Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:26 PM GMT

PDB ID	:	1ARO
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

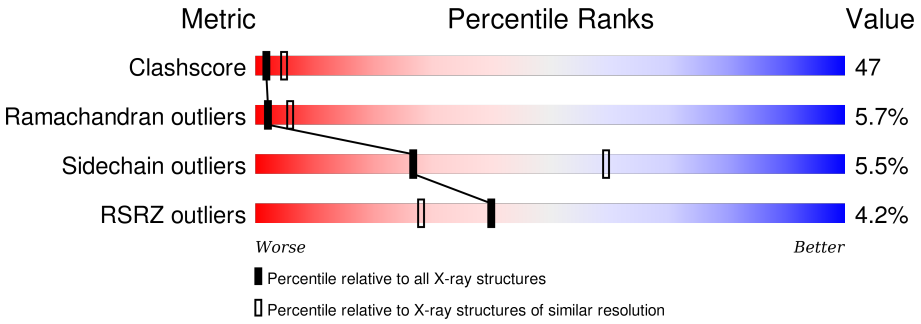
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	P	883	4% 37% 43% 7% • 12%
2	L	151	2% 42% 48% 9% •

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	UNP P00573
P	839	SER	CYS	ENGINEERED	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 (three-letter code: HG) (formula: Hg).

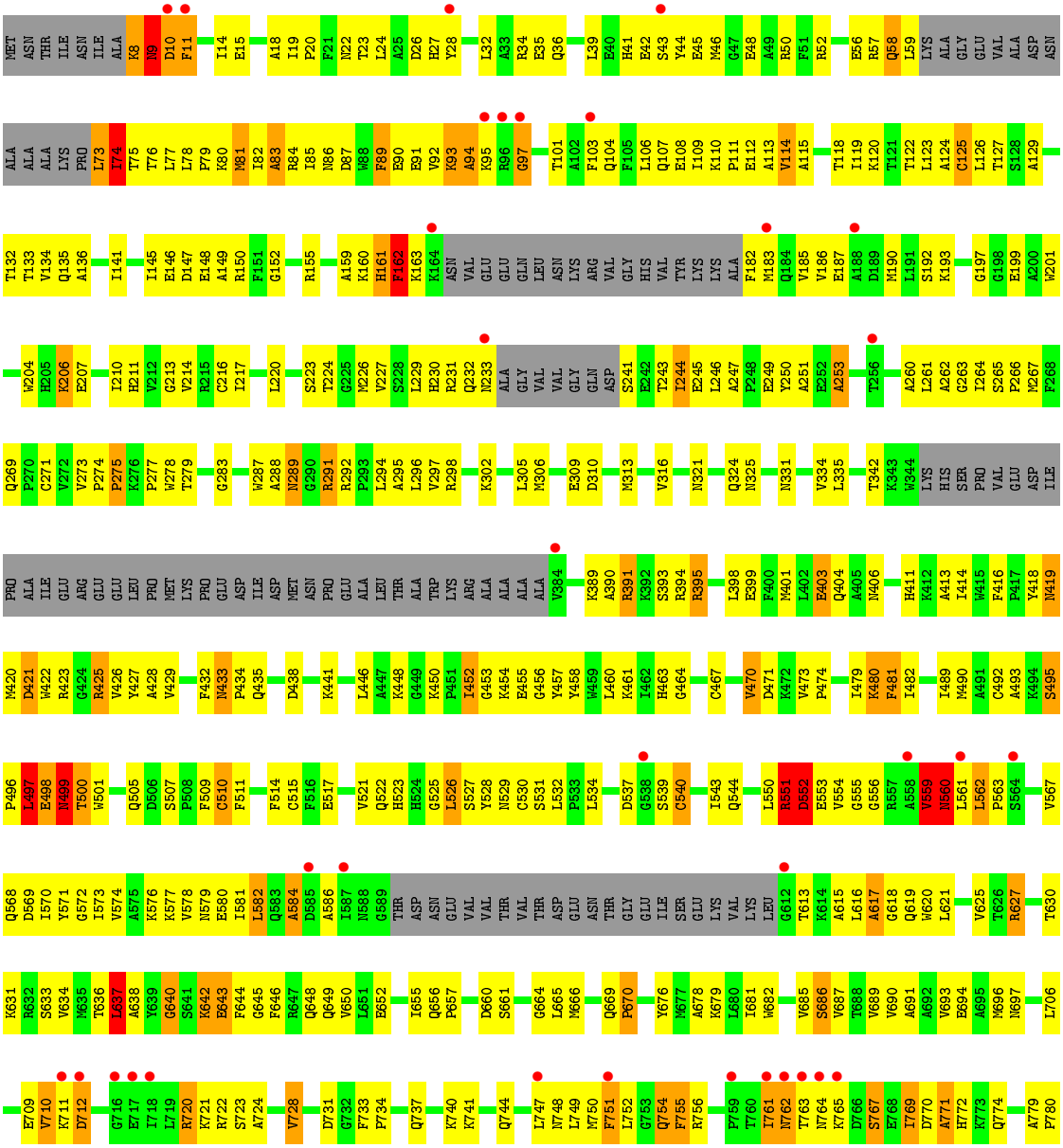
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	6	Total	Hg	0	0
			6	6		
3	L	1	Total	Hg	0	0
			1	1		

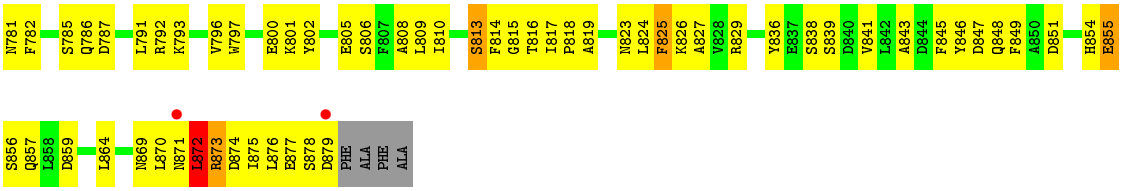
3 Residue-property plots (i)

