



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:20 PM UTC

PDB ID : 7DRR / pdb_00007drr
Title : Structure of SspE-R100A protein
Authors : Haiyan, G.; Jinchuan, Z.; Chen, S.; Wang, L.; Wu, G.
Deposited on : 2020-12-29
Resolution : 3.48 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

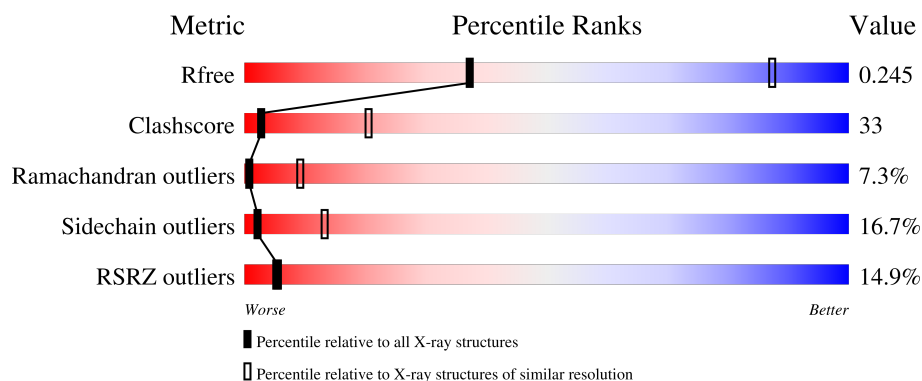
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 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	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)

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	771	
1	B	771	
1	C	771	
1	D	771	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24524 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 SspE protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	771	Total	C	N	O	S	0	0	0
			6131	3869	1076	1166	20			
1	A	771	Total	C	N	O	S	0	0	0
			6131	3869	1076	1166	20			
1	B	771	Total	C	N	O	S	0	0	0
			6131	3869	1076	1166	20			
1	C	771	Total	C	N	O	S	0	0	0
			6131	3869	1076	1166	20			

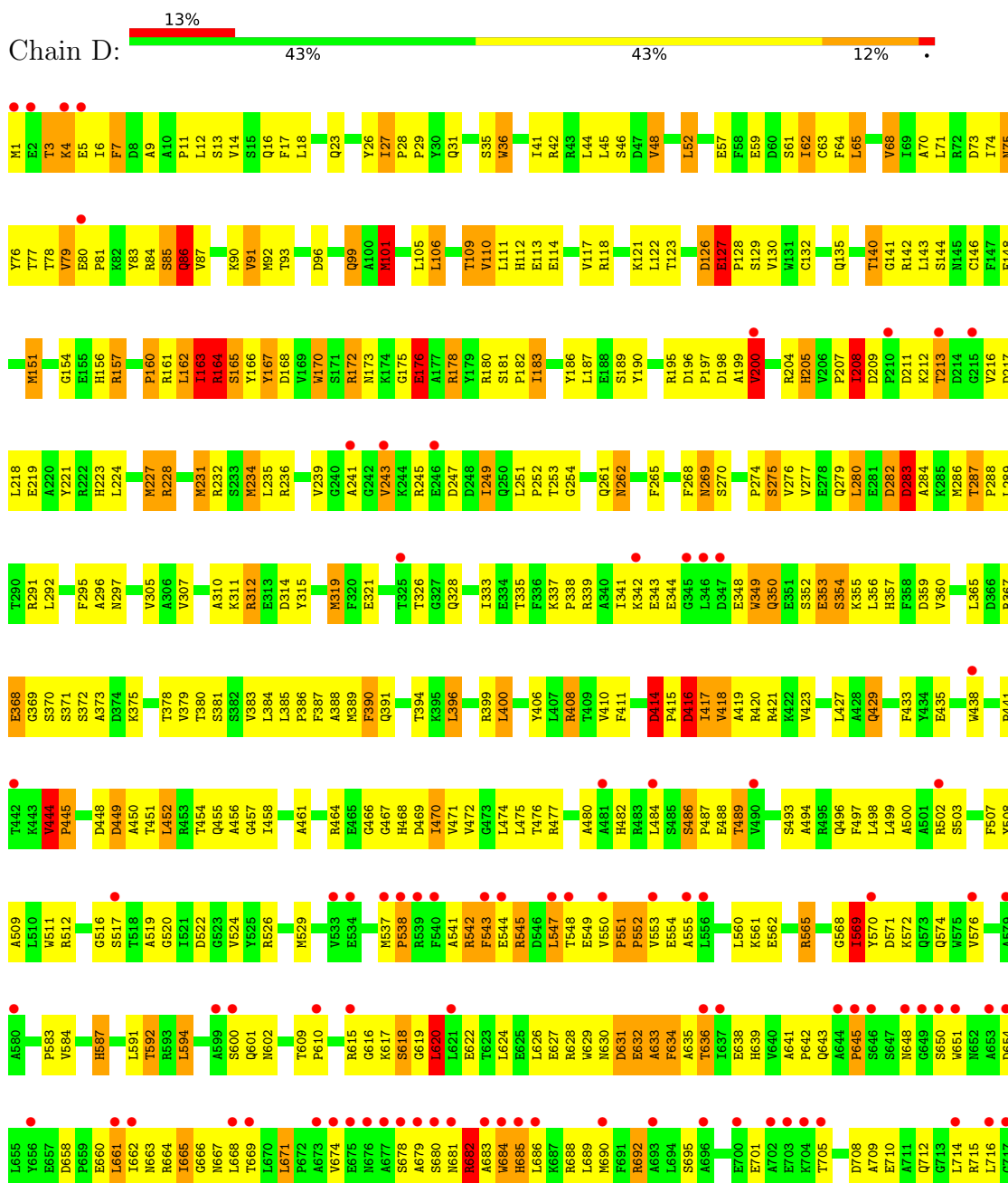
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	100	ALA	ARG	engineered mutation	UNP A0A6I8WFL9
A	100	ALA	ARG	engineered mutation	UNP A0A6I8WFL9
B	100	ALA	ARG	engineered mutation	UNP A0A6I8WFL9
C	100	ALA	ARG	engineered mutation	UNP A0A6I8WFL9

3 Residue-property plots

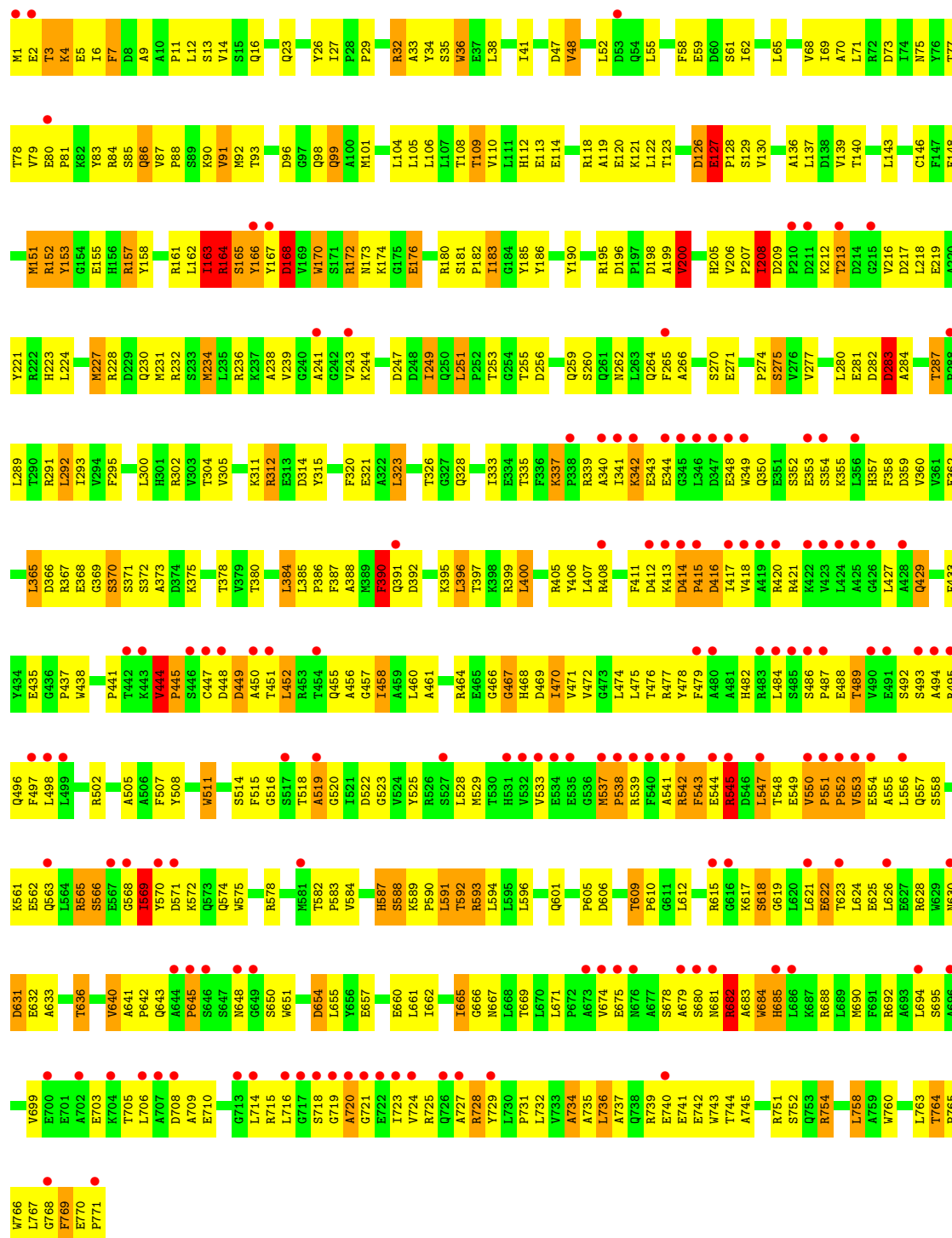
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

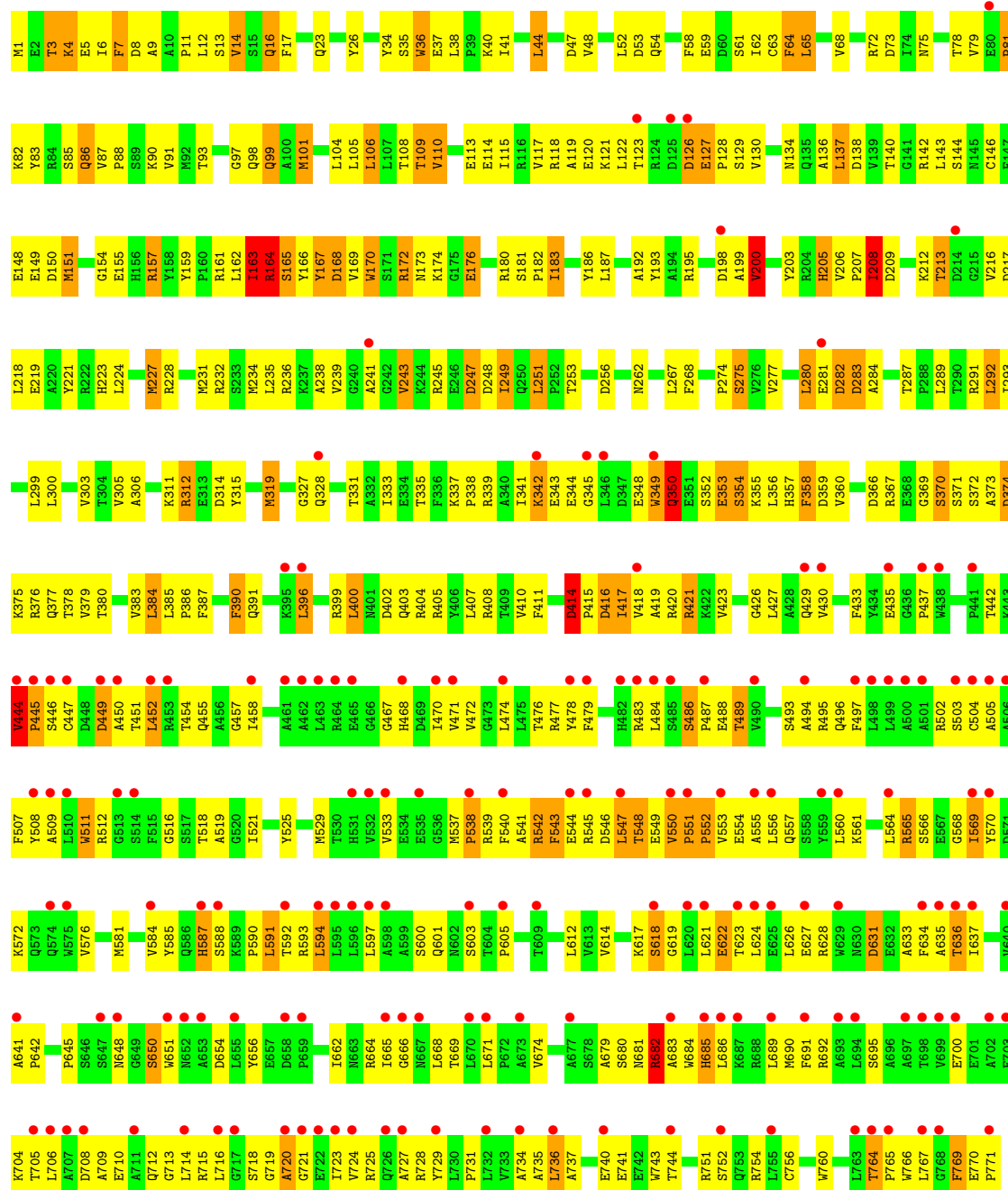




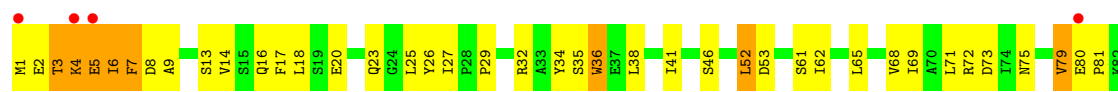
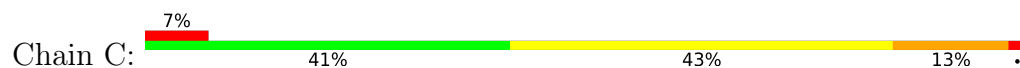
● Molecule 1: SspE protein

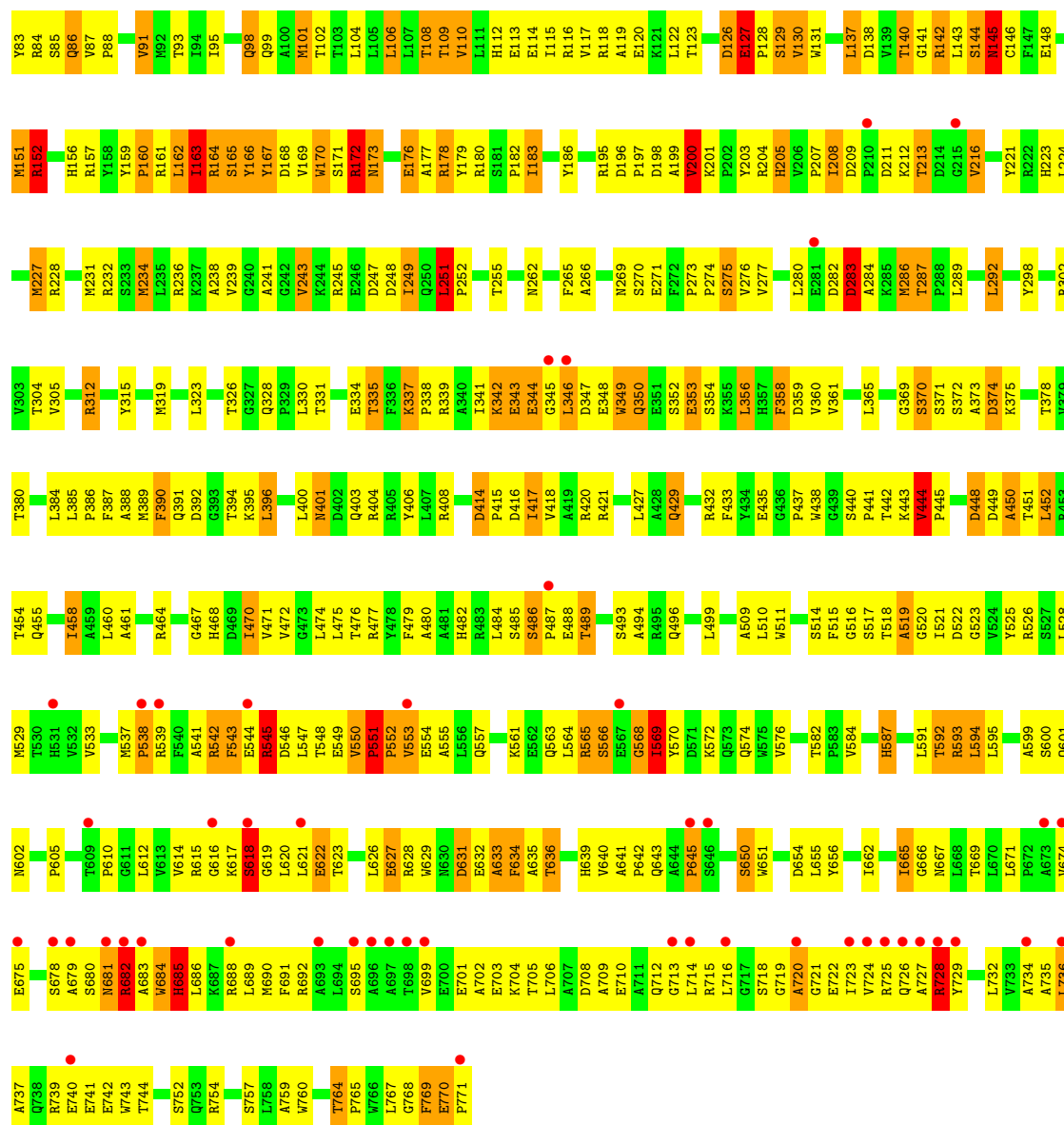


● Molecule 1: SspE protein



• Molecule 1: SspE protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.03Å 137.97Å 292.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.54 – 3.48 36.54 – 3.48	Depositor EDS
% Data completeness (in resolution range)	93.3 (36.54-3.48) 93.3 (36.54-3.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.5	Depositor
R, R_{free}	0.224 , 0.294 0.240 , 0.245	Depositor DCC
R_{free} test set	2673 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 67.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	24524	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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	0.63	0/6266	0.99	9/8508 (0.1%)
1	B	0.63	0/6266	0.95	6/8508 (0.1%)
1	C	0.87	1/6266 (0.0%)	1.16	15/8508 (0.2%)
1	D	0.69	2/6266 (0.0%)	1.05	16/8508 (0.2%)
All	All	0.71	3/25064 (0.0%)	1.04	46/34032 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	6
1	D	0	1
All	All	0	9

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	127	GLU	C-N	6.57	1.43	1.33
1	C	145	ASN	CA-C	-6.49	1.41	1.52
1	D	170	TRP	CG-CD2	-5.34	1.34	1.43

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	151	MET	CA-C-N	-9.99	106.05	122.54
1	C	151	MET	C-N-CA	-9.99	106.05	122.54
1	D	151	MET	CA-C-N	-9.40	107.92	122.49
1	D	151	MET	C-N-CA	-9.40	107.92	122.49
1	D	319	MET	CB-CG-SD	-8.81	86.26	112.70
1	B	151	MET	CA-C-N	-7.05	110.06	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	MET	C-N-CA	-7.05	110.06	122.26
1	D	178	ARG	CB-CG-CD	-7.00	95.19	111.30
1	A	416	ASP	CA-C-N	6.96	134.51	121.97
1	A	416	ASP	C-N-CA	6.96	134.51	121.97
1	C	345	GLY	N-CA-C	-6.94	93.17	113.30
1	D	170	TRP	CA-CB-CG	6.87	126.65	113.60
1	D	85	SER	CA-C-N	-6.79	109.25	122.62
1	D	85	SER	C-N-CA	-6.79	109.25	122.62
1	C	251	LEU	CA-CB-CG	6.54	139.20	116.30
1	D	121	LYS	O-C-N	-6.52	113.92	122.59
1	C	152	ARG	CB-CG-CD	-6.22	97.00	111.30
1	B	170	TRP	CA-CB-CG	6.13	125.24	113.60
1	C	178	ARG	CB-CG-CD	-6.04	97.40	111.30
1	A	170	TRP	CA-CB-CG	5.97	124.94	113.60
1	B	251	LEU	CA-CB-CG	5.83	136.71	116.30
1	B	319	MET	CB-CG-SD	-5.76	95.41	112.70
1	D	176	GLU	N-CA-C	5.73	123.01	110.80
1	C	142	ARG	NE-CZ-NH1	-5.68	115.82	121.50
1	C	545	ARG	CA-C-N	-5.55	110.02	119.35
1	C	545	ARG	C-N-CA	-5.55	110.02	119.35
1	D	86	GLN	CB-CG-CD	-5.45	103.33	112.60
1	C	178	ARG	CA-CB-CG	5.43	124.97	114.10
1	C	172	ARG	CG-CD-NE	5.43	123.94	112.00
1	A	337	LYS	CD-CE-NZ	5.38	129.11	111.90
1	C	346	LEU	CA-CB-CG	5.34	135.00	116.30
1	D	178	ARG	CG-CD-NE	5.32	123.71	112.00
1	C	170	TRP	CA-CB-CG	5.32	123.71	113.60
1	D	162	LEU	CA-C-N	-5.32	112.40	121.97
1	D	162	LEU	C-N-CA	-5.32	112.40	121.97
1	A	593	ARG	CG-CD-NE	-5.31	100.32	112.00
1	A	556	LEU	CA-CB-CG	5.26	134.72	116.30
1	D	101	MET	CB-CG-SD	-5.26	96.92	112.70
1	D	417	ILE	N-CA-C	-5.23	98.46	109.34
1	B	345	GLY	N-CA-C	-5.23	98.14	113.30
1	A	545	ARG	CA-C-N	-5.22	111.57	121.54
1	A	545	ARG	C-N-CA	-5.22	111.57	121.54
1	C	283	ASP	N-CA-C	5.14	121.75	110.80
1	A	126	ASP	N-CA-C	-5.13	106.57	114.16
1	D	368	GLU	CA-CB-CG	-5.09	103.91	114.10
1	C	417	ILE	N-CA-C	-5.03	98.88	109.34

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	PRO	Peptide
1	A	553	VAL	Peptide
1	C	173	ASN	Peptide
1	C	344	GLU	Peptide
1	C	551	PRO	Peptide
1	C	553	VAL	Peptide
1	C	681	ASN	Peptide
1	C	79	VAL	Peptide
1	D	175	GLY	Peptide

5.2 Too-close contacts [i](#)

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	6131	0	6038	397	1
1	B	6131	0	6038	392	1
1	C	6131	0	6038	444	2
1	D	6131	0	6038	401	2
All	All	24524	0	24152	1616	3

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 33.

