



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:42 AM UTC

PDB ID : 1XDO / pdb_00001xdo
Title : Crystal Structure of Escherichia coli Polyphosphate Kinase
Authors : Zhu, Y.; Huang, W.; Lee, S.S.; Xu, W.
Deposited on : 2004-09-07
Resolution : 3.00 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

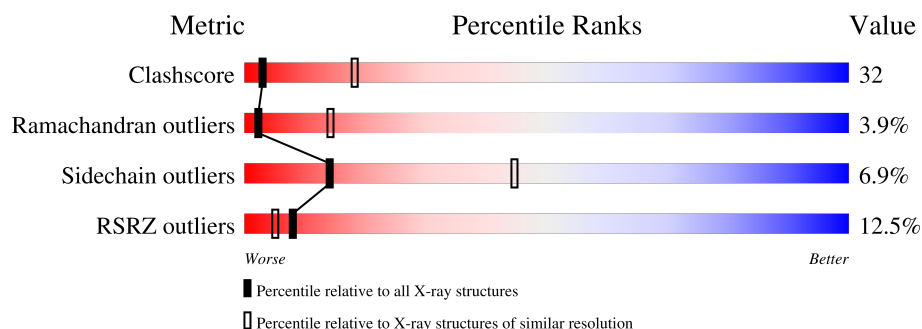
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	687	12% 48% 44% 8%
1	B	687	13% 47% 46% 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11234 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.

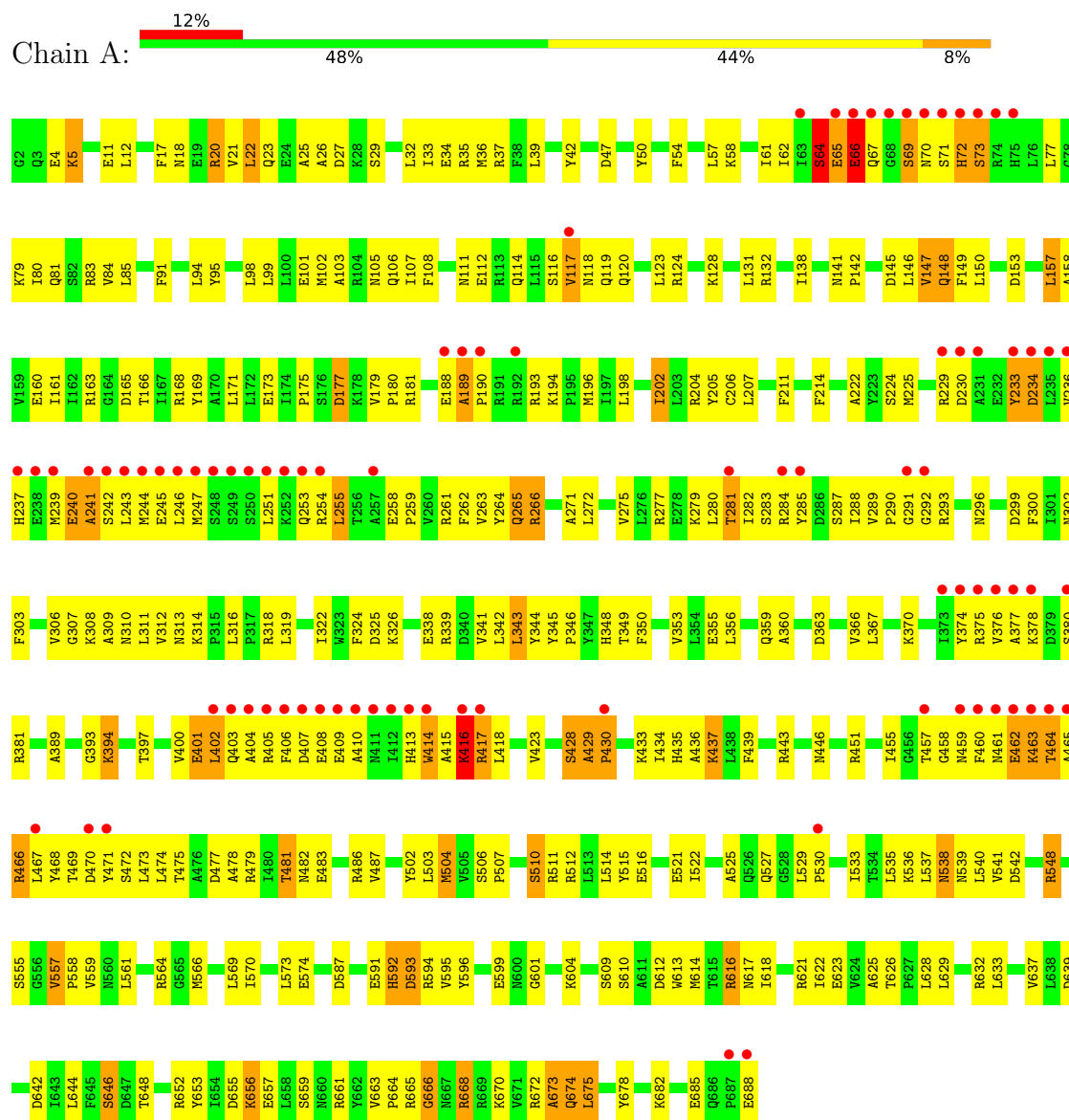
- Molecule 1 is a protein called Polyphosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	687	Total	C	N	O	S	0	0	0
			5617	3568	1008	1025	16			
1	B	687	Total	C	N	O	S	0	0	0
			5617	3568	1008	1025	16			

3 Residue-property plots

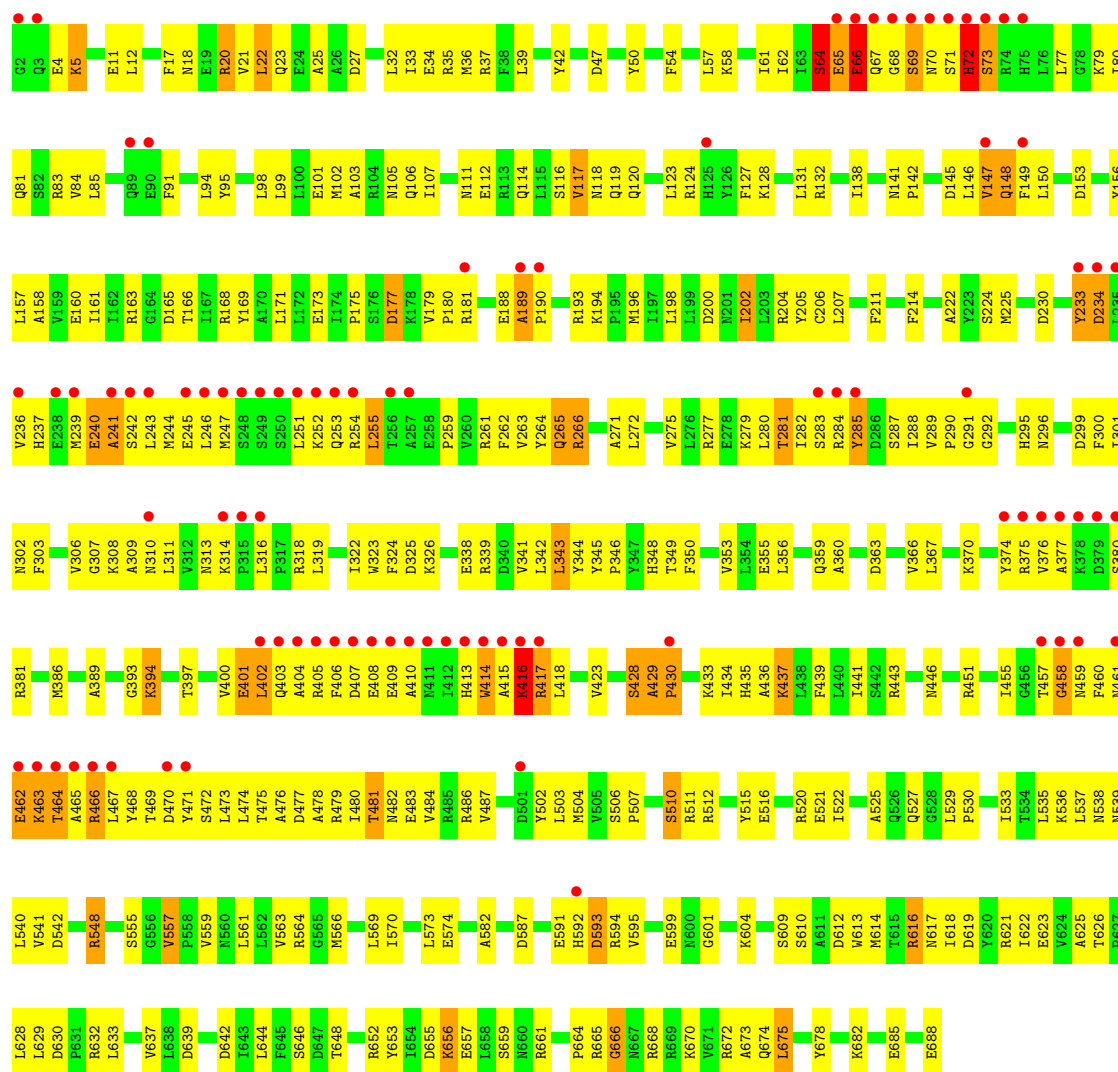
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Polyphosphate kinase



• Molecule 1: Polyphosphate kinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	154.00Å 154.00Å 155.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.00-3.00) 88.4 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 2.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.255 , 0.273 0.267 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.028 for -h,l,k 0.017 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	11234	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.55	0/5735	1.04	28/7772 (0.4%)
1	B	0.56	0/5735	1.04	31/7772 (0.4%)
All	All	0.55	0/11470	1.04	59/15544 (0.4%)

