



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:40 PM UTC

PDB ID : 4GZZ / pdb_00004gzz
Title : Crystal structures of bacterial RNA Polymerase paused elongation complexes
Authors : Weixlbaumer, A.; Leon, K.; Landick, R.; Darst, S.A.
Deposited on : 2012-09-06
Resolution : 4.29 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

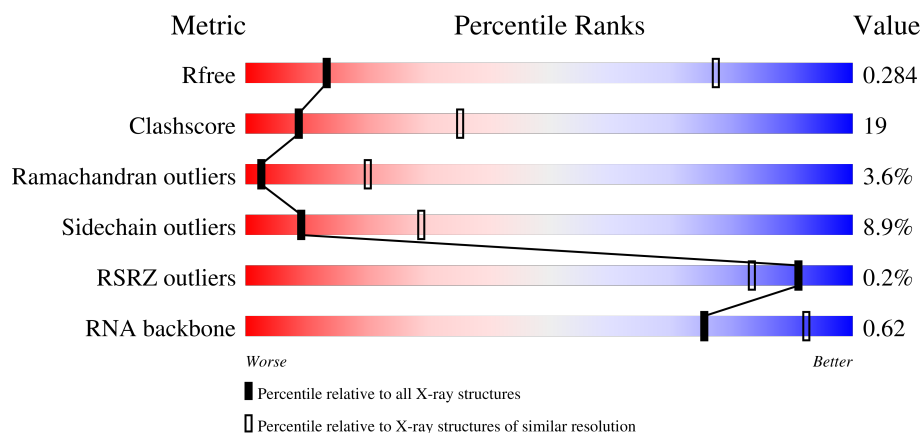
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.29 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)
RNA backbone	3983	1036 (5.50-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	315	42% 26% • 29%
1	B	315	47% 23% • 29%
2	C	1119	53% 38% 6% •
3	D	1534	49% 34% 5% • 11%

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Mol	Chain	Length	Quality of chain
4	E	99	41%41%10%6%
5	N	13	46%38%15%
6	R	16	6%44%6%44%
7	T	22	50%50%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 24400 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			
1	B	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1083	Total	C	N	O	S	0	0	0
			8548	5412	1524	1588	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1358	Total	C	N	O	S	0	0	0
			10714	6780	1900	2001	33			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1525	HIS	-	expression tag	UNP Q8RQE8
D	1526	HIS	-	expression tag	UNP Q8RQE8
D	1527	HIS	-	expression tag	UNP Q8RQE8
D	1528	HIS	-	expression tag	UNP Q8RQE8
D	1529	HIS	-	expression tag	UNP Q8RQE8
D	1530	HIS	-	expression tag	UNP Q8RQE8
D	1531	HIS	-	expression tag	UNP Q8RQE8
D	1532	HIS	-	expression tag	UNP Q8RQE8
D	1533	HIS	-	expression tag	UNP Q8RQE8
D	1534	HIS	-	expression tag	UNP Q8RQE8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			754	481	131	138	4			

- Molecule 5 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	N	11	Total	C	N	O	P	0	0	0
			225	107	43	64	11			

- Molecule 6 is a RNA chain called RNA transcript.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	R	9	Total	C	N	O	P	0	0	0
			191	85	31	66	9			

- Molecule 7 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	T	22	Total	C	N	O	P	0	0	0
			447	213	81	131	22			

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		

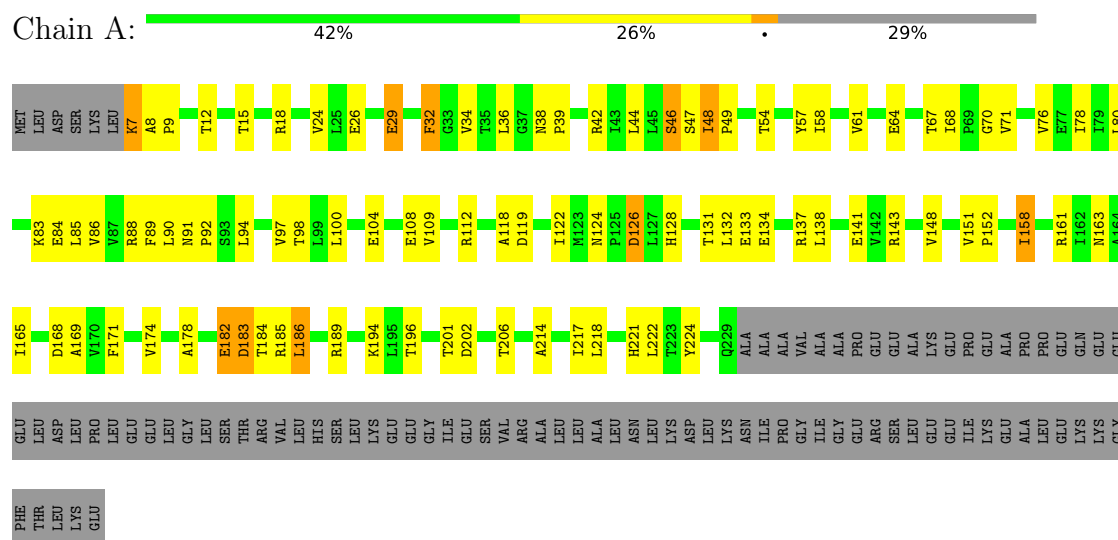
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total	Mg	0	0
			1	1		

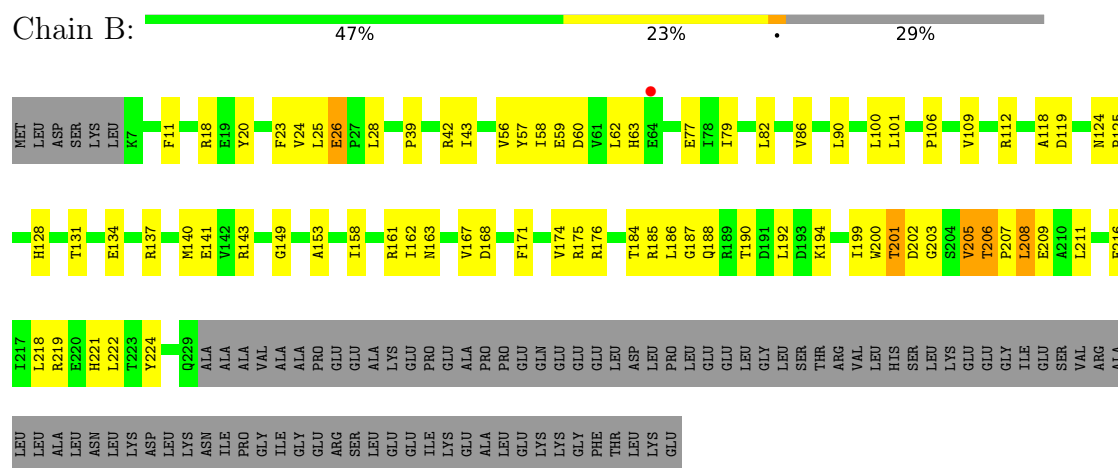
3 Residue-property plots

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

• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 2: DNA-directed RNA polymerase subunit beta

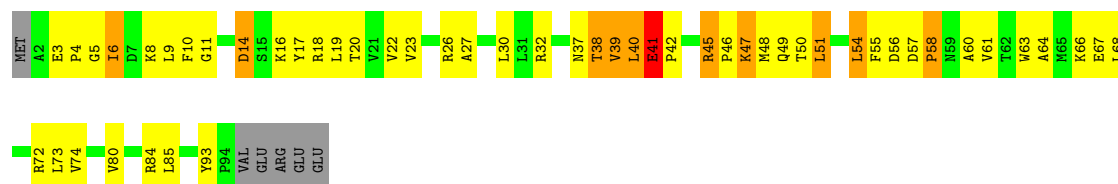








- Molecule 4: DNA-directed RNA polymerase subunit omega



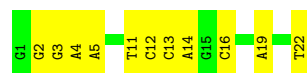
- Molecule 5: non-template DNA



- Molecule 6: RNA transcript



- Molecule 7: template DNA



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	286.55Å 286.55Å 199.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.78 – 4.29 38.78 – 4.29	Depositor EDS
% Data completeness (in resolution range)	99.0 (38.78-4.29) 87.7 (38.78-4.29)	Depositor EDS
R_{merge}	0.44	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 4.28Å)	Xtriage
Refinement program	PHENIX 1.8_1069, CNS	Depositor
R, R_{free}	0.234 , 0.285 0.236 , 0.284	Depositor DCC
R_{free} test set	2074 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å ²)	164.3	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 80.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24400	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	0/1791	0.82	1/2436 (0.0%)
1	B	0.37	0/1791	0.82	2/2436 (0.1%)
2	C	0.38	0/8711	0.86	20/11784 (0.2%)
3	D	0.38	0/10897	0.83	16/14726 (0.1%)
4	E	0.37	0/768	0.91	4/1035 (0.4%)
5	N	0.10	0/252	0.51	0/386
6	R	0.10	0/212	0.22	0/328
7	T	0.13	0/500	0.54	0/768
All	All	0.37	0/24922	0.83	43/33899 (0.1%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	705	ALA	CA-C-N	-10.62	106.56	119.84
3	D	705	ALA	C-N-CA	-10.62	106.56	119.84
2	C	726	ILE	CA-C-N	7.64	129.40	119.84
2	C	726	ILE	C-N-CA	7.64	129.40	119.84
2	C	247	PRO	N-CA-C	7.46	119.81	110.70
2	C	792	VAL	CA-C-N	7.28	127.87	120.38
2	C	792	VAL	C-N-CA	7.28	127.87	120.38
3	D	827	ILE	N-CA-C	7.12	117.11	110.42
4	E	41	GLU	CA-C-N	-6.97	111.13	119.84
4	E	41	GLU	C-N-CA	-6.97	111.13	119.84
1	B	26	GLU	N-CA-C	6.93	114.45	108.22
2	C	728	HIS	N-CA-C	6.81	122.13	113.55
2	C	247	PRO	CA-C-N	-6.71	111.45	119.84
2	C	247	PRO	C-N-CA	-6.71	111.45	119.84
3	D	80	VAL	N-CA-C	6.64	117.60	107.77
3	D	1188	VAL	N-CA-C	6.62	117.09	108.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	593	ASN	CA-C-N	6.61	128.10	119.84
3	D	593	ASN	C-N-CA	6.61	128.10	119.84
2	C	1111	ILE	N-CA-C	-6.09	107.92	113.71
2	C	177	GLU	CA-C-N	6.09	127.45	119.84
2	C	177	GLU	C-N-CA	6.09	127.45	119.84
2	C	118	ILE	CA-C-N	6.03	126.35	119.83
2	C	118	ILE	C-N-CA	6.03	126.35	119.83
3	D	1340	GLY	CA-C-N	6.02	125.73	119.05
3	D	1340	GLY	C-N-CA	6.02	125.73	119.05
2	C	151	ASP	CA-C-N	5.70	126.97	119.84
2	C	151	ASP	C-N-CA	5.70	126.97	119.84
3	D	51	GLY	CA-C-N	5.64	126.89	119.84
3	D	51	GLY	C-N-CA	5.64	126.89	119.84
2	C	601	GLY	N-CA-C	5.57	117.51	110.38
3	D	528	VAL	N-CA-C	5.49	116.03	108.12
2	C	258	TYR	N-CA-C	-5.39	106.90	112.93
3	D	183	GLU	N-CA-C	5.31	116.69	107.93
3	D	81	THR	N-CA-C	-5.27	101.63	109.96
1	B	118	ALA	CB-CA-C	-5.16	110.21	117.23
1	A	183	ASP	N-CA-C	5.10	114.88	108.45
4	E	45	ARG	CA-C-N	5.10	125.01	119.76
4	E	45	ARG	C-N-CA	5.10	125.01	119.76
2	C	52	PHE	CA-C-N	-5.04	113.54	119.84
2	C	52	PHE	C-N-CA	-5.04	113.54	119.84
2	C	284	ARG	N-CA-C	5.04	117.46	109.50
3	D	1231	GLU	CA-C-N	-5.03	113.56	119.84
3	D	1231	GLU	C-N-CA	-5.03	113.56	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1759	0	1805	66	0
1	B	1759	0	1805	51	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	8548	0	8650	381	0
3	D	10714	0	10936	427	1
4	E	754	0	769	41	0
5	N	225	0	124	3	0
6	R	191	0	95	10	0
7	T	447	0	248	10	0
8	D	2	0	0	0	0
9	D	1	0	0	0	0
All	All	24400	0	24432	912	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 19.