All (1616) 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:D:126:ASP:HB3	1:D:129:SER:HB3	1.37	1.05
1:A:126:ASP:HB3	1:A:129:SER:HB3	1.36	1.04
1:C:173:ASN:HB2	1:C:176:GLU:OE2	1.57	1.02
1:D:183:ILE:HD12	1:D:183:ILE:H	1.26	0.98
1:C:243:VAL:HG11	1:C:245:ARG:HH21	1.27	0.96
1:A:182:PRO:HB2	1:A:224:LEU:HD13	1.51	0.93
1:A:688:ARG:NH1	1:A:740:GLU:OE2	2.01	0.93
1:A:32:ARG:O	1:A:164:ARG:NH2	2.04	0.91
1:A:612:LEU:HB3	1:A:754:ARG:HD3	1.50	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:692:ARG:HG3	1:D:737:ALA:HB1	1.53	0.89
1:C:688:ARG:NH1	1:C:740:GLU:OE2	2.05	0.89
1:B:126:ASP:HB3	1:B:129:SER:HB3	1.50	0.89
1:A:628:ARG:HA	1:A:631:ASP:HB2	1.55	0.89
1:B:612:LEU:HB3	1:B:754:ARG:HD3	1.55	0.89
1:D:622:GLU:O	1:D:628:ARG:NH1	2.07	0.88
1:D:724:VAL:HG12	1:D:725:ARG:HG3	1.55	0.88
1:C:628:ARG:HA	1:C:631:ASP:HB2	1.53	0.88
1:C:614:VAL:HG12	1:C:754:ARG:HH11	1.38	0.87
1:A:339:ARG:HG2	1:A:408:ARG:HH22	1.39	0.87
1:D:367:ARG:NH1	1:D:435:GLU:OE2	2.09	0.86
1:D:113:GLU:OE2	1:D:232:ARG:NH2	2.07	0.86
1:A:449:ASP:HB3	1:A:452:LEU:HB2	1.57	0.85
1:C:223:HIS:HE1	1:C:227:MET:HE2	1.41	0.85
1:A:484:LEU:HB3	1:A:548:THR:HG22	1.58	0.85
1:C:1:MET:HA	1:C:4:LYS:HB2	1.56	0.85
1:C:106:LEU:HB3	1:C:231:MET:HE1	1.57	0.85
1:C:441:PRO:HG2	1:C:461:ALA:HB2	1.59	0.85
1:B:565:ARG:HH21	1:B:771:PRO:HB3	1.41	0.85
1:C:183:ILE:H	1:C:183:ILE:HD12	1.42	0.85
1:D:114:GLU:OE1	1:D:118:ARG:NH1	2.08	0.85
1:A:339:ARG:HG2	1:A:408:ARG:NH2	1.91	0.84
1:A:455:GLN:OE1	1:A:502:ARG:NH2	2.10	0.84
1:A:496:GLN:HA	1:A:553:VAL:HG13	1.59	0.84
1:A:385:LEU:HD22	1:A:396:LEU:HB3	1.60	0.83
1:C:161:ARG:O	1:C:162:LEU:HB2	1.77	0.83
1:B:477:ARG:HD3	1:B:542:ARG:H	1.42	0.83
1:B:628:ARG:HA	1:B:631:ASP:HB2	1.59	0.83
1:D:161:ARG:O	1:D:162:LEU:HB2	1.79	0.82
1:A:449:ASP:O	1:A:452:LEU:N	2.12	0.82
1:A:715:ARG:HB3	1:A:719:GLY:HA2	1.61	0.82
1:C:622:GLU:O	1:C:628:ARG:NH1	2.13	0.82
1:C:477:ARG:HD3	1:C:542:ARG:H	1.45	0.82
1:B:614:VAL:HG12	1:B:754:ARG:HH11	1.44	0.81
1:C:223:HIS:CE1	1:C:227:MET:HE2	2.15	0.81
1:C:17:PHE:CE2	1:C:101:MET:HE3	2.14	0.81
1:C:680:SER:HA	1:C:690:MET:HE1	1.61	0.81
1:D:617:LYS:O	1:D:619:GLY:N	2.13	0.81
1:A:208:ILE:HG21	1:A:221:TYR:CD2	2.15	0.81
1:A:692:ARG:HG3	1:A:737:ALA:HB1	1.60	0.81
1:B:9:ALA:HB3	1:C:9:ALA:HB3	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:THR:O	1:C:5:GLU:N	2.14	0.81
1:D:209:ASP:OD1	1:D:212:LYS:N	2.13	0.81
1:D:9:ALA:HB3	1:A:9:ALA:HB3	1.61	0.81
1:A:680:SER:O	1:A:682:ARG:NH2	2.13	0.80
1:A:208:ILE:HG21	1:A:221:TYR:HD2	1.47	0.80
1:A:542:ARG:HE	1:A:547:LEU:HD12	1.47	0.80
1:A:1:MET:HA	1:A:4:LYS:HB2	1.64	0.79
1:D:469:ASP:O	1:D:472:VAL:HG23	1.82	0.79
1:D:628:ARG:HA	1:D:631:ASP:HB2	1.64	0.79
1:D:111:LEU:HD22	1:D:296:ALA:HB2	1.65	0.79
1:D:208:ILE:HG21	1:D:221:TYR:CD2	2.18	0.79
1:C:692:ARG:HG3	1:C:737:ALA:HB1	1.63	0.79
1:A:173:ASN:HB2	1:A:176:GLU:OE2	1.83	0.78
1:A:12:LEU:HA	1:A:16:GLN:HE21	1.49	0.78
1:D:760:TRP:O	1:D:764:THR:OG1	2.02	0.78
1:A:337:LYS:HZ1	1:A:358:PHE:HD1	1.29	0.78
1:C:485:SER:OG	1:C:489:THR:OG1	2.00	0.78
1:B:715:ARG:HB3	1:B:719:GLY:HA2	1.64	0.78
1:A:477:ARG:HD3	1:A:542:ARG:H	1.49	0.78
1:D:161:ARG:HA	1:D:170:TRP:HH2	1.48	0.78
1:C:651:TRP:NE1	1:C:683:ALA:HA	1.99	0.78
1:B:692:ARG:HG3	1:B:737:ALA:HB1	1.66	0.77
1:C:344:GLU:OE1	1:C:421:ARG:NH2	2.17	0.77
1:C:511:TRP:HH2	1:C:519:ALA:HB3	1.50	0.77
1:C:617:LYS:O	1:C:619:GLY:N	2.17	0.77
1:C:474:LEU:N	1:C:529:MET:HE1	1.99	0.77
1:D:110:VAL:HA	1:D:228:ARG:HH11	1.49	0.77
1:A:196:ASP:HB3	1:A:199:ALA:HB2	1.67	0.77
1:A:542:ARG:HD3	1:A:547:LEU:H	1.50	0.77
1:B:161:ARG:O	1:B:162:LEU:HB2	1.84	0.77
1:D:715:ARG:HB3	1:D:719:GLY:HA2	1.67	0.77
1:C:127:GLU:HB3	1:C:128:PRO:HD2	1.67	0.77
1:D:474:LEU:O	1:D:477:ARG:HB3	1.84	0.77
1:C:612:LEU:HB3	1:C:754:ARG:HD3	1.65	0.77
1:C:474:LEU:H	1:C:529:MET:HE1	1.48	0.76
1:C:665:ILE:HD13	1:C:665:ILE:H	1.51	0.76
1:B:47:ASP:OD1	1:B:399:ARG:NH2	2.19	0.76
1:C:208:ILE:HG13	1:C:209:ASP:H	1.47	0.76
1:A:724:VAL:HG12	1:A:725:ARG:HG3	1.67	0.76
1:B:58:PHE:CE2	1:B:405:ARG:HD3	2.20	0.76
1:B:680:SER:O	1:B:682:ARG:NH2	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:ASN:HB2	1:D:176:GLU:OE2	1.85	0.76
1:A:477:ARG:NH2	1:A:547:LEU:O	2.18	0.76
1:B:312:ARG:HD3	1:B:315:TYR:CE2	2.21	0.76
1:A:3:THR:O	1:A:5:GLU:N	2.19	0.76
1:B:3:THR:O	1:B:5:GLU:N	2.19	0.75
1:C:511:TRP:CH2	1:C:519:ALA:HB3	2.21	0.75
1:D:110:VAL:HG12	1:D:228:ARG:HE	1.50	0.75
1:D:543:PHE:O	1:D:545:ARG:NH2	2.16	0.75
1:B:344:GLU:OE1	1:B:421:ARG:NH2	2.19	0.75
1:A:128:PRO:HG3	1:A:275:SER:HB2	1.67	0.75
1:D:3:THR:O	1:D:5:GLU:N	2.20	0.75
1:A:126:ASP:CB	1:A:129:SER:HB3	2.14	0.75
1:A:570:TYR:HB2	1:A:769:PHE:HZ	1.52	0.74
1:B:565:ARG:HG2	1:B:570:TYR:CE2	2.22	0.74
1:C:343:GLU:OE2	1:C:420:ARG:CZ	2.35	0.74
1:D:183:ILE:H	1:D:183:ILE:CD1	1.98	0.74
1:D:680:SER:O	1:D:682:ARG:NH2	2.20	0.74
1:B:26:TYR:HD2	1:B:93:THR:HG22	1.53	0.73
1:C:553:VAL:HB	1:C:554:GLU:HG3	1.68	0.73
1:D:5:GLU:O	1:D:7:PHE:N	2.20	0.73
1:C:167:TYR:CZ	1:C:216:VAL:HG22	2.24	0.73
1:C:390:PHE:HE1	1:C:542:ARG:HG2	1.54	0.73
1:B:36:TRP:CD1	1:B:99:GLN:HG2	2.23	0.73
1:A:183:ILE:H	1:A:183:ILE:HD12	1.53	0.73
1:D:86:GLN:HE22	1:D:172:ARG:H	1.37	0.73
1:C:213:THR:O	1:C:213:THR:OG1	2.05	0.73
1:A:553:VAL:HB	1:A:554:GLU:HG3	1.71	0.73
1:B:5:GLU:O	1:B:7:PHE:N	2.20	0.72
1:C:127:GLU:HB3	1:C:128:PRO:CD	2.18	0.72
1:C:474:LEU:O	1:C:477:ARG:HB3	1.89	0.72
1:B:73:ASP:OD2	1:B:78:THR:OG1	2.05	0.72
1:C:544:GLU:HB2	1:C:545:ARG:NH2	2.05	0.72
1:C:232:ARG:HD3	1:C:236:ARG:CZ	2.20	0.72
1:D:552:PRO:HG2	1:D:555:ALA:H	1.53	0.72
1:B:12:LEU:HB3	1:B:16:GLN:HG3	1.71	0.72
1:B:617:LYS:O	1:B:619:GLY:N	2.23	0.72
1:A:470:ILE:HG21	1:A:522:ASP:HA	1.71	0.72
1:B:312:ARG:HD3	1:B:315:TYR:HE2	1.56	0.71
1:B:710:GLU:HA	1:B:714:LEU:H	1.55	0.71
1:A:544:GLU:HB2	1:A:545:ARG:NH2	2.05	0.71
1:C:715:ARG:HB3	1:C:719:GLY:HA2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:529:MET:SD	1:D:541:ALA:HB2	2.31	0.71
1:D:449:ASP:O	1:D:451:THR:N	2.23	0.71
1:C:544:GLU:HB2	1:C:545:ARG:HH22	1.56	0.71
1:B:37:GLU:H	1:B:40:LYS:HZ1	1.38	0.71
1:B:182:PRO:HD3	1:B:221:TYR:HE1	1.55	0.71
1:D:375:LYS:O	1:D:378:THR:HG22	1.91	0.71
1:C:680:SER:O	1:C:682:ARG:NH2	2.23	0.71
1:A:341:ILE:HG12	1:A:349:TRP:CZ2	2.25	0.71
1:B:7:PHE:C	1:B:7:PHE:CD2	2.69	0.71
1:B:333:ILE:HD12	1:B:380:THR:HG23	1.73	0.71
1:D:651:TRP:NE1	1:D:683:ALA:HA	2.05	0.70
1:B:385:LEU:HD22	1:B:396:LEU:HB3	1.73	0.70
1:D:127:GLU:HB3	1:D:128:PRO:HD2	1.73	0.70
1:A:617:LYS:O	1:A:619:GLY:N	2.24	0.70
1:C:172:ARG:HH11	1:C:172:ARG:HG3	1.56	0.70
1:C:517:SER:O	1:C:519:ALA:N	2.24	0.70
1:A:118:ARG:HB2	1:A:289:LEU:HD13	1.71	0.70
1:A:208:ILE:HD13	1:A:209:ASP:H	1.55	0.70
1:B:151:MET:HB3	1:B:172:ARG:HH11	1.57	0.70
1:D:720:ALA:HB1	1:D:723:ILE:HD12	1.73	0.70
1:A:387:PHE:CE2	1:A:427:LEU:HG	2.26	0.70
1:C:113:GLU:O	1:C:117:VAL:HG12	1.91	0.70
1:B:208:ILE:HD13	1:B:209:ASP:H	1.56	0.70
1:C:520:GLY:O	1:C:523:GLY:N	2.25	0.70
1:D:3:THR:HG22	1:A:16:GLN:HE22	1.57	0.70
1:A:12:LEU:HB3	1:A:16:GLN:HG3	1.72	0.70
1:A:47:ASP:OD1	1:A:399:ARG:NH2	2.24	0.70
1:A:391:GLN:OE1	1:A:542:ARG:NH1	2.24	0.70
1:C:3:THR:O	1:C:3:THR:OG1	2.05	0.70
1:A:161:ARG:O	1:A:162:LEU:HB2	1.90	0.70
1:C:496:GLN:HA	1:C:553:VAL:HG13	1.73	0.69
1:B:183:ILE:HD12	1:B:183:ILE:H	1.57	0.69
1:D:326:THR:HG21	1:A:323:LEU:O	1.92	0.69
1:D:449:ASP:O	1:D:452:LEU:N	2.26	0.69
1:A:674:VAL:HG11	1:A:679:ALA:H	1.58	0.69
1:D:73:ASP:OD2	1:D:78:THR:OG1	2.10	0.69
1:A:412:ASP:OD1	1:A:420:ARG:NH2	2.26	0.69
1:B:148:GLU:OE1	1:B:195:ARG:NH1	2.26	0.69
1:C:651:TRP:CZ3	1:C:684:TRP:HB2	2.28	0.69
1:D:484:LEU:HB3	1:D:548:THR:HG22	1.75	0.69
1:A:36:TRP:CD1	1:A:99:GLN:HG2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:SER:OG	1:A:619:GLY:N	2.26	0.69
1:C:209:ASP:OD1	1:C:212:LYS:N	2.26	0.69
1:A:572:LYS:HE2	1:A:760:TRP:CZ3	2.27	0.69
1:B:417:ILE:HG23	1:B:418:VAL:HG23	1.75	0.69
1:D:12:LEU:HB3	1:D:16:GLN:HG3	1.75	0.68
1:C:538:PRO:HB3	1:C:550:VAL:HG22	1.75	0.68
1:D:441:PRO:HG2	1:D:461:ALA:HB2	1.75	0.68
1:A:412:ASP:HA	1:A:420:ARG:HH21	1.58	0.68
1:D:641:ALA:HB3	1:D:667:ASN:HD21	1.58	0.68
1:B:418:VAL:HA	1:B:421:ARG:HD2	1.76	0.68
1:B:705:THR:HA	1:B:708:ASP:HB2	1.75	0.68
1:B:127:GLU:OE2	1:B:128:PRO:HD3	1.94	0.68
1:C:183:ILE:H	1:C:183:ILE:CD1	2.07	0.68
1:C:674:VAL:HG11	1:C:679:ALA:H	1.59	0.68
1:A:621:LEU:HD12	1:A:729:TYR:HD2	1.58	0.68
1:B:525:TYR:O	1:B:529:MET:HG2	1.94	0.68
1:C:705:THR:HA	1:C:708:ASP:HB2	1.74	0.68
1:B:208:ILE:HG21	1:B:221:TYR:CD2	2.29	0.68
1:B:651:TRP:CZ3	1:B:684:TRP:HB2	2.29	0.68
1:B:213:THR:O	1:B:213:THR:OG1	2.11	0.67
1:C:470:ILE:HD12	1:C:522:ASP:OD2	1.94	0.67
1:D:208:ILE:HG21	1:D:221:TYR:HD2	1.58	0.67
1:A:114:GLU:OE1	1:A:118:ARG:NH1	2.26	0.67
1:A:239:VAL:HG12	1:A:251:LEU:HD21	1.76	0.67
1:C:666:GLY:H	1:C:752:SER:HB3	1.59	0.67
1:A:666:GLY:H	1:A:752:SER:HB3	1.59	0.67
1:A:414:ASP:O	1:A:416:ASP:N	2.26	0.67
1:A:511:TRP:CZ3	1:A:519:ALA:HB3	2.29	0.67
1:C:168:ASP:OD1	1:C:180:ARG:N	2.24	0.67
1:A:414:ASP:OD2	1:A:416:ASP:OD2	2.12	0.67
1:B:113:GLU:OE2	1:B:232:ARG:NH2	2.28	0.67
1:D:542:ARG:HE	1:D:547:LEU:HD12	1.58	0.67
1:D:728:ARG:HD3	1:D:729:TYR:N	2.09	0.67
1:C:126:ASP:HB3	1:C:129:SER:HB3	1.77	0.67
1:D:418:VAL:H	1:D:421:ARG:HD2	1.60	0.67
1:D:7:PHE:HD1	1:D:319:MET:SD	2.18	0.67
1:C:486:SER:O	1:C:488:GLU:N	2.28	0.67
1:C:599:ALA:HB2	1:C:759:ALA:HB2	1.77	0.67
1:B:474:LEU:O	1:B:477:ARG:HB3	1.93	0.67
1:B:564:LEU:HB3	1:B:570:TYR:HB3	1.77	0.67
1:C:4:LYS:O	1:C:5:GLU:HG3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:680:SER:HA	1:D:690:MET:HE1	1.75	0.67
1:A:105:LEU:HD23	1:A:162:LEU:HD12	1.77	0.66
1:B:680:SER:HA	1:B:690:MET:HE1	1.76	0.66
1:C:437:PRO:HD3	1:C:479:PHE:CE2	2.29	0.66
1:D:11:PRO:O	1:D:12:LEU:HD23	1.95	0.66
1:D:438:TRP:CE3	1:D:464:ARG:HG3	2.31	0.66
1:D:445:PRO:HG3	1:D:497:PHE:HD1	1.60	0.66
1:B:128:PRO:HD3	1:B:275:SER:HB2	1.77	0.66
1:B:390:PHE:HE1	1:B:542:ARG:HG2	1.59	0.66
1:B:454:THR:HG21	1:B:627:GLU:OE2	1.95	0.66
1:A:120:GLU:HG2	1:A:200:VAL:HG11	1.76	0.66
1:A:641:ALA:H	1:A:667:ASN:HD21	1.44	0.66
1:C:449:ASP:O	1:C:451:THR:N	2.28	0.66
1:C:634:PHE:HD1	1:C:634:PHE:H	1.42	0.66
1:A:651:TRP:CZ3	1:A:684:TRP:HB2	2.31	0.66
1:C:114:GLU:OE1	1:C:118:ARG:NH1	2.28	0.66
1:A:83:TYR:CZ	1:A:176:GLU:HB2	2.31	0.66
1:B:208:ILE:HG21	1:B:221:TYR:HD2	1.60	0.65
1:C:387:PHE:CE2	1:C:427:LEU:HG	2.31	0.65
1:C:538:PRO:HB2	1:C:550:VAL:HG13	1.78	0.65
1:C:621:LEU:HD12	1:C:729:TYR:HD2	1.61	0.65
1:D:321:GLU:OE2	1:A:400:LEU:HB2	1.97	0.65
1:A:344:GLU:OE1	1:A:421:ARG:NH2	2.29	0.65
1:C:374:ASP:OD1	1:C:374:ASP:N	2.30	0.65
1:B:173:ASN:HB2	1:B:176:GLU:OE2	1.96	0.65
1:D:477:ARG:HD3	1:D:541:ALA:HA	1.79	0.65
1:A:445:PRO:HD3	1:A:497:PHE:HE1	1.61	0.65
1:B:449:ASP:O	1:B:451:THR:N	2.30	0.65
1:B:486:SER:O	1:B:488:GLU:N	2.30	0.65
1:B:489:THR:O	1:B:489:THR:OG1	2.15	0.65
1:A:168:ASP:OD1	1:A:180:ARG:N	2.28	0.65
1:A:391:GLN:O	1:A:391:GLN:NE2	2.29	0.65
1:D:551:PRO:HB2	1:D:552:PRO:HD3	1.79	0.65
1:B:3:THR:O	1:B:3:THR:OG1	2.11	0.65
1:C:458:ILE:HD11	1:C:629:TRP:HB2	1.78	0.65
1:D:634:PHE:HD1	1:D:634:PHE:H	1.43	0.65
1:B:4:LYS:O	1:B:5:GLU:HG3	1.97	0.65
1:B:538:PRO:HB2	1:B:550:VAL:HG13	1.78	0.65
1:B:375:LYS:HA	1:B:378:THR:HG22	1.79	0.65
1:B:505:ALA:O	1:B:508:TYR:HB3	1.97	0.65
1:A:127:GLU:HB3	1:A:128:PRO:HD2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:PHE:CE2	1:D:427:LEU:HG	2.33	0.64
1:C:265:PHE:CZ	1:C:271:GLU:HG3	2.31	0.64
1:D:496:GLN:HA	1:D:553:VAL:HG13	1.79	0.64
1:A:561:LYS:NZ	1:A:768:GLY:O	2.27	0.64
1:C:17:PHE:HE2	1:C:101:MET:HE3	1.57	0.64
1:D:27:ILE:HB	1:D:164:ARG:HA	1.80	0.64
1:A:705:THR:HA	1:A:708:ASP:HB2	1.78	0.64
1:B:477:ARG:CZ	1:B:542:ARG:HB3	2.26	0.64
1:C:391:GLN:O	1:C:391:GLN:NE2	2.31	0.64
1:B:7:PHE:C	1:B:7:PHE:HD2	2.05	0.64
1:B:355:LYS:HD2	1:B:359:ASP:OD2	1.97	0.64
1:C:180:ARG:HH12	1:C:212:LYS:HE2	1.62	0.64
1:A:87:VAL:HG22	1:A:88:PRO:HD2	1.78	0.64
1:C:396:LEU:HD11	1:C:403:GLN:HA	1.77	0.64
1:D:389:MET:HE1	1:D:526:ARG:HD3	1.80	0.64
1:D:390:PHE:CE1	1:D:542:ARG:HG2	2.32	0.64
1:A:26:TYR:HD2	1:A:93:THR:HG22	1.63	0.64
1:A:168:ASP:OD1	1:A:181:SER:N	2.29	0.64
1:A:474:LEU:O	1:A:477:ARG:HB3	1.98	0.64
1:A:621:LEU:HD12	1:A:729:TYR:CD2	2.33	0.64
1:A:486:SER:O	1:A:488:GLU:N	2.31	0.64
1:B:26:TYR:OH	1:B:165:SER:HB3	1.98	0.64
1:C:243:VAL:HG11	1:C:245:ARG:NH2	2.09	0.63
1:A:3:THR:O	1:A:3:THR:OG1	2.16	0.63
1:A:13:SER:OG	1:A:16:GLN:HG2	1.99	0.63
1:A:669:THR:HG22	1:A:732:LEU:HD13	1.80	0.63
1:B:86:GLN:HE22	1:B:172:ARG:H	1.46	0.63
1:C:438:TRP:CE3	1:C:464:ARG:HG3	2.33	0.63
1:D:385:LEU:HD22	1:D:396:LEU:HB3	1.79	0.63
1:D:511:TRP:HH2	1:D:519:ALA:HB3	1.64	0.63
1:A:339:ARG:CG	1:A:408:ARG:HH22	2.10	0.63
1:C:514:SER:OG	1:C:515:PHE:N	2.29	0.63
1:C:631:ASP:C	1:C:633:ALA:H	2.07	0.63
1:D:163:ILE:O	1:D:168:ASP:OD2	2.17	0.63
1:C:282:ASP:O	1:C:284:ALA:N	2.32	0.63
1:C:681:ASN:OD1	1:C:682:ARG:N	2.32	0.63
1:D:23:GLN:HG3	1:D:90:LYS:HD3	1.78	0.63
1:D:86:GLN:NE2	1:D:172:ARG:HD3	2.14	0.63
1:D:284:ALA:O	1:D:286:MET:N	2.32	0.63
1:C:390:PHE:CE1	1:C:542:ARG:HG2	2.34	0.63
1:C:651:TRP:HE1	1:C:683:ALA:HA	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ARG:HB2	1:B:289:LEU:HD13	1.79	0.63
1:B:151:MET:HB3	1:B:172:ARG:NH1	2.12	0.63
1:D:396:LEU:HD21	1:D:406:TYR:CG	2.34	0.63
1:A:584:VAL:HG12	1:A:592:THR:HG22	1.81	0.63
1:A:760:TRP:O	1:A:764:THR:OG1	2.15	0.63
1:B:385:LEU:CD2	1:B:396:LEU:HB3	2.28	0.63
1:B:442:THR:HA	1:B:626:LEU:HD21	1.81	0.63
1:B:477:ARG:HD3	1:B:542:ARG:N	2.12	0.63
1:C:584:VAL:HG12	1:C:592:THR:HG22	1.80	0.63
1:D:276:VAL:HG12	1:D:280:LEU:HD22	1.81	0.62
1:D:208:ILE:HG23	1:D:209:ASP:N	2.14	0.62
1:C:13:SER:OG	1:C:16:GLN:HG2	1.98	0.62
1:C:352:SER:O	1:C:354:SER:N	2.31	0.62
1:C:489:THR:OG1	1:C:489:THR:O	2.17	0.62
1:C:433:PHE:CG	1:C:476:THR:HG22	2.33	0.62
1:C:545:ARG:NH2	1:C:545:ARG:H	1.97	0.62
1:D:172:ARG:HG3	1:D:172:ARG:HH11	1.63	0.62
1:B:36:TRP:HE3	1:B:41:ILE:HD13	1.65	0.62
1:C:449:ASP:O	1:C:452:LEU:N	2.32	0.62
1:B:720:ALA:HB1	1:B:723:ILE:HB	1.80	0.62
1:C:546:ASP:HB3	1:C:549:GLU:HG2	1.81	0.62
1:A:355:LYS:HD2	1:A:359:ASP:OD2	2.00	0.62
1:B:449:ASP:O	1:B:452:LEU:N	2.32	0.62
1:D:349:TRP:O	1:D:349:TRP:CD1	2.53	0.62
1:D:600:SER:HB3	1:D:732:LEU:HD21	1.82	0.62
1:D:7:PHE:C	1:D:7:PHE:CD2	2.78	0.62
1:A:605:PRO:HB3	1:A:735:ALA:HB2	1.81	0.62
1:C:688:ARG:HD3	1:C:692:ARG:HH12	1.64	0.61
1:B:411:PHE:HA	1:B:423:VAL:HG11	1.83	0.61
1:D:458:ILE:HG13	1:D:629:TRP:HB2	1.82	0.61
1:D:610:PRO:O	1:D:739:ARG:HB2	2.01	0.61
1:A:34:TYR:HD2	1:A:224:LEU:HD12	1.65	0.61
1:D:127:GLU:HB3	1:D:128:PRO:CD	2.30	0.61
1:D:584:VAL:HG12	1:D:592:THR:HG22	1.83	0.61
1:C:724:VAL:HG12	1:C:725:ARG:HG3	1.80	0.61
1:A:33:ALA:HA	1:A:164:ARG:NH2	2.16	0.61
1:A:441:PRO:HG2	1:A:461:ALA:HB2	1.83	0.61
1:C:127:GLU:OE2	1:C:127:GLU:C	2.44	0.61
1:A:333:ILE:HD12	1:A:365:LEU:HD21	1.83	0.61
1:B:26:TYR:O	1:B:93:THR:HA	2.01	0.61
1:B:380:THR:O	1:B:384:LEU:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:LEU:HD11	1:D:231:MET:HG2	1.83	0.61
1:D:565:ARG:HG2	1:D:570:TYR:CE2	2.35	0.61
1:A:153:TYR:CD1	1:B:134:ASN:HB3	2.35	0.61
1:C:728:ARG:HD3	1:C:729:TYR:N	2.15	0.61
1:A:232:ARG:HD3	1:A:236:ARG:CZ	2.30	0.61
1:D:208:ILE:CD1	1:D:209:ASP:H	2.14	0.61
1:A:208:ILE:HG23	1:A:209:ASP:N	2.15	0.61
1:A:551:PRO:HB2	1:A:552:PRO:HD3	1.83	0.60
1:A:570:TYR:HB2	1:A:769:PHE:CZ	2.36	0.60
1:C:688:ARG:CZ	1:C:740:GLU:OE2	2.49	0.60
1:A:11:PRO:O	1:A:12:LEU:HD23	2.01	0.60
1:A:433:PHE:HE2	1:A:438:TRP:NE1	1.99	0.60
1:A:543:PHE:C	1:A:543:PHE:HD2	2.10	0.60
1:C:522:ASP:OD1	1:C:522:ASP:N	2.33	0.60
1:D:631:ASP:O	1:D:633:ALA:N	2.34	0.60
1:A:452:LEU:HB3	1:A:498:LEU:HD13	1.83	0.60
1:B:143:LEU:O	1:B:146:CYS:CB	2.50	0.60
1:B:533:VAL:O	1:B:538:PRO:HD2	2.01	0.60
1:B:516:GLY:O	1:B:587:HIS:NE2	2.33	0.60
1:D:636:THR:HB	1:D:671:LEU:O	2.01	0.60
1:A:489:THR:O	1:A:489:THR:OG1	2.19	0.60
1:A:565:ARG:HG2	1:A:570:TYR:CE2	2.35	0.60
1:C:682:ARG:HE	1:C:716:LEU:HD13	1.65	0.60
1:D:283:ASP:HA	1:D:287:THR:HB	1.83	0.60
1:B:114:GLU:OE1	1:B:118:ARG:NH1	2.33	0.60
1:B:357:HIS:O	1:B:360:VAL:HB	2.01	0.60
1:C:349:TRP:O	1:C:349:TRP:CD1	2.55	0.60
1:D:26:TYR:OH	1:D:165:SER:HB3	2.01	0.60
1:D:583:PRO:HG3	1:D:660:GLU:HG2	1.84	0.60
1:B:377:GLN:HE22	1:B:403:GLN:HE22	1.50	0.60
1:B:474:LEU:H	1:B:529:MET:HE1	1.67	0.60
1:B:729:TYR:CE2	1:B:731:PRO:HG3	2.37	0.60
1:C:471:VAL:HG12	1:C:475:LEU:HG	1.84	0.60
1:C:484:LEU:HB3	1:C:548:THR:HG22	1.84	0.60
1:A:433:PHE:HE2	1:A:438:TRP:CD1	2.19	0.60
1:B:1:MET:HA	1:B:4:LYS:HB2	1.82	0.60
1:C:113:GLU:OE1	1:C:228:ARG:NH1	2.35	0.60
1:D:52:LEU:HD13	1:D:252:PRO:HD2	1.84	0.60
1:D:390:PHE:HE1	1:D:542:ARG:HG2	1.67	0.60
1:A:674:VAL:HG11	1:A:679:ALA:N	2.16	0.60
1:B:542:ARG:HE	1:B:547:LEU:HD12	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:674:VAL:HG11	1:C:679:ALA:N	2.17	0.60
1:D:489:THR:O	1:D:489:THR:OG1	2.16	0.59
1:B:561:LYS:HE3	1:B:769:PHE:HA	1.82	0.59
1:A:163:ILE:HG13	1:A:170:TRP:CH2	2.37	0.59
1:A:217:ASP:C	1:A:219:GLU:H	2.09	0.59
1:B:26:TYR:CZ	1:B:79:VAL:HA	2.37	0.59
1:C:433:PHE:CD1	1:C:476:THR:HG22	2.37	0.59
1:C:715:ARG:HG2	1:C:720:ALA:HB2	1.84	0.59
1:D:542:ARG:O	1:D:542:ARG:HG3	2.03	0.59
1:A:720:ALA:HB1	1:A:723:ILE:HD12	1.83	0.59
1:B:372:SER:OG	1:B:373:ALA:N	2.33	0.59
1:C:477:ARG:NE	1:C:542:ARG:HB3	2.16	0.59
1:D:674:VAL:HG11	1:D:679:ALA:H	1.67	0.59
1:C:5:GLU:O	1:C:7:PHE:N	2.29	0.59
1:C:764:THR:O	1:C:769:PHE:HB2	2.02	0.59
1:D:414:ASP:HB3	1:D:419:ALA:HB1	1.84	0.59
1:D:651:TRP:CZ3	1:D:684:TRP:HB2	2.37	0.59
1:D:651:TRP:HE1	1:D:683:ALA:HA	1.68	0.59
1:A:682:ARG:HE	1:A:716:LEU:HD13	1.67	0.59
1:B:449:ASP:HB3	1:B:452:LEU:HB2	1.84	0.59
1:B:621:LEU:HD12	1:B:729:TYR:HD2	1.68	0.59
1:D:274:PRO:HA	1:D:277:VAL:HG22	1.83	0.59
1:B:689:LEU:HB3	1:B:709:ALA:HB2	1.83	0.59
1:A:344:GLU:OE2	1:A:352:SER:HB2	2.03	0.59
