



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:09 AM UTC

PDB ID : 1XDV / pdb_00001xdv
Title : Experimentally Phased Structure of Human the Son of Sevenless protein at 4.1 Ang.
Authors : Sondermann, H.; Soisson, S.M.; Boykevisch, S.; Yang, S.S.; Bar-Sagi, D.; Kuriyan, J.
Deposited on : 2004-09-08
Resolution : 4.10 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

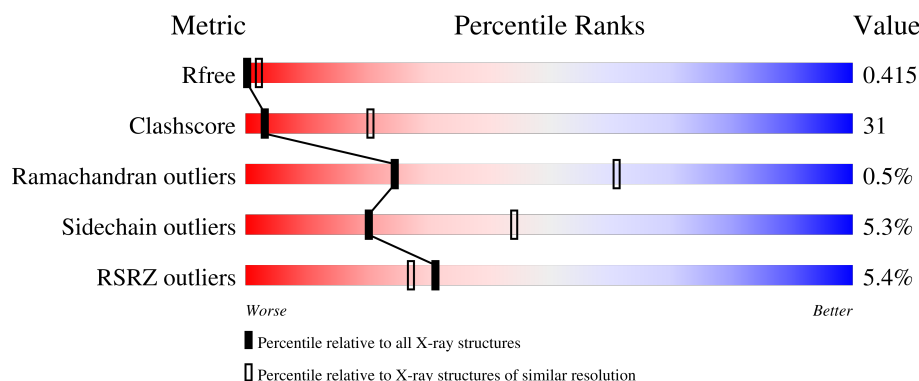
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	847	5% 57% 29% • 11%
1	B	847	4% 55% 30% • 10%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12516 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.

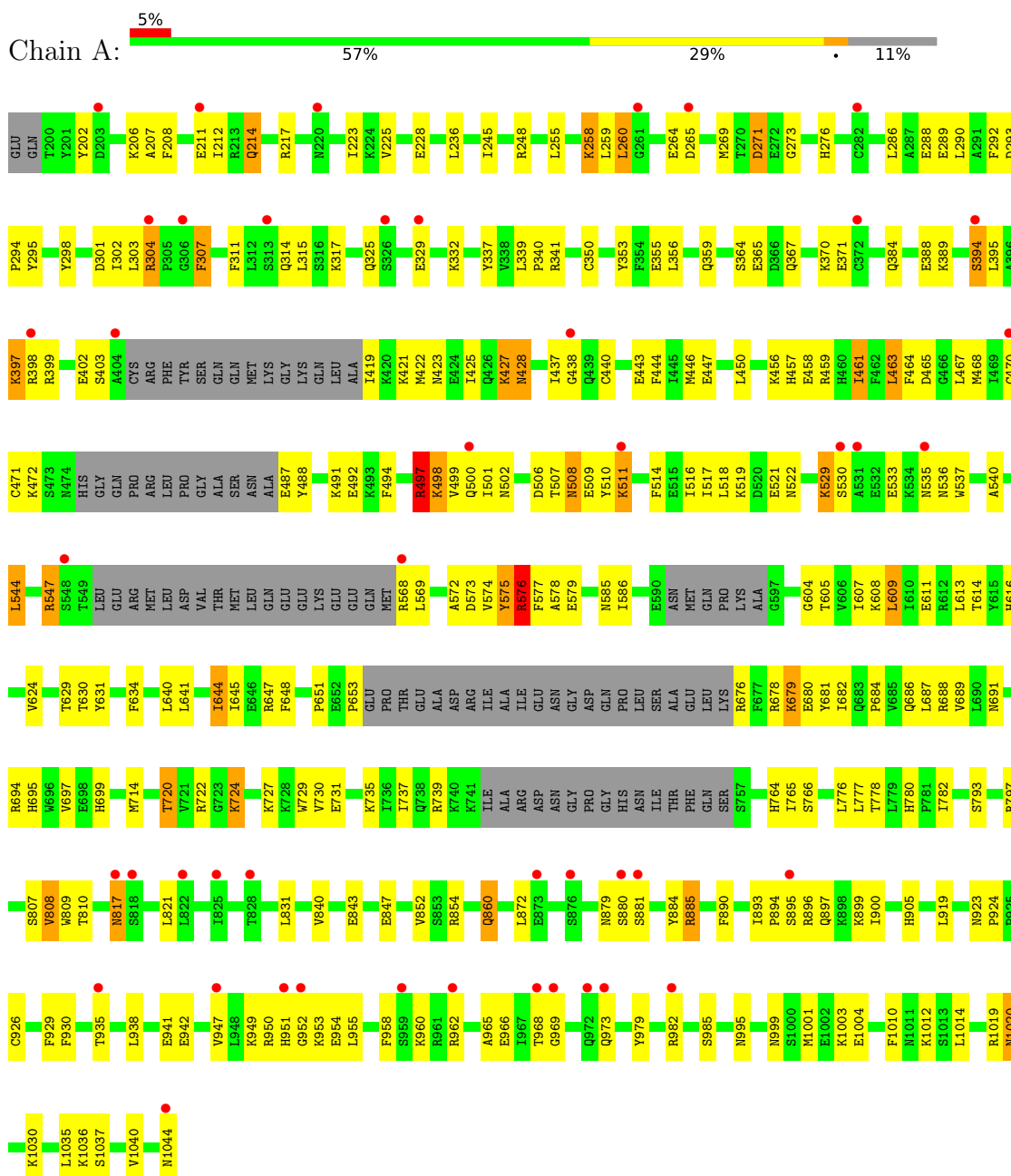
- Molecule 1 is a protein called Son of sevenless protein homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	758	Total	C	N	O	S	0	0	0
			6254	4009	1066	1151	28			
1	B	759	Total	C	N	O	S	0	0	0
			6262	4015	1067	1152	28			

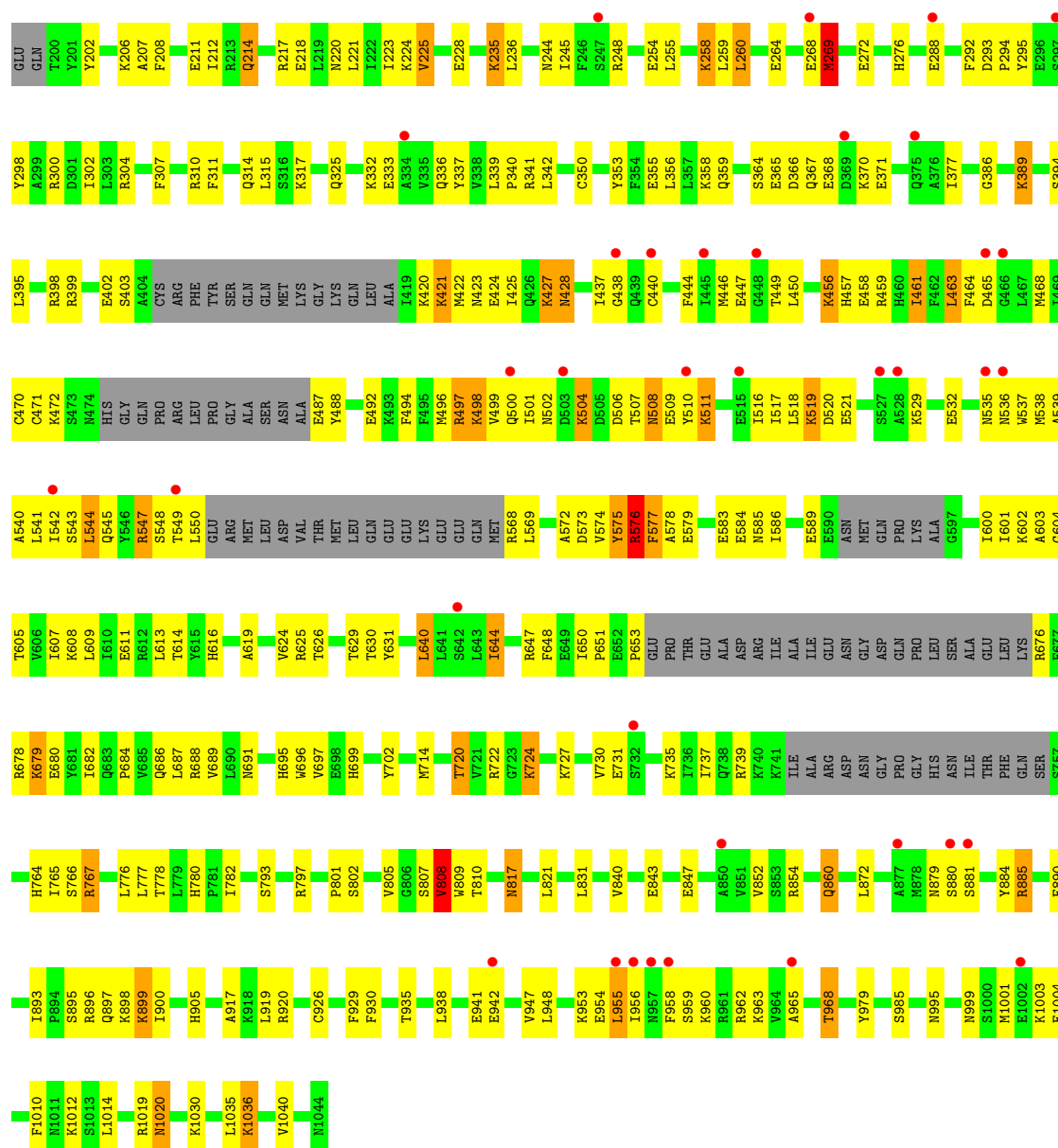
3 Residue-property plots

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: Son of sevenless protein homolog 1



• Molecule 1: Son of sevenless protein homolog 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.03Å 124.71Å 245.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 4.10 8.00 – 4.10	Depositor EDS
% Data completeness (in resolution range)	91.0 (8.00-4.10) 80.5 (8.00-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.84 (at 4.14Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.433 , 0.449 0.403 , 0.415	Depositor DCC
R_{free} test set	1858 reflections (9.84%)	wwPDB-VP
Wilson B-factor (Å ²)	110.0	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.59	EDS
Total number of atoms	12516	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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	0.47	2/6390 (0.0%)	0.94	20/8615 (0.2%)
1	B	0.48	3/6398 (0.0%)	0.95	19/8626 (0.2%)
All	All	0.47	5/12788 (0.0%)	0.94	39/17241 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	427	LYS	CA-C	-10.02	1.38	1.52
1	A	427	LYS	CA-C	-9.97	1.38	1.52
1	A	428	ASN	N-CA	-9.04	1.35	1.46
1	B	428	ASN	N-CA	-9.03	1.35	1.46
1	B	269	MET	CG-SD	7.05	1.98	1.80

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	576	ARG	N-CA-C	10.49	122.09	108.24
1	A	576	ARG	N-CA-C	10.48	122.08	108.24
1	B	679	LYS	N-CA-C	-9.28	103.05	114.75
1	A	679	LYS	N-CA-C	-9.22	103.14	114.75
1	B	577	PHE	N-CA-C	-8.62	102.31	112.92
1	A	577	PHE	N-CA-C	-8.61	102.33	112.92
1	B	427	LYS	N-CA-C	7.02	121.70	113.20
1	A	427	LYS	N-CA-C	7.00	121.68	113.20
1	B	1020	ASN	N-CA-C	6.81	124.86	109.81
1	A	1020	ASN	N-CA-C	6.80	124.84	109.81
1	A	461	ILE	N-CA-C	6.20	117.05	108.12
1	B	461	ILE	N-CA-C	6.14	116.96	108.12
1	A	631	TYR	N-CA-C	6.09	118.88	111.82
1	B	631	TYR	N-CA-C	6.07	118.86	111.82
1	B	394	SER	N-CA-C	5.98	118.29	111.11
1	A	394	SER	N-CA-C	5.98	118.28	111.11
1	A	817	ASN	N-CA-C	5.71	119.97	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	817	ASN	N-CA-C	5.66	119.91	112.89
1	B	930	PHE	N-CA-C	5.56	117.42	111.36
1	A	930	PHE	N-CA-C	5.53	117.38	111.36
1	B	985	SER	N-CA-C	5.50	117.98	111.33
1	A	225	VAL	N-CA-C	5.43	116.50	111.45
1	B	225	VAL	N-CA-C	5.43	116.50	111.45
1	A	985	SER	N-CA-C	5.40	117.86	111.33
1	B	307	PHE	N-CA-C	5.38	117.59	111.02
1	A	307	PHE	N-CA-C	5.37	117.57	111.02
1	B	843	GLU	N-CA-C	5.37	117.89	111.71
1	A	223	ILE	N-CA-C	5.35	115.56	110.53
1	B	223	ILE	N-CA-C	5.32	115.53	110.53
1	A	843	GLU	N-CA-C	5.31	117.81	111.71
1	B	776	LEU	N-CA-C	5.26	118.49	111.75
1	A	776	LEU	N-CA-C	5.23	118.44	111.75
1	A	995	ASN	CA-C-N	5.06	124.51	119.24
1	A	995	ASN	C-N-CA	5.06	124.51	119.24
1	B	808	VAL	N-CA-C	5.04	118.12	111.17
1	A	467	LEU	N-CA-C	5.03	117.36	108.75
1	B	995	ASN	CA-C-N	5.01	124.45	119.24
1	B	995	ASN	C-N-CA	5.01	124.45	119.24
1	A	214	GLN	N-CA-C	-5.00	105.73	111.14

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	6254	0	6262	393	122
1	B	6262	0	6267	484	116
All	All	12516	0	12529	781	122

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 31.