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	350	PHE	N-CA-C	-8.35	102.99	113.01
1	B	350	PHE	N-CA-C	-8.27	103.09	113.01
1	B	466	ARG	N-CA-C	8.26	123.13	112.89
1	B	467	LEU	N-CA-C	-8.18	103.51	113.97
1	A	467	LEU	N-CA-C	-8.06	103.65	113.97
1	A	466	ARG	N-CA-C	7.96	122.76	112.89
1	B	381	ARG	N-CA-C	-7.88	103.67	113.28
1	A	381	ARG	N-CA-C	-7.13	104.58	113.28
1	A	266	ARG	N-CA-C	7.09	119.91	111.33
1	A	138	ILE	N-CA-C	-6.99	97.66	107.80
1	B	266	ARG	N-CA-C	6.89	119.66	111.33
1	B	138	ILE	N-CA-C	-6.88	97.83	107.80
1	A	70	ASN	N-CA-C	6.86	118.67	110.44
1	B	593	ASP	CA-C-N	-6.79	113.35	122.72
1	B	593	ASP	C-N-CA	-6.79	113.35	122.72
1	B	70	ASN	N-CA-C	6.78	118.57	110.44
1	B	593	ASP	CA-CB-CG	6.76	119.36	112.60
1	A	73	SER	N-CA-C	6.50	118.91	111.11
1	B	73	SER	N-CA-C	6.48	118.88	111.11
1	A	593	ASP	CA-CB-CG	6.29	118.89	112.60
1	B	165	ASP	N-CA-C	-6.13	106.06	112.93
1	A	64	SER	N-CA-C	-6.02	104.41	110.97
1	A	165	ASP	N-CA-C	-5.90	106.32	112.93
1	B	64	SER	N-CA-C	-5.88	104.56	110.97
1	A	463	LYS	N-CA-C	-5.83	106.29	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	463	LYS	N-CA-C	-5.64	106.06	113.12
1	A	211	PHE	N-CA-C	5.63	121.18	113.97
1	A	557	VAL	CA-C-N	5.51	126.35	120.13
1	A	557	VAL	C-N-CA	5.51	126.35	120.13
1	A	202	ILE	N-CA-C	-5.50	105.00	111.00
1	A	475	THR	N-CA-C	5.38	117.24	109.07
1	A	592	HIS	CA-C-O	5.38	124.81	118.90
1	A	380	SER	N-CA-C	5.37	117.82	110.24
1	A	504	MET	N-CA-C	-5.37	99.97	108.73
1	B	202	ILE	N-CA-C	-5.36	105.16	111.00
1	B	458	GLY	N-CA-C	-5.31	106.42	112.79
1	B	401	GLU	N-CA-C	-5.27	101.87	110.20
1	B	475	THR	N-CA-C	5.25	117.06	109.07
1	B	252	LYS	N-CA-C	-5.21	105.67	111.36
1	B	20	ARG	N-CA-C	-5.21	105.60	111.28
1	B	521	GLU	N-CA-C	-5.20	105.50	111.07
1	B	557	VAL	CA-C-N	5.20	126.00	120.13
1	B	557	VAL	C-N-CA	5.20	126.00	120.13
1	B	211	PHE	N-CA-C	5.19	120.61	113.97
1	B	476	ALA	N-CA-C	-5.11	105.95	113.61
1	A	538	ASN	N-CA-C	-5.10	107.19	113.41
1	A	72	HIS	CA-C-N	5.10	127.42	120.54
1	A	72	HIS	C-N-CA	5.10	127.42	120.54
1	B	72	HIS	CA-C-N	5.08	127.40	120.54
1	B	72	HIS	C-N-CA	5.08	127.40	120.54
1	B	380	SER	N-CA-C	5.08	117.41	110.24
1	A	401	GLU	N-CA-C	-5.08	102.18	110.20
1	A	319	LEU	N-CA-C	5.08	118.49	109.96
1	A	596	TYR	O-C-N	-5.07	117.38	123.31
1	A	521	GLU	N-CA-C	-5.04	105.68	111.07
1	A	20	ARG	N-CA-C	-5.03	105.80	111.28
1	B	595	VAL	CA-CB-CG2	5.02	118.94	110.40
1	B	319	LEU	N-CA-C	5.02	118.39	109.96
1	B	619	ASP	N-CA-C	5.00	121.07	114.12

