



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:06 PM UTC

PDB ID : 7DRS / pdb_00007drs
Title : Structure of SspE_40224
Authors : Haiyan, G.; Jinchuan, Z.; Chen, S.; Wang, L.; Wu, G.
Deposited on : 2020-12-29
Resolution : 3.42 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

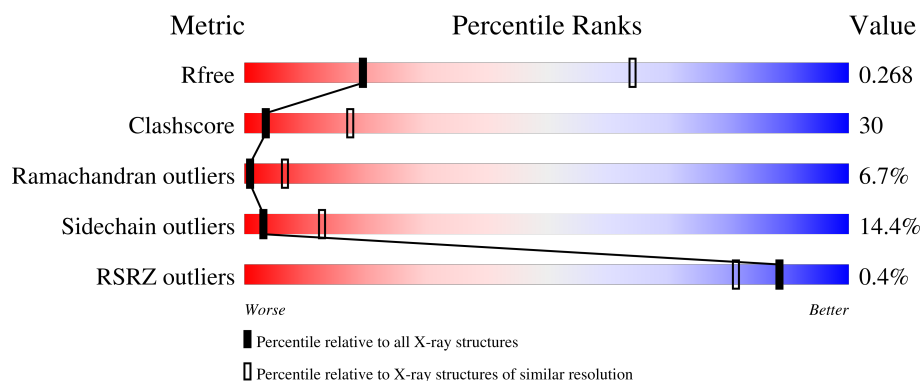
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

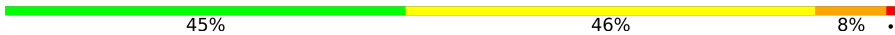
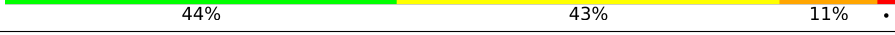
The reported resolution of this entry is 3.42 Å.

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	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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 24548 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.

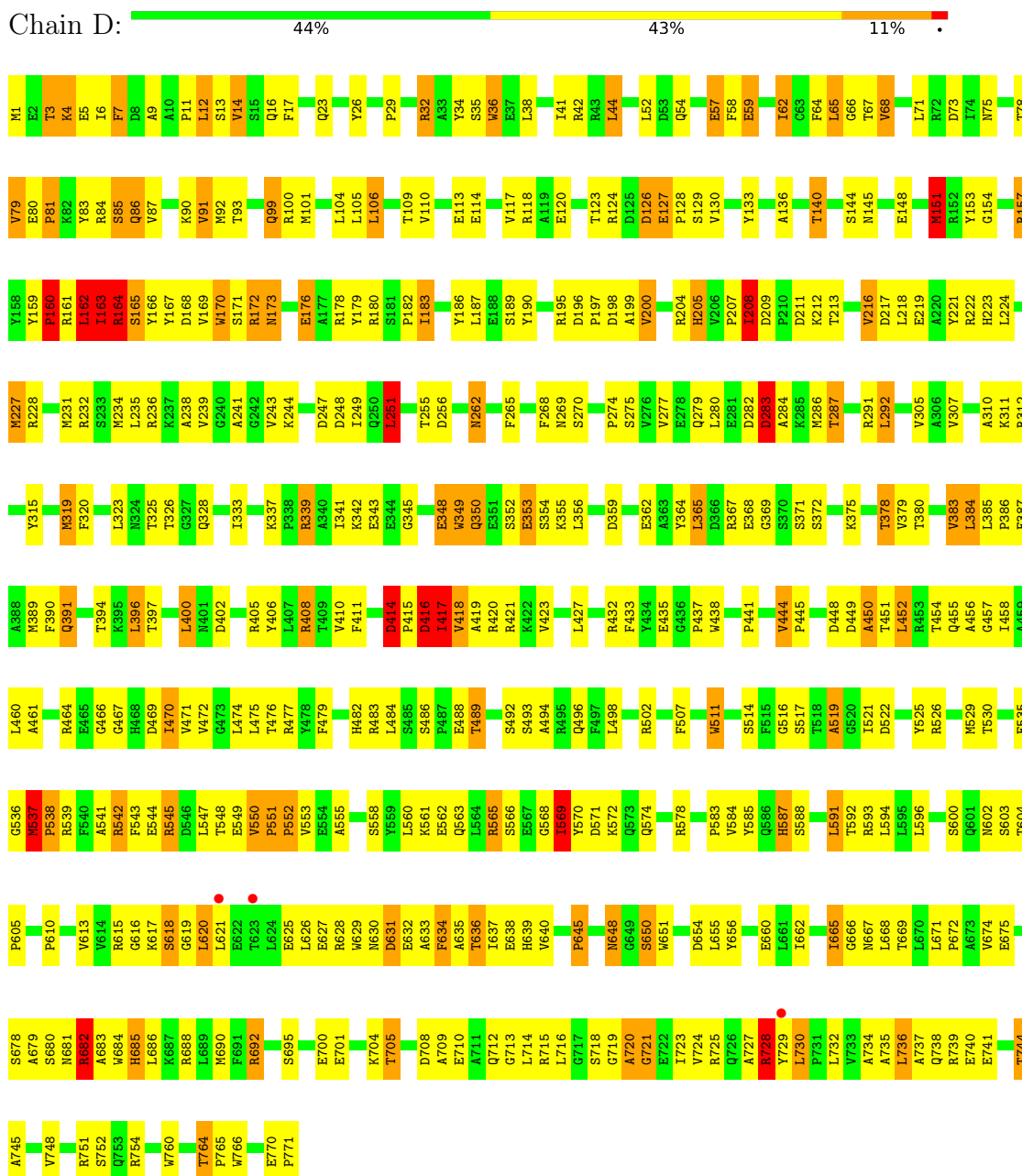
- Molecule 1 is a protein called SspE protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	771	Total	C	N	O	S	0	0	0
			6137	3872	1079	1166	20			
1	A	771	Total	C	N	O	S	0	0	0
			6137	3872	1079	1166	20			
1	B	771	Total	C	N	O	S	0	0	0
			6137	3872	1079	1166	20			
1	C	771	Total	C	N	O	S	0	0	0
			6137	3872	1079	1166	20			

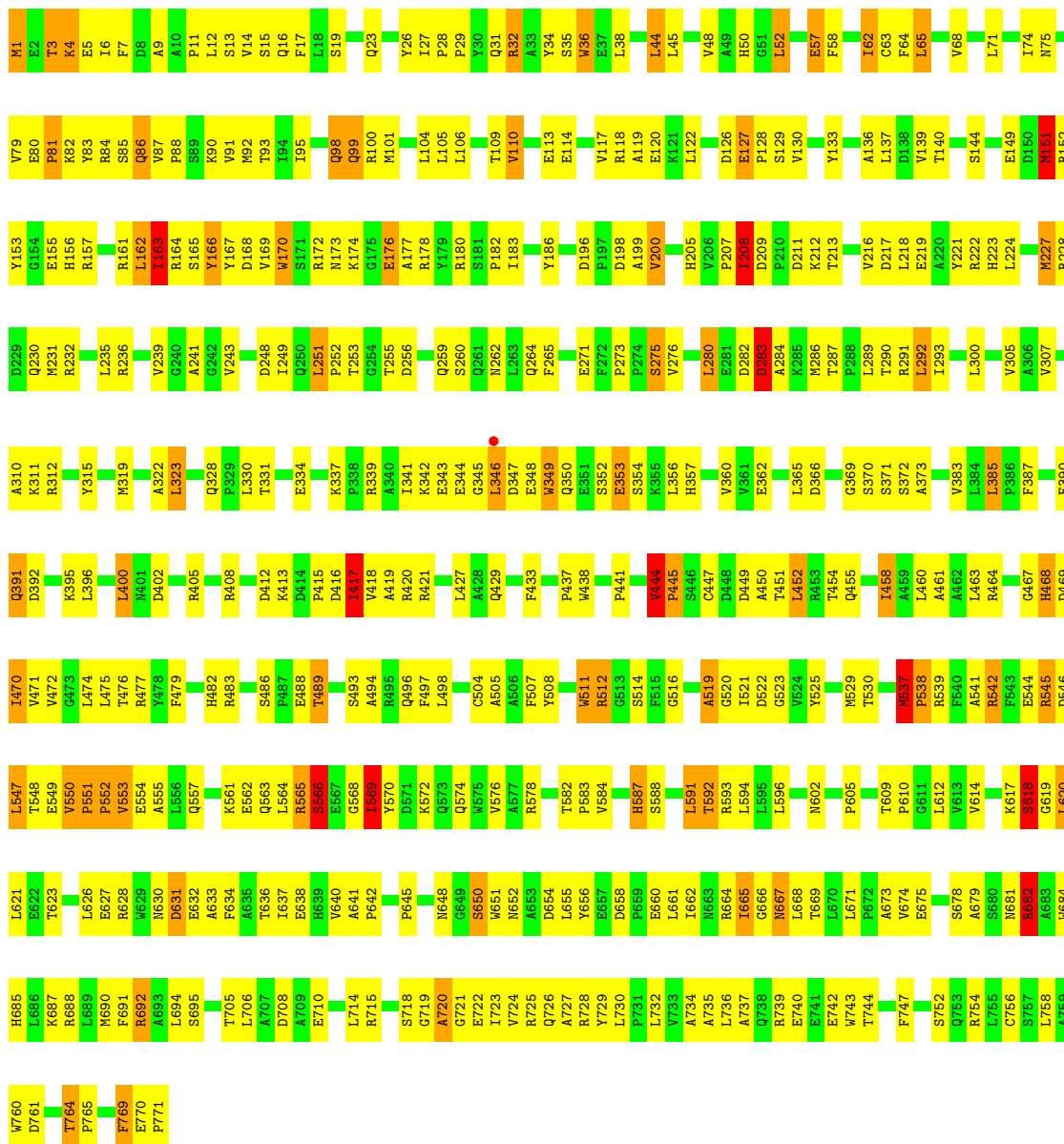
3 Residue-property plots

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.

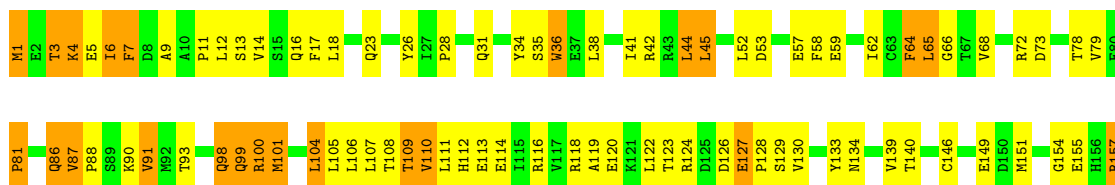
• Molecule 1: SspE protein

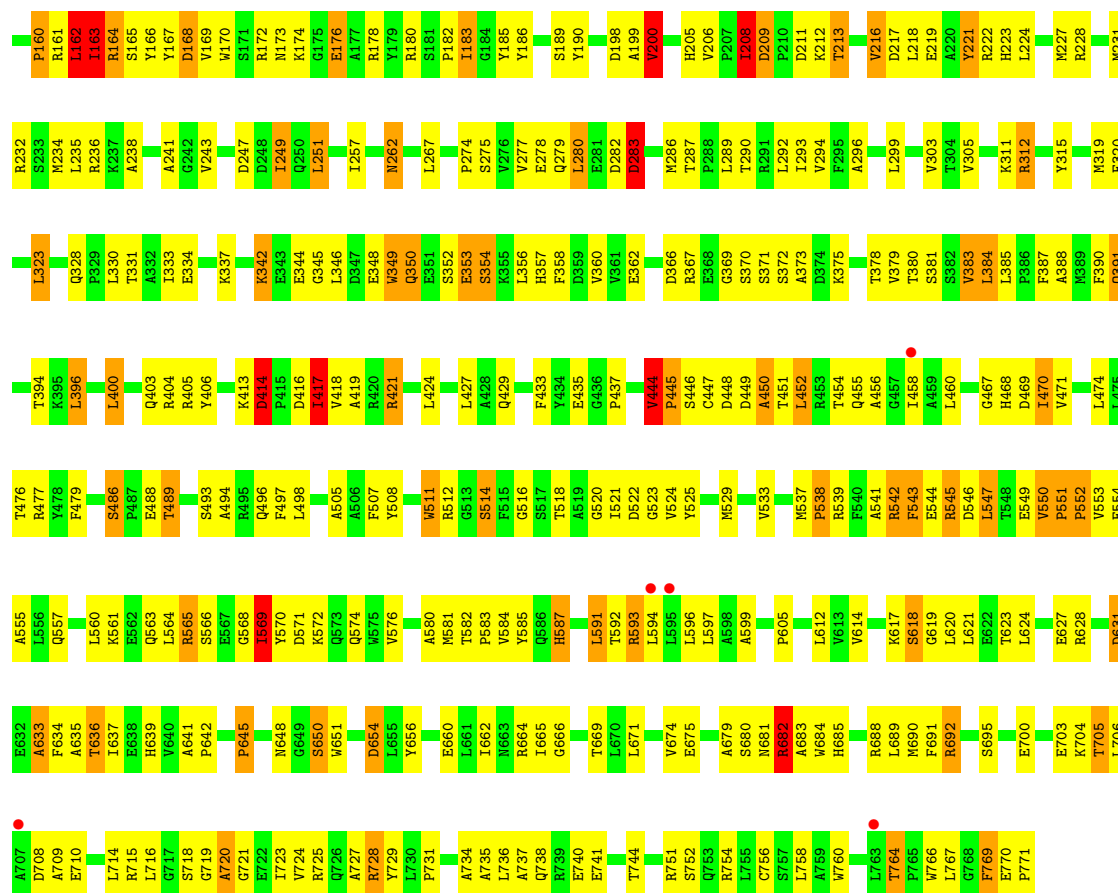


- Molecule 1: SspE protein

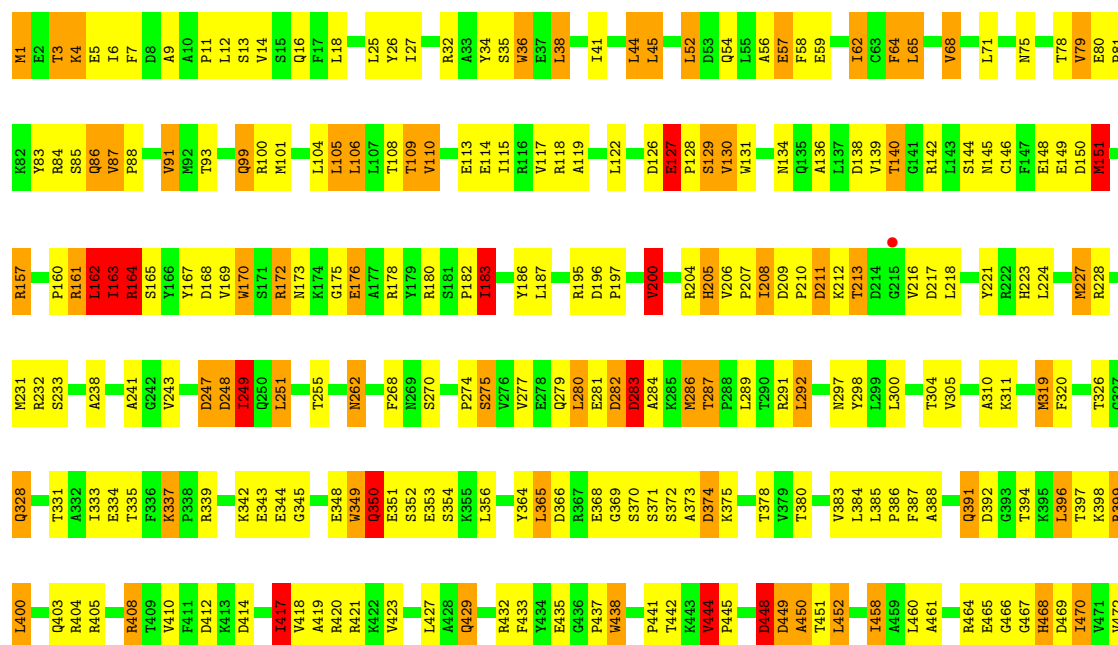
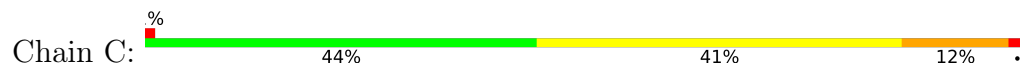