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

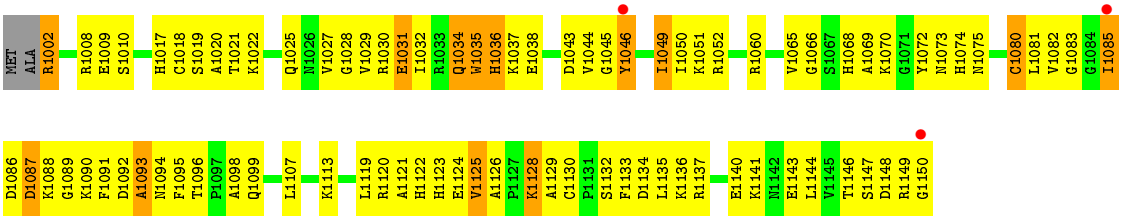
- Molecule 1: T7 RNA POLYMERASE

Chain P:





• Molecule 2: T7 LYSOZYME



4 Data and refinement statistics (i)

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 33.50 – 2.78	Depositor EDS
% Data completeness (in resolution range)	93.9 (30.00-2.80) 90.1 (33.50-2.78)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	0.54 (at 2.76Å)	Xtriage
Refinement program	CNS, X-PLOR	Depositor
R, R_{free}	0.262 , 0.309 0.276 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
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 , 83.4	EDS
Estimated twinning fraction	0.025 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 36539 reflections	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.69	14/6261 (0.2%)	1.05	41/8460 (0.5%)
2	L	0.57	1/1210 (0.1%)	0.81	1/1630 (0.1%)
All	All	0.68	15/7471 (0.2%)	1.01	42/10090 (0.4%)

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 (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	74	ILE	N-CA	14.10	1.74	1.46
1	P	559	VAL	C-N	-13.68	1.02	1.34
1	P	499	ASN	C-N	-10.51	1.09	1.34
1	P	497	LEU	C-N	-9.12	1.13	1.34
1	P	74	ILE	CA-CB	9.09	1.75	1.54
1	P	58	GLN	C-O	8.59	1.39	1.23
1	P	58	GLN	CG-CD	8.50	1.70	1.51
1	P	58	GLN	CD-NE2	7.72	1.52	1.32
1	P	9	ASN	C-N	-7.14	1.17	1.34
1	P	560	ASN	C-N	6.66	1.49	1.34
1	P	58	GLN	CA-C	-6.26	1.36	1.52
1	P	8	LYS	C-N	-6.25	1.19	1.34
2	L	1080	CYS	CB-SG	5.93	1.92	1.82
1	P	58	GLN	N-CA	-5.56	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	74	ILE	CB-CG1	5.35	1.69	1.54

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	8	LYS	O-C-N	-20.13	90.50	122.70
1	P	559	VAL	O-C-N	-17.78	94.25	122.70
1	P	559	VAL	C-N-CA	14.85	158.83	121.70
1	P	498	GLU	CB-CA-C	-13.31	83.79	110.40
1	P	499	ASN	CB-CA-C	13.18	136.76	110.40
1	P	559	VAL	CA-C-N	12.02	143.65	117.20
1	P	8	LYS	C-N-CA	11.86	151.35	121.70
1	P	58	GLN	CB-CA-C	-10.69	89.02	110.40
1	P	497	LEU	O-C-N	-10.34	106.16	122.70
1	P	497	LEU	C-N-CA	8.47	142.88	121.70
1	P	8	LYS	CA-C-N	8.12	135.06	117.20
1	P	74	ILE	C-N-CA	8.12	141.99	121.70
1	P	74	ILE	CA-CB-CG1	7.87	125.96	111.00
1	P	74	ILE	N-CA-C	-7.86	89.79	111.00
1	P	498	GLU	N-CA-CB	7.82	124.68	110.60
1	P	244	ILE	CB-CA-C	-7.63	96.33	111.60
1	P	552	ASP	N-CA-CB	7.45	124.01	110.60
1	P	872	LEU	CA-CB-CG	7.40	132.33	115.30
1	P	74	ILE	CA-C-N	-7.29	101.17	117.20
1	P	74	ILE	CB-CA-C	-7.28	97.04	111.60
1	P	11	PHE	CB-CA-C	-7.26	95.87	110.40
1	P	10	ASP	CB-CA-C	-7.22	95.95	110.40
1	P	499	ASN	O-C-N	-7.18	111.21	122.70
1	P	74	ILE	CG1-CB-CG2	-7.09	95.81	111.40
1	P	97	GLY	N-CA-C	6.91	130.38	113.10
1	P	9	ASN	CA-C-N	6.65	131.82	117.20
1	P	10	ASP	N-CA-CB	-6.53	98.84	110.60
1	P	499	ASN	CA-C-N	6.38	131.24	117.20
1	P	74	ILE	N-CA-CB	6.35	125.40	110.80
1	P	499	ASN	C-N-CA	6.27	137.38	121.70
1	P	162	PHE	N-CA-CB	6.03	121.46	110.60
1	P	9	ASN	C-N-CA	5.96	136.59	121.70
1	P	551	ARG	CB-CA-C	5.50	121.41	110.40
1	P	74	ILE	CA-C-O	5.47	131.58	120.10
1	P	813	SER	N-CA-C	-5.40	96.42	111.00
1	P	640	GLY	N-CA-C	-5.36	99.69	113.10
2	L	1080	CYS	CA-CB-SG	5.27	123.48	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	767	SER	N-CA-C	5.26	125.21	111.00
1	P	751	PHE	N-CA-C	5.26	125.19	111.00
1	P	107	GLN	N-CA-C	5.15	124.91	111.00
1	P	279	THR	N-CA-C	-5.08	97.30	111.00
1	P	497	LEU	CA-C-N	5.03	128.26	117.20

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	Mainchain,Peptide
1	P	499	ASN	Peptide
1	P	559	VAL	Mainchain,Peptide
1	P	74	ILE	Mainchain
1	P	8	LYS	Mainchain,Peptide
1	P	9	ASN	Mainchain

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	P	6124	0	6086	580	1
2	L	1183	0	1156	88	0
3	L	1	0	0	0	0
3	P	6	0	0	2	0
All	All	7314	0	7242	662	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 47.