All (781) 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:269:MET:CE	1:A:729:TRP:CZ2	1.75	1.68
1:A:1019:ARG:HH22	1:B:905:HIS:CE1	1.17	1.60
1:A:269:MET:HE3	1:A:729:TRP:CZ2	1.06	1.58
1:B:269:MET:CG	1:B:691:ASN:HD21	0.94	1.58
1:B:342:LEU:HD21	1:B:550:LEU:CD1	1.20	1.58
1:A:630:THR:HG22	1:A:969:GLY:CA	1.24	1.56
1:A:630:THR:CG2	1:A:969:GLY:HA3	1.26	1.54
1:B:268:GLU:CD	1:B:619:ALA:CB	1.78	1.53
1:B:602:LYS:HE2	1:B:948:LEU:CD1	1.36	1.51
1:A:905:HIS:CD2	1:B:1019:ARG:HH12	1.32	1.48
1:B:342:LEU:CD2	1:B:550:LEU:HD13	1.43	1.46
1:B:402:GLU:CG	1:B:536:ASN:HA	1.45	1.46
1:A:905:HIS:CE1	1:B:1019:ARG:HH22	1.32	1.44
1:A:304:ARG:NH2	1:A:399:ARG:NH1	1.63	1.44
1:B:342:LEU:CD2	1:B:550:LEU:CD1	1.97	1.43
1:A:1019:ARG:HH12	1:B:905:HIS:CD2	1.37	1.42
1:B:402:GLU:OE2	1:B:536:ASN:N	1.58	1.35
1:A:269:MET:CE	1:A:729:TRP:CE2	2.12	1.33
1:A:269:MET:HE3	1:A:729:TRP:CH2	1.64	1.31
1:A:1019:ARG:NH2	1:B:905:HIS:CE1	1.96	1.29
1:B:398:ARG:HG2	1:B:532:GLU:OE2	1.13	1.29
1:A:269:MET:CG	1:A:691:ASN:HD21	1.48	1.26
1:A:269:MET:HG2	1:A:691:ASN:ND2	1.52	1.25
1:B:630:THR:CA	1:B:805:VAL:HG11	1.66	1.24
1:B:217:ARG:NE	1:B:548:SER:O	1.68	1.24
1:A:905:HIS:CD2	1:B:1019:ARG:NH1	2.08	1.22
1:A:304:ARG:NE	1:A:307:PHE:HB2	1.54	1.21
1:A:1019:ARG:NH1	1:B:905:HIS:CD2	2.07	1.21
1:A:935:THR:OG1	1:B:1004:GLU:OE2	1.60	1.20
1:A:905:HIS:CE1	1:B:1019:ARG:NH2	2.10	1.20
1:A:942:GLU:OE1	1:B:999:ASN:ND2	1.77	1.18
1:B:337:TYR:CB	1:B:538:MET:HE3	1.73	1.17
1:B:342:LEU:HD22	1:B:550:LEU:CD2	1.73	1.17
1:A:304:ARG:CD	1:A:307:PHE:HB2	1.75	1.16
1:B:337:TYR:HB3	1:B:538:MET:HE3	1.20	1.16
1:B:584:GLU:HG2	1:B:953:LYS:CD	1.76	1.16
1:B:269:MET:HG2	1:B:691:ASN:ND2	1.41	1.14
1:A:304:ARG:CZ	1:A:307:PHE:HB2	1.78	1.13
1:A:634:PHE:HB2	1:A:958:PHE:CZ	1.83	1.13
1:B:342:LEU:HD22	1:B:550:LEU:HD22	1.14	1.13
1:B:268:GLU:OE2	1:B:619:ALA:HB1	0.95	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:MET:HE2	1:A:729:TRP:CZ2	1.82	1.12
1:B:342:LEU:HD13	1:B:550:LEU:HD21	1.26	1.12
1:B:402:GLU:HG2	1:B:536:ASN:HA	1.30	1.12
1:B:584:GLU:HG2	1:B:953:LYS:HD2	1.16	1.12
1:B:268:GLU:CD	1:B:619:ALA:HB1	1.57	1.11
1:B:268:GLU:OE2	1:B:619:ALA:CB	1.78	1.11
1:B:604:GLY:H	1:B:956:ILE:HB	1.01	1.11
1:B:268:GLU:CD	1:B:619:ALA:HB3	1.72	1.11
1:A:884:TYR:CE2	1:B:885:ARG:HB3	1.85	1.11
1:B:402:GLU:CG	1:B:536:ASN:CA	2.14	1.10
1:A:629:THR:CG2	1:A:969:GLY:O	2.00	1.09
1:A:269:MET:HE2	1:A:729:TRP:CE2	1.82	1.09
1:B:602:LYS:CE	1:B:948:LEU:HD11	1.83	1.09
1:B:341:ARG:HG2	1:B:539:ALA:CA	1.48	1.09
1:B:630:THR:HA	1:B:805:VAL:HG11	1.09	1.09
1:B:337:TYR:CG	1:B:538:MET:HE2	1.89	1.07
1:B:341:ARG:CG	1:B:539:ALA:HA	1.81	1.07
1:A:506:ASP:OD1	1:A:508:ASN:HB3	1.54	1.07
1:B:602:LYS:CE	1:B:948:LEU:CD1	2.31	1.07
1:B:218:GLU:HG2	1:B:550:LEU:HA	1.32	1.07
1:A:885:ARG:HB3	1:B:884:TYR:CE2	1.89	1.06
1:B:341:ARG:HG2	1:B:539:ALA:HA	1.34	1.06
1:B:604:GLY:N	1:B:956:ILE:HB	1.71	1.06
1:B:506:ASP:OD2	1:B:508:ASN:HB3	1.56	1.05
1:B:602:LYS:HE2	1:B:948:LEU:HD12	1.31	1.04
1:B:217:ARG:HH21	1:B:548:SER:C	1.65	1.04
1:B:217:ARG:CZ	1:B:548:SER:O	2.05	1.04
1:B:398:ARG:CG	1:B:532:GLU:OE2	2.06	1.04
1:A:304:ARG:CZ	1:A:307:PHE:CB	2.36	1.04
1:A:938:LEU:HD21	1:B:999:ASN:HB2	1.41	1.03
1:A:905:HIS:ND1	1:B:1019:ARG:NH2	2.06	1.03
1:B:342:LEU:HD21	1:B:550:LEU:HD11	1.05	1.02
1:A:499:VAL:HG23	1:A:517:ILE:HB	1.39	1.02
1:B:342:LEU:CD1	1:B:550:LEU:HD21	1.89	1.02
1:B:217:ARG:NH2	1:B:548:SER:O	1.92	1.02
1:A:303:LEU:HA	1:A:304:ARG:HH21	1.24	1.01
1:A:905:HIS:CE1	1:B:1014:LEU:HD11	1.93	1.01
1:B:767:ARG:HH11	1:B:767:ARG:H	1.02	1.00
1:A:885:ARG:HB3	1:B:884:TYR:HE2	1.20	1.00
1:A:884:TYR:HE2	1:B:885:ARG:HB3	1.16	1.00
1:B:269:MET:CB	1:B:691:ASN:HD21	1.74	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:GLU:CG	1:B:953:LYS:HD2	1.91	1.00
1:B:602:LYS:HE2	1:B:948:LEU:HD11	1.04	0.99
1:B:268:GLU:CD	1:B:619:ALA:HB2	1.88	0.98
1:B:341:ARG:CG	1:B:539:ALA:CA	2.17	0.97
1:B:337:TYR:CG	1:B:538:MET:CE	2.47	0.97
1:A:935:THR:HG1	1:B:1004:GLU:CD	1.73	0.97
1:A:1004:GLU:CD	1:B:935:THR:HG1	1.71	0.97
1:B:337:TYR:CB	1:B:538:MET:CE	2.43	0.97
1:A:1004:GLU:OE2	1:B:935:THR:OG1	1.82	0.97
1:A:810:THR:HG22	1:B:1001:MET:HE3	1.46	0.96
1:A:1019:ARG:NH2	1:B:905:HIS:ND1	2.03	0.96
1:B:604:GLY:H	1:B:956:ILE:CB	1.78	0.96
1:A:634:PHE:HB2	1:A:958:PHE:HZ	1.22	0.96
1:B:601:ILE:O	1:B:958:PHE:HB3	1.67	0.94
1:A:630:THR:HB	1:A:965:ALA:O	1.68	0.94
1:B:583:GLU:O	1:B:955:LEU:HD21	1.68	0.94
1:A:304:ARG:HH11	1:A:307:PHE:H	0.94	0.94
1:B:269:MET:HB3	1:B:691:ASN:OD1	1.64	0.94
1:A:337:TYR:OH	1:A:502:ASN:ND2	2.01	0.94
1:A:999:ASN:ND2	1:B:942:GLU:OE1	1.99	0.93
1:B:269:MET:HG2	1:B:691:ASN:HD21	0.77	0.93
1:B:342:LEU:CD2	1:B:550:LEU:CD2	2.47	0.93
1:A:269:MET:HG2	1:A:691:ASN:HD21	0.78	0.93
1:A:269:MET:SD	1:A:687:LEU:HD11	2.09	0.93
1:A:1001:MET:HE3	1:B:810:THR:HG22	1.48	0.93
1:B:422:MET:HE3	1:B:437:ILE:HG22	1.50	0.93
1:B:499:VAL:HG12	1:B:517:ILE:HB	1.51	0.93
1:A:905:HIS:CG	1:B:1019:ARG:HH22	1.88	0.92
1:A:935:THR:OG1	1:B:1004:GLU:CD	2.11	0.92
1:A:269:MET:CE	1:A:729:TRP:HZ2	1.77	0.92
1:A:302:ILE:O	1:A:304:ARG:NH2	2.02	0.92
1:B:630:THR:HA	1:B:805:VAL:CG1	1.99	0.92
1:A:304:ARG:NH1	1:A:307:PHE:CB	2.31	0.91
1:A:422:MET:HE3	1:A:437:ILE:HG22	1.50	0.91
1:A:301:ASP:O	1:A:304:ARG:HG3	1.70	0.91
1:A:629:THR:HG22	1:A:969:GLY:O	1.68	0.91
1:B:268:GLU:CG	1:B:619:ALA:HB2	1.99	0.91
1:B:402:GLU:CD	1:B:536:ASN:N	2.29	0.91
1:B:337:TYR:HB3	1:B:538:MET:CE	2.00	0.91
1:B:342:LEU:HD21	1:B:550:LEU:HD13	0.99	0.91
1:B:496:MET:HA	1:B:498:LYS:HZ3	1.34	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:LYS:HE3	1:B:377:ILE:HD13	1.53	0.90
1:B:218:GLU:HG2	1:B:550:LEU:CA	2.01	0.90
1:A:629:THR:HG22	1:A:969:GLY:C	1.95	0.90
1:B:398:ARG:HG2	1:B:532:GLU:CD	1.97	0.90
1:B:269:MET:CG	1:B:691:ASN:ND2	1.78	0.89
1:B:630:THR:CB	1:B:805:VAL:HG11	2.03	0.89
1:B:402:GLU:CD	1:B:536:ASN:CA	2.45	0.89
1:A:304:ARG:NH1	1:A:307:PHE:HB3	1.88	0.88
1:B:402:GLU:CD	1:B:536:ASN:HA	1.98	0.88
1:B:337:TYR:CD1	1:B:538:MET:HE2	2.09	0.88
1:A:304:ARG:HH11	1:A:307:PHE:N	1.71	0.88
1:A:614:THR:HG23	1:A:688:ARG:HB2	1.56	0.87
1:B:268:GLU:OE1	1:B:619:ALA:HB3	1.72	0.87
1:A:1019:ARG:HH22	1:B:905:HIS:CG	1.92	0.87
1:A:881:SER:N	1:B:881:SER:OG	2.08	0.87
1:A:269:MET:CE	1:A:687:LEU:HD11	2.05	0.85
1:B:614:THR:HG23	1:B:688:ARG:HB2	1.56	0.85
1:A:303:LEU:HA	1:A:304:ARG:NH2	1.90	0.85
1:B:269:MET:CB	1:B:691:ASN:ND2	2.34	0.85
1:A:905:HIS:NE2	1:B:1014:LEU:CD1	2.40	0.85
1:A:881:SER:OG	1:B:881:SER:N	2.10	0.85
1:A:1014:LEU:HD11	1:B:905:HIS:CE1	2.12	0.85
1:A:896:ARG:O	1:A:899:LYS:HG2	1.78	0.84
1:B:268:GLU:CG	1:B:619:ALA:CB	2.56	0.83
1:A:303:LEU:CA	1:A:304:ARG:HH21	1.91	0.83
1:A:1019:ARG:NH1	1:B:905:HIS:NE2	2.18	0.83
1:A:1019:ARG:NH2	1:B:905:HIS:CG	2.47	0.82
1:A:630:THR:HG22	1:A:969:GLY:N	1.93	0.82
1:A:905:HIS:CG	1:B:1019:ARG:NH2	2.47	0.82
1:A:304:ARG:NE	1:A:304:ARG:N	2.28	0.82
1:B:202:TYR:O	1:B:206:LYS:HG3	1.80	0.81
1:B:341:ARG:CZ	1:B:539:ALA:H	1.94	0.81
1:B:499:VAL:CG1	1:B:517:ILE:HB	2.10	0.81
1:B:366:ASP:OD2	1:B:368:GLU:HG2	1.79	0.81
1:A:446:MET:HE2	1:A:540:ALA:HB3	1.63	0.80
1:B:341:ARG:HG2	1:B:539:ALA:C	2.06	0.80
1:B:767:ARG:HH11	1:B:767:ARG:N	1.80	0.80
1:A:269:MET:HE2	1:A:729:TRP:NE1	1.94	0.80
1:A:304:ARG:NH1	1:A:307:PHE:H	1.78	0.80
1:A:202:TYR:O	1:A:206:LYS:HG3	1.81	0.80
1:A:1004:GLU:CD	1:B:935:THR:OG1	2.21	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:ASP:OD2	1:B:508:ASN:CB	2.29	0.79
1:B:446:MET:HE2	1:B:540:ALA:HB3	1.63	0.79
1:A:938:LEU:HD21	1:B:999:ASN:CB	2.13	0.79
1:B:402:GLU:OE2	1:B:535:ASN:C	2.26	0.79
1:B:220:ASN:HB3	1:B:224:LYS:NZ	1.98	0.78
1:B:584:GLU:HG2	1:B:953:LYS:CG	2.14	0.78
1:B:498:LYS:HG3	1:B:518:LEU:HD13	1.63	0.78
1:A:929:PHE:CE1	1:B:1003:LYS:HE3	2.19	0.78
1:A:304:ARG:CZ	1:A:307:PHE:HB3	2.12	0.78
1:A:905:HIS:NE2	1:B:1014:LEU:HD13	1.98	0.78
1:A:629:THR:OG1	1:A:973:GLN:OE1	2.00	0.77
1:A:341:ARG:NH2	1:A:536:ASN:OD1	2.17	0.77
1:A:519:LYS:HD3	1:A:519:LYS:H	1.50	0.77
1:B:268:GLU:HG2	1:B:619:ALA:HB2	1.65	0.77
1:B:342:LEU:CD2	1:B:550:LEU:HD22	2.06	0.77
1:B:496:MET:HA	1:B:498:LYS:NZ	1.99	0.77
1:A:1019:ARG:CZ	1:B:905:HIS:CD2	2.67	0.76
1:B:630:THR:HG22	1:B:805:VAL:CG2	2.15	0.76
1:A:697:VAL:HG11	1:A:737:ILE:HG12	1.67	0.76
1:B:498:LYS:O	1:B:498:LYS:HE2	1.84	0.76
1:A:999:ASN:HB2	1:B:938:LEU:HD21	1.67	0.76
1:B:342:LEU:HD22	1:B:550:LEU:HD13	1.65	0.76
1:B:767:ARG:H	1:B:767:ARG:NH1	1.82	0.76
1:A:304:ARG:CD	1:A:307:PHE:CB	2.63	0.76
1:A:634:PHE:CB	1:A:958:PHE:CZ	2.68	0.76
1:A:446:MET:HE1	1:A:537:TRP:HA	1.68	0.76
1:A:1019:ARG:NH2	1:B:905:HIS:NE2	2.34	0.76
1:B:601:ILE:O	1:B:958:PHE:CD2	2.38	0.75
1:A:544:LEU:HA	1:A:547:ARG:HH12	1.50	0.75
1:B:697:VAL:HG11	1:B:737:ILE:HG12	1.67	0.75