1:A:544:GLU:HB2	1:A:545:ARG:HH22	1.67	0.59
1:B:299:LEU:HD12	1:B:303:VAL:HG21	1.83	0.59
1:B:474:LEU:HG	1:B:529:MET:SD	2.42	0.59
1:C:144:SER:C	1:C:146:CYS:H	2.10	0.59
1:C:167:TYR:OH	1:C:216:VAL:HG13	2.02	0.59
1:D:643:GLN:O	1:D:645:PRO:HD3	2.02	0.59
1:D:68:VAL:HG11	1:D:101:MET:HE2	1.85	0.58
1:D:343:GLU:OE2	1:D:420:ARG:CZ	2.51	0.58
1:C:234:MET:HG2	1:C:249:ILE:HD11	1.85	0.58
1:A:433:PHE:CG	1:A:476:THR:HG22	2.38	0.58
1:B:642:PRO:O	1:B:656:TYR:OH	2.19	0.58
1:C:551:PRO:HB2	1:C:552:PRO:HD3	1.85	0.58
1:D:26:TYR:HD2	1:D:93:THR:HG22	1.67	0.58
1:D:496:GLN:HG2	1:D:553:VAL:HG22	1.85	0.58
1:D:537:MET:HB2	1:D:538:PRO:HD3	1.86	0.58
1:A:569:ILE:HD12	1:A:578:ARG:NH2	2.18	0.58
1:B:182:PRO:HD3	1:B:221:TYR:CE1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:VAL:HA	1:C:421:ARG:HD2	1.84	0.58
1:D:132:CYS:SG	1:D:289:LEU:HD23	2.43	0.58
1:D:544:GLU:HB2	1:D:545:ARG:NH2	2.19	0.58
1:D:686:LEU:HD21	1:D:712:GLN:HB3	1.84	0.58
1:C:109:THR:HG22	1:C:228:ARG:HE	1.68	0.58
1:D:163:ILE:HD12	1:D:170:TRP:CD2	2.39	0.58
1:C:5:GLU:C	1:C:7:PHE:H	2.12	0.58
1:C:699:VAL:HG12	1:C:703:GLU:HG3	1.84	0.58
1:D:80:GLU:OE1	1:A:342:LYS:HG3	2.04	0.58
1:B:353:GLU:O	1:B:356:LEU:HB2	2.03	0.58
1:D:70:ALA:HB3	1:D:92:MET:HE3	1.86	0.58
1:C:238:ALA:HB2	1:C:249:ILE:HD13	1.85	0.58
1:D:615:ARG:HG2	1:D:616:GLY:H	1.69	0.58
1:D:163:ILE:HD12	1:D:170:TRP:CE2	2.39	0.57
1:B:86:GLN:NE2	1:B:172:ARG:H	2.01	0.57
1:B:551:PRO:HB2	1:B:552:PRO:HD3	1.85	0.57
1:C:151:MET:HG3	1:C:159:TYR:CZ	2.39	0.57
1:C:552:PRO:HG2	1:C:555:ALA:H	1.69	0.57
1:A:474:LEU:N	1:A:529:MET:HE1	2.19	0.57
1:B:418:VAL:H	1:B:421:ARG:HD2	1.68	0.57
1:A:86:GLN:HE22	1:A:172:ARG:H	1.51	0.57
1:A:151:MET:HB3	1:A:172:ARG:NH1	2.20	0.57
1:B:710:GLU:OE2	1:B:715:ARG:NE	2.37	0.57
1:A:445:PRO:HG3	1:A:497:PHE:CD1	2.39	0.57
1:A:543:PHE:C	1:A:543:PHE:CD2	2.83	0.57
1:A:551:PRO:HB2	1:A:552:PRO:CD	2.35	0.57
1:A:643:GLN:O	1:A:645:PRO:HD3	2.05	0.57
1:B:710:GLU:HG2	1:B:715:ARG:HG3	1.85	0.57
1:C:168:ASP:HA	1:C:178:ARG:O	2.04	0.57
1:A:372:SER:OG	1:A:373:ALA:N	2.34	0.57
1:A:511:TRP:HZ3	1:A:519:ALA:HB3	1.68	0.57
1:C:342:LYS:O	1:C:343:GLU:HG2	2.05	0.57
1:C:642:PRO:HD3	1:C:651:TRP:CZ2	2.39	0.57
1:D:449:ASP:HB3	1:D:452:LEU:HB2	1.87	0.57
1:D:679:ALA:HA	1:D:716:LEU:O	2.05	0.57
1:D:729:TYR:CE2	1:D:731:PRO:HG3	2.40	0.57
1:A:438:TRP:CE3	1:A:464:ARG:HG3	2.39	0.57
1:A:533:VAL:O	1:A:538:PRO:HD2	2.05	0.57
1:D:186:TYR:OH	1:D:228:ARG:HD2	2.04	0.57
1:D:549:GLU:HB2	1:D:550:VAL:HG23	1.86	0.57
1:D:666:GLY:H	1:D:752:SER:HB3	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:710:GLU:HG2	1:D:715:ARG:HG3	1.87	0.57
1:A:155:GLU:HG3	1:A:174:LYS:HE2	1.87	0.57
1:C:477:ARG:CZ	1:C:542:ARG:HB3	2.35	0.57
1:C:612:LEU:HD13	1:C:754:ARG:HD2	1.87	0.57
1:A:5:GLU:O	1:A:7:PHE:N	2.32	0.57
1:A:507:PHE:CZ	1:A:511:TRP:HD1	2.23	0.57
1:A:516:GLY:O	1:A:587:HIS:NE2	2.38	0.57
1:B:477:ARG:HD3	1:B:541:ALA:HA	1.87	0.57
1:A:449:ASP:O	1:A:451:THR:N	2.38	0.56
1:B:108:THR:HB	1:B:143:LEU:HD22	1.86	0.56
1:B:312:ARG:NH1	1:B:314:ASP:OD1	2.37	0.56
1:B:418:VAL:CA	1:B:421:ARG:HD2	2.36	0.56
1:C:36:TRP:HE3	1:C:41:ILE:HD13	1.69	0.56
1:C:665:ILE:H	1:C:665:ILE:CD1	2.13	0.56
1:B:349:TRP:O	1:B:349:TRP:CD1	2.58	0.56
1:D:183:ILE:HD12	1:D:183:ILE:N	2.09	0.56
1:D:190:TYR:CD1	1:D:190:TYR:C	2.83	0.56
1:D:423:VAL:HA	1:D:542:ARG:HH22	1.70	0.56
1:A:58:PHE:CE2	1:A:405:ARG:HD3	2.40	0.56
1:A:563:GLN:O	1:A:566:SER:OG	2.22	0.56
1:B:455:GLN:HG2	1:B:624:LEU:O	2.05	0.56
1:C:128:PRO:HD3	1:C:275:SER:HB2	1.88	0.56
1:C:631:ASP:O	1:C:633:ALA:N	2.38	0.56
1:A:445:PRO:HD3	1:A:497:PHE:CE1	2.41	0.56
1:A:507:PHE:CZ	1:A:511:TRP:CD1	2.93	0.56
1:B:26:TYR:CD2	1:B:93:THR:HG22	2.36	0.56
1:B:143:LEU:O	1:B:146:CYS:HB3	2.05	0.56
1:B:457:GLY:HA3	1:B:626:LEU:HD22	1.87	0.56
1:B:715:ARG:HG2	1:B:720:ALA:HB2	1.87	0.56
1:C:270:SER:OG	1:C:271:GLU:N	2.38	0.56
1:C:415:PRO:O	1:C:420:ARG:NH1	2.38	0.56
1:D:36:TRP:HE3	1:D:41:ILE:HD13	1.70	0.56
1:D:355:LYS:HD2	1:D:359:ASP:OD2	2.05	0.56
1:A:228:ARG:HD3	1:A:228:ARG:C	2.29	0.56
1:A:238:ALA:HB2	1:A:249:ILE:CD1	2.35	0.56
1:B:173:ASN:ND2	1:B:176:GLU:OE2	2.35	0.56
1:B:180:ARG:HH12	1:B:212:LYS:HE2	1.70	0.56
1:B:516:GLY:C	1:B:587:HIS:HE2	2.13	0.56
1:C:542:ARG:O	1:C:542:ARG:HG3	2.05	0.56
1:A:239:VAL:HA	1:A:291:ARG:NH1	2.20	0.56
1:B:183:ILE:HG13	1:B:224:LEU:CD1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:GLN:HA	1:B:553:VAL:HG13	1.88	0.56
1:B:692:ARG:NH2	1:B:740:GLU:OE1	2.39	0.56
1:C:372:SER:OG	1:C:373:ALA:N	2.31	0.56
1:D:168:ASP:HA	1:D:178:ARG:O	2.04	0.56
1:D:763:LEU:O	1:D:766:TRP:HB2	2.06	0.56
1:A:88:PRO:HG2	1:A:91:VAL:HG12	1.88	0.56
1:B:651:TRP:CH2	1:B:684:TRP:HB2	2.41	0.56
1:B:669:THR:CG2	1:B:751:ARG:HH22	2.19	0.56
1:C:341:ILE:HG12	1:C:349:TRP:CZ2	2.40	0.56
1:C:375:LYS:HA	1:C:378:THR:HG22	1.87	0.56
1:C:684:TRP:HE1	1:C:742:GLU:HA	1.71	0.56
1:D:48:VAL:HG22	1:D:295:PHE:CE1	2.41	0.56
1:D:562:GLU:HG2	1:D:565:ARG:NH1	2.21	0.56
1:B:26:TYR:CE2	1:B:79:VAL:HA	2.41	0.56
1:C:339:ARG:HG2	1:C:408:ARG:CZ	2.35	0.56
1:A:375:LYS:HA	1:A:378:THR:HG22	1.88	0.56
1:A:565:ARG:HH21	1:A:771:PRO:HB3	1.71	0.56
1:D:312:ARG:HD3	1:D:315:TYR:CE2	2.41	0.56
1:A:561:LYS:HE3	1:A:769:PHE:HA	1.87	0.56
1:A:709:ALA:HB3	1:A:714:LEU:HD22	1.87	0.56
1:C:496:GLN:NE2	1:C:553:VAL:HG22	2.20	0.56
1:C:561:LYS:NZ	1:C:768:GLY:O	2.33	0.56
1:D:282:ASP:O	1:D:284:ALA:N	2.38	0.55
1:D:343:GLU:OE2	1:D:420:ARG:NH1	2.39	0.55
1:A:496:GLN:HG2	1:A:553:VAL:HG22	1.88	0.55
1:B:149:GLU:HG2	1:B:150:ASP:N	2.21	0.55
1:B:208:ILE:HG23	1:B:209:ASP:N	2.21	0.55
1:B:239:VAL:HA	1:B:291:ARG:HH12	1.71	0.55
1:A:123:THR:O	1:A:123:THR:OG1	2.24	0.55
1:B:155:GLU:H	1:B:174:LYS:HE2	1.70	0.55
1:B:110:VAL:CG2	1:B:235:LEU:HD12	2.36	0.55
1:C:26:TYR:CZ	1:C:79:VAL:HA	2.41	0.55
1:A:433:PHE:CE2	1:A:438:TRP:CD1	2.94	0.55
1:B:11:PRO:O	1:B:12:LEU:HD23	2.06	0.55
1:B:496:GLN:HG2	1:B:553:VAL:HG13	1.87	0.55
1:C:87:VAL:HG13	1:C:88:PRO:O	2.06	0.55
1:C:144:SER:C	1:C:146:CYS:N	2.63	0.55
1:C:433:PHE:CE2	1:C:438:TRP:CD1	2.94	0.55
1:A:561:LYS:HD2	1:A:767:LEU:HB3	1.89	0.55
1:B:163:ILE:O	1:B:168:ASP:OD2	2.25	0.55
1:C:186:TYR:CE2	1:C:205:HIS:CD2	2.93	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:ARG:NH1	1:D:213:THR:HG22	2.22	0.55
1:B:127:GLU:HB3	1:B:128:PRO:HD2	1.89	0.55
1:B:551:PRO:HB2	1:B:552:PRO:CD	2.37	0.55
1:C:602:ASN:OD1	1:C:622:GLU:HG3	2.06	0.55
1:D:388:ALA:HA	1:D:406:TYR:OH	2.07	0.55
1:D:682:ARG:HE	1:D:716:LEU:HD13	1.72	0.55
1:A:180:ARG:NH1	1:A:213:THR:HG22	2.22	0.55
1:A:681:ASN:OD1	1:A:682:ARG:N	2.39	0.55
1:B:343:GLU:OE2	1:B:420:ARG:CZ	2.55	0.55
1:B:488:GLU:HG2	1:B:489:THR:N	2.22	0.55
1:D:84:ARG:O	1:D:85:SER:C	2.49	0.55
1:D:454:THR:HG21	1:D:627:GLU:OE2	2.07	0.55
1:D:511:TRP:CH2	1:D:519:ALA:HB3	2.42	0.55
1:A:260:SER:O	1:A:264:GLN:HG3	2.07	0.55
1:B:78:THR:OG1	1:B:93:THR:HG21	2.06	0.55
1:C:143:LEU:O	1:C:146:CYS:HB3	2.07	0.55
1:C:709:ALA:HB1	1:C:714:LEU:HB2	1.89	0.55
1:A:151:MET:O	1:A:157:ARG:HD3	2.07	0.55
1:A:441:PRO:O	1:A:444:VAL:HG22	2.06	0.55
1:B:486:SER:HB3	1:B:488:GLU:OE2	2.06	0.55
1:C:496:GLN:HG2	1:C:553:VAL:HG13	1.89	0.55
1:C:684:TRP:HD1	1:C:742:GLU:OE2	1.90	0.55
1:D:565:ARG:HG2	1:D:570:TYR:HE2	1.71	0.55
1:A:119:ALA:O	1:A:122:LEU:HB2	2.07	0.55
1:B:572:LYS:HE2	1:B:760:TRP:CZ3	2.41	0.55
1:B:593:ARG:HH21	1:B:635:ALA:HB1	1.72	0.55
1:C:182:PRO:HG2	1:C:183:ILE:HD12	1.88	0.55
1:B:355:LYS:HD2	1:B:359:ASP:CG	2.32	0.54
1:B:538:PRO:HB3	1:B:550:VAL:HG22	1.89	0.54
1:C:631:ASP:C	1:C:633:ALA:N	2.65	0.54
1:D:715:ARG:HG2	1:D:720:ALA:HB2	1.89	0.54
1:A:589:LYS:HA	1:A:592:THR:HG23	1.88	0.54
1:B:642:PRO:HD3	1:B:651:TRP:CZ2	2.41	0.54
1:C:665:ILE:HG12	1:C:752:SER:HB2	1.88	0.54
1:D:208:ILE:HD12	1:D:209:ASP:H	1.72	0.54
1:D:333:ILE:HD12	1:D:380:THR:HG23	1.89	0.54
1:D:561:LYS:HE2	1:D:771:PRO:HD2	1.90	0.54
1:D:674:VAL:HG13	1:D:678:SER:H	1.72	0.54
1:A:114:GLU:OE2	1:A:236:ARG:NE	2.30	0.54
1:A:496:GLN:CA	1:A:553:VAL:HG13	2.34	0.54
1:C:537:MET:HB2	1:C:538:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:PHE:HD1	1:B:319:MET:SD	2.31	0.54
1:C:433:PHE:C	1:C:433:PHE:CD2	2.86	0.54
1:C:458:ILE:CD1	1:C:629:TRP:HB2	2.37	0.54
1:D:164:ARG:NH1	1:D:183:ILE:HD11	2.22	0.54
1:D:516:GLY:O	1:D:587:HIS:NE2	2.41	0.54
1:A:127:GLU:HB3	1:A:128:PRO:CD	2.37	0.54
1:A:164:ARG:NH1	1:A:183:ILE:HD11	2.22	0.54
1:D:486:SER:O	1:D:488:GLU:N	2.40	0.54
1:D:507:PHE:CD1	1:D:560:LEU:HD22	2.42	0.54
1:A:666:GLY:HA2	1:A:751:ARG:HD3	1.89	0.54
1:D:474:LEU:N	1:D:529:MET:HE1	2.22	0.54
1:A:367:ARG:NH1	1:A:435:GLU:OE2	2.41	0.54
1:A:455:GLN:HG2	1:A:624:LEU:O	2.08	0.54
1:A:710:GLU:HG2	1:A:715:ARG:HG3	1.88	0.54
1:B:127:GLU:HB3	1:B:128:PRO:CD	2.38	0.54
1:B:565:ARG:NH2	1:B:771:PRO:HB3	2.18	0.54
1:C:86:GLN:HE22	1:C:172:ARG:H	1.54	0.54
1:D:196:ASP:OD1	1:D:197:PRO:HD2	2.08	0.54
1:D:208:ILE:HG23	1:D:209:ASP:HB3	1.90	0.54
1:D:433:PHE:CB	1:D:476:THR:HG22	2.38	0.54
1:C:551:PRO:HB2	1:C:552:PRO:CD	2.38	0.54
1:A:488:GLU:HG2	1:A:489:THR:N	2.22	0.54
1:C:488:GLU:HG2	1:C:489:THR:HG22	1.89	0.54
1:D:180:ARG:HH11	1:D:213:THR:HG22	1.72	0.53
1:B:122:LEU:HD22	1:B:129:SER:OG	2.07	0.53
1:C:312:ARG:HB3	1:C:312:ARG:HH11	1.72	0.53
1:C:543:PHE:C	1:C:543:PHE:HD2	2.15	0.53
1:A:181:SER:HB2	1:A:182:PRO:HD2	1.90	0.53
1:B:312:ARG:HB2	1:B:315:TYR:CD2	2.43	0.53
1:C:437:PRO:HB2	1:C:460:LEU:CD1	2.37	0.53
1:A:120:GLU:C	1:A:122:LEU:H	2.16	0.53
1:A:253:THR:N	1:A:256:ASP:OD2	2.19	0.53
1:B:120:GLU:C	1:B:122:LEU:H	2.16	0.53
1:B:239:VAL:HA	1:B:291:ARG:NH1	2.24	0.53
1:B:387:PHE:CD2	1:B:427:LEU:HG	2.42	0.53
1:B:496:GLN:HG2	1:B:553:VAL:HG22	1.90	0.53
1:B:576:VAL:HG13	1:B:756:CYS:HB2	1.90	0.53
1:D:339:ARG:HG2	1:D:408:ARG:NH1	2.24	0.53
1:C:570:TYR:N	1:C:570:TYR:CD2	2.76	0.53
1:C:667:ASN:ND2	1:C:743:TRP:HE1	2.06	0.53
1:C:710:GLU:HG2	1:C:715:ARG:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:544:GLU:HB2	1:D:545:ARG:HH22	1.73	0.53
1:A:27:ILE:HB	1:A:164:ARG:HA	1.89	0.53
1:A:484:LEU:HD23	1:A:548:THR:HG22	1.91	0.53
1:A:688:ARG:HB3	1:A:692:ARG:CZ	2.39	0.53
1:B:414:ASP:HB3	1:B:419:ALA:CB	2.39	0.53
1:C:683:ALA:O	1:C:685:HIS:N	2.42	0.53
1:D:239:VAL:HA	1:D:291:ARG:NH1	2.24	0.53
1:D:262:ASN:ND2	1:D:262:ASN:H	2.06	0.53
1:A:4:LYS:O	1:A:5:GLU:HG3	2.07	0.53
1:A:605:PRO:HG3	1:A:734:ALA:HB3	1.90	0.53
1:A:734:ALA:O	1:A:736:LEU:N	2.36	0.53
1:D:74:ILE:HG23	1:D:75:ASN:OD1	2.09	0.53
1:B:161:ARG:HA	1:B:170:TRP:HH2	1.74	0.53
1:C:143:LEU:O	1:C:146:CYS:CB	2.57	0.53
1:C:509:ALA:HB2	1:C:594:LEU:HD12	1.90	0.53
1:C:554:GLU:HA	1:C:557:GLN:HG3	1.90	0.53
1:A:390:PHE:CD1	1:A:390:PHE:C	2.86	0.53
1:B:119:ALA:O	1:B:122:LEU:HB2	2.09	0.53
1:C:148:GLU:OE1	1:C:195:ARG:NH1	2.36	0.53
1:C:510:LEU:HD12	1:C:564:LEU:HD11	1.89	0.53
1:C:550:VAL:HG13	1:C:551:PRO:HA	1.90	0.53
1:C:692:ARG:HG3	1:C:737:ALA:CB	2.36	0.53
1:D:232:ARG:HD3	1:D:236:ARG:CZ	2.39	0.53
1:A:764:THR:N	1:A:765:PRO:HD2	2.24	0.53
1:B:477:ARG:NE	1:B:542:ARG:HB3	2.24	0.53
1:B:557:GLN:O	1:B:561:LYS:HD3	2.09	0.53
1:B:561:LYS:HD2	1:B:767:LEU:HB3	1.90	0.53
1:C:437:PRO:HD3	1:C:479:PHE:HE2	1.73	0.53
1:A:282:ASP:O	1:A:284:ALA:N	2.42	0.53
1:D:123:THR:O	1:D:129:SER:OG	2.12	0.52
1:D:143:LEU:O	1:D:146:CYS:CB	2.57	0.52
1:D:662:ILE:HD12	1:D:662:ILE:H	1.73	0.52
1:B:81:PRO:HG2	1:B:169:VAL:HG22	1.91	0.52
1:B:390:PHE:CD1	1:B:390:PHE:C	2.87	0.52
1:C:675:GLU:O	1:C:680:SER:OG	2.24	0.52
1:B:228:ARG:HD3	1:B:228:ARG:C	2.34	0.52
1:B:344:GLU:CD	1:B:421:ARG:HH21	2.17	0.52
1:B:415:PRO:O	1:B:420:ARG:NH1	2.42	0.52
1:B:418:VAL:N	1:B:421:ARG:HD2	2.25	0.52
1:C:543:PHE:C	1:C:543:PHE:CD2	2.87	0.52
1:D:385:LEU:CD2	1:D:396:LEU:HB3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:630:ASN:O	1:D:632:GLU:N	2.43	0.52
1:A:445:PRO:HG3	1:A:497:PHE:HD1	1.74	0.52
1:C:209:ASP:O	1:C:209:ASP:CG	2.51	0.52
1:D:228:ARG:C	1:D:228:ARG:HD3	2.35	0.52
1:B:444:VAL:HG12	1:B:445:PRO:HD3	1.90	0.52
1:B:557:GLN:HB3	1:B:767:LEU:O	2.10	0.52
1:B:706:LEU:HD12	1:B:714:LEU:HD23	1.91	0.52
1:C:682:ARG:HB2	1:C:686:LEU:HB2	1.92	0.52
1:C:701:GLU:HA	1:C:704:LYS:HB2	1.91	0.52
1:A:542:ARG:HD3	1:A:547:LEU:N	2.21	0.52
1:B:35:SER:O	1:B:36:TRP:C	2.52	0.52
1:C:343:GLU:OE2	1:C:420:ARG:NH1	2.42	0.52
1:C:401:ASN:H	1:C:401:ASN:ND2	2.06	0.52
1:A:622:GLU:O	1:A:628:ARG:NH1	2.42	0.52
1:B:123:THR:O	1:B:129:SER:OG	2.18	0.52
1:B:671:LEU:HD11	1:B:691:PHE:HE1	1.74	0.52
1:D:418:VAL:HG23	1:D:421:ARG:HH11	1.75	0.52
1:A:113:GLU:OE2	1:A:232:ARG:NH2	2.43	0.52
1:A:457:GLY:C	1:A:626:LEU:HB2	2.34	0.52
1:A:562:GLU:HG2	1:A:565:ARG:NH1	2.25	0.52
1:D:268:PHE:O	1:D:270:SER:N	2.42	0.52
1:A:255:THR:O	1:A:259:GLN:HG3	2.10	0.52
1:A:312:ARG:NH1	1:A:314:ASP:OD2	2.42	0.52
1:A:654:ASP:HB2	1:A:745:ALA:HB2	1.91	0.52
1:B:34:TYR:CD2	1:B:224:LEU:HD12	2.44	0.52
1:B:507:PHE:HB2	1:B:560:LEU:HD13	1.92	0.52
1:B:605:PRO:HB3	1:B:735:ALA:HB2	1.92	0.52
1:C:760:TRP:O	1:C:764:THR:OG1	2.27	0.52
1:D:537:MET:CB	1:D:538:PRO:HD3	2.40	0.52
1:D:705:THR:HA	1:D:708:ASP:HB2	1.92	0.52
1:A:433:PHE:O	1:A:437:PRO:HD2	2.09	0.52
1:A:525:TYR:O	1:A:529:MET:HG2	2.10	0.52
1:B:418:VAL:HA	1:B:421:ARG:CD	2.40	0.52
1:C:138:ASP:CG	1:C:142:ARG:HH12	2.17	0.52
1:C:326:THR:O	1:C:326:THR:HG23	2.09	0.52
1:B:151:MET:HE2	1:B:159:TYR:CE2	2.45	0.52
1:B:337:LYS:HE2	1:B:358:PHE:CE1	2.45	0.52
1:C:86:GLN:NE2	1:C:172:ARG:HD3	2.25	0.52
1:C:208:ILE:HG12	1:C:221:TYR:CE2	2.45	0.52
1:D:710:GLU:HA	1:D:714:LEU:H	1.76	0.51
1:A:396:LEU:HD12	1:A:397:THR:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:VAL:HG13	1:B:591:LEU:HD13	1.90	0.51
1:A:537:MET:CB	1:A:538:PRO:HD3	2.41	0.51
1:A:545:ARG:NH2	1:A:545:ARG:H	2.08	0.51
1:B:681:ASN:OD1	1:B:682:ARG:N	2.44	0.51
1:C:167:TYR:CE1	1:C:216:VAL:HG22	2.45	0.51
1:D:457:GLY:C	1:D:626:LEU:HB2	2.36	0.51
1:D:686:LEU:HD21	1:D:712:GLN:CB	2.40	0.51
1:B:455:GLN:NE2	1:B:766:TRP:HZ2	2.08	0.51
1:B:539:ARG:O	1:B:550:VAL:HG11	2.10	0.51
1:C:84:ARG:O	1:C:85:SER:C	2.52	0.51
1:C:472:VAL:O	1:C:476:THR:HG23	2.09	0.51
1:D:339:ARG:HG2	1:D:408:ARG:CZ	2.40	0.51
1:D:472:VAL:O	1:D:476:THR:HG23	2.09	0.51
1:A:35:SER:O	1:A:36:TRP:C	2.54	0.51
1:A:265:PHE:CZ	1:A:271:GLU:HG3	2.46	0.51
1:B:17:PHE:HE2	1:B:101:MET:SD	2.33	0.51
1:B:183:ILE:HG13	1:B:224:LEU:HD11	1.92	0.51
1:C:106:LEU:HD21	1:C:224:LEU:HG	1.92	0.51
1:C:212:LYS:C	1:C:213:THR:HG23	2.35	0.51
1:C:429:GLN:HG2	1:C:480:ALA:HB2	1.92	0.51
1:C:511:TRP:CE3	1:C:521:ILE:HG12	2.45	0.51
1:C:545:ARG:H	1:C:545:ARG:HH21	1.59	0.51
1:B:104:LEU:HD21	1:B:299:LEU:HD11	1.91	0.51
1:C:35:SER:O	1:C:36:TRP:C	2.54	0.51
1:C:538:PRO:HB2	1:C:550:VAL:CG1	2.41	0.51
1:C:722:GLU:O	1:C:726:GLN:NE2	2.44	0.51
1:D:353:GLU:O	1:D:356:LEU:HB2	2.10	0.51
1:D:445:PRO:HG3	1:D:497:PHE:CD1	2.45	0.51
1:D:511:TRP:HZ3	1:D:517:SER:O	1.92	0.51
1:B:23:GLN:O	1:B:161:ARG:NH1	2.43	0.51
1:B:208:ILE:CD1	1:B:209:ASP:H	2.21	0.51
1:C:73:ASP:HB3	1:C:91:VAL:CG2	2.41	0.51
1:C:120:GLU:HG2	1:C:200:VAL:HG11	1.92	0.51
1:C:600:SER:HB3	1:C:732:LEU:HD21	1.92	0.51
1:D:207:PRO:O	1:D:208:ILE:HG22	2.10	0.51
1:D:626:LEU:HD12	1:D:626:LEU:O	2.11	0.51
1:D:728:ARG:HD3	1:D:728:ARG:C	2.36	0.51
1:C:83:TYR:CD1	1:C:169:VAL:HG11	2.46	0.51
1:A:720:ALA:HB1	1:A:723:ILE:HB	1.93	0.51
1:C:106:LEU:O	1:C:110:VAL:HG12	2.11	0.51
1:D:415:PRO:O	1:D:420:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LEU:HB3	1:A:93:THR:OG1	2.11	0.51
1:A:312:ARG:HD3	1:A:315:TYR:CE2	2.45	0.51
1:A:413:LYS:O	1:A:415:PRO:HD3	2.11	0.51
1:C:32:ARG:O	1:C:164:ARG:NH2	2.44	0.51
1:C:148:GLU:CD	1:C:195:ARG:NH1	2.69	0.51
1:C:418:VAL:HA	1:C:421:ARG:CD	2.40	0.51
1:C:477:ARG:HD3	1:C:542:ARG:N	2.22	0.51
1:A:541:ALA:O	1:A:542:ARG:C	2.54	0.51
1:B:109:THR:HG23	1:B:228:ARG:HH11	1.76	0.51
1:B:584:VAL:HG12	1:B:592:THR:HG22	1.91	0.51
1:C:417:ILE:HD12	1:C:420:ARG:HB2	1.93	0.51
1:C:452:LEU:HD11	1:C:499:LEU:HD23	1.93	0.51
1:C:636:THR:CG2	1:C:675:GLU:HG2	2.41	0.51
1:C:641:ALA:HA	1:C:651:TRP:CH2	2.47	0.50
1:D:62:ILE:HG22	1:A:315:TYR:CE1	2.45	0.50
1:D:73:ASP:HB3	1:D:91:VAL:HG22	1.94	0.50
1:D:199:ALA:O	1:D:200:VAL:HB	2.11	0.50
1:D:641:ALA:N	1:D:667:ASN:OD1	2.44	0.50
1:A:456:ALA:HB3	1:A:498:LEU:HD22	1.93	0.50
1:B:180:ARG:HH22	1:B:212:LYS:NZ	2.09	0.50
1:B:674:VAL:HG11	1:B:679:ALA:N	2.27	0.50
1:C:621:LEU:HD12	1:C:729:TYR:CD2	2.43	0.50
1:D:148:GLU:OE1	1:D:195:ARG:NH1	2.42	0.50
1:D:312:ARG:NH1	1:D:314:ASP:OD1	2.44	0.50
1:D:538:PRO:HB2	1:D:550:VAL:HG13	1.93	0.50
1:D:674:VAL:HG11	1:D:679:ALA:N	2.26	0.50
1:B:180:ARG:O	1:B:221:TYR:OH	2.25	0.50
1:D:4:LYS:O	1:D:5:GLU:HG3	2.11	0.50
1:C:385:LEU:CD2	1:C:396:LEU:HB3	2.42	0.50
1:D:630:ASN:O	1:D:632:GLU:HG3	2.12	0.50
1:D:631:ASP:C	1:D:633:ALA:H	2.18	0.50
1:A:26:TYR:CZ	1:A:79:VAL:HG12	2.45	0.50
1:B:64:PHE:HE1	1:B:306:ALA:HB2	1.75	0.50
1:B:299:LEU:HA	1:B:303:VAL:HG23	1.93	0.50
1:C:163:ILE:O	1:C:168:ASP:OD2	2.29	0.50
1:D:477:ARG:NH1	1:D:542:ARG:H	2.09	0.50
1:A:84:ARG:O	1:A:85:SER:C	2.53	0.50
1:A:414:ASP:C	1:A:416:ASP:H	2.18	0.50
1:A:484:LEU:HD21	1:A:547:LEU:HD23	1.94	0.50
1:A:542:ARG:NE	1:A:547:LEU:HD12	2.22	0.50
1:B:674:VAL:HG11	1:B:679:ALA:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:561:LYS:HD2	1:C:767:LEU:HB3	1.94	0.50
1:D:135:GLN:HG2	1:D:268:PHE:HE2	1.76	0.50
1:D:470:ILE:HG21	1:D:522:ASP:HA	1.93	0.50
1:A:341:ILE:HG12	1:A:349:TRP:CE2	2.47	0.50
1:C:112:HIS:O	1:C:116:ARG:HB2	2.12	0.50
1:C:120:GLU:CD	1:C:200:VAL:HG21	2.37	0.50
1:D:326:THR:HG23	1:D:326:THR:O	2.12	0.50
1:D:471:VAL:HG12	1:D:475:LEU:HG	1.92	0.50
1:A:339:ARG:HG2	1:A:408:ARG:CZ	2.41	0.50
1:A:478:TYR:OH	1:A:551:PRO:HG2	2.12	0.50
1:A:683:ALA:O	1:A:685:HIS:N	2.44	0.50
1:B:437:PRO:HG3	1:B:479:PHE:HE2	1.77	0.50
1:C:35:SER:O	1:C:223:HIS:NE2	2.44	0.50
1:C:433:PHE:CB	1:C:476:THR:HG22	2.41	0.50
1:D:172:ARG:HG3	1:D:172:ARG:NH1	2.27	0.50
1:B:341:ILE:HG12	1:B:349:TRP:CE2	2.46	0.50