All (662) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:74:ILE:N	1:P:74:ILE:CA	1.74	1.45
1:P:73:LEU:C	1:P:74:ILE:HA	1.18	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	1.20
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:58:GLN:C	1:P:59:LEU:N	2.01	1.14
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:401:MET:HE1	1:P:432:PHE:HA	1.35	1.06
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:74:ILE:N	1:P:74:ILE:C	2.29	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:74:ILE:CB	1:P:74:ILE:C	2.44	0.84
1:P:298:ARG:NH1	1:P:419:ASN:HB3	1.92	0.84
2:L:1091:PHE:HB2	2:L:1132:SER:HB2	1.60	0.84
1:P:19:ILE:H	1:P:19:ILE:HD12	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:HB	1:P:74:ILE:CA	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: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: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:93:LYS:O	1:P:95:LYS:N	2.14	0.80
1:P:93:LYS:C	1:P:95:LYS:H	1.86	0.80
1:P:125:CYS:HG	3:P:904:HG:HG	1.24	0.79
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: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
1:P:500:THR:O	1:P:500:THR:HG22	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:473:VAL:HG22	1:P:474:PRO:CD	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:147:ASP:OD1	1:P:292:ARG:HD2	1.84	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:871:ASN:HB2	1:P:875:ILE:CG2	2.13	0.77
1:P:631:LYS:HA	1:P:634:VAL:HG12	1.67	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: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:643:GLU:HA	1:P:646:PHE:CD1	2.20	0.76
1:P:422:TRP:CE2	1:P:423:ARG:HG3	2.21	0.76
1:P:233:ASN:C	1:P:756:ARG:O	2.25	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
1:P:185:VAL:O	1:P:185:VAL:HG12	1.84	0.75
1:P:579:ASN:OD1	1:P:625:VAL:HB	1.87	0.74
2:L:1028:GLY:H	2:L:1031:GLU:HG2	1.52	0.74
1:P:810:ILE:HG13	1:P:813:SER:OG	1.87	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:CG2	1:P:74:ILE:CA	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:186:VAL:CG2	1:P:325:ASN:OD1	2.36	0.73
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: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:855:GLU:OE1	2:L:1030:ARG:HD2	1.90	0.71
1:P:627:ARG:HH11	1:P:627:ARG:HG2	1.54	0.71
1:P:562:LEU:CG	1:P:876:LEU:HD11	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:871:ASN:CB	1:P:875:ILE:HG12	2.21	0.70
1:P:631:LYS:HA	1:P:634:VAL:CG1	2.21	0.70
1:P:433:ASN:ND2	1:P:435:GLN:H	1.88	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:638:ALA:HA	1:P:696:MET:HE1	1.73	0.70
1:P:84:ARG:CG	1:P:223:SER:HB3	2.20	0.70
1:P:433:ASN:C	1:P:433:ASN:HD22	1.93	0.70
1:P:298:ARG:HH11	1:P:298:ARG:HG3	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:616:LEU:C	1:P:618:GLY:H	1.96	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: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:577:LYS:NZ	1:P:581:ILE:HD11	2.08	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:160:LYS:C	1:P:162:PHE:N	2.46	0.67
1:P:664:GLY:HA2	1:P:666:MET:SD	2.34	0.67
1:P:391:ARG:HH11	1:P:391:ARG:HB3	1.60	0.67
1:P:108:GLU:HG2	1:P:108:GLU:O	1.94	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:HG22	1:P:636:THR:O	1.93	0.66
1:P:15:GLU:O	1:P:19:ILE:CD1	2.42	0.66
1:P:458:TYR:CD1	1:P:479:ILE:HD11	2.31	0.66
1:P:227:VAL:HG12	1:P:246:LEU:HD23	1.78	0.66
1:P:441:LYS:HE2	1:P:810:ILE:HD12	1.77	0.65
1:P:230:HIS:O	1:P:231:ARG:HB3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:42:GLU:HG2	1:P:50:ARG:NH1	2.12	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:58:GLN:O	1:P:59:LEU:N	2.28	0.65
1:P:19:ILE:HG21	1:P:192:SER:HB3	1.78	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:740:LYS:HB3	1:P:767:SER:HB2	1.79	0.64
1:P:148:GLU:O	1:P:152:GLY:N	2.30	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
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
2:L:1046:TYR:CZ	2:L:1080:CYS:SG	2.92	0.62
1:P:206:LYS:HB2	1:P:206:LYS:NZ	2.14	0.62
1:P:829:ARG:HD2	1:P:877:GLU:HA	1.81	0.62
1:P:42:GLU:O	1:P:120:LYS:HE3	1.98	0.62
1:P:160:LYS:O	1:P:161:HIS:C	2.38	0.62
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:186:VAL:HG21	1:P:325:ASN:CG	2.20	0.62