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	5617	0	5456	351	0
1	B	5617	0	5456	359	0
All	All	11234	0	10912	707	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (707) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:ARG:HD3	1:A:612:ASP:OD1	1.47	1.13
1:B:437:LYS:HZ2	1:B:459:ASN:HB3	1.07	1.10
1:A:437:LYS:HZ2	1:A:459:ASN:HB3	1.01	1.10
1:B:461:ASN:HB3	1:B:464:THR:HB	1.31	1.09
1:A:437:LYS:HG2	1:A:459:ASN:HA	1.14	1.06
1:B:437:LYS:HG2	1:B:459:ASN:HA	1.12	1.06
1:A:402:LEU:HD23	1:A:402:LEU:H	1.20	1.06
1:A:461:ASN:HB3	1:A:464:THR:HB	1.34	1.06
1:B:376:VAL:HG12	1:B:460:PHE:HB2	1.35	1.05
1:B:402:LEU:HD23	1:B:402:LEU:H	1.22	1.04
1:A:376:VAL:HG12	1:A:460:PHE:HB2	1.34	1.02
1:A:318:ARG:HH22	1:A:465:ALA:HB1	1.25	1.01
1:A:436:ALA:C	1:A:437:LYS:HD2	1.84	1.01
1:B:436:ALA:C	1:B:437:LYS:HD2	1.86	1.00
1:B:318:ARG:HH22	1:B:465:ALA:HB1	1.23	0.99
1:A:344:TYR:H	1:A:348:HIS:HD2	1.10	0.95
1:A:470:ASP:OD2	1:A:592:HIS:HB3	1.66	0.94
1:B:470:ASP:OD2	1:B:592:HIS:HB3	1.68	0.93
1:B:111:ASN:H	1:B:114:GLN:HE21	1.11	0.93
1:B:284:ARG:HG3	1:B:285:TYR:H	1.34	0.92
1:B:240:GLU:HB3	1:B:244:MET:H	1.35	0.92
1:A:111:ASN:H	1:A:114:GLN:HE21	1.11	0.92
1:A:240:GLU:HB3	1:A:244:MET:H	1.34	0.91
1:B:665:ARG:HH21	1:B:670:LYS:HG3	1.36	0.91
1:B:344:TYR:H	1:B:348:HIS:HD2	1.11	0.91
1:B:437:LYS:HE3	1:B:458:GLY:C	1.96	0.89
1:A:408:GLU:HG3	1:A:409:GLU:H	1.38	0.89
1:A:548:ARG:HG2	1:A:548:ARG:HH11	1.34	0.89
1:B:548:ARG:HG2	1:B:548:ARG:HH11	1.35	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:TYR:CZ	1:A:290:PRO:HB3	2.09	0.88
1:A:12:LEU:HD22	1:A:83:ARG:NH1	1.88	0.88
1:A:437:LYS:HE3	1:A:458:GLY:C	1.98	0.88
1:B:12:LEU:HD22	1:B:83:ARG:NH1	1.88	0.88
1:B:429:ALA:HB1	1:B:430:PRO:HD2	1.56	0.87
1:B:408:GLU:HG3	1:B:409:GLU:H	1.39	0.87
1:A:284:ARG:HG3	1:A:285:TYR:H	1.35	0.87
1:A:429:ALA:HB1	1:A:430:PRO:HD2	1.57	0.86
1:A:437:LYS:NZ	1:A:459:ASN:HB3	1.90	0.86
1:A:537:LEU:HA	1:A:594:ARG:HG2	1.54	0.86
1:A:284:ARG:HG3	1:A:285:TYR:HD1	1.41	0.85
1:A:437:LYS:HZ2	1:A:459:ASN:CB	1.89	0.84
1:A:665:ARG:HH21	1:A:670:LYS:HG3	1.40	0.84
1:B:437:LYS:NZ	1:B:459:ASN:HB3	1.91	0.84
1:B:284:ARG:HG3	1:B:285:TYR:HD1	1.41	0.84
1:B:264:TYR:CZ	1:B:290:PRO:HB3	2.13	0.84
1:B:594:ARG:HD3	1:B:612:ASP:OD1	1.77	0.83
1:A:437:LYS:HG2	1:A:459:ASN:CA	2.05	0.82
1:A:458:GLY:HA3	1:A:470:ASP:OD1	1.79	0.81
1:B:458:GLY:HA3	1:B:470:ASP:OD1	1.80	0.81
1:A:464:THR:O	1:A:468:TYR:HB2	1.82	0.80
1:B:64:SER:HB3	1:B:69:SER:HB3	1.64	0.80
1:B:437:LYS:HG2	1:B:459:ASN:CA	2.03	0.80
1:A:360:ALA:HA	1:A:366:VAL:HG21	1.65	0.79
1:A:65:GLU:HA	1:A:69:SER:OG	1.81	0.79
1:A:32:LEU:HD13	1:A:101:GLU:OE2	1.83	0.78
1:A:437:LYS:CG	1:A:459:ASN:HA	2.08	0.78
1:A:242:SER:O	1:A:246:LEU:HG	1.82	0.78
1:B:116:SER:O	1:B:120:GLN:HG3	1.82	0.78
1:A:116:SER:O	1:A:120:GLN:HG3	1.82	0.78
1:B:242:SER:O	1:B:246:LEU:HG	1.83	0.78
1:B:179:VAL:HG13	1:B:180:PRO:HD2	1.65	0.77
1:B:464:THR:O	1:B:468:TYR:HB2	1.84	0.77
1:B:65:GLU:O	1:B:67:GLN:N	2.17	0.77
1:B:402:LEU:HD23	1:B:402:LEU:N	1.99	0.77
1:B:65:GLU:HA	1:B:69:SER:OG	1.84	0.77
1:A:65:GLU:O	1:A:67:GLN:N	2.17	0.76
1:A:594:ARG:HH11	1:A:612:ASP:CG	1.94	0.76
1:B:32:LEU:HD13	1:B:101:GLU:OE2	1.85	0.76
1:A:402:LEU:HD23	1:A:402:LEU:N	1.98	0.76
1:B:437:LYS:CG	1:B:459:ASN:HA	2.06	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:VAL:HG13	1:A:180:PRO:HD2	1.67	0.76
1:A:116:SER:OG	1:A:119:GLN:HG3	1.86	0.76
1:A:64:SER:HB3	1:A:69:SER:HB3	1.65	0.75
1:B:665:ARG:NH2	1:B:670:LYS:HG3	2.02	0.75
1:B:360:ALA:HA	1:B:366:VAL:HG21	1.67	0.75
1:A:112:GLU:HB2	1:A:205:TYR:HB2	1.69	0.74
1:B:111:ASN:N	1:B:114:GLN:HE21	1.86	0.74
1:A:181:ARG:HH12	1:A:296:ASN:HB2	1.53	0.74
1:B:537:LEU:HA	1:B:594:ARG:HG2	1.69	0.73
1:B:112:GLU:HB2	1:B:205:TYR:HB2	1.70	0.73
1:A:196:MET:HE1	1:A:306:VAL:HG21	1.70	0.73
1:A:237:HIS:HB2	1:A:244:MET:SD	2.29	0.73
1:A:266:ARG:NH1	1:A:291:GLY:HA2	2.03	0.73
1:A:470:ASP:CG	1:A:592:HIS:HB3	2.14	0.73
1:A:224:SER:H	1:A:265:GLN:NE2	1.86	0.73
1:B:116:SER:OG	1:B:119:GLN:HG3	1.89	0.73
1:A:307:GLY:HA3	1:A:311:LEU:HD12	1.71	0.72
1:A:429:ALA:HB1	1:A:430:PRO:CD	2.19	0.72
1:B:429:ALA:HB1	1:B:430:PRO:CD	2.18	0.72
1:B:307:GLY:HA3	1:B:311:LEU:HD12	1.72	0.72
1:B:470:ASP:CG	1:B:592:HIS:HB3	2.13	0.72
1:B:266:ARG:NH1	1:B:291:GLY:HA2	2.05	0.72
1:B:344:TYR:HE2	1:B:593:ASP:OD1	1.73	0.72
1:A:344:TYR:H	1:A:348:HIS:CD2	2.01	0.72
1:B:659:SER:OG	1:B:661:ARG:HG3	1.90	0.72
1:B:665:ARG:O	1:B:665:ARG:HG3	1.89	0.72
1:B:196:MET:HE1	1:B:306:VAL:HG21	1.72	0.71
1:B:237:HIS:HB2	1:B:244:MET:SD	2.30	0.71
1:B:181:ARG:HH12	1:B:296:ASN:HB2	1.54	0.71
1:B:437:LYS:HD3	1:B:458:GLY:O	1.91	0.71
1:A:111:ASN:N	1:A:114:GLN:HE21	1.86	0.71
1:B:224:SER:H	1:B:265:GLN:NE2	1.88	0.70
1:B:326:LYS:HE2	1:B:688:GLU:OE2	1.91	0.70
1:B:344:TYR:H	1:B:348:HIS:CD2	2.02	0.70
1:A:665:ARG:O	1:A:665:ARG:HG3	1.89	0.70
1:B:204:ARG:HH12	1:B:265:GLN:HE22	1.40	0.70
1:B:402:LEU:O	1:B:403:GLN:HG3	1.92	0.69
1:A:326:LYS:HE2	1:A:688:GLU:OE2	1.91	0.69
1:A:207:LEU:HD11	1:A:222:ALA:HB2	1.75	0.69
1:A:587:ASP:HB3	1:A:674:GLN:OE1	1.92	0.69
1:A:22:LEU:HD22	1:A:94:LEU:HD12	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:LEU:HD11	1:B:222:ALA:HB2	1.74	0.69
1:A:659:SER:OG	1:A:661:ARG:HG3	1.93	0.69
1:A:251:LEU:O	1:A:255:LEU:HB2	1.93	0.69
1:A:339:ARG:HD2	1:A:632:ARG:NH1	2.07	0.69
1:B:240:GLU:HB3	1:B:244:MET:N	2.07	0.69
1:A:111:ASN:H	1:A:114:GLN:NE2	1.89	0.69
1:A:402:LEU:HD21	1:A:428:SER:O	1.93	0.69
1:B:402:LEU:H	1:B:402:LEU:CD2	2.04	0.69
1:A:402:LEU:O	1:A:403:GLN:HG3	1.92	0.68
1:B:587:ASP:HB3	1:B:674:GLN:OE1	1.93	0.68
1:A:665:ARG:NH2	1:A:670:LYS:HG3	2.06	0.68
1:B:402:LEU:HD21	1:B:428:SER:O	1.93	0.68
1:B:251:LEU:O	1:B:255:LEU:HB2	1.93	0.68
1:A:163:ARG:O	1:A:166:THR:HB	1.92	0.68
1:A:402:LEU:H	1:A:402:LEU:CD2	2.02	0.68
1:A:318:ARG:HH22	1:A:465:ALA:CB	2.05	0.67
1:A:569:LEU:C	1:A:569:LEU:HD23	2.19	0.67
1:A:204:ARG:HH12	1:A:265:GLN:HE22	1.43	0.67
1:A:318:ARG:NH2	1:A:465:ALA:HB1	2.05	0.67
1:B:163:ARG:O	1:B:166:THR:HB	1.93	0.67
1:B:318:ARG:NH2	1:B:465:ALA:HB1	2.04	0.67
1:A:483:GLU:HB3	1:A:503:LEU:HD22	1.76	0.67
1:B:504:MET:HB3	1:B:625:ALA:HB3	1.77	0.67
1:A:240:GLU:HB3	1:A:244:MET:N	2.06	0.66
1:B:65:GLU:N	1:B:69:SER:HB3	2.10	0.66
1:B:111:ASN:H	1:B:114:GLN:NE2	1.89	0.66
1:B:569:LEU:HD23	1:B:569:LEU:C	2.20	0.66
1:A:240:GLU:CB	1:A:244:MET:HB2	2.24	0.66
1:B:240:GLU:CB	1:B:244:MET:HB2	2.25	0.66
1:B:141:ASN:HB3	1:B:142:PRO:HD2	1.78	0.66
1:A:141:ASN:HB3	1:A:142:PRO:HD2	1.77	0.65
1:A:65:GLU:N	1:A:69:SER:HB3	2.11	0.65
1:A:196:MET:HE1	1:A:306:VAL:CG2	2.26	0.65
1:A:594:ARG:NH1	1:A:612:ASP:OD2	2.29	0.65
1:B:339:ARG:HD2	1:B:632:ARG:NH1	2.11	0.65
1:A:504:MET:HB3	1:A:625:ALA:HB3	1.78	0.65
1:A:181:ARG:HH12	1:A:296:ASN:CB	2.10	0.65
1:A:376:VAL:CG1	1:A:460:PHE:HB2	2.18	0.65
1:B:181:ARG:HH12	1:B:296:ASN:CB	2.10	0.65
1:A:405:ARG:HG2	1:A:433:LYS:NZ	2.12	0.64
1:A:35:ARG:NH2	1:A:101:GLU:OE2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ARG:HG2	1:A:266:ARG:HH11	1.62	0.64
1:B:95:TYR:CE2	1:B:99:LEU:HD11	2.32	0.64
1:B:266:ARG:HH11	1:B:266:ARG:HG2	1.62	0.64
1:B:318:ARG:HH22	1:B:465:ALA:CB	2.05	0.64
1:B:644:LEU:HD23	1:B:673:ALA:HB1	1.79	0.64
1:A:644:LEU:HD23	1:A:673:ALA:HB1	1.80	0.64
1:A:437:LYS:HD3	1:A:458:GLY:O	1.97	0.64
1:A:408:GLU:HG3	1:A:409:GLU:N	2.12	0.64
1:A:284:ARG:HG3	1:A:285:TYR:N	2.11	0.64
1:B:22:LEU:HD22	1:B:94:LEU:HD12	1.78	0.63
1:B:196:MET:HE1	1:B:306:VAL:CG2	2.29	0.63
1:B:344:TYR:CE2	1:B:593:ASP:OD1	2.50	0.63
1:A:405:ARG:HE	1:A:621:ARG:HH22	1.47	0.63
1:A:196:MET:CE	1:A:306:VAL:HG21	2.28	0.63
1:A:548:ARG:HH11	1:A:548:ARG:CG	2.11	0.63
1:B:405:ARG:HG2	1:B:433:LYS:NZ	2.14	0.63
1:A:80:ILE:O	1:A:84:VAL:HG23	1.99	0.63
1:B:34:GLU:HG3	1:B:313:ASN:ND2	2.14	0.63
1:A:262:PHE:HD2	1:A:288:ILE:HG23	1.64	0.62
1:B:483:GLU:HB3	1:B:503:LEU:HD22	1.80	0.62