1:C:539:ARG:O	1:C:550:VAL:HG11	2.11	0.50
1:D:744:THR:O	1:D:748:VAL:HG23	2.12	0.49
1:A:13:SER:H	1:A:16:GLN:NE2	2.10	0.49
1:A:153:TYR:CE2	1:A:172:ARG:HG3	2.47	0.49
1:A:208:ILE:CD1	1:A:209:ASP:H	2.25	0.49
1:A:542:ARG:HD2	1:A:544:GLU:O	2.12	0.49
1:A:549:GLU:HB2	1:A:550:VAL:HG23	1.93	0.49
1:A:552:PRO:HG2	1:A:555:ALA:H	1.76	0.49
1:B:217:ASP:O	1:B:218:LEU:HB2	2.12	0.49
1:B:581:MET:SD	1:B:664:ARG:NH1	2.84	0.49
1:C:679:ALA:HA	1:C:716:LEU:O	2.12	0.49
1:C:703:GLU:OE2	1:C:725:ARG:NE	2.43	0.49
1:D:204:ARG:O	1:D:205:HIS:CB	2.61	0.49
1:D:344:GLU:OE1	1:D:421:ARG:NH2	2.45	0.49
1:D:477:ARG:HD3	1:D:542:ARG:H	1.76	0.49
1:D:493:SER:OG	1:D:494:ALA:N	2.44	0.49
1:A:337:LYS:NZ	1:A:358:PHE:CD1	2.72	0.49
1:B:163:ILE:HD12	1:B:170:TRP:CD2	2.47	0.49
1:C:477:ARG:CZ	1:C:542:ARG:CB	2.90	0.49
1:D:204:ARG:O	1:D:205:HIS:HB2	2.12	0.49
1:A:29:PRO:HG3	1:A:80:GLU:HG3	1.94	0.49
1:A:674:VAL:HG13	1:A:678:SER:HB3	1.94	0.49
1:C:52:LEU:HB2	1:C:298:TYR:CG	2.48	0.49
1:C:165:SER:O	1:C:166:TYR:HB2	2.12	0.49
1:C:196:ASP:OD1	1:C:197:PRO:HD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:LYS:C	1:C:343:GLU:HG2	2.37	0.49
1:C:650:SER:OG	1:C:651:TRP:N	2.45	0.49
1:D:164:ARG:HH12	1:D:183:ILE:HD11	1.76	0.49
1:C:709:ALA:CB	1:C:714:LEU:HB2	2.42	0.49
1:D:62:ILE:HG22	1:A:315:TYR:HE1	1.77	0.49
1:D:602:ASN:HB2	1:D:620:LEU:HB3	1.94	0.49
1:A:180:ARG:HH12	1:A:212:LYS:HE2	1.78	0.49
1:A:615:ARG:NH1	1:A:758:LEU:HG	2.28	0.49
1:B:342:LYS:HG3	1:C:80:GLU:OE1	2.12	0.49
1:B:414:ASP:HB3	1:B:419:ALA:HB1	1.94	0.49
1:B:713:GLY:O	1:B:716:LEU:HG	2.12	0.49
1:C:119:ALA:O	1:C:122:LEU:HB2	2.13	0.49
1:A:36:TRP:HE3	1:A:41:ILE:HD13	1.77	0.49
1:A:610:PRO:O	1:A:739:ARG:HB2	2.12	0.49
1:A:729:TYR:CE2	1:A:731:PRO:HG3	2.48	0.49
1:B:542:ARG:HG3	1:B:542:ARG:O	2.11	0.49
1:C:86:GLN:NE2	1:C:172:ARG:H	2.10	0.49
1:C:706:LEU:O	1:C:710:GLU:HG3	2.12	0.49
1:D:669:THR:HG23	1:D:751:ARG:HH22	1.78	0.49
1:B:341:ILE:HG12	1:B:349:TRP:CZ2	2.48	0.49
1:C:433:PHE:HE2	1:C:438:TRP:CD1	2.31	0.49
1:D:337:LYS:HE3	1:D:337:LYS:HB2	1.47	0.49
1:B:400:LEU:HD13	1:B:400:LEU:HA	1.55	0.49
1:B:400:LEU:HB3	1:B:404:ARG:NH2	2.27	0.49
1:B:512:ARG:HB3	1:B:591:LEU:HD11	1.95	0.49
1:C:199:ALA:C	1:C:201:LYS:H	2.20	0.49
1:D:500:ALA:O	1:D:503:SER:OG	2.26	0.49
1:D:551:PRO:HB2	1:D:552:PRO:CD	2.42	0.49
1:A:355:LYS:HD2	1:A:359:ASP:CG	2.38	0.49
1:B:109:THR:HG22	1:B:228:ARG:HE	1.77	0.49
1:C:557:GLN:O	1:C:561:LYS:HD3	2.13	0.49
1:C:605:PRO:HB3	1:C:735:ALA:HB2	1.94	0.49
1:D:217:ASP:O	1:D:218:LEU:HB2	2.12	0.49
1:D:764:THR:N	1:D:765:PRO:HD2	2.27	0.49
1:A:667:ASN:O	1:A:667:ASN:ND2	2.45	0.49
1:A:699:VAL:HG12	1:A:703:GLU:HG3	1.95	0.49
1:C:25:LEU:O	1:C:162:LEU:HA	2.12	0.49
1:C:211:ASP:OD1	1:C:211:ASP:O	2.30	0.49
1:C:390:PHE:CD1	1:C:390:PHE:C	2.91	0.49
1:C:593:ARG:HH21	1:C:635:ALA:HB1	1.77	0.49
1:C:688:ARG:HB3	1:C:692:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:728:ARG:HD3	1:C:729:TYR:H	1.78	0.49
1:D:5:GLU:C	1:D:7:PHE:N	2.71	0.48
1:D:253:THR:HA	1:D:291:ARG:NE	2.28	0.48
1:D:418:VAL:N	1:D:421:ARG:HD2	2.27	0.48
1:A:153:TYR:CE1	1:B:134:ASN:HB3	2.47	0.48
1:B:35:SER:N	1:B:99:GLN:OE1	2.32	0.48
1:B:101:MET:HA	1:B:101:MET:HE3	1.94	0.48
1:B:149:GLU:HB2	1:B:161:ARG:NH2	2.28	0.48
1:B:553:VAL:HB	1:B:554:GLU:HG3	1.94	0.48
1:C:38:LEU:HG	1:C:38:LEU:O	2.13	0.48
1:C:720:ALA:HB1	1:C:723:ILE:HB	1.95	0.48
1:D:126:ASP:OD1	1:D:126:ASP:O	2.31	0.48
1:D:385:LEU:HB2	1:D:386:PRO:HD3	1.95	0.48
1:B:543:PHE:C	1:B:543:PHE:CD2	2.92	0.48
1:B:572:LYS:HB3	1:B:760:TRP:CZ3	2.48	0.48
1:C:389:MET:HE1	1:C:526:ARG:HD3	1.95	0.48
1:D:1:MET:HA	1:D:4:LYS:HB2	1.94	0.48
1:D:65:LEU:HD23	1:D:65:LEU:HA	1.62	0.48
1:D:212:LYS:HB3	1:D:213:THR:H	1.42	0.48
1:D:631:ASP:C	1:D:633:ALA:N	2.70	0.48
1:A:73:ASP:OD2	1:A:78:THR:OG1	2.31	0.48
1:A:655:LEU:HD23	1:A:745:ALA:HA	1.95	0.48
1:B:173:ASN:HB2	1:B:176:GLU:CD	2.37	0.48
1:B:203:TYR:CE2	1:B:205:HIS:HB2	2.48	0.48
1:B:417:ILE:HG13	1:B:421:ARG:CZ	2.43	0.48
1:C:116:ARG:HH22	1:C:199:ALA:HB3	1.77	0.48
1:C:576:VAL:HG11	1:C:757:SER:OG	2.13	0.48
1:D:601:GLN:O	1:D:602:ASN:C	2.56	0.48
1:D:701:GLU:O	1:D:705:THR:OG1	2.28	0.48
1:A:357:HIS:O	1:A:360:VAL:HB	2.14	0.48
1:A:505:ALA:O	1:A:508:TYR:HB3	2.13	0.48
1:A:623:THR:O	1:A:625:GLU:N	2.44	0.48
1:B:186:TYR:OH	1:B:228:ARG:HD2	2.13	0.48
1:C:488:GLU:HG2	1:C:489:THR:N	2.27	0.48
1:C:636:THR:HG23	1:C:675:GLU:HG2	1.95	0.48
1:D:142:ARG:NH2	1:D:297:ASN:OD1	2.47	0.48
1:D:538:PRO:HB3	1:D:550:VAL:HG22	1.95	0.48
1:A:109:THR:CG2	1:A:228:ARG:HE	2.26	0.48
1:A:266:ALA:HB1	1:A:302:ARG:NH1	2.28	0.48
1:B:144:SER:C	1:B:146:CYS:H	2.21	0.48
1:B:390:PHE:C	1:B:390:PHE:HD1	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:THR:O	1:B:626:LEU:N	2.45	0.48
1:B:689:LEU:HD13	1:B:709:ALA:HA	1.94	0.48
1:D:372:SER:OG	1:D:375:LYS:HB3	2.14	0.48
1:B:400:LEU:O	1:B:403:GLN:N	2.46	0.48
1:B:621:LEU:HD12	1:B:729:TYR:CD2	2.46	0.48
1:B:634:PHE:HD1	1:B:634:PHE:H	1.60	0.48
1:C:208:ILE:HG21	1:C:221:TYR:CD2	2.48	0.48
1:D:156:HIS:O	1:D:172:ARG:HA	2.14	0.48
1:B:73:ASP:OD1	1:B:73:ASP:C	2.56	0.48
1:C:454:THR:HG21	1:C:627:GLU:OE2	2.13	0.48
1:D:261:GLN:CD	1:D:261:GLN:H	2.22	0.48
1:A:575:TRP:CZ3	1:A:760:TRP:HB2	2.49	0.48
1:B:7:PHE:CD2	1:B:8:ASP:N	2.82	0.48
1:C:104:LEU:O	1:C:108:THR:HG23	2.14	0.48
1:C:601:GLN:HA	1:C:623:THR:OG1	2.14	0.48
1:A:390:PHE:C	1:A:390:PHE:HD1	2.22	0.48
1:A:514:SER:O	1:A:582:THR:HG21	2.14	0.48
1:C:26:TYR:CE1	1:C:79:VAL:HG12	2.49	0.48
1:C:312:ARG:HH11	1:C:312:ARG:CB	2.26	0.48
1:C:361:VAL:HG21	1:C:427:LEU:HB3	1.96	0.48
1:D:35:SER:HB2	1:D:99:GLN:OE1	2.14	0.48
1:D:76:TYR:HB3	1:D:79:VAL:HG21	1.96	0.48
1:D:617:LYS:CG	1:D:620:LEU:HB2	2.43	0.48
1:B:138:ASP:CG	1:B:142:ARG:HH12	2.22	0.48
1:B:163:ILE:HD12	1:B:170:TRP:CE2	2.49	0.48
1:C:122:LEU:HD22	1:C:129:SER:HB2	1.96	0.48
1:D:496:GLN:HG2	1:D:553:VAL:HG13	1.95	0.47
1:B:7:PHE:O	1:B:8:ASP:HB2	2.14	0.47
1:B:339:ARG:HG2	1:B:408:ARG:CZ	2.43	0.47
1:B:379:VAL:O	1:B:383:VAL:HG12	2.14	0.47
1:C:8:ASP:C	1:C:8:ASP:OD1	2.57	0.47
1:D:29:PRO:HG3	1:D:80:GLU:HG3	1.96	0.47
1:D:140:THR:HG22	1:D:141:GLY:N	2.29	0.47
1:D:617:LYS:HG2	1:D:620:LEU:HB2	1.96	0.47
1:D:642:PRO:HD3	1:D:651:TRP:CZ2	2.49	0.47
1:B:447:CYS:HB2	1:B:494:ALA:HB1	1.96	0.47
1:B:518:THR:HG22	1:B:521:ILE:HD12	1.95	0.47
1:C:151:MET:SD	1:C:151:MET:N	2.84	0.47
1:C:171:SER:OG	1:C:176:GLU:HG2	2.14	0.47
1:C:448:ASP:O	1:C:450:ALA:N	2.47	0.47
1:C:496:GLN:CA	1:C:553:VAL:HG13	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:688:ARG:HD3	1:C:692:ARG:NH1	2.27	0.47
1:D:127:GLU:OE2	1:D:128:PRO:HD3	2.15	0.47
1:D:411:PHE:O	1:D:420:ARG:HG2	2.15	0.47
1:D:553:VAL:HB	1:D:554:GLU:HG3	1.96	0.47
1:B:212:LYS:HB3	1:B:213:THR:H	1.48	0.47
1:B:445:PRO:HG3	1:B:497:PHE:HD1	1.78	0.47
1:C:525:TYR:O	1:C:529:MET:HG2	2.14	0.47
1:A:709:ALA:HB1	1:A:714:LEU:HD13	1.96	0.47
1:C:388:ALA:HA	1:C:406:TYR:OH	2.14	0.47
1:D:232:ARG:HD3	1:D:236:ARG:NH2	2.30	0.47
1:D:683:ALA:O	1:D:685:HIS:N	2.47	0.47
1:A:471:VAL:HG12	1:A:475:LEU:HG	1.97	0.47
1:A:514:SER:OG	1:A:515:PHE:N	2.47	0.47
1:A:538:PRO:HB3	1:A:550:VAL:HG22	1.97	0.47
1:B:106:LEU:HB3	1:B:231:MET:HE1	1.95	0.47
1:B:127:GLU:OE2	1:B:275:SER:OG	2.23	0.47
1:B:154:GLY:O	1:B:157:ARG:HB2	2.15	0.47
1:C:203:TYR:CE2	1:C:205:HIS:HB2	2.49	0.47
1:C:565:ARG:O	1:C:568:GLY:N	2.47	0.47
1:D:482:HIS:HA	1:D:493:SER:OG	2.14	0.47
1:A:238:ALA:HB2	1:A:249:ILE:HD13	1.96	0.47
1:A:274:PRO:HA	1:A:277:VAL:HG22	1.95	0.47
1:A:292:LEU:HD12	1:A:292:LEU:HA	1.66	0.47
1:A:417:ILE:HG23	1:A:418:VAL:HG23	1.96	0.47
1:A:447:CYS:HB2	1:A:494:ALA:HB1	1.95	0.47
1:B:126:ASP:CB	1:B:129:SER:HB3	2.35	0.47
1:B:367:ARG:NH1	1:B:435:GLU:OE2	2.47	0.47
1:B:468:HIS:NE2	1:B:521:ILE:HG21	2.29	0.47
1:C:342:LYS:HE3	1:C:342:LYS:HA	1.97	0.47
1:D:5:GLU:CD	1:D:311:LYS:HB2	2.40	0.47
1:D:127:GLU:OE2	1:D:127:GLU:C	2.58	0.47
1:D:689:LEU:HD13	1:D:709:ALA:HA	1.95	0.47
1:A:641:ALA:N	1:A:667:ASN:HD21	2.10	0.47
1:A:690:MET:HB2	1:A:690:MET:HE3	1.73	0.47
1:A:690:MET:O	1:A:694:LEU:HD12	2.15	0.47
1:B:192:ALA:HA	1:B:195:ARG:NH2	2.29	0.47
1:B:601:GLN:HG2	1:B:622:GLU:HG2	1.97	0.47
1:B:662:ILE:HD12	1:B:662:ILE:H	1.80	0.47
1:C:516:GLY:HA2	1:C:587:HIS:NE2	2.29	0.47
1:C:610:PRO:O	1:C:739:ARG:HB2	2.15	0.47
1:C:655:LEU:HB2	1:C:656:TYR:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:ASP:HB3	1:D:91:VAL:CG2	2.45	0.47
1:D:617:LYS:HB3	1:D:620:LEU:HB2	1.97	0.47
1:A:26:TYR:CE2	1:A:79:VAL:HA	2.50	0.47
1:A:642:PRO:HD3	1:A:651:TRP:CZ2	2.49	0.47
1:A:681:ASN:H	1:A:690:MET:HE1	1.80	0.47
1:B:282:ASP:O	1:B:284:ALA:N	2.48	0.47
1:C:151:MET:HE2	1:C:159:TYR:CD2	2.49	0.47
1:C:341:ILE:HG12	1:C:349:TRP:CE2	2.50	0.47
1:C:390:PHE:HD2	1:C:476:THR:OG1	1.98	0.47
1:C:723:ILE:HG12	1:C:726:GLN:HE22	1.79	0.47
1:D:59:GLU:H	1:D:59:GLU:HG3	1.47	0.47
1:A:136:ALA:HB2	1:A:293:ILE:HD11	1.97	0.47
1:A:340:ALA:HB2	1:A:411:PHE:CZ	2.50	0.47
1:A:386:PRO:HB3	1:A:472:VAL:HB	1.96	0.47
1:A:488:GLU:HG2	1:A:489:THR:HG22	1.97	0.47
1:B:548:THR:OG1	1:B:549:GLU:N	2.47	0.47
1:C:123:THR:O	1:C:123:THR:OG1	2.31	0.47
1:C:160:PRO:N	1:C:170:TRP:HZ3	2.12	0.47
1:C:344:GLU:OE2	1:C:352:SER:HB2	2.15	0.47
1:C:715:ARG:HG2	1:C:720:ALA:CB	2.45	0.47
1:C:764:THR:N	1:C:765:PRO:HD2	2.30	0.47
1:A:352:SER:O	1:A:354:SER:N	2.48	0.47
1:A:387:PHE:CD2	1:A:427:LEU:HG	2.50	0.47
1:A:437:PRO:HB2	1:A:460:LEU:HD13	1.97	0.47
1:A:529:MET:SD	1:A:541:ALA:HB2	2.55	0.47
1:B:155:GLU:HG3	1:B:174:LYS:HE2	1.97	0.47
1:B:418:VAL:HG22	1:B:421:ARG:HH11	1.80	0.47
1:B:455:GLN:CD	1:B:766:TRP:HZ2	2.23	0.47
1:B:507:PHE:CB	1:B:560:LEU:HD13	2.45	0.47
1:B:666:GLY:H	1:B:752:SER:HB3	1.80	0.47
1:C:120:GLU:C	1:C:122:LEU:H	2.23	0.47
1:C:331:THR:HB	1:C:380:THR:HG21	1.97	0.47
1:C:689:LEU:HB3	1:C:709:ALA:HB2	1.97	0.47
1:D:312:ARG:HB2	1:D:315:TYR:CD2	2.50	0.46
1:D:639:HIS:HA	1:D:667:ASN:O	2.15	0.46
1:A:539:ARG:O	1:A:550:VAL:HG11	2.15	0.46
1:B:691:PHE:CE2	1:B:736:LEU:HD13	2.51	0.46
1:C:440:SER:C	1:C:442:THR:H	2.23	0.46
1:D:375:LYS:HA	1:D:378:THR:HG22	1.96	0.46
1:A:239:VAL:HA	1:A:291:ARG:HH12	1.80	0.46
1:B:484:LEU:CD2	1:B:548:THR:HG22	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:ARG:HA	1:B:682:ARG:HD3	1.40	0.46
1:C:312:ARG:HD3	1:C:315:TYR:CE2	2.50	0.46
1:D:113:GLU:O	1:D:117:VAL:HG12	2.15	0.46
1:D:542:ARG:HD2	1:D:544:GLU:O	2.14	0.46
1:A:437:PRO:HG3	1:A:479:PHE:HE2	1.80	0.46
1:A:615:ARG:HH22	1:A:758:LEU:C	2.23	0.46
1:B:312:ARG:CB	1:B:312:ARG:HH11	2.28	0.46
1:B:570:TYR:HD1	1:B:769:PHE:CZ	2.33	0.46
1:A:13:SER:H	1:A:16:GLN:HE21	1.63	0.46
1:A:312:ARG:HB2	1:A:315:TYR:HD2	1.80	0.46
1:A:433:PHE:CE2	1:A:438:TRP:NE1	2.81	0.46
1:A:588:SER:OG	1:A:591:LEU:HB2	2.15	0.46
1:B:54:GLN:NE2	1:B:402:ASP:OD1	2.48	0.46
1:B:509:ALA:HB2	1:B:594:LEU:HD12	1.97	0.46
1:C:34:TYR:CD2	1:C:224:LEU:HD12	2.49	0.46
1:D:183:ILE:CD1	1:D:183:ILE:N	2.75	0.46
1:D:239:VAL:HA	1:D:291:ARG:HH12	1.79	0.46
1:D:415:PRO:HA	1:D:420:ARG:CZ	2.46	0.46
1:A:270:SER:HB2	1:B:85:SER:HA	1.96	0.46
1:A:326:THR:HG23	1:A:326:THR:O	2.16	0.46
1:A:569:ILE:HG12	1:A:574:GLN:CD	2.41	0.46
1:B:110:VAL:HG12	1:B:228:ARG:NE	2.30	0.46
1:B:228:ARG:HD3	1:B:228:ARG:O	2.15	0.46
1:B:709:ALA:HB3	1:B:714:LEU:HD22	1.97	0.46
1:C:27:ILE:HB	1:C:164:ARG:HA	1.98	0.46
1:D:161:ARG:HA	1:D:170:TRP:CH2	2.39	0.46
1:A:163:ILE:HD12	1:A:170:TRP:CD2	2.51	0.46
1:B:396:LEU:HD11	1:B:403:GLN:HG2	1.97	0.46
1:C:284:ALA:O	1:C:286:MET:N	2.46	0.46
1:C:615:ARG:HG2	1:C:616:GLY:H	1.80	0.46
1:A:152:ARG:HD2	1:B:138:ASP:HA	1.98	0.46
1:A:380:THR:O	1:A:384:LEU:HB2	2.16	0.46
1:A:520:GLY:O	1:A:522:ASP:N	2.49	0.46
1:A:537:MET:HE2	1:A:537:MET:HB3	1.65	0.46
1:A:565:ARG:HH21	1:A:771:PRO:CB	2.28	0.46
1:C:20:GLU:HB3	1:C:23:GLN:HB2	1.96	0.46
1:C:292:LEU:HD12	1:C:292:LEU:HA	1.48	0.46
1:C:390:PHE:HD2	1:C:476:THR:HG1	1.63	0.46
1:C:602:ASN:HB2	1:C:620:LEU:HB3	1.97	0.46
1:D:182:PRO:HB2	1:D:224:LEU:HD13	1.97	0.46
1:A:163:ILE:O	1:A:164:ARG:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:TYR:OH	1:A:206:VAL:O	2.33	0.46
1:A:583:PRO:HD3	1:A:660:GLU:OE1	2.16	0.46
1:B:109:THR:CG2	1:B:228:ARG:HE	2.29	0.46
1:B:337:LYS:HB3	1:B:338:PRO:HD3	1.97	0.46
1:B:503:SER:HB2	1:B:767:LEU:HD23	1.98	0.46
1:B:684:TRP:CE2	1:B:743:TRP:HB2	2.51	0.46
1:B:706:LEU:HD13	1:B:723:ILE:HG22	1.97	0.46
1:C:83:TYR:CE2	1:C:176:GLU:HB2	2.51	0.46
1:C:162:LEU:O	1:C:163:ILE:HG12	2.16	0.46
1:C:684:TRP:O	1:C:684:TRP:CG	2.68	0.46
1:B:167:TYR:CD1	1:B:167:TYR:N	2.84	0.46
1:B:344:GLU:O	1:B:349:TRP:HB3	2.15	0.46
1:B:356:LEU:O	1:B:359:ASP:HB2	2.16	0.46
1:C:391:GLN:O	1:C:391:GLN:CD	2.59	0.46
1:C:563:GLN:O	1:C:566:SER:OG	2.33	0.46
1:D:110:VAL:HA	1:D:228:ARG:NH1	2.24	0.46
1:D:208:ILE:HG23	1:D:209:ASP:CB	2.46	0.46
1:D:449:ASP:C	1:D:451:THR:N	2.74	0.46
1:D:664:ARG:O	1:D:668:LEU:HG	2.16	0.46
1:A:433:PHE:C	1:A:433:PHE:CD2	2.93	0.46
1:A:477:ARG:NE	1:A:542:ARG:HB3	2.30	0.46
1:A:584:VAL:HG13	1:A:591:LEU:HD13	1.98	0.46
1:B:87:VAL:HG22	1:B:88:PRO:HD2	1.98	0.46
1:B:292:LEU:HD12	1:B:292:LEU:HA	1.58	0.46
1:B:552:PRO:HG2	1:B:555:ALA:H	1.80	0.46
1:B:664:ARG:O	1:B:668:LEU:HG	2.15	0.46
1:C:337:LYS:NZ	1:C:337:LYS:HB2	2.28	0.46
1:D:283:ASP:HA	1:D:287:THR:CB	2.46	0.45
1:A:396:LEU:HD12	1:A:397:THR:N	2.31	0.45
1:B:760:TRP:O	1:B:764:THR:OG1	2.31	0.45
1:C:186:TYR:CZ	1:C:205:HIS:HD2	2.35	0.45
1:C:228:ARG:HD3	1:C:228:ARG:C	2.40	0.45
1:C:517:SER:C	1:C:519:ALA:N	2.74	0.45
1:C:643:GLN:O	1:C:645:PRO:HD3	2.17	0.45
1:D:681:ASN:OD1	1:D:682:ARG:N	2.49	0.45
1:D:692:ARG:HG3	1:D:737:ALA:CB	2.37	0.45
1:A:388:ALA:HA	1:A:406:TYR:OH	2.16	0.45
1:A:469:ASP:N	1:A:469:ASP:OD1	2.48	0.45
1:B:355:LYS:HD2	1:B:359:ASP:OD1	2.15	0.45
1:D:416:ASP:HB2	1:D:417:ILE:H	1.35	0.45
1:A:369:GLY:O	1:A:371:SER:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:ALA:HA	1:B:651:TRP:CH2	2.51	0.45
1:C:686:LEU:HD21	1:C:712:GLN:HB3	1.98	0.45
1:C:710:GLU:OE2	1:C:715:ARG:NE	2.49	0.45
1:D:163:ILE:O	1:D:164:ARG:HB2	2.16	0.45
1:D:234:MET:HG2	1:D:249:ILE:HD11	1.99	0.45
1:D:243:VAL:HG11	1:D:245:ARG:HH21	1.81	0.45
1:D:572:LYS:HB3	1:D:760:TRP:CZ3	2.52	0.45
1:D:594:LEU:HD23	1:D:594:LEU:HA	1.81	0.45
1:A:371:SER:OG	1:A:375:LYS:HG2	2.17	0.45
1:A:538:PRO:HB2	1:A:550:VAL:HG13	1.98	0.45
1:A:565:ARG:O	1:A:566:SER:C	2.60	0.45
1:B:433:PHE:O	1:B:437:PRO:HD2	2.17	0.45
1:C:239:VAL:HG11	1:C:292:LEU:HD13	1.98	0.45
1:C:441:PRO:O	1:C:444:VAL:HG22	2.16	0.45
1:C:493:SER:OG	1:C:494:ALA:N	2.50	0.45
1:C:688:ARG:HB3	1:C:692:ARG:CZ	2.47	0.45
1:D:16:GLN:HE22	1:A:3:THR:HG22	1.81	0.45
1:D:352:SER:O	1:D:354:SER:N	2.50	0.45
1:D:414:ASP:HB3	1:D:419:ALA:CB	2.46	0.45
1:D:709:ALA:CB	1:D:714:LEU:HB2	2.47	0.45
1:A:183:ILE:HG13	1:A:224:LEU:CD1	2.47	0.45
1:C:284:ALA:C	1:C:286:MET:H	2.25	0.45
1:C:548:THR:OG1	1:C:549:GLU:N	2.49	0.45
1:A:238:ALA:HB2	1:A:249:ILE:HD12	1.97	0.45
1:B:182:PRO:HB2	1:B:224:LEU:HD13	1.99	0.45
1:B:636:THR:HB	1:B:671:LEU:O	2.17	0.45
1:D:3:THR:O	1:D:3:THR:OG1	2.35	0.45
1:D:86:GLN:NE2	1:D:172:ARG:H	2.11	0.45
1:D:455:GLN:HG2	1:D:624:LEU:O	2.17	0.45
1:D:634:PHE:CD1	1:D:634:PHE:N	2.82	0.45
1:A:163:ILE:O	1:A:168:ASP:OD2	2.35	0.45
1:A:209:ASP:OD1	1:A:212:LYS:N	2.50	0.45
1:C:5:GLU:CD	1:C:6:ILE:N	2.75	0.45
1:C:26:TYR:CE2	1:C:79:VAL:HA	2.52	0.45
1:C:496:GLN:CD	1:C:553:VAL:HG22	2.42	0.45
1:D:339:ARG:HB3	1:D:408:ARG:HH22	1.82	0.45
1:D:632:GLU:HA	1:D:635:ALA:HB3	1.99	0.45
1:A:38:LEU:HD13	1:A:230:GLN:OE1	2.17	0.45
1:A:337:LYS:HB2	1:A:337:LYS:HE3	1.46	0.45
1:A:565:ARG:HH21	1:A:771:PRO:CG	2.30	0.45
1:B:181:SER:HB2	1:B:182:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:588:SER:OG	1:B:591:LEU:HB2	2.16	0.45
1:C:18:LEU:HA	1:C:18:LEU:HD23	1.78	0.45
1:D:499:LEU:HA	1:D:502:ARG:HD3	1.99	0.45
1:B:407:LEU:HD23	1:B:407:LEU:HA	1.63	0.45
1:C:760:TRP:CZ2	1:C:764:THR:HG21	2.52	0.45
1:D:26:TYR:CE2	1:D:79:VAL:HA	2.52	0.44
1:D:387:PHE:CD1	1:D:387:PHE:C	2.95	0.44
1:D:469:ASP:OD1	1:D:469:ASP:N	2.49	0.44
1:D:665:ILE:HG13	1:D:756:CYS:SG	2.57	0.44
1:D:764:THR:O	1:D:769:PHE:HB2	2.17	0.44
1:A:606:ASP:OD2	1:A:609:THR:OG1	2.34	0.44
1:A:682:ARG:HD3	1:A:682:ARG:HA	1.57	0.44
1:B:243:VAL:HG11	1:B:245:ARG:HH21	1.81	0.44
1:C:390:PHE:C	1:C:390:PHE:HD1	2.25	0.44
1:C:669:THR:HG21	1:C:736:LEU:HD12	1.99	0.44
1:C:682:ARG:HG3	1:C:686:LEU:HD13	1.99	0.44
1:D:641:ALA:HA	1:D:651:TRP:CZ3	2.52	0.44
1:D:669:THR:CG2	1:D:751:ARG:HH22	2.29	0.44
1:C:339:ARG:HB3	1:C:408:ARG:HH22	1.81	0.44
1:D:522:ASP:OD1	1:D:522:ASP:N	2.49	0.44
1:A:433:PHE:CD1	1:A:476:THR:HG22	2.52	0.44
1:A:596:LEU:HD23	1:A:596:LEU:HA	1.77	0.44
1:A:709:ALA:HB1	1:A:714:LEU:HB2	1.99	0.44
1:B:764:THR:N	1:B:765:PRO:HD2	2.32	0.44
1:C:234:MET:CG	1:C:249:ILE:HD11	2.47	0.44
1:D:284:ALA:C	1:D:286:MET:H	2.23	0.44
1:D:385:LEU:HD22	1:D:396:LEU:CB	2.47	0.44
1:D:400:LEU:HA	1:D:400:LEU:HD13	1.60	0.44
1:D:429:GLN:HG2	1:D:480:ALA:HB2	1.99	0.44
1:D:441:PRO:O	1:D:444:VAL:HG22	2.17	0.44
1:A:460:LEU:HD23	1:A:460:LEU:HA	1.71	0.44
1:B:720:ALA:HB1	1:B:723:ILE:HD12	2.00	0.44
1:C:87:VAL:HG22	1:C:88:PRO:HD2	1.99	0.44
1:C:359:ASP:O	1:C:360:VAL:C	2.61	0.44
1:C:470:ILE:HG21	1:C:522:ASP:HA	1.98	0.44
1:C:665:ILE:HD13	1:C:665:ILE:N	2.26	0.44
1:C:689:LEU:HD13	1:C:709:ALA:HA	1.99	0.44
1:D:208:ILE:HG21	1:D:221:TYR:CE2	2.53	0.44
1:A:86:GLN:NE2	1:A:172:ARG:H	2.16	0.44
1:B:13:SER:OG	1:B:16:GLN:HG2	2.16	0.44
1:B:319:MET:HE2	1:B:319:MET:HB3	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:TRP:HA	1:B:352:SER:OG	2.18	0.44
1:C:537:MET:CB	1:C:538:PRO:HD3	2.48	0.44
1:D:162:LEU:HD23	1:D:162:LEU:HA	1.67	0.44
1:D:265:PHE:O	1:D:269:ASN:N	2.51	0.44
1:D:678:SER:OG	1:D:721:GLY:HA3	2.16	0.44
1:A:5:GLU:OE2	1:A:311:LYS:HB2	2.18	0.44
1:A:162:LEU:HD23	1:A:162:LEU:HA	1.44	0.44
1:A:186:TYR:OH	1:A:228:ARG:HD2	2.16	0.44
1:B:369:GLY:O	1:B:371:SER:N	2.51	0.44
1:B:537:MET:HE2	1:B:537:MET:HB3	1.87	0.44
1:C:113:GLU:OE2	1:C:232:ARG:NH2	2.50	0.44