1:P:160:LYS:O	1:P:162:PHE:N	2.33	0.62
1:P:74:ILE:HG13	1:P:74:ILE:O	1.99	0.62
2:L:1137:ARG:HH11	2:L:1141:LYS:HE3	1.64	0.62
2:L:1125:VAL:O	2:L:1125:VAL:HG12	1.98	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:335:LEU:HD11	1:P:406:ASN:HD21	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:118:THR:HG23	1:P:141:ILE:HD13	1.84	0.60
1:P:636:THR:HG22	1:P:640:GLY:CA	2.31	0.60
1:P:631:LYS:CA	1:P:634:VAL:HG12	2.31	0.60
1:P:9:ASN:O	1:P:11:PHE:N	2.35	0.60
1:P:810:ILE:O	1:P:813:SER:OG	2.20	0.60
2:L:1134:ASP:OD1	2:L:1137:ARG:HB2	2.01	0.60
1:P:457:TYR:CD1	1:P:521:VAL:HG11	2.36	0.60
1:P:872:LEU:O	1:P:874:ASP:N	2.35	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:298:ARG:HH12	1:P:419:ASN:CB	2.12	0.59
1:P:249:GLU:HG3	1:P:250:TYR:H	1.67	0.59
1:P:797:TRP:NE1	1:P:801:LYS:HG3	2.18	0.59
2:L:1034:GLN:C	2:L:1034:GLN:HE21	2.05	0.59
1:P:737:GLN:NE2	1:P:781:ASN:OD1	2.35	0.59
1:P:550:LEU:CD1	1:P:691:ALA:HB1	2.25	0.59
1:P:446:LEU:HB2	1:P:531:SER:O	2.02	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:28:TYR:HD1	1:P:185:VAL:CG2	2.15	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:28:TYR:CD2	1:P:183:MET:HE3	2.39	0.58
1:P:288:ALA:O	1:P:291:ARG:HG2	2.03	0.58
1:P:613:THR:C	1:P:615:ALA:H	2.04	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:CD1	1:P:19:ILE:H	2.15	0.57
1:P:631:LYS:O	1:P:634:VAL:HG12	2.05	0.57
1:P:104:GLN:O	1:P:104:GLN:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:28:TYR:HD2	1:P:32:LEU:HD13	1.68	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:120:LYS:NZ	1:P:267:MET:HA	2.19	0.57
1:P:720:ARG:HD3	2:L:1034:GLN:OE1	2.04	0.57
1:P:335:LEU:HD21	1:P:406:ASN:HD22	1.69	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:433:ASN:C	1:P:433:ASN:ND2	2.57	0.56
1:P:230:HIS:HD2	1:P:245:GLU:HG3	1.57	0.56
1:P:111:PRO:HA	1:P:114:VAL:HB	1.86	0.56
2:L:1132:SER:O	2:L:1147:SER:O	2.23	0.56
1:P:740:LYS:HB3	1:P:767:SER:CB	2.35	0.56
1:P:543:ILE:HG22	1:P:559:VAL:HG21	1.87	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
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:871:ASN:HB2	1:P:875:ILE:HG12	1.86	0.56
2:L:1133:PHE:HE1	2:L:1135:LEU:HD12	1.71	0.56
1:P:550:LEU:O	1:P:551:ARG:HB2	2.06	0.56
1:P:77:LEU:HD21	1:P:250:TYR:CZ	2.40	0.56
1:P:793:LYS:NZ	1:P:793:LYS:HB3	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:682:TRP:HA	1:P:685:VAL:HG22	1.88	0.55
1:P:571:TYR:CD1	1:P:631:LYS:HB2	2.41	0.55
1:P:390:ALA:O	1:P:394:ARG:HG3	2.06	0.55
1:P:452:ILE:H	1:P:452:ILE:CD1	1.98	0.55
1:P:249:GLU:HG3	1:P:250:TYR:HD1	1.70	0.55
2:L:1141:LYS:C	2:L:1143:GLU:H	2.09	0.55
1:P:574:VAL:O	1:P:578:VAL:HG23	2.07	0.55
2:L:1135:LEU:N	2:L:1150:GLY:O	2.34	0.55
1:P:182:PHE:HE2	1:P:413:ALA:HB2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:74:ILE:N	1:P:75:THR:HG1	2.05	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: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:162:PHE:CD2	1:P:163:LYS:CA	2.89	0.54
1:P:85:ILE:HD12	1:P:115:ALA:HB2	1.89	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:616:LEU:C	1:P:618:GLY:N	2.61	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: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:101:THR:O	1:P:101:THR:HG22	2.06	0.54
1:P:452:ILE:CD1	1:P:528:TYR:O	2.56	0.54
1:P:455:GLU:O	1:P:456:GLY:C	2.45	0.54
1:P:637:LEU:O	1:P:696:MET:HE2	2.08	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: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
1:P:93:LYS:C	1:P:95:LYS:N	2.51	0.53
2:L:1008:ARG:HD2	2:L:1075:ASN:HA	1.88	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:182:PHE:CE2	1:P:413:ALA:HB2	2.43	0.53
1:P:160:LYS:O	1:P:162:PHE:HA	2.09	0.53
1:P:129:ALA:HB2	1:P:393:SER:OG	2.09	0.53
1:P:331:ASN:OD1	1:P:334:VAL:HG23	2.08	0.53
1:P:45:GLU:HB3	1:P:155:ARG:HH21	1.73	0.53
1:P:747:LEU:HD21	1:P:761:ILE:HD11	1.90	0.53
1:P:570:ILE:HG23	1:P:571:TYR:N	2.24	0.53
1:P:744:GLN:HA	1:P:764:ASN:ND2	2.23	0.53
1:P:480:LYS:O	1:P:482:ILE:N	2.42	0.53
2:L:1068:HIS:CG	2:L:1069:ALA:N	2.77	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:480:LYS:O	1:P:481:PHE:C	2.47	0.52
1:P:35:GLU:OE2	1:P:411:HIS:HE1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:1072:TYR:HE2	2:L:1125:VAL:HG11	1.73	0.52