- Molecule 1: SspE protein





• Molecule 1: SspE protein



Q473	L474	L475	T476	R477	Y478	F479	A480	A481	H482	R483	L484	S485	S486	P487	E488	T489	S492	S493	Q496	F497	L498	L499	A500	A501	C504	A509	L510	W511	S514	G520	I521	D522	G523	V524	Y525	R526	M529	T530	V533	M537	P538	R539	F540	A541	R542	F543	E544	R545	D546	L547			
L621	E622	T623	L626	E627	R628	W629	M630	D631	E632	A633	F634	A635	T636	I637	E638	H639	V640	A641	P642	P645	M648	G649	S650	W651	M652	A653	D654	I662	M663	R664	I665	G666	M667	L668	T669	L670	L671	V674	E675	S678	A679	S680	M681	R682	A683	W684	H685	L686	K687	R688	L689	M690	F691
R692	S695	T705	L706	A707	D708	A709	E710	G713	L714	R715	L716	G717	S718	G719	A720	G721	E722	I723	Q726	A727	R728	Y729	L732	V733	A734	A735	L736	Q737	Q738	R739	E740	E741	E742	W743	T744	R751	S752	Q753	R754	L755	C756	A759	W760	T764	P765	W766	L767	G768	F769	E770	P771		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.08Å 138.15Å 293.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.14 – 3.42 46.14 – 3.42	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.14-3.42) 99.7 (46.14-3.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.5	Depositor
R, R_{free}	0.212 , 0.264 0.221 , 0.268	Depositor DCC
R_{free} test set	3032 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	121.6	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 126.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24548	wwPDB-VP
Average B, all atoms (Å ²)	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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	0.59	0/6272	0.91	7/8515 (0.1%)
1	B	0.57	1/6272 (0.0%)	0.88	9/8515 (0.1%)
1	C	0.76	3/6272 (0.0%)	1.06	25/8515 (0.3%)
1	D	0.66	2/6272 (0.0%)	1.00	16/8515 (0.2%)
All	All	0.65	6/25088 (0.0%)	0.97	57/34060 (0.2%)

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	B	0	1
1	C	0	5
1	D	0	3
All	All	0	11

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	209	ASP	C-O	6.25	1.27	1.23
1	C	151	MET	CG-SD	-5.72	1.66	1.80
1	D	145	ASN	CA-C	5.49	1.62	1.52
1	C	161	ARG	CB-CG	-5.33	1.36	1.52
1	D	170	TRP	CG-CD2	-5.12	1.34	1.43
1	C	170	TRP	CG-CD2	-5.01	1.34	1.43

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	145	ASN	CA-C-O	8.74	132.69	119.23
1	C	151	MET	CA-C-N	-7.74	108.86	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	151	MET	C-N-CA	-7.74	108.86	122.26
1	C	345	GLY	N-CA-C	-7.16	92.53	113.30
1	A	417	ILE	N-CA-C	-6.55	95.72	109.34
1	B	251	LEU	CA-CB-CG	6.52	139.12	116.30
1	B	345	GLY	N-CA-C	-6.48	94.52	113.30
1	C	162	LEU	CA-C-N	-6.48	110.31	121.97
1	C	162	LEU	C-N-CA	-6.48	110.31	121.97
1	C	170	TRP	CA-CB-CG	6.47	125.90	113.60
1	C	200	VAL	CA-C-N	6.46	139.30	120.97
1	C	200	VAL	C-N-CA	6.46	139.30	120.97
1	D	178	ARG	CB-CG-CD	-6.38	96.64	111.30
1	D	417	ILE	N-CA-C	-6.20	96.45	109.34
1	A	170	TRP	CA-CB-CG	5.96	124.92	113.60
1	B	417	ILE	N-CA-C	-5.78	97.31	109.34
1	B	178	ARG	CB-CG-CD	-5.78	98.00	111.30
1	C	178	ARG	CA-CB-CG	5.72	125.53	114.10
1	C	178	ARG	CB-CG-CD	-5.68	98.24	111.30
1	D	162	LEU	CA-C-N	-5.66	111.78	121.97
1	D	162	LEU	C-N-CA	-5.66	111.78	121.97
1	B	346	LEU	CA-CB-CG	5.66	136.11	116.30
1	D	345	GLY	N-CA-C	-5.64	96.94	113.30
1	C	545	ARG	CA-C-N	-5.63	111.85	121.08
1	C	545	ARG	C-N-CA	-5.63	111.85	121.08
1	A	345	GLY	N-CA-C	-5.61	97.04	113.30
1	C	251	LEU	CA-CB-CG	5.58	135.85	116.30
1	D	251	LEU	CA-CB-CG	5.58	135.83	116.30
1	A	346	LEU	CA-CB-CG	5.57	135.79	116.30
1	C	417	ILE	N-CA-C	-5.49	97.91	109.34
1	B	100	ARG	CG-CD-NE	-5.49	99.93	112.00
1	D	144	SER	CA-C-N	-5.45	111.42	122.31
1	D	144	SER	C-N-CA	-5.45	111.42	122.31
1	C	183	ILE	CB-CA-C	-5.44	104.89	112.02
1	C	227	MET	CG-SD-CE	-5.43	88.95	100.90
1	C	210	PRO	N-CA-C	-5.38	106.85	113.84
1	B	162	LEU	CA-C-N	-5.37	112.30	121.97
1	B	162	LEU	C-N-CA	-5.37	112.30	121.97
1	C	145	ASN	CA-C-O	5.36	127.48	119.23
1	B	178	ARG	CA-CB-CG	5.35	124.81	114.10
1	D	151	MET	CA-C-N	-5.32	113.05	122.26
1	D	151	MET	C-N-CA	-5.32	113.05	122.26
1	C	161	ARG	N-CA-C	-5.29	101.49	109.85
1	A	537	MET	CB-CG-SD	-5.26	96.92	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	416	ASP	CA-C-N	5.23	131.39	121.97
1	D	416	ASP	C-N-CA	5.23	131.39	121.97
1	C	249	ILE	CG1-CB-CG2	-5.22	95.05	110.70
1	C	291	ARG	NE-CZ-NH1	-5.21	116.29	121.50
1	C	319	MET	CB-CG-SD	-5.16	97.21	112.70
1	A	151	MET	CA-C-N	-5.08	114.17	122.54
1	A	151	MET	C-N-CA	-5.08	114.17	122.54
1	C	233	SER	CA-CB-OG	-5.07	100.96	111.10
1	C	438	TRP	CA-CB-CG	-5.06	103.98	113.60
1	D	319	MET	CB-CG-SD	-5.05	97.55	112.70
1	C	351	GLU	N-CA-C	-5.03	98.13	108.53
1	D	85	SER	CA-C-N	-5.00	112.76	122.62
1	D	85	SER	C-N-CA	-5.00	112.76	122.62

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	PRO	Peptide
1	A	553	VAL	Peptide
1	B	160	PRO	Peptide
1	C	151	MET	Peptide
1	C	160	PRO	Peptide
1	C	551	PRO	Peptide
1	C	553	VAL	Peptide
1	C	79	VAL	Peptide
1	D	160	PRO	Peptide
1	D	173	ASN	Peptide
1	D	79	VAL	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6137	0	6046	353	1
1	B	6137	0	6046	367	1
1	C	6137	0	6046	369	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	6137	0	6046	379	2
All	All	24548	0	24184	1444	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 30.