1:C:163:ILE:HG13	1:C:170:TRP:CZ2	2.52	0.44
1:D:27:ILE:O	1:D:164:ARG:HA	2.17	0.44
1:A:78:THR:OG1	1:A:93:THR:HG21	2.17	0.44
1:A:742:GLU:HG3	1:A:743:TRP:H	1.83	0.44
1:B:374:ASP:OD1	1:B:374:ASP:N	2.38	0.44
1:C:369:GLY:O	1:C:370:SER:HB3	2.18	0.44
1:C:474:LEU:HA	1:C:474:LEU:HD23	1.62	0.44
1:C:572:LYS:HE2	1:C:760:TRP:CZ3	2.52	0.44
1:D:85:SER:HA	1:C:270:SER:HB2	2.00	0.44
1:D:173:ASN:HB2	1:D:176:GLU:CD	2.42	0.44
1:D:187:LEU:HA	1:D:187:LEU:HD23	1.77	0.44
1:D:372:SER:OG	1:D:373:ALA:N	2.48	0.44
1:A:474:LEU:H	1:A:529:MET:HE1	1.82	0.44
1:A:571:ASP:O	1:A:572:LYS:C	2.60	0.44
1:A:740:GLU:HB3	1:A:741:GLU:H	1.65	0.44
1:B:110:VAL:HG12	1:B:228:ARG:HE	1.81	0.44
1:B:232:ARG:HD3	1:B:236:ARG:CZ	2.48	0.44
1:B:682:ARG:HH21	1:B:716:LEU:HD13	1.82	0.44
1:C:72:ARG:HG3	1:C:72:ARG:O	2.17	0.44
1:C:283:ASP:O	1:C:287:THR:HB	2.17	0.44
1:C:283:ASP:OD2	1:C:283:ASP:N	2.51	0.44
1:B:136:ALA:O	1:B:137:LEU:C	2.60	0.44
1:C:458:ILE:HG12	1:C:626:LEU:HA	1.98	0.44
1:C:640:VAL:HG21	1:C:743:TRP:CH2	2.53	0.44
1:D:143:LEU:O	1:D:146:CYS:HB3	2.18	0.43
1:D:221:TYR:CD1	1:D:221:TYR:N	2.85	0.43
1:D:287:THR:N	1:D:288:PRO:CD	2.81	0.43
1:D:456:ALA:HB3	1:D:498:LEU:HD22	1.99	0.43
1:D:665:ILE:HD13	1:D:665:ILE:H	1.83	0.43
1:A:239:VAL:HG11	1:A:292:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:GLU:O	1:A:545:ARG:C	2.60	0.43
1:B:115:ILE:HD13	1:B:293:ILE:HG12	1.99	0.43
1:B:618:SER:OG	1:B:619:GLY:N	2.51	0.43
1:C:98:GLN:HE21	1:C:98:GLN:HB2	1.56	0.43
1:C:274:PRO:HA	1:C:277:VAL:HG22	2.00	0.43
1:C:414:ASP:O	1:C:416:ASP:N	2.50	0.43
1:C:593:ARG:NH2	1:C:635:ALA:HB1	2.33	0.43
1:D:661:LEU:O	1:D:663:ASN:N	2.50	0.43
1:D:682:ARG:HB3	1:D:683:ALA:H	1.51	0.43
1:B:349:TRP:O	1:B:350:GLN:HG2	2.18	0.43
1:B:373:ALA:O	1:B:376:ARG:HB3	2.18	0.43
1:B:590:PRO:HA	1:B:593:ARG:HB2	2.00	0.43
1:B:724:VAL:HG12	1:B:725:ARG:HG3	1.99	0.43
1:C:130:VAL:O	1:C:131:TRP:C	2.61	0.43
1:C:159:TYR:HB3	1:C:170:TRP:CZ3	2.53	0.43
1:C:335:THR:HG21	1:C:404:ARG:HE	1.83	0.43
1:C:339:ARG:HB3	1:C:408:ARG:NH2	2.33	0.43
1:D:13:SER:HB3	1:A:2:GLU:HG2	2.00	0.43
1:D:28:PRO:HD2	1:D:31:GLN:HG2	2.00	0.43
1:D:154:GLY:O	1:D:157:ARG:HB2	2.18	0.43
1:D:390:PHE:CD1	1:D:390:PHE:C	2.97	0.43
1:D:520:GLY:O	1:D:524:VAL:HG23	2.17	0.43
1:D:537:MET:HE2	1:D:537:MET:HB3	1.59	0.43
1:A:223:HIS:CE1	1:A:227:MET:SD	3.11	0.43
1:A:671:LEU:HD23	1:A:671:LEU:HA	1.69	0.43
1:B:149:GLU:HG2	1:B:150:ASP:H	1.82	0.43
1:C:83:TYR:HD1	1:C:169:VAL:HG11	1.82	0.43
1:C:162:LEU:HA	1:C:162:LEU:HD23	1.67	0.43
1:C:207:PRO:O	1:C:208:ILE:HG22	2.18	0.43
1:C:396:LEU:HD21	1:C:406:TYR:CG	2.53	0.43
1:C:674:VAL:HG13	1:C:678:SER:HB3	2.00	0.43
1:D:618:SER:OG	1:D:619:GLY:N	2.50	0.43
1:A:706:LEU:O	1:A:710:GLU:HG3	2.18	0.43
1:B:59:GLU:H	1:B:59:GLU:HG3	1.58	0.43
1:D:217:ASP:C	1:D:219:GLU:H	2.25	0.43
1:D:420:ARG:O	1:D:423:VAL:HB	2.19	0.43
1:D:682:ARG:HD3	1:D:682:ARG:HA	1.36	0.43
1:A:636:THR:OG1	1:A:675:GLU:HG2	2.19	0.43
1:A:662:ILE:HA	1:A:667:ASN:OD1	2.18	0.43
1:B:44:LEU:HD21	1:B:65:LEU:HD21	2.01	0.43
1:B:280:LEU:O	1:B:281:GLU:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LEU:HB2	1:C:298:TYR:CD2	2.53	0.43
1:C:443:LYS:O	1:C:444:VAL:C	2.61	0.43
1:C:734:ALA:O	1:C:736:LEU:N	2.43	0.43
1:D:31:GLN:OE1	1:D:31:GLN:HA	2.19	0.43
1:D:337:LYS:HB3	1:D:338:PRO:HD3	1.99	0.43
1:D:502:ARG:NH2	1:D:766:TRP:HE1	2.17	0.43
1:A:217:ASP:C	1:A:219:GLU:N	2.77	0.43
1:A:493:SER:OG	1:A:494:ALA:N	2.52	0.43
1:B:472:VAL:O	1:B:476:THR:HG23	2.19	0.43
1:B:493:SER:OG	1:B:494:ALA:N	2.51	0.43
1:B:686:LEU:HD21	1:B:712:GLN:CB	2.48	0.43
1:C:437:PRO:HB2	1:C:460:LEU:HD12	1.99	0.43
1:D:17:PHE:CE2	1:D:101:MET:HE3	2.53	0.43
1:D:128:PRO:HD3	1:D:275:SER:HB2	2.00	0.43
1:D:235:LEU:HD23	1:D:235:LEU:HA	1.87	0.43
1:D:387:PHE:HE2	1:D:427:LEU:N	2.15	0.43
1:D:541:ALA:O	1:D:542:ARG:C	2.61	0.43
1:A:168:ASP:CG	1:A:181:SER:H	2.24	0.43
1:A:429:GLN:OE1	1:A:429:GLN:HA	2.18	0.43
1:A:484:LEU:CD2	1:A:547:LEU:HD23	2.48	0.43
1:A:688:ARG:CZ	1:A:740:GLU:OE2	2.64	0.43
1:B:385:LEU:HB2	1:B:386:PRO:HD3	2.00	0.43
1:B:650:SER:OG	1:B:683:ALA:HB1	2.19	0.43
1:B:683:ALA:O	1:B:685:HIS:N	2.50	0.43
1:B:706:LEU:HD22	1:B:724:VAL:HA	1.99	0.43
1:C:127:GLU:OE2	1:C:128:PRO:N	2.51	0.43
1:C:353:GLU:O	1:C:356:LEU:HB2	2.18	0.43
1:C:564:LEU:HB3	1:C:570:TYR:HB3	2.00	0.43
1:C:569:ILE:HG12	1:C:574:GLN:CD	2.44	0.43
1:C:699:VAL:HA	1:C:702:ALA:HB3	2.01	0.43
1:D:68:VAL:HA	1:D:96:ASP:O	2.19	0.43
1:A:34:TYR:CD2	1:A:224:LEU:HD12	2.49	0.43
1:A:55:LEU:HD11	1:A:302:ARG:NH2	2.34	0.43
1:A:244:LYS:HB2	1:A:244:LYS:HE3	1.92	0.43
1:B:26:TYR:HB3	1:B:93:THR:HG22	2.01	0.43
1:B:231:MET:HE3	1:B:231:MET:HB2	1.75	0.43
1:C:5:GLU:C	1:C:7:PHE:N	2.72	0.43
1:C:26:TYR:CD1	1:C:79:VAL:HG12	2.54	0.43
1:C:639:HIS:HA	1:C:667:ASN:O	2.19	0.43
1:D:369:GLY:O	1:D:371:SER:N	2.52	0.43
1:A:165:SER:O	1:A:166:TYR:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ILE:O	1:A:418:VAL:HB	2.18	0.43
1:B:83:TYR:HD1	1:B:169:VAL:HG11	1.84	0.43
1:B:199:ALA:O	1:B:200:VAL:HB	2.19	0.43
1:C:186:TYR:CZ	1:C:205:HIS:CD2	3.07	0.43
1:C:760:TRP:CE2	1:C:764:THR:HG21	2.54	0.43
1:D:106:LEU:HB3	1:D:231:MET:HE1	2.00	0.43
1:D:144:SER:C	1:D:146:CYS:H	2.26	0.43
1:D:684:TRP:O	1:D:684:TRP:CG	2.72	0.43
1:D:740:GLU:HB3	1:D:741:GLU:H	1.70	0.43
1:B:113:GLU:O	1:B:117:VAL:HG12	2.19	0.43
1:B:238:ALA:HB2	1:B:249:ILE:HD13	2.01	0.43
1:B:312:ARG:HH12	1:B:314:ASP:CG	2.27	0.43
1:B:375:LYS:O	1:B:378:THR:HG22	2.19	0.43
1:B:623:THR:HG22	1:B:634:PHE:HZ	1.84	0.43
1:B:740:GLU:HB3	1:B:741:GLU:H	1.68	0.43
1:C:337:LYS:O	1:C:338:PRO:C	2.60	0.43
1:D:36:TRP:O	1:D:227:MET:HE2	2.19	0.42
1:D:71:LEU:HD12	1:D:310:ALA:O	2.18	0.42
1:D:389:MET:HE1	1:D:526:ARG:HH11	1.84	0.42
1:D:561:LYS:CE	1:D:771:PRO:HD2	2.49	0.42
1:A:342:LYS:O	1:A:343:GLU:HG2	2.19	0.42
1:A:395:LYS:HG3	1:A:395:LYS:O	2.19	0.42
1:A:455:GLN:HB3	1:A:502:ARG:HE	1.84	0.42
1:B:113:GLU:OE1	1:B:228:ARG:NH1	2.51	0.42
1:B:344:GLU:HG3	1:B:354:SER:OG	2.19	0.42
1:B:366:ASP:O	1:B:370:SER:HB2	2.18	0.42
1:C:251:LEU:HB2	1:C:252:PRO:HD2	2.00	0.42
1:D:5:GLU:OE2	1:D:311:LYS:HB2	2.19	0.42
1:D:83:TYR:OH	1:D:176:GLU:HB2	2.19	0.42
1:D:181:SER:HB2	1:D:182:PRO:HD2	2.01	0.42
1:D:488:GLU:HG2	1:D:489:THR:N	2.33	0.42
1:A:283:ASP:O	1:A:287:THR:HB	2.19	0.42
1:A:578:ARG:O	1:A:582:THR:HG23	2.19	0.42
1:B:150:ASP:OD1	1:B:151:MET:O	2.37	0.42
1:D:433:PHE:CG	1:D:476:THR:HG22	2.54	0.42
1:D:470:ILE:H	1:D:470:ILE:HG12	1.59	0.42
1:A:96:ASP:HB2	1:A:320:PHE:CE2	2.54	0.42
1:A:520:GLY:O	1:A:523:GLY:N	2.51	0.42
1:B:338:PRO:CG	1:C:29:PRO:HG2	2.50	0.42
1:B:414:ASP:HB2	1:B:544:GLU:OE2	2.19	0.42
1:B:486:SER:O	1:B:489:THR:N	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:LEU:HD13	1:B:766:TRP:CH2	2.55	0.42
1:B:666:GLY:O	1:B:751:ARG:HD2	2.20	0.42
1:C:544:GLU:O	1:C:545:ARG:C	2.63	0.42
1:C:565:ARG:HA	1:C:570:TYR:CE2	2.55	0.42
1:C:617:LYS:CG	1:C:620:LEU:HB2	2.48	0.42
1:C:650:SER:OG	1:C:683:ALA:HB1	2.18	0.42
1:D:455:GLN:O	1:D:458:ILE:HG22	2.19	0.42
1:D:543:PHE:HD2	1:D:543:PHE:C	2.27	0.42
1:D:734:ALA:O	1:D:737:ALA:N	2.52	0.42
1:B:299:LEU:HA	1:B:303:VAL:CG2	2.48	0.42
1:B:331:THR:HB	1:B:380:THR:HG21	2.00	0.42
1:B:356:LEU:HD23	1:B:356:LEU:HA	1.85	0.42
1:B:396:LEU:CD1	1:B:403:GLN:HG2	2.49	0.42
1:B:495:ARG:O	1:B:496:GLN:C	2.62	0.42
1:B:709:ALA:CB	1:B:714:LEU:HB2	2.49	0.42
1:C:172:ARG:HG3	1:C:172:ARG:NH1	2.30	0.42
1:C:369:GLY:O	1:C:371:SER:N	2.50	0.42
1:C:416:ASP:HB2	1:C:417:ILE:H	1.47	0.42
1:C:433:PHE:CE2	1:C:438:TRP:NE1	2.88	0.42
1:C:533:VAL:O	1:C:538:PRO:HD2	2.19	0.42
1:C:561:LYS:HE2	1:C:771:PRO:HD2	2.02	0.42
1:C:595:LEU:HD23	1:C:595:LEU:HA	1.85	0.42
1:C:713:GLY:O	1:C:716:LEU:HG	2.19	0.42
1:C:740:GLU:HB3	1:C:741:GLU:H	1.68	0.42
1:D:417:ILE:C	1:D:419:ALA:N	2.77	0.42
1:D:507:PHE:CG	1:D:560:LEU:HD22	2.53	0.42
1:A:139:VAL:HG12	1:A:143:LEU:HD12	2.00	0.42
1:A:458:ILE:N	1:A:626:LEU:HB2	2.34	0.42
1:A:561:LYS:HD2	1:A:767:LEU:O	2.19	0.42
1:B:274:PRO:HA	1:B:277:VAL:HG22	2.01	0.42
1:B:682:ARG:HE	1:B:716:LEU:HD13	1.84	0.42
1:C:69:ILE:O	1:C:95:ILE:N	2.50	0.42
1:C:152:ARG:HE	1:C:152:ARG:HB2	1.43	0.42
1:C:163:ILE:HG23	1:C:163:ILE:HD13	1.77	0.42
1:C:496:GLN:HG2	1:C:553:VAL:HG22	2.02	0.42
1:D:682:ARG:HE	1:D:716:LEU:CD1	2.32	0.42
1:A:251:LEU:O	1:A:291:ARG:NH2	2.51	0.42
1:A:312:ARG:CB	1:A:312:ARG:HH11	2.31	0.42
1:B:5:GLU:OE2	1:B:311:LYS:HB2	2.19	0.42
1:B:541:ALA:O	1:B:542:ARG:C	2.61	0.42
1:B:565:ARG:HG2	1:B:570:TYR:CZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:GLU:O	1:B:628:ARG:NH1	2.47	0.42
1:C:164:ARG:NH1	1:C:183:ILE:HD11	2.34	0.42
1:C:401:ASN:H	1:C:401:ASN:HD22	1.67	0.42
1:C:617:LYS:HG2	1:C:620:LEU:HB2	2.02	0.42
1:C:769:PHE:O	1:C:770:GLU:HG2	2.19	0.42
1:D:7:PHE:C	1:D:7:PHE:HD2	2.25	0.42
1:D:468:HIS:HD2	1:D:512:ARG:HH21	1.68	0.42
1:D:615:ARG:HG2	1:D:616:GLY:N	2.34	0.42
1:D:734:ALA:O	1:D:736:LEU:N	2.45	0.42
1:A:104:LEU:O	1:A:105:LEU:C	2.62	0.42
1:A:569:ILE:HG12	1:A:574:GLN:OE1	2.18	0.42
1:B:97:GLY:O	1:B:99:GLN:N	2.53	0.42
1:C:266:ALA:HB1	1:C:302:ARG:NH1	2.34	0.42
1:C:429:GLN:HG2	1:C:480:ALA:CB	2.49	0.42
1:A:127:GLU:C	1:A:127:GLU:OE2	2.63	0.42
1:B:223:HIS:CE1	1:B:227:MET:HG2	2.54	0.42
1:B:700:GLU:O	1:B:704:LYS:HD2	2.19	0.42
1:C:71:LEU:HB3	1:C:93:THR:OG1	2.20	0.42
1:C:151:MET:HB3	1:C:172:ARG:CZ	2.50	0.42
1:C:204:ARG:O	1:C:205:HIS:CB	2.67	0.42
1:C:542:ARG:NH1	1:C:544:GLU:O	2.53	0.42
1:C:634:PHE:CD1	1:C:634:PHE:N	2.82	0.42
1:D:27:ILE:CG1	1:D:162:LEU:HD22	2.49	0.42
1:A:300:LEU:HD23	1:A:300:LEU:HA	1.78	0.42
1:A:337:LYS:NZ	1:A:362:GLU:CD	2.77	0.42
1:A:516:GLY:O	1:A:587:HIS:CD2	2.73	0.42
1:A:589:LYS:N	1:A:590:PRO:HD2	2.34	0.42
1:A:630:ASN:O	1:A:632:GLU:N	2.53	0.42
1:B:44:LEU:O	1:B:48:VAL:HG12	2.20	0.42
1:B:282:ASP:OD1	1:B:282:ASP:N	2.53	0.42
1:B:488:GLU:CD	1:B:489:THR:HG22	2.44	0.42
1:B:529:MET:HA	1:B:540:PHE:HB3	2.02	0.42
1:B:585:TYR:CD1	1:B:637:ILE:HG21	2.54	0.42
1:C:273:PRO:HG2	1:C:276:VAL:CG2	2.50	0.42
1:C:514:SER:O	1:C:582:THR:HG21	2.20	0.42
1:C:576:VAL:HG21	1:C:757:SER:HA	2.01	0.42
1:D:128:PRO:HG3	1:D:275:SER:HB2	2.02	0.42
1:D:477:ARG:CZ	1:D:542:ARG:H	2.32	0.42
1:D:688:ARG:HD3	1:D:692:ARG:HH12	1.85	0.42
1:A:26:TYR:CE1	1:A:79:VAL:HG12	2.55	0.42
1:A:400:LEU:HD13	1:A:400:LEU:HA	1.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ASP:O	1:A:472:VAL:HG23	2.20	0.42
1:A:472:VAL:O	1:A:476:THR:HG23	2.20	0.42
1:B:13:SER:O	1:B:14:VAL:C	2.62	0.42
1:B:471:VAL:HG13	1:B:504:CYS:SG	2.60	0.42
1:B:486:SER:HB3	1:B:488:GLU:CD	2.45	0.42
1:C:38:LEU:N	1:C:227:MET:HE3	2.35	0.42
1:C:541:ALA:O	1:C:542:ARG:C	2.63	0.42
1:C:715:ARG:HB3	1:C:719:GLY:CA	2.48	0.42
1:D:29:PRO:HB2	1:D:166:TYR:CE2	2.55	0.41
1:D:162:LEU:O	1:D:163:ILE:HG13	2.20	0.41
1:A:59:GLU:H	1:A:59:GLU:HG3	1.56	0.41
1:A:148:GLU:OE1	1:A:195:ARG:NH1	2.45	0.41
1:B:207:PRO:O	1:B:208:ILE:HG22	2.19	0.41
1:B:605:PRO:HG3	1:B:734:ALA:HB3	2.02	0.41
1:D:167:TYR:CD1	1:D:167:TYR:N	2.88	0.41
1:D:180:ARG:HD3	1:D:213:THR:CG2	2.49	0.41
1:A:70:ALA:HB3	1:A:92:MET:HE3	2.01	0.41
1:A:231:MET:HB2	1:A:231:MET:HE3	1.70	0.41
1:A:234:MET:HE2	1:A:234:MET:HB2	1.93	0.41
1:A:636:THR:HB	1:A:671:LEU:O	2.20	0.41
1:A:651:TRP:CH2	1:A:684:TRP:HB2	2.55	0.41
1:B:128:PRO:CD	1:B:275:SER:HB2	2.48	0.41
1:B:337:LYS:HE2	1:B:358:PHE:CD1	2.55	0.41
1:C:52:LEU:HD13	1:C:52:LEU:C	2.45	0.41
1:C:83:TYR:CZ	1:C:176:GLU:HB2	2.55	0.41
1:C:337:LYS:NZ	1:C:358:PHE:CD1	2.86	0.41
1:D:123:THR:O	1:D:123:THR:OG1	2.29	0.41
1:D:161:ARG:CA	1:D:170:TRP:HH2	2.25	0.41
1:D:390:PHE:HD1	1:D:391:GLN:N	2.19	0.41
1:A:763:LEU:O	1:A:766:TRP:HB2	2.21	0.41
1:B:352:SER:O	1:B:354:SER:N	2.53	0.41
1:B:426:GLY:O	1:B:430:VAL:HG23	2.20	0.41
1:C:140:THR:HG22	1:C:141:GLY:N	2.35	0.41
1:C:395:LYS:HG3	1:C:395:LYS:O	2.20	0.41
1:C:565:ARG:O	1:C:566:SER:C	2.63	0.41
1:D:379:VAL:O	1:D:383:VAL:HG12	2.20	0.41
1:A:482:HIS:HA	1:A:493:SER:CB	2.50	0.41
1:A:557:GLN:O	1:A:561:LYS:HD3	2.21	0.41
1:A:665:ILE:C	1:A:667:ASN:H	2.28	0.41
1:B:104:LEU:HD23	1:B:104:LEU:HA	1.64	0.41
1:B:217:ASP:C	1:B:219:GLU:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:ASP:O	1:C:284:ALA:C	2.63	0.41
1:C:339:ARG:HG2	1:C:408:ARG:NH1	2.35	0.41
1:C:440:SER:C	1:C:442:THR:N	2.78	0.41
1:C:617:LYS:HA	1:C:617:LYS:HD2	1.90	0.41
1:C:662:ILE:HD12	1:C:662:ILE:H	1.85	0.41
1:C:723:ILE:HG12	1:C:726:GLN:NE2	2.35	0.41
1:D:337:LYS:O	1:D:341:ILE:HG13	2.21	0.41
1:D:720:ALA:HB1	1:D:723:ILE:HB	2.02	0.41
1:A:366:ASP:O	1:A:370:SER:HB2	2.20	0.41
1:B:377:GLN:HE22	1:B:403:GLN:NE2	2.16	0.41
1:C:330:LEU:HB3	1:C:334:GLU:OE1	2.21	0.41
1:C:666:GLY:N	1:C:752:SER:HB3	2.31	0.41
1:D:576:VAL:HG13	1:D:756:CYS:HB2	2.02	0.41
1:D:658:ASP:OD2	1:D:664:ARG:NH2	2.54	0.41
1:D:665:ILE:HG12	1:D:752:SER:HB2	2.02	0.41
1:D:715:ARG:HG2	1:D:720:ALA:CB	2.49	0.41
1:A:48:VAL:HG22	1:A:295:PHE:CE1	2.56	0.41
1:A:444:VAL:HB	1:A:445:PRO:CD	2.50	0.41
1:A:666:GLY:O	1:A:751:ARG:HD2	2.21	0.41
1:A:709:ALA:CB	1:A:714:LEU:HB2	2.49	0.41
1:B:339:ARG:HG2	1:B:408:ARG:NH1	2.36	0.41
1:D:253:THR:O	1:D:254:GLY:C	2.63	0.41
1:A:217:ASP:O	1:A:218:LEU:HB2	2.21	0.41
1:A:312:ARG:HD3	1:A:315:TYR:HE2	1.86	0.41
1:A:337:LYS:HZ3	1:A:362:GLU:CD	2.29	0.41
1:A:466:GLY:O	1:A:467:GLY:O	2.38	0.41
1:B:38:LEU:O	1:B:38:LEU:HG	2.21	0.41
1:B:87:VAL:HG13	1:B:88:PRO:O	2.21	0.41
1:B:247:ASP:CG	1:B:248:ASP:H	2.28	0.41
1:B:455:GLN:OE1	1:B:502:ARG:NH2	2.48	0.41
1:C:482:HIS:HA	1:C:493:SER:HB2	2.02	0.41
1:C:691:PHE:CD2	1:C:736:LEU:HD13	2.54	0.41
1:D:35:SER:O	1:D:223:HIS:NE2	2.48	0.41
1:D:387:PHE:CD2	1:D:427:LEU:HG	2.55	0.41
1:D:445:PRO:CD	1:D:498:LEU:HD21	2.51	0.41
1:A:168:ASP:OD1	1:A:168:ASP:N	2.54	0.41
1:A:375:LYS:O	1:A:378:THR:HG22	2.20	0.41
1:A:495:ARG:O	1:A:496:GLN:C	2.63	0.41
1:A:584:VAL:HG21	1:A:665:ILE:HD13	2.01	0.41
1:B:11:PRO:HB3	1:C:7:PHE:CD2	2.55	0.41
1:B:162:LEU:HD23	1:B:162:LEU:HA	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:GLN:HE21	1:B:542:ARG:HH12	1.68	0.41
1:B:417:ILE:HD12	1:B:420:ARG:HB2	2.03	0.41
1:B:511:TRP:HH2	1:B:519:ALA:HB3	1.86	0.41
1:C:391:GLN:OE1	1:C:542:ARG:NH1	2.53	0.41
1:D:9:ALA:HA	1:D:307:VAL:O	2.21	0.41
1:D:83:TYR:CZ	1:D:176:GLU:HB2	2.56	0.41
1:D:112:HIS:NE2	1:D:140:THR:HG23	2.35	0.41
1:D:160:PRO:O	1:D:170:TRP:CZ3	2.74	0.41
1:D:339:ARG:HG2	1:D:408:ARG:NH2	2.36	0.41
1:D:357:HIS:O	1:D:360:VAL:HB	2.20	0.41
1:D:433:PHE:HB3	1:D:476:THR:HG22	2.02	0.41
1:D:543:PHE:C	1:D:543:PHE:CD2	2.98	0.41
1:D:572:LYS:HE2	1:D:760:TRP:CZ3	2.56	0.41
1:D:633:ALA:HB3	1:D:634:PHE:HD1	1.84	0.41
1:A:407:LEU:HA	1:A:407:LEU:HD23	1.78	0.41
1:A:479:PHE:O	1:A:479:PHE:CD1	2.74	0.41
1:A:640:VAL:HG11	1:A:743:TRP:CE2	2.56	0.41
1:B:72:ARG:CZ	1:B:90:LYS:HG3	2.51	0.41
1:C:86:GLN:CD	1:C:172:ARG:HD3	2.45	0.41
1:C:228:ARG:HA	1:C:231:MET:HE2	2.03	0.41
1:C:432:ARG:O	1:C:435:GLU:N	2.50	0.41
1:C:433:PHE:HE2	1:C:438:TRP:NE1	2.19	0.41
1:D:42:ARG:HA	1:D:234:MET:HE3	2.03	0.41
1:A:108:THR:HB	1:A:143:LEU:HD22	2.03	0.41
1:A:123:THR:O	1:A:129:SER:OG	2.28	0.41
1:B:449:ASP:C	1:B:451:THR:N	2.78	0.41
1:C:137:LEU:O	1:C:138:ASP:C	2.63	0.41
1:C:156:HIS:ND1	1:C:177:ALA:HB3	2.36	0.41
1:C:706:LEU:HD22	1:C:724:VAL:HA	2.03	0.41
1:D:282:ASP:OD1	1:D:282:ASP:N	2.54	0.40
1:D:451:THR:O	1:D:455:GLN:HG3	2.21	0.40
1:D:508:TYR:O	1:D:509:ALA:C	2.63	0.40
1:D:571:ASP:O	1:D:572:LYS:C	2.64	0.40
1:D:638:GLU:O	1:D:668:LEU:HA	2.21	0.40
1:A:112:HIS:HD1	1:A:190:TYR:HE1	1.69	0.40
1:A:486:SER:HB3	1:A:488:GLU:CD	2.45	0.40
1:A:492:SER:O	1:A:496:GLN:HG3	2.21	0.40
1:A:715:ARG:HG2	1:A:720:ALA:HB2	2.03	0.40
1:B:300:LEU:HD23	1:B:300:LEU:HA	1.82	0.40
1:B:478:TYR:OH	1:B:556:LEU:HG	2.21	0.40
1:C:104:LEU:HA	1:C:104:LEU:HD23	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ILE:HG23	1:C:289:LEU:HD11	2.03	0.40
1:D:209:ASP:O	1:D:209:ASP:CG	2.65	0.40
1:D:417:ILE:C	1:D:419:ALA:H	2.29	0.40
1:D:538:PRO:HB2	1:D:550:VAL:CG1	2.51	0.40
1:A:212:LYS:HB3	1:A:213:THR:H	1.57	0.40
1:A:274:PRO:O	1:A:277:VAL:HG22	2.22	0.40
1:C:148:GLU:OE2	1:C:195:ARG:NH1	2.55	0.40
1:C:182:PRO:HB2	1:C:224:LEU:HD13	2.02	0.40
1:C:211:ASP:O	1:C:212:LYS:HG2	2.20	0.40
1:D:18:LEU:HD23	1:D:18:LEU:HA	1.82	0.40
1:D:106:LEU:O	1:D:109:THR:HG22	2.22	0.40
1:D:617:LYS:HD2	1:D:617:LYS:HA	1.89	0.40
1:A:157:ARG:HD2	1:A:158:TYR:CE2	2.57	0.40
1:A:414:ASP:C	1:A:416:ASP:N	2.79	0.40
1:A:542:ARG:O	1:A:542:ARG:HG3	2.19	0.40
1:B:187:LEU:HD23	1:B:187:LEU:HA	1.65	0.40
1:B:253:THR:O	1:B:256:ASP:HB2	2.20	0.40
1:B:337:LYS:O	1:B:338:PRO:C	2.63	0.40
1:B:372:SER:OG	1:B:375:LYS:HB3	2.21	0.40
1:B:416:ASP:HB2	1:B:417:ILE:H	1.28	0.40
1:B:474:LEU:HD12	1:B:525:TYR:CD1	2.56	0.40
1:B:543:PHE:C	1:B:543:PHE:HD2	2.29	0.40
1:B:597:LEU:HD22	1:B:623:THR:HB	2.03	0.40
1:B:600:SER:HA	1:B:603:SER:OG	2.21	0.40
1:C:337:LYS:HB2	1:C:337:LYS:HZ2	1.86	0.40
1:C:346:LEU:HB3	1:C:347:ASP:H	1.69	0.40
1:C:386:PRO:O	1:C:389:MET:HB2	2.22	0.40
1:C:417:ILE:HD12	1:C:417:ILE:HA	1.59	0.40
1:A:69:ILE:HD13	1:A:69:ILE:HG21	1.91	0.40
1:B:65:LEU:HD22	1:B:65:LEU:O	2.21	0.40
1:B:163:ILE:O	1:B:164:ARG:HB2	2.21	0.40
1:C:451:THR:O	1:C:455:GLN:HG3	2.21	0.40
1:C:549:GLU:O	1:C:550:VAL:HB	2.21	0.40
1:C:641:ALA:N	1:C:667:ASN:OD1	2.50	0.40
1:D:417:ILE:HD12	1:D:417:ILE:HA	1.71	0.40
1:D:477:ARG:NE	1:D:542:ARG:HB3	2.36	0.40
1:D:569:ILE:HD13	1:D:574:GLN:HB3	2.02	0.40
1:D:728:ARG:HD3	1:D:729:TYR:H	1.83	0.40
1:A:23:GLN:HG3	1:A:90:LYS:HD3	2.04	0.40
1:A:158:TYR:CD2	1:A:158:TYR:N	2.90	0.40
1:A:484:LEU:CD2	1:A:548:THR:HG22	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:LEU:HB2	1:B:268:PHE:CD1	2.56	0.40
1:B:474:LEU:HG	1:B:529:MET:CE	2.51	0.40
1:C:122:LEU:HD23	1:C:122:LEU:HA	1.78	0.40
1:C:145:ASN:OD1	1:C:145:ASN:N	2.55	0.40
1:C:164:ARG:HH12	1:C:183:ILE:HD11	1.85	0.40
1:C:168:ASP:OD1	1:C:179:TYR:HA	2.21	0.40
1:C:228:ARG:HA	1:C:231:MET:CE	2.50	0.40
1:C:618:SER:OG	1:C:619:GLY:N	2.54	0.40