All (912) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:428:ARG:HH12	3:D:1086:LEU:HD21	1.24	0.98
2:C:610:ARG:HG3	2:C:610:ARG:HH11	1.27	0.96
2:C:846:LYS:NZ	6:R:29:U:OP1	1.99	0.96
1:B:188:GLN:O	3:D:646:LYS:NZ	2.00	0.94
1:A:80:LEU:HD21	2:C:573:ARG:HH11	1.34	0.92
2:C:194:VAL:HG21	2:C:224:GLU:HG3	1.57	0.87
3:D:808:THR:H	3:D:809:PRO:HD2	1.37	0.86
3:D:925:GLU:O	3:D:929:ARG:NH1	2.08	0.86
2:C:274:ARG:NH1	2:C:284:ARG:HH12	1.72	0.86
2:C:388:ARG:NH1	7:T:22:DT:OP1	2.09	0.85
3:D:1486:VAL:HG11	4:E:22:VAL:HG13	1.58	0.85
3:D:629:SER:HB3	3:D:726:ILE:HG12	1.61	0.81
3:D:1128:VAL:HG23	3:D:1133:ARG:HH22	1.43	0.81
1:A:34:VAL:HG21	2:C:939:ARG:HE	1.45	0.81
2:C:738:ASP:HB2	2:C:744:ARG:HB3	1.61	0.81
2:C:274:ARG:HH12	2:C:284:ARG:HH12	1.26	0.80
2:C:290:LEU:HD13	2:C:302:VAL:HG12	1.64	0.80
3:D:501:ALA:HB1	3:D:1453:ALA:HB2	1.64	0.80
2:C:224:GLU:HB3	2:C:227:PHE:HB3	1.62	0.80
1:A:151:VAL:HB	1:A:169:ALA:HB3	1.64	0.79
2:C:292:ARG:NH1	2:C:294:GLU:HB2	1.97	0.78
3:D:136:ASP:HB2	3:D:137:PRO:HD2	1.66	0.78
3:D:161:LEU:O	3:D:397:LYS:NZ	2.17	0.78
2:C:1008:ARG:HD2	2:C:1026:GLN:HB3	1.66	0.77
2:C:292:ARG:HH12	2:C:294:GLU:HB2	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1106:VAL:HG12	3:D:1220:ALA:HA	1.63	0.77
3:D:213:VAL:HG11	3:D:385:VAL:HA	1.67	0.77
2:C:1008:ARG:HH12	2:C:1011:GLY:N	1.82	0.76
1:A:18:ARG:HG3	1:A:206:THR:HG22	1.67	0.76
1:A:108:GLU:HG2	1:A:131:THR:HG22	1.67	0.76
3:D:1209:LEU:HD11	4:E:16:LYS:HD2	1.67	0.76
1:A:182:GLU:HB2	1:A:194:LYS:HD3	1.69	0.75
2:C:1051:GLU:HG3	2:C:1055:LEU:HD23	1.67	0.75
2:C:584:GLU:HB3	2:C:666:LEU:H	1.52	0.75
2:C:1103:ASP:HB3	2:C:1105:LYS:HZ1	1.50	0.75
2:C:720:GLU:O	2:C:820:ARG:NH2	2.20	0.74
2:C:52:PHE:HE1	2:C:98:LEU:HD13	1.53	0.74
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.70	0.74
2:C:437:ARG:HD3	2:C:467:ILE:HB	1.68	0.74
1:B:205:VAL:HG13	1:B:209:GLU:HB2	1.69	0.74
2:C:714:ASP:OD1	2:C:820:ARG:NH1	2.21	0.74
3:D:983:LEU:HD13	3:D:988:ARG:HB2	1.69	0.74
2:C:1103:ASP:HB3	2:C:1105:LYS:NZ	2.03	0.74
2:C:239:PHE:HB2	2:C:251:ASP:HB3	1.71	0.73
1:B:79:ILE:HA	1:B:82:LEU:HD12	1.71	0.73
2:C:610:ARG:HH11	2:C:610:ARG:CG	2.02	0.73
2:C:1105:LYS:NZ	2:C:1107:ASN:HB2	2.03	0.73
2:C:726:ILE:HD13	2:C:754:ILE:HD13	1.71	0.72
3:D:1165:TYR:HB3	3:D:1207:TYR:HE1	1.54	0.72
3:D:1283:ILE:HD11	3:D:1290:LEU:HD12	1.72	0.72
2:C:670:GLN:NE2	2:C:699:PHE:O	2.22	0.72
2:C:290:LEU:HD11	2:C:301:GLU:H	1.55	0.72
2:C:334:ARG:HH12	2:C:415:PRO:HG2	1.55	0.72
2:C:224:GLU:O	2:C:228:ALA:N	2.21	0.72
2:C:435:TYR:OH	2:C:533:ASP:OD2	2.04	0.71
2:C:1048:THR:N	3:D:758:GLU:OE2	2.21	0.71
3:D:1194:CYS:SG	3:D:1195:GLN:N	2.63	0.71
3:D:127:LEU:HG	3:D:152:LEU:HD12	1.72	0.70
2:C:274:ARG:HH12	2:C:284:ARG:NH1	1.87	0.70
2:C:23:VAL:HA	2:C:121:MET:HE1	1.73	0.70
3:D:210:ARG:HB3	3:D:388:HIS:HB2	1.74	0.70
3:D:805:GLU:OE2	3:D:816:HIS:NE2	2.25	0.70
3:D:52:PRO:HG2	3:D:80:VAL:HG13	1.74	0.69
3:D:148:GLU:HB3	3:D:151:GLN:HB2	1.72	0.69
3:D:557:LEU:HD21	3:D:566:ILE:HG22	1.74	0.69
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:701:LEU:HB3	3:D:713:ILE:HD11	1.74	0.69
3:D:165:LYS:HE3	3:D:200:ASP:HB2	1.75	0.69
2:C:290:LEU:HD21	2:C:300:ASP:HB2	1.74	0.69
2:C:579:VAL:O	2:C:842:ARG:NH2	2.26	0.69
1:A:58:ILE:HB	1:A:61:VAL:HB	1.74	0.68
1:A:104:GLU:HB3	1:A:137:ARG:HG3	1.74	0.68
2:C:674:VAL:HG22	2:C:869:VAL:HB	1.75	0.68
3:D:798:GLU:HB2	3:D:828:LYS:HE3	1.76	0.68
3:D:852:ALA:HB1	3:D:857:ILE:HD11	1.74	0.68
2:C:260:LEU:HD22	2:C:288:ARG:HH22	1.58	0.68
3:D:346:ARG:NH1	3:D:347:VAL:O	2.27	0.68
4:E:46:PRO:HG3	4:E:66:LYS:HD3	1.76	0.68
2:C:22:GLN:NE2	2:C:136:ILE:O	2.25	0.68
2:C:976:ASP:OD1	2:C:978:ARG:NH1	2.26	0.68
3:D:169:TYR:HB3	3:D:195:VAL:HG11	1.75	0.68
2:C:212:GLY:HA2	2:C:218:VAL:HG21	1.75	0.68
2:C:734:LEU:HG	2:C:737:LEU:HD12	1.74	0.67
3:D:568:ARG:NH1	3:D:571:LYS:HE3	2.09	0.67
3:D:135:LEU:HD23	3:D:148:GLU:HB2	1.74	0.67
2:C:274:ARG:HH12	2:C:284:ARG:HH22	1.43	0.67
3:D:820:GLU:HB2	3:D:836:VAL:HG21	1.76	0.67
1:B:90:LEU:HB2	1:B:119:ASP:HB3	1.76	0.66
2:C:845:ASN:HB2	2:C:884:GLN:NE2	2.11	0.66
2:C:292:ARG:HG3	2:C:292:ARG:HH11	1.58	0.66
3:D:1495:ILE:HG23	4:E:84:ARG:HD3	1.75	0.66
4:E:54:LEU:HG	4:E:58:PRO:HG2	1.76	0.66
1:B:59:GLU:HB3	1:B:137:ARG:HH12	1.61	0.66
3:D:493:ARG:NH2	3:D:1389:LEU:O	2.27	0.66
2:C:30:LEU:HB3	2:C:44:ILE:HD12	1.78	0.66
2:C:115:LEU:HA	2:C:375:SER:HB2	1.78	0.65
2:C:101:ILE:HD12	2:C:107:LEU:HD22	1.78	0.65
2:C:265:ARG:HH11	2:C:267:TYR:HD1	1.45	0.65
2:C:1105:LYS:HZ1	2:C:1107:ASN:HB2	1.62	0.65
2:C:185:LYS:HG2	2:C:190:LYS:HG2	1.79	0.65
2:C:787:ASP:OD1	2:C:791:ARG:NH2	2.29	0.65
3:D:568:ARG:HH11	3:D:571:LYS:HE3	1.61	0.65
1:B:175:ARG:N	1:B:200:TRP:O	2.29	0.65
2:C:824:ARG:NH2	2:C:826:TYR:OH	2.29	0.65
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.79	0.65
3:D:645:PRO:HG2	3:D:648:MET:HG3	1.78	0.65
3:D:1147:ARG:HD3	3:D:1188:VAL:HG21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:770:LEU:HD12	3:D:1211:MET:HA	1.80	0.64
3:D:1273:VAL:HG12	3:D:1274:ILE:H	1.62	0.64
2:C:292:ARG:HB3	2:C:299:LYS:HZ2	1.62	0.64
3:D:1147:ARG:HE	3:D:1364:HIS:HE1	1.44	0.64
2:C:428:ARG:NH1	3:D:1086:LEU:HD21	2.06	0.64
3:D:783:ARG:HH11	3:D:783:ARG:HG2	1.62	0.64
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	1.79	0.64
3:D:1273:VAL:HG21	3:D:1305:LEU:HD12	1.79	0.64
2:C:95:TYR:HD1	2:C:112:GLU:HB3	1.61	0.64
2:C:690:ILE:HG23	2:C:852:ILE:HG23	1.79	0.64
3:D:988:ARG:HA	3:D:991:GLN:HB2	1.79	0.64
6:R:24:U:O4	7:T:19:DA:N1	2.31	0.64
2:C:668:LEU:O	2:C:995:MET:HB3	1.97	0.63
3:D:362:GLU:O	3:D:364:GLY:N	2.22	0.63
3:D:414:ARG:HG3	3:D:433:GLY:H	1.63	0.63
3:D:950:GLY:N	3:D:953:ASP:OD2	2.30	0.63
3:D:1213:ARG:HH22	4:E:11:GLY:HA2	1.63	0.63
4:E:48:MET:HB2	4:E:54:LEU:HB2	1.81	0.63
6:R:24:U:H3	7:T:19:DA:H2	1.45	0.63
2:C:1008:ARG:HH12	2:C:1010:THR:C	2.06	0.63
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.79	0.63
3:D:129:PHE:HB3	3:D:572:ARG:HG3	1.81	0.63
3:D:700:VAL:HG12	3:D:749:VAL:HG12	1.81	0.63
2:C:86:LYS:HD3	2:C:813:VAL:HG12	1.81	0.62
2:C:1009:SER:HA	3:D:625:TYR:HA	1.81	0.62
1:A:71:VAL:HG11	1:A:78:ILE:HD11	1.81	0.62
2:C:144:PRO:HB3	2:C:164:PRO:HA	1.82	0.62
2:C:264:PRO:HB2	2:C:289:THR:HG21	1.79	0.62
2:C:658:GLY:N	2:C:661:SER:OG	2.32	0.62
2:C:580:MET:HB2	2:C:584:GLU:OE2	1.99	0.62
3:D:163:TYR:O	3:D:165:LYS:N	2.29	0.62
1:B:62:LEU:HD23	1:B:163:ASN:HD22	1.65	0.62
2:C:744:ARG:HG3	2:C:747:ALA:HB2	1.81	0.62
3:D:1314:LYS:NZ	3:D:1316:GLY:HA3	2.14	0.62
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.81	0.62
2:C:309:TYR:CZ	2:C:321:GLU:HB3	2.35	0.62
3:D:501:ALA:O	3:D:505:SER:OG	2.15	0.61
3:D:1354:LYS:HA	3:D:1357:ARG:HD2	1.81	0.61
3:D:115:LEU:HD21	3:D:468:LEU:HD22	1.81	0.61
3:D:1294:VAL:HG11	3:D:1319:VAL:HG11	1.82	0.61
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:274:ARG:HH12	2:C:284:ARG:NH2	1.98	0.61
2:C:505:GLY:O	2:C:506:ASN:ND2	2.31	0.61
3:D:1232:PRO:HB2	3:D:1361:VAL:HG11	1.81	0.61
2:C:873:PRO:HB3	3:D:949:ILE:HG12	1.81	0.61
2:C:165:LEU:HG	2:C:166:PRO:HA	1.82	0.61
2:C:299:LYS:HZ2	2:C:299:LYS:HB3	1.64	0.61
2:C:599:GLU:OE2	2:C:651:LYS:HD2	2.01	0.61
2:C:953:VAL:HG13	2:C:966:LEU:HD13	1.81	0.61
2:C:267:TYR:HB2	2:C:272:ALA:HB3	1.82	0.60
3:D:1405:GLU:HA	3:D:1409:ALA:HB3	1.81	0.60
1:A:112:ARG:NH2	1:A:126:ASP:OD1	2.35	0.60
2:C:578:VAL:HG13	2:C:579:VAL:HG23	1.83	0.60
2:C:607:ASP:OD1	2:C:608:GLY:N	2.34	0.60
3:D:87:ARG:HD2	3:D:88:TYR:CE1	2.37	0.60
3:D:543:LEU:HD13	3:D:581:LEU:HA	1.84	0.60
2:C:259:GLY:HA2	2:C:291:ALA:HB2	1.83	0.60
3:D:917:GLN:HB3	3:D:921:ARG:NH1	2.17	0.60
3:D:473:LEU:HD23	3:D:499:VAL:HG21	1.84	0.60
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.83	0.60
2:C:7:GLY:HA3	2:C:904:PRO:HG2	1.83	0.60
2:C:184:MET:HB2	2:C:193:LEU:HB2	1.84	0.60
2:C:230:ARG:HB3	2:C:233:GLU:HB2	1.84	0.60
2:C:759:THR:HG22	2:C:787:ASP:HA	1.84	0.60
3:D:184:GLU:HA	3:D:202:VAL:HA	1.82	0.60
3:D:1479:ASP:OD2	3:D:1482:ARG:NH2	2.34	0.60
3:D:18:ILE:HG23	3:D:518:PRO:HG3	1.83	0.60
2:C:978:ARG:CG	2:C:978:ARG:HH11	2.15	0.59
3:D:612:GLY:O	3:D:616:GLN:NE2	2.35	0.59
2:C:437:ARG:NH1	2:C:491:GLU:OE1	2.26	0.59
3:D:165:LYS:O	3:D:395:VAL:HG23	2.02	0.59
3:D:760:ARG:HD3	4:E:61:VAL:HG11	1.83	0.59
4:E:39:VAL:O	4:E:72:ARG:NH1	2.35	0.59
2:C:265:ARG:NH1	2:C:267:TYR:HD1	2.00	0.59
1:B:149:GLY:H	1:B:171:PHE:HB2	1.66	0.59