All (1444) 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:C:223:HIS:HE1	1:C:227:MET:HE2	1.19	1.07
1:C:628:ARG:HA	1:C:631:ASP:HB2	1.44	0.99
1:A:418:VAL:H	1:A:421:ARG:HD2	1.25	0.98
1:B:126:ASP:HB3	1:B:129:SER:HB3	1.45	0.98
1:A:126:ASP:HB3	1:A:129:SER:HB3	1.44	0.96
1:D:126:ASP:HB3	1:D:129:SER:HB3	1.47	0.95
1:C:114:GLU:OE1	1:C:118:ARG:NH1	2.00	0.95
1:C:173:ASN:HB2	1:C:176:GLU:OE2	1.67	0.95
1:A:553:VAL:HB	1:A:554:GLU:HG3	1.51	0.93
1:D:692:ARG:HG3	1:D:737:ALA:HB1	1.50	0.92
1:C:680:SER:HA	1:C:690:MET:HE1	1.51	0.92
1:A:584:VAL:HG12	1:A:592:THR:HG22	1.49	0.92
1:D:628:ARG:HA	1:D:631:ASP:HB2	1.49	0.92
1:D:1:MET:HA	1:D:4:LYS:HB2	1.51	0.92
1:C:223:HIS:CE1	1:C:227:MET:HE2	2.05	0.91
1:A:496:GLN:HA	1:A:553:VAL:HG13	1.53	0.90
1:B:703:GLU:OE2	1:B:725:ARG:NE	2.05	0.89
1:B:477:ARG:HD3	1:B:542:ARG:H	1.37	0.89
1:A:688:ARG:NH1	1:A:740:GLU:OE2	2.05	0.89
1:D:474:LEU:O	1:D:477:ARG:HB3	1.75	0.87
1:B:628:ARG:HA	1:B:631:ASP:HB2	1.57	0.86
1:D:724:VAL:HG12	1:D:725:ARG:HG3	1.58	0.85
1:A:391:GLN:O	1:A:391:GLN:NE2	2.08	0.85
1:C:126:ASP:HB3	1:C:129:SER:HB3	1.57	0.85
1:B:593:ARG:HH21	1:B:635:ALA:HB1	1.42	0.84
1:B:183:ILE:HD12	1:B:183:ILE:H	1.42	0.84
1:D:543:PHE:O	1:D:545:ARG:NH2	2.11	0.83
1:C:208:ILE:HG13	1:C:209:ASP:H	1.43	0.83
1:A:208:ILE:HD13	1:A:209:ASP:H	1.43	0.83
1:A:593:ARG:HG3	1:A:637:ILE:HD11	1.61	0.83
1:B:612:LEU:HB3	1:B:754:ARG:HD3	1.61	0.83
1:C:496:GLN:HA	1:C:553:VAL:HG13	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:ALA:H	1:A:667:ASN:HD21	1.25	0.82
1:D:385:LEU:HD22	1:D:396:LEU:HB3	1.62	0.81
1:A:433:PHE:CG	1:A:476:THR:HG22	2.14	0.81
1:D:552:PRO:HG2	1:D:555:ALA:H	1.46	0.81
1:D:182:PRO:HD3	1:D:221:TYR:HE1	1.45	0.81
1:A:692:ARG:HG3	1:A:737:ALA:HB1	1.63	0.81
1:A:114:GLU:OE1	1:A:118:ARG:NH1	2.14	0.80
1:C:183:ILE:H	1:C:183:ILE:HD12	1.46	0.80
1:A:612:LEU:HB3	1:A:754:ARG:HD3	1.61	0.80
1:C:692:ARG:HG3	1:C:737:ALA:HB1	1.64	0.80
1:B:208:ILE:HD13	1:B:209:ASP:H	1.47	0.80
1:D:173:ASN:HB2	1:D:176:GLU:OE2	1.83	0.79
1:A:182:PRO:HB2	1:A:224:LEU:HD13	1.63	0.79
1:A:391:GLN:OE1	1:A:542:ARG:NH1	2.14	0.79
1:B:682:ARG:HH21	1:B:716:LEU:HD13	1.46	0.79
1:C:1:MET:HA	1:C:4:LYS:HB2	1.62	0.79
1:B:36:TRP:CD1	1:B:99:GLN:HG2	2.18	0.78
1:C:474:LEU:O	1:C:477:ARG:HB3	1.83	0.78
1:D:114:GLU:OE1	1:D:118:ARG:NH1	2.16	0.78
1:B:565:ARG:HG2	1:B:570:TYR:CE2	2.18	0.78
1:D:42:ARG:HA	1:D:234:MET:HE1	1.63	0.78
1:C:36:TRP:CD1	1:C:99:GLN:HG2	2.19	0.78
1:B:571:ASP:OD2	1:B:574:GLN:NE2	2.16	0.77
1:D:496:GLN:HA	1:D:553:VAL:HG13	1.66	0.77
1:B:710:GLU:HA	1:B:714:LEU:H	1.50	0.77
1:C:612:LEU:HB3	1:C:754:ARG:HD3	1.66	0.77
1:D:124:ARG:HD3	1:D:133:TYR:CD2	2.19	0.77
1:A:1:MET:HA	1:A:4:LYS:HB2	1.66	0.77
1:A:565:ARG:HG2	1:A:570:TYR:CE2	2.20	0.77
1:C:638:GLU:OE2	1:C:687:LYS:NZ	2.18	0.77
1:A:715:ARG:HB3	1:A:719:GLY:HA2	1.67	0.77
1:C:391:GLN:O	1:C:391:GLN:NE2	2.17	0.77
1:D:720:ALA:HB1	1:D:723:ILE:HD12	1.64	0.77
1:D:469:ASP:O	1:D:472:VAL:HG23	1.85	0.77
1:D:680:SER:O	1:D:682:ARG:NH2	2.17	0.76
1:A:196:ASP:HB3	1:A:199:ALA:HB2	1.67	0.76
1:D:223:HIS:HE1	1:D:227:MET:HE2	1.51	0.76
1:A:412:ASP:OD1	1:A:420:ARG:NH2	2.19	0.76
1:C:433:PHE:CG	1:C:476:THR:HG22	2.20	0.76
1:B:525:TYR:O	1:B:529:MET:HG2	1.86	0.76
1:C:484:LEU:HB3	1:C:548:THR:HG22	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ASN:HB2	1:A:176:GLU:OE2	1.85	0.75
1:A:479:PHE:CE1	1:A:483:ARG:HD2	2.20	0.75
1:D:12:LEU:HB3	1:D:16:GLN:HG3	1.67	0.75
1:C:388:ALA:HB2	1:C:396:LEU:HD23	1.68	0.75
1:C:715:ARG:HB3	1:C:719:GLY:HA2	1.69	0.75
1:D:367:ARG:NH1	1:D:435:GLU:OE2	2.20	0.74
1:D:389:MET:HE1	1:D:526:ARG:HD3	1.67	0.74
1:A:477:ARG:HD3	1:A:542:ARG:H	1.51	0.74
1:B:110:VAL:HA	1:B:228:ARG:HH11	1.52	0.74
1:D:168:ASP:OD1	1:D:180:ARG:N	2.19	0.74
1:A:552:PRO:HG2	1:A:555:ALA:H	1.52	0.74
1:A:617:LYS:O	1:A:619:GLY:N	2.21	0.74
1:A:525:TYR:O	1:A:529:MET:HG2	1.87	0.74
1:B:42:ARG:HA	1:B:234:MET:HE1	1.68	0.74
1:C:5:GLU:O	1:C:7:PHE:N	2.19	0.74
1:C:161:ARG:O	1:C:162:LEU:HB2	1.87	0.74
1:A:128:PRO:HG3	1:A:275:SER:HB2	1.70	0.73
1:C:614:VAL:HG12	1:C:754:ARG:HH11	1.52	0.73
1:D:106:LEU:HB3	1:D:231:MET:HE1	1.69	0.73
1:B:34:TYR:HD2	1:B:224:LEU:HD12	1.51	0.73
1:C:4:LYS:O	1:C:5:GLU:HG3	1.89	0.73
1:C:68:VAL:HG11	1:C:101:MET:HE3	1.69	0.73
1:C:35:SER:O	1:C:223:HIS:NE2	2.22	0.73
1:D:183:ILE:HD12	1:D:183:ILE:H	1.53	0.73
1:A:565:ARG:HH21	1:A:771:PRO:HB3	1.53	0.72
1:C:470:ILE:HD12	1:C:522:ASP:OD2	1.88	0.72
1:B:280:LEU:HD21	1:B:290:THR:HG21	1.70	0.72
1:D:525:TYR:O	1:D:529:MET:HG2	1.89	0.72
1:C:544:GLU:HB2	1:C:545:ARG:NH2	2.05	0.72
1:C:684:TRP:HD1	1:C:742:GLU:OE2	1.72	0.72
1:D:584:VAL:HG12	1:D:592:THR:HG22	1.72	0.72
1:D:680:SER:HA	1:D:690:MET:HE1	1.71	0.72
1:D:454:THR:HG21	1:D:627:GLU:OE2	1.89	0.72
1:A:223:HIS:CE1	1:A:227:MET:HE2	2.24	0.72
1:A:339:ARG:HG2	1:A:408:ARG:NH2	2.04	0.72
1:D:208:ILE:HG21	1:D:221:TYR:CD2	2.25	0.71
1:A:36:TRP:CD1	1:A:99:GLN:HG2	2.25	0.71
1:A:208:ILE:HG21	1:A:221:TYR:CD2	2.26	0.71
1:A:666:GLY:H	1:A:752:SER:HB3	1.55	0.71
1:B:9:ALA:HB3	1:C:9:ALA:HB3	1.71	0.71
1:D:617:LYS:O	1:D:619:GLY:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:HD13	1:A:252:PRO:HD2	1.71	0.71
1:A:628:ARG:HA	1:A:631:ASP:HB2	1.71	0.71
1:B:715:ARG:HB3	1:B:719:GLY:HA2	1.72	0.71
1:A:470:ILE:HG21	1:A:522:ASP:HA	1.72	0.71
1:B:3:THR:O	1:B:5:GLU:N	2.23	0.71
1:C:705:THR:HA	1:C:708:ASP:HB2	1.73	0.71
1:D:391:GLN:O	1:D:391:GLN:NE2	2.24	0.71
1:B:1:MET:HA	1:B:4:LYS:HB2	1.73	0.71
1:D:312:ARG:HD3	1:D:315:TYR:CE2	2.26	0.71
1:D:470:ILE:HG21	1:D:522:ASP:HA	1.73	0.71
1:C:441:PRO:HG2	1:C:461:ALA:HB2	1.73	0.71
1:D:283:ASP:HA	1:D:287:THR:HB	1.72	0.71
1:B:614:VAL:HG12	1:B:754:ARG:HH11	1.55	0.70
1:A:127:GLU:OE2	1:A:128:PRO:HD3	1.90	0.70
1:A:280:LEU:HD21	1:A:290:THR:HG21	1.73	0.70
1:B:505:ALA:O	1:B:508:TYR:HB3	1.91	0.70
1:C:651:TRP:CZ3	1:C:684:TRP:HB2	2.26	0.70
1:C:688:ARG:NH1	1:C:740:GLU:OE2	2.24	0.70
1:B:120:GLU:HG2	1:B:200:VAL:HG11	1.73	0.70
1:C:617:LYS:O	1:C:619:GLY:N	2.24	0.70
1:B:86:GLN:NE2	1:B:172:ARG:HG2	2.07	0.70
1:B:564:LEU:HB3	1:B:570:TYR:HB3	1.74	0.70
1:C:622:GLU:O	1:C:628:ARG:NH1	2.24	0.70
1:D:477:ARG:HD3	1:D:542:ARG:H	1.57	0.70
1:D:617:LYS:HB3	1:D:620:LEU:HB2	1.73	0.70
1:B:396:LEU:HD11	1:B:403:GLN:HG2	1.74	0.69
1:D:9:ALA:HB3	1:A:9:ALA:HB3	1.75	0.69
1:A:605:PRO:HB3	1:A:735:ALA:HB2	1.74	0.69
1:C:538:PRO:HB2	1:C:550:VAL:HG13	1.73	0.69
1:A:50:HIS:NE2	1:A:402:ASP:OD1	2.25	0.69
1:D:529:MET:SD	1:D:541:ALA:HB2	2.33	0.69
1:A:13:SER:H	1:A:16:GLN:HE21	1.38	0.69
1:C:385:LEU:HD22	1:C:396:LEU:HB3	1.75	0.69
1:A:27:ILE:HB	1:A:164:ARG:HA	1.75	0.69
1:C:3:THR:O	1:C:5:GLU:N	2.26	0.69
1:C:3:THR:O	1:C:3:THR:OG1	2.10	0.68
1:D:438:TRP:CE3	1:D:464:ARG:HG3	2.29	0.68
1:D:634:PHE:HD1	1:D:634:PHE:H	1.38	0.68
1:B:3:THR:O	1:B:3:THR:OG1	2.11	0.68
1:D:760:TRP:O	1:D:764:THR:OG1	2.11	0.68
1:D:715:ARG:HB3	1:D:719:GLY:HA2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ARG:NH1	1:B:435:GLU:OE2	2.26	0.68
1:C:418:VAL:H	1:C:421:ARG:HD2	1.59	0.68
1:C:545:ARG:NH2	1:C:545:ARG:H	1.92	0.68
1:B:380:THR:O	1:B:384:LEU:HB2	1.94	0.68
1:C:545:ARG:H	1:C:545:ARG:HH21	1.42	0.68
1:D:113:GLU:OE2	1:D:232:ARG:NH2	2.27	0.67
1:A:11:PRO:O	1:A:12:LEU:HD23	1.94	0.67
1:A:385:LEU:HD22	1:A:396:LEU:HB3	1.76	0.67
1:B:4:LYS:O	1:B:5:GLU:HG3	1.95	0.67
1:B:110:VAL:HG12	1:B:228:ARG:HE	1.59	0.67
1:B:651:TRP:CZ3	1:B:684:TRP:HB2	2.29	0.67
1:B:584:VAL:HG13	1:B:591:LEU:HD13	1.77	0.67
1:A:612:LEU:HD13	1:A:754:ARG:HD2	1.77	0.67
1:C:544:GLU:HB2	1:C:545:ARG:HH22	1.58	0.67
1:B:418:VAL:H	1:B:421:ARG:HD2	1.59	0.67
1:A:418:VAL:N	1:A:421:ARG:HD2	2.06	0.67
1:C:138:ASP:CG	1:C:142:ARG:HH12	2.03	0.67
1:D:36:TRP:CD1	1:D:99:GLN:HG2	2.30	0.67
1:C:474:LEU:H	1:C:529:MET:HE1	1.59	0.67
1:C:542:ARG:NH1	1:C:544:GLU:O	2.28	0.67
1:D:418:VAL:H	1:D:421:ARG:HD2	1.59	0.67
1:C:636:THR:HG23	1:C:675:GLU:HG2	1.77	0.67
1:D:551:PRO:HB2	1:D:552:PRO:HD3	1.76	0.66
1:B:710:GLU:HG2	1:B:715:ARG:HG3	1.77	0.66
1:C:553:VAL:HB	1:C:554:GLU:HG3	1.77	0.66
1:C:642:PRO:HD3	1:C:651:TRP:CZ2	2.29	0.66
1:D:364:TYR:CE1	1:D:368:GLU:HG3	2.31	0.66
1:A:3:THR:O	1:A:5:GLU:N	2.27	0.66
1:B:474:LEU:HG	1:B:529:MET:SD	2.35	0.66
1:B:58:PHE:CE2	1:B:405:ARG:HD3	2.29	0.66
1:B:561:LYS:HE3	1:B:769:PHE:HA	1.77	0.66
1:C:584:VAL:HG12	1:C:592:THR:HG22	1.78	0.66
1:A:724:VAL:HG12	1:A:725:ARG:HG3	1.78	0.66
1:B:486:SER:HB3	1:B:488:GLU:OE2	1.95	0.66
1:C:180:ARG:HH12	1:C:212:LYS:HE2	1.61	0.66
1:C:605:PRO:HB3	1:C:735:ALA:HB2	1.78	0.66
1:D:68:VAL:HG11	1:D:101:MET:HE3	1.78	0.65
1:A:651:TRP:CZ3	1:A:684:TRP:HB2	2.32	0.65
1:C:182:PRO:HD3	1:C:221:TYR:HE1	1.61	0.65
1:C:344:GLU:OE1	1:C:421:ARG:NH2	2.28	0.65
1:D:565:ARG:HG2	1:D:570:TYR:CE2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ASP:OD2	1:B:283:ASP:N	2.29	0.65
1:A:127:GLU:HB3	1:A:128:PRO:HD2	1.77	0.65
1:C:400:LEU:HD12	1:C:404:ARG:HH21	1.61	0.65
1:B:477:ARG:HD3	1:B:542:ARG:N	2.10	0.65
1:B:689:LEU:HB3	1:B:709:ALA:HB2	1.77	0.65
1:D:127:GLU:OE2	1:D:128:PRO:HD3	1.97	0.65
1:A:705:THR:HA	1:A:708:ASP:HB2	1.78	0.65
1:B:34:TYR:CD2	1:B:224:LEU:HD12	2.31	0.65
1:B:538:PRO:HB2	1:B:550:VAL:HG13	1.78	0.65
1:B:605:PRO:HG3	1:B:734:ALA:HB3	1.78	0.65
1:C:343:GLU:OE2	1:C:420:ARG:CZ	2.45	0.65
1:D:489:THR:O	1:D:489:THR:OG1	2.15	0.65
1:C:113:GLU:O	1:C:117:VAL:HG12	1.97	0.65
1:C:543:PHE:O	1:C:545:ARG:NH2	2.28	0.65
1:C:128:PRO:HD3	1:C:275:SER:HB2	1.78	0.65
1:C:213:THR:O	1:C:213:THR:OG1	2.14	0.65
1:A:472:VAL:O	1:A:476:THR:HG23	1.97	0.64
1:A:542:ARG:HD3	1:A:547:LEU:H	1.61	0.64
1:B:692:ARG:NH2	1:B:740:GLU:OE1	2.30	0.64
1:C:183:ILE:H	1:C:183:ILE:CD1	2.10	0.64
1:A:217:ASP:C	1:A:219:GLU:H	2.06	0.64