All (3) 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:D:85:SER:N	1:C:211:ASP:OD2[4_457]	2.06	0.14
1:D:84:ARG:N	1:C:211:ASP:OD2[4_457]	2.15	0.05
1:A:657:GLU:OE1	1:B:236:ARG:NH1[4_447]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

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	769/771 (100%)	598 (78%)	112 (15%)	59 (8%)	1	8
1	B	769/771 (100%)	597 (78%)	122 (16%)	50 (6%)	1	11
1	C	769/771 (100%)	601 (78%)	109 (14%)	59 (8%)	1	8
1	D	769/771 (100%)	600 (78%)	113 (15%)	56 (7%)	1	9
All	All	3076/3084 (100%)	2396 (78%)	456 (15%)	224 (7%)	1	9

All (224) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	4	LYS
1	D	36	TRP
1	D	127	GLU
1	D	200	VAL
1	D	205	HIS
1	D	208	ILE
1	D	283	ASP
1	D	353	GLU
1	D	538	PRO
1	D	551	PRO
1	D	552	PRO
1	D	565	ARG
1	D	618	SER
1	D	631	ASP
1	D	633	ALA
1	D	645	PRO
1	D	650	SER
1	D	682	ARG
1	D	727	ALA
1	A	4	LYS
1	A	6	ILE
1	A	127	GLU
1	A	200	VAL
1	A	205	HIS
1	A	208	ILE
1	A	241	ALA
1	A	283	ASP
1	A	353	GLU
1	A	414	ASP
1	A	444	VAL
1	A	445	PRO
1	A	538	PRO
1	A	551	PRO
1	A	552	PRO
1	A	565	ARG
1	A	618	SER
1	A	631	ASP
1	A	633	ALA
1	A	645	PRO
1	A	650	SER
1	A	682	ARG
1	A	727	ALA
1	B	4	LYS