3:D:1174:LEU:HD22	3:D:1183:ILE:HD11	1.85	0.59
2:C:165:LEU:HD21	2:C:418:LEU:HD11	1.85	0.59
3:D:565:ILE:HD12	3:D:565:ILE:H	1.66	0.59
2:C:408:ARG:NH2	2:C:456:ALA:O	2.36	0.59
3:D:734:GLU:OE2	3:D:780:LYS:NZ	2.36	0.59
2:C:146:VAL:HG22	2:C:162:ILE:HG12	1.85	0.58
3:D:614:PHE:HB3	3:D:1439:SER:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:618:LEU:HD11	3:D:1467:ILE:HG12	1.84	0.58
1:A:80:LEU:HD21	2:C:573:ARG:NH1	2.12	0.58
2:C:443:THR:HG22	2:C:453:THR:HG22	1.85	0.58
3:D:647:ARG:NH1	3:D:724:GLN:OE1	2.36	0.58
2:C:604:ALA:HB3	2:C:612:VAL:HB	1.85	0.58
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.84	0.58
2:C:223:ASP:OD1	2:C:224:GLU:HG2	2.04	0.58
2:C:755:LEU:HD11	2:C:825:VAL:HG11	1.85	0.58
3:D:1161:GLU:HB2	3:D:1164:ARG:HB2	1.85	0.58
2:C:38:LYS:HD2	2:C:39:ARG:NH1	2.18	0.58
2:C:216:GLU:O	2:C:218:VAL:N	2.37	0.58
1:B:206:THR:HG22	1:B:207:PRO:HD2	1.84	0.58
3:D:58:CYS:SG	3:D:59:ALA:N	2.77	0.58
3:D:660:LYS:HG3	3:D:694:VAL:HG12	1.86	0.58
4:E:14:ASP:OD1	4:E:14:ASP:N	2.30	0.58
3:D:1031:ASN:OD1	3:D:1033:GLN:NE2	2.36	0.57
2:C:18:LEU:HD21	2:C:542:VAL:HG11	1.86	0.57
2:C:537:LYS:HG2	2:C:905:ILE:HG12	1.86	0.57
3:D:520:LEU:HB3	3:D:525:ARG:HD3	1.85	0.57
2:C:473:ARG:HA	2:C:531:PHE:HA	1.85	0.57
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.86	0.57
2:C:52:PHE:CE1	2:C:98:LEU:HD13	2.36	0.57
3:D:368:VAL:HB	3:D:377:VAL:HG12	1.86	0.57
3:D:783:ARG:HG2	3:D:783:ARG:NH1	2.20	0.57
1:A:9:PRO:HG2	1:B:224:TYR:CE2	2.40	0.57
3:D:1480:PHE:O	4:E:18:ARG:NH1	2.38	0.57
1:A:85:LEU:HA	1:A:124:ASN:HD22	1.70	0.57
2:C:841:ASN:OD1	2:C:844:GLY:N	2.35	0.57
1:A:18:ARG:HH21	1:A:88:ARG:HD2	1.70	0.57
1:A:104:GLU:OE1	1:A:137:ARG:NH1	2.37	0.57
2:C:710:ILE:HD11	2:C:758:ARG:HH21	1.69	0.57
2:C:429:ASP:OD2	3:D:1079:LYS:HD3	2.05	0.56
3:D:1394:VAL:HB	3:D:1397:LYS:HG2	1.87	0.56
3:D:1418:LYS:HD3	3:D:1419:PRO:HD2	1.86	0.56
3:D:1458:GLU:O	3:D:1460:ILE:N	2.37	0.56
1:A:143:ARG:HH12	1:A:158:ILE:HD12	1.69	0.56
2:C:274:ARG:NH1	2:C:284:ARG:NH1	2.47	0.56
3:D:783:ARG:HD3	3:D:1029:ARG:HG2	1.86	0.56
1:B:174:VAL:HA	1:B:201:THR:HA	1.86	0.56
2:C:601:GLY:HA3	2:C:614:ARG:O	2.05	0.56
2:C:66:LEU:HD12	2:C:98:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:204:GLN:NE2	2:C:228:ALA:O	2.38	0.56
2:C:292:ARG:HB3	2:C:299:LYS:HB3	1.87	0.56
2:C:689:VAL:HB	2:C:870:ILE:HB	1.86	0.56
2:C:845:ASN:HB2	2:C:884:GLN:HE22	1.71	0.56
3:D:172:PRO:HG2	3:D:175:VAL:HG21	1.87	0.56
3:D:1131:SER:HB2	3:D:1133:ARG:NH2	2.21	0.56
2:C:858:MET:HG3	2:C:859:PRO:HD2	1.87	0.56
3:D:180:LYS:NZ	3:D:388:HIS:HE1	2.03	0.56
2:C:324:ASP:O	2:C:330:ASN:ND2	2.39	0.56
2:C:437:ARG:HG3	2:C:437:ARG:HH11	1.70	0.56
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.88	0.56
2:C:756:VAL:O	2:C:789:SER:HB3	2.06	0.56
3:D:179:VAL:HG13	3:D:183:GLU:HB3	1.87	0.56
2:C:437:ARG:HG2	2:C:469:THR:HG23	1.87	0.56
3:D:180:LYS:HZ1	3:D:388:HIS:HE1	1.54	0.56
3:D:210:ARG:HH21	3:D:346:ARG:HD3	1.71	0.56
2:C:9:ILE:HG12	2:C:907:ASP:CG	2.31	0.55
1:A:132:LEU:HD21	1:A:138:LEU:HD23	1.88	0.55
2:C:145:GLY:H	2:C:163:ILE:HG23	1.71	0.55
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.42	0.55
2:C:91:GLN:HA	2:C:119:PRO:HA	1.88	0.55
4:E:72:ARG:HB2	4:E:73:LEU:HD12	1.88	0.55
3:D:345:TYR:CZ	3:D:377:VAL:HB	2.41	0.55
1:A:57:TYR:HE1	1:A:163:ASN:HB2	1.72	0.55
2:C:5:ARG:HG2	2:C:902:ILE:HB	1.89	0.55
3:D:792:ILE:HD13	3:D:941:PHE:CD2	2.40	0.55
3:D:1277:ILE:HG13	3:D:1301:LYS:HZ1	1.71	0.55
1:A:7:LYS:HD3	1:A:186:LEU:HD22	1.88	0.55
1:A:143:ARG:NH1	1:A:158:ILE:HD12	2.22	0.55
2:C:326:ASP:HB2	2:C:331:ARG:NH1	2.22	0.55
3:D:22:SER:OG	3:D:92:HIS:ND1	2.38	0.55
3:D:1236:LEU:HD23	3:D:1359:GLN:HG3	1.88	0.55
2:C:200:LEU:HD22	2:C:300:ASP:HB3	1.89	0.55
3:D:182:GLY:HA2	3:D:203:ALA:O	2.07	0.55
3:D:800:LYS:NZ	3:D:804:LEU:HD13	2.22	0.55
2:C:194:VAL:HG12	2:C:221:LEU:HB2	1.89	0.55
1:A:29:GLU:OE2	1:A:189:ARG:HD2	2.07	0.54
1:B:185:ARG:NH2	3:D:688:TRP:HB3	2.23	0.54
2:C:512:ARG:HB3	2:C:523:ILE:HD11	1.89	0.54
2:C:739:GLU:HB2	2:C:742:VAL:HB	1.89	0.54
3:D:165:LYS:HD2	3:D:397:LYS:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:801:GLY:HA3	3:D:825:ALA:HA	1.88	0.54
3:D:1107:VAL:O	3:D:1218:GLY:N	2.37	0.54
3:D:1128:VAL:HG23	3:D:1133:ARG:NH2	2.18	0.54
3:D:494:LYS:HB2	3:D:494:LYS:NZ	2.23	0.54
3:D:1425:THR:O	3:D:1429:LEU:HB2	2.08	0.54
2:C:46:ALA:HB1	2:C:266:ARG:NH1	2.23	0.54
2:C:292:ARG:NH1	2:C:292:ARG:HG3	2.23	0.54
3:D:484:PRO:HB3	3:D:488:ARG:NE	2.22	0.54
3:D:486:ARG:HE	3:D:489:ARG:HD2	1.71	0.54
3:D:764:LEU:HD23	3:D:766:ALA:H	1.71	0.54
1:B:216:GLU:OE2	1:B:219:ARG:NH2	2.41	0.54
2:C:54:ILE:HG22	2:C:66:LEU:HD23	1.89	0.54
2:C:398:THR:HG21	2:C:567:GLN:HA	1.89	0.54
2:C:140:ILE:HG12	2:C:333:ILE:HG12	1.90	0.54
3:D:139:GLY:HA2	3:D:452:ILE:HG12	1.90	0.54
3:D:421:LEU:HB2	3:D:427:VAL:HG12	1.88	0.54
3:D:607:LEU:HD23	3:D:614:PHE:HE1	1.73	0.54
3:D:1277:ILE:HG13	3:D:1301:LYS:NZ	2.23	0.54
3:D:784:ASP:HB3	3:D:939:PHE:CE1	2.42	0.54
3:D:842:VAL:HG12	3:D:865:THR:HB	1.90	0.54
3:D:52:PRO:HG3	3:D:78:VAL:HG13	1.90	0.54
1:A:174:VAL:HA	1:A:201:THR:HG22	1.89	0.54
2:C:97:ARG:HG2	2:C:111:ASP:HB3	1.89	0.54
2:C:18:LEU:HD22	2:C:404:LEU:HD21	1.89	0.53
2:C:233:GLU:N	2:C:233:GLU:OE1	2.41	0.53
3:D:165:LYS:HB2	3:D:397:LYS:HB2	1.90	0.53
2:C:146:VAL:HB	2:C:281:LEU:HD11	1.89	0.53
2:C:1038:TRP:HB3	3:D:1227:GLN:HE21	1.73	0.53
2:C:274:ARG:HH12	2:C:284:ARG:CZ	2.21	0.53
2:C:580:MET:O	2:C:903:SER:N	2.35	0.53
3:D:361:VAL:HG13	3:D:365:ASP:HB2	1.91	0.53
3:D:626:SER:OG	3:D:627:GLY:N	2.42	0.53
2:C:274:ARG:HH21	2:C:278:GLU:HB2	1.73	0.53
3:D:664:LYS:NZ	3:D:693:GLU:OE2	2.41	0.53
3:D:1396:GLU:HA	3:D:1399:ASP:OD2	2.08	0.53
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.91	0.53
2:C:158:TYR:HD1	2:C:314:THR:HG22	1.73	0.53
3:D:1281:VAL:O	3:D:1315:ASP:HA	2.09	0.53
2:C:987:ILE:HA	3:D:948:THR:HG21	1.90	0.53
3:D:955:VAL:HB	3:D:1011:PHE:HE1	1.73	0.53
3:D:1281:VAL:HG11	3:D:1313:VAL:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:260:LEU:HD13	2:C:261:ILE:HG13	1.91	0.53
1:A:85:LEU:HD12	1:A:124:ASN:HB3	1.90	0.52
2:C:255:ALA:HB1	2:C:298:PHE:CE1	2.44	0.52
3:D:153:LEU:HD23	3:D:153:LEU:H	1.73	0.52
3:D:155:ASP:O	3:D:159:ARG:HG2	2.09	0.52
3:D:367:ILE:HG13	3:D:377:VAL:HG13	1.90	0.52
2:C:375:SER:O	2:C:375:SER:OG	2.24	0.52
2:C:713:ARG:HA	2:C:819:VAL:HA	1.90	0.52
1:B:163:ASN:OD1	1:B:163:ASN:N	2.43	0.52
2:C:48:PHE:O	2:C:52:PHE:HB2	2.10	0.52
3:D:960:LYS:NZ	3:D:1063:GLU:OE2	2.39	0.52
3:D:1258:ARG:NH1	3:D:1262:LEU:HD11	2.24	0.52
2:C:44:ILE:HG23	2:C:344:PHE:CE2	2.45	0.52
2:C:404:LEU:HD22	2:C:591:SER:HB3	1.90	0.52
3:D:832:ARG:NE	3:D:833:GLU:OE2	2.42	0.52
4:E:54:LEU:HD23	4:E:58:PRO:HD2	1.89	0.52
1:B:24:VAL:HG11	1:B:194:LYS:HZ1	1.75	0.52
2:C:489:THR:HG23	2:C:490:GLU:HG3	1.92	0.52
4:E:17:TYR:O	4:E:20:THR:OG1	2.21	0.52
2:C:564:MET:HE2	2:C:846:LYS:HG2	1.91	0.52
2:C:602:GLU:H	2:C:614:ARG:HB3	1.74	0.52
2:C:873:PRO:HB2	3:D:1023:MET:HE1	1.92	0.52
1:B:25:LEU:HD23	1:B:28:LEU:HD21	1.92	0.52
1:B:106:PRO:HG3	1:B:134:GLU:OE2	2.08	0.52
1:B:185:ARG:HB3	1:B:190:THR:HG23	1.92	0.52
2:C:428:ARG:HB3	2:C:450:GLY:HA3	1.91	0.52
2:C:806:LEU:HB2	2:C:822:VAL:HG22	1.91	0.52
3:D:397:LYS:HD3	3:D:448:GLU:HB3	1.90	0.52
3:D:800:LYS:HZ2	3:D:804:LEU:HD13	1.74	0.52
1:A:133:GLU:HG2	1:A:134:GLU:H	1.74	0.52
2:C:144:PRO:HA	2:C:163:ILE:HG23	1.90	0.52
3:D:637:LEU:HB2	3:D:641:GLN:HG3	1.92	0.52
3:D:1155:VAL:HG23	3:D:1156:LEU:H	1.73	0.52
1:B:101:LEU:HD21	1:B:109:VAL:HG11	1.92	0.52
2:C:504:GLU:HG3	2:C:509:ALA:HB2	1.91	0.52
2:C:236:ILE:HA	2:C:251:ASP:OD2	2.10	0.51
3:D:127:LEU:HD23	3:D:134:VAL:HB	1.91	0.51
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.39	0.51
3:D:19:ARG:NH1	3:D:19:ARG:HB2	2.25	0.51
3:D:925:GLU:OE1	4:E:6:ILE:N	2.44	0.51
1:B:185:ARG:HH11	3:D:692:GLU:CD	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1088:LEU:HD13	3:D:613:ARG:HG3	1.92	0.51
3:D:87:ARG:HB2	3:D:523:ASP:HB3	1.93	0.51
3:D:111:LYS:HD2	3:D:1452:ILE:HD13	1.93	0.51
1:B:58:ILE:HG23	1:B:140:MET:HB3	1.91	0.51
2:C:124:ASP:OD2	2:C:125:GLY:N	2.44	0.51
2:C:186:VAL:O	2:C:188:LYS:N	2.43	0.51
2:C:338:GLU:HA	2:C:341:THR:HG22	1.93	0.51
2:C:540:PHE:HB3	2:C:544:THR:HB	1.92	0.51
3:D:82:LYS:C	3:D:84:ILE:H	2.18	0.51
4:E:54:LEU:HA	4:E:58:PRO:HG2	1.93	0.51
2:C:1009:SER:HB2	3:D:625:TYR:CD1	2.45	0.51
3:D:28:LYS:C	3:D:548:ILE:HG21	2.35	0.51