1:A:95:TYR:CE2	1:A:99:LEU:HD11	2.34	0.62
1:B:284:ARG:HG3	1:B:285:TYR:N	2.10	0.62
1:A:437:LYS:HE3	1:A:459:ASN:N	2.13	0.62
1:B:413:HIS:HA	1:B:416:LYS:HE3	1.81	0.62
1:B:262:PHE:HD2	1:B:288:ILE:HG23	1.65	0.62
1:B:437:LYS:HE3	1:B:459:ASN:N	2.14	0.62
1:A:34:GLU:HG3	1:A:313:ASN:ND2	2.14	0.61
1:A:413:HIS:HA	1:A:416:LYS:HE3	1.81	0.61
1:B:376:VAL:CG1	1:B:460:PHE:HB2	2.20	0.61
1:B:483:GLU:O	1:B:487:VAL:HG23	2.00	0.61
1:A:266:ARG:CZ	1:A:291:GLY:HA2	2.30	0.61
1:A:20:ARG:HG2	1:A:652:ARG:HD2	1.82	0.61
1:A:436:ALA:C	1:A:437:LYS:CD	2.69	0.61
1:B:116:SER:C	1:B:118:ASN:H	2.09	0.61
1:A:116:SER:C	1:A:118:ASN:H	2.09	0.61
1:B:95:TYR:CZ	1:B:99:LEU:HD11	2.36	0.61
1:A:483:GLU:O	1:A:487:VAL:HG23	2.01	0.60
1:B:64:SER:OG	1:B:69:SER:HA	2.01	0.60
1:A:22:LEU:HD22	1:A:94:LEU:CD1	2.31	0.60
1:A:27:ASP:O	1:A:35:ARG:HD3	2.01	0.60
1:B:437:LYS:HB3	1:B:460:PHE:CE1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:GLU:HB2	1:A:244:MET:HB2	1.82	0.60
1:B:173:GLU:O	1:B:175:PRO:HD3	2.02	0.60
1:B:240:GLU:HB2	1:B:244:MET:HB2	1.82	0.60
1:B:20:ARG:HG2	1:B:652:ARG:HD2	1.83	0.60
1:B:266:ARG:CZ	1:B:291:GLY:HA2	2.32	0.60
1:B:405:ARG:HE	1:B:621:ARG:HH22	1.48	0.60
1:A:370:LYS:HG2	1:A:397:THR:HB	1.84	0.60
1:A:506:SER:O	1:A:622:ILE:HA	2.02	0.60
1:B:437:LYS:CD	1:B:458:GLY:O	2.49	0.60
1:A:393:GLY:O	1:A:394:LYS:O	2.19	0.60
1:B:80:ILE:O	1:B:84:VAL:HG23	2.01	0.60
1:B:241:ALA:O	1:B:245:GLU:HG3	2.02	0.60
1:A:241:ALA:O	1:A:245:GLU:HG3	2.02	0.60
1:A:66:GLU:HG3	1:A:251:LEU:HD22	1.84	0.60
1:A:473:LEU:C	1:A:474:LEU:HD22	2.26	0.60
1:B:196:MET:CE	1:B:306:VAL:HG21	2.30	0.60
1:A:478:ALA:HA	1:A:481:THR:HB	1.83	0.60
1:B:370:LYS:HG2	1:B:397:THR:HB	1.84	0.60
1:A:120:GLN:HB3	1:A:205:TYR:OH	2.02	0.59
1:A:266:ARG:NH1	1:A:266:ARG:HG2	2.16	0.59
1:A:348:HIS:HE1	1:A:685:GLU:OE1	1.84	0.59
1:A:437:LYS:HB3	1:A:460:PHE:CE1	2.37	0.59
1:B:266:ARG:NH1	1:B:266:ARG:HG2	2.16	0.59
1:B:533:ILE:HB	1:B:559:VAL:HG22	1.85	0.59
1:A:539:ASN:ND2	1:A:566:MET:H	2.01	0.59
1:B:437:LYS:HZ2	1:B:459:ASN:CB	1.99	0.59
1:A:189:ALA:HB3	1:A:190:PRO:CD	2.33	0.59
1:B:402:LEU:N	1:B:402:LEU:CD2	2.66	0.59
1:A:339:ARG:HD2	1:A:632:ARG:HH12	1.66	0.58
1:B:437:LYS:HD2	1:B:437:LYS:N	2.18	0.58
1:B:27:ASP:O	1:B:35:ARG:HD3	2.03	0.58
1:B:120:GLN:HB3	1:B:205:TYR:OH	2.02	0.58
1:B:348:HIS:HE1	1:B:685:GLU:OE1	1.85	0.58
1:A:95:TYR:CZ	1:A:99:LEU:HD11	2.38	0.58
1:B:189:ALA:HB3	1:B:190:PRO:CD	2.33	0.58
1:A:594:ARG:HD3	1:A:612:ASP:CG	2.26	0.58
1:A:307:GLY:HA3	1:A:311:LEU:CD1	2.34	0.58
1:B:529:LEU:HB3	1:B:530:PRO:HD2	1.85	0.58
1:B:539:ASN:ND2	1:B:566:MET:H	2.01	0.58
1:B:478:ALA:HA	1:B:481:THR:HB	1.85	0.58
1:B:506:SER:HB2	1:B:623:GLU:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ALA:HB2	1:B:462:GLU:H	1.69	0.58
1:B:506:SER:O	1:B:622:ILE:HA	2.04	0.58
1:A:64:SER:OG	1:A:69:SER:HA	2.03	0.57
1:A:377:ALA:HB2	1:A:462:GLU:H	1.69	0.57
1:A:512:ARG:HG2	1:A:516:GLU:OE2	2.04	0.57
1:B:402:LEU:HG	1:B:403:GLN:OE1	2.03	0.57
1:B:539:ASN:HD22	1:B:566:MET:H	1.52	0.57
1:A:173:GLU:O	1:A:175:PRO:HD3	2.04	0.57
1:A:402:LEU:HG	1:A:403:GLN:OE1	2.04	0.57
1:A:529:LEU:HB3	1:A:530:PRO:HD2	1.86	0.57
1:B:307:GLY:HA3	1:B:311:LEU:CD1	2.35	0.57
1:A:435:HIS:O	1:A:437:LYS:HE2	2.04	0.57
1:B:512:ARG:HG2	1:B:516:GLU:OE2	2.04	0.57
1:B:515:TYR:CD2	1:B:548:ARG:HG3	2.39	0.57
1:A:436:ALA:CA	1:A:437:LYS:HD2	2.34	0.57
1:B:408:GLU:HG3	1:B:409:GLU:N	2.14	0.57
1:A:285:TYR:H	1:A:285:TYR:HD1	1.52	0.56
1:B:469:THR:C	1:B:470:ASP:OD2	2.48	0.56
1:A:345:TYR:CE1	1:A:472:SER:HB2	2.40	0.56
1:B:473:LEU:C	1:B:474:LEU:HD22	2.30	0.56
1:A:233:TYR:O	1:A:234:ASP:HB2	2.05	0.56
1:A:240:GLU:HA	1:A:243:LEU:HB2	1.86	0.56
1:A:515:TYR:CD2	1:A:548:ARG:HG3	2.40	0.56
1:A:539:ASN:HD22	1:A:566:MET:H	1.52	0.56
1:A:570:ILE:HG23	1:A:656:LYS:HB3	1.86	0.56
1:B:17:PHE:HA	1:B:20:ARG:CZ	2.35	0.56
1:B:548:ARG:HH11	1:B:548:ARG:CG	2.12	0.56
1:A:355:GLU:O	1:A:359:GLN:HG3	2.05	0.56
1:B:233:TYR:O	1:B:234:ASP:HB2	2.04	0.56
1:A:179:VAL:CG1	1:A:180:PRO:HD2	2.36	0.56
1:A:537:LEU:HA	1:A:594:ARG:CG	2.31	0.56
1:B:435:HIS:O	1:B:437:LYS:HE2	2.04	0.56
1:B:22:LEU:HD22	1:B:94:LEU:CD1	2.35	0.56
1:A:17:PHE:HA	1:A:20:ARG:CZ	2.36	0.56
1:A:25:ALA:O	1:A:35:ARG:HD2	2.05	0.56
1:B:25:ALA:O	1:B:35:ARG:HD2	2.06	0.56
1:A:204:ARG:HH12	1:A:265:GLN:NE2	2.04	0.56
1:B:81:GLN:O	1:B:85:LEU:HG	2.07	0.56
1:B:35:ARG:NH2	1:B:101:GLU:OE2	2.38	0.55
1:B:179:VAL:CG1	1:B:180:PRO:HD2	2.34	0.55
1:B:204:ARG:HH12	1:B:265:GLN:NE2	2.02	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:ASP:OD1	1:A:479:ARG:HB2	2.06	0.55
1:B:271:ALA:O	1:B:275:VAL:HG23	2.07	0.55
1:B:285:TYR:H	1:B:285:TYR:HD1	1.52	0.55
1:B:405:ARG:HG2	1:B:433:LYS:HZ3	1.70	0.55
1:A:437:LYS:CD	1:A:437:LYS:N	2.69	0.55
1:A:62:ILE:HA	1:A:65:GLU:OE1	2.07	0.55
1:A:377:ALA:N	1:A:461:ASN:HA	2.21	0.55
1:A:437:LYS:CD	1:A:458:GLY:O	2.55	0.55
1:B:437:LYS:CD	1:B:437:LYS:N	2.70	0.55
1:A:469:THR:C	1:A:470:ASP:OD2	2.50	0.55
1:B:240:GLU:HA	1:B:243:LEU:HB2	1.88	0.55
1:B:468:TYR:HD2	1:B:592:HIS:HB2	1.72	0.55
1:B:570:ILE:HG23	1:B:656:LYS:HB3	1.88	0.55
1:B:37:ARG:HA	1:B:300:PHE:O	2.08	0.55
1:B:393:GLY:O	1:B:394:LYS:O	2.25	0.55
1:A:468:TYR:HD2	1:A:592:HIS:HB2	1.71	0.54
1:A:338:GLU:HG3	1:A:339:ARG:HG3	1.90	0.54
1:A:437:LYS:HD2	1:A:437:LYS:N	2.19	0.54
1:B:66:GLU:HG3	1:B:251:LEU:HD22	1.88	0.54
1:A:271:ALA:O	1:A:275:VAL:HG23	2.07	0.54
1:B:339:ARG:HD2	1:B:632:ARG:HH12	1.71	0.54
1:A:160:GLU:HG3	1:A:169:TYR:HE2	1.72	0.54
1:B:160:GLU:HG3	1:B:169:TYR:HE2	1.72	0.54
1:B:254:ARG:O	1:B:254:ARG:HD3	2.07	0.54
1:B:377:ALA:N	1:B:461:ASN:HA	2.22	0.54
1:B:455:ILE:HG21	1:B:626:THR:OG1	2.08	0.54
1:A:254:ARG:O	1:A:254:ARG:HD3	2.08	0.54
1:B:345:TYR:CE1	1:B:472:SER:HB2	2.42	0.54
1:A:67:GLN:HE22	1:A:246:LEU:CD1	2.22	0.53
1:B:436:ALA:CA	1:B:437:LYS:HD2	2.37	0.53
1:B:477:ASP:OD1	1:B:479:ARG:HB2	2.08	0.53
1:A:375:ARG:HG2	1:A:407:ASP:HB2	1.90	0.53
1:B:375:ARG:CD	1:B:407:ASP:HB2	2.38	0.53
1:B:511:ARG:HD2	1:B:515:TYR:CZ	2.44	0.53
1:B:599:GLU:OE2	1:B:604:LYS:NZ	2.34	0.53
1:A:656:LYS:HG3	1:A:657:GLU:OE1	2.08	0.53
1:B:510:SER:HB3	1:B:618:ILE:HG23	1.90	0.53
1:B:665:ARG:HG2	1:B:665:ARG:HH11	1.72	0.53
1:A:375:ARG:CD	1:A:407:ASP:HB2	2.37	0.53
1:A:510:SER:HB3	1:A:618:ILE:HG23	1.89	0.53
1:A:533:ILE:HB	1:A:559:VAL:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:GLN:O	1:A:85:LEU:HG	2.09	0.53
1:B:39:LEU:HD11	1:B:98:LEU:HD12	1.91	0.53
1:B:338:GLU:HG3	1:B:339:ARG:HG3	1.91	0.53
1:B:587:ASP:HB3	1:B:674:GLN:CD	2.34	0.53
1:A:402:LEU:N	1:A:402:LEU:CD2	2.64	0.52
1:B:263:VAL:HA	1:B:289:VAL:O	2.09	0.52
1:A:61:ILE:HG23	1:A:73:SER:CB	2.39	0.52
1:B:239:MET:O	1:B:241:ALA:N	2.39	0.52
1:B:539:ASN:HD22	1:B:566:MET:HB2	1.74	0.52
1:B:628:LEU:CD1	1:B:637:VAL:HG21	2.39	0.52
1:A:375:ARG:CG	1:A:407:ASP:HB2	2.39	0.52
1:A:37:ARG:HA	1:A:300:PHE:O	2.10	0.52
1:B:61:ILE:HG23	1:B:73:SER:CB	2.39	0.52
1:B:247:MET:SD	1:B:251:LEU:HD23	2.49	0.52
1:A:455:ILE:HG21	1:A:626:THR:OG1	2.10	0.52
1:B:62:ILE:HA	1:B:65:GLU:OE1	2.09	0.52
1:B:284:ARG:NH1	1:B:284:ARG:HB2	2.25	0.52
1:B:436:ALA:C	1:B:437:LYS:CD	2.72	0.52
1:B:642:ASP:O	1:B:646:SER:HB3	2.10	0.52
1:A:123:LEU:HD22	1:A:202:ILE:HG23	1.92	0.52
1:B:12:LEU:HD22	1:B:83:ARG:HH11	1.70	0.52
1:A:587:ASP:HB3	1:A:674:GLN:CD	2.34	0.52
1:B:656:LYS:HG3	1:B:657:GLU:OE1	2.10	0.52
1:A:359:GLN:HB3	1:B:214:PHE:CZ	2.45	0.51
1:A:628:LEU:CD1	1:A:637:VAL:HG21	2.40	0.51
1:A:66:GLU:CG	1:A:251:LEU:HD22	2.40	0.51
1:A:284:ARG:HB2	1:A:284:ARG:NH1	2.25	0.51
1:A:405:ARG:HG2	1:A:433:LYS:HZ3	1.73	0.51
1:B:403:GLN:OE1	1:B:430:PRO:O	2.28	0.51
1:A:469:THR:O	1:A:470:ASP:OD2	2.28	0.51
1:B:67:GLN:HE22	1:B:246:LEU:CD1	2.23	0.51
1:A:665:ARG:HG2	1:A:665:ARG:HH11	1.74	0.51
1:B:639:ASP:O	1:B:642:ASP:HB2	2.11	0.51
1:A:239:MET:O	1:A:241:ALA:N	2.39	0.51
1:B:177:ASP:N	1:B:177:ASP:OD1	2.41	0.51
1:B:281:THR:O	1:B:281:THR:HG22	2.11	0.51