1:A:258:LYS:HE2	1:A:286:LEU:HD21	1.68	0.75
1:A:942:GLU:CD	1:B:999:ASN:ND2	2.44	0.75
1:B:446:MET:HE1	1:B:537:TRP:HA	1.68	0.74
1:B:498:LYS:HG3	1:B:518:LEU:HA	1.69	0.74
1:B:342:LEU:HD13	1:B:550:LEU:CD2	2.11	0.74
1:A:1003:LYS:HE3	1:B:929:PHE:CE1	2.21	0.74
1:B:342:LEU:CD2	1:B:550:LEU:CG	2.66	0.74
1:B:402:GLU:OE2	1:B:536:ASN:CA	2.34	0.74
1:B:583:GLU:O	1:B:955:LEU:CD2	2.35	0.74
1:B:584:GLU:CG	1:B:953:LYS:CD	2.57	0.74
1:A:341:ARG:HH12	1:A:535:ASN:HB3	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:SER:C	1:B:881:SER:HG	1.95	0.73
1:A:884:TYR:OH	1:B:885:ARG:HD2	1.87	0.73
1:B:342:LEU:HD22	1:B:550:LEU:CG	2.18	0.73
1:A:422:MET:CE	1:A:437:ILE:HG22	2.20	0.72
1:A:634:PHE:CB	1:A:958:PHE:HZ	2.01	0.72
1:A:506:ASP:CG	1:A:508:ASN:HB3	2.13	0.72
1:B:218:GLU:HG2	1:B:550:LEU:C	2.15	0.72
1:A:905:HIS:NE2	1:B:1019:ARG:NH1	2.27	0.72
1:B:508:ASN:O	1:B:509:GLU:HG3	1.90	0.72
1:A:905:HIS:NE2	1:B:1014:LEU:HD11	2.04	0.72
1:A:1019:ARG:HH22	1:B:905:HIS:ND1	1.29	0.71
1:A:269:MET:O	1:A:694:ARG:NH1	2.23	0.71
1:B:244:ASN:HB3	1:B:310:ARG:NH2	2.06	0.71
1:B:300:ARG:O	1:B:304:ARG:HG3	1.90	0.71
1:B:207:ALA:O	1:B:211:GLU:HG3	1.91	0.71
1:B:221:LEU:HD13	1:B:549:THR:OG1	1.90	0.70
1:A:265:ASP:HB3	1:A:687:LEU:HD21	1.72	0.70
1:B:220:ASN:HB3	1:B:224:LYS:HZ2	1.55	0.70
1:B:702:TYR:CE1	1:B:802:SER:OG	2.14	0.70
1:A:207:ALA:O	1:A:211:GLU:HG3	1.91	0.70
1:A:881:SER:HG	1:B:880:SER:C	1.98	0.70
1:B:342:LEU:HD22	1:B:550:LEU:CD1	2.09	0.70
1:B:422:MET:CE	1:B:437:ILE:HG22	2.20	0.70
1:A:879:ASN:HB3	1:B:1010:PHE:CZ	2.27	0.70
1:A:905:HIS:CD2	1:B:1019:ARG:CZ	2.74	0.69
1:A:880:SER:C	1:B:881:SER:OG	2.34	0.69
1:B:421:LYS:HE2	1:B:421:LYS:HA	1.73	0.69
1:A:604:GLY:O	1:A:962:ARG:NH2	2.26	0.69
1:A:304:ARG:HD3	1:A:307:PHE:HB2	1.69	0.69
1:A:355:GLU:HG3	1:A:359:GLN:HE21	1.58	0.69
1:A:500:GLN:OE1	1:A:516:ILE:HG12	1.93	0.69
1:B:629:THR:HG22	1:B:805:VAL:HG21	1.74	0.69
1:A:507:THR:C	1:A:509:GLU:H	1.99	0.69
1:A:679:LYS:HD2	1:A:679:LYS:O	1.93	0.69
1:A:498:LYS:HG2	1:A:518:LEU:HA	1.75	0.68
1:B:507:THR:C	1:B:509:GLU:H	1.99	0.68
1:B:947:VAL:HG11	1:B:954:GLU:HG3	1.76	0.68
1:A:498:LYS:HG2	1:A:518:LEU:HD23	1.75	0.68
1:B:355:GLU:HG3	1:B:359:GLN:HE21	1.58	0.68
1:A:1019:ARG:HH22	1:B:905:HIS:CD2	2.11	0.68
1:B:214:GLN:HE22	1:B:550:LEU:C	2.00	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602:LYS:C	1:B:958:PHE:CB	2.66	0.68
1:A:881:SER:OG	1:B:880:SER:C	2.37	0.68
1:B:342:LEU:HD23	1:B:550:LEU:HD13	1.66	0.68
1:B:601:ILE:O	1:B:958:PHE:CB	2.41	0.68
1:B:602:LYS:HA	1:B:958:PHE:HB3	1.76	0.68
1:B:629:THR:HG23	1:B:801:PRO:HB2	1.76	0.68
1:B:568:ARG:C	1:B:569:LEU:HD22	2.18	0.67
1:B:679:LYS:HD2	1:B:679:LYS:O	1.93	0.67
1:A:634:PHE:HB2	1:A:958:PHE:CE2	2.28	0.67
1:B:602:LYS:C	1:B:958:PHE:HB2	2.17	0.67
1:A:568:ARG:C	1:A:569:LEU:HD22	2.18	0.67
1:B:341:ARG:CZ	1:B:539:ALA:N	2.54	0.67
1:A:276:HIS:HE1	1:A:365:GLU:H	1.42	0.67
1:B:547:ARG:HB3	1:B:547:ARG:NH1	2.09	0.67
1:A:840:VAL:HG13	1:A:1012:LYS:HB3	1.76	0.67
1:B:220:ASN:O	1:B:224:LYS:HG2	1.95	0.67
1:A:341:ARG:HG3	1:A:403:SER:OG	1.95	0.67
1:A:929:PHE:HE1	1:B:1003:LYS:HE3	1.59	0.67
1:A:1019:ARG:NH2	1:B:905:HIS:CD2	2.62	0.67
1:A:609:LEU:CD2	1:A:962:ARG:NH1	2.58	0.66
1:A:529:LYS:HE3	1:A:533:GLU:OE2	1.95	0.66
1:A:630:THR:HG23	1:A:969:GLY:HA3	1.62	0.66
1:B:840:VAL:HG13	1:B:1012:LYS:HB3	1.76	0.66
1:B:276:HIS:HE1	1:B:365:GLU:H	1.42	0.66
1:A:1003:LYS:CE	1:B:929:PHE:HE1	2.08	0.66
1:B:341:ARG:HG3	1:B:403:SER:OG	1.95	0.66
1:A:947:VAL:HG11	1:A:954:GLU:HG3	1.76	0.66
1:B:602:LYS:CA	1:B:958:PHE:HB3	2.25	0.66
1:A:1019:ARG:CZ	1:B:905:HIS:NE2	2.59	0.66
1:A:506:ASP:OD1	1:A:508:ASN:CB	2.38	0.65
1:A:1014:LEU:CD1	1:B:905:HIS:NE2	2.59	0.65
1:A:1003:LYS:HE3	1:B:929:PHE:CZ	2.30	0.65
1:B:614:THR:HG21	1:B:689:VAL:HG23	1.78	0.65
1:B:314:GLN:NE2	1:B:317:LYS:NZ	2.44	0.65
1:A:885:ARG:HD2	1:B:884:TYR:OH	1.96	0.65
1:A:614:THR:HG21	1:A:689:VAL:HG23	1.77	0.65
1:A:314:GLN:NE2	1:A:317:LYS:NZ	2.44	0.65
1:A:544:LEU:HA	1:A:547:ARG:NH1	2.11	0.65
1:A:547:ARG:HH11	1:A:547:ARG:HB2	1.62	0.65
1:A:929:PHE:HE1	1:B:1003:LYS:CE	2.10	0.65
1:B:793:SER:O	1:B:797:ARG:HG3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:GLN:NE2	1:B:502:ASN:ND2	2.45	0.65
1:B:500:GLN:NE2	1:B:545:GLN:HB2	2.12	0.65
1:A:269:MET:HG2	1:A:691:ASN:CG	2.21	0.64
1:A:446:MET:HE2	1:A:540:ALA:CB	2.27	0.64
1:B:589:GLU:OE1	1:B:959:SER:HB2	1.97	0.64
1:A:793:SER:O	1:A:797:ARG:HG3	1.97	0.64
1:B:269:MET:CB	1:B:691:ASN:CG	2.69	0.64
1:B:629:THR:HG23	1:B:801:PRO:CB	2.28	0.64
1:A:630:THR:CB	1:A:969:GLY:HA3	2.20	0.64
1:B:614:THR:O	1:B:614:THR:HG22	1.98	0.64
1:B:500:GLN:OE1	1:B:545:GLN:HB2	1.98	0.64
1:B:444:PHE:HZ	1:B:447:GLU:HB2	1.62	0.64
1:A:303:LEU:CA	1:A:304:ARG:NH2	2.57	0.64
1:A:884:TYR:CE2	1:B:885:ARG:CB	2.73	0.64
1:B:602:LYS:O	1:B:956:ILE:O	2.13	0.64
1:B:603:ALA:CA	1:B:956:ILE:HB	2.27	0.64
1:A:459:ARG:HG2	1:A:459:ARG:HH11	1.63	0.64
1:A:398:ARG:HH21	1:A:398:ARG:HA	1.62	0.63
1:B:446:MET:HE2	1:B:540:ALA:CB	2.27	0.63
1:A:444:PHE:HZ	1:A:447:GLU:HB2	1.62	0.63
1:A:614:THR:HG22	1:A:614:THR:O	1.98	0.63
1:A:905:HIS:HE1	1:B:1014:LEU:HD11	1.59	0.63
1:B:547:ARG:HH11	1:B:548:SER:N	1.97	0.63
1:B:780:HIS:CE1	1:B:782:ILE:HD12	2.34	0.63
1:A:1010:PHE:CZ	1:B:879:ASN:HB3	2.33	0.63
1:A:269:MET:HE1	1:A:729:TRP:CE2	2.30	0.63
1:A:269:MET:HB3	1:A:694:ARG:HH12	1.64	0.63
1:A:419:ILE:HG13	1:A:422:MET:SD	2.39	0.63
1:B:630:THR:CB	1:B:805:VAL:CG1	2.75	0.63
1:A:402:GLU:CG	1:A:536:ASN:OD1	2.46	0.63
1:B:269:MET:HB3	1:B:691:ASN:CG	2.24	0.62
1:A:780:HIS:CE1	1:A:782:ILE:HD12	2.33	0.62
1:B:235:LYS:HD3	1:B:235:LYS:H	1.64	0.62
1:A:301:ASP:O	1:A:304:ARG:CG	2.46	0.62
1:B:458:GLU:O	1:B:458:GLU:CD	2.42	0.62
1:B:333:GLU:HG2	1:B:501:ILE:HG13	1.81	0.62
1:B:500:GLN:HE22	1:B:545:GLN:HB2	1.62	0.62
1:A:609:LEU:HD22	1:A:962:ARG:NH1	2.15	0.62
1:B:459:ARG:HH11	1:B:459:ARG:HG2	1.63	0.62
1:B:629:THR:O	1:B:805:VAL:HG21	1.99	0.62
1:A:735:LYS:HD2	1:A:739:ARG:NH2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:LEU:HD12	1:B:461:ILE:HD12	1.83	0.61
1:B:342:LEU:CD2	1:B:550:LEU:HD11	1.94	0.61
1:B:367:GLN:O	1:B:371:GLU:HG2	2.01	0.61
1:A:547:ARG:NH1	1:A:547:ARG:HB2	2.16	0.61
1:A:905:HIS:CD2	1:B:1019:ARG:HH22	2.17	0.61
1:B:584:GLU:CD	1:B:953:LYS:HD2	2.25	0.61
1:B:218:GLU:CG	1:B:550:LEU:C	2.74	0.61
1:B:735:LYS:HD2	1:B:739:ARG:NH2	2.15	0.61
1:A:271:ASP:CG	1:A:273:GLY:H	2.08	0.61
1:A:364:SER:HB3	1:A:370:LYS:HG2	1.82	0.61
1:A:302:ILE:C	1:A:304:ARG:HE	2.09	0.61
1:B:260:LEU:HD22	1:B:264:GLU:HG3	1.83	0.61
1:B:341:ARG:HH12	1:B:535:ASN:HA	1.66	0.61
1:A:629:THR:HG21	1:A:973:GLN:HB2	1.83	0.60
1:B:506:ASP:CG	1:B:508:ASN:HB3	2.24	0.60
1:A:260:LEU:HD22	1:A:264:GLU:HG3	1.83	0.60
1:A:364:SER:HB3	1:A:370:LYS:CG	2.32	0.60
1:A:450:LEU:HD12	1:A:461:ILE:HD12	1.83	0.60
1:B:777:LEU:HD23	1:B:854:ARG:HG3	1.83	0.60
1:A:304:ARG:NE	1:A:304:ARG:H	1.98	0.60
1:A:367:GLN:O	1:A:371:GLU:HG2	2.01	0.60
1:A:840:VAL:CG1	1:A:1012:LYS:HB3	2.32	0.60
1:A:905:HIS:CE1	1:B:1014:LEU:CD1	2.73	0.60
1:B:364:SER:HB3	1:B:370:LYS:CG	2.32	0.60
1:A:446:MET:HE3	1:A:463:LEU:HD12	1.83	0.60
1:A:777:LEU:HD23	1:A:854:ARG:HG3	1.83	0.60
1:B:840:VAL:CG1	1:B:1012:LYS:HB3	2.32	0.60
1:B:917:ALA:HA	1:B:920:ARG:NH2	2.17	0.60
1:A:885:ARG:CB	1:B:884:TYR:CE2	2.77	0.59
1:B:224:LYS:HG3	1:B:225:VAL:HG23	1.84	0.59
1:B:221:LEU:HD23	1:B:550:LEU:CD2	2.33	0.59
1:A:810:THR:HG22	1:B:1001:MET:CE	2.29	0.59
1:A:999:ASN:ND2	1:B:942:GLU:CD	2.60	0.59
1:B:364:SER:HB3	1:B:370:LYS:HG2	1.83	0.59
1:B:446:MET:HE3	1:B:463:LEU:HD12	1.83	0.59
1:B:456:LYS:H	1:B:456:LYS:HE3	1.67	0.59
1:B:630:THR:HG22	1:B:805:VAL:HG21	1.85	0.59
1:A:260:LEU:O	1:A:264:GLU:HG3	2.03	0.59
1:A:905:HIS:CD2	1:B:1019:ARG:NH2	2.70	0.59
1:A:1014:LEU:HD13	1:B:905:HIS:NE2	2.18	0.59
1:B:428:ASN:ND2	1:B:487:GLU:N	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:GLU:HG3	1:B:625:ARG:NH2	2.17	0.58
1:A:575:TYR:HD2	1:A:651:PRO:HG2	1.69	0.58
1:B:644:ILE:HG23	1:B:689:VAL:HG13	1.85	0.58
1:A:629:THR:HG22	1:A:969:GLY:CA	2.33	0.58
1:B:575:TYR:HD2	1:B:651:PRO:HG2	1.69	0.58
1:B:260:LEU:O	1:B:264:GLU:HG3	2.03	0.58
1:A:644:ILE:HG23	1:A:689:VAL:HG13	1.85	0.58
1:B:258:LYS:HA	1:B:258:LYS:NZ	2.19	0.58
1:B:269:MET:HE1	1:B:691:ASN:N	2.19	0.58
1:A:269:MET:HE1	1:A:687:LEU:HD11	1.84	0.58
1:A:630:THR:CG2	1:A:969:GLY:CA	2.17	0.57
1:B:337:TYR:HB2	1:B:538:MET:HE3	1.79	0.57
1:A:428:ASN:ND2	1:A:487:GLU:N	2.51	0.57
1:B:456:LYS:H	1:B:456:LYS:CE	2.17	0.57
1:B:519:LYS:HB2	1:B:519:LYS:NZ	2.19	0.57
1:A:506:ASP:OD1	1:A:510:TYR:CE2	2.57	0.57
1:A:629:THR:O	1:A:969:GLY:HA2	2.04	0.57
1:A:1014:LEU:HD11	1:B:905:HIS:NE2	2.19	0.57
1:B:500:GLN:CD	1:B:545:GLN:HB2	2.29	0.57
1:A:498:LYS:HB2	1:A:517:ILE:O	2.04	0.57