3:D:525:ARG:NH1	3:D:541:ASN:OD1	2.44	0.51
3:D:550:ARG:HH11	3:D:573:MET:HB3	1.75	0.51
3:D:957:PRO:HG3	3:D:1007:VAL:HA	1.93	0.51
1:A:44:LEU:HD23	1:A:48:ILE:HD11	1.91	0.51
1:A:98:THR:HG22	1:A:143:ARG:HG3	1.92	0.51
2:C:35:PRO:HD2	2:C:38:LYS:HG3	1.93	0.51
2:C:37:GLU:OE2	2:C:38:LYS:HG2	2.10	0.51
2:C:442:GLU:HG2	2:C:454:SER:HB2	1.92	0.51
2:C:18:LEU:HB3	2:C:404:LEU:HD11	1.93	0.51
2:C:48:PHE:HB3	2:C:52:PHE:HD2	1.76	0.51
2:C:978:ARG:HH11	2:C:978:ARG:HG2	1.76	0.51
3:D:458:ALA:HB2	3:D:575:GLN:HE22	1.76	0.51
3:D:616:GLN:HG3	3:D:621:LYS:NZ	2.26	0.51
4:E:26:ARG:HH21	4:E:30:LEU:HD13	1.76	0.51
2:C:141:HIS:HB2	2:C:418:LEU:HD22	1.92	0.51
2:C:284:ARG:NH1	2:C:285:LEU:H	2.09	0.51
2:C:1095:LEU:HD23	3:D:101:HIS:HE2	1.74	0.51
2:C:46:ALA:HB1	2:C:266:ARG:HH12	1.76	0.50
1:A:58:ILE:HG21	1:A:68:ILE:HD11	1.93	0.50
2:C:141:HIS:HE1	2:C:334:ARG:HG3	1.76	0.50
2:C:259:GLY:CA	2:C:291:ALA:HB2	2.41	0.50
3:D:1197:ARG:HB3	3:D:1396:GLU:CD	2.37	0.50
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.47	0.50
2:C:458:TYR:HB3	2:C:470:PRO:HG3	1.93	0.50
2:C:610:ARG:HG3	2:C:610:ARG:NH1	2.08	0.50
3:D:415:VAL:HG21	3:D:421:LEU:HD21	1.92	0.50
3:D:695:ILE:HG13	3:D:696:HIS:H	1.76	0.50
3:D:728:LEU:HD21	3:D:736:PHE:HZ	1.75	0.50
1:B:221:HIS:HA	1:B:224:TYR:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:38:LYS:NZ	2:C:38:LYS:HB3	2.27	0.50
2:C:521:PRO:HG3	3:D:1068:LEU:HD21	1.94	0.50
2:C:606:VAL:H	2:C:645:VAL:HG22	1.76	0.50
2:C:680:ASP:H	3:D:943:THR:HG21	1.76	0.50
2:C:1004:LYS:HD3	3:D:744:GLN:OE1	2.12	0.50
3:D:483:HIS:HB2	3:D:484:PRO:HD3	1.94	0.50
2:C:89:THR:HG22	2:C:129:ILE:HA	1.92	0.50
2:C:139:GLN:OE1	2:C:334:ARG:NH1	2.45	0.50
3:D:103:TRP:NE1	3:D:604:THR:OG1	2.41	0.50
1:B:176:ARG:NH2	3:D:888:GLU:OE2	2.45	0.50
2:C:1:MET:O	2:C:899:GLN:HA	2.12	0.50
2:C:636:ALA:HB3	2:C:703:ILE:HG13	1.93	0.50
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.93	0.50
3:D:690:ALA:O	3:D:694:VAL:HG13	2.12	0.50
3:D:1278:ASP:OD2	3:D:1278:ASP:N	2.40	0.50
3:D:1453:ALA:O	3:D:1455:LYS:N	2.44	0.50
1:B:184:THR:O	1:B:192:LEU:HB2	2.11	0.49
2:C:718:GLY:HA3	2:C:761:PHE:CD2	2.47	0.49
3:D:1213:ARG:NH2	4:E:10:PHE:O	2.45	0.49
1:A:38:ASN:O	1:A:42:ARG:HG2	2.12	0.49
2:C:649:VAL:HG12	2:C:653:ASP:HB3	1.94	0.49
3:D:1369:GLU:HA	3:D:1372:VAL:HG12	1.93	0.49
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.94	0.49
2:C:363:SER:H	2:C:371:LYS:HE3	1.77	0.49
3:D:101:HIS:ND1	3:D:582:LEU:HD13	2.27	0.49
3:D:758:GLU:O	3:D:762:GLN:HG2	2.12	0.49
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.92	0.49
2:C:733:ALA:HB1	2:C:754:ILE:HD12	1.93	0.49
2:C:1067:TYR:O	2:C:1071:ILE:HG12	2.12	0.49
3:D:191:LEU:HG	3:D:197:SER:HB2	1.94	0.49
3:D:628:ARG:HH12	7:T:16:DC:H2"	1.76	0.49
2:C:893:ALA:HB2	2:C:918:LEU:HD23	1.94	0.49
3:D:646:LYS:HB3	3:D:688:TRP:CH2	2.47	0.49
1:B:24:VAL:HG11	1:B:194:LYS:NZ	2.27	0.49
2:C:919:ALA:HB2	2:C:968:LEU:HD21	1.94	0.49
3:D:126:VAL:HG13	3:D:132:TYR:HD2	1.78	0.49
3:D:1008:PHE:HZ	3:D:1032:PRO:HA	1.78	0.49
2:C:1006:HIS:HB2	3:D:628:ARG:HG2	1.94	0.49
3:D:116:LEU:O	3:D:118:LEU:HG	2.12	0.49
4:E:5:GLY:HA3	4:E:8:LYS:HE3	1.93	0.49
2:C:175:GLU:OE1	2:C:190:LYS:NZ	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:443:THR:CG2	2:C:453:THR:HG22	2.43	0.49
3:D:365:ASP:O	3:D:379:ALA:HB2	2.13	0.49
3:D:505:SER:OG	3:D:1453:ALA:HA	2.13	0.49
2:C:113:VAL:O	2:C:115:LEU:N	2.43	0.49
1:B:60:ASP:OD1	1:B:60:ASP:N	2.46	0.48
2:C:1103:ASP:OD2	2:C:1104:GLU:N	2.40	0.48
2:C:1105:LYS:HZ3	2:C:1107:ASN:HB2	1.76	0.48
3:D:802:ALA:HB3	3:D:824:ASN:HB3	1.95	0.48
3:D:1336:LEU:HD13	3:D:1376:MET:HE1	1.95	0.48
2:C:42:VAL:HA	2:C:46:ALA:HB2	1.94	0.48
2:C:295:ASP:C	2:C:297:GLU:H	2.20	0.48
2:C:876:VAL:HG11	3:D:949:ILE:HG21	1.95	0.48
2:C:999:HIS:CE1	6:R:28:C:H4'	2.47	0.48
3:D:50:PHE:CD1	3:D:522:PRO:HD3	2.48	0.48
3:D:152:LEU:CD2	3:D:152:LEU:H	2.26	0.48
2:C:69:LEU:HD13	2:C:99:GLN:HG2	1.95	0.48
4:E:47:LYS:HB3	4:E:55:PHE:CE2	2.48	0.48
6:R:22:U:H2'	6:R:23:G:C8	2.48	0.48
2:C:292:ARG:NH2	2:C:294:GLU:OE1	2.46	0.48
3:D:615:ARG:NE	3:D:1439:SER:O	2.41	0.48
3:D:1041:LEU:H	3:D:1041:LEU:HD22	1.77	0.48
1:A:7:LYS:NZ	1:A:7:LYS:HB3	2.28	0.48
2:C:726:ILE:HD11	2:C:754:ILE:HG21	1.94	0.48
2:C:1005:MET:HB2	3:D:724:GLN:HE22	1.78	0.48
3:D:136:ASP:CB	3:D:137:PRO:HD2	2.40	0.48
3:D:1457:ASP:OD2	3:D:1464:GLU:OE2	2.31	0.48
3:D:1495:ILE:HD12	4:E:84:ARG:HG2	1.94	0.48
2:C:185:LYS:HD2	2:C:190:LYS:HE2	1.95	0.48
2:C:210:GLU:HG2	2:C:304:LEU:HD21	1.96	0.48
3:D:719:VAL:O	3:D:721:VAL:HG23	2.14	0.48
3:D:784:ASP:HB3	3:D:939:PHE:HE1	1.78	0.48
3:D:1372:VAL:HG23	3:D:1375:MET:HE2	1.96	0.48
3:D:152:LEU:H	3:D:152:LEU:HD23	1.78	0.48
3:D:970:LYS:HE3	3:D:974:ILE:HD11	1.96	0.48
2:C:678:PRO:HA	2:C:683:ASN:HD21	1.78	0.48
3:D:207:PHE:O	3:D:390:PRO:HA	2.14	0.48
3:D:546:ARG:HA	3:D:549:ASN:HB2	1.96	0.48
3:D:704:ARG:NH2	3:D:743:ASP:OD2	2.47	0.48
2:C:193:LEU:HD21	2:C:307:LEU:HD21	1.96	0.48
3:D:119:SER:HB2	3:D:123:LEU:HB2	1.96	0.48
3:D:433:GLY:HA3	3:D:447:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1108:ARG:HH21	3:D:1198:TYR:C	2.22	0.48
1:B:57:TYR:CD2	1:B:161:ARG:HG3	2.49	0.48
1:B:100:LEU:HD23	1:B:141:GLU:HB3	1.95	0.48
2:C:1008:ARG:HH21	2:C:1020:PRO:HB3	1.78	0.48
3:D:417:PRO:HG3	3:D:431:VAL:HA	1.96	0.48
3:D:584:ASN:OD1	3:D:590:PRO:HD2	2.14	0.48
3:D:832:ARG:O	3:D:834:THR:N	2.47	0.48
3:D:704:ARG:HG2	3:D:736:PHE:O	2.14	0.47
3:D:1349:VAL:HG22	3:D:1368:ILE:HG22	1.96	0.47
3:D:1412:LYS:C	3:D:1414:PRO:HD3	2.39	0.47
2:C:45:GLN:O	2:C:48:PHE:HB2	2.13	0.47
3:D:607:LEU:HD23	3:D:614:PHE:CE1	2.48	0.47
3:D:1258:ARG:HG3	3:D:1258:ARG:HH11	1.78	0.47
3:D:1481:VAL:HG13	4:E:18:ARG:HA	1.96	0.47
4:E:51:LEU:HD23	4:E:51:LEU:H	1.78	0.47
2:C:19:THR:HG21	2:C:124:ASP:O	2.14	0.47
3:D:47:GLU:HG2	3:D:52:PRO:HA	1.95	0.47
3:D:543:LEU:HG	3:D:600:LEU:HD12	1.96	0.47
3:D:1107:VAL:HA	3:D:1200:VAL:O	2.15	0.47
3:D:1309:ALA:HB1	3:D:1326:THR:HG23	1.96	0.47
2:C:162:ILE:HB	2:C:172:ILE:HB	1.96	0.47
2:C:1055:LEU:HD11	2:C:1066:ALA:HB2	1.97	0.47
3:D:1128:VAL:HG12	3:D:1129:THR:H	1.79	0.47
2:C:577:PRO:HB2	2:C:580:MET:HB3	1.97	0.47
3:D:190:GLU:HG2	3:D:196:VAL:HG22	1.96	0.47
3:D:827:ILE:O	3:D:835:SER:OG	2.24	0.47
1:A:42:ARG:NH1	2:C:978:ARG:HA	2.29	0.47
2:C:274:ARG:NH1	2:C:284:ARG:HH22	2.10	0.47
2:C:471:TYR:CE2	2:C:496:ILE:HG21	2.49	0.47
2:C:971:LYS:HA	2:C:988:VAL:HA	1.95	0.47
3:D:100:ALA:HB2	3:D:513:ILE:HG13	1.95	0.47
3:D:1008:PHE:CZ	3:D:1032:PRO:HA	2.49	0.47
3:D:1165:TYR:HB3	3:D:1207:TYR:CE1	2.42	0.47
3:D:1261:GLU:OE2	3:D:1269:LYS:HG3	2.14	0.47
1:A:54:THR:HG21	1:A:158:ILE:HD12	1.97	0.47
3:D:163:TYR:C	3:D:165:LYS:H	2.21	0.47
3:D:212:ARG:HB3	3:D:388:HIS:CD2	2.49	0.47
3:D:474:GLU:O	3:D:478:LEU:HB2	2.14	0.47
3:D:565:ILE:O	3:D:569:ASN:HB2	2.14	0.47
3:D:890:VAL:O	3:D:926:LYS:NZ	2.48	0.47
3:D:1278:ASP:HA	3:D:1319:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:23:VAL:HG13	4:E:64:ALA:HB3	1.97	0.47
2:C:73:LEU:HB2	2:C:93:PRO:O	2.15	0.47
2:C:700:TYR:HB2	2:C:833:LEU:HB2	1.96	0.47
3:D:616:GLN:HG3	3:D:621:LYS:HZ3	1.80	0.47
3:D:707:THR:HG23	3:D:712:GLY:HA3	1.97	0.47
3:D:1003:VAL:O	3:D:1007:VAL:HG23	2.15	0.47
3:D:1315:ASP:OD2	3:D:1315:ASP:N	2.47	0.47
4:E:37:ASN:HB3	4:E:93:TYR:CZ	2.50	0.47
1:A:83:LYS:HD3	1:A:168:ASP:HB2	1.96	0.47
3:D:46:ASP:OD2	3:D:48:ARG:HB3	2.15	0.47
3:D:853:VAL:HG11	3:D:860:LEU:HG	1.97	0.47
4:E:22:VAL:CG1	4:E:68:LEU:HD21	2.45	0.47
1:A:91:ASN:CG	1:A:92:PRO:HD2	2.40	0.46
2:C:205:GLU:H	2:C:205:GLU:HG3	1.50	0.46
2:C:409:ARG:HA	2:C:454:SER:HA	1.95	0.46
3:D:185:VAL:CG2	3:D:203:ALA:HB2	2.46	0.46
3:D:565:ILE:HD12	3:D:565:ILE:N	2.30	0.46
3:D:989:TYR:O	3:D:993:LEU:HG	2.15	0.46
3:D:1106:VAL:HG11	3:D:1474:ALA:HB2	1.96	0.46
3:D:1282:ARG:HB2	3:D:1293:PHE:O	2.15	0.46
1:B:23:PHE:CD2	1:B:211:LEU:HD22	2.50	0.46
1:B:185:ARG:HD3	3:D:692:GLU:OE2	2.13	0.46
2:C:121:MET:HE2	2:C:121:MET:HB3	1.78	0.46
2:C:216:GLU:C	2:C:218:VAL:H	2.22	0.46
3:D:808:THR:H	3:D:809:PRO:CD	2.17	0.46
2:C:1051:GLU:OE1	3:D:752:SER:HB3	2.15	0.46
3:D:807:ALA:HA	3:D:833:GLU:CD	2.40	0.46
3:D:1272:ALA:O	3:D:1325:LEU:HD23	2.15	0.46
2:C:475:VAL:O	2:C:477:GLY:N	2.48	0.46
2:C:744:ARG:HH11	2:C:747:ALA:HB2	1.79	0.46
2:C:880:MET:HE2	2:C:880:MET:HB2	1.87	0.46
2:C:1073:GLY:HA3	3:D:659:LYS:HG2	1.97	0.46
3:D:560:GLN:HG3	3:D:561:GLY:H	1.79	0.46