1:A:544:GLU:HB2	1:A:545:ARG:NH2	2.13	0.64
1:B:87:VAL:HG22	1:B:88:PRO:HD2	1.78	0.64
1:B:666:GLY:H	1:B:752:SER:HB3	1.63	0.64
1:D:538:PRO:HB3	1:D:550:VAL:HG22	1.80	0.64
1:B:12:LEU:HB3	1:B:16:GLN:HG3	1.80	0.64
1:C:634:PHE:HD1	1:C:634:PHE:H	1.43	0.64
1:A:441:PRO:HG2	1:A:461:ALA:HB2	1.79	0.64
1:A:449:ASP:O	1:A:451:THR:N	2.30	0.64
1:B:206:VAL:O	1:B:208:ILE:N	2.28	0.64
1:C:228:ARG:HA	1:C:231:MET:HE3	1.77	0.64
1:B:650:SER:OG	1:B:683:ALA:HB1	1.98	0.64
1:C:477:ARG:HD3	1:C:542:ARG:H	1.63	0.64
1:D:458:ILE:HG13	1:D:629:TRP:HB2	1.79	0.64
1:A:529:MET:SD	1:A:541:ALA:HB2	2.38	0.64
1:B:680:SER:HA	1:B:690:MET:HE1	1.80	0.64
1:B:127:GLU:HB3	1:B:128:PRO:HD2	1.80	0.64
1:B:238:ALA:HB2	1:B:249:ILE:HD13	1.79	0.64
1:D:4:LYS:O	1:D:5:GLU:HG3	1.98	0.63
1:D:199:ALA:O	1:D:200:VAL:HB	1.98	0.63
1:A:417:ILE:C	1:A:419:ALA:H	2.06	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:LEU:O	1:A:569:ILE:N	2.31	0.63
1:C:561:LYS:NZ	1:C:768:GLY:O	2.25	0.63
1:B:565:ARG:HH21	1:B:771:PRO:HB3	1.64	0.63
1:A:12:LEU:HB3	1:A:16:GLN:HG3	1.80	0.63
1:A:674:VAL:HG11	1:A:679:ALA:H	1.64	0.63
1:B:98:GLN:OE1	1:B:99:GLN:N	2.30	0.63
1:B:706:LEU:HD12	1:B:714:LEU:HD23	1.81	0.63
1:D:208:ILE:HG21	1:D:221:TYR:HD2	1.62	0.63
1:D:449:ASP:O	1:D:451:THR:N	2.32	0.63
1:C:369:GLY:O	1:C:371:SER:N	2.31	0.63
1:C:680:SER:O	1:C:682:ARG:NH2	2.31	0.63
1:D:474:LEU:N	1:D:529:MET:HE1	2.14	0.63
1:A:542:ARG:HD2	1:A:544:GLU:O	1.99	0.63
1:A:710:GLU:HG2	1:A:715:ARG:HG3	1.81	0.63
1:B:104:LEU:HD21	1:B:299:LEU:HD11	1.79	0.63
1:C:651:TRP:NE1	1:C:683:ALA:HA	2.14	0.63
1:D:441:PRO:HG2	1:D:461:ALA:HB2	1.81	0.63
1:D:665:ILE:HD13	1:D:665:ILE:H	1.63	0.63
1:A:106:LEU:HB3	1:A:231:MET:HE1	1.80	0.63
1:B:127:GLU:HB3	1:B:128:PRO:CD	2.29	0.63
1:B:180:ARG:HH12	1:B:212:LYS:HE2	1.63	0.63
1:B:636:THR:HB	1:B:671:LEU:O	1.99	0.63
1:C:127:GLU:HB3	1:C:128:PRO:CD	2.29	0.63
1:C:485:SER:OG	1:C:489:THR:OG1	2.17	0.63
1:B:86:GLN:HE21	1:B:172:ARG:HG2	1.64	0.62
1:C:59:GLU:HG2	1:C:262:ASN:HB3	1.81	0.62
1:A:681:ASN:OD1	1:A:682:ARG:N	2.32	0.62
1:B:489:THR:O	1:B:489:THR:OG1	2.17	0.62
1:A:417:ILE:O	1:A:419:ALA:N	2.31	0.62
1:D:163:ILE:HD13	1:D:168:ASP:HB3	1.82	0.62
1:A:27:ILE:HD13	1:A:98:GLN:NE2	2.15	0.62
1:A:511:TRP:CH2	1:A:519:ALA:HB3	2.35	0.62
1:A:153:TYR:CD1	1:B:134:ASN:HB3	2.35	0.62
1:B:576:VAL:HG13	1:B:756:CYS:HB2	1.81	0.62
1:B:312:ARG:HD3	1:B:315:TYR:CE2	2.35	0.62
1:B:369:GLY:O	1:B:371:SER:N	2.33	0.62
1:C:477:ARG:CZ	1:C:542:ARG:HB3	2.29	0.62
1:D:569:ILE:HG23	1:D:574:GLN:HB3	1.82	0.62
1:D:389:MET:HE1	1:D:526:ARG:HH11	1.64	0.62
1:D:542:ARG:HD2	1:D:544:GLU:O	2.00	0.62
1:A:463:LEU:HD21	1:A:505:ALA:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:492:SER:O	1:D:496:GLN:HG3	2.00	0.61
1:A:417:ILE:C	1:A:419:ALA:N	2.57	0.61
1:D:182:PRO:HD3	1:D:221:TYR:CE1	2.32	0.61
1:A:642:PRO:O	1:A:656:TYR:OH	2.18	0.61
1:A:760:TRP:O	1:A:764:THR:OG1	2.18	0.61
1:D:274:PRO:HA	1:D:277:VAL:HG22	1.80	0.61
1:D:325:THR:HB	1:A:100:ARG:HH22	1.65	0.61
1:D:681:ASN:OD1	1:D:682:ARG:N	2.33	0.61
1:B:44:LEU:HD21	1:B:65:LEU:HD21	1.81	0.61
1:B:474:LEU:O	1:B:477:ARG:HB3	2.01	0.61
1:C:136:ALA:O	1:C:140:THR:HB	2.01	0.61
1:C:612:LEU:HD13	1:C:754:ARG:HD2	1.82	0.61
1:D:701:GLU:O	1:D:705:THR:OG1	2.19	0.61
1:B:518:THR:HG22	1:B:521:ILE:HD12	1.82	0.61
1:C:54:GLN:OE1	1:C:405:ARG:NH1	2.33	0.61
1:D:163:ILE:O	1:D:168:ASP:OD2	2.19	0.61
1:A:12:LEU:HA	1:A:16:GLN:HE21	1.65	0.61
1:B:551:PRO:HB2	1:B:552:PRO:HD3	1.83	0.61
1:D:7:PHE:C	1:D:7:PHE:CD2	2.79	0.61
1:B:349:TRP:CD1	1:B:349:TRP:C	2.79	0.61
1:B:474:LEU:H	1:B:529:MET:HE1	1.66	0.61
1:B:636:THR:HG21	1:B:675:GLU:HG2	1.83	0.61
1:C:452:LEU:HD11	1:C:499:LEU:HD23	1.82	0.61
1:A:23:GLN:O	1:A:161:ARG:NH1	2.34	0.61
1:A:32:ARG:O	1:A:164:ARG:NH2	2.34	0.61
1:B:354:SER:HB3	1:B:424:LEU:HD12	1.83	0.61
1:B:57:GLU:HG2	1:B:58:PHE:CE2	2.36	0.60
1:C:352:SER:O	1:C:354:SER:N	2.34	0.60
1:C:387:PHE:CE2	1:C:427:LEU:HG	2.36	0.60
1:A:228:ARG:HD3	1:A:228:ARG:C	2.26	0.60
1:C:520:GLY:O	1:C:523:GLY:N	2.35	0.60
1:C:83:TYR:CD1	1:C:169:VAL:HG11	2.37	0.60
1:C:539:ARG:O	1:C:550:VAL:HG11	2.00	0.60
1:D:71:LEU:HD12	1:D:310:ALA:O	2.01	0.60
1:D:600:SER:HB3	1:D:732:LEU:HD21	1.82	0.60
1:A:163:ILE:O	1:A:164:ARG:HB2	2.02	0.60
1:A:341:ILE:HG12	1:A:349:TRP:CZ2	2.37	0.60
1:A:477:ARG:CZ	1:A:542:ARG:HB3	2.32	0.60
1:B:539:ARG:O	1:B:550:VAL:HG11	2.02	0.60
1:C:552:PRO:HG2	1:C:555:ALA:H	1.66	0.60
1:A:283:ASP:OD2	1:A:283:ASP:N	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:GLN:CD	1:A:553:VAL:HG22	2.26	0.60
1:A:602:ASN:HB2	1:A:620:LEU:HB3	1.84	0.60
1:A:474:LEU:N	1:A:529:MET:HE1	2.17	0.60
1:A:588:SER:OG	1:A:591:LEU:HB2	2.02	0.60
1:C:710:GLU:HG2	1:C:715:ARG:HG3	1.84	0.60
1:D:411:PHE:O	1:D:420:ARG:HG2	2.02	0.59
1:B:163:ILE:O	1:B:168:ASP:OD2	2.20	0.59
1:B:533:VAL:O	1:B:538:PRO:HD2	2.01	0.59
1:B:715:ARG:HG2	1:B:720:ALA:HB2	1.84	0.59
1:D:636:THR:HB	1:D:671:LEU:O	2.02	0.59
1:A:128:PRO:HB3	1:A:276:VAL:HG22	1.83	0.59
1:C:474:LEU:N	1:C:529:MET:HE1	2.16	0.59
1:D:414:ASP:HB3	1:D:419:ALA:HB1	1.84	0.59
1:B:319:MET:HE3	1:C:64:PHE:CZ	2.37	0.59
1:B:163:ILE:HD12	1:B:170:TRP:CE2	2.37	0.59
1:C:438:TRP:CE3	1:C:464:ARG:HG3	2.38	0.59
1:A:551:PRO:HB2	1:A:552:PRO:HD3	1.85	0.59
1:A:570:TYR:HB2	1:A:769:PHE:HZ	1.67	0.59
1:D:26:TYR:HD2	1:D:93:THR:HG22	1.66	0.59
1:D:764:THR:N	1:D:765:PRO:HD2	2.18	0.59
1:A:474:LEU:O	1:A:477:ARG:HB3	2.02	0.59
1:B:5:GLU:OE2	1:B:311:LYS:HB2	2.03	0.59
1:A:83:TYR:CZ	1:A:176:GLU:HB2	2.38	0.59
1:A:449:ASP:O	1:A:452:LEU:N	2.32	0.58
1:D:127:GLU:HB3	1:D:128:PRO:HD2	1.85	0.58
1:D:216:VAL:HG12	1:D:217:ASP:H	1.68	0.58
1:D:437:PRO:HB2	1:D:460:LEU:HD13	1.85	0.58
1:A:127:GLU:HB3	1:A:128:PRO:CD	2.32	0.58
1:C:57:GLU:HG2	1:C:58:PHE:CE2	2.38	0.58
1:C:545:ARG:HH21	1:C:545:ARG:N	2.01	0.58
1:C:667:ASN:ND2	1:C:743:TRP:HE1	2.01	0.58
1:D:432:ARG:NH2	1:D:435:GLU:OE1	2.36	0.58
1:B:692:ARG:HG3	1:B:737:ALA:HB1	1.85	0.58
1:D:565:ARG:HG2	1:D:570:TYR:HE2	1.69	0.58
1:A:13:SER:H	1:A:16:GLN:NE2	2.01	0.58
1:C:525:TYR:O	1:C:529:MET:HG2	2.02	0.58
1:B:16:GLN:HE22	1:C:3:THR:HG22	1.69	0.58
1:B:208:ILE:HG21	1:B:221:TYR:CD2	2.39	0.58
1:B:449:ASP:O	1:B:451:THR:N	2.37	0.58
1:C:449:ASP:O	1:C:451:THR:N	2.36	0.58
1:A:4:LYS:O	1:A:5:GLU:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ARG:HD3	1:A:236:ARG:CZ	2.33	0.58
1:D:349:TRP:CD1	1:D:349:TRP:C	2.81	0.58
1:D:705:THR:HA	1:D:708:ASP:HB2	1.86	0.58
1:A:57:GLU:HG2	1:A:58:PHE:CE2	2.38	0.58
1:C:208:ILE:HG21	1:C:221:TYR:CD2	2.38	0.58
1:D:209:ASP:OD1	1:D:212:LYS:N	2.36	0.58
1:D:484:LEU:HB3	1:D:548:THR:HG22	1.86	0.58
1:B:391:GLN:O	1:B:391:GLN:NE2	2.37	0.58
1:C:468:HIS:HE2	1:C:521:ILE:HG21	1.69	0.58
1:D:484:LEU:HD22	1:D:547:LEU:HD23	1.84	0.58
1:D:538:PRO:HB2	1:D:550:VAL:HG13	1.85	0.58
1:D:3:THR:O	1:D:5:GLU:N	2.36	0.58
1:D:472:VAL:O	1:D:476:THR:HG23	2.04	0.58
1:A:417:ILE:HG13	1:A:421:ARG:NH1	2.19	0.57
1:B:64:PHE:CE2	1:C:319:MET:HG2	2.39	0.57
1:A:29:PRO:HB3	1:A:165:SER:HB2	1.85	0.57
1:A:520:GLY:O	1:A:523:GLY:N	2.38	0.57
1:C:26:TYR:CE2	1:C:79:VAL:HA	2.39	0.57
1:C:34:TYR:CD2	1:C:224:LEU:HD12	2.39	0.57
1:D:219:GLU:HA	1:D:222:ARG:HD2	1.85	0.57
1:B:114:GLU:OE1	1:B:118:ARG:NH1	2.37	0.57
1:B:208:ILE:HG21	1:B:221:TYR:HD2	1.68	0.57
1:B:257:ILE:HD13	1:B:294:VAL:HG21	1.87	0.57
1:C:148:GLU:OE2	1:C:195:ARG:NH1	2.37	0.57
1:C:417:ILE:O	1:C:419:ALA:N	2.31	0.57
1:D:397:THR:OG1	1:D:402:ASP:OD2	2.20	0.57
1:D:605:PRO:HB3	1:D:735:ALA:HB2	1.86	0.57
1:A:449:ASP:HB3	1:A:452:LEU:HB2	1.84	0.57
1:A:562:GLU:HG2	1:A:565:ARG:NH1	2.20	0.57
1:A:722:GLU:O	1:A:726:GLN:NE2	2.37	0.57
1:C:475:LEU:HD21	1:C:504:CYS:SG	2.44	0.57
1:D:127:GLU:HB3	1:D:128:PRO:CD	2.34	0.57
1:A:496:GLN:CA	1:A:553:VAL:HG13	2.32	0.57
1:A:486:SER:O	1:A:488:GLU:N	2.38	0.57
1:B:57:GLU:HG2	1:B:58:PHE:CD2	2.39	0.57
1:C:682:ARG:HE	1:C:716:LEU:HD13	1.69	0.57
1:D:544:GLU:HB2	1:D:545:ARG:NH2	2.20	0.57
1:A:516:GLY:O	1:A:587:HIS:NE2	2.37	0.57
1:C:283:ASP:OD2	1:C:283:ASP:N	2.37	0.57
1:B:471:VAL:HG22	1:B:525:TYR:CZ	2.40	0.56
1:C:13:SER:OG	1:C:16:GLN:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:HIS:HE1	1:D:227:MET:CE	2.16	0.56
1:D:549:GLU:HG3	1:D:550:VAL:HG23	1.86	0.56
1:D:688:ARG:NH1	1:D:740:GLU:OE2	2.38	0.56
1:A:572:LYS:HE2	1:A:760:TRP:CZ3	2.39	0.56
1:A:706:LEU:HD12	1:A:714:LEU:HD23	1.86	0.56
1:B:128:PRO:HD3	1:B:275:SER:HB2	1.86	0.56
1:B:650:SER:OG	1:B:651:TRP:N	2.39	0.56
1:C:26:TYR:CD1	1:C:163:ILE:HG22	2.39	0.56
1:C:83:TYR:CE2	1:C:176:GLU:HB2	2.39	0.56
1:C:186:TYR:CE2	1:C:205:HIS:CD2	2.93	0.56
1:C:666:GLY:H	1:C:752:SER:HB3	1.69	0.56
1:D:682:ARG:HH21	1:D:716:LEU:HD13	1.71	0.56
1:A:161:ARG:O	1:A:162:LEU:HB2	2.05	0.56
1:B:219:GLU:HA	1:B:222:ARG:HD2	1.87	0.56
1:B:372:SER:OG	1:B:373:ALA:N	2.37	0.56
1:A:13:SER:OG	1:A:16:GLN:HG2	2.05	0.56
1:A:208:ILE:HD12	1:A:221:TYR:CE2	2.41	0.56
1:B:385:LEU:HD22	1:B:396:LEU:HB3	1.86	0.56
1:B:581:MET:SD	1:B:664:ARG:NH1	2.79	0.56
1:B:669:THR:CG2	1:B:751:ARG:HH22	2.18	0.56
1:C:510:LEU:HD13	1:C:564:LEU:HD21	1.88	0.56
1:A:155:GLU:HB2	1:A:174:LYS:HG2	1.88	0.56
1:C:87:VAL:HG13	1:C:88:PRO:O	2.06	0.56
1:C:168:ASP:OD1	1:C:180:ARG:N	2.38	0.56
1:C:720:ALA:HB1	1:C:723:ILE:HB	1.88	0.56
1:B:706:LEU:HD13	1:B:723:ILE:HG22	1.87	0.56
1:C:100:ARG:HG3	1:C:100:ARG:HH11	1.71	0.56
1:D:343:GLU:OE2	1:D:420:ARG:CZ	2.53	0.56
1:D:387:PHE:CE2	1:D:427:LEU:HG	2.40	0.56
1:A:488:GLU:HG2	1:A:489:THR:N	2.19	0.56
1:B:705:THR:HA	1:B:708:ASP:HB2	1.88	0.56
1:C:163:ILE:O	1:C:164:ARG:HB2	2.04	0.56
1:A:720:ALA:HB1	1:A:723:ILE:HD12	1.87	0.55
1:B:113:GLU:OE2	1:B:232:ARG:NH2	2.39	0.55
1:B:617:LYS:O	1:B:619:GLY:N	2.39	0.55
1:C:59:GLU:HG2	1:C:262:ASN:CB	2.36	0.55