1:B:276:HIS:CE1	1:B:365:GLU:H	2.22	0.57
1:B:497:ARG:H	1:B:498:LYS:HD3	1.70	0.57
1:A:905:HIS:NE2	1:B:1019:ARG:NH2	2.48	0.57
1:B:217:ARG:NH2	1:B:548:SER:C	2.44	0.57
1:B:428:ASN:HD21	1:B:487:GLU:N	2.03	0.57
1:B:767:ARG:NH1	1:B:767:ARG:HB2	2.20	0.57
1:B:235:LYS:HD3	1:B:235:LYS:N	2.20	0.56
1:A:419:ILE:HG13	1:A:422:MET:HB2	1.87	0.56
1:A:1003:LYS:CE	1:B:929:PHE:CE1	2.84	0.56
1:B:314:GLN:NE2	1:B:317:LYS:HZ1	2.02	0.56
1:B:423:ASN:O	1:B:427:LYS:HD3	2.04	0.56
1:A:630:THR:HG22	1:A:969:GLY:C	2.19	0.56
1:B:314:GLN:HE22	1:B:317:LYS:NZ	2.04	0.56
1:B:547:ARG:HH11	1:B:547:ARG:C	2.13	0.56
1:A:456:LYS:HD2	1:A:457:HIS:CD2	2.39	0.56
1:A:860:GLN:HG3	1:A:900:ILE:HD13	1.87	0.56
1:B:269:MET:CE	1:B:691:ASN:N	2.66	0.56
1:A:302:ILE:C	1:A:304:ARG:HH21	2.13	0.56
1:A:276:HIS:CE1	1:A:365:GLU:H	2.22	0.56
1:A:419:ILE:CG1	1:A:422:MET:HB2	2.36	0.56
1:A:428:ASN:HD21	1:A:487:GLU:N	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:GLN:HE22	1:A:317:LYS:NZ	2.04	0.56
1:A:929:PHE:CZ	1:B:1003:LYS:HE3	2.40	0.56
1:A:421:LYS:HZ1	1:A:425:ILE:HD11	1.72	0.55
1:B:221:LEU:HD23	1:B:550:LEU:HD23	1.88	0.55
1:B:601:ILE:C	1:B:958:PHE:HB3	2.29	0.55
1:B:602:LYS:CE	1:B:948:LEU:HD12	2.17	0.55
1:B:860:GLN:HG3	1:B:900:ILE:HD13	1.87	0.55
1:A:507:THR:O	1:A:509:GLU:N	2.39	0.55
1:A:611:GLU:HA	1:A:647:ARG:NH1	2.22	0.55
1:B:235:LYS:NZ	1:B:235:LYS:HB2	2.21	0.55
1:A:629:THR:HG21	1:A:969:GLY:O	2.00	0.55
1:B:342:LEU:CD1	1:B:550:LEU:CD2	2.74	0.55
1:B:269:MET:CA	1:B:691:ASN:ND2	2.69	0.55
1:B:403:SER:OG	1:B:539:ALA:HB1	2.06	0.55
1:B:601:ILE:O	1:B:958:PHE:HD2	1.87	0.55
1:A:302:ILE:O	1:A:304:ARG:CZ	2.55	0.55
1:B:269:MET:HA	1:B:691:ASN:ND2	2.22	0.55
1:B:504:LYS:HE3	1:B:504:LYS:HA	1.89	0.55
1:B:547:ARG:HD2	1:B:547:ARG:O	2.06	0.55
1:A:269:MET:SD	1:A:687:LEU:HD21	2.47	0.54
1:A:766:SER:OG	1:A:778:THR:HB	2.07	0.54
1:B:766:SER:OG	1:B:778:THR:HB	2.08	0.54
1:B:947:VAL:HG11	1:B:954:GLU:CG	2.37	0.54
1:A:499:VAL:CG2	1:A:517:ILE:HB	2.25	0.54
1:B:221:LEU:CD1	1:B:549:THR:OG1	2.54	0.54
1:B:629:THR:HG21	1:B:968:THR:HG21	1.89	0.54
1:B:630:THR:HG22	1:B:805:VAL:CG1	2.38	0.54
1:B:519:LYS:O	1:B:519:LYS:HD3	2.06	0.54
1:B:630:THR:HG22	1:B:805:VAL:HG22	1.88	0.54
1:B:547:ARG:HB3	1:B:547:ARG:HH11	1.73	0.54
1:A:458:GLU:CD	1:A:458:GLU:H	2.16	0.54
1:A:1036:LYS:HD3	1:A:1037:SER:O	2.08	0.54
1:B:258:LYS:HA	1:B:258:LYS:HZ2	1.73	0.54
1:B:272:GLU:HG3	1:B:625:ARG:HH22	1.71	0.54
1:A:397:LYS:NZ	1:A:397:LYS:HB3	2.24	0.53
1:A:568:ARG:HH21	1:A:568:ARG:HG3	1.73	0.53
1:B:456:LYS:HG2	1:B:457:HIS:ND1	2.22	0.53
1:B:611:GLU:HA	1:B:647:ARG:NH1	2.22	0.53
1:A:314:GLN:HE22	1:A:317:LYS:HZ3	1.55	0.53
1:A:402:GLU:HG3	1:A:536:ASN:OD1	2.07	0.53
1:A:511:LYS:HD2	1:A:511:LYS:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:LYS:HD2	1:B:518:LEU:HD13	1.89	0.53
1:A:303:LEU:C	1:A:304:ARG:NH2	2.66	0.53
1:B:498:LYS:CG	1:B:518:LEU:HD13	2.33	0.53
1:B:603:ALA:C	1:B:956:ILE:HB	2.31	0.53
1:A:269:MET:CG	1:A:691:ASN:ND2	2.33	0.53
1:A:498:LYS:CG	1:A:518:LEU:HD23	2.38	0.53
1:B:603:ALA:HA	1:B:956:ILE:HB	1.91	0.53
1:A:304:ARG:NH1	1:A:307:PHE:HB2	2.09	0.53
1:A:421:LYS:NZ	1:A:425:ILE:HD11	2.24	0.53
1:B:604:GLY:H	1:B:956:ILE:CG1	2.22	0.53
1:A:394:SER:O	1:A:398:ARG:HG2	2.09	0.53
1:A:947:VAL:HG11	1:A:954:GLU:CG	2.37	0.53
1:B:695:HIS:CD2	1:B:699:HIS:HD2	2.27	0.53
1:B:963:LYS:HB3	1:B:963:LYS:HZ2	1.73	0.53
1:B:245:ILE:HD11	1:B:314:GLN:HG2	1.91	0.53
1:A:653:PRO:HD3	1:A:678:ARG:NH1	2.24	0.52
1:A:245:ILE:HD11	1:A:314:GLN:HG2	1.91	0.52
1:A:304:ARG:NH2	1:A:399:ARG:HH11	1.92	0.52
1:B:1036:LYS:NZ	1:B:1036:LYS:HB2	2.23	0.52
1:B:653:PRO:HD3	1:B:678:ARG:NH1	2.24	0.52
1:B:398:ARG:CG	1:B:532:GLU:CD	2.72	0.52
1:B:402:GLU:OE2	1:B:536:ASN:CG	2.53	0.52
1:B:449:THR:HG23	1:B:458:GLU:OE1	2.09	0.52
1:B:568:ARG:HG3	1:B:568:ARG:HH21	1.73	0.52
1:B:568:ARG:O	1:B:569:LEU:HD13	2.09	0.52
1:A:500:GLN:C	1:A:501:ILE:HD12	2.35	0.52
1:A:905:HIS:NE2	1:B:1019:ARG:CZ	2.72	0.52
1:B:311:PHE:O	1:B:315:LEU:HD13	2.09	0.52
1:A:519:LYS:H	1:A:519:LYS:CD	2.22	0.52
1:B:402:GLU:CD	1:B:535:ASN:C	2.75	0.52
1:A:518:LEU:HB2	1:A:521:GLU:HB2	1.91	0.52
1:A:684:PRO:O	1:A:688:ARG:HG2	2.10	0.52
1:A:568:ARG:O	1:A:569:LEU:HD13	2.09	0.52
1:A:695:HIS:CD2	1:A:699:HIS:HD2	2.27	0.52
1:A:780:HIS:HE1	1:A:782:ILE:HD12	1.74	0.52
1:B:500:GLN:C	1:B:501:ILE:HD12	2.35	0.51
1:B:511:LYS:HD2	1:B:511:LYS:O	2.09	0.51
1:B:601:ILE:O	1:B:958:PHE:CG	2.63	0.51
1:B:890:PHE:HA	1:B:893:ILE:HD12	1.93	0.51
1:A:311:PHE:O	1:A:315:LEU:HD13	2.09	0.51
1:B:507:THR:C	1:B:509:GLU:N	2.67	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:684:PRO:O	1:B:688:ARG:HG2	2.10	0.51
1:A:780:HIS:HE1	1:A:782:ILE:CD1	2.24	0.50
1:A:884:TYR:CZ	1:B:885:ARG:HD2	2.45	0.50
1:B:507:THR:O	1:B:509:GLU:N	2.40	0.50
1:A:727:LYS:O	1:A:731:GLU:HG3	2.12	0.50
1:B:602:LYS:CA	1:B:958:PHE:CB	2.89	0.50
1:A:890:PHE:HA	1:A:893:ILE:HD12	1.93	0.50
1:A:1001:MET:CE	1:B:810:THR:HG22	2.32	0.50
1:A:206:LYS:NZ	1:A:206:LYS:HB3	2.26	0.50
1:A:304:ARG:CZ	1:A:304:ARG:N	2.74	0.50
1:A:304:ARG:HD3	1:A:307:PHE:CB	2.36	0.50
1:B:896:ARG:HH11	1:B:896:ARG:HG2	1.77	0.50
1:A:648:PHE:HE2	1:A:722:ARG:NH1	2.09	0.50
1:A:896:ARG:HG2	1:A:896:ARG:HH11	1.77	0.50
1:B:630:THR:HB	1:B:805:VAL:CG1	2.41	0.50
1:B:727:LYS:O	1:B:731:GLU:HG3	2.12	0.50
1:A:399:ARG:O	1:A:402:GLU:HB3	2.12	0.50
1:B:399:ARG:O	1:B:402:GLU:HB3	2.12	0.50
1:A:314:GLN:NE2	1:A:317:LYS:HZ1	2.09	0.50
1:B:506:ASP:C	1:B:508:ASN:N	2.68	0.50
1:B:780:HIS:HE1	1:B:782:ILE:HD12	1.74	0.50
1:A:905:HIS:HE1	1:B:1010:PHE:HE2	1.60	0.50
1:B:780:HIS:HE1	1:B:782:ILE:CD1	2.24	0.50
1:A:999:ASN:CB	1:B:938:LEU:HD21	2.38	0.49
1:A:926:CYS:HA	1:A:979:TYR:OH	2.13	0.49
1:A:1001:MET:HE3	1:B:810:THR:CG2	2.32	0.49
1:B:468:MET:HE1	1:B:516:ILE:HD12	1.94	0.49
1:B:496:MET:CA	1:B:498:LYS:HZ3	2.17	0.49
1:B:579:GLU:O	1:B:608:LYS:HE2	2.12	0.49
1:B:648:PHE:HE2	1:B:722:ARG:NH1	2.09	0.49
1:A:579:GLU:O	1:A:608:LYS:HE2	2.12	0.49
1:B:498:LYS:HD3	1:B:498:LYS:N	2.26	0.49
1:B:926:CYS:HA	1:B:979:TYR:OH	2.13	0.49
1:A:500:GLN:HE22	1:A:516:ILE:CG1	2.25	0.49
1:A:629:THR:CG2	1:A:969:GLY:C	2.67	0.49
1:A:304:ARG:HE	1:A:304:ARG:H	1.60	0.49
1:A:507:THR:C	1:A:509:GLU:N	2.67	0.49
1:A:720:THR:O	1:A:722:ARG:HD3	2.13	0.49
1:B:547:ARG:C	1:B:547:ARG:HD2	2.37	0.49
1:B:808:VAL:HG11	1:B:817:ASN:HB3	1.95	0.49
1:A:446:MET:CE	1:A:463:LEU:HD12	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ASP:C	1:A:508:ASN:N	2.68	0.49
1:A:613:LEU:HD11	1:A:624:VAL:HA	1.94	0.49
1:A:1003:LYS:HE2	1:B:929:PHE:HE1	1.76	0.49
1:B:446:MET:CE	1:B:463:LEU:HD12	2.43	0.49
1:B:269:MET:SD	1:B:687:LEU:HG	2.53	0.48
1:B:499:VAL:HG23	1:B:545:GLN:HE22	1.79	0.48
1:B:720:THR:O	1:B:722:ARG:HD3	2.13	0.48
1:A:808:VAL:HG11	1:A:817:ASN:HB3	1.95	0.48
1:A:575:TYR:O	1:A:576:ARG:HG2	2.14	0.48
1:A:586:ILE:HG13	1:A:608:LYS:HG2	1.94	0.48
1:B:613:LEU:HD11	1:B:624:VAL:HA	1.94	0.48
1:B:202:TYR:CE2	1:B:206:LYS:HD2	2.48	0.48
1:B:603:ALA:CA	1:B:956:ILE:CB	2.89	0.48
1:B:603:ALA:CB	1:B:955:LEU:C	2.62	0.48
1:A:265:ASP:HB3	1:A:687:LEU:CD2	2.41	0.48
1:B:456:LYS:HE3	1:B:456:LYS:N	2.28	0.48
1:B:519:LYS:O	1:B:520:ASP:CG	2.56	0.48
1:A:468:MET:HE1	1:A:516:ILE:HD12	1.94	0.48
1:A:568:ARG:HH12	1:A:616:HIS:CE1	2.32	0.48
1:B:576:ARG:HB3	1:B:578:ALA:H	1.78	0.48
1:B:260:LEU:HD22	1:B:264:GLU:CG	2.44	0.48
1:B:498:LYS:HG2	1:B:517:ILE:O	2.14	0.48
1:A:468:MET:HE1	1:A:516:ILE:CD1	2.44	0.48
1:B:496:MET:SD	1:B:498:LYS:NZ	2.86	0.48
1:A:423:ASN:O	1:A:427:LYS:HG3	2.14	0.48
1:A:443:GLU:HG2	1:A:444:PHE:N	2.29	0.48
1:A:735:LYS:HE3	1:A:739:ARG:HH21	1.79	0.48
1:B:543:SER:HA	1:B:550:LEU:HD12	1.96	0.48
1:B:603:ALA:HB3	1:B:955:LEU:C	2.39	0.48
1:B:586:ILE:HG13	1:B:608:LYS:HG2	1.94	0.47
1:B:963:LYS:HB3	1:B:963:LYS:NZ	2.28	0.47
1:A:941:GLU:HA	1:A:960:LYS:HE3	1.96	0.47
1:B:221:LEU:HD22	1:B:549:THR:C	2.31	0.47
1:B:314:GLN:HE22	1:B:317:LYS:HZ3	1.62	0.47
1:B:337:TYR:C	1:B:542:ILE:HG13	2.39	0.47
1:B:676:ARG:HG2	1:B:676:ARG:HH11	1.79	0.47
1:A:269:MET:HG3	1:A:691:ASN:HD21	1.61	0.47
1:B:468:MET:HE1	1:B:516:ILE:CD1	2.44	0.47
1:B:584:GLU:CG	1:B:953:LYS:CE	2.92	0.47
1:B:941:GLU:HA	1:B:960:LYS:HE3	1.96	0.47
1:A:547:ARG:HH11	1:A:547:ARG:CB	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:ARG:HB3	1:A:578:ALA:H	1.78	0.47
1:B:506:ASP:OD2	1:B:510:TYR:CE2	2.67	0.47
1:B:575:TYR:O	1:B:576:ARG:HG2	2.14	0.47
1:B:735:LYS:HE3	1:B:739:ARG:HH21	1.79	0.47
1:A:735:LYS:O	1:A:735:LYS:HD3	2.15	0.47
1:A:519:LYS:HD3	1:A:519:LYS:N	2.25	0.47
1:B:310:ARG:HG2	1:B:310:ARG:HH21	1.79	0.47
1:B:499:VAL:HG11	1:B:517:ILE:HD12	1.97	0.47
1:A:217:ARG:HG3	1:A:217:ARG:HH11	1.80	0.47
1:A:304:ARG:HD2	1:A:307:PHE:N	2.30	0.47
1:A:935:THR:CB	1:B:1004:GLU:OE2	2.58	0.47