3:D:1112:CYS:HB2	3:D:1195:GLN:HG2	1.98	0.46
1:B:11:PHE:CE1	1:B:23:PHE:HB3	2.51	0.46
2:C:1051:GLU:OE2	3:D:751:LEU:HB2	2.15	0.46
3:D:355:VAL:HG11	3:D:385:VAL:HG11	1.98	0.46
3:D:1401:GLU:CD	3:D:1415:VAL:HG22	2.40	0.46
2:C:255:ALA:HB1	2:C:298:PHE:HE1	1.80	0.46
2:C:260:LEU:HG	2:C:291:ALA:HB3	1.98	0.46
3:D:648:MET:HB3	3:D:648:MET:HE2	1.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ARG:HH22	2:C:939:ARG:NH2	2.14	0.46
2:C:36:PRO:HB2	2:C:70:GLU:CD	2.41	0.46
2:C:838:LYS:HE3	3:D:741:ASP:O	2.15	0.46
2:C:949:LYS:HD3	3:D:796:ARG:NH1	2.31	0.46
3:D:65:ARG:HD2	3:D:65:ARG:HA	1.65	0.46
3:D:539:ASP:HB3	3:D:600:LEU:HB3	1.97	0.46
3:D:602:SER:O	3:D:606:ILE:HG12	2.15	0.46
3:D:978:TYR:HB2	3:D:983:LEU:HD11	1.97	0.46
3:D:1225:ALA:O	3:D:1229:ILE:HG13	2.16	0.46
3:D:1422:MET:HB2	3:D:1426:LYS:HD3	1.97	0.46
1:A:89:PHE:HE1	1:A:97:VAL:HB	1.79	0.46
2:C:676:ILE:HG23	2:C:988:VAL:HG13	1.97	0.46
2:C:726:ILE:HD12	2:C:734:LEU:HD11	1.97	0.46
2:C:892:LEU:HD23	2:C:918:LEU:HD22	1.98	0.46
3:D:179:VAL:HG11	3:D:203:ALA:HB3	1.96	0.46
3:D:214:GLU:HB3	3:D:340:THR:OG1	2.15	0.46
3:D:1018:ASN:HD21	3:D:1020:LEU:HB3	1.81	0.46
3:D:1119:SER:HB2	3:D:1185:GLU:HB3	1.97	0.46
3:D:1146:GLY:HA3	3:D:1207:TYR:HB2	1.98	0.46
2:C:288:ARG:HD3	2:C:288:ARG:H	1.81	0.46
2:C:715:THR:OG1	2:C:718:GLY:O	2.34	0.46
2:C:874:LEU:HD21	3:D:787:LEU:HD22	1.98	0.46
3:D:57:GLU:HG2	3:D:58:CYS:N	2.30	0.46
3:D:352:ASN:ND2	3:D:371:ILE:HG12	2.30	0.46
2:C:15:LEU:O	2:C:586:ARG:NH2	2.49	0.45
2:C:260:LEU:O	2:C:262:ALA:N	2.45	0.45
2:C:358:ARG:HD3	2:C:372:LEU:HA	1.98	0.45
2:C:957:LYS:HD3	2:C:961:GLU:HB3	1.98	0.45
3:D:81:THR:HG22	3:D:82:LYS:H	1.81	0.45
1:B:186:LEU:O	1:B:188:GLN:NE2	2.50	0.45
2:C:395:LYS:HE3	2:C:407:LYS:HZ3	1.81	0.45
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.97	0.45
3:D:63:TYR:HB3	3:D:68:PHE:CE1	2.51	0.45
3:D:613:ARG:NH1	3:D:616:GLN:HG2	2.30	0.45
3:D:709:HIS:ND1	3:D:1231:GLU:HG3	2.32	0.45
3:D:739:ASP:OD2	3:D:741:ASP:OD2	2.33	0.45
3:D:1388:ARG:HD2	3:D:1388:ARG:N	2.31	0.45
3:D:1435:LEU:HB2	3:D:1464:GLU:HG3	1.98	0.45
1:A:49:PRO:HA	1:A:148:VAL:HG22	1.99	0.45
2:C:136:ILE:HB	2:C:336:VAL:HG13	1.98	0.45
2:C:274:ARG:HG2	2:C:285:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:86:ARG:O	3:D:522:PRO:HD2	2.16	0.45
3:D:416:ALA:HB3	3:D:419:ASP:OD1	2.17	0.45
3:D:792:ILE:HD13	3:D:941:PHE:HD2	1.82	0.45
3:D:1136:LYS:HB3	3:D:1139:ASP:OD2	2.16	0.45
3:D:1310:ARG:NH1	3:D:1327:ARG:NH1	2.65	0.45
3:D:1371:VAL:O	3:D:1375:MET:HG3	2.16	0.45
4:E:45:ARG:HH21	4:E:63:TRP:HH2	1.63	0.45
2:C:431:HIS:N	2:C:434:HIS:HD2	2.15	0.45
3:D:554:LEU:HD13	3:D:570:GLU:HB3	1.99	0.45
3:D:800:LYS:HG2	3:D:804:LEU:HD22	1.98	0.45
4:E:27:ALA:HB1	4:E:60:ALA:HB1	1.97	0.45
2:C:196:LEU:HA	2:C:199:VAL:HG23	1.97	0.45
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.99	0.45
2:C:1109:VAL:HG22	3:D:2:LYS:HB2	1.99	0.45
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.52	0.45
3:D:583:ASP:OD2	3:D:604:THR:HG21	2.17	0.45
2:C:642:ARG:NE	2:C:657:ASP:OD2	2.50	0.45
3:D:41:ARG:HE	3:D:41:ARG:HB3	1.59	0.45
3:D:496:LEU:HD21	3:D:1388:ARG:HH21	1.82	0.45
3:D:792:ILE:HG13	3:D:793:THR:HG23	1.99	0.45
3:D:939:PHE:O	3:D:943:THR:HG23	2.17	0.45
7:T:2:DG:H2''	7:T:3:DG:C8	2.52	0.45
2:C:98:LEU:HD12	2:C:99:GLN:N	2.32	0.45
2:C:512:ARG:HD3	2:C:512:ARG:HA	1.77	0.45
2:C:842:ARG:HH11	2:C:842:ARG:HB3	1.81	0.45
3:D:527:MET:SD	3:D:537:THR:HB	2.57	0.45
3:D:978:TYR:HB2	3:D:988:ARG:HD3	1.99	0.45
3:D:1044:LEU:HD23	3:D:1044:LEU:H	1.82	0.45
3:D:1294:VAL:HG12	3:D:1295:GLU:N	2.31	0.45
4:E:22:VAL:HG11	4:E:68:LEU:HD21	1.97	0.45
2:C:281:LEU:HD13	2:C:281:LEU:H	1.82	0.45
2:C:693:GLU:HA	2:C:696:LYS:HD2	1.99	0.45
3:D:39:PRO:HD3	3:D:53:ILE:HG21	1.99	0.45
3:D:53:ILE:HA	3:D:86:ARG:HH11	1.82	0.45
2:C:69:LEU:O	2:C:97:ARG:HB2	2.17	0.45
2:C:572:ILE:HG13	2:C:573:ARG:H	1.82	0.45
3:D:660:LYS:O	3:D:664:LYS:HG3	2.16	0.45
3:D:1283:ILE:HG13	3:D:1292:VAL:HG22	1.98	0.45
1:A:169:ALA:HB1	1:A:171:PHE:CE2	2.52	0.45
2:C:393:GLN:HG2	6:R:25:G:O2'	2.16	0.45
2:C:77:PRO:HD2	2:C:91:GLN:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:284:ARG:CG	2:C:301:GLU:HG2	2.47	0.44
2:C:1031:ARG:HB3	7:T:16:DC:OP1	2.17	0.44
2:C:225:SER:O	2:C:229:MET:HB2	2.16	0.44
2:C:431:HIS:CG	2:C:432:ARG:N	2.85	0.44
3:D:168:THR:HA	3:D:394:LEU:HB3	1.99	0.44
2:C:584:GLU:H	2:C:584:GLU:CD	2.25	0.44
2:C:722:ILE:HA	2:C:758:ARG:HB3	1.99	0.44
2:C:974:LEU:HD12	2:C:974:LEU:HA	1.84	0.44
3:D:1149:LEU:HD21	3:D:1166:LEU:HD11	1.99	0.44
3:D:1294:VAL:O	3:D:1295:GLU:HB2	2.17	0.44
1:A:70:GLY:HA2	1:A:133:GLU:HB3	1.99	0.44
3:D:829:VAL:O	3:D:831:GLY:N	2.47	0.44
3:D:890:VAL:HG11	3:D:922:LEU:HD13	1.99	0.44
3:D:1394:VAL:HG21	3:D:1432:LYS:NZ	2.32	0.44
3:D:1435:LEU:HD23	3:D:1464:GLU:O	2.16	0.44
2:C:387:SER:OG	2:C:388:ARG:NH2	2.50	0.44
2:C:743:VAL:HG11	2:C:755:LEU:HD12	2.00	0.44
1:A:36:LEU:C	1:A:39:PRO:HD2	2.42	0.44
1:A:133:GLU:OE2	2:C:605:LYS:HB3	2.18	0.44
1:B:201:THR:HG22	1:B:202:ASP:H	1.83	0.44
2:C:397:GLU:HG2	2:C:403:SER:OG	2.18	0.44
2:C:503:LEU:HD23	2:C:508:ILE:HA	1.99	0.44
2:C:675:ALA:HB2	2:C:867:VAL:HG21	1.99	0.44
2:C:724:ARG:HB2	2:C:741:GLY:H	1.83	0.44
2:C:863:ASP:C	2:C:865:THR:H	2.26	0.44
3:D:1071:PHE:O	3:D:1074:SER:OG	2.33	0.44
3:D:11:ALA:HA	3:D:1451:ALA:O	2.17	0.44
3:D:205:TYR:CD1	3:D:390:PRO:HG3	2.53	0.44
3:D:808:THR:N	3:D:809:PRO:HD2	2.18	0.44
1:B:208:LEU:HD13	1:B:208:LEU:HA	1.86	0.44
2:C:56:GLU:OE2	2:C:359:MET:HE2	2.18	0.44
2:C:274:ARG:HH22	2:C:284:ARG:NH2	2.16	0.44
2:C:468:ARG:NE	2:C:485:TYR:O	2.51	0.44
2:C:1017:THR:OG1	2:C:1019:GLN:HG2	2.17	0.44
4:E:47:LYS:HB3	4:E:55:PHE:HE2	1.83	0.44
2:C:141:HIS:CE1	2:C:334:ARG:HG3	2.52	0.44
3:D:353:VAL:HG22	3:D:368:VAL:HG22	1.99	0.44
3:D:825:ALA:HA	3:D:826:PRO:HD2	1.88	0.44
3:D:961:LYS:O	3:D:965:GLU:HB2	2.18	0.44
3:D:1127:GLU:HB3	3:D:1133:ARG:CZ	2.48	0.44
2:C:108:ILE:HG13	2:C:366:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:468:ARG:HD3	2:C:485:TYR:HB3	1.99	0.43
3:D:553:ARG:NH2	3:D:570:GLU:OE2	2.51	0.43
3:D:710:ARG:C	3:D:712:GLY:H	2.25	0.43
3:D:1314:LYS:HZ1	3:D:1316:GLY:HA3	1.83	0.43
3:D:1466:VAL:HG22	3:D:1472:ILE:HG22	2.00	0.43
2:C:64:LEU:HD13	2:C:359:MET:SD	2.58	0.43
2:C:727:PRO:HG2	2:C:759:THR:HG21	1.99	0.43
3:D:796:ARG:HB2	3:D:828:LYS:HG2	2.00	0.43
3:D:31:THR:OG1	3:D:32:ILE:N	2.39	0.43
3:D:1301:LYS:HD2	3:D:1303:TYR:CE1	2.54	0.43
1:A:122:ILE:HG22	1:A:124:ASN:H	1.84	0.43
2:C:100:LEU:HB3	2:C:368:THR:OG1	2.19	0.43
2:C:250:ARG:O	2:C:254:VAL:HG23	2.18	0.43
2:C:842:ARG:HH11	2:C:842:ARG:CB	2.31	0.43
2:C:1023:GLY:HA2	2:C:1026:GLN:O	2.19	0.43
3:D:708:LEU:HD21	3:D:1091:SER:HB2	1.99	0.43
3:D:1280:VAL:HG23	3:D:1282:ARG:HG3	2.00	0.43
3:D:1314:LYS:HZ2	3:D:1316:GLY:HA3	1.81	0.43
2:C:2:GLU:HG3	2:C:899:GLN:HB3	1.99	0.43
2:C:13:ILE:HA	2:C:14:PRO:HD3	1.90	0.43
3:D:58:CYS:HA	3:D:78:VAL:HG11	2.01	0.43
3:D:414:ARG:HG3	3:D:433:GLY:N	2.30	0.43
6:R:26:U:H2'	6:R:27:G:H8	1.84	0.43
1:B:186:LEU:O	1:B:188:GLN:N	2.52	0.43
2:C:54:ILE:CG2	2:C:66:LEU:HD23	2.49	0.43
2:C:146:VAL:HA	2:C:161:SER:O	2.18	0.43
2:C:327:HIS:C	2:C:329:GLY:H	2.26	0.43
2:C:1019:GLN:HA	2:C:1020:PRO:HD3	1.76	0.43
2:C:1034:GLU:OE2	3:D:1096:ARG:NH1	2.52	0.43
2:C:1076:VAL:HB	3:D:752:SER:HA	2.00	0.43
3:D:184:GLU:CD	3:D:202:VAL:HG12	2.44	0.43
3:D:465:LEU:HD22	3:D:509:PRO:HB2	1.99	0.43
3:D:966:GLU:HA	3:D:969:ARG:HG2	2.00	0.43
3:D:1295:GLU:HB3	3:D:1296:SER:H	1.49	0.43
4:E:38:THR:HG23	4:E:41:GLU:HG2	2.01	0.43
1:A:32:PHE:CE2	1:B:43:ILE:HG12	2.54	0.43
2:C:56:GLU:HB2	2:C:64:LEU:HB3	2.00	0.43
2:C:358:ARG:HD3	2:C:371:LYS:O	2.19	0.43
2:C:700:TYR:HB3	2:C:996:LYS:HE3	2.00	0.43
3:D:178:LEU:HD13	3:D:178:LEU:HA	1.83	0.43
3:D:458:ALA:HB2	3:D:575:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.99	0.43
3:D:1312:LEU:HD11	3:D:1327:ARG:HE	1.82	0.43
3:D:1381:VAL:HG23	3:D:1391:GLU:O	2.19	0.43
6:R:22:U:H2'	6:R:23:G:H8	1.82	0.43
1:B:59:GLU:HB3	1:B:137:ARG:NH1	2.31	0.43
2:C:272:ALA:HB1	2:C:276:LYS:HZ1	1.84	0.43
2:C:434:HIS:ND1	2:C:438:ILE:HD12	2.34	0.43
2:C:540:PHE:CE2	2:C:906:PHE:HE2	2.37	0.43
3:D:32:ILE:HG21	3:D:37:LEU:HD13	2.01	0.43
1:B:153:ALA:HB2	1:B:168:ASP:N	2.34	0.43
3:D:15:PRO:HB3	3:D:19:ARG:HH22	1.83	0.43
3:D:24:GLY:HA3	3:D:49:ILE:HG12	1.99	0.43
3:D:760:ARG:NH2	4:E:3:GLU:OE1	2.46	0.43
2:C:136:ILE:HD11	2:C:386:PHE:CE1	2.54	0.42