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Mol	Chain	Res	Type
1	B	6	ILE
1	B	127	GLU
1	B	200	VAL
1	B	208	ILE
1	B	241	ALA
1	B	283	ASP
1	B	353	GLU
1	B	444	VAL
1	B	445	PRO
1	B	467	GLY
1	B	538	PRO
1	B	551	PRO
1	B	552	PRO
1	B	565	ARG
1	B	618	SER
1	B	633	ALA
1	B	645	PRO
1	B	650	SER
1	B	682	ARG
1	B	770	GLU
1	C	4	LYS
1	C	127	GLU
1	C	208	ILE
1	C	247	ASP
1	C	283	ASP
1	C	353	GLU
1	C	414	ASP
1	C	444	VAL
1	C	445	PRO
1	C	538	PRO
1	C	551	PRO
1	C	552	PRO
1	C	618	SER
1	C	631	ASP
1	C	633	ALA
1	C	645	PRO
1	C	650	SER
1	C	682	ARG
1	C	727	ALA
1	C	770	GLU
1	D	6	ILE
1	D	81	PRO

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Mol	Chain	Res	Type
1	D	126	ASP
1	D	164	ARG
1	D	241	ALA
1	D	444	VAL
1	D	445	PRO
1	D	450	ALA
1	D	467	GLY
1	D	685	HIS
1	D	695	SER
1	D	720	ALA
1	D	721	GLY
1	A	36	TRP
1	A	450	ALA
1	A	467	GLY
1	A	685	HIS
1	A	695	SER
1	A	721	GLY
1	A	770	GLU
1	B	36	TRP
1	B	81	PRO
1	B	205	HIS
1	B	247	ASP
1	B	450	ALA
1	B	631	ASP
1	B	685	HIS
1	B	695	SER
1	B	721	GLY
1	C	6	ILE
1	C	36	TRP
1	C	200	VAL
1	C	205	HIS
1	C	450	ALA
1	C	467	GLY
1	C	518	THR
1	C	565	ARG
1	C	587	HIS
1	C	685	HIS
1	C	695	SER
1	C	720	ALA
1	C	721	GLY
1	D	569	ILE
1	D	587	HIS

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Mol	Chain	Res	Type
1	D	632	GLU
1	D	684	TRP
1	D	718	SER
1	D	728	ARG
1	D	770	GLU
1	A	164	ARG
1	A	370	SER
1	A	569	ILE
1	A	648	ASN
1	A	718	SER
1	A	720	ALA
1	B	121	LYS
1	B	164	ARG
1	B	370	SER
1	B	587	HIS
1	B	718	SER
1	B	720	ALA
1	B	727	ALA
1	C	81	PRO
1	C	164	ARG
1	C	241	ALA
1	C	350	GLN
1	C	568	GLY
1	C	632	GLU
1	C	684	TRP
1	C	718	SER
1	D	247	ASP
1	D	350	GLN
1	D	370	SER
1	D	390	PHE
1	A	247	ASP
1	A	390	PHE
1	A	448	ASP
1	A	519	ALA
1	A	566	SER
1	A	587	HIS
1	A	684	TRP
1	A	734	ALA
1	B	350	GLN
1	B	568	GLY
1	B	569	ILE
1	C	126	ASP

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Mol	Chain	Res	Type
1	C	269	ASN
1	C	448	ASP
1	C	519	ALA
1	C	569	ILE
1	D	414	ASP
1	D	448	ASP
1	D	620	LEU
1	D	648	ASN
1	D	736	LEU
1	A	81	PRO
1	A	121	LYS
1	A	163	ILE
1	A	281	GLU
1	A	350	GLN
1	A	392	ASP
1	A	487	PRO
1	A	728	ARG
1	B	126	ASP
1	B	163	ILE
1	B	390	PHE
1	B	414	ASP
1	B	487	PRO
1	B	648	ASN
1	C	5	GLU
1	C	160	PRO
1	C	166	TYR
1	C	248	ASP
1	C	392	ASP
1	C	545	ARG
1	C	566	SER
1	C	728	ARG
1	D	57	GLU
1	D	163	ILE
1	D	416	ASP
1	A	166	TYR
1	A	168	ASP
1	A	518	THR
1	B	166	TYR
1	C	162	LEU
1	C	370	SER
1	C	487	PRO
1	D	160	PRO

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Mol	Chain	Res	Type
1	D	568	GLY
1	C	163	ILE
1	C	550	VAL
1	A	640	VAL
1	B	550	VAL
1	D	418	VAL
1	D	487	PRO
1	D	466	GLY
1	A	568	GLY
1	B	327	GLY
1	B	417	ILE
1	A	415	PRO
1	A	550	VAL

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	650/650 (100%)	545 (84%)	105 (16%)	2	14
1	B	650/650 (100%)	546 (84%)	104 (16%)	2	14
1	C	650/650 (100%)	540 (83%)	110 (17%)	2	13
1	D	650/650 (100%)	535 (82%)	115 (18%)	2	10
All	All	2600/2600 (100%)	2166 (83%)	434 (17%)	2	13

All (434) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3	THR
1	D	7	PHE
1	D	14	VAL
1	D	27	ILE
1	D	44	LEU
1	D	46	SER
1	D	48	VAL
1	D	52	LEU

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Mol	Chain	Res	Type
1	D	61	SER
1	D	62	ILE
1	D	63	CYS
1	D	64	PHE
1	D	65	LEU
1	D	68	VAL
1	D	75	ASN
1	D	77	THR
1	D	79	VAL
1	D	86	GLN
1	D	87	VAL
1	D	91	VAL
1	D	99	GLN
1	D	101	MET
1	D	105	LEU
1	D	106	LEU
1	D	109	THR
1	D	110	VAL
1	D	122	LEU
1	D	127	GLU
1	D	130	VAL
1	D	140	THR
1	D	151	MET
1	D	157	ARG
1	D	163	ILE
1	D	164	ARG
1	D	165	SER
1	D	167	TYR
1	D	172	ARG
1	D	176	GLU
1	D	183	ILE
1	D	189	SER
1	D	198	ASP
1	D	200	VAL
1	D	208	ILE
1	D	211	ASP
1	D	213	THR
1	D	216	VAL
1	D	227	MET
1	D	228	ARG
1	D	231	MET
1	D	234	MET

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Mol	Chain	Res	Type
1	D	243	VAL
1	D	249	ILE
1	D	251	LEU
1	D	262	ASN
1	D	269	ASN
1	D	275	SER
1	D	279	GLN
1	D	280	LEU
1	D	282	ASP
1	D	283	ASP
1	D	287	THR
1	D	292	LEU
1	D	305	VAL
1	D	312	ARG
1	D	328	GLN
1	D	335	THR
1	D	342	LYS
1	D	348	GLU
1	D	349	TRP
1	D	350	GLN
1	D	354	SER
1	D	365	LEU
1	D	368	GLU
1	D	381	SER
1	D	384	LEU
1	D	394	THR
1	D	396	LEU
1	D	399	ARG
1	D	400	LEU
1	D	408	ARG
1	D	410	VAL
1	D	414	ASP
1	D	416	ASP
1	D	429	GLN
1	D	444	VAL
1	D	449	ASP
1	D	452	LEU
1	D	470	ILE
1	D	486	SER
1	D	489	THR
1	D	542	ARG
1	D	543	PHE

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Mol	Chain	Res	Type
1	D	545	ARG
1	D	547	LEU
1	D	569	ILE
1	D	591	LEU
1	D	592	THR
1	D	594	LEU
1	D	609	THR
1	D	620	LEU
1	D	634	PHE
1	D	636	THR
1	D	654	ASP
1	D	661	LEU
1	D	665	ILE
1	D	671	LEU
1	D	682	ARG
1	D	692	ARG
1	D	728	ARG
1	D	730	LEU
1	D	736	LEU
1	D	744	THR
1	D	754	ARG
1	D	764	THR
1	D	766	TRP
1	A	3	THR
1	A	7	PHE
1	A	14	VAL
1	A	32	ARG
1	A	48	VAL
1	A	52	LEU
1	A	61	SER
1	A	62	ILE
1	A	65	LEU
1	A	68	VAL
1	A	75	ASN
1	A	77	THR
1	A	86	GLN
1	A	91	VAL
1	A	98	GLN
1	A	99	GLN
1	A	101	MET
1	A	106	LEU
1	A	109	THR