1:B:375:ARG:HD3	1:B:404:ALA:HB1	1.92	0.51
1:B:375:ARG:CG	1:B:407:ASP:HB2	2.40	0.51
1:B:672:ARG:HD3	1:B:675:LEU:HD12	1.91	0.51
1:A:23:GLN:OE1	1:A:652:ARG:HD3	2.11	0.51
1:A:263:VAL:HA	1:A:289:VAL:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:SER:OG	1:A:610:SER:N	2.43	0.51
1:A:247:MET:SD	1:A:251:LEU:HD23	2.51	0.51
1:B:117:VAL:HG12	1:B:117:VAL:O	2.11	0.51
1:A:628:LEU:HD11	1:A:637:VAL:HG21	1.92	0.51
1:A:111:ASN:CG	1:A:114:GLN:HG3	2.36	0.51
1:A:599:GLU:OE2	1:A:604:LYS:NZ	2.36	0.51
1:B:415:ALA:O	1:B:416:LYS:C	2.54	0.51
1:B:79:LYS:O	1:B:83:ARG:HD3	2.11	0.50
1:B:628:LEU:HD11	1:B:637:VAL:HG21	1.91	0.50
1:A:111:ASN:OD1	1:A:114:GLN:HG3	2.10	0.50
1:A:506:SER:HB2	1:A:623:GLU:HB2	1.94	0.50
1:B:194:LYS:HD2	1:B:306:VAL:CG1	2.42	0.50
1:A:103:ALA:HA	1:A:107:ILE:O	2.11	0.50
1:B:439:PHE:CD1	1:B:439:PHE:C	2.88	0.50
1:A:614:MET:HB2	1:A:617:ASN:HD22	1.77	0.50
1:A:672:ARG:HD3	1:A:675:LEU:HD12	1.91	0.50
1:B:609:SER:OG	1:B:610:SER:N	2.44	0.50
1:A:236:VAL:HG12	1:A:236:VAL:O	2.12	0.50
1:A:642:ASP:O	1:A:646:SER:HB3	2.12	0.50
1:B:375:ARG:HG2	1:B:407:ASP:HB2	1.92	0.50
1:B:614:MET:HB2	1:B:617:ASN:HD22	1.77	0.50
1:A:418:LEU:HB3	1:A:423:VAL:HB	1.94	0.50
1:A:39:LEU:HD22	1:A:91:PHE:CE1	2.47	0.50
1:A:639:ASP:O	1:A:642:ASP:HB2	2.11	0.50
1:B:73:SER:O	1:B:77:LEU:HD23	2.11	0.50
1:B:236:VAL:O	1:B:236:VAL:HG12	2.12	0.50
1:B:71:SER:O	1:B:73:SER:N	2.40	0.49
1:B:111:ASN:CG	1:B:114:GLN:HG3	2.37	0.49
1:B:233:TYR:CG	1:B:234:ASP:N	2.80	0.49
1:A:281:THR:HG22	1:A:281:THR:O	2.12	0.49
1:B:469:THR:O	1:B:470:ASP:OD2	2.30	0.49
1:A:194:LYS:HD2	1:A:306:VAL:CG1	2.42	0.49
1:B:355:GLU:O	1:B:359:GLN:HG3	2.11	0.49
1:B:434:ILE:HA	1:B:622:ILE:HB	1.94	0.49
1:B:457:THR:CG2	1:B:471:TYR:HB2	2.42	0.49
1:A:240:GLU:HB3	1:A:244:MET:HB2	1.94	0.49
1:A:393:GLY:O	1:A:394:LYS:C	2.56	0.49
1:A:439:PHE:CD1	1:A:439:PHE:C	2.90	0.49
1:A:479:ARG:NH1	1:A:629:LEU:HD13	2.27	0.49
1:B:161:ILE:HB	1:B:168:ARG:HB2	1.94	0.49
1:B:418:LEU:HB3	1:B:423:VAL:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ASN:O	1:B:106:GLN:HB2	2.13	0.49
1:B:367:LEU:O	1:B:394:LYS:HA	2.13	0.49
1:A:264:TYR:CE2	1:A:290:PRO:HB3	2.47	0.49
1:A:79:LYS:O	1:A:83:ARG:HD3	2.12	0.49
1:A:233:TYR:CG	1:A:234:ASP:N	2.80	0.49
1:A:540:LEU:CD2	1:A:561:LEU:HD13	2.42	0.49
1:B:61:ILE:HG23	1:B:73:SER:HB2	1.95	0.49
1:B:66:GLU:CG	1:B:251:LEU:HD22	2.43	0.49
1:B:400:VAL:HG23	1:B:400:VAL:O	2.13	0.49
1:B:666:GLY:C	1:B:668:ARG:H	2.21	0.49
1:B:4:GLU:O	1:B:5:LYS:C	2.56	0.49
1:B:111:ASN:OD1	1:B:114:GLN:HG3	2.13	0.49
1:A:117:VAL:HG12	1:A:117:VAL:O	2.13	0.49
1:A:344:TYR:N	1:A:348:HIS:HD2	1.94	0.49
1:A:415:ALA:O	1:A:416:LYS:C	2.56	0.49
1:A:457:THR:CG2	1:A:471:TYR:HB2	2.43	0.49
1:B:405:ARG:HH22	1:B:616:ARG:HE	1.60	0.49
1:B:413:HIS:O	1:B:415:ALA:N	2.41	0.48
1:A:161:ILE:HB	1:A:168:ARG:HB2	1.96	0.48
1:B:240:GLU:HB3	1:B:244:MET:HB2	1.94	0.48
1:A:429:ALA:O	1:A:430:PRO:C	2.57	0.48
1:A:479:ARG:HG2	1:A:502:TYR:OH	2.14	0.48
1:B:103:ALA:HA	1:B:107:ILE:O	2.13	0.48
1:B:648:THR:HG22	1:B:668:ARG:HH21	1.79	0.48
1:A:4:GLU:O	1:A:5:LYS:C	2.56	0.48
1:B:61:ILE:CG2	1:B:73:SER:HB2	2.43	0.48
1:B:233:TYR:CD1	1:B:234:ASP:N	2.82	0.48
1:B:306:VAL:HG12	1:B:306:VAL:O	2.13	0.48
1:A:61:ILE:CG2	1:A:73:SER:HB2	2.44	0.48
1:A:158:ALA:HA	1:A:171:LEU:HD23	1.96	0.48
1:A:177:ASP:OD1	1:A:177:ASP:N	2.41	0.48
1:B:374:TYR:CD2	1:B:437:LYS:NZ	2.82	0.48
1:B:401:GLU:HA	1:B:428:SER:HB3	1.96	0.48
1:B:451:ARG:HB2	1:B:481:THR:CG2	2.43	0.48
1:A:12:LEU:HD22	1:A:83:ARG:HH11	1.70	0.48
1:A:403:GLN:OE1	1:A:430:PRO:O	2.31	0.48
1:A:405:ARG:HH22	1:A:616:ARG:HE	1.59	0.48
1:B:468:TYR:HD2	1:B:592:HIS:CG	2.32	0.48
1:A:36:MET:O	1:A:39:LEU:HB2	2.14	0.48
1:B:538:ASN:HB2	1:B:612:ASP:OD1	2.14	0.48
1:B:539:ASN:ND2	1:B:566:MET:HE3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:ARG:HG2	1:A:548:ARG:NH1	2.12	0.48
1:B:81:GLN:O	1:B:81:GLN:HG2	2.14	0.48
1:A:73:SER:O	1:A:77:LEU:HD23	2.13	0.47
1:A:214:PHE:CZ	1:B:359:GLN:HB3	2.49	0.47
1:B:461:ASN:OD1	1:B:463:LYS:HB2	2.14	0.47
1:B:536:LYS:NZ	1:B:591:GLU:OE1	2.42	0.47
1:A:401:GLU:HA	1:A:428:SER:HB3	1.97	0.47
1:B:39:LEU:HD22	1:B:91:PHE:CE1	2.50	0.47
1:A:375:ARG:HD3	1:A:404:ALA:HB1	1.95	0.47
1:B:194:LYS:HD2	1:B:306:VAL:HG11	1.95	0.47
1:A:233:TYR:CD1	1:A:234:ASP:N	2.82	0.47
1:A:511:ARG:HD2	1:A:515:TYR:CZ	2.50	0.47
1:A:389:ALA:HB1	1:A:394:LYS:HG3	1.96	0.47
1:B:301:ILE:HG22	1:B:301:ILE:O	2.14	0.47
1:A:39:LEU:HD11	1:A:98:LEU:HD12	1.96	0.47
1:A:461:ASN:OD1	1:A:463:LYS:HB2	2.15	0.47
1:A:539:ASN:ND2	1:A:566:MET:HE3	2.30	0.47
1:A:71:SER:O	1:A:73:SER:N	2.41	0.47
1:A:400:VAL:HG23	1:A:400:VAL:O	2.14	0.47
1:A:415:ALA:C	1:A:417:ARG:N	2.73	0.47
1:A:539:ASN:HD22	1:A:566:MET:HB2	1.80	0.47
1:B:207:LEU:HD11	1:B:222:ALA:CB	2.42	0.47
1:B:344:TYR:N	1:B:348:HIS:HD2	1.95	0.47
1:B:393:GLY:O	1:B:394:LYS:C	2.57	0.47
1:A:557:VAL:HA	1:A:558:PRO:HD3	1.73	0.47
1:B:120:GLN:O	1:B:124:ARG:HG3	2.14	0.47
1:B:415:ALA:C	1:B:417:ARG:N	2.72	0.47
1:A:538:ASN:HB2	1:A:612:ASP:OD1	2.15	0.47
1:B:23:GLN:OE1	1:B:652:ARG:HD3	2.14	0.47
1:B:405:ARG:HH21	1:B:616:ARG:HD2	1.80	0.47
1:A:194:LYS:HD2	1:A:306:VAL:HG11	1.96	0.47
1:A:207:LEU:HD11	1:A:222:ALA:CB	2.42	0.47
1:A:648:THR:HG22	1:A:668:ARG:HH21	1.79	0.47
1:A:666:GLY:C	1:A:668:ARG:H	2.21	0.46
1:B:548:ARG:CG	1:B:548:ARG:NH1	2.75	0.46
1:A:105:ASN:O	1:A:106:GLN:HB2	2.16	0.46
1:A:511:ARG:NH1	1:A:542:ASP:OD1	2.44	0.46
1:B:285:TYR:N	1:B:285:TYR:CD1	2.83	0.46
1:B:540:LEU:CD2	1:B:561:LEU:HD13	2.45	0.46
1:A:413:HIS:O	1:A:415:ALA:N	2.39	0.46
1:A:11:GLU:HG2	1:A:57:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LYS:O	1:A:310:ASN:N	2.49	0.46
1:A:374:TYR:CG	1:A:375:ARG:N	2.82	0.46
1:B:363:ASP:OD2	1:B:443:ARG:NH1	2.45	0.46
1:B:415:ALA:O	1:B:417:ARG:N	2.47	0.46
1:A:61:ILE:HG23	1:A:73:SER:HB2	1.97	0.46
1:A:416:LYS:H	1:A:416:LYS:HG2	1.61	0.46
1:B:18:ASN:O	1:B:21:VAL:HB	2.16	0.46
1:B:374:TYR:CG	1:B:375:ARG:N	2.83	0.46
1:B:429:ALA:O	1:B:430:PRO:C	2.59	0.46
1:A:18:ASN:O	1:A:21:VAL:HB	2.16	0.46
1:A:318:ARG:NH1	1:A:466:ARG:HG2	2.30	0.46
1:A:477:ASP:OD2	1:A:479:ARG:NH2	2.48	0.46
1:B:261:ARG:HG2	1:B:287:SER:HB3	1.98	0.46
1:B:570:ILE:HG22	1:B:573:LEU:HG	1.96	0.46
1:A:363:ASP:O	1:A:394:LYS:NZ	2.48	0.46
1:A:415:ALA:O	1:A:417:ARG:N	2.48	0.46
1:B:345:TYR:O	1:B:469:THR:HA	2.15	0.46
1:B:128:LYS:HG2	1:B:132:ARG:HH21	1.81	0.46
1:B:506:SER:HA	1:B:507:PRO:HA	1.72	0.46
1:A:405:ARG:NH2	1:A:616:ARG:HE	2.14	0.45
1:A:405:ARG:NH2	1:A:616:ARG:NE	2.64	0.45
1:B:405:ARG:NH2	1:B:616:ARG:NE	2.64	0.45
1:A:374:TYR:CD2	1:A:437:LYS:NZ	2.84	0.45
1:A:405:ARG:HH21	1:A:616:ARG:HD2	1.81	0.45
1:B:64:SER:CB	1:B:69:SER:HA	2.46	0.45
1:B:83:ARG:HH11	1:B:83:ARG:HG2	1.81	0.45
1:B:158:ALA:HA	1:B:171:LEU:HD23	1.97	0.45
1:B:470:ASP:OD1	1:B:592:HIS:HB3	2.16	0.45
1:A:644:LEU:HD23	1:A:673:ALA:CB	2.46	0.45
1:B:264:TYR:CE2	1:B:290:PRO:HB3	2.51	0.45
1:B:405:ARG:NH2	1:B:616:ARG:HE	2.14	0.45
1:A:66:GLU:HB2	1:A:251:LEU:HD22	1.99	0.45
1:B:145:ASP:O	1:B:146:LEU:C	2.59	0.45
1:A:306:VAL:O	1:A:306:VAL:HG12	2.16	0.45
1:B:116:SER:C	1:B:118:ASN:N	2.75	0.45
1:B:548:ARG:HG2	1:B:548:ARG:NH1	2.14	0.45
1:A:265:GLN:HG3	1:A:292:GLY:O	2.17	0.45
1:B:36:MET:O	1:B:39:LEU:HB2	2.16	0.45
1:B:190:PRO:HG2	1:B:193:ARG:HD2	1.98	0.45
1:B:592:HIS:HD2	1:B:594:ARG:HH22	1.65	0.45
1:A:145:ASP:CG	1:A:145:ASP:O	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:TYR:O	1:A:469:THR:HA	2.17	0.45
1:A:522:ILE:HG23	1:A:555:SER:CB	2.46	0.45
1:A:405:ARG:HG2	1:A:433:LYS:HZ2	1.81	0.45
1:B:451:ARG:HG2	1:B:451:ARG:HH11	1.81	0.45
1:B:510:SER:O	1:B:511:ARG:C	2.59	0.45
1:B:533:ILE:O	1:B:559:VAL:HA	2.17	0.45
1:A:64:SER:CB	1:A:69:SER:HA	2.47	0.45
1:B:11:GLU:HG2	1:B:57:LEU:HD22	1.98	0.45
1:B:146:LEU:O	1:B:147:VAL:C	2.59	0.45
1:A:451:ARG:HB2	1:A:481:THR:CG2	2.46	0.44
1:B:477:ASP:OD2	1:B:479:ARG:NH2	2.49	0.44