2:C:462:ASP:OD2	2:C:468:ARG:NH1	2.52	0.42
3:D:123:LEU:HG	3:D:152:LEU:HD21	2.00	0.42
3:D:148:GLU:OE2	3:D:153:LEU:HD22	2.18	0.42
3:D:462:GLN:O	3:D:466:LYS:HG3	2.19	0.42
1:A:32:PHE:CZ	1:B:43:ILE:HG12	2.54	0.42
1:A:89:PHE:HB3	1:A:94:LEU:HD12	2.01	0.42
2:C:56:GLU:HA	2:C:356:ARG:HH12	1.84	0.42
2:C:355:VAL:HG23	2:C:372:LEU:HB3	2.01	0.42
2:C:542:VAL:HA	2:C:545:ASN:HB2	1.99	0.42
2:C:565:GLN:H	2:C:565:GLN:HG2	1.64	0.42
2:C:1008:ARG:HD3	2:C:1028:GLY:N	2.35	0.42
3:D:729:HIS:HE2	3:D:935:LYS:HD2	1.84	0.42
3:D:908:LYS:HB2	3:D:1027:GLY:HA3	2.01	0.42
1:B:20:TYR:HA	1:B:199:ILE:O	2.19	0.42
2:C:184:MET:HB2	2:C:184:MET:HE2	1.85	0.42
2:C:603:VAL:HB	2:C:647:GLN:H	1.84	0.42
2:C:1016:ILE:HG13	2:C:1017:THR:HG22	2.00	0.42
3:D:176:ASP:HB3	3:D:177:ALA:H	1.55	0.42
3:D:908:LYS:HB2	3:D:1027:GLY:CA	2.48	0.42
3:D:968:ASP:HA	3:D:971:LEU:HD23	2.01	0.42
3:D:1198:TYR:OH	3:D:1432:LYS:NZ	2.52	0.42
3:D:1209:LEU:C	3:D:1211:MET:H	2.27	0.42
3:D:1325:LEU:HD22	3:D:1325:LEU:H	1.84	0.42
4:E:3:GLU:HB2	4:E:6:ILE:CG2	2.50	0.42
1:B:11:PHE:HE1	1:B:23:PHE:HB3	1.84	0.42
2:C:274:ARG:HB2	2:C:285:LEU:HD22	2.01	0.42
2:C:891:GLY:O	2:C:991:GLN:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:420:VAL:HG22	3:D:428:LYS:HZ3	1.85	0.42
3:D:952:ASP:HA	3:D:1062:ARG:HH11	1.84	0.42
3:D:1394:VAL:HG21	3:D:1432:LYS:HZ1	1.83	0.42
4:E:57:ASP:N	4:E:58:PRO:HD3	2.35	0.42
1:A:24:VAL:HG22	1:A:196:THR:HG22	2.01	0.42
1:A:57:TYR:CD2	1:A:161:ARG:HG3	2.54	0.42
1:A:143:ARG:NH1	1:A:158:ILE:HG21	2.35	0.42
2:C:442:GLU:OE2	2:C:543:ASN:ND2	2.43	0.42
2:C:1105:LYS:H	2:C:1105:LYS:HD3	1.84	0.42
3:D:57:GLU:HG3	3:D:64:LYS:HD2	2.02	0.42
3:D:131:LYS:HB2	3:D:568:ARG:HG2	2.01	0.42
3:D:157:GLU:HA	3:D:160:GLU:HG2	2.01	0.42
3:D:983:LEU:H	3:D:983:LEU:HG	1.60	0.42
2:C:238:LEU:HD21	2:C:242:LEU:HD13	2.02	0.42
2:C:425:PHE:H	2:C:428:ARG:HD2	1.84	0.42
2:C:1046:ALA:HB2	3:D:1472:ILE:HG13	2.02	0.42
2:C:1073:GLY:CA	3:D:659:LYS:HG2	2.50	0.42
2:C:1103:ASP:CG	2:C:1104:GLU:H	2.26	0.42
3:D:206:ARG:HG2	3:D:392:SER:HB2	2.01	0.42
3:D:462:GLN:HG2	3:D:466:LYS:HE3	2.02	0.42
4:E:9:LEU:HD23	4:E:19:LEU:HD11	2.00	0.42
7:T:13:DC:H2"	7:T:14:DA:OP2	2.18	0.42
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.91	0.42
1:A:84:GLU:O	1:A:124:ASN:ND2	2.52	0.42
2:C:846:LYS:NZ	6:R:29:U:P	2.90	0.42
2:C:1094:ALA:HB2	3:D:520:LEU:HD12	2.02	0.42
3:D:904:VAL:HB	3:D:905:PRO:HD2	2.02	0.42
3:D:1301:LYS:HD3	3:D:1301:LYS:HA	1.94	0.42
2:C:292:ARG:CB	2:C:299:LYS:HZ2	2.30	0.42
2:C:344:PHE:CE1	2:C:378:LEU:HD11	2.55	0.42
3:D:205:TYR:CE1	3:D:390:PRO:HG3	2.54	0.42
3:D:466:LYS:HG2	3:D:510:GLU:HB3	2.02	0.42
3:D:1462:LEU:O	3:D:1465:ASN:N	2.53	0.42
5:N:7:DG:H2"	5:N:8:DA:C8	2.54	0.42
2:C:148:PHE:CE2	2:C:309:TYR:HD2	2.38	0.42
2:C:267:TYR:CB	2:C:272:ALA:HB3	2.50	0.42
3:D:841:TYR:HB3	3:D:843:PHE:CZ	2.55	0.42
3:D:1307:LYS:HD3	3:D:1307:LYS:C	2.45	0.42
3:D:1398:TRP:CE3	3:D:1398:TRP:HA	2.55	0.42
1:A:128:HIS:NE2	1:A:131:THR:HG23	2.35	0.42
1:B:18:ARG:NH2	1:B:203:GLY:O	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:184:MET:HE2	2:C:193:LEU:HD12	2.00	0.42
2:C:810:ASP:HB2	2:C:813:VAL:HG13	2.02	0.42
2:C:889:HIS:O	2:C:918:LEU:HD21	2.20	0.42
3:D:171:LEU:HD23	3:D:171:LEU:HA	1.94	0.42
3:D:568:ARG:HA	3:D:571:LYS:HG3	2.01	0.42
4:E:47:LYS:HA	4:E:54:LEU:HB3	2.01	0.42
7:T:3:DG:H2"	7:T:4:DA:C8	2.55	0.42
1:A:178:ALA:HB2	2:C:864:GLY:CA	2.50	0.41
2:C:328:LEU:C	2:C:330:ASN:H	2.26	0.41
2:C:910:LYS:O	2:C:914:ILE:HG12	2.20	0.41
3:D:131:LYS:HG3	3:D:568:ARG:HG2	2.02	0.41
3:D:832:ARG:HA	3:D:832:ARG:HD2	1.74	0.41
3:D:1042:ARG:NH1	3:D:1073:SER:HB3	2.35	0.41
2:C:9:ILE:HG12	2:C:907:ASP:OD2	2.19	0.41
2:C:301:GLU:O	2:C:305:PRO:HD2	2.21	0.41
2:C:759:THR:HB	2:C:785:VAL:HG22	2.02	0.41
2:C:794:PRO:HG3	2:C:1026:GLN:C	2.45	0.41
2:C:1008:ARG:NH1	2:C:1011:GLY:N	2.59	0.41
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	2.01	0.41
2:C:1038:TRP:HH2	3:D:1096:ARG:HA	1.85	0.41
3:D:881:LEU:O	3:D:885:ILE:HG13	2.20	0.41
3:D:1280:VAL:O	3:D:1294:VAL:HG13	2.20	0.41
2:C:118:ILE:HA	2:C:119:PRO:HD3	1.80	0.41
2:C:181:VAL:HA	2:C:220:GLY:O	2.20	0.41
2:C:352:ALA:O	2:C:355:VAL:HG12	2.20	0.41
2:C:473:ARG:HB2	2:C:473:ARG:NH1	2.35	0.41
3:D:29:PRO:HB3	3:D:548:ILE:HB	2.01	0.41
3:D:129:PHE:C	3:D:568:ARG:HH21	2.27	0.41
4:E:80:VAL:HG11	4:E:85:LEU:HD23	2.01	0.41
1:A:90:LEU:HB3	1:A:119:ASP:HB3	2.03	0.41
1:A:183:ASP:OD1	1:A:183:ASP:N	2.53	0.41
2:C:334:ARG:HH11	2:C:418:LEU:CD1	2.34	0.41
2:C:1056:LYS:HB3	3:D:624:ASP:HB2	2.03	0.41
2:C:1103:ASP:N	2:C:1107:ASN:O	2.53	0.41
3:D:357:GLU:OE2	3:D:386:HIS:ND1	2.37	0.41
3:D:877:PRO:HA	3:D:880:ILE:HG22	2.02	0.41
2:C:327:HIS:CE1	2:C:489:THR:HA	2.56	0.41
2:C:724:ARG:HB2	2:C:741:GLY:N	2.36	0.41
2:C:1101:THR:HG21	2:C:1111:ILE:HD11	2.02	0.41
3:D:32:ILE:HG22	3:D:33:ASN:O	2.20	0.41
3:D:1289:LYS:NZ	3:D:1304:LYS:HB2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:THR:HB	2:C:627:ARG:HD3	2.02	0.41
1:A:221:HIS:HA	1:A:224:TYR:CD2	2.56	0.41
2:C:969:GLN:HG2	3:D:952:ASP:OD2	2.21	0.41
3:D:161:LEU:HD23	3:D:162:ARG:HG2	2.02	0.41
3:D:426:LYS:HE2	3:D:426:LYS:HB3	1.90	0.41
3:D:760:ARG:HH21	4:E:3:GLU:CD	2.27	0.41
3:D:1291:SER:HA	3:D:1302:GLU:OE2	2.20	0.41
3:D:1412:LYS:HD3	3:D:1412:LYS:HA	1.47	0.41
1:B:11:PHE:HB2	1:B:25:LEU:HD12	2.02	0.41
2:C:246:ASP:HA	2:C:247:PRO:HD3	1.70	0.41
2:C:749:VAL:HA	2:C:753:ASP:OD2	2.19	0.41
3:D:568:ARG:HA	3:D:568:ARG:HD2	1.97	0.41
3:D:764:LEU:O	3:D:768:ASN:ND2	2.45	0.41
3:D:1004:THR:HG23	3:D:1036:ARG:HB2	2.03	0.41
4:E:41:GLU:H	4:E:41:GLU:HG3	1.56	0.41
7:T:11:DT:H2''	7:T:12:DC:O5'	2.21	0.41
2:C:572:ILE:HG13	2:C:573:ARG:N	2.35	0.41
3:D:31:THR:HG1	3:D:32:ILE:H	1.68	0.41
3:D:1142:ALA:HB1	3:D:1364:HIS:HA	2.03	0.41
3:D:1290:LEU:HD21	3:D:1305:LEU:HD13	2.02	0.41
7:T:4:DA:H2''	7:T:5:DA:C8	2.56	0.41
1:A:46:SER:OG	1:A:47:SER:N	2.52	0.41
1:A:141:GLU:OE1	1:A:141:GLU:N	2.53	0.41
1:A:151:VAL:HA	1:A:152:PRO:HD2	1.93	0.41
1:B:77:GLU:OE2	3:D:867:ARG:NH1	2.54	0.41
2:C:78:PHE:HA	2:C:79:PRO:HD3	1.88	0.41
2:C:137:VAL:HG23	2:C:391:LEU:HD23	2.02	0.41
2:C:177:GLU:HG2	2:C:178:PRO:HD2	2.03	0.41
2:C:214:TYR:HD1	2:C:215:GLY:H	1.69	0.41
3:D:704:ARG:HG3	3:D:705:ALA:N	2.36	0.41
3:D:984:THR:HG22	3:D:987:GLU:CD	2.46	0.41
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	2.03	0.41
3:D:1407:LEU:HD23	3:D:1407:LEU:HA	1.91	0.41
3:D:1458:GLU:O	3:D:1460:ILE:HG22	2.20	0.41
3:D:1492:LEU:O	3:D:1496:GLU:HB2	2.21	0.41
4:E:26:ARG:NH1	4:E:73:LEU:HD21	2.35	0.41
5:N:3:DA:H2''	5:N:4:DA:C8	2.56	0.41
6:R:26:U:H2'	6:R:27:G:C8	2.56	0.41
1:B:56:VAL:HG23	1:B:167:VAL:HG21	2.02	0.41
2:C:73:LEU:HD22	2:C:94:LEU:HA	2.03	0.41
2:C:1071:ILE:HD13	2:C:1071:ILE:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:352:ASN:CG	3:D:371:ILE:HG12	2.46	0.41
3:D:1197:ARG:HH21	3:D:1198:TYR:HE2	1.69	0.41
2:C:378:LEU:O	2:C:382:ILE:HG12	2.21	0.40
2:C:682:TYR:HA	3:D:633:VAL:HG11	2.02	0.40
3:D:108:VAL:HB	3:D:109:PRO:HD3	2.02	0.40
3:D:470:LEU:H	3:D:470:LEU:HG	1.69	0.40
3:D:502:PHE:CZ	3:D:512:MET:HE2	2.56	0.40
1:A:26:GLU:OE2	1:A:185:ARG:HB2	2.21	0.40
2:C:219:GLN:O	2:C:223:ASP:OD2	2.38	0.40
2:C:257:VAL:O	2:C:264:PRO:HD3	2.21	0.40
3:D:465:LEU:HD13	3:D:509:PRO:O	2.22	0.40
3:D:629:SER:OG	3:D:630:VAL:N	2.55	0.40
3:D:983:LEU:CD1	3:D:988:ARG:HB2	2.44	0.40
1:A:42:ARG:HE	2:C:856:GLU:HB2	1.84	0.40
1:A:86:VAL:HG21	1:A:202:ASP:HB2	2.04	0.40
1:A:100:LEU:HD22	1:A:141:GLU:HG3	2.02	0.40
1:A:214:ALA:HA	1:A:217:ILE:HD12	2.03	0.40
2:C:216:GLU:C	2:C:218:VAL:N	2.79	0.40
2:C:1097:LEU:HD11	3:D:103:TRP:CZ3	2.56	0.40
3:D:834:THR:HB	3:D:838:ARG:HD2	2.04	0.40
3:D:1310:ARG:HH11	3:D:1327:ARG:NH1	2.20	0.40
3:D:1311:LEU:HA	3:D:1325:LEU:O	2.20	0.40
5:N:6:DA:H2"	5:N:7:DG:C8	2.56	0.40
2:C:184:MET:O	2:C:190:LYS:HA	2.21	0.40
2:C:442:GLU:HG2	2:C:454:SER:CB	2.51	0.40
3:D:801:GLY:HA3	3:D:826:PRO:HD2	2.04	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:B:143:ARG:NH1	3:D:1297:GLU:OE2[3_455]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/315 (70%)	186 (84%)	29 (13%)	6 (3%)	4	25
1	B	221/315 (70%)	193 (87%)	25 (11%)	3 (1%)	9	39
2	C	1077/1119 (96%)	897 (83%)	144 (13%)	36 (3%)	3	21
3	D	1352/1534 (88%)	1097 (81%)	198 (15%)	57 (4%)	2	17
4	E	91/99 (92%)	73 (80%)	13 (14%)	5 (6%)	1	15
All	All	2962/3382 (88%)	2446 (83%)	409 (14%)	107 (4%)	2	20