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Mol	Chain	Res	Type
1	A	110	VAL
1	A	127	GLU
1	A	130	VAL
1	A	137	LEU
1	A	140	THR
1	A	146	CYS
1	A	151	MET
1	A	152	ARG
1	A	153	TYR
1	A	157	ARG
1	A	163	ILE
1	A	164	ARG
1	A	165	SER
1	A	167	TYR
1	A	168	ASP
1	A	172	ARG
1	A	176	GLU
1	A	183	ILE
1	A	198	ASP
1	A	200	VAL
1	A	208	ILE
1	A	213	THR
1	A	216	VAL
1	A	227	MET
1	A	234	MET
1	A	243	VAL
1	A	249	ILE
1	A	251	LEU
1	A	262	ASN
1	A	275	SER
1	A	280	LEU
1	A	283	ASP
1	A	287	THR
1	A	292	LEU
1	A	304	THR
1	A	305	VAL
1	A	312	ARG
1	A	321	GLU
1	A	323	LEU
1	A	328	GLN
1	A	335	THR
1	A	342	LYS

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Mol	Chain	Res	Type
1	A	348	GLU
1	A	365	LEU
1	A	368	GLU
1	A	384	LEU
1	A	390	PHE
1	A	396	LEU
1	A	400	LEU
1	A	429	GLN
1	A	444	VAL
1	A	449	ASP
1	A	452	LEU
1	A	458	ILE
1	A	468	HIS
1	A	470	ILE
1	A	489	THR
1	A	511	TRP
1	A	528	LEU
1	A	537	MET
1	A	542	ARG
1	A	543	PHE
1	A	545	ARG
1	A	547	LEU
1	A	558	SER
1	A	569	ILE
1	A	588	SER
1	A	591	LEU
1	A	592	THR
1	A	593	ARG
1	A	594	LEU
1	A	601	GLN
1	A	609	THR
1	A	622	GLU
1	A	636	THR
1	A	654	ASP
1	A	661	LEU
1	A	665	ILE
1	A	682	ARG
1	A	728	ARG
1	A	736	LEU
1	A	744	THR
1	A	754	ARG
1	A	758	LEU

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Mol	Chain	Res	Type
1	A	764	THR
1	A	769	PHE
1	B	3	THR
1	B	7	PHE
1	B	14	VAL
1	B	16	GLN
1	B	44	LEU
1	B	52	LEU
1	B	53	ASP
1	B	61	SER
1	B	62	ILE
1	B	63	CYS
1	B	64	PHE
1	B	65	LEU
1	B	68	VAL
1	B	75	ASN
1	B	82	LYS
1	B	86	GLN
1	B	91	VAL
1	B	98	GLN
1	B	99	GLN
1	B	101	MET
1	B	105	LEU
1	B	106	LEU
1	B	109	THR
1	B	110	VAL
1	B	130	VAL
1	B	137	LEU
1	B	140	THR
1	B	157	ARG
1	B	163	ILE
1	B	164	ARG
1	B	165	SER
1	B	167	TYR
1	B	168	ASP
1	B	172	ARG
1	B	176	GLU
1	B	183	ILE
1	B	193	TYR
1	B	198	ASP
1	B	200	VAL
1	B	206	VAL

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Mol	Chain	Res	Type
1	B	208	ILE
1	B	213	THR
1	B	216	VAL
1	B	227	MET
1	B	234	MET
1	B	243	VAL
1	B	249	ILE
1	B	251	LEU
1	B	262	ASN
1	B	275	SER
1	B	280	LEU
1	B	282	ASP
1	B	283	ASP
1	B	287	THR
1	B	292	LEU
1	B	305	VAL
1	B	312	ARG
1	B	328	GLN
1	B	335	THR
1	B	342	LYS
1	B	348	GLU
1	B	349	TRP
1	B	350	GLN
1	B	354	SER
1	B	358	PHE
1	B	374	ASP
1	B	384	LEU
1	B	396	LEU
1	B	400	LEU
1	B	410	VAL
1	B	414	ASP
1	B	416	ASP
1	B	421	ARG
1	B	429	GLN
1	B	444	VAL
1	B	446	SER
1	B	449	ASP
1	B	452	LEU
1	B	458	ILE
1	B	470	ILE
1	B	483	ARG
1	B	486	SER

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Mol	Chain	Res	Type
1	B	489	THR
1	B	511	TRP
1	B	542	ARG
1	B	543	PHE
1	B	545	ARG
1	B	546	ASP
1	B	547	LEU
1	B	548	THR
1	B	566	SER
1	B	569	ILE
1	B	591	LEU
1	B	594	LEU
1	B	622	GLU
1	B	636	THR
1	B	654	ASP
1	B	665	ILE
1	B	682	ARG
1	B	728	ARG
1	B	736	LEU
1	B	744	THR
1	B	764	THR
1	B	769	PHE
1	C	2	GLU
1	C	3	THR
1	C	7	PHE
1	C	14	VAL
1	C	46	SER
1	C	52	LEU
1	C	53	ASP
1	C	61	SER
1	C	62	ILE
1	C	65	LEU
1	C	68	VAL
1	C	75	ASN
1	C	86	GLN
1	C	91	VAL
1	C	98	GLN
1	C	99	GLN
1	C	101	MET
1	C	102	THR
1	C	106	LEU
1	C	108	THR

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Mol	Chain	Res	Type
1	C	109	THR
1	C	110	VAL
1	C	127	GLU
1	C	129	SER
1	C	130	VAL
1	C	137	LEU
1	C	140	THR
1	C	144	SER
1	C	145	ASN
1	C	152	ARG
1	C	157	ARG
1	C	163	ILE
1	C	165	SER
1	C	167	TYR
1	C	172	ARG
1	C	176	GLU
1	C	183	ILE
1	C	198	ASP
1	C	200	VAL
1	C	213	THR
1	C	216	VAL
1	C	227	MET
1	C	234	MET
1	C	243	VAL
1	C	249	ILE
1	C	251	LEU
1	C	255	THR
1	C	262	ASN
1	C	275	SER
1	C	280	LEU
1	C	283	ASP
1	C	286	MET
1	C	287	THR
1	C	292	LEU
1	C	304	THR
1	C	305	VAL
1	C	312	ARG
1	C	319	MET
1	C	323	LEU
1	C	328	GLN
1	C	335	THR
1	C	337	LYS

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Mol	Chain	Res	Type
1	C	342	LYS
1	C	343	GLU
1	C	348	GLU
1	C	349	TRP
1	C	350	GLN
1	C	356	LEU
1	C	358	PHE
1	C	365	LEU
1	C	374	ASP
1	C	384	LEU
1	C	390	PHE
1	C	394	THR
1	C	396	LEU
1	C	400	LEU
1	C	401	ASN
1	C	429	GLN
1	C	444	VAL
1	C	452	LEU
1	C	458	ILE
1	C	468	HIS
1	C	470	ILE
1	C	486	SER
1	C	489	THR
1	C	528	LEU
1	C	542	ARG
1	C	543	PHE
1	C	545	ARG
1	C	547	LEU
1	C	569	ILE
1	C	591	LEU
1	C	592	THR
1	C	593	ARG
1	C	594	LEU
1	C	618	SER
1	C	622	GLU
1	C	627	GLU
1	C	634	PHE
1	C	636	THR
1	C	654	ASP
1	C	665	ILE
1	C	671	LEU
1	C	682	ARG

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Mol	Chain	Res	Type
1	C	685	HIS
1	C	728	ARG
1	C	736	LEU
1	C	744	THR
1	C	764	THR
1	C	769	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	16	GLN
1	D	50	HIS
1	D	350	GLN
1	D	377	GLN
1	D	403	GLN
1	D	574	GLN
1	A	16	GLN
1	A	98	GLN
1	A	205	HIS
1	A	301	HIS
1	A	377	GLN
1	A	403	GLN
1	A	531	HIS
1	A	557	GLN
1	A	667	ASN
1	B	134	ASN
1	B	328	GLN
1	B	377	GLN
1	B	531	HIS
1	B	663	ASN
1	C	50	HIS
1	C	98	GLN
1	C	350	GLN
1	C	401	ASN
1	C	557	GLN
1	C	676	ASN
1	C	712	GLN

5.3.3 RNA ⓘ

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	771/771 (100%)	0.92	140 (18%) 3 4	22, 75, 151, 187	0
1	B	771/771 (100%)	1.09	168 (21%) 2 2	16, 102, 186, 207	0
1	C	771/771 (100%)	0.34	52 (6%) 24 15	4, 50, 132, 180	0
1	D	771/771 (100%)	0.70	101 (13%) 7 6	8, 76, 152, 195	0
All	All	3084/3084 (100%)	0.76	461 (14%) 5 5	4, 72, 168, 207	0

All (461) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	714	LEU	7.4
1	B	763	LEU	6.9
1	B	533	VAL	6.9
1	A	544	GLU	6.8
1	D	729	TYR	6.5
1	B	595	LEU	5.8
1	B	723	ILE	5.7
1	A	540	PHE	5.6
1	B	458	ILE	5.2
1	D	621	LEU	5.2
1	B	597	LEU	5.2
1	D	538	PRO	5.1
1	B	346	LEU	5.1
1	B	497	PHE	5.0
1	A	542	ARG	5.0
1	A	771	PRO	5.0
1	A	494	ALA	5.0
1	B	509	ALA	4.9
1	A	547	LEU	4.9
1	A	484	LEU	4.9
1	A	345	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	531	HIS	4.8
1	B	722	GLU	4.8
1	A	414	ASP	4.8
1	A	716	LEU	4.8
1	B	462	ALA	4.7
1	C	215	GLY	4.7
1	B	702	ALA	4.7
1	A	714	LEU	4.6
1	C	697	ALA	4.6
1	B	441	PRO	4.6
1	C	727	ALA	4.5
1	B	503	SER	4.4
1	B	500	ALA	4.4
1	A	210	PRO	4.4
1	C	674	VAL	4.4
1	A	487	PRO	4.4
1	A	213	THR	4.3
1	C	80	GLU	4.3
1	D	246	GLU	4.3
1	D	714	LEU	4.2
1	D	726	GLN	4.2
1	B	532	VAL	4.2
1	D	215	GLY	4.2
1	A	723	ILE	4.2
1	C	210	PRO	4.2
1	D	717	GLY	4.2
1	A	675	GLU	4.1
1	D	723	ILE	4.1
1	B	689	LEU	4.1
1	D	484	LEU	4.0
1	D	724	VAL	4.0
1	A	211	ASP	4.0
1	D	80	GLU	4.0
1	A	552	PRO	4.0
1	B	624	LEU	4.0
1	A	553	VAL	4.0
1	A	568	GLY	4.0
1	D	674	VAL	3.9
1	A	215	GLY	3.9
1	A	719	GLY	3.9
1	B	499	LEU	3.9
1	B	596	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	699	VAL	3.9
1	B	535	GLU	3.9
1	B	637	ILE	3.9
1	B	711	ALA	3.9
1	B	569	ILE	3.9
1	D	615	ARG	3.8
1	B	736	LEU	3.8
1	C	716	LEU	3.8
1	D	677	ALA	3.8
1	B	444	VAL	3.8
1	D	681	ASN	3.8
1	A	533	VAL	3.7
1	D	346	LEU	3.7
1	B	506	ALA	3.7
1	D	210	PRO	3.7
1	D	684	TRP	3.7
1	A	346	LEU	3.7
1	B	80	GLU	3.7
1	A	541	ALA	3.7
1	D	676	ASN	3.7
1	A	353	GLU	3.6
1	A	674	VAL	3.6
1	A	551	PRO	3.6
1	C	696	ALA	3.6
1	B	281	GLU	3.6
1	A	686	LEU	3.6
1	D	345	GLY	3.6
1	D	703	GLU	3.6
1	B	418	VAL	3.5
1	B	694	LEU	3.5
1	A	729	TYR	3.5
1	C	726	GLN	3.5
1	B	767	LEU	3.5
1	A	681	ASN	3.5
1	C	531	HIS	3.5
1	A	1	MET	3.5
1	C	1	MET	3.5
1	A	448	ASP	3.5
1	C	724	VAL	3.5
1	B	594	LEU	3.5
1	A	420	ARG	3.5
1	B	629	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	621	LEU	3.4
1	B	732	LEU	3.4
1	B	508	TYR	3.4
1	D	683	ALA	3.4
1	B	531	HIS	3.4
1	B	647	SER	3.4
1	A	539	ARG	3.4
1	B	501	ALA	3.4
1	A	417	ILE	3.4
1	B	764	THR	3.4
1	B	479	PHE	3.4
1	B	345	GLY	3.4
1	A	418	VAL	3.3
1	A	535	GLU	3.3
1	D	502	ARG	3.3
1	C	771	PRO	3.3
1	D	716	LEU	3.3
1	A	532	VAL	3.3
1	A	480	ALA	3.3
1	C	698	THR	3.3
1	B	670	LEU	3.3
1	B	640	VAL	3.3
1	C	693	ALA	3.3
1	B	666	GLY	3.3
1	B	634	PHE	3.3
1	B	450	ALA	3.3
1	B	727	ALA	3.3
1	B	729	TYR	3.2
1	C	618	SER	3.2
1	A	499	LEU	3.2
1	C	346	LEU	3.2
1	A	391	GLN	3.2
1	D	678	SER	3.2
1	D	702	ALA	3.2
1	B	505	ALA	3.2
1	B	544	GLU	3.2
1	D	727	ALA	3.2
1	B	700	GLU	3.2
1	A	726	GLN	3.2
1	D	599	ALA	3.2
1	D	342	LYS	3.1
1	A	649	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	681	ASN	3.1
1	B	705	THR	3.1
1	A	708	ASP	3.1
1	C	538	PRO	3.1
1	A	425	ALA	3.1
1	B	714	LEU	3.1
1	A	485	SER	3.1
1	B	651	TRP	3.1
1	B	498	LEU	3.1
1	C	713	GLY	3.1
1	A	354	SER	3.1
1	A	727	ALA	3.0
1	B	484	LEU	3.0
1	B	618	SER	3.0
1	B	461	ALA	3.0
1	A	495	ARG	3.0
1	A	644	ALA	3.0
1	B	653	ALA	3.0
1	B	765	PRO	3.0
1	D	539	ARG	3.0
1	D	649	GLY	3.0
1	B	474	LEU	3.0
1	B	538	PRO	3.0
1	A	679	ALA	3.0
1	A	166	TYR	3.0
1	B	698	THR	3.0
1	A	645	PRO	2.9
1	D	653	ALA	2.9
1	D	553	VAL	2.9
1	C	544	GLU	2.9
1	D	533	VAL	2.9
1	B	396	LEU	2.9
1	A	648	ASN	2.9
1	D	675	GLU	2.9
1	B	513	GLY	2.9
1	C	725	ARG	2.9
1	A	567	GLU	2.9
1	B	752	SER	2.9
1	B	342	LYS	2.9
1	C	675	GLU	2.9
1	A	490	VAL	2.9
1	B	540	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	342	LYS	2.9
1	D	746	GLU	2.8
1	A	724	VAL	2.8
1	A	419	ALA	2.8
1	A	443	LYS	2.8
1	A	497	PHE	2.8
1	B	510	LEU	2.8
1	C	723	ILE	2.8
1	D	650	SER	2.8
1	A	718	SER	2.8
1	B	677	ALA	2.8
1	C	688	ARG	2.8
1	B	214	ASP	2.8
1	D	686	LEU	2.8
1	B	547	LEU	2.8
1	C	679	ALA	2.8
1	A	243	VAL	2.8
1	C	609	THR	2.8
1	A	570	TYR	2.8
1	D	725	ARG	2.8
1	B	494	ALA	2.8
1	D	770	GLU	2.8
1	D	347	ASP	2.7
1	B	721	GLY	2.7
1	D	570	TYR	2.7
1	A	428	ALA	2.7
1	B	768	GLY	2.7
1	A	571	ASP	2.7
1	B	468	HIS	2.7
1	B	555	ALA	2.7
1	D	576	VAL	2.7
1	A	288	PRO	2.7
1	D	543	PHE	2.7
1	A	722	GLU	2.7
1	D	481	ALA	2.7
1	D	696	ALA	2.7
1	B	659	PRO	2.7
1	B	771	PRO	2.7
1	C	539	ARG	2.7
1	D	718	SER	2.7
1	A	356	LEU	2.7
1	D	637	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	349	TRP	2.7
1	A	486	SER	2.7
1	B	708	ASP	2.7
1	A	415	PRO	2.6
1	D	1	MET	2.6
1	D	213	THR	2.6
1	A	673	ALA	2.6
1	B	446	SER	2.6
1	B	471	VAL	2.6
1	B	648	ASN	2.6
1	D	700	GLU	2.6
1	B	625	GLU	2.6
1	D	645	PRO	2.6
1	A	563	GLN	2.6
1	A	621	LEU	2.6
1	C	683	ALA	2.6
1	A	615	ARG	2.6
1	B	687	LYS	2.6
1	D	690	MET	2.6
1	B	126	ASP	2.6
1	B	717	GLY	2.6
1	B	452	LEU	2.6
1	A	423	VAL	2.6
1	A	581	MET	2.6
1	B	478	TYR	2.6
1	C	487	PRO	2.6
1	A	412	ASP	2.6
1	B	449	ASP	2.6
1	D	661	LEU	2.6
1	A	80	GLU	2.6
1	B	349	TRP	2.5
1	B	504	CYS	2.5
1	A	446	SER	2.5
1	A	646	SER	2.5
1	C	621	LEU	2.5
1	D	580	ALA	2.5
1	A	700	GLU	2.5
1	D	669	THR	2.5
1	B	575	TRP	2.5
1	B	545	ARG	2.5
1	B	724	VAL	2.5
1	A	740	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	703	GLU	2.5
1	A	537	MET	2.5
1	B	671	LEU	2.5
1	D	517	SER	2.5
1	B	490	VAL	2.5
1	C	553	VAL	2.5
1	A	519	ALA	2.5
1	B	734	ALA	2.5
1	A	344	GLU	2.5
1	D	654	ASP	2.5
1	A	676	ASN	2.5
1	B	685	HIS	2.5
1	D	600	SER	2.5
1	D	644	ALA	2.5
1	D	679	ALA	2.5
1	A	491	GLU	2.5
1	D	547	LEU	2.5
1	D	610	PRO	2.5
1	A	538	PRO	2.5
1	B	553	VAL	2.5
1	A	422	LYS	2.4
1	B	667	ASN	2.4
1	D	705	THR	2.4
1	A	442	THR	2.4
1	B	550	VAL	2.4
1	C	5	GLU	2.4
1	C	281	GLU	2.4
1	C	678	SER	2.4
1	A	704	LYS	2.4
1	B	564	LEU	2.4
1	D	651	TRP	2.4
1	B	487	PRO	2.4
1	A	713	GLY	2.4
1	D	720	ALA	2.4
1	A	707	ALA	2.4
1	B	328	GLN	2.4
1	A	348	GLU	2.4
1	B	438	TRP	2.4
1	A	426	GLY	2.4
1	B	635	ALA	2.4
1	B	673	ALA	2.4
1	B	683	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	2	GLU	2.4
1	A	556	LEU	2.4
1	B	560	LEU	2.4
1	B	627	GLU	2.4
1	B	686	LEU	2.4
1	C	736	LEU	2.4
1	B	437	PRO	2.4
1	B	587	HIS	2.4
1	B	665	ILE	2.4
1	B	693	ALA	2.4
1	A	483	ARG	2.4
1	A	706	LEU	2.4
1	D	243	VAL	2.4
1	D	550	VAL	2.4
1	A	447	CYS	2.4
1	B	592	THR	2.3
1	D	555	ALA	2.3
1	A	685	HIS	2.3
1	A	702	ALA	2.3
1	B	570	TYR	2.3
1	B	556	LEU	2.3
1	B	726	GLN	2.3
1	C	699	VAL	2.3
1	A	517	SER	2.3
1	B	485	SER	2.3
1	D	442	THR	2.3
1	A	545	ARG	2.3
1	B	697	ALA	2.3
1	B	198	ASP	2.3
1	D	540	PHE	2.3
1	B	574	GLN	2.3
1	D	534	GLU	2.3
1	C	740	GLU	2.3
1	A	550	VAL	2.3
1	B	453	ARG	2.3
1	B	605	PRO	2.3
1	D	662	ILE	2.3
1	A	717	GLY	2.3
1	D	673	ALA	2.3
1	C	646	SER	2.3
1	C	734	ALA	2.3
1	D	668	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	626	LEU	2.3
1	B	655	LEU	2.3
1	A	554	GLU	2.3
1	B	445	PRO	2.3
1	A	241	ALA	2.3
1	B	641	ALA	2.3
1	A	451	THR	2.3
1	A	527	SER	2.3
1	B	620	LEU	2.3
1	A	413	LYS	2.3
1	C	4	LYS	2.3
1	A	721	GLY	2.3
1	B	603	SER	2.3
1	D	648	ASN	2.3
1	D	5	GLU	2.2
1	D	742	GLU	2.2
1	B	707	ALA	2.2
1	D	438	TRP	2.2
1	D	646	SER	2.2
1	D	680	SER	2.2
1	B	125	ASP	2.2
1	D	771	PRO	2.2
1	A	720	ALA	2.2
1	D	325	THR	2.2
1	D	548	THR	2.2
1	A	493	SER	2.2
1	B	584	VAL	2.2
1	B	652	ASN	2.2
1	A	616	GLY	2.2
1	B	716	LEU	2.2
1	C	729	TYR	2.2
1	D	200	VAL	2.2
1	B	429	GLN	2.2
1	A	630	ASN	2.2
1	B	465	GLU	2.2
1	B	706	LEU	2.2
1	B	598	ALA	2.2
1	C	720	ALA	2.2
1	A	454	THR	2.2
1	A	623	THR	2.2
1	B	636	THR	2.2
1	B	559	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	680	SER	2.2
1	D	556	LEU	2.2
1	B	755	LEU	2.2
1	D	693	ALA	2.2
1	A	768	GLY	2.2
1	C	345	GLY	2.2
1	D	490	VAL	2.1
1	B	623	THR	2.1
1	D	656	TYR	2.1
1	B	470	ILE	2.1
1	B	463	LEU	2.1
1	D	704	LYS	2.1
1	D	544	GLU	2.1
1	D	579	ALA	2.1
1	B	483	ARG	2.1
1	C	567	GLU	2.1
1	B	691	PHE	2.1
1	D	685	HIS	2.1
1	B	430	VAL	2.1
1	D	4	LYS	2.1
1	D	241	ALA	2.1
1	B	464	ARG	2.1
1	C	728	ARG	2.1
1	D	2	GLU	2.1
1	A	534	GLU	2.1
1	C	616	GLY	2.1
1	B	658	ASP	2.1
1	D	636	THR	2.1
1	A	694	LEU	2.1
1	B	123	THR	2.1
1	B	609	THR	2.1
1	C	695	SER	2.1
1	A	53	ASP	2.1
1	B	744	THR	2.1
1	A	265	PHE	2.1
1	A	338	PRO	2.1
1	C	645	PRO	2.1
1	D	751	ARG	2.1
1	A	341	ILE	2.1
1	D	537	MET	2.1
1	B	447	CYS	2.1
1	A	340	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	720	ALA	2.1
1	B	588	SER	2.0
1	A	347	ASP	2.0
1	A	450	ALA	2.0
1	C	673	ALA	2.0
1	A	479	PHE	2.0
1	B	740	GLU	2.0
1	A	408	ARG	2.0
1	B	514	SER	2.0
1	B	482	HIS	2.0
1	A	696	ALA	2.0
1	B	241	ALA	2.0
1	A	167	TYR	2.0
1	D	769	PHE	2.0
1	B	395	LYS	2.0
1	B	551	PRO	2.0
1	B	435	GLU	2.0
1	C	682	ARG	2.0
1	A	424	LEU	2.0
1	A	498	LEU	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.