1:A:451:ARG:HH11	1:A:451:ARG:HG2	1.81	0.44
1:B:22:LEU:HG	1:B:42:TYR:CE1	2.53	0.44
1:B:308:LYS:O	1:B:310:ASN:N	2.50	0.44
1:B:339:ARG:HE	1:B:339:ARG:HB3	1.44	0.44
1:B:341:VAL:HG12	1:B:343:LEU:HD13	1.99	0.44
1:A:32:LEU:HD13	1:A:101:GLU:CD	2.42	0.44
1:A:190:PRO:HG2	1:A:193:ARG:HD2	1.99	0.44
1:A:83:ARG:HH11	1:A:83:ARG:HG2	1.81	0.44
1:A:150:LEU:HD22	1:A:280:LEU:HD21	1.98	0.44
1:A:262:PHE:HD2	1:A:288:ILE:CG2	2.31	0.44
1:A:506:SER:HA	1:A:507:PRO:HA	1.70	0.44
1:B:206:CYS:O	1:B:207:LEU:C	2.61	0.44
1:B:389:ALA:HB1	1:B:394:LYS:HG3	1.98	0.44
1:B:594:ARG:HD3	1:B:612:ASP:CG	2.42	0.44
1:A:302:ASN:O	1:A:303:PHE:C	2.61	0.44
1:A:367:LEU:O	1:A:394:LYS:HA	2.18	0.44
1:A:533:ILE:O	1:A:559:VAL:HA	2.17	0.44
1:A:599:GLU:HG3	1:A:601:GLY:O	2.16	0.44
1:B:302:ASN:O	1:B:303:PHE:C	2.59	0.44
1:B:318:ARG:NH1	1:B:466:ARG:HG2	2.32	0.44
1:A:145:ASP:O	1:A:146:LEU:C	2.60	0.44
1:A:266:ARG:HG2	1:A:291:GLY:HA2	2.00	0.44
1:A:285:TYR:N	1:A:285:TYR:CD1	2.83	0.44
1:A:434:ILE:HA	1:A:622:ILE:HB	1.99	0.44
1:B:32:LEU:HD21	1:B:102:MET:HA	2.00	0.44
1:B:64:SER:HB3	1:B:69:SER:CB	2.44	0.44
1:A:341:VAL:HG12	1:A:343:LEU:HD13	2.00	0.44
1:A:363:ASP:OD2	1:A:443:ARG:NH1	2.49	0.44
1:A:377:ALA:HB2	1:A:462:GLU:N	2.32	0.44
1:A:481:THR:HG22	1:A:482:ASN:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:PHE:HD2	1:B:288:ILE:CG2	2.31	0.44
1:B:377:ALA:HB2	1:B:462:GLU:N	2.33	0.44
1:A:120:GLN:O	1:A:124:ARG:HG3	2.18	0.44
1:A:470:ASP:OD1	1:A:592:HIS:HB3	2.18	0.44
1:B:50:TYR:OH	1:B:84:VAL:HG11	2.18	0.44
1:A:230:ASP:OD1	1:A:259:PRO:HG2	2.18	0.43
1:A:536:LYS:NZ	1:A:591:GLU:OE1	2.45	0.43
1:B:324:PHE:CE1	1:B:341:VAL:HG11	2.53	0.43
1:B:599:GLU:HG3	1:B:601:GLY:O	2.18	0.43
1:B:653:TYR:CE1	1:B:664:PRO:HD3	2.53	0.43
1:A:50:TYR:OH	1:A:84:VAL:HG11	2.18	0.43
1:A:284:ARG:HG3	1:A:285:TYR:CD1	2.34	0.43
1:A:541:VAL:O	1:A:542:ASP:C	2.61	0.43
1:B:67:GLN:HE22	1:B:246:LEU:HD13	1.83	0.43
1:B:265:GLN:HG3	1:B:292:GLY:O	2.19	0.43
1:B:541:VAL:O	1:B:542:ASP:C	2.61	0.43
1:A:67:GLN:HE22	1:A:246:LEU:HD13	1.82	0.43
1:B:457:THR:HG21	1:B:471:TYR:HB2	2.00	0.43
1:B:480:ILE:O	1:B:484:VAL:HG23	2.18	0.43
1:A:33:ILE:HB	1:A:311:LEU:O	2.18	0.43
1:A:81:GLN:O	1:A:81:GLN:HG2	2.18	0.43
1:A:206:CYS:O	1:A:207:LEU:C	2.61	0.43
1:B:150:LEU:HD22	1:B:280:LEU:HD21	2.00	0.43
1:B:325:ASP:O	1:B:326:LYS:C	2.61	0.43
1:B:408:GLU:C	1:B:410:ALA:H	2.26	0.43
1:B:437:LYS:HB3	1:B:460:PHE:CD1	2.53	0.43
1:A:261:ARG:HG2	1:A:287:SER:HB3	1.98	0.43
1:A:548:ARG:CG	1:A:548:ARG:NH1	2.73	0.43
1:B:181:ARG:O	1:B:198:LEU:HD23	2.19	0.43
1:B:266:ARG:HG2	1:B:291:GLY:HA2	2.01	0.43
1:B:644:LEU:HD23	1:B:673:ALA:CB	2.46	0.43
1:A:324:PHE:CE1	1:A:341:VAL:HG11	2.54	0.43
1:A:325:ASP:O	1:A:326:LYS:C	2.61	0.43
1:A:344:TYR:HE2	1:A:593:ASP:OD1	2.01	0.43
1:B:594:ARG:HH11	1:B:612:ASP:CG	2.26	0.43
1:A:128:LYS:HG2	1:A:132:ARG:HH21	1.84	0.43
1:A:408:GLU:C	1:A:410:ALA:H	2.25	0.43
1:B:145:ASP:O	1:B:145:ASP:CG	2.61	0.43
1:B:295:HIS:O	1:B:296:ASN:HB2	2.19	0.43
1:B:522:ILE:HG23	1:B:555:SER:CB	2.49	0.43
1:A:35:ARG:HH22	1:A:101:GLU:CD	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLU:HG3	1:A:169:TYR:CE2	2.54	0.43
1:A:339:ARG:HE	1:A:339:ARG:HB3	1.46	0.43
1:A:672:ARG:O	1:A:673:ALA:C	2.62	0.43
1:B:123:LEU:HD22	1:B:202:ILE:HG23	2.00	0.43
1:B:479:ARG:HG2	1:B:502:TYR:OH	2.18	0.43
1:A:54:PHE:CD2	1:A:58:LYS:HE3	2.54	0.43
1:A:363:ASP:HB2	1:B:214:PHE:CD2	2.54	0.43
1:A:374:TYR:HD1	1:A:401:GLU:CD	2.26	0.43
1:A:653:TYR:CE1	1:A:664:PRO:HD3	2.54	0.43
1:B:66:GLU:HB2	1:B:251:LEU:HD22	2.00	0.43
1:B:308:LYS:HB2	1:B:310:ASN:ND2	2.33	0.43
1:B:353:VAL:HG13	1:B:439:PHE:HE2	1.84	0.43
1:B:451:ARG:HB2	1:B:481:THR:HG21	2.01	0.43
1:B:537:LEU:O	1:B:563:VAL:HA	2.18	0.43
1:A:32:LEU:HD21	1:A:102:MET:HA	2.01	0.42
1:B:17:PHE:HA	1:B:20:ARG:NH2	2.34	0.42
1:B:512:ARG:O	1:B:516:GLU:HG3	2.19	0.42
1:A:147:VAL:HG22	1:A:279:LYS:O	2.19	0.42
1:B:323:TRP:CH2	1:B:339:ARG:HD3	2.55	0.42
1:B:374:TYR:HD1	1:B:401:GLU:CD	2.27	0.42
1:A:181:ARG:O	1:A:198:LEU:HD23	2.20	0.42
1:B:32:LEU:HD13	1:B:101:GLU:CD	2.42	0.42
1:A:146:LEU:O	1:A:147:VAL:C	2.61	0.42
1:B:656:LYS:HB2	1:B:656:LYS:HE2	1.79	0.42
1:A:233:TYR:HE1	1:A:236:VAL:HB	1.85	0.42
1:A:312:VAL:HG12	1:A:313:ASN:N	2.35	0.42
1:A:429:ALA:O	1:A:430:PRO:O	2.38	0.42
1:B:64:SER:O	1:B:69:SER:N	2.53	0.42
1:B:233:TYR:HE1	1:B:236:VAL:HB	1.85	0.42
1:B:253:GLN:NE2	1:B:253:GLN:C	2.77	0.42
1:B:525:ALA:HB2	1:B:557:VAL:HG22	2.01	0.42
1:A:131:LEU:O	1:A:132:ARG:C	2.62	0.42
1:B:131:LEU:O	1:B:132:ARG:C	2.62	0.42
1:B:479:ARG:NH1	1:B:629:LEU:HD13	2.34	0.42
1:B:511:ARG:NH1	1:B:542:ASP:OD1	2.45	0.42
1:B:561:LEU:HB2	1:B:582:ALA:CB	2.49	0.42
1:A:22:LEU:HG	1:A:42:TYR:CE1	2.55	0.42
1:A:570:ILE:HG22	1:A:573:LEU:HG	2.02	0.42
1:A:64:SER:O	1:A:69:SER:N	2.53	0.41
1:B:200:ASP:OD2	1:B:200:ASP:N	2.53	0.41
1:A:656:LYS:HB2	1:A:656:LYS:HE2	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LEU:HG	1:B:42:TYR:CD1	2.55	0.41
1:B:147:VAL:HG22	1:B:279:LYS:O	2.20	0.41
1:B:342:LEU:HB3	1:B:633:LEU:HD22	2.02	0.41
1:A:253:GLN:C	1:A:253:GLN:NE2	2.78	0.41
1:B:160:GLU:HG3	1:B:169:TYR:CE2	2.54	0.41
1:B:437:LYS:CE	1:B:458:GLY:C	2.82	0.41
1:A:265:GLN:HG3	1:A:293:ARG:HA	2.02	0.41
1:A:342:LEU:HB3	1:A:633:LEU:HD22	2.03	0.41
1:B:54:PHE:CD2	1:B:58:LYS:HE3	2.54	0.41
1:B:386:MET:HE2	1:B:386:MET:N	2.35	0.41
1:B:441:ILE:O	1:B:451:ARG:HA	2.20	0.41
1:B:609:SER:HA	1:B:625:ALA:HA	2.01	0.41
1:A:64:SER:C	1:A:69:SER:HB3	2.46	0.41
1:A:345:TYR:HE1	1:A:472:SER:HB2	1.86	0.41
1:A:437:LYS:HB3	1:A:460:PHE:CD1	2.55	0.41
1:B:481:THR:HG22	1:B:482:ASN:N	2.35	0.41
1:B:535:LEU:HD11	1:B:613:TRP:CH2	2.55	0.41
1:A:378:LYS:HE2	1:A:378:LYS:HB3	1.92	0.41
1:B:64:SER:C	1:B:69:SER:HB3	2.45	0.41
1:B:127:PHE:CD1	1:B:127:PHE:C	2.98	0.41
1:B:561:LEU:HB2	1:B:582:ALA:HB2	2.03	0.41
1:A:27:ASP:CG	1:A:29:SER:HG	2.28	0.41
1:A:655:ASP:C	1:A:657:GLU:H	2.28	0.41
1:B:95:TYR:O	1:B:99:LEU:HG	2.19	0.41
1:B:156:TYR:CE2	1:B:173:GLU:HB2	2.55	0.41
1:B:375:ARG:HD2	1:B:407:ASP:HB2	2.03	0.41
1:B:655:ASP:C	1:B:657:GLU:H	2.28	0.41
1:A:148:GLN:O	1:A:150:LEU:N	2.53	0.41
1:A:510:SER:O	1:A:511:ARG:C	2.64	0.41
1:B:540:LEU:HD23	1:B:561:LEU:HD13	2.03	0.41
1:A:240:GLU:HB3	1:A:244:MET:CB	2.51	0.41
1:A:281:THR:O	1:A:283:SER:N	2.54	0.41
1:A:413:HIS:C	1:A:415:ALA:H	2.28	0.41
1:A:457:THR:HG21	1:A:471:TYR:HB2	2.02	0.41
1:A:525:ALA:C	1:A:527:GLN:H	2.28	0.41
1:B:281:THR:O	1:B:283:SER:N	2.54	0.41
1:B:346:PRO:HD2	1:B:469:THR:HG22	2.01	0.41
1:A:26:ALA:HA	1:A:94:LEU:HD21	2.03	0.41
1:A:514:LEU:O	1:A:515:TYR:C	2.63	0.41
1:A:535:LEU:HD11	1:A:613:TRP:CH2	2.55	0.41
1:B:33:ILE:HB	1:B:311:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:TYR:CE1	1:B:682:LYS:HD3	2.57	0.41
1:A:67:GLN:HE22	1:A:246:LEU:HD12	1.86	0.40
1:B:148:GLN:O	1:B:150:LEU:N	2.54	0.40
1:B:375:ARG:CD	1:B:404:ALA:HB1	2.51	0.40
1:B:506:SER:HB2	1:B:623:GLU:CB	2.52	0.40
1:A:157:LEU:HA	1:A:157:LEU:HD12	1.87	0.40
1:A:229:ARG:HE	1:A:258:GLU:HG3	1.86	0.40
1:A:308:LYS:HB2	1:A:310:ASN:ND2	2.36	0.40
1:A:346:PRO:HD2	1:A:469:THR:HG22	2.04	0.40
1:B:416:LYS:H	1:B:416:LYS:HG2	1.59	0.40
1:A:107:ILE:C	1:A:108:PHE:CD1	2.99	0.40
1:B:64:SER:O	1:B:68:GLY:C	2.64	0.40
1:B:194:LYS:CE	1:B:306:VAL:HG12	2.51	0.40
1:B:525:ALA:C	1:B:527:GLN:H	2.29	0.40
1:A:479:ARG:HG2	1:A:502:TYR:CZ	2.56	0.40
1:A:663:VAL:HA	1:A:664:PRO:HD3	1.87	0.40
1:A:678:TYR:CZ	1:A:682:LYS:HD3	2.57	0.40
1:B:230:ASP:OD1	1:B:259:PRO:HG2	2.21	0.40
1:B:520:ARG:HB2	1:B:520:ARG:NH1	2.36	0.40
1:A:353:VAL:HG13	1:A:439:PHE:HE2	1.86	0.40
1:A:375:ARG:HD2	1:A:407:ASP:HB2	2.04	0.40
1:B:630:ASP:C	1:B:630:ASP:OD2	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	685/687 (100%)	585 (85%)	73 (11%)	27 (4%)	2	14
1	B	685/687 (100%)	582 (85%)	77 (11%)	26 (4%)	2	15
All	All	1370/1374 (100%)	1167 (85%)	150 (11%)	53 (4%)	2	14