1:P:808:ALA:O	1:P:814:PHE:HA	2.09	0.52
1:P:856:SER:HA	1:P:859:ASP:CG	2.30	0.52
2:L:1060:ARG:HH11	2:L:1066:GLY:HA2	1.73	0.52
1:P:425:ARG:HB2	1:P:427:TYR:HE1	1.75	0.52
2:L:1020:ALA:HB1	2:L:1085:ILE:CD1	2.22	0.52
1:P:855:GLU:HA	2:L:1030:ARG:CD	2.40	0.52
1:P:553:GLU:O	1:P:556:GLY:N	2.42	0.52
1:P:132:THR:CG2	1:P:244:ILE:CG2	2.88	0.52
1:P:132:THR:HG21	1:P:244:ILE:CG2	2.39	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
2:L:1122:HIS:C	2:L:1124:GLU:H	2.12	0.52
1:P:797:TRP:CD1	1:P:801:LYS:HG3	2.46	0.51
1:P:571:TYR:HD1	1:P:634:VAL:CG1	2.23	0.51
1:P:133:THR:O	1:P:134:VAL:C	2.49	0.51
1:P:77:LEU:O	1:P:81:MET:HB2	2.10	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:14:ILE:O	1:P:15:GLU:C	2.49	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:186:VAL:HG21	1:P:325:ASN:OD1	2.10	0.51
1:P:18:ALA:HB1	1:P:22:ASN:ND2	2.26	0.51
1:P:232:GLN:NE2	1:P:755:PHE:CE1	2.79	0.51
1:P:43:SER:HA	1:P:120:LYS:NZ	2.26	0.51
1:P:148:GLU:HA	1:P:148:GLU:OE1	2.10	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:220:LEU:HD21	1:P:226:MET:HE2	1.91	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:532:LEU:C	1:P:532:LEU:HD23	2.31	0.50
1:P:655:ILE:HG22	1:P:656:GLN:N	2.26	0.50
1:P:553:GLU:HG3	1:P:870:LEU:HD12	1.92	0.50
1:P:826:LYS:HA	1:P:829:ARG:NH1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:537:ASP:OD1	1:P:813:SER:HB3	2.12	0.50
1:P:616:LEU:HD12	1:P:676:TYR:HB2	1.93	0.50
1:P:586:ALA:HB3	1:P:617:ALA:CB	2.38	0.50
1:P:620:TRP:CZ2	1:P:655:ILE:HD11	2.47	0.50
1:P:122:THR:O	1:P:126:LEU:HD13	2.10	0.50
1:P:870:LEU:O	1:P:871:ASN:C	2.49	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
2:L:1002:ARG:NH1	2:L:1002:ARG:CG	2.73	0.50
1:P:721:LYS:HG2	1:P:722:ARG:N	2.27	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:294:LEU:HD21	1:P:429:VAL:HG21	1.93	0.50
1:P:685:VAL:C	1:P:687:VAL:H	2.14	0.50
1:P:747:LEU:HG	1:P:761:ILE:HG13	1.94	0.50
1:P:634:VAL:O	1:P:634:VAL:HG22	2.11	0.50
1:P:627:ARG:NH1	1:P:627:ARG:HG2	2.26	0.50
1:P:232:GLN:CD	1:P:755:PHE:CE1	2.85	0.50
1:P:306:MET:CE	1:P:309:GLU:OE1	2.60	0.50
2:L:1146:THR:O	2:L:1147:SER:HB2	2.11	0.50
1:P:855:GLU:HA	2:L:1030:ARG:HD2	1.94	0.50
1:P:572:GLY:HA2	1:P:627:ARG:HB3	1.94	0.50
1:P:89:PHE:O	1:P:103:PHE:CZ	2.61	0.50
1:P:74:ILE:HD12	1:P:74:ILE:O	2.11	0.49
1:P:452:ILE:HG22	1:P:456:GLY:CA	2.36	0.49
1:P:106:LEU:O	1:P:109:ILE:HB	2.12	0.49
1:P:582:LEU:O	1:P:586:ALA:HB3	2.11	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:631:LYS:C	1:P:634:VAL:HG12	2.32	0.49
1:P:769:ILE:HG22	1:P:770:ASP:N	2.27	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: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:806:SER:O	1:P:816:THR:HG23	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:124:ALA:O	1:P:127:THR:HB	2.12	0.49
2:L:1002:ARG:NH1	2:L:1002:ARG:HG2	2.20	0.49
1:P:706:LEU:HD11	1:P:849:PHE:CG	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:90:GLU:HA	1:P:93:LYS:HB2	1.94	0.49
1:P:450:LYS:O	1:P:529:ASN:HA	2.12	0.49
1:P:693:VAL:HG13	1:P:694:GLU:N	2.27	0.49
1:P:422:TRP:CD2	1:P:423:ARG:HG3	2.48	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:73:LEU:HB2	1:P:260:ALA:HB1	1.95	0.48
1:P:58:GLN:O	1:P:58:GLN:HG2	2.08	0.48
1:P:643:GLU:CA	1:P:646:PHE:CD1	2.94	0.48
1:P:249:GLU:HG3	1:P:250:TYR:N	2.27	0.48
1:P:463:HIS:CG	1:P:534:LEU:HD22	2.49	0.48
1:P:399:GLU:O	1:P:403:GLU:OE2	2.30	0.48
1:P:571:TYR:CD1	1:P:634:VAL:CG1	2.96	0.48
2:L:1074:HIS:CE1	2:L:1075:ASN:OD1	2.66	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:872:LEU:O	1:P:873:ARG:C	2.51	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
1:P:856:SER:O	1:P:857:GLN:C	2.50	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:HD12	1:P:769:ILE:H	1.79	0.48
1:P:243:THR:O	1:P:243:THR:HG22	2.14	0.47
1:P:418:TYR:CE2	1:P:428:ALA:HB2	2.50	0.47
1:P:132:THR:HB	1:P:244:ILE:HG22	1.87	0.47
1:P:109:ILE:CD1	1:P:145:ILE:CG2	2.92	0.47
1:P:58:GLN:CA	1:P:59:LEU:N	2.75	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:525:GLY:C	1:P:527:SER:H	2.17	0.47
1:P:509:PHE:C	1:P:511:PHE:H	2.18	0.47
1:P:190:MET:O	1:P:190:MET:HG2	2.14	0.47
1:P:44:TYR:CD1	1:P:44:TYR:N	2.82	0.47
1:P:871:ASN:O	1:P:872:LEU:C	2.51	0.47
1:P:685:VAL:HG23	1:P:686:SER:N	2.30	0.47