1:D:537:MET:CB	1:D:538:PRO:HD3	2.37	0.55
1:D:588:SER:OG	1:D:591:LEU:HB2	2.06	0.55
1:A:578:ARG:O	1:A:582:THR:HG23	2.06	0.55
1:B:333:ILE:HD12	1:B:380:THR:HG23	1.87	0.55
1:B:682:ARG:NH2	1:B:716:LEU:HD13	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:538:PRO:HB3	1:C:550:VAL:HG22	1.88	0.55
1:C:688:ARG:HD3	1:C:692:ARG:HH12	1.72	0.55
1:D:86:GLN:OE1	1:D:171:SER:HB2	2.06	0.55
1:D:605:PRO:HG3	1:D:734:ALA:HB3	1.88	0.55
1:A:477:ARG:NH2	1:A:547:LEU:O	2.39	0.55
1:B:760:TRP:O	1:B:764:THR:OG1	2.25	0.55
1:C:130:VAL:O	1:C:134:ASN:ND2	2.39	0.55
1:C:621:LEU:HD12	1:C:729:TYR:HD2	1.72	0.55
1:C:722:GLU:O	1:C:726:GLN:NE2	2.39	0.55
1:D:232:ARG:HD3	1:D:236:ARG:CZ	2.36	0.55
1:B:149:GLU:HB2	1:B:161:ARG:NH2	2.21	0.55
1:B:168:ASP:OD1	1:B:180:ARG:N	2.33	0.55
1:B:455:GLN:O	1:B:458:ILE:HG22	2.07	0.55
1:C:364:TYR:CE1	1:C:368:GLU:HG3	2.41	0.55
1:D:496:GLN:HG2	1:D:553:VAL:HG22	1.87	0.55
1:A:493:SER:OG	1:A:494:ALA:N	2.39	0.55
1:A:621:LEU:HD12	1:A:729:TYR:HD2	1.71	0.55
1:B:34:TYR:CE1	1:B:36:TRP:HB2	2.42	0.55
1:B:86:GLN:HB3	1:B:172:ARG:HH21	1.71	0.55
1:B:414:ASP:HB3	1:B:419:ALA:CB	2.37	0.55
1:D:26:TYR:CE2	1:D:79:VAL:HA	2.42	0.55
1:A:438:TRP:CE3	1:A:464:ARG:HG3	2.42	0.55
1:B:583:PRO:HG3	1:B:660:GLU:HG2	1.87	0.55
1:C:630:ASN:O	1:C:632:GLU:HG3	2.05	0.55
1:D:284:ALA:O	1:D:286:MET:N	2.34	0.55
1:D:551:PRO:HB2	1:D:552:PRO:CD	2.36	0.55
1:D:628:ARG:HA	1:D:631:ASP:CB	2.30	0.55
1:C:127:GLU:HB3	1:C:128:PRO:HD2	1.88	0.55
1:C:565:ARG:HH21	1:C:771:PRO:HB3	1.72	0.55
1:A:605:PRO:HA	1:A:735:ALA:HB2	1.88	0.55
1:A:674:VAL:HG13	1:A:678:SER:HB3	1.89	0.55
1:B:593:ARG:NH2	1:B:635:ALA:HB1	2.18	0.55
1:B:634:PHE:HD1	1:B:634:PHE:H	1.54	0.55
1:D:516:GLY:O	1:D:587:HIS:NE2	2.39	0.55
1:C:57:GLU:HG2	1:C:58:PHE:CD2	2.42	0.55
1:C:408:ARG:HD3	1:C:412:ASP:OD2	2.07	0.55
1:A:113:GLU:O	1:A:117:VAL:HG12	2.06	0.55
1:A:180:ARG:NH1	1:A:213:THR:HG22	2.21	0.55
1:A:489:THR:O	1:A:489:THR:OG1	2.25	0.55
1:C:119:ALA:O	1:C:122:LEU:HB2	2.07	0.55
1:D:217:ASP:C	1:D:219:GLU:H	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:SER:OG	1:D:375:LYS:HB3	2.07	0.54
1:B:542:ARG:HE	1:B:547:LEU:HD12	1.72	0.54
1:B:38:LEU:N	1:B:227:MET:HE1	2.22	0.54
1:C:374:ASP:OD1	1:C:374:ASP:N	2.39	0.54
1:D:120:GLU:HG2	1:D:200:VAL:HG11	1.88	0.54
1:A:120:GLU:HG2	1:A:200:VAL:HG11	1.90	0.54
1:B:414:ASP:HB3	1:B:419:ALA:HB1	1.88	0.54
1:C:18:LEU:HB2	1:C:146:CYS:SG	2.47	0.54
1:C:496:GLN:CA	1:C:553:VAL:HG13	2.35	0.54
1:D:312:ARG:HD3	1:D:315:TYR:CD2	2.42	0.54
1:D:632:GLU:HA	1:D:635:ALA:HB3	1.88	0.54
1:A:26:TYR:HD2	1:A:93:THR:HG22	1.71	0.54
1:A:507:PHE:CZ	1:A:511:TRP:HD1	2.25	0.54
1:C:526:ARG:O	1:C:530:THR:HG23	2.07	0.54
1:C:636:THR:CG2	1:C:675:GLU:HG2	2.37	0.54
1:D:161:ARG:HA	1:D:170:TRP:HH2	1.73	0.54
1:D:630:ASN:O	1:D:632:GLU:N	2.40	0.54
1:A:569:ILE:HG23	1:A:574:GLN:HB3	1.90	0.54
1:C:437:PRO:HD3	1:C:479:PHE:CE2	2.42	0.54
1:C:565:ARG:O	1:C:568:GLY:N	2.41	0.54
1:C:605:PRO:HG3	1:C:734:ALA:HB3	1.89	0.54
1:C:674:VAL:HG11	1:C:679:ALA:H	1.72	0.54
1:B:186:TYR:OH	1:B:228:ARG:HD2	2.06	0.54
1:C:343:GLU:OE2	1:C:420:ARG:NH1	2.40	0.54
1:B:557:GLN:O	1:B:561:LYS:HD3	2.08	0.54
1:B:570:TYR:HD1	1:B:769:PHE:CZ	2.25	0.54
1:C:344:GLU:OE2	1:C:352:SER:HB2	2.08	0.54
1:C:561:LYS:HD2	1:C:767:LEU:HB3	1.89	0.54
1:D:621:LEU:HD12	1:D:729:TYR:CD2	2.42	0.54
1:D:688:ARG:HD3	1:D:692:ARG:HH12	1.73	0.54
1:A:437:PRO:HB2	1:A:460:LEU:HD13	1.89	0.54
1:B:724:VAL:HG12	1:B:725:ARG:HG3	1.90	0.54
1:C:148:GLU:CD	1:C:195:ARG:NH1	2.66	0.54
1:A:87:VAL:HG22	1:A:88:PRO:HD2	1.89	0.54
1:B:36:TRP:HE3	1:B:41:ILE:HD13	1.73	0.54
1:B:645:PRO:HB2	1:B:648:ASN:HA	1.90	0.54
1:C:104:LEU:O	1:C:108:THR:HG23	2.08	0.54
1:D:565:ARG:HH21	1:D:771:PRO:HB3	1.73	0.54
1:B:344:GLU:OE1	1:B:421:ARG:NH2	2.41	0.54
1:B:417:ILE:HG13	1:B:421:ARG:NH1	2.23	0.54
1:C:126:ASP:O	1:C:128:PRO:HD2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:PRO:HG2	1:D:179:TYR:CD1	2.42	0.53
1:A:260:SER:O	1:A:264:GLN:HG3	2.08	0.53
1:A:284:ALA:O	1:A:286:MET:N	2.36	0.53
1:B:549:GLU:HG3	1:B:550:VAL:HG23	1.89	0.53
1:A:474:LEU:H	1:A:529:MET:HE1	1.71	0.53
1:A:688:ARG:CZ	1:A:740:GLU:OE2	2.56	0.53
1:D:651:TRP:CZ3	1:D:684:TRP:HB2	2.44	0.53
1:A:118:ARG:HB2	1:A:289:LEU:HD13	1.90	0.53
1:C:163:ILE:O	1:C:168:ASP:OD2	2.26	0.53
1:A:416:ASP:HB2	1:A:419:ALA:HB3	1.90	0.53
1:A:662:ILE:HD12	1:A:662:ILE:H	1.73	0.53
1:B:612:LEU:HD13	1:B:754:ARG:HD2	1.89	0.53
1:C:88:PRO:HG2	1:C:91:VAL:HG12	1.90	0.53
1:D:415:PRO:O	1:D:420:ARG:NH1	2.42	0.53
1:C:441:PRO:O	1:C:444:VAL:HG22	2.09	0.53
1:D:674:VAL:HG11	1:D:679:ALA:H	1.72	0.53
1:B:228:ARG:HA	1:B:231:MET:HE3	1.90	0.53
1:B:542:ARG:HG3	1:B:542:ARG:HH11	1.74	0.53
1:D:35:SER:O	1:D:223:HIS:NE2	2.36	0.53
1:A:511:TRP:CD2	1:A:521:ILE:HG12	2.44	0.53
1:D:86:GLN:CB	1:D:172:ARG:HE	2.21	0.53
1:A:315:TYR:O	1:A:319:MET:HG3	2.09	0.53
1:B:486:SER:O	1:B:488:GLU:N	2.42	0.53
1:B:669:THR:HG23	1:B:751:ARG:HH12	1.73	0.53
1:C:509:ALA:HA	1:C:591:LEU:HD21	1.91	0.53
1:C:551:PRO:HB2	1:C:552:PRO:HD3	1.89	0.53
1:A:557:GLN:O	1:A:561:LYS:HD3	2.09	0.52
1:C:674:VAL:HG11	1:C:679:ALA:N	2.24	0.52
1:D:81:PRO:HD3	1:D:166:TYR:H	1.73	0.52
1:A:26:TYR:CE2	1:A:79:VAL:HA	2.45	0.52
1:A:479:PHE:HE1	1:A:483:ARG:HD2	1.69	0.52
1:B:5:GLU:O	1:B:7:PHE:N	2.40	0.52
1:B:729:TYR:CE2	1:B:731:PRO:HG3	2.44	0.52
1:A:674:VAL:HG11	1:A:679:ALA:N	2.23	0.52
1:B:1:MET:SD	1:C:62:ILE:HD13	2.49	0.52
1:B:106:LEU:O	1:B:109:THR:HG22	2.09	0.52
1:B:163:ILE:O	1:B:164:ARG:HB2	2.09	0.52
1:B:163:ILE:HD12	1:B:170:TRP:CD2	2.44	0.52
1:D:715:ARG:HG2	1:D:720:ALA:HB2	1.91	0.52
1:A:454:THR:HG21	1:A:627:GLU:OE2	2.09	0.52
1:B:621:LEU:HD13	1:B:728:ARG:HH12	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:ARG:NH2	1:A:545:ARG:H	2.08	0.52
1:A:546:ASP:O	1:A:548:THR:N	2.40	0.52
1:B:6:ILE:HG22	1:B:7:PHE:HB3	1.92	0.52
1:B:537:MET:CB	1:B:538:PRO:HD3	2.40	0.52
1:C:180:ARG:HD3	1:C:213:THR:HG22	1.92	0.52
1:D:3:THR:O	1:D:3:THR:OG1	2.27	0.52
1:D:715:ARG:HG2	1:D:720:ALA:CB	2.40	0.52
1:A:79:VAL:HG23	1:A:82:LYS:HD3	1.91	0.52
1:A:81:PRO:O	1:A:169:VAL:HG13	2.10	0.52
1:B:375:LYS:HA	1:B:378:THR:HG22	1.91	0.52
1:C:83:TYR:HD1	1:C:169:VAL:HG11	1.74	0.52
1:C:537:MET:HB2	1:C:538:PRO:HD3	1.92	0.52
1:C:764:THR:O	1:C:769:PHE:HB2	2.10	0.52
1:D:84:ARG:HG3	1:D:84:ARG:O	2.08	0.52
1:D:223:HIS:CE1	1:D:227:MET:HE2	2.38	0.52
1:D:471:VAL:HG12	1:D:475:LEU:HG	1.92	0.52
1:D:630:ASN:O	1:D:632:GLU:HG3	2.10	0.52
1:A:209:ASP:OD1	1:A:212:LYS:N	2.43	0.52
1:A:764:THR:N	1:A:765:PRO:HD2	2.25	0.52
1:C:115:ILE:HG23	1:C:289:LEU:HD11	1.92	0.52
1:C:228:ARG:HD3	1:C:228:ARG:C	2.35	0.52
1:C:569:ILE:HG23	1:C:574:GLN:HB3	1.92	0.52
1:A:27:ILE:HD13	1:A:98:GLN:HE21	1.73	0.52
1:A:282:ASP:N	1:A:282:ASP:OD1	2.42	0.52
1:D:7:PHE:HD1	1:D:319:MET:SD	2.33	0.52
1:A:605:PRO:CB	1:A:735:ALA:HB2	2.39	0.52
1:B:488:GLU:HG2	1:B:489:THR:N	2.24	0.52
1:B:496:GLN:HG2	1:B:553:VAL:HG13	1.92	0.52
1:C:433:PHE:CB	1:C:476:THR:HG22	2.39	0.52
1:C:537:MET:CB	1:C:538:PRO:HD3	2.40	0.52
1:D:32:ARG:O	1:D:164:ARG:NH2	2.43	0.51
1:D:161:ARG:O	1:D:162:LEU:HB2	2.09	0.51
1:D:186:TYR:OH	1:D:228:ARG:HD2	2.11	0.51
1:D:196:ASP:OD1	1:D:197:PRO:HD2	2.09	0.51
1:D:474:LEU:H	1:D:529:MET:HE1	1.74	0.51
1:B:474:LEU:HG	1:B:529:MET:CE	2.40	0.51
1:B:584:VAL:HG12	1:B:592:THR:HG22	1.92	0.51
1:C:163:ILE:HD13	1:C:168:ASP:HB3	1.93	0.51
1:C:486:SER:O	1:C:488:GLU:N	2.43	0.51
1:C:615:ARG:HG2	1:C:616:GLY:H	1.75	0.51
1:D:375:LYS:O	1:D:378:THR:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:456:ALA:HB3	1:D:498:LEU:HD22	1.92	0.51
1:D:662:ILE:HD12	1:D:662:ILE:H	1.73	0.51
1:B:13:SER:OG	1:B:16:GLN:HG2	2.11	0.51
1:C:38:LEU:N	1:C:227:MET:HE1	2.25	0.51
1:A:3:THR:O	1:A:3:THR:OG1	2.26	0.51
1:B:417:ILE:O	1:B:419:ALA:N	2.37	0.51
1:B:433:PHE:CG	1:B:476:THR:HG22	2.44	0.51
1:B:437:PRO:HG3	1:B:479:PHE:HE2	1.75	0.51
1:D:34:TYR:CD2	1:D:224:LEU:HD12	2.45	0.51
1:D:85:SER:C	1:D:86:GLN:HG3	2.35	0.51
1:D:583:PRO:HG3	1:D:660:GLU:HG2	1.93	0.51
1:D:154:GLY:O	1:D:157:ARG:HB2	2.11	0.51
1:D:339:ARG:HG2	1:D:408:ARG:CZ	2.41	0.51
1:A:58:PHE:CE2	1:A:405:ARG:HD3	2.45	0.51
1:B:623:THR:HG22	1:B:634:PHE:HZ	1.75	0.51
1:D:458:ILE:HD11	1:D:629:TRP:HE3	1.75	0.51
1:D:602:ASN:HB2	1:D:620:LEU:HB3	1.91	0.51
1:D:603:SER:HB3	1:D:613:VAL:CG1	2.40	0.51
1:A:636:THR:OG1	1:A:675:GLU:HG2	2.11	0.51
1:B:414:ASP:OD1	1:B:544:GLU:OE2	2.29	0.51
1:D:452:LEU:HB3	1:D:498:LEU:HD13	1.92	0.51
1:A:161:ARG:HA	1:A:170:TRP:HH2	1.75	0.51
1:A:621:LEU:HD12	1:A:729:TYR:CD2	2.44	0.51
1:B:23:GLN:O	1:B:161:ARG:NH1	2.44	0.51
1:B:337:LYS:HZ2	1:B:362:GLU:CD	2.19	0.51
1:A:688:ARG:HB3	1:A:692:ARG:CZ	2.41	0.51
1:C:681:ASN:OD1	1:C:682:ARG:N	2.43	0.51
1:C:706:LEU:O	1:C:710:GLU:HG3	2.10	0.51
1:A:496:GLN:NE2	1:A:553:VAL:HG22	2.25	0.51
1:A:561:LYS:O	1:A:564:LEU:N	2.44	0.51
1:B:182:PRO:HD3	1:B:221:TYR:CE1	2.45	0.51
1:B:353:GLU:O	1:B:356:LEU:HB2	2.11	0.51
1:D:57:GLU:HG2	1:D:58:PHE:CD2	2.46	0.51
1:D:62:ILE:HG22	1:A:315:TYR:CE1	2.46	0.51
1:C:86:GLN:HE22	1:C:172:ARG:H	1.57	0.51
1:C:337:LYS:NZ	1:C:337:LYS:HB2	2.26	0.51
1:D:54:GLN:OE1	1:D:405:ARG:NH1	2.44	0.50
1:A:344:GLU:O	1:A:349:TRP:HB3	2.11	0.50
1:B:173:ASN:HB2	1:B:176:GLU:OE2	2.11	0.50
1:A:433:PHE:O	1:A:437:PRO:HD2	2.11	0.50
1:C:650:SER:OG	1:C:683:ALA:HB1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:ILE:HD12	1:A:578:ARG:NH2	2.26	0.50
1:B:516:GLY:O	1:B:587:HIS:NE2	2.45	0.50
1:B:537:MET:HB2	1:B:538:PRO:HD3	1.93	0.50
1:C:56:ALA:O	1:C:262:ASN:ND2	2.44	0.50
1:C:274:PRO:HA	1:C:277:VAL:HG22	1.92	0.50
1:C:692:ARG:HG3	1:C:737:ALA:CB	2.38	0.50
1:D:84:ARG:O	1:D:85:SER:C	2.54	0.50
1:D:486:SER:O	1:D:488:GLU:N	2.45	0.50