1:B:457:HIS:NE2	1:B:459:ARG:NH1	2.63	0.47
1:A:260:LEU:HD22	1:A:264:GLU:CG	2.44	0.47
1:B:626:THR:HG23	1:B:965:ALA:HB2	1.96	0.47
1:B:807:SER:HA	1:B:809:TRP:CZ3	2.50	0.47
1:A:500:GLN:CD	1:A:516:ILE:HG12	2.38	0.47
1:B:568:ARG:HH12	1:B:616:HIS:CE1	2.32	0.47
1:A:630:THR:HG21	1:A:966:GLU:O	2.15	0.46
1:A:421:LYS:O	1:A:425:ILE:HG13	2.15	0.46
1:B:228:GLU:HA	1:B:228:GLU:OE1	2.15	0.46
1:B:421:LYS:O	1:B:425:ILE:HG13	2.15	0.46
1:A:202:TYR:CD2	1:A:206:LYS:HD2	2.50	0.46
1:A:530:SER:OG	1:A:533:GLU:HG3	2.15	0.46
1:A:676:ARG:HG2	1:A:676:ARG:HH11	1.79	0.46
1:A:879:ASN:CG	1:B:1010:PHE:CZ	2.93	0.46
1:A:1014:LEU:HD11	1:B:905:HIS:HE1	1.75	0.46
1:A:510:TYR:O	1:A:510:TYR:CD1	2.69	0.46
1:A:630:THR:O	1:A:965:ALA:HB1	2.14	0.46
1:A:905:HIS:CG	1:B:1019:ARG:CZ	2.98	0.46
1:B:498:LYS:CG	1:B:517:ILE:O	2.64	0.46
1:A:605:THR:HG22	1:A:607:ILE:H	1.80	0.46
1:A:506:ASP:OD2	1:A:506:ASP:O	2.33	0.46
1:B:735:LYS:CE	1:B:739:ARG:HH21	2.28	0.46
1:A:398:ARG:HH21	1:A:398:ARG:CA	2.28	0.46
1:A:735:LYS:CE	1:A:739:ARG:HH21	2.28	0.46
1:B:457:HIS:CD2	1:B:472:LYS:HG3	2.51	0.46
1:A:519:LYS:O	1:A:521:GLU:HG2	2.16	0.46
1:A:807:SER:HA	1:A:809:TRP:CZ3	2.50	0.46
1:B:468:MET:HE2	1:B:494:PHE:HD2	1.81	0.46
1:A:258:LYS:HE2	1:A:286:LEU:CD2	2.40	0.46
1:A:879:ASN:CB	1:B:1010:PHE:CZ	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ARG:HG3	1:B:217:ARG:HH11	1.80	0.46
1:B:272:GLU:CG	1:B:625:ARG:NH2	2.79	0.46
1:B:510:TYR:CD1	1:B:510:TYR:O	2.69	0.46
1:A:228:GLU:OE1	1:A:228:GLU:HA	2.15	0.45
1:A:389:LYS:HD3	1:A:389:LYS:C	2.41	0.45
1:A:458:GLU:HG2	1:A:458:GLU:O	2.17	0.45
1:A:468:MET:HE2	1:A:494:PHE:HD2	1.81	0.45
1:B:341:ARG:HG3	1:B:539:ALA:HB1	1.07	0.45
1:B:847:GLU:HG2	1:B:1035:LEU:HD21	1.98	0.45
1:A:269:MET:SD	1:A:687:LEU:CD1	2.95	0.45
1:A:500:GLN:NE2	1:A:516:ILE:HG12	2.32	0.45
1:B:605:THR:HG22	1:B:607:ILE:H	1.80	0.45
1:B:735:LYS:O	1:B:735:LYS:HD3	2.15	0.45
1:A:202:TYR:CE2	1:A:206:LYS:HD2	2.51	0.45
1:A:497:ARG:NH2	1:A:519:LYS:HB3	2.31	0.45
1:B:584:GLU:HG2	1:B:953:LYS:HG3	1.97	0.45
1:A:629:THR:HG23	1:A:969:GLY:O	2.04	0.45
1:B:254:GLU:O	1:B:258:LYS:HG2	2.17	0.45
1:B:499:VAL:CG1	1:B:517:ILE:HD12	2.46	0.45
1:B:519:LYS:HD3	1:B:520:ASP:OD2	2.17	0.45
1:A:398:ARG:HB3	1:A:398:ARG:NH2	2.31	0.45
1:A:470:CYS:HB2	1:A:492:GLU:HB2	1.99	0.45
1:A:609:LEU:HD21	1:A:962:ARG:NH1	2.32	0.45
1:A:682:ILE:HG23	1:A:686:GLN:HE21	1.82	0.45
1:B:202:TYR:CD2	1:B:206:LYS:HD2	2.52	0.45
1:B:650:ILE:HA	1:B:651:PRO:HD3	1.82	0.45
1:A:929:PHE:CE1	1:B:1003:LYS:CE	2.89	0.45
1:B:506:ASP:C	1:B:508:ASN:H	2.25	0.45
1:B:767:ARG:N	1:B:767:ARG:HD3	2.31	0.45
1:A:389:LYS:HD3	1:A:389:LYS:O	2.16	0.45
1:B:421:LYS:NZ	1:B:425:ILE:HG13	2.32	0.45
1:A:471:CYS:HB3	1:A:488:TYR:HB3	2.00	0.44
1:B:471:CYS:HB3	1:B:488:TYR:HB3	1.99	0.44
1:B:574:VAL:HG12	1:B:574:VAL:O	2.17	0.44
1:A:506:ASP:C	1:A:508:ASN:H	2.25	0.44
1:A:574:VAL:HG12	1:A:574:VAL:O	2.17	0.44
1:B:341:ARG:NH2	1:B:536:ASN:C	2.71	0.44
1:A:724:LYS:NZ	1:A:727:LYS:NZ	2.65	0.44
1:A:456:LYS:O	1:A:456:LYS:HD3	2.18	0.44
1:A:609:LEU:HD21	1:A:962:ARG:HH11	1.82	0.44
1:A:885:ARG:HD2	1:B:884:TYR:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:724:LYS:NZ	1:B:727:LYS:NZ	2.65	0.44
1:A:236:LEU:O	1:A:317:LYS:NZ	2.51	0.44
1:A:568:ARG:NH1	1:A:616:HIS:CE1	2.86	0.44
1:B:236:LEU:O	1:B:317:LYS:NZ	2.51	0.44
1:B:676:ARG:HD3	1:B:676:ARG:N	2.33	0.44
1:A:394:SER:HA	1:A:397:LYS:HZ2	1.83	0.44
1:A:676:ARG:HD3	1:A:676:ARG:N	2.33	0.44
1:A:847:GLU:HG2	1:A:1035:LEU:HD21	1.98	0.44
1:B:298:TYR:CE2	1:B:302:ILE:HG13	2.52	0.44
1:B:402:GLU:OE2	1:B:535:ASN:HB2	2.18	0.44
1:B:572:ALA:C	1:B:574:VAL:H	2.26	0.44
1:A:364:SER:HB3	1:A:370:LYS:HG3	1.99	0.44
1:A:500:GLN:HE22	1:A:516:ILE:HG12	1.82	0.44
1:A:722:ARG:HD3	1:A:722:ARG:N	2.33	0.44
1:B:457:HIS:NE2	1:B:472:LYS:HD2	2.33	0.44
1:B:498:LYS:CD	1:B:518:LEU:HD13	2.47	0.44
1:B:568:ARG:NH1	1:B:616:HIS:CE1	2.86	0.44
1:A:298:TYR:CE2	1:A:302:ILE:HG13	2.52	0.43
1:A:457:HIS:CD2	1:A:472:LYS:NZ	2.86	0.43
1:A:609:LEU:CD2	1:A:962:ARG:HH11	2.31	0.43
1:B:470:CYS:HB2	1:B:492:GLU:HB2	1.99	0.43
1:A:248:ARG:HA	1:A:248:ARG:NE	2.33	0.43
1:A:942:GLU:OE2	1:B:999:ASN:ND2	2.52	0.43
1:B:364:SER:HB3	1:B:370:LYS:HG3	1.99	0.43
1:B:682:ILE:HG23	1:B:686:GLN:HE21	1.82	0.43
1:B:872:LEU:HD12	1:B:929:PHE:CG	2.53	0.43
1:B:358:LYS:HA	1:B:358:LYS:HE2	2.01	0.43
1:B:422:MET:HG2	1:B:464:PHE:HE2	1.83	0.43
1:A:459:ARG:HG2	1:A:459:ARG:NH1	2.32	0.43
1:A:647:ARG:HA	1:A:647:ARG:HD2	1.92	0.43
1:B:248:ARG:HA	1:B:248:ARG:NE	2.33	0.43
1:B:511:LYS:HD2	1:B:511:LYS:C	2.43	0.43
1:A:872:LEU:HD12	1:A:929:PHE:CG	2.53	0.43
1:A:1010:PHE:HE2	1:B:905:HIS:HE1	1.66	0.43
1:A:511:LYS:HD2	1:A:511:LYS:C	2.43	0.43
1:A:879:ASN:CG	1:B:1010:PHE:CE2	2.97	0.43
1:B:292:PHE:HE2	1:B:353:TYR:CE2	2.36	0.43
1:A:208:PHE:CE1	1:A:353:TYR:HE1	2.37	0.43
1:A:293:ASP:N	1:A:294:PRO:CD	2.82	0.43
1:A:576:ARG:HH22	1:A:647:ARG:C	2.27	0.43
1:B:208:PHE:CE1	1:B:353:TYR:HE1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:722:ARG:HD3	1:B:722:ARG:N	2.33	0.43
1:A:339:LEU:N	1:A:340:PRO:HD2	2.34	0.43
1:A:422:MET:HG2	1:A:464:PHE:HE2	1.83	0.43
1:B:500:GLN:OE1	1:B:541:LEU:O	2.37	0.43
1:A:506:ASP:OD1	1:A:510:TYR:CD2	2.72	0.42
1:A:1019:ARG:CZ	1:B:905:HIS:CG	2.99	0.42
1:B:293:ASP:N	1:B:294:PRO:CD	2.82	0.42
1:B:339:LEU:N	1:B:340:PRO:HD2	2.34	0.42
1:B:422:MET:HG2	1:B:464:PHE:CE2	2.54	0.42
1:A:271:ASP:OD2	1:A:273:GLY:N	2.51	0.42
1:A:422:MET:HG2	1:A:464:PHE:CE2	2.54	0.42
1:B:341:ARG:NH2	1:B:539:ALA:H	2.14	0.42
1:A:292:PHE:HE2	1:A:353:TYR:CE2	2.36	0.42
1:A:341:ARG:NH2	1:A:536:ASN:HA	2.34	0.42
1:A:419:ILE:HG12	1:A:419:ILE:O	2.19	0.42
1:B:576:ARG:HH22	1:B:647:ARG:C	2.27	0.42
1:B:630:THR:CG2	1:B:805:VAL:HG11	2.49	0.42
1:A:500:GLN:NE2	1:A:514:PHE:HD1	2.18	0.42
1:A:714:MET:HE3	1:A:714:MET:HB3	1.89	0.42
1:A:777:LEU:HA	1:A:854:ARG:NH1	2.35	0.42
1:A:325:GLN:HG3	1:A:332:LYS:HD2	2.02	0.42
1:A:395:LEU:N	1:A:395:LEU:HD22	2.35	0.42
1:B:516:ILE:HG22	1:B:518:LEU:HD22	2.01	0.42
1:A:572:ALA:C	1:A:574:VAL:H	2.26	0.42
1:A:852:VAL:HG11	1:A:893:ILE:HD11	2.01	0.42
1:A:764:HIS:CG	1:A:765:ILE:H	2.38	0.42
1:B:506:ASP:OD1	1:B:510:TYR:CG	2.73	0.42
1:B:603:ALA:HA	1:B:956:ILE:CB	2.48	0.42
1:B:852:VAL:HG11	1:B:893:ILE:HD11	2.01	0.42
1:A:572:ALA:O	1:A:573:ASP:HB3	2.20	0.42
1:A:935:THR:OG1	1:B:1004:GLU:CG	2.68	0.42
1:B:777:LEU:HA	1:B:854:ARG:NH1	2.34	0.42
1:B:395:LEU:N	1:B:395:LEU:HD22	2.35	0.42
1:B:585:ASN:HB3	1:B:608:LYS:HG2	2.02	0.42
1:B:764:HIS:CG	1:B:765:ILE:N	2.88	0.42
1:A:304:ARG:CZ	1:A:399:ARG:NH1	2.65	0.41
1:A:465:ASP:HA	1:A:544:LEU:HD21	2.02	0.41
1:A:847:GLU:CD	1:A:1030:LYS:H	2.28	0.41
1:B:572:ALA:O	1:B:573:ASP:HB3	2.20	0.41
1:A:780:HIS:HE1	1:A:782:ILE:CG1	2.33	0.41
1:B:420:LYS:O	1:B:424:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:MET:HE1	1:B:438:GLY:HA2	2.02	0.41
1:B:630:THR:CG2	1:B:805:VAL:CG1	2.98	0.41
1:B:780:HIS:HE1	1:B:782:ILE:CG1	2.33	0.41
1:B:519:LYS:HB2	1:B:519:LYS:HZ3	1.85	0.41
1:B:325:GLN:HG3	1:B:332:LYS:HD2	2.02	0.41
1:B:506:ASP:OD1	1:B:506:ASP:O	2.39	0.41
1:A:544:LEU:CA	1:A:547:ARG:HH12	2.26	0.41
1:B:465:ASP:HA	1:B:544:LEU:HD21	2.02	0.41
1:B:852:VAL:CG1	1:B:893:ILE:HD11	2.51	0.41
1:B:896:ARG:HG3	1:B:897:GLN:N	2.36	0.41
1:A:459:ARG:NE	1:A:492:GLU:OE1	2.54	0.41
1:A:852:VAL:CG1	1:A:893:ILE:HD11	2.50	0.41
1:B:518:LEU:HB2	1:B:521:GLU:HB2	2.02	0.41
1:B:600:ILE:HG23	1:B:962:ARG:HH12	1.77	0.41
1:B:847:GLU:CD	1:B:1030:LYS:H	2.28	0.41
1:A:295:TYR:CD1	1:A:350:CYS:HB2	2.55	0.41
1:A:371:GLU:HA	1:A:371:GLU:OE1	2.21	0.41
1:A:923:ASN:HA	1:A:924:PRO:HD2	1.85	0.41
1:B:714:MET:HE3	1:B:714:MET:HB3	1.89	0.41
1:A:630:THR:HG22	1:A:969:GLY:HA3	0.52	0.41
1:A:1004:GLU:CG	1:B:935:THR:OG1	2.68	0.41
1:B:212:ILE:CG2	1:B:260:LEU:HG	2.51	0.41
1:B:295:TYR:CD1	1:B:350:CYS:HB2	2.55	0.41
1:B:547:ARG:NH1	1:B:548:SER:N	2.64	0.41
1:B:640:LEU:HD13	1:B:696:TRP:CZ3	2.56	0.41
1:A:896:ARG:HG3	1:A:897:GLN:N	2.36	0.41
1:B:508:ASN:C	1:B:510:TYR:H	2.29	0.41
1:A:212:ILE:CG2	1:A:260:LEU:HG	2.51	0.40
1:B:244:ASN:HB3	1:B:310:ARG:CZ	2.50	0.40
1:B:371:GLU:HA	1:B:371:GLU:OE1	2.21	0.40
1:B:459:ARG:NE	1:B:492:GLU:OE1	2.54	0.40
1:A:422:MET:HE1	1:A:438:GLY:HA2	2.02	0.40
1:A:508:ASN:C	1:A:510:TYR:H	2.29	0.40
1:A:585:ASN:HB3	1:A:608:LYS:HG2	2.02	0.40
1:B:421:LYS:HZ3	1:B:425:ILE:HG13	1.84	0.40
1:A:641:LEU:O	1:A:645:ILE:HG13	2.21	0.40
1:B:235:LYS:HB2	1:B:235:LYS:HZ2	1.84	0.40
1:A:458:GLU:CD	1:A:458:GLU:N	2.79	0.40
1:A:568:ARG:NH1	1:A:681:TYR:CD2	2.88	0.40
1:B:498:LYS:HB2	1:B:517:ILE:O	2.20	0.40
1:B:576:ARG:HD3	1:B:577:PHE:H	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:THR:HG23	1:B:801:PRO:HB3	1.99	0.40
1:A:947:VAL:HG12	1:A:949:LYS:HZ2	1.87	0.40