1:P:266:PRO:CD	1:P:404:GLN:HE21	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:877:GLU:C	1:P:879:ASP:N	2.66	0.47
1:P:28:TYR:HD1	1:P:185:VAL:HG23	1.79	0.47
1:P:871:ASN:HB3	1:P:875:ILE:HG12	1.94	0.47
1:P:648:GLN:O	1:P:652:GLU:CB	2.55	0.47
2:L:1046:TYR:CE2	2:L:1080:CYS:SG	3.08	0.47
1:P:448:LYS:NZ	1:P:805:GLU:OE1	2.36	0.47
1:P:23:THR:O	1:P:27:HIS:HB2	2.14	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: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
1:P:74:ILE:CD1	1:P:74:ILE:O	2.63	0.46
1:P:553:GLU:O	1:P:555:GLY:N	2.48	0.46
1:P:553:GLU:CG	1:P:870:LEU:HD12	2.44	0.46
1:P:401:MET:SD	1:P:432:PHE:HA	2.55	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: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:537:ASP:OD1	1:P:813:SER:CB	2.64	0.46
1:P:260:ALA:C	1:P:262:ALA:H	2.19	0.46
2:L:1113:LYS:O	2:L:1113:LYS:CG	2.63	0.46
1:P:678:ALA:O	1:P:679:LYS:C	2.54	0.46
2:L:1027:VAL:HA	2:L:1031:GLU:HG3	1.96	0.46
1:P:413:ALA:O	1:P:414:ILE:HG23	2.15	0.46
1:P:15:GLU:O	1:P:19:ILE:HD13	2.15	0.46
1:P:297:VAL:HG13	1:P:421:ASP:O	2.16	0.46
1:P:78:LEU:O	1:P:82:ILE:HG13	2.14	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:1081:LEU:HD22	2:L:1099:GLN:HE21	1.81	0.46
2:L:1068:HIS:CG	2:L:1069:ALA:H	2.34	0.46
1:P:230:HIS:CG	1:P:245:GLU:HG3	2.42	0.45
1:P:419:ASN:HD22	1:P:419:ASN:HA	1.54	0.45
1:P:416:PHE:CE2	1:P:433:ASN:HA	2.51	0.45
1:P:395:ARG:HG2	1:P:395:ARG:NH1	2.31	0.45
1:P:420:MET:HA	1:P:425:ARG:O	2.16	0.45
1:P:791:LEU:O	1:P:792:ARG:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:206:LYS:HZ3	1:P:206:LYS:HB2	1.82	0.45
2:L:1113:LYS:HG2	2:L:1113:LYS:O	2.17	0.45
1:P:749:LEU:HD23	1:P:751:PHE:HE1	1.81	0.45
1:P:543:ILE:O	1:P:543:ILE:HG22	2.17	0.45
1:P:73:LEU:N	1:P:74:ILE:N	2.64	0.45
1:P:643:GLU:HA	1:P:646:PHE:HD1	1.74	0.45
1:P:489:ILE:O	1:P:492:CYS:HB2	2.17	0.45
2:L:1017:HIS:ND1	2:L:1130:CYS:CB	2.80	0.45
1:P:824:LEU:O	1:P:827:ALA:HB3	2.16	0.45
1:P:74:ILE:HG21	1:P:263:GLY:H	1.82	0.45
1:P:76:THR:C	1:P:79:PRO:HD2	2.37	0.45
1:P:818:PRO:O	1:P:819:ALA:C	2.55	0.45
1:P:552:ASP:O	1:P:552:ASP:OD1	2.35	0.45
2:L:1134:ASP:HA	2:L:1149:ARG:O	2.16	0.45
1:P:109:ILE:HG22	1:P:114:VAL:HG23	1.98	0.45
1:P:824:LEU:O	1:P:827:ALA:N	2.49	0.45
1:P:92:VAL:C	1:P:94:ALA:H	2.20	0.45
1:P:26:ASP:OD1	1:P:26:ASP:O	2.35	0.45
1:P:761:ILE:O	1:P:762:ASN:C	2.55	0.45
1:P:185:VAL:HB	1:P:274:PRO:CB	2.41	0.45
1:P:20:PRO:HG3	1:P:289:ASN:HB2	1.99	0.45
1:P:637:LEU:O	1:P:696:MET:CE	2.64	0.45
1:P:246:LEU:O	1:P:247:ALA:C	2.53	0.45
1:P:814:PHE:HE2	1:P:824:LEU:CD2	2.29	0.45
1:P:728:VAL:N	1:P:848:GLN:HE22	2.01	0.45
1:P:425:ARG:HD2	1:P:427:TYR:OH	2.17	0.45
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
1:P:77:LEU:CD2	1:P:224:THR:HB	2.47	0.44
2:L:1137:ARG:CD	2:L:1141:LYS:HD2	2.39	0.44
1:P:562:LEU:O	1:P:876:LEU:HG	2.16	0.44
1:P:642:LYS:HA	1:P:682:TRP:CE3	2.51	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:232:GLN:CD	1:P:755:PHE:CD1	2.91	0.44
1:P:616:LEU:HD12	1:P:676:TYR:CG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:786:GLN:O	1:P:787:ASP:C	2.56	0.44
1:P:56:GLU:O	1:P:59:LEU:N	2.50	0.44
1:P:15:GLU:O	1:P:18:ALA:HB3	2.18	0.44
1:P:617:ALA:O	1:P:621:LEU:HD12	2.18	0.44
1:P:577:LYS:O	1:P:581:ILE:HG13	2.18	0.44
1:P:723:SER:OG	1:P:724:ALA:N	2.51	0.44
2:L:1089:GLY:O	2:L:1090:LYS:HD3	2.17	0.44
1:P:298:ARG:NH1	1:P:298:ARG:HG3	2.28	0.44
2:L:1029:VAL:CG1	2:L:1030:ARG:N	2.80	0.44
1:P:45:GLU:HB3	1:P:155:ARG:NH2	2.32	0.44
1:P:470:VAL:O	1:P:470:VAL:HG12	2.17	0.44
1:P:697:ASN:HD22	1:P:697:ASN:N	2.16	0.44
1:P:463:HIS:CD2	1:P:467:CYS:SG	3.10	0.44
1:P:118:THR:CG2	1:P:216:CYS:HB3	2.47	0.44
1:P:770:ASP:OD1	1:P:770:ASP:O	2.35	0.44
1:P:877:GLU:C	1:P:879:ASP:H	2.21	0.44
1:P:770:ASP:O	1:P:772:HIS:N	2.51	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:637:LEU:HA	1:P:637:LEU:HD12	1.61	0.44
1:P:869:ASN:OD1	1:P:869:ASN:O	2.36	0.44
1:P:36:GLN:O	1:P:39:LEU:HB3	2.17	0.43
1:P:855:GLU:OE1	2:L:1031:GLU:OE2	2.36	0.43
1:P:108:GLU:CG	1:P:108:GLU:O	2.65	0.43
2:L:1022:LYS:H	2:L:1025:GLN:NE2	2.14	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: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:455:GLU:O	1:P:458:TYR:HB3	2.17	0.43
1:P:19:ILE:N	1:P:19:ILE:HD12	2.21	0.43
1:P:422:TRP:CZ2	1:P:423:ARG:HG3	2.54	0.43