1:D:610:PRO:O	1:D:739:ARG:HB2	2.11	0.50
1:B:282:ASP:OD1	1:B:282:ASP:N	2.44	0.50
1:C:5:GLU:CD	1:C:311:LYS:HB2	2.36	0.50
1:B:11:PRO:O	1:B:12:LEU:HD23	2.11	0.50
1:B:418:VAL:N	1:B:421:ARG:HD2	2.27	0.50
1:C:45:LEU:N	1:C:45:LEU:HD23	2.26	0.50
1:A:35:SER:O	1:A:223:HIS:NE2	2.37	0.50
1:B:26:TYR:CZ	1:B:79:VAL:HA	2.47	0.50
1:D:385:LEU:HB2	1:D:386:PRO:HD3	1.94	0.50
1:A:576:VAL:HG13	1:A:756:CYS:HB2	1.94	0.50
1:C:472:VAL:O	1:C:476:THR:HG23	2.11	0.50
1:B:5:GLU:CD	1:B:311:LYS:HB2	2.36	0.50
1:B:213:THR:O	1:B:213:THR:OG1	2.21	0.50
1:B:238:ALA:HB2	1:B:249:ILE:CD1	2.42	0.50
1:B:671:LEU:HD11	1:B:691:PHE:HE1	1.77	0.50
1:D:36:TRP:HE3	1:D:41:ILE:HD13	1.76	0.50
1:D:78:THR:O	1:D:80:GLU:HG2	2.12	0.50
1:D:681:ASN:H	1:D:690:MET:HE1	1.77	0.50
1:B:585:TYR:HA	1:B:592:THR:HG21	1.94	0.50
1:C:448:ASP:O	1:C:450:ALA:N	2.45	0.50
1:D:83:TYR:HD1	1:D:169:VAL:HG11	1.77	0.49
1:D:511:TRP:HH2	1:D:519:ALA:HB3	1.76	0.49
1:A:569:ILE:CG2	1:A:574:GLN:HB3	2.42	0.49
1:A:634:PHE:HD1	1:A:634:PHE:H	1.60	0.49
1:B:280:LEU:HD13	1:B:286:MET:HE2	1.93	0.49
1:B:477:ARG:CZ	1:B:542:ARG:HB3	2.42	0.49
1:C:149:GLU:HB2	1:C:161:ARG:NH2	2.27	0.49
1:A:265:PHE:CZ	1:A:271:GLU:HG3	2.47	0.49
1:C:86:GLN:NE2	1:C:172:ARG:H	2.09	0.49
1:D:207:PRO:O	1:D:208:ILE:HG22	2.13	0.49
1:D:511:TRP:CD2	1:D:521:ILE:HG12	2.48	0.49
1:D:744:THR:O	1:D:748:VAL:HG23	2.12	0.49
1:B:557:GLN:HB3	1:B:767:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:ARG:NH2	1:B:771:PRO:HB3	2.26	0.49
1:C:452:LEU:HB3	1:C:498:LEU:HD13	1.94	0.49
1:C:538:PRO:CB	1:C:550:VAL:HG22	2.42	0.49
1:A:496:GLN:HG2	1:A:553:VAL:HG22	1.93	0.49
1:B:180:ARG:HH22	1:B:212:LYS:NZ	2.10	0.49
1:B:444:VAL:HG12	1:B:445:PRO:HD3	1.94	0.49
1:C:496:GLN:CD	1:C:553:VAL:HG22	2.38	0.49
1:D:479:PHE:HE1	1:D:483:ARG:NE	2.10	0.49
1:A:13:SER:N	1:A:16:GLN:HE21	2.08	0.49
1:A:565:ARG:HH21	1:A:771:PRO:CB	2.23	0.49
1:C:217:ASP:O	1:C:218:LEU:HB2	2.12	0.49
1:C:593:ARG:HH21	1:C:635:ALA:HB1	1.77	0.49
1:C:662:ILE:HD12	1:C:662:ILE:H	1.78	0.49
1:D:239:VAL:HG11	1:D:292:LEU:HD13	1.94	0.49
1:D:326:THR:HG21	1:A:323:LEU:O	2.12	0.49
1:D:621:LEU:HD12	1:D:729:TYR:HD2	1.77	0.49
1:C:148:GLU:OE1	1:C:195:ARG:NH1	2.44	0.49
1:C:509:ALA:HB2	1:C:594:LEU:HD12	1.93	0.49
1:C:570:TYR:N	1:C:570:TYR:CD2	2.80	0.49
1:C:709:ALA:HB1	1:C:714:LEU:HB2	1.94	0.49
1:A:113:GLU:OE2	1:A:232:ARG:NH2	2.46	0.49
1:A:126:ASP:OD1	1:A:126:ASP:O	2.31	0.49
1:A:239:VAL:HG11	1:A:292:LEU:HD13	1.93	0.49
1:A:458:ILE:N	1:A:626:LEU:HB2	2.28	0.49
1:B:123:THR:O	1:B:129:SER:OG	2.23	0.49
1:B:570:TYR:HD1	1:B:769:PHE:HZ	1.59	0.49
1:B:642:PRO:HD3	1:B:651:TRP:CZ2	2.48	0.49
1:C:583:PRO:HB2	1:C:586:GLN:HG3	1.95	0.49
1:C:641:ALA:HA	1:C:651:TRP:CH2	2.47	0.49
1:B:86:GLN:NE2	1:B:172:ARG:H	2.10	0.49
1:B:569:ILE:HG12	1:B:574:GLN:HB3	1.95	0.49
1:C:282:ASP:OD1	1:C:282:ASP:N	2.46	0.49
1:C:546:ASP:O	1:C:548:THR:N	2.44	0.49
1:C:631:ASP:C	1:C:633:ALA:H	2.21	0.49
1:D:433:PHE:CG	1:D:476:THR:HG22	2.48	0.49
1:D:569:ILE:HD12	1:D:578:ARG:NH2	2.28	0.49
1:D:151:MET:SD	1:D:151:MET:N	2.85	0.49
1:D:728:ARG:HD3	1:D:729:TYR:N	2.27	0.49
1:A:163:ILE:O	1:A:168:ASP:OD2	2.31	0.49
1:C:36:TRP:HE3	1:C:41:ILE:HD13	1.78	0.49
1:D:603:SER:HB3	1:D:613:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:GLU:HB2	1:A:545:ARG:HH22	1.77	0.48
1:B:155:GLU:H	1:B:174:LYS:HE2	1.77	0.48
1:B:681:ASN:O	1:B:682:ARG:HB2	2.13	0.48
1:B:110:VAL:CG2	1:B:235:LEU:HD12	2.43	0.48
1:B:654:ASP:OD1	1:B:654:ASP:N	2.47	0.48
1:D:5:GLU:CD	1:D:311:LYS:HB2	2.38	0.48
1:A:706:LEU:HG	1:A:710:GLU:OE2	2.13	0.48
1:B:354:SER:HB3	1:B:424:LEU:CD1	2.42	0.48
1:C:449:ASP:O	1:C:452:LEU:N	2.41	0.48
1:C:529:MET:HB3	1:C:541:ALA:HB2	1.96	0.48
1:D:389:MET:CE	1:D:526:ARG:HH11	2.26	0.48
1:D:728:ARG:HD3	1:D:729:TYR:H	1.78	0.48
1:A:29:PRO:HG3	1:A:80:GLU:HG3	1.93	0.48
1:C:52:LEU:HD23	1:C:298:TYR:CD1	2.49	0.48
1:C:106:LEU:O	1:C:110:VAL:HG12	2.13	0.48
1:C:636:THR:HB	1:C:671:LEU:O	2.13	0.48
1:D:562:GLU:HG2	1:D:565:ARG:NH1	2.28	0.48
1:A:638:GLU:OE2	1:A:687:LYS:NZ	2.46	0.48
1:A:665:ILE:CD1	1:A:665:ILE:H	2.27	0.48
1:B:445:PRO:HG3	1:B:497:PHE:HD1	1.79	0.48
1:B:514:SER:O	1:B:582:THR:HG21	2.14	0.48
1:B:572:LYS:HE2	1:B:760:TRP:CZ3	2.48	0.48
1:B:669:THR:HG21	1:B:751:ARG:HH22	1.78	0.48
1:C:588:SER:OG	1:C:591:LEU:HB2	2.14	0.48
1:D:365:LEU:HD12	1:D:379:VAL:HG12	1.95	0.48
1:A:516:GLY:O	1:A:587:HIS:CD2	2.66	0.48
1:D:213:THR:O	1:D:213:THR:OG1	2.30	0.48
1:D:674:VAL:HG13	1:D:678:SER:H	1.78	0.48
1:A:57:GLU:HG2	1:A:58:PHE:CD2	2.49	0.48
1:B:26:TYR:CE2	1:B:79:VAL:HA	2.49	0.48
1:B:524:VAL:HG22	1:B:563:GLN:NE2	2.29	0.48
1:D:190:TYR:CD1	1:D:190:TYR:C	2.92	0.48
1:D:666:GLY:H	1:D:752:SER:HB3	1.79	0.48
1:B:319:MET:HB3	1:B:319:MET:HE2	1.53	0.48
1:B:496:GLN:NE2	1:B:553:VAL:HG22	2.29	0.48
1:C:371:SER:OG	1:C:375:LYS:HG2	2.14	0.48
1:C:469:ASP:O	1:C:472:VAL:HG23	2.14	0.48
1:C:520:GLY:O	1:C:521:ILE:C	2.56	0.48
1:D:228:ARG:C	1:D:228:ARG:HD3	2.39	0.48
1:A:400:LEU:HD13	1:A:400:LEU:HA	1.75	0.48
1:B:34:TYR:HD1	1:B:99:GLN:OE1	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ILE:HB	1:C:164:ARG:HA	1.95	0.48
1:C:65:LEU:HD23	1:C:65:LEU:HA	1.61	0.48
1:C:372:SER:OG	1:C:373:ALA:N	2.43	0.48
1:C:555:ALA:HA	1:C:558:SER:OG	2.14	0.48
1:B:636:THR:CG2	1:B:675:GLU:HG2	2.43	0.48
1:B:709:ALA:HB3	1:B:714:LEU:HD22	1.95	0.48
1:B:720:ALA:HB1	1:B:723:ILE:HD12	1.95	0.48
1:C:470:ILE:HG21	1:C:522:ASP:HA	1.95	0.48
1:D:113:GLU:O	1:D:117:VAL:HG12	2.14	0.47
1:D:406:TYR:CZ	1:D:410:VAL:HG21	2.49	0.47
1:D:502:ARG:CZ	1:D:766:TRP:CD1	2.97	0.47
1:D:511:TRP:CH2	1:D:519:ALA:HB3	2.49	0.47
1:D:526:ARG:O	1:D:530:THR:HG23	2.14	0.47
1:A:369:GLY:O	1:A:371:SER:N	2.44	0.47
1:C:25:LEU:O	1:C:162:LEU:HA	2.14	0.47
1:C:465:GLU:CD	1:C:629:TRP:HE1	2.22	0.47
1:C:554:GLU:HA	1:C:557:GLN:HG3	1.97	0.47
1:C:642:PRO:HD3	1:C:651:TRP:CE2	2.48	0.47
1:C:650:SER:OG	1:C:651:TRP:N	2.45	0.47
1:D:9:ALA:CB	1:A:9:ALA:HB3	2.42	0.47
1:D:315:TYR:HE1	1:A:62:ILE:HG22	1.79	0.47
1:D:432:ARG:HD3	1:D:483:ARG:HH12	1.79	0.47
1:A:610:PRO:HB2	1:A:739:ARG:HA	1.95	0.47
1:B:164:ARG:NH1	1:B:183:ILE:HD11	2.28	0.47
1:C:268:PHE:O	1:C:270:SER:HB3	2.13	0.47
1:C:417:ILE:C	1:C:419:ALA:H	2.22	0.47
1:C:417:ILE:C	1:C:419:ALA:N	2.72	0.47
1:D:5:GLU:O	1:D:7:PHE:N	2.48	0.47
1:A:331:THR:N	1:A:334:GLU:OE1	2.47	0.47
1:B:217:ASP:O	1:B:218:LEU:HB2	2.13	0.47
1:C:488:GLU:HG2	1:C:489:THR:HG22	1.94	0.47
1:D:34:TYR:HD2	1:D:224:LEU:HD12	1.80	0.47
1:D:136:ALA:O	1:D:140:THR:HB	2.14	0.47
1:D:596:LEU:HD21	1:D:665:ILE:HG22	1.96	0.47
1:A:357:HIS:O	1:A:360:VAL:HB	2.15	0.47
1:A:496:GLN:CG	1:A:553:VAL:HG22	2.45	0.47
1:A:605:PRO:CA	1:A:735:ALA:HB2	2.43	0.47
1:B:161:ARG:O	1:B:162:LEU:HB2	2.13	0.47
1:B:700:GLU:HG2	1:B:704:LYS:HE3	1.96	0.47
1:C:709:ALA:CB	1:C:714:LEU:HB2	2.44	0.47
1:A:217:ASP:C	1:A:219:GLU:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:THR:HG21	1:B:627:GLU:OE2	2.15	0.47
1:B:512:ARG:NE	1:B:518:THR:HG23	2.30	0.47
1:C:11:PRO:O	1:C:12:LEU:HD23	2.14	0.47
1:C:204:ARG:O	1:C:205:HIS:CB	2.63	0.47
1:C:247:ASP:N	1:C:247:ASP:OD1	2.46	0.47
1:C:484:LEU:CB	1:C:548:THR:HG22	2.40	0.47
1:D:26:TYR:CZ	1:D:79:VAL:HA	2.50	0.47
1:D:674:VAL:HG11	1:D:679:ALA:N	2.30	0.47
1:B:86:GLN:HE22	1:B:172:ARG:H	1.63	0.47
1:B:124:ARG:HD3	1:B:133:TYR:CD2	2.50	0.47
1:B:682:ARG:HE	1:B:716:LEU:HD13	1.78	0.47
1:C:706:LEU:HG	1:C:710:GLU:OE2	2.15	0.47
1:D:714:LEU:O	1:D:714:LEU:HG	2.13	0.47
1:A:469:ASP:O	1:A:471:VAL:N	2.47	0.47
1:A:512:ARG:NH1	1:A:588:SER:HB3	2.30	0.47
1:A:537:MET:HE2	1:A:537:MET:HB3	1.54	0.47
1:A:549:GLU:HG3	1:A:550:VAL:HG23	1.96	0.47
1:B:199:ALA:O	1:B:200:VAL:HB	2.15	0.47
1:B:507:PHE:CD1	1:B:560:LEU:HB3	2.50	0.47
1:B:544:GLU:HB2	1:B:545:ARG:NH2	2.30	0.47
1:B:642:PRO:O	1:B:656:TYR:OH	2.26	0.47
1:C:128:PRO:CD	1:C:275:SER:HB2	2.44	0.47
1:C:208:ILE:HG13	1:C:209:ASP:N	2.21	0.47
1:C:599:ALA:HB2	1:C:759:ALA:HB2	1.97	0.47
1:D:651:TRP:NE1	1:D:683:ALA:HA	2.29	0.47
1:A:186:TYR:OH	1:A:228:ARG:HD2	2.14	0.47
1:B:449:ASP:O	1:B:452:LEU:N	2.46	0.47
1:C:32:ARG:O	1:C:164:ARG:NH2	2.47	0.47
1:D:569:ILE:HD13	1:D:574:GLN:HB3	1.96	0.47
1:D:585:TYR:CD1	1:D:637:ILE:HG21	2.50	0.47
1:A:474:LEU:HG	1:A:529:MET:CE	2.45	0.47
1:B:366:ASP:O	1:B:370:SER:HB2	2.15	0.47
1:B:580:ALA:O	1:B:664:ARG:HD3	2.15	0.47
1:C:580:ALA:O	1:C:664:ARG:HD3	2.15	0.47
1:D:678:SER:OG	1:D:721:GLY:HA3	2.15	0.47
1:A:339:ARG:HG2	1:A:408:ARG:HH22	1.77	0.47
1:A:658:ASP:OD2	1:A:664:ARG:NH2	2.48	0.47
1:B:11:PRO:HB3	1:C:7:PHE:CD2	2.51	0.47
1:B:26:TYR:CE2	1:B:165:SER:HB3	2.50	0.47
1:B:400:LEU:HD13	1:B:400:LEU:HA	1.70	0.47
1:B:552:PRO:HG2	1:B:555:ALA:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:TYR:CZ	1:C:79:VAL:HA	2.49	0.47
1:C:375:LYS:O	1:C:378:THR:HG22	2.15	0.47
1:C:458:ILE:HD11	1:C:629:TRP:HB2	1.97	0.47
1:D:239:VAL:HG12	1:D:251:LEU:HD21	1.97	0.46
1:D:283:ASP:HA	1:D:287:THR:CB	2.43	0.46
1:D:337:LYS:O	1:D:341:ILE:HG13	2.15	0.46
1:D:339:ARG:HG2	1:D:408:ARG:NH2	2.30	0.46
1:D:605:PRO:HA	1:D:613:VAL:HG22	1.97	0.46
1:A:537:MET:HB2	1:A:538:PRO:HD3	1.96	0.46
1:A:665:ILE:H	1:A:665:ILE:HD13	1.80	0.46
1:B:539:ARG:NH1	1:B:543:PHE:HD1	2.14	0.46
1:B:688:ARG:HD3	1:B:692:ARG:HH22	1.80	0.46
1:C:601:GLN:HG2	1:C:622:GLU:HG2	1.97	0.46
1:C:728:ARG:HD3	1:C:729:TYR:N	2.30	0.46
1:D:380:THR:HG22	1:D:384:LEU:HD22	1.97	0.46
1:D:415:PRO:HA	1:D:420:ARG:CZ	2.45	0.46
1:A:339:ARG:CG	1:A:408:ARG:HH22	2.28	0.46
1:B:38:LEU:H	1:B:227:MET:HE1	1.79	0.46
1:B:455:GLN:HG2	1:B:624:LEU:O	2.15	0.46
1:B:474:LEU:HG	1:B:529:MET:HE1	1.97	0.46
1:C:148:GLU:CD	1:C:195:ARG:HH12	2.22	0.46
1:D:208:ILE:HG23	1:D:209:ASP:N	2.28	0.46
1:D:282:ASP:N	1:D:282:ASP:OD1	2.48	0.46