All (122) 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:A:293:ASP:OD2	1:B:300:ARG:NE[2_765]	0.38	1.82
1:A:894:PRO:C	1:B:575:TYR:OH[3_755]	0.54	1.66
1:A:949:LYS:CA	1:B:573:ASP:OD2[1_655]	0.56	1.64
1:A:953:LYS:CA	1:B:574:VAL:CG2[1_655]	0.66	1.54
1:A:953:LYS:N	1:B:574:VAL:CA[1_655]	0.67	1.53
1:A:953:LYS:CG	1:B:574:VAL:CG1[1_655]	0.72	1.48
1:A:949:LYS:CB	1:B:573:ASP:CG[1_655]	0.74	1.46
1:A:895:SER:N	1:B:575:TYR:CZ[3_755]	0.75	1.45
1:A:575:TYR:CE2	1:B:895:SER:O[3_845]	0.76	1.44
1:A:521:GLU:OE2	1:B:727:LYS:NZ[3_855]	0.84	1.36
1:A:953:LYS:CA	1:B:574:VAL:CB[1_655]	0.97	1.23
1:A:952:GLY:CA	1:B:575:TYR:N[1_655]	0.98	1.22
1:A:953:LYS:C	1:B:574:VAL:CG2[1_655]	0.98	1.22
1:A:952:GLY:C	1:B:574:VAL:CA[1_655]	1.06	1.14
1:A:575:TYR:OH	1:B:898:LYS:N[3_845]	1.12	1.08
1:A:953:LYS:N	1:B:574:VAL:CB[1_655]	1.12	1.08
1:A:288:GLU:O	1:B:389:LYS:NZ[2_765]	1.17	1.03
1:A:575:TYR:CE1	1:B:898:LYS:C[3_845]	1.17	1.03
1:A:575:TYR:OH	1:B:897:GLN:C[3_845]	1.18	1.02
1:A:651:PRO:CB	1:B:899:LYS:NZ[3_845]	1.18	1.02
1:A:952:GLY:C	1:B:574:VAL:N[1_655]	1.18	1.02
1:A:949:LYS:CB	1:B:573:ASP:OD2[1_655]	1.20	1.00
1:A:575:TYR:CE1	1:B:898:LYS:CA[3_845]	1.22	0.98
1:A:293:ASP:CG	1:B:300:ARG:NE[2_765]	1.23	0.97
1:A:953:LYS:CB	1:B:574:VAL:CG1[1_655]	1.25	0.95
1:A:895:SER:N	1:B:575:TYR:CE1[3_755]	1.30	0.90
1:A:895:SER:OG	1:B:575:TYR:CD1[3_755]	1.30	0.90
1:A:521:GLU:OE2	1:B:727:LYS:CE[3_855]	1.31	0.89
1:A:293:ASP:OD2	1:B:300:ARG:CZ[2_765]	1.32	0.88
1:A:894:PRO:CA	1:B:575:TYR:OH[3_755]	1.36	0.84
1:A:288:GLU:C	1:B:389:LYS:NZ[2_765]	1.42	0.78
1:A:894:PRO:C	1:B:575:TYR:CZ[3_755]	1.42	0.78
1:A:517:ILE:CG2	1:A:1044:ASN:ND2[1_655]	1.43	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:SER:N	1:B:575:TYR:OH[3_755]	1.45	0.75
1:A:952:GLY:CA	1:B:574:VAL:C[1_655]	1.46	0.74
1:A:951:HIS:O	1:B:574:VAL:O[1_655]	1.49	0.71
1:A:651:PRO:CG	1:B:899:LYS:NZ[3_845]	1.50	0.70
1:A:575:TYR:CE1	1:B:899:LYS:N[3_845]	1.53	0.67
1:A:575:TYR:CZ	1:B:898:LYS:N[3_845]	1.54	0.66
1:A:894:PRO:O	1:B:575:TYR:OH[3_755]	1.54	0.66
1:A:575:TYR:CD2	1:B:895:SER:O[3_845]	1.55	0.65
1:A:953:LYS:CD	1:B:574:VAL:CG1[1_655]	1.57	0.63
1:A:949:LYS:C	1:B:573:ASP:OD2[1_655]	1.58	0.62
1:A:949:LYS:CB	1:B:573:ASP:OD1[1_655]	1.62	0.58
1:A:953:LYS:N	1:B:574:VAL:N[1_655]	1.62	0.58
1:A:952:GLY:C	1:B:574:VAL:C[1_655]	1.63	0.57
1:A:575:TYR:CE1	1:B:898:LYS:CB[3_845]	1.65	0.55
1:A:952:GLY:CA	1:B:574:VAL:N[1_655]	1.65	0.55
1:A:521:GLU:CD	1:B:727:LYS:NZ[3_855]	1.72	0.48
1:A:521:GLU:CA	1:B:724:LYS:NZ[3_855]	1.73	0.47
1:A:575:TYR:CD2	1:B:899:LYS:CD[3_845]	1.73	0.47
1:A:575:TYR:CG	1:B:899:LYS:CD[3_845]	1.73	0.47
1:A:895:SER:OG	1:B:575:TYR:CG[3_755]	1.73	0.47
1:A:288:GLU:O	1:B:389:LYS:CE[2_765]	1.74	0.46
1:A:575:TYR:CZ	1:B:899:LYS:N[3_845]	1.74	0.46
1:A:949:LYS:CA	1:B:573:ASP:CG[1_655]	1.74	0.46
1:A:949:LYS:CB	1:B:573:ASP:CB[1_655]	1.74	0.46
1:A:521:GLU:OE2	1:B:727:LYS:CD[3_855]	1.77	0.43
1:A:575:TYR:CD2	1:B:899:LYS:CE[3_845]	1.77	0.43
1:A:575:TYR:OH	1:B:897:GLN:CA[3_845]	1.79	0.41
1:A:289:GLU:N	1:B:389:LYS:NZ[2_765]	1.80	0.40
1:A:293:ASP:OD2	1:B:300:ARG:CD[2_765]	1.80	0.40
1:A:951:HIS:O	1:B:574:VAL:C[1_655]	1.80	0.40
1:A:952:GLY:C	1:B:574:VAL:CB[1_655]	1.80	0.40
1:A:954:GLU:N	1:B:574:VAL:CG2[1_655]	1.80	0.40
1:A:575:TYR:CZ	1:B:895:SER:O[3_845]	1.81	0.39
1:A:651:PRO:CG	1:B:899:LYS:CE[3_845]	1.83	0.37
1:A:952:GLY:CA	1:B:574:VAL:CA[1_655]	1.83	0.37
1:A:952:GLY:N	1:B:575:TYR:N[1_655]	1.84	0.36
1:A:952:GLY:N	1:B:573:ASP:O[1_655]	1.86	0.34
1:A:953:LYS:N	1:B:574:VAL:CG2[1_655]	1.87	0.33
1:A:953:LYS:CB	1:B:574:VAL:CB[1_655]	1.87	0.33
1:A:575:TYR:CB	1:B:899:LYS:CD[3_845]	1.88	0.32
1:A:949:LYS:CG	1:B:573:ASP:CB[1_655]	1.89	0.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:TYR:CE2	1:B:895:SER:C[3_845]	1.90	0.30
1:A:953:LYS:CA	1:B:574:VAL:CG1[1_655]	1.90	0.30
1:A:293:ASP:CG	1:B:300:ARG:CZ[2_765]	1.91	0.29
1:A:952:GLY:N	1:B:574:VAL:C[1_655]	1.92	0.28
1:A:575:TYR:OH	1:B:897:GLN:N[3_845]	1.93	0.27
1:A:575:TYR:CE1	1:B:898:LYS:N[3_845]	1.94	0.26
1:A:895:SER:N	1:B:575:TYR:CE2[3_755]	1.94	0.26
1:A:575:TYR:CD1	1:B:898:LYS:CB[3_845]	1.96	0.24
1:A:894:PRO:CA	1:B:575:TYR:CZ[3_755]	1.96	0.24
1:A:895:SER:CA	1:B:575:TYR:CE1[3_755]	1.97	0.23
1:A:953:LYS:CB	1:B:574:VAL:CG2[1_655]	1.97	0.23
1:A:949:LYS:CD	1:B:573:ASP:CB[1_655]	1.98	0.22
1:A:289:GLU:OE1	1:B:389:LYS:CG[2_765]	1.99	0.21
1:A:522:ASN:N	1:B:724:LYS:CD[3_855]	1.99	0.21
1:A:949:LYS:N	1:B:573:ASP:OD2[1_655]	1.99	0.21
1:A:329:GLU:CG	1:A:982:ARG:NE[1_655]	2.01	0.19
1:A:289:GLU:CA	1:B:389:LYS:NZ[2_765]	2.02	0.18
1:A:290:LEU:CD1	1:B:386:GLY:O[2_765]	2.03	0.17
1:A:575:TYR:CD1	1:B:898:LYS:C[3_845]	2.03	0.17
1:A:575:TYR:CZ	1:B:898:LYS:CA[3_845]	2.03	0.17
1:A:952:GLY:O	1:B:574:VAL:N[1_655]	2.04	0.16
1:A:953:LYS:O	1:B:574:VAL:CG2[1_655]	2.04	0.16
1:A:950:ARG:NH1	1:B:579:GLU:OE2[1_655]	2.05	0.15
1:A:951:HIS:C	1:B:574:VAL:C[1_655]	2.05	0.15
1:A:952:GLY:CA	1:B:573:ASP:C[1_655]	2.08	0.12
1:A:388:GLU:OE1	1:A:507:THR:O[4_466]	2.09	0.11
1:A:894:PRO:CB	1:B:575:TYR:OH[3_755]	2.09	0.11
1:A:949:LYS:CG	1:B:573:ASP:CG[1_655]	2.09	0.11
1:A:293:ASP:OD2	1:B:300:ARG:NH2[2_765]	2.10	0.10
1:A:491:LYS:NZ	1:B:288:GLU:OE1[3_855]	2.10	0.10
1:A:953:LYS:CA	1:B:574:VAL:CA[1_655]	2.10	0.10
1:A:894:PRO:C	1:B:575:TYR:CE1[3_755]	2.12	0.08
1:A:952:GLY:C	1:B:575:TYR:N[1_655]	2.12	0.08
1:A:575:TYR:CD1	1:B:899:LYS:N[3_845]	2.13	0.07
1:A:521:GLU:CD	1:B:724:LYS:NZ[3_855]	2.14	0.06
1:A:952:GLY:N	1:B:574:VAL:CA[1_655]	2.14	0.06
1:A:329:GLU:CG	1:A:982:ARG:CZ[1_655]	2.15	0.05
1:A:651:PRO:CB	1:B:899:LYS:CE[3_845]	2.15	0.05
1:A:953:LYS:N	1:B:574:VAL:C[1_655]	2.15	0.05
1:A:289:GLU:OE1	1:B:389:LYS:CD[2_765]	2.16	0.04
1:A:329:GLU:CG	1:A:982:ARG:CD[1_655]	2.16	0.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:SER:CA	1:B:575:TYR:CZ[3_755]	2.16	0.04
1:A:952:GLY:O	1:B:574:VAL:CB[1_655]	2.16	0.04
1:A:293:ASP:OD1	1:B:300:ARG:CZ[2_765]	2.17	0.03
1:A:384:GLN:NE2	1:A:509:GLU:CD[4_466]	2.17	0.03
1:A:575:TYR:CZ	1:B:898:LYS:C[3_845]	2.18	0.02
1:A:293:ASP:CG	1:B:300:ARG:CD[2_765]	2.19	0.01
1:A:895:SER:OG	1:B:575:TYR:CE1[3_755]	2.19	0.01