1:P:579:ASN:OD1	1:P:625:VAL:CB	2.63	0.43
1:P:710:VAL:HG12	1:P:712:ASP:H	1.84	0.43
1:P:438:ASP:HA	1:P:441:LYS:HB2	2.00	0.43
2:L:1034:GLN:O	2:L:1035:TRP:C	2.56	0.43
1:P:162:PHE:CG	1:P:163:LYS:N	2.60	0.43
1:P:685:VAL:C	1:P:687:VAL:N	2.72	0.43
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:146:GLU:O	1:P:149:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:490:MET:O	1:P:493:ALA:HB2	2.19	0.43
1:P:496:PRO:HG2	1:P:497:LEU:N	2.34	0.43
1:P:265:SER:HB3	1:P:269:GLN:OE1	2.19	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:141:ILE:O	1:P:145:ILE:HG12	2.18	0.43
1:P:123:LEU:HD12	1:P:264:ILE:HG21	2.01	0.43
1:P:552:ASP:OD1	1:P:552:ASP:C	2.56	0.42
1:P:836:TYR:HE1	1:P:841:VAL:HG21	1.82	0.42
1:P:85:ILE:HD13	1:P:114:VAL:HG12	2.00	0.42
1:P:391:ARG:HD2	1:P:391:ARG:C	2.40	0.42
1:P:774:GLN:OE1	1:P:774:GLN:HA	2.19	0.42
1:P:460:LEU:O	1:P:463:HIS:HB3	2.18	0.42
1:P:298:ARG:NH1	1:P:419:ASN:CB	2.73	0.42
1:P:120:LYS:HZ1	1:P:267:MET:HA	1.83	0.42
1:P:36:GLN:OE1	1:P:36:GLN:HA	2.20	0.42
1:P:313:MET:SD	1:P:316:VAL:HG21	2.59	0.42
1:P:854:HIS:O	1:P:855:GLU:C	2.57	0.42
1:P:74:ILE:N	1:P:75:THR:CG2	2.78	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
1:P:109:ILE:HD13	1:P:145:ILE:CG2	2.50	0.42
2:L:1009:GLU:O	2:L:1010:SER:HB3	2.20	0.42
1:P:534:LEU:HD11	1:P:818:PRO:CG	2.37	0.42
2:L:1141:LYS:C	2:L:1143:GLU:N	2.73	0.42
1:P:619:GLN:O	1:P:666:MET:HG3	2.19	0.42
2:L:1034:GLN:HE22	2:L:1038:GLU:HG3	1.85	0.42
2:L:1018:CYS:O	2:L:1019:SER:C	2.57	0.42
1:P:782:PHE:HE1	1:P:845:PHE:CE1	2.37	0.42
1:P:877:GLU:H	1:P:877:GLU:HG2	1.63	0.42
1:P:80:LYS:O	1:P:83:ALA:HB3	2.19	0.42
2:L:1136:LYS:HE2	2:L:1140:GLU:OE2	2.19	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:159:ALA:O	1:P:162:PHE:O	2.38	0.42
1:P:19:ILE:O	1:P:20:PRO:C	2.56	0.42
1:P:669:GLN:HA	1:P:670:PRO:HD2	1.77	0.42
1:P:657:PRO:O	1:P:660:ASP:OD1	2.38	0.42
1:P:211:HIS:HA	1:P:214:VAL:CG1	2.49	0.42
2:L:1120:ARG:HH21	2:L:1125:VAL:HG21	1.84	0.42
1:P:150:ARG:CG	1:P:150:ARG:O	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:39:LEU:CD1	1:P:269:GLN:NE2	2.83	0.41
1:P:642:LYS:C	1:P:644:PHE:N	2.73	0.41
1:P:275:PRO:HG2	1:P:324:GLN:HG2	2.02	0.41
1:P:39:LEU:HD11	1:P:269:GLN:NE2	2.35	0.41
1:P:113:ALA:O	1:P:114:VAL:C	2.57	0.41
1:P:211:HIS:O	1:P:214:VAL:CG1	2.68	0.41
2:L:1126:ALA:C	2:L:1128:LYS:H	2.24	0.41
1:P:426:VAL:O	1:P:426:VAL:HG23	2.20	0.41
1:P:685:VAL:O	1:P:687:VAL:N	2.53	0.41
1:P:576:LYS:CG	1:P:577:LYS:N	2.83	0.41
2:L:1086:ASP:OD1	2:L:1087:ASP:N	2.53	0.41
1:P:873:ARG:HA	1:P:873:ARG:HD3	1.90	0.41
1:P:495:SER:OG	1:P:496:PRO:HD3	2.20	0.41
1:P:77:LEU:HD21	1:P:250:TYR:OH	2.20	0.41
1:P:816:THR:HG22	1:P:817:ILE:N	2.23	0.41
1:P:826:LYS:HG2	1:P:829:ARG:NH2	2.16	0.41
1:P:505:GLN:HG3	1:P:511:PHE:CD2	2.56	0.41
1:P:335:LEU:HD21	1:P:406:ASN:ND2	2.35	0.41
1:P:550:LEU:HA	1:P:550:LEU:HD23	1.75	0.41
1:P:422:TRP:CZ2	1:P:423:ARG:HD3	2.55	0.41
1:P:185:VAL:H	1:P:274:PRO:CG	2.28	0.41
1:P:800:GLU:O	1:P:801:LYS:C	2.58	0.41
1:P:791:LEU:HD11	1:P:809:LEU:HD22	2.02	0.41
1:P:571:TYR:CG	1:P:631:LYS:HB2	2.55	0.41
1:P:613:THR:C	1:P:615:ALA:N	2.72	0.41
1:P:543:ILE:HG22	1:P:559:VAL:CG2	2.51	0.41
2:L:1123:HIS:HD1	2:L:1123:HIS:C	2.22	0.41
1:P:779:ALA:N	1:P:780:PRO:HD2	2.36	0.41
1:P:873:ARG:C	1:P:875:ILE:H	2.22	0.41
1:P:829:ARG:HH11	1:P:829:ARG:HB2	1.85	0.41
1:P:42:GLU:CG	1:P:50:ARG:NH1	2.83	0.41
2:L:1050:ILE:HG22	2:L:1099:GLN:HG3	2.02	0.40
1:P:109:ILE:CD1	1:P:145:ILE:HG22	2.51	0.40
1:P:83:ALA:O	1:P:84:ARG:C	2.59	0.40
1:P:514:PHE:O	1:P:515:CYS:C	2.60	0.40
1:P:731:ASP:CG	1:P:792:ARG:HH21	2.24	0.40
1:P:733:PHE:HA	1:P:734:PRO:HD3	1.69	0.40
2:L:1037:LYS:HE2	2:L:1037:LYS:HB3	1.85	0.40
1:P:480:LYS:C	1:P:482:ILE:N	2.72	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1090:LYS:HA	2:L:1090:LYS:HD3	1.87	0.40
1:P:45:GLU:CB	1:P:155:ARG:NH2	2.85	0.40
1:P:185:VAL:O	1:P:187:GLU:CD	2.60	0.40
1:P:464:GLY:HA2	1:P:467:CYS:SG	2.62	0.40
1:P:80:LYS:HD2	1:P:224:THR:HG22	2.02	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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	P	760/883 (86%)	591 (78%)	120 (16%)	49 (6%)	2 4
2	L	147/151 (97%)	110 (75%)	34 (23%)	3 (2%)	9 30
All	All	907/1034 (88%)	701 (77%)	154 (17%)	52 (6%)	2 6