1:B:267:LEU:CD1	1:B:294:VAL:HG13	2.46	0.46
1:B:388:ALA:HA	1:B:406:TYR:OH	2.15	0.46
1:C:284:ALA:O	1:C:286:MET:N	2.48	0.46
1:C:349:TRP:CD1	1:C:349:TRP:C	2.94	0.46
1:C:396:LEU:HD11	1:C:403:GLN:HA	1.97	0.46
1:D:68:VAL:CG1	1:D:101:MET:HE3	2.45	0.46
1:D:162:LEU:HD23	1:D:162:LEU:HA	1.50	0.46
1:D:538:PRO:CB	1:D:550:VAL:HG22	2.44	0.46
1:D:615:ARG:HG2	1:D:616:GLY:N	2.30	0.46
1:A:538:PRO:HB2	1:A:550:VAL:HG13	1.97	0.46
1:A:610:PRO:O	1:A:739:ARG:HB2	2.15	0.46
1:B:280:LEU:HD12	1:B:280:LEU:HA	1.77	0.46
1:B:507:PHE:CZ	1:B:511:TRP:HD1	2.33	0.46
1:B:542:ARG:HD2	1:B:544:GLU:O	2.15	0.46
1:C:442:THR:HG22	1:C:626:LEU:HD21	1.96	0.46
1:D:239:VAL:HA	1:D:291:ARG:NH1	2.30	0.46
1:A:101:MET:HE3	1:A:101:MET:HA	1.96	0.46
1:B:161:ARG:HA	1:B:170:TRP:HH2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:ARG:HG2	1:B:720:ALA:CB	2.44	0.46
1:C:231:MET:HE3	1:C:231:MET:HB2	1.82	0.46
1:D:212:LYS:HB3	1:D:213:THR:H	1.47	0.46
1:A:669:THR:HG22	1:A:732:LEU:HD13	1.98	0.46
1:B:337:LYS:HE2	1:B:358:PHE:CD1	2.51	0.46
1:C:665:ILE:HG12	1:C:752:SER:HB2	1.98	0.46
1:D:26:TYR:O	1:D:93:THR:HA	2.16	0.46
1:D:457:GLY:C	1:D:626:LEU:HB2	2.41	0.46
1:D:482:HIS:HA	1:D:493:SER:OG	2.16	0.46
1:C:452:LEU:HD11	1:C:499:LEU:CD2	2.46	0.46
1:C:522:ASP:OD1	1:C:522:ASP:N	2.47	0.46
1:C:541:ALA:O	1:C:542:ARG:C	2.59	0.46
1:C:585:TYR:HA	1:C:592:THR:HG21	1.98	0.46
1:C:669:THR:CG2	1:C:751:ARG:HH22	2.29	0.46
1:C:690:MET:HE3	1:C:690:MET:HB2	1.76	0.46
1:D:537:MET:HB2	1:D:538:PRO:HD3	1.98	0.46
1:D:636:THR:CG2	1:D:675:GLU:HG2	2.45	0.46
1:A:71:LEU:HD12	1:A:310:ALA:O	2.15	0.46
1:A:445:PRO:HD3	1:A:497:PHE:HE1	1.81	0.46
1:A:682:ARG:HA	1:A:682:ARG:HD3	1.52	0.46
1:D:448:ASP:OD2	1:D:449:ASP:N	2.49	0.46
1:D:544:GLU:HB2	1:D:545:ARG:HH22	1.81	0.46
1:A:5:GLU:OE2	1:A:311:LYS:HB2	2.15	0.46
1:A:110:VAL:CG2	1:A:235:LEU:HD12	2.45	0.46
1:A:441:PRO:O	1:A:444:VAL:HG22	2.15	0.46
1:A:537:MET:CB	1:A:538:PRO:HD3	2.46	0.46
1:B:688:ARG:NH1	1:B:740:GLU:OE2	2.49	0.46
1:C:164:ARG:HH11	1:C:164:ARG:HG3	1.79	0.46
1:C:549:GLU:HG3	1:C:550:VAL:HG23	1.97	0.46
1:D:148:GLU:OE1	1:D:195:ARG:NH1	2.49	0.46
1:D:645:PRO:HG3	1:D:656:TYR:OH	2.15	0.46
1:A:612:LEU:HB3	1:A:754:ARG:CD	2.39	0.46
1:B:139:VAL:HG21	1:B:293:ILE:HG23	1.98	0.46
1:B:445:PRO:HG3	1:B:497:PHE:CD1	2.51	0.46
1:B:445:PRO:HB2	1:B:446:SER:H	1.62	0.46
1:B:538:PRO:HB3	1:B:550:VAL:HG22	1.98	0.46
1:C:691:PHE:HD2	1:C:736:LEU:HD22	1.79	0.46
1:D:537:MET:HE2	1:D:537:MET:HB3	1.52	0.45
1:B:651:TRP:CH2	1:B:684:TRP:HB2	2.51	0.45
1:C:349:TRP:O	1:C:350:GLN:HB2	2.16	0.45
1:A:208:ILE:HG23	1:A:209:ASP:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:LYS:C	1:A:343:GLU:HG2	2.40	0.45
1:A:469:ASP:C	1:A:471:VAL:N	2.72	0.45
1:B:26:TYR:O	1:B:93:THR:HA	2.16	0.45
1:B:35:SER:O	1:B:223:HIS:CE1	2.69	0.45
1:D:247:ASP:OD1	1:D:247:ASP:N	2.48	0.45
1:D:634:PHE:HB3	1:D:730:LEU:HD22	1.99	0.45
1:B:576:VAL:HG13	1:B:756:CYS:CB	2.45	0.45
1:B:691:PHE:CE2	1:B:736:LEU:HD13	2.52	0.45
1:C:86:GLN:CD	1:C:172:ARG:HD3	2.40	0.45
1:C:331:THR:N	1:C:334:GLU:OE1	2.45	0.45
1:C:333:ILE:HD12	1:C:380:THR:HG23	1.97	0.45
1:D:163:ILE:O	1:D:164:ARG:HB2	2.14	0.45
1:A:319:MET:HE2	1:A:319:MET:HB3	1.59	0.45
1:A:542:ARG:HE	1:A:547:LEU:HD12	1.80	0.45
1:B:417:ILE:HG13	1:B:421:ARG:CZ	2.47	0.45
1:C:612:LEU:HB3	1:C:754:ARG:CD	2.43	0.45
1:C:682:ARG:HB2	1:C:686:LEU:HB2	1.99	0.45
1:D:610:PRO:HB2	1:D:739:ARG:HA	1.98	0.45
1:D:685:HIS:O	1:D:688:ARG:HB2	2.17	0.45
1:B:78:THR:OG1	1:B:93:THR:HG21	2.16	0.45
1:B:689:LEU:HD13	1:B:709:ALA:HA	1.99	0.45
1:D:284:ALA:C	1:D:286:MET:H	2.22	0.45
1:D:682:ARG:NH2	1:D:716:LEU:HD13	2.31	0.45
1:D:682:ARG:HA	1:D:682:ARG:HD3	1.49	0.45
1:D:682:ARG:HB3	1:D:683:ALA:H	1.46	0.45
1:B:221:TYR:N	1:B:221:TYR:CD1	2.84	0.45
1:B:274:PRO:O	1:B:277:VAL:HG22	2.17	0.45
1:B:493:SER:OG	1:B:494:ALA:N	2.49	0.45
1:D:204:ARG:O	1:D:205:HIS:CB	2.65	0.45
1:D:692:ARG:NE	1:D:737:ALA:O	2.49	0.45
1:A:15:SER:HB2	1:A:300:LEU:HD22	1.98	0.45
1:A:84:ARG:O	1:A:84:ARG:HG3	2.15	0.45
1:A:460:LEU:HD23	1:A:460:LEU:HA	1.69	0.45
1:B:496:GLN:HA	1:B:553:VAL:HG13	1.97	0.45
1:A:452:LEU:HD22	1:A:452:LEU:HA	1.78	0.45
1:A:538:PRO:HB3	1:A:550:VAL:HG22	1.98	0.45
1:B:208:ILE:HG23	1:B:209:ASP:N	2.31	0.45
1:B:455:GLN:CD	1:B:766:TRP:HZ2	2.24	0.45
1:C:397:THR:OG1	1:C:399:ARG:HG3	2.16	0.45
1:D:65:LEU:HA	1:D:65:LEU:HD23	1.58	0.45
1:A:208:ILE:HD13	1:A:209:ASP:N	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ASP:N	1:A:469:ASP:OD1	2.48	0.45
1:A:618:SER:OG	1:A:619:GLY:N	2.49	0.45
1:C:100:ARG:HG3	1:C:100:ARG:NH1	2.31	0.45
1:D:7:PHE:HE2	1:A:11:PRO:HD3	1.81	0.45
1:A:163:ILE:HD12	1:A:170:TRP:CD2	2.51	0.45
1:A:251:LEU:O	1:A:291:ARG:NH2	2.40	0.45
1:A:413:LYS:O	1:A:415:PRO:HD3	2.17	0.45
1:B:118:ARG:HB2	1:B:289:LEU:HD13	1.98	0.45
1:B:223:HIS:NE2	1:B:227:MET:HE2	2.32	0.45
1:B:356:LEU:HA	1:B:356:LEU:HD23	1.67	0.45
1:B:681:ASN:OD1	1:B:682:ARG:N	2.50	0.45
1:C:728:ARG:HD3	1:C:729:TYR:H	1.82	0.45
1:A:84:ARG:O	1:A:85:SER:C	2.59	0.44
1:A:136:ALA:HB2	1:A:293:ILE:HD11	1.99	0.44
1:A:312:ARG:HD3	1:A:315:TYR:CE2	2.52	0.44
1:B:110:VAL:HA	1:B:228:ARG:NH1	2.28	0.44
1:B:662:ILE:HD12	1:B:662:ILE:H	1.81	0.44
1:D:11:PRO:C	1:D:12:LEU:HD23	2.42	0.44
1:A:213:THR:O	1:A:213:THR:OG1	2.34	0.44
1:C:600:SER:HB3	1:C:732:LEU:HD21	1.99	0.44
1:D:59:GLU:HG2	1:D:262:ASN:HB3	2.00	0.44
1:D:369:GLY:O	1:D:371:SER:N	2.46	0.44
1:D:448:ASP:O	1:D:450:ALA:N	2.50	0.44
1:D:522:ASP:OD1	1:D:522:ASP:N	2.51	0.44
1:D:710:GLU:HG2	1:D:715:ARG:HG3	1.99	0.44
1:A:28:PRO:HG2	1:A:31:GLN:HG2	1.98	0.44
1:A:482:HIS:HA	1:A:493:SER:HB2	1.98	0.44
1:B:417:ILE:HD12	1:B:417:ILE:HA	1.83	0.44
1:C:78:THR:OG1	1:C:93:THR:HG21	2.18	0.44
1:C:551:PRO:HB2	1:C:552:PRO:CD	2.48	0.44
1:C:557:GLN:O	1:C:561:LYS:HD3	2.16	0.44
1:D:417:ILE:O	1:D:419:ALA:N	2.46	0.44
1:D:417:ILE:HD12	1:D:417:ILE:HA	1.73	0.44
1:D:700:GLU:HG2	1:D:704:LYS:HE3	1.98	0.44
1:B:104:LEU:O	1:B:108:THR:HG23	2.18	0.44
1:B:212:LYS:HB3	1:B:213:THR:H	1.45	0.44
1:B:320:PHE:HD1	1:B:320:PHE:O	2.00	0.44
1:B:352:SER:O	1:B:353:GLU:C	2.61	0.44
1:B:396:LEU:CD1	1:B:403:GLN:HG2	2.45	0.44
1:B:413:LYS:HD3	1:B:544:GLU:OE1	2.16	0.44
1:B:452:LEU:HB3	1:B:498:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:GLU:OE2	1:C:232:ARG:NH2	2.50	0.44
1:C:452:LEU:HD22	1:C:452:LEU:HA	1.80	0.44
1:C:615:ARG:HG2	1:C:616:GLY:N	2.32	0.44
1:D:165:SER:O	1:D:166:TYR:HB2	2.17	0.44
1:D:337:LYS:HE3	1:D:337:LYS:HB2	1.57	0.44
1:D:530:THR:O	1:D:539:ARG:NH1	2.51	0.44
1:A:165:SER:O	1:A:166:TYR:HB2	2.17	0.44
1:A:530:THR:O	1:A:539:ARG:HD2	2.18	0.44
1:A:584:VAL:HG13	1:A:591:LEU:HD13	1.99	0.44
1:B:112:HIS:O	1:B:116:ARG:HB2	2.17	0.44
1:C:496:GLN:HG2	1:C:553:VAL:HG22	2.00	0.44
1:D:348:GLU:O	1:D:348:GLU:HG2	2.18	0.44
1:D:416:ASP:HB2	1:D:417:ILE:O	2.18	0.44
1:D:617:LYS:CB	1:D:620:LEU:HB2	2.44	0.44
1:D:648:ASN:C	1:D:650:SER:N	2.74	0.44
1:A:273:PRO:HG2	1:A:276:VAL:CG2	2.48	0.44
1:A:710:GLU:HA	1:A:714:LEU:H	1.83	0.44
1:B:372:SER:OG	1:B:375:LYS:HB3	2.18	0.44
1:B:682:ARG:HB3	1:B:683:ALA:H	1.49	0.44
1:C:71:LEU:HD12	1:C:310:ALA:O	2.18	0.44
1:D:333:ILE:HD12	1:D:380:THR:HG23	2.00	0.44
1:B:122:LEU:HD22	1:B:129:SER:OG	2.17	0.44
1:B:416:ASP:HB2	1:B:417:ILE:H	1.56	0.44
1:B:418:VAL:HA	1:B:421:ARG:CD	2.48	0.44
1:B:488:GLU:CD	1:B:489:THR:HG22	2.43	0.44
1:B:537:MET:HB3	1:B:537:MET:HE2	1.72	0.44
1:B:561:LYS:HG2	1:B:769:PHE:CE1	2.52	0.44
1:C:26:TYR:O	1:C:93:THR:HA	2.18	0.44
1:C:161:ARG:HA	1:C:170:TRP:HH2	1.81	0.44
1:A:5:GLU:O	1:A:7:PHE:N	2.51	0.44
1:A:356:LEU:HD23	1:A:356:LEU:HA	1.59	0.44
1:A:650:SER:OG	1:A:651:TRP:N	2.51	0.44
1:B:232:ARG:HD3	1:B:236:ARG:CZ	2.47	0.44
1:B:605:PRO:HA	1:B:735:ALA:HB2	2.00	0.44
1:C:109:THR:HG22	1:C:228:ARG:HE	1.82	0.44
1:C:496:GLN:HA	1:C:553:VAL:CG1	2.42	0.44
1:D:186:TYR:CZ	1:D:205:HIS:HD2	2.35	0.44
1:D:385:LEU:CD2	1:D:396:LEU:HB3	2.42	0.44
1:D:400:LEU:HD13	1:D:400:LEU:HA	1.62	0.44
1:A:387:PHE:CE2	1:A:427:LEU:HG	2.53	0.44
1:A:452:LEU:HB3	1:A:498:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:GLN:O	1:A:566:SER:OG	2.33	0.44
1:A:638:GLU:O	1:A:668:LEU:HA	2.18	0.44
1:B:111:LEU:HD22	1:B:296:ALA:HB2	1.98	0.44
1:C:26:TYR:HD2	1:C:93:THR:HG22	1.83	0.44
1:C:44:LEU:HD21	1:C:65:LEU:HD21	1.98	0.44
1:D:57:GLU:HG2	1:D:58:PHE:CE2	2.53	0.43
1:D:163:ILE:HD11	1:D:179:TYR:CE1	2.53	0.43
1:D:482:HIS:CE1	1:D:494:ALA:HB2	2.53	0.43
1:D:561:LYS:HE2	1:D:771:PRO:HD2	2.00	0.43
1:A:168:ASP:HA	1:A:178:ARG:O	2.18	0.43
1:A:468:HIS:CE1	1:A:508:TYR:HB2	2.53	0.43
1:B:81:PRO:HG2	1:B:169:VAL:HG22	2.00	0.43
1:B:379:VAL:O	1:B:383:VAL:HG12	2.18	0.43
1:C:488:GLU:HG2	1:C:489:THR:N	2.33	0.43
1:D:187:LEU:HD23	1:D:187:LEU:HA	1.74	0.43
1:D:569:ILE:HB	1:D:578:ARG:NH1	2.33	0.43
1:D:569:ILE:CG2	1:D:574:GLN:HB3	2.47	0.43
1:D:625:GLU:OE1	1:D:628:ARG:NH1	2.52	0.43
1:D:679:ALA:HA	1:D:716:LEU:O	2.18	0.43
1:D:709:ALA:O	1:D:713:GLY:N	2.50	0.43
1:B:11:PRO:HB3	1:C:7:PHE:CE2	2.52	0.43
1:B:127:GLU:OE2	1:B:128:PRO:HD3	2.18	0.43
1:B:217:ASP:C	1:B:219:GLU:H	2.26	0.43
1:B:507:PHE:HB2	1:B:560:LEU:HD13	1.99	0.43
1:C:339:ARG:HG2	1:C:408:ARG:CZ	2.49	0.43
1:D:64:PHE:CZ	1:A:319:MET:HE3	2.53	0.43
1:D:231:MET:HE3	1:D:231:MET:HB2	1.77	0.43
1:D:433:PHE:CB	1:D:476:THR:HG22	2.49	0.43
1:D:571:ASP:O	1:D:572:LYS:C	2.62	0.43
1:D:638:GLU:O	1:D:668:LEU:HA	2.19	0.43
1:A:353:GLU:HB2	1:A:421:ARG:HE	1.83	0.43
1:A:390:PHE:CD1	1:A:390:PHE:C	2.96	0.43
1:A:743:TRP:CZ3	1:A:747:PHE:HE2	2.36	0.43
1:B:543:PHE:C	1:B:543:PHE:CD2	2.96	0.43
1:C:149:GLU:HG2	1:C:150:ASP:N	2.32	0.43
1:C:542:ARG:O	1:C:542:ARG:HG3	2.15	0.43
1:C:610:PRO:O	1:C:739:ARG:HB2	2.18	0.43
1:C:669:THR:HG21	1:C:736:LEU:HD12	1.99	0.43