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	GLU
1	A	66	GLU
1	A	234	ASP
1	A	241	ALA
1	A	394	LYS
1	A	414	TRP
1	A	430	PRO
1	B	65	GLU
1	B	66	GLU
1	B	241	ALA
1	B	394	LYS
1	B	414	TRP
1	B	430	PRO
1	A	117	VAL
1	A	147	VAL
1	A	149	PHE
1	A	188	GLU
1	A	189	ALA
1	A	309	ALA
1	A	510	SER
1	B	117	VAL
1	B	147	VAL
1	B	149	PHE
1	B	188	GLU
1	B	189	ALA
1	B	234	ASP
1	B	309	ALA
1	A	281	THR
1	A	446	ASN
1	B	281	THR
1	B	446	ASN
1	B	510	SER
1	A	5	LYS
1	A	148	GLN
1	A	240	GLU
1	A	282	ILE
1	A	416	LYS
1	A	574	GLU
1	B	5	LYS
1	B	240	GLU
1	B	282	ILE
1	B	416	LYS

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Mol	Chain	Res	Type
1	B	574	GLU
1	A	429	ALA
1	A	674	GLN
1	B	72	HIS
1	B	148	GLN
1	B	322	ILE
1	B	429	ALA
1	A	673	ALA
1	A	322	ILE
1	A	666	GLY
1	B	666	GLY