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	744/847 (88%)	709 (95%)	31 (4%)	4 (0%)	24	61
1	B	745/847 (88%)	710 (95%)	31 (4%)	4 (0%)	24	61
All	All	1489/1694 (88%)	1419 (95%)	62 (4%)	8 (0%)	24	61

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1020	ASN
1	B	1020	ASN
1	A	497	ARG
1	A	508	ASN
1	B	497	ARG
1	B	508	ASN
1	A	440	CYS
1	B	440	CYS

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	698/773 (90%)	664 (95%)	34 (5%)	22	46
1	B	699/773 (90%)	659 (94%)	40 (6%)	18	43
All	All	1397/1546 (90%)	1323 (95%)	74 (5%)	20	44

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	GLN
1	A	255	LEU
1	A	258	LYS
1	A	259	LEU
1	A	260	LEU
1	A	271	ASP
1	A	304	ARG
1	A	356	LEU
1	A	397	LYS
1	A	463	LEU
1	A	497	ARG
1	A	498	LYS
1	A	511	LYS
1	A	529	LYS
1	A	544	LEU
1	A	547	ARG
1	A	575	TYR
1	A	576	ARG
1	A	609	LEU
1	A	640	LEU
1	A	644	ILE
1	A	680	GLU
1	A	720	THR
1	A	724	LYS
1	A	730	VAL
1	A	808	VAL
1	A	821	LEU
1	A	831	LEU
1	A	860	GLN
1	A	885	ARG
1	A	919	LEU