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	P	563	PRO
1	P	761	ILE

5.3.2 Protein sidechains (i)

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	642/729 (88%)	608 (95%)	34 (5%)	28	61
2	L	124/125 (99%)	116 (94%)	8 (6%)	21	52
All	All	766/854 (90%)	724 (94%)	42 (6%)	27	59

All (42) 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	162	PHE
1	P	206	LYS
1	P	289	ASN
1	P	291	ARG
1	P	296	LEU
1	P	310	ASP
1	P	391	ARG
1	P	395	ARG
1	P	403	GLU
1	P	419	ASN
1	P	421	ASP
1	P	433	ASN
1	P	452	ILE
1	P	471	ASP
1	P	480	LYS

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Mol	Chain	Res	Type
1	P	510	CYS
1	P	552	ASP
1	P	562	LEU
1	P	627	ARG
1	P	637	LEU
1	P	712	ASP
1	P	720	ARG
1	P	728	VAL
1	P	748	ASN
1	P	754	GLN
1	P	825	PHE
1	P	847	ASP
1	P	851	ASP
2	L	1002	ARG
2	L	1031	GLU
2	L	1034	GLN
2	L	1035	TRP
2	L	1036	HIS
2	L	1049	ILE
2	L	1085	ILE
2	L	1128	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	36	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
1	P	406	ASN
1	P	411	HIS
1	P	419	ASN
1	P	433	ASN
1	P	499	ASN
1	P	544	GLN
1	P	545	HIS
1	P	560	ASN

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Mol	Chain	Res	Type
1	P	648	GLN
1	P	697	ASN
1	P	737	GLN
1	P	744	GLN
1	P	758	GLN
1	P	764	ASN
1	P	781	ASN
1	P	784	HIS
1	P	790	HIS
1	P	811	HIS
1	P	848	GLN
1	P	857	GLN
1	P	869	ASN
2	L	1007	GLN
2	L	1017	HIS
2	L	1025	GLN
2	L	1034	GLN
2	L	1036	HIS
2	L	1039	GLN
2	L	1074	HIS
2	L	1101	GLN
2	L	1122	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 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.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	P	774/883 (87%)	0.01	36 (4%) 35 24	19, 77, 112, 123	41 (5%)
2	L	149/151 (98%)	-0.22	3 (2%) 68 58	46, 66, 105, 114	5 (3%)
All	All	923/1034 (89%)	-0.02	39 (4%) 40 28	19, 75, 110, 123	46 (4%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	233	ASN	6.7
1	P	717	GLU	6.4
1	P	712	ASP	4.7
1	P	711	LYS	4.6
1	P	751	PHE	4.6
1	P	718	ILE	3.9
1	P	879	ASP	3.8
1	P	759	PRO	3.7
1	P	10	ASP	3.5
1	P	585	ASP	3.5
1	P	612	GLY	3.4
1	P	716	GLY	3.3
1	P	43	SER	3.2
1	P	188	ALA	3.2
1	P	762	ASN	3.2
1	P	97	GLY	3.2
1	P	183	MET	3.1
1	P	561	LEU	3.1
1	P	765	LYS	3.1
1	P	11	PHE	2.9
1	P	28	TYR	2.9
1	P	747	LEU	2.9
1	P	96	ARG	2.8
1	P	164	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	P	384	VAL	2.6
1	P	587	ILE	2.5
1	P	564	SER	2.4
2	L	1046	TYR	2.4
2	L	1150	GLY	2.4
1	P	95	LYS	2.3
1	P	764	ASN	2.2
1	P	558	ALA	2.2
2	L	1085	ILE	2.1
1	P	538	GLY	2.1
1	P	761	ILE	2.1
1	P	871	ASN	2.1
1	P	763	THR	2.1
1	P	103	PHE	2.0
1	P	256	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	HG	L	903	1/1	0.97	0.11	-1.02	113,113,113,113	0
3	HG	P	907	1/1	0.99	0.04	-4.30	159,159,159,159	0
3	HG	P	908	1/1	0.99	0.03	-4.50	199,199,199,199	0
3	HG	P	905	1/1	0.99	0.12	-	83,83,83,83	0
3	HG	P	906	1/1	0.95	0.16	-	136,136,136,136	0
3	HG	P	904	1/1	0.99	0.15	-	87,87,87,87	0
3	HG	P	909	1/1	0.95	0.15	-	199,199,199,199	0

6.5 Other polymers (i)

There are no such residues in this entry.