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ALA
1	A	184	THR
2	C	2	GLU
2	C	111	ASP
2	C	164	PRO
2	C	213	ALA
2	C	217	LEU
2	C	262	ALA
3	D	117	ASP
3	D	165	LYS
3	D	176	ASP
3	D	363	ALA
3	D	705	ALA
3	D	808	THR
3	D	823	LEU
3	D	1067	VAL
3	D	1273	VAL
3	D	1294	VAL
3	D	1295	GLU
3	D	1327	ARG
3	D	1433	SER
3	D	1454	GLY
3	D	1459	LEU
1	A	29	GLU
2	C	96	ALA
2	C	114	PHE
2	C	248	PRO
2	C	320	HIS

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Mol	Chain	Res	Type
2	C	476	GLY
2	C	517	ARG
2	C	984	GLU
3	D	55	ASP
3	D	82	LYS
3	D	137	PRO
3	D	594	PRO
3	D	824	ASN
3	D	1205	TYR
1	A	48	ILE
1	B	125	PRO
2	C	231	PRO
2	C	244	PRO
2	C	274	ARG
2	C	367	LEU
2	C	542	VAL
2	C	815	LEU
3	D	164	GLY
3	D	200	ASP
3	D	345	TYR
3	D	374	GLU
3	D	417	PRO
3	D	560	GLN
3	D	616	GLN
3	D	806	PHE
3	D	830	ALA
3	D	844	ALA
3	D	1128	VAL
3	D	1284	GLU
3	D	1287	GLU
3	D	1302	GLU
4	E	4	PRO
4	E	42	PRO
4	E	50	THR
1	A	186	LEU
2	C	33	ASP
2	C	187	ASN
2	C	188	LYS
2	C	315	ALA
2	C	864	GLY
3	D	406	ASP
3	D	425	GLY