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Mol	Chain	Res	Type
1	A	955	LEU
1	A	968	THR
1	A	1040	VAL
1	B	214	GLN
1	B	235	LYS
1	B	255	LEU
1	B	258	LYS
1	B	259	LEU
1	B	260	LEU
1	B	269	MET
1	B	356	LEU
1	B	389	LYS
1	B	421	LYS
1	B	456	LYS
1	B	463	LEU
1	B	498	LYS
1	B	504	LYS
1	B	511	LYS
1	B	519	LYS
1	B	529	LYS
1	B	544	LEU
1	B	547	ARG
1	B	575	TYR
1	B	576	ARG
1	B	609	LEU
1	B	640	LEU
1	B	644	ILE
1	B	680	GLU
1	B	720	THR
1	B	724	LYS
1	B	730	VAL
1	B	767	ARG
1	B	808	VAL
1	B	821	LEU
1	B	831	LEU
1	B	860	GLN
1	B	885	ARG
1	B	899	LYS
1	B	919	LEU
1	B	955	LEU
1	B	968	THR
1	B	1036	LYS

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Mol	Chain	Res	Type
1	B	1040	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	ASN
1	A	244	ASN
1	A	276	HIS
1	A	314	GLN
1	A	359	GLN
1	A	375	GLN
1	A	428	ASN
1	A	457	HIS
1	A	500	GLN
1	A	508	ASN
1	A	585	ASN
1	A	683	GLN
1	A	686	GLN
1	A	691	ASN
1	A	695	HIS
1	A	699	HIS
1	A	863	GLN
1	A	866	ASN
1	A	888	HIS
1	A	936	ASN
1	B	214	GLN
1	B	240	ASN
1	B	244	ASN
1	B	276	HIS
1	B	314	GLN
1	B	336	GLN
1	B	352	HIS
1	B	359	GLN
1	B	375	GLN
1	B	428	ASN
1	B	508	ASN
1	B	585	ASN
1	B	683	GLN
1	B	686	GLN
1	B	691	ASN
1	B	695	HIS
1	B	699	HIS

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Mol	Chain	Res	Type
1	B	770	HIS
1	B	863	GLN
1	B	866	ASN
1	B	888	HIS
1	B	936	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	758/847 (89%)	0.66	46 (6%) 27 25	27, 27, 27, 27	0
1	B	759/847 (89%)	0.58	36 (4%) 36 30	27, 27, 27, 27	0
All	All	1517/1694 (89%)	0.62	82 (5%) 31 27	27, 27, 27, 27	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	261	GLY	6.0
1	B	549	THR	5.2
1	A	959	SER	4.7
1	B	466	GLY	4.6
1	A	952	GLY	3.9
1	B	268	GLU	3.9
1	B	957	ASN	3.9
1	A	951	HIS	3.7
1	B	528	ALA	3.7
1	A	265	ASP	3.5
1	B	465	ASP	3.4
1	B	500	GLN	3.4
1	B	965	ALA	3.3
1	A	935	THR	3.2
1	A	973	GLN	3.2
1	B	880	SER	3.1
1	B	536	ASN	3.1
1	B	527	SER	3.1
1	B	375	GLN	3.0
1	B	642	SER	3.0
1	A	304	ARG	2.9
1	A	969	GLY	2.9
1	A	947	VAL	2.9
1	B	942	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	955	LEU	2.9
1	B	732	SER	2.8
1	B	958	PHE	2.8
1	A	825	ILE	2.8
1	A	404	ALA	2.8
1	B	881	SER	2.8
1	B	297	SER	2.7
1	A	1044	ASN	2.7
1	A	828	THR	2.7
1	B	440	CYS	2.7
1	A	282	CYS	2.6
1	B	503	ASP	2.6
1	A	548	SER	2.6
1	A	470	CYS	2.6
1	B	510	TYR	2.6
1	B	1002	GLU	2.6
1	A	438	GLY	2.6
1	A	500	GLN	2.5
1	B	877	ALA	2.5
1	A	972	GLN	2.5
1	B	448	GLY	2.5
1	A	818	SER	2.5
1	A	220	ASN	2.5
1	A	372	CYS	2.4
1	B	369	ASP	2.4
1	B	535	ASN	2.4
1	A	394	SER	2.4
1	A	880	SER	2.4
1	A	822	LEU	2.3
1	B	445	ILE	2.3
1	A	568	ARG	2.3
1	A	535	ASN	2.3
1	B	288	GLU	2.3
1	A	876	SER	2.3
1	A	203	ASP	2.3
1	A	895	SER	2.3
1	A	398	ARG	2.3
1	A	881	SER	2.2
1	A	329	GLU	2.2
1	A	306	GLY	2.2
1	A	982	ARG	2.2
1	B	438	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	530	SER	2.2
1	A	873	GLU	2.2
1	B	850	ALA	2.1
1	A	313	SER	2.1
1	A	326	SER	2.1
1	B	542	ILE	2.1
1	A	817	ASN	2.1
1	B	334	ALA	2.1
1	A	511	LYS	2.1
1	B	956	ILE	2.1
1	A	211	GLU	2.1
1	A	531	ALA	2.0
1	A	962	ARG	2.0
1	B	515	GLU	2.0
1	B	247	SER	2.0
1	A	968	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.