	613	THR	3.5
1	P	220	LEU	3.4
1	P	10	ASP	3.3
1	P	578	VAL	3.3
1	P	540	CYS	3.3
1	P	586	ALA	3.2
1	P	96	ARG	3.1
1	P	138	ALA	3.1
1	P	107	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	P	711	LYS	3.1
1	P	561	LEU	3.0
1	P	403	GLU	3.0
1	P	718	ILE	3.0
1	P	499	ASN	2.9
1	P	498	GLU	2.9
1	P	710	VAL	2.8
1	P	243	THR	2.8
1	P	29	GLY	2.8
1	P	186	VAL	2.8
1	P	257	ARG	2.7
1	P	231	ARG	2.7
1	P	384	VAL	2.7
1	P	11	PHE	2.7
1	P	404	GLN	2.7
1	P	615	ALA	2.7
1	P	97	GLY	2.7
1	P	614	LYS	2.6
1	P	759	PRO	2.6
1	P	187	GLU	2.6
1	P	245	GLU	2.6
1	P	637	LEU	2.6
1	P	9	ASN	2.6
1	P	585	ASP	2.5
1	P	632	ARG	2.5
1	P	507	SER	2.5
1	P	487	GLU	2.5
1	P	33	ALA	2.4
1	P	83	ALA	2.4
1	P	560	ASN	2.4
1	P	640	GLY	2.4
1	P	815	GLY	2.4
1	P	51	PHE	2.3
1	P	25	ALA	2.3
1	P	750	MET	2.3
1	P	141	ILE	2.3
1	P	678	ALA	2.3
1	P	537	ASP	2.3
1	P	624	GLY	2.3
1	P	760	THR	2.2
1	P	541	SER	2.2
1	P	401	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	P	619	GLN	2.2
1	P	34	ARG	2.2
1	P	49	ALA	2.2
1	P	136	ALA	2.2
1	P	74	ILE	2.2
1	P	162	PHE	2.2
1	P	659	ILE	2.1
1	P	461	LYS	2.1
1	P	393	SER	2.1
1	P	660	ASP	2.1
1	P	500	THR	2.1
1	P	188	ALA	2.1
1	P	751	PHE	2.1
1	P	93	LYS	2.0
1	P	588	ASN	2.0
1	P	253	ALA	2.0
1	P	636	THR	2.0
1	P	631	LYS	2.0

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	HG	P	909	1/1	0.93	0.10	199,199,199,199	0
3	HG	P	908	1/1	0.94	0.20	199,199,199,199	0
3	HG	P	906	1/1	0.95	0.06	136,136,136,136	0
3	HG	P	907	1/1	0.97	0.21	159,159,159,159	0
3	HG	P	904	1/1	0.99	0.04	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HG	P	905	1/1	0.99	0.03	83,83,83,83	0
3	HG	L	903	1/1	0.99	0.03	113,113,113,113	0

5.5 Other polymers [i](#)

There are no such residues in this entry.