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Mol	Chain	Res	Type
3	D	832	ARG
3	D	1129	THR
3	D	1269	LYS
3	D	1385	GLY
2	C	39	ARG
2	C	369	PRO
2	C	680	ASP
2	C	795	GLY
3	D	410	SER
3	D	522	PRO
3	D	722	GLU
3	D	1317	ASP
2	C	272	ALA
2	C	999	HIS
3	D	146	PRO
3	D	601	ARG
3	D	735	ALA
3	D	1197	ARG
4	E	58	PRO
1	B	187	GLY
2	C	905	ILE
3	D	182	GLY
3	D	1032	PRO
2	C	52	PHE
2	C	152	PRO
2	C	983	ILE
3	D	109	PRO
3	D	1155	VAL
3	D	1411	GLY
1	B	158	ILE
3	D	208	PRO
3	D	1306	PRO
2	C	376	ARG
4	E	41	GLU
1	A	109	VAL
2	C	261	ILE
3	D	809	PRO

5.3.2 Protein sidechains

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	196/273 (72%)	187 (95%)	9 (5%)	24	46
1	B	196/273 (72%)	186 (95%)	10 (5%)	21	44
2	C	912/941 (97%)	831 (91%)	81 (9%)	9	29
3	D	1147/1289 (89%)	1034 (90%)	113 (10%)	7	24
4	E	82/88 (93%)	69 (84%)	13 (16%)	2	13
All	All	2533/2864 (88%)	2307 (91%)	226 (9%)	9	29

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	12	THR
1	A	15	THR
1	A	32	PHE
1	A	46	SER
1	A	126	ASP
1	A	158	ILE
1	A	165	ILE
1	A	182	GLU
1	B	26	GLU
1	B	63	HIS
1	B	86	VAL
1	B	112	ARG
1	B	124	ASN
1	B	162	ILE
1	B	201	THR
1	B	205	VAL
1	B	206	THR
1	B	208	LEU
2	C	30	LEU
2	C	38	LYS
2	C	39	ARG
2	C	81	ASP
2	C	94	LEU
2	C	98	LEU
2	C	104	ASP
2	C	112	GLU

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Mol	Chain	Res	Type
2	C	118	ILE
2	C	127	PHE
2	C	135	VAL
2	C	154	ARG
2	C	157	ARG
2	C	189	ARG
2	C	193	LEU
2	C	205	GLU
2	C	206	THR
2	C	214	TYR
2	C	232	GLU
2	C	243	ARG
2	C	267	TYR
2	C	274	ARG
2	C	281	LEU
2	C	284	ARG
2	C	289	THR
2	C	295	ASP
2	C	299	LYS
2	C	300	ASP
2	C	303	PHE
2	C	306	THR
2	C	307	LEU
2	C	321	GLU
2	C	350	ARG
2	C	367	LEU
2	C	375	SER
2	C	376	ARG
2	C	378	LEU
2	C	388	ARG
2	C	391	LEU
2	C	393	GLN
2	C	394	PHE
2	C	402	SER
2	C	403	SER
2	C	473	ARG
2	C	474	VAL
2	C	481	ASP
2	C	506	ASN
2	C	559	LEU
2	C	567	GLN
2	C	583	LEU

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Mol	Chain	Res	Type
2	C	610	ARG
2	C	620	LEU
2	C	626	ARG
2	C	627	ARG
2	C	649	VAL
2	C	676	ILE
2	C	690	ILE
2	C	699	PHE
2	C	703	ILE
2	C	728	HIS
2	C	810	ASP
2	C	813	VAL
2	C	835	VAL
2	C	842	ARG
2	C	855	VAL
2	C	865	THR
2	C	880	MET
2	C	899	GLN
2	C	907	ASP
2	C	911	GLU
2	C	953	VAL
2	C	966	LEU
2	C	978	ARG
2	C	988	VAL
2	C	995	MET
2	C	1000	MET
2	C	1001	VAL
2	C	1008	ARG
2	C	1021	LEU
2	C	1099	VAL
2	C	1105	LYS
3	D	5	VAL
3	D	41	ARG
3	D	57	GLU
3	D	60	CYS
3	D	64	LYS
3	D	72	VAL
3	D	74	GLU
3	D	75	ARG
3	D	79	GLU
3	D	80	VAL
3	D	85	VAL

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Mol	Chain	Res	Type
3	D	87	ARG
3	D	107	ASP
3	D	124	GLU
3	D	127	LEU
3	D	142	LEU
3	D	145	VAL
3	D	149	LYS
3	D	152	LEU
3	D	153	LEU
3	D	161	LEU
3	D	165	LYS
3	D	166	GLN
3	D	176	ASP
3	D	178	LEU
3	D	185	VAL
3	D	186	VAL
3	D	202	VAL
3	D	340	THR
3	D	347	VAL
3	D	372	ASP
3	D	394	LEU
3	D	400	VAL
3	D	408	GLU
3	D	435	VAL
3	D	449	SER
3	D	468	LEU
3	D	470	LEU
3	D	494	LYS
3	D	507	ASN
3	D	520	LEU
3	D	567	ILE
3	D	642	CYS
3	D	686	GLU
3	D	687	VAL
3	D	692	GLU
3	D	694	VAL
3	D	724	GLN
3	D	734	GLU
3	D	783	ARG
3	D	804	LEU
3	D	808	THR
3	D	813	LEU

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Mol	Chain	Res	Type
3	D	817	GLU
3	D	823	LEU
3	D	828	LYS
3	D	833	GLU
3	D	857	ILE
3	D	892	ASP
3	D	902	LEU
3	D	926	LYS
3	D	935	LYS
3	D	971	LEU
3	D	972	LEU
3	D	983	LEU
3	D	991	GLN
3	D	1012	GLU
3	D	1013	GLU
3	D	1041	LEU
3	D	1044	LEU
3	D	1058	ARG
3	D	1079	LYS
3	D	1083	ASP
3	D	1106	VAL
3	D	1109	GLU
3	D	1115	THR
3	D	1129	THR
3	D	1151	ARG
3	D	1155	VAL
3	D	1162	GLU
3	D	1197	ARG
3	D	1207	TYR
3	D	1209	LEU
3	D	1235	GLN
3	D	1262	LEU
3	D	1273	VAL
3	D	1277	ILE
3	D	1278	ASP
3	D	1283	ILE
3	D	1284	GLU
3	D	1292	VAL
3	D	1296	SER
3	D	1299	PHE
3	D	1304	LYS
3	D	1305	LEU

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Mol	Chain	Res	Type
3	D	1307	LYS
3	D	1314	LYS
3	D	1315	ASP
3	D	1325	LEU
3	D	1327	ARG
3	D	1342	GLU
3	D	1373	ARG
3	D	1389	LEU
3	D	1410	GLU
3	D	1412	LYS
3	D	1424	VAL
3	D	1433	SER
3	D	1435	LEU
3	D	1441	GLN
3	D	1478	SER
3	D	1484	THR
3	D	1488	ASP
3	D	1492	LEU
4	E	6	ILE
4	E	14	ASP
4	E	32	ARG
4	E	38	THR
4	E	39	VAL
4	E	40	LEU
4	E	41	GLU
4	E	47	LYS
4	E	49	GLN
4	E	51	LEU
4	E	54	LEU
4	E	56	ASP
4	E	74	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	124	ASN
1	B	156	HIS
1	B	188	GLN
2	C	141	HIS
2	C	179	ASN
2	C	431	HIS

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Mol	Chain	Res	Type
2	C	434	HIS
2	C	500	ASN
2	C	538	GLN
2	C	609	ASN
2	C	639	GLN
2	C	884	GLN
2	C	1100	GLN
3	D	125	GLN
3	D	350	HIS
3	D	388	HIS
3	D	575	GLN
3	D	611	GLN
3	D	640	HIS
3	D	641	GLN
3	D	1031	ASN
3	D	1033	GLN
3	D	1124	GLN
3	D	1227	GLN
3	D	1235	GLN
3	D	1374	GLN
3	D	1465	ASN
3	D	1489	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	R	8/16 (50%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	R	22	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	223/315 (70%)	-0.74	0	100 100	52, 116, 169, 205	0
1	B	223/315 (70%)	-0.66	1 (0%)	88 77	53, 107, 163, 198	0
2	C	1083/1119 (96%)	-0.60	1 (0%)	92 88	34, 108, 177, 264	0
3	D	1358/1534 (88%)	-0.62	4 (0%)	90 80	31, 110, 196, 250	0
4	E	93/99 (93%)	-0.66	0	100 100	65, 121, 179, 228	0
5	N	11/13 (84%)	-0.26	0	100 100	340, 362, 386, 405	0
6	R	9/16 (56%)	-0.66	0	100 100	201, 206, 235, 243	0
7	T	22/22 (100%)	-0.15	0	100 100	219, 336, 388, 406	0
All	All	3022/3433 (88%)	-0.62	6 (0%)	91 83	31, 111, 192, 406	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	802	ALA	3.6
2	C	302	VAL	2.6
3	D	777	PRO	2.5
3	D	393	ILE	2.2
3	D	949	ILE	2.1
1	B	64	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	ZN	D	1601	1/1	0.92	0.11	70,70,70,70	0
9	MG	D	1603	1/1	0.95	0.04	70,70,70,70	0
8	ZN	D	1602	1/1	1.00	0.02	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.