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	566/619 (91%)	526 (93%)	40 (7%)	13	43
1	B	566/619 (91%)	528 (93%)	38 (7%)	15	46
All	All	1132/1238 (91%)	1054 (93%)	78 (7%)	14	45

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	47	ASP
1	A	64	SER
1	A	66	GLU
1	A	69	SER
1	A	72	HIS
1	A	153	ASP
1	A	157	LEU
1	A	177	ASP
1	A	225	MET
1	A	233	TYR
1	A	255	LEU

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Mol	Chain	Res	Type
1	A	265	GLN
1	A	272	LEU
1	A	277	ARG
1	A	299	ASP
1	A	314	LYS
1	A	316	LEU
1	A	343	LEU
1	A	349	THR
1	A	356	LEU
1	A	402	LEU
1	A	406	PHE
1	A	414	TRP
1	A	416	LYS
1	A	417	ARG
1	A	428	SER
1	A	437	LYS
1	A	462	GLU
1	A	464	THR
1	A	481	THR
1	A	486	ARG
1	A	548	ARG
1	A	564	ARG
1	A	595	VAL
1	A	616	ARG
1	A	646	SER
1	A	656	LYS
1	A	668	ARG
1	A	675	LEU
1	B	22	LEU
1	B	47	ASP
1	B	64	SER
1	B	66	GLU
1	B	69	SER
1	B	72	HIS
1	B	153	ASP
1	B	157	LEU
1	B	177	ASP
1	B	225	MET
1	B	233	TYR
1	B	255	LEU
1	B	265	GLN
1	B	272	LEU

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Mol	Chain	Res	Type
1	B	277	ARG
1	B	285	TYR
1	B	299	ASP
1	B	314	LYS
1	B	316	LEU
1	B	343	LEU
1	B	349	THR
1	B	356	LEU
1	B	402	LEU
1	B	406	PHE
1	B	414	TRP
1	B	416	LYS
1	B	417	ARG
1	B	428	SER
1	B	437	LYS
1	B	462	GLU
1	B	464	THR
1	B	481	THR
1	B	486	ARG
1	B	548	ARG
1	B	564	ARG
1	B	616	ARG
1	B	656	LYS
1	B	675	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	70	ASN
1	A	72	HIS
1	A	75	HIS
1	A	114	GLN
1	A	120	GLN
1	A	253	GLN
1	A	265	GLN
1	A	270	ASN
1	A	310	ASN
1	A	348	HIS
1	A	459	ASN
1	A	526	GLN
1	A	527	GLN

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Mol	Chain	Res	Type
1	A	539	ASN
1	A	560	ASN
1	A	617	ASN
1	B	67	GLN
1	B	70	ASN
1	B	72	HIS
1	B	75	HIS
1	B	114	GLN
1	B	120	GLN
1	B	253	GLN
1	B	265	GLN
1	B	270	ASN
1	B	310	ASN
1	B	348	HIS
1	B	459	ASN
1	B	526	GLN
1	B	527	GLN
1	B	539	ASN
1	B	560	ASN
1	B	617	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	687/687 (100%)	0.62	84 (12%) 8 5	7, 35, 95, 135	0
1	B	687/687 (100%)	0.66	88 (12%) 7 5	12, 35, 97, 133	0
All	All	1374/1374 (100%)	0.64	172 (12%) 8 5	7, 35, 97, 135	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	465	ALA	8.7
1	A	412	ILE	8.6
1	A	410	ALA	8.5
1	B	465	ALA	8.1
1	A	69	SER	6.7
1	A	376	VAL	6.5
1	A	464	THR	6.2
1	A	73	SER	6.1
1	B	412	ILE	6.1
1	B	376	VAL	6.1
1	A	66	GLU	6.0
1	A	242	SER	5.9
1	B	464	THR	5.5
1	A	71	SER	5.4
1	B	73	SER	5.2
1	B	2	GLY	5.1
1	A	411	ASN	5.1
1	B	410	ALA	5.0
1	B	69	SER	4.9
1	B	415	ALA	4.9
1	B	66	GLU	4.9
1	B	242	SER	4.8
1	B	406	PHE	4.8
1	B	457	THR	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	246	LEU	4.7
1	B	430	PRO	4.6
1	B	243	LEU	4.5
1	B	236	VAL	4.4
1	A	406	PHE	4.4
1	A	375	ARG	4.4
1	A	67	GLN	4.3
1	A	374	TYR	4.3
1	B	461	ASN	4.2
1	A	461	ASN	4.2
1	B	407	ASP	4.2
1	A	241	ALA	4.2
1	B	405	ARG	4.1
1	B	374	TYR	4.1
1	A	243	LEU	4.1
1	A	74	ARG	4.1
1	A	408	GLU	4.0
1	B	409	GLU	4.0
1	A	190	PRO	4.0
1	B	463	LYS	4.0
1	B	67	GLN	4.0
1	B	241	ALA	3.9
1	A	245	GLU	3.9
1	B	459	ASN	3.8
1	A	72	HIS	3.8
1	B	72	HIS	3.8
1	A	467	LEU	3.8
1	B	315	PRO	3.8
1	B	411	ASN	3.7
1	B	413	HIS	3.7
1	A	405	ARG	3.7
1	A	65	GLU	3.6
1	B	375	ARG	3.6
1	A	189	ALA	3.6
1	A	404	ALA	3.5
1	B	235	LEU	3.5
1	B	378	LYS	3.5
1	B	285	TYR	3.5
1	A	235	LEU	3.5
1	B	71	SER	3.5
1	B	65	GLU	3.4
1	A	285	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	233	TYR	3.4
1	A	377	ALA	3.4
1	A	407	ASP	3.4
1	A	246	LEU	3.4
1	A	430	PRO	3.4
1	B	403	GLN	3.4
1	A	459	ASN	3.3
1	B	470	ASP	3.2
1	A	68	GLY	3.2
1	A	253	GLN	3.2
1	B	233	TYR	3.2
1	A	247	MET	3.2
1	B	74	ARG	3.2
1	B	377	ALA	3.2
1	B	250	SER	3.1
1	B	189	ALA	3.1
1	A	250	SER	3.1
1	A	236	VAL	3.1
1	B	252	LYS	3.1
1	A	75	HIS	3.1
1	B	467	LEU	3.1
1	A	70	ASN	3.1
1	A	192	ARG	3.1
1	B	458	GLY	3.0
1	B	402	LEU	3.0
1	A	413	HIS	3.0
1	B	253	GLN	3.0
1	B	466	ARG	3.0
1	A	254	ARG	3.0
1	A	234	ASP	3.0
1	B	3	GLN	3.0
1	A	249	SER	3.0
1	A	237	HIS	2.9
1	B	314	LYS	2.9
1	A	403	GLN	2.9
1	B	414	TRP	2.9
1	A	238	GLU	2.9
1	B	68	GLY	2.9
1	B	404	ALA	2.8
1	B	190	PRO	2.8
1	A	281	THR	2.8
1	A	688	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	462	GLU	2.8
1	B	234	ASP	2.7
1	B	408	GLU	2.7
1	B	416	LYS	2.7
1	A	257	ALA	2.7
1	B	75	HIS	2.7
1	A	460	PHE	2.7
1	B	238	GLU	2.7
1	B	249	SER	2.7
1	B	147	VAL	2.7
1	A	402	LEU	2.7
1	A	252	LYS	2.7
1	A	414	TRP	2.7
1	A	292	GLY	2.6
1	B	471	TYR	2.6
1	A	251	LEU	2.6
1	A	470	ASP	2.6
1	B	310	ASN	2.6
1	B	125	HIS	2.6
1	B	239	MET	2.5
1	B	245	GLU	2.5
1	B	251	LEU	2.5
1	B	248	SER	2.5
1	A	463	LYS	2.5
1	B	254	ARG	2.5
1	B	316	LEU	2.5
1	B	256	THR	2.5
1	A	378	LYS	2.5
1	A	248	SER	2.4
1	B	247	MET	2.4
1	B	257	ALA	2.4
1	A	416	LYS	2.4
1	A	188	GLU	2.4
1	A	229	ARG	2.4
1	B	283	SER	2.4
1	A	284	ARG	2.4
1	A	291	GLY	2.4
1	A	687	PRO	2.4
1	B	592	HIS	2.3
1	A	457	THR	2.3
1	B	70	ASN	2.3
1	A	239	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	471	TYR	2.2
1	B	291	GLY	2.2
1	A	409	GLU	2.2
1	A	373	ILE	2.2
1	A	244	MET	2.2
1	A	231	ALA	2.2
1	B	90	GLU	2.2
1	A	230	ASP	2.2
1	B	501	ASP	2.2
1	B	379	ASP	2.1
1	A	63	ILE	2.1
1	A	417	ARG	2.1
1	B	284	ARG	2.1
1	B	417	ARG	2.1
1	A	530	PRO	2.1
1	A	117	VAL	2.1
1	B	462	GLU	2.1
1	A	380	SER	2.1
1	B	181	ARG	2.1
1	B	380	SER	2.0
1	B	149	PHE	2.0
1	B	89	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.