1:D:7:PHE:CE2	1:A:11:PRO:HD3	2.53	0.43
1:D:11:PRO:O	1:D:12:LEU:HD23	2.19	0.43
1:D:13:SER:OG	1:D:16:GLN:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:PHE:O	1:D:269:ASN:N	2.51	0.43
1:D:418:VAL:N	1:D:421:ARG:HD2	2.31	0.43
1:D:571:ASP:O	1:D:574:GLN:N	2.51	0.43
1:D:650:SER:OG	1:D:651:TRP:N	2.50	0.43
1:D:710:GLU:HA	1:D:714:LEU:H	1.84	0.43
1:A:352:SER:O	1:A:354:SER:N	2.52	0.43
1:A:614:VAL:HG12	1:A:754:ARG:HH11	1.83	0.43
1:B:17:PHE:CE2	1:B:101:MET:HE2	2.54	0.43
1:C:331:THR:O	1:C:335:THR:HG23	2.18	0.43
1:C:433:PHE:CD1	1:C:476:THR:HG22	2.51	0.43
1:D:26:TYR:CD2	1:D:93:THR:HG22	2.50	0.43
1:D:29:PRO:HG3	1:D:80:GLU:HG3	2.00	0.43
1:D:78:THR:OG1	1:D:93:THR:HG21	2.18	0.43
1:D:352:SER:O	1:D:354:SER:N	2.52	0.43
1:A:23:GLN:OE1	1:A:92:MET:HG3	2.19	0.43
1:A:235:LEU:O	1:A:236:ARG:C	2.61	0.43
1:A:395:LYS:HG3	1:A:395:LYS:O	2.17	0.43
1:C:187:LEU:HD23	1:C:187:LEU:HA	1.66	0.43
1:D:186:TYR:CZ	1:D:205:HIS:CD2	3.06	0.43
1:D:320:PHE:C	1:D:320:PHE:CD1	2.95	0.43
1:D:666:GLY:O	1:D:751:ARG:HD2	2.18	0.43
1:B:228:ARG:HD3	1:B:228:ARG:C	2.43	0.43
1:C:162:LEU:HA	1:C:162:LEU:HD23	1.84	0.43
1:C:666:GLY:N	1:C:752:SER:HB3	2.34	0.43
1:D:92:MET:HE3	1:D:92:MET:HB3	1.59	0.43
1:D:565:ARG:O	1:D:568:GLY:N	2.51	0.43
1:A:149:GLU:OE1	1:A:151:MET:SD	2.77	0.43
1:A:156:HIS:ND1	1:A:177:ALA:HB3	2.34	0.43
1:A:482:HIS:HA	1:A:493:SER:CB	2.49	0.43
1:B:320:PHE:CD1	1:B:320:PHE:C	2.96	0.43
1:B:469:ASP:C	1:B:471:VAL:N	2.74	0.43
1:C:44:LEU:CD2	1:C:65:LEU:HD21	2.48	0.43
1:C:110:VAL:HG21	1:C:232:ARG:HA	2.00	0.43
1:C:139:VAL:HG22	1:C:297:ASN:OD1	2.19	0.43
1:C:164:ARG:HH11	1:C:164:ARG:CG	2.31	0.43
1:C:533:VAL:O	1:C:538:PRO:HD2	2.19	0.43
1:C:654:ASP:OD1	1:C:654:ASP:N	2.49	0.43
1:D:59:GLU:HG2	1:D:262:ASN:CB	2.49	0.43
1:D:353:GLU:HB2	1:D:421:ARG:HE	1.83	0.43
1:D:433:PHE:CE2	1:D:438:TRP:CD1	3.07	0.43
1:A:455:GLN:O	1:A:458:ILE:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ASP:O	1:A:472:VAL:HG23	2.19	0.43
1:D:339:ARG:HG2	1:D:408:ARG:NH1	2.33	0.43
1:A:113:GLU:OE1	1:A:232:ARG:NH2	2.52	0.43
1:A:223:HIS:HE1	1:A:227:MET:HE2	1.79	0.43
1:A:511:TRP:CZ3	1:A:519:ALA:HB3	2.54	0.43
1:B:455:GLN:NE2	1:B:766:TRP:HZ2	2.17	0.43
1:B:541:ALA:O	1:B:542:ARG:C	2.61	0.43
1:C:638:GLU:O	1:C:668:LEU:HA	2.19	0.43
1:A:15:SER:O	1:A:19:SER:OG	2.36	0.43
1:A:551:PRO:HB2	1:A:552:PRO:CD	2.47	0.43
1:C:576:VAL:HG13	1:C:756:CYS:HB2	2.00	0.43
1:D:11:PRO:HB3	1:A:7:PHE:CE2	2.54	0.42
1:D:59:GLU:HG2	1:D:262:ASN:CG	2.43	0.42
1:D:615:ARG:HG2	1:D:616:GLY:H	1.84	0.42
1:A:477:ARG:HD3	1:A:542:ARG:N	2.28	0.42
1:B:87:VAL:HG13	1:B:88:PRO:O	2.19	0.42
1:B:417:ILE:C	1:B:419:ALA:N	2.77	0.42
1:B:468:HIS:NE2	1:B:521:ILE:HG21	2.34	0.42
1:B:554:GLU:HA	1:B:557:GLN:HG3	2.01	0.42
1:C:385:LEU:N	1:C:386:PRO:CD	2.82	0.42
1:C:684:TRP:HE1	1:C:742:GLU:HA	1.83	0.42
1:D:172:ARG:H	1:D:172:ARG:HD3	1.84	0.42
1:D:268:PHE:O	1:D:270:SER:N	2.52	0.42
1:D:391:GLN:OE1	1:D:542:ARG:NH1	2.51	0.42
1:B:72:ARG:NH1	1:B:90:LYS:HA	2.34	0.42
1:B:106:LEU:HB3	1:B:231:MET:HE1	2.00	0.42
1:B:470:ILE:H	1:B:470:ILE:HG12	1.57	0.42
1:B:522:ASP:OD1	1:B:522:ASP:N	2.52	0.42
1:C:760:TRP:CZ2	1:C:764:THR:HG21	2.54	0.42
1:D:7:PHE:C	1:D:7:PHE:HD2	2.25	0.42
1:D:123:THR:O	1:D:123:THR:OG1	2.33	0.42
1:D:235:LEU:O	1:D:238:ALA:N	2.49	0.42
1:D:604:THR:O	1:D:613:VAL:HG13	2.19	0.42
1:B:59:GLU:HG2	1:B:262:ASN:CB	2.49	0.42
1:B:447:CYS:HB2	1:B:494:ALA:HB1	2.01	0.42
1:B:520:GLY:O	1:B:523:GLY:N	2.53	0.42
1:B:709:ALA:CB	1:B:714:LEU:HB2	2.49	0.42
1:D:379:VAL:O	1:D:383:VAL:HG12	2.19	0.42
1:A:232:ARG:HD3	1:A:236:ARG:NH2	2.35	0.42
1:A:366:ASP:O	1:A:370:SER:HB2	2.19	0.42
1:A:565:ARG:O	1:A:566:SER:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:VAL:HB	1:A:667:ASN:ND2	2.35	0.42
1:B:119:ALA:O	1:B:122:LEU:HB2	2.19	0.42
1:C:433:PHE:CE2	1:C:438:TRP:NE1	2.87	0.42
1:C:561:LYS:HE3	1:C:769:PHE:HA	2.01	0.42
1:C:617:LYS:O	1:C:618:SER:C	2.62	0.42
1:D:26:TYR:HB3	1:D:93:THR:HG22	2.02	0.42
1:D:59:GLU:H	1:D:59:GLU:HG3	1.46	0.42
1:D:244:LYS:HA	1:D:248:ASP:OD2	2.20	0.42
1:D:356:LEU:HD23	1:D:356:LEU:HA	1.88	0.42
1:A:114:GLU:HB3	1:A:292:LEU:HD23	2.01	0.42
1:A:139:VAL:HG21	1:A:293:ILE:HG23	2.00	0.42
1:A:337:LYS:O	1:A:341:ILE:HG13	2.20	0.42
1:B:740:GLU:HB3	1:B:741:GLU:H	1.66	0.42
1:C:105:LEU:HD13	1:C:105:LEU:HA	1.80	0.42
1:C:183:ILE:HD12	1:C:183:ILE:N	2.24	0.42
1:C:492:SER:O	1:C:496:GLN:HG3	2.19	0.42
1:D:11:PRO:HB3	1:A:7:PHE:CD2	2.54	0.42
1:D:565:ARG:O	1:D:566:SER:C	2.62	0.42
1:A:162:LEU:HD23	1:A:162:LEU:HA	1.65	0.42
1:B:235:LEU:O	1:B:236:ARG:C	2.63	0.42
1:C:128:PRO:O	1:C:131:TRP:HB3	2.19	0.42
1:C:280:LEU:C	1:C:282:ASP:N	2.77	0.42
1:C:437:PRO:HB2	1:C:460:LEU:CD1	2.50	0.42
1:D:386:PRO:O	1:D:389:MET:N	2.53	0.42
1:D:734:ALA:O	1:D:736:LEU:N	2.44	0.42
1:A:26:TYR:O	1:A:93:THR:HA	2.20	0.42
1:A:133:TYR:CZ	1:A:137:LEU:HD11	2.55	0.42
1:A:511:TRP:CE3	1:A:521:ILE:HD11	2.54	0.42
1:B:58:PHE:HE2	1:B:405:ARG:HD3	1.81	0.42
1:B:247:ASP:OD1	1:B:247:ASP:N	2.50	0.42
1:D:390:PHE:CD1	1:D:390:PHE:C	2.98	0.42
1:A:122:LEU:HD22	1:A:129:SER:OG	2.19	0.42
1:A:300:LEU:HA	1:A:300:LEU:HD23	1.63	0.42
1:A:341:ILE:HG12	1:A:349:TRP:CE2	2.55	0.42
1:A:372:SER:OG	1:A:373:ALA:N	2.50	0.42
1:A:433:PHE:CB	1:A:476:THR:HG22	2.48	0.42
1:A:542:ARG:O	1:A:542:ARG:HG3	2.12	0.42
1:B:28:PRO:HG2	1:B:31:GLN:HG2	2.01	0.42
1:B:45:LEU:HD21	1:B:107:LEU:HD13	2.02	0.42
1:B:623:THR:HG22	1:B:634:PHE:CZ	2.54	0.42
1:B:639:HIS:HB3	1:B:641:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:LEU:HB3	1:C:16:GLN:HG3	2.02	0.42
1:C:186:TYR:OH	1:C:228:ARG:HD2	2.19	0.42
1:C:460:LEU:HD21	1:C:501:ALA:HB1	2.02	0.42
1:C:496:GLN:CG	1:C:553:VAL:HG22	2.50	0.42
1:C:537:MET:HB3	1:C:537:MET:HE2	1.51	0.42
1:C:631:ASP:C	1:C:633:ALA:N	2.78	0.42
1:D:17:PHE:CD1	1:D:307:VAL:HG21	2.55	0.42
1:D:23:GLN:HG3	1:D:90:LYS:HD3	2.02	0.42
1:D:535:GLU:HG3	1:D:536:GLY:N	2.34	0.42
1:A:346:LEU:HB3	1:A:347:ASP:H	1.69	0.42
1:A:433:PHE:CD2	1:A:476:THR:HG22	2.54	0.42
1:B:112:HIS:NE2	1:B:140:THR:HG23	2.35	0.42
1:B:216:VAL:HG12	1:B:217:ASP:H	1.85	0.42
1:B:315:TYR:O	1:B:319:MET:HG3	2.20	0.42
1:B:337:LYS:HE3	1:B:337:LYS:HB2	1.30	0.42
1:B:357:HIS:O	1:B:360:VAL:HB	2.20	0.42
1:B:674:VAL:HG11	1:B:679:ALA:H	1.85	0.42
1:C:196:ASP:OD1	1:C:197:PRO:HD2	2.20	0.42
1:C:300:LEU:HD23	1:C:300:LEU:HA	1.68	0.42
1:C:610:PRO:HB2	1:C:738:GLN:O	2.19	0.42
1:C:628:ARG:CA	1:C:631:ASP:HB2	2.33	0.42
1:C:651:TRP:CH2	1:C:684:TRP:HB2	2.54	0.42
1:D:292:LEU:HD12	1:D:292:LEU:HA	1.87	0.42
1:D:639:HIS:HA	1:D:667:ASN:O	2.20	0.42
1:D:671:LEU:HD23	1:D:671:LEU:HA	1.67	0.42
1:A:337:LYS:HZ2	1:A:362:GLU:CD	2.28	0.42
1:A:445:PRO:HG3	1:A:497:PHE:HD1	1.84	0.42
1:A:655:LEU:HB2	1:A:656:TYR:CD1	2.54	0.42
1:B:221:TYR:N	1:B:221:TYR:HD1	2.17	0.42
1:C:764:THR:N	1:C:765:PRO:HD2	2.35	0.42
1:D:555:ALA:HA	1:D:558:SER:OG	2.20	0.41
1:D:569:ILE:HB	1:D:578:ARG:CZ	2.50	0.41
1:D:610:PRO:HB2	1:D:738:GLN:O	2.19	0.41
1:A:44:LEU:HA	1:A:44:LEU:HD22	1.80	0.41
1:A:152:ARG:HH21	1:A:152:ARG:HD3	1.64	0.41
1:A:445:PRO:HG3	1:A:497:PHE:CD1	2.55	0.41
1:A:630:ASN:O	1:A:632:GLU:N	2.53	0.41
1:A:665:ILE:HG12	1:A:752:SER:HB2	2.02	0.41
1:A:690:MET:O	1:A:694:LEU:HD12	2.20	0.41
1:B:342:LYS:HG3	1:C:80:GLU:OE1	2.18	0.41
1:B:631:ASP:C	1:B:633:ALA:H	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:GLU:C	1:C:7:PHE:N	2.77	0.41
1:C:420:ARG:O	1:C:423:VAL:HB	2.19	0.41
1:C:682:ARG:HD3	1:C:682:ARG:HA	1.57	0.41
1:D:218:LEU:O	1:D:222:ARG:HG3	2.20	0.41
1:D:239:VAL:HG21	1:D:292:LEU:HD22	2.02	0.41
1:D:417:ILE:C	1:D:419:ALA:N	2.78	0.41
1:D:679:ALA:HB2	1:D:720:ALA:HA	2.01	0.41
1:A:35:SER:N	1:A:99:GLN:OE1	2.35	0.41
1:A:155:GLU:HG3	1:A:174:LYS:HE2	2.02	0.41
1:A:690:MET:HB2	1:A:690:MET:HE3	1.70	0.41
1:B:128:PRO:HG3	1:B:275:SER:HB2	2.03	0.41
1:B:631:ASP:C	1:B:633:ALA:N	2.78	0.41
1:C:365:LEU:O	1:C:369:GLY:N	2.37	0.41
1:C:429:GLN:HG2	1:C:480:ALA:CB	2.50	0.41
1:C:569:ILE:HG12	1:C:574:GLN:CD	2.45	0.41
1:D:13:SER:O	1:D:14:VAL:C	2.62	0.41
1:D:217:ASP:C	1:D:219:GLU:N	2.77	0.41
1:D:451:THR:O	1:D:455:GLN:HG3	2.20	0.41
1:D:488:GLU:HG2	1:D:489:THR:N	2.34	0.41
1:D:655:LEU:HD23	1:D:745:ALA:HA	2.01	0.41
1:D:679:ALA:CB	1:D:720:ALA:HA	2.50	0.41
1:A:34:TYR:CD2	1:A:224:LEU:HD12	2.55	0.41
1:A:38:LEU:HD13	1:A:230:GLN:OE1	2.19	0.41
1:A:742:GLU:HG3	1:A:743:TRP:H	1.85	0.41
1:B:23:GLN:HG3	1:B:90:LYS:HD3	2.03	0.41
1:B:299:LEU:HA	1:B:303:VAL:CG2	2.50	0.41
1:B:387:PHE:CD2	1:B:427:LEU:HG	2.56	0.41
1:B:448:ASP:O	1:B:450:ALA:N	2.54	0.41
1:C:432:ARG:HA	1:C:435:GLU:OE1	2.20	0.41
1:C:511:TRP:CD2	1:C:521:ILE:HG12	2.55	0.41
1:C:595:LEU:HD23	1:C:595:LEU:HA	1.73	0.41
1:D:159:TYR:OH	1:D:171:SER:HA	2.21	0.41
1:A:17:PHE:CE1	1:A:307:VAL:HG21	2.56	0.41
1:A:253:THR:O	1:A:256:ASP:HB2	2.20	0.41
1:A:542:ARG:HD3	1:A:547:LEU:N	2.32	0.41
1:B:190:TYR:CD1	1:B:190:TYR:C	2.99	0.41
1:B:381:SER:OG	1:B:403:GLN:OE1	2.36	0.41
1:B:682:ARG:HD3	1:B:682:ARG:HA	1.62	0.41
1:C:1:MET:HA	1:C:4:LYS:CB	2.41	0.41
1:C:328:GLN:N	1:C:328:GLN:CD	2.78	0.41
1:D:67:THR:H	1:D:100:ARG:NH1	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:ASP:HB3	1:D:91:VAL:HG22	2.03	0.41
1:D:235:LEU:O	1:D:236:ARG:C	2.63	0.41
1:D:507:PHE:O	1:D:511:TRP:HB2	2.20	0.41
1:A:74:ILE:HD12	1:A:74:ILE:HA	1.78	0.41
1:A:153:TYR:CE1	1:B:134:ASN:HB3	2.55	0.41
1:A:583:PRO:HD3	1:A:660:GLU:OE1	2.21	0.41
1:A:617:LYS:HB3	1:A:620:LEU:HB2	2.02	0.41
1:B:151:MET:O	1:B:157:ARG:HD3	2.20	0.41
1:C:713:GLY:O	1:C:716:LEU:HG	2.20	0.41
1:D:12:LEU:HD12	1:D:17:PHE:HA	2.02	0.41
1:D:44:LEU:HD21	1:D:65:LEU:HD21	2.02	0.41
1:D:565:ARG:HH21	1:D:771:PRO:CB	2.33	0.41
1:B:41:ILE:H	1:B:41:ILE:HG12	1.66	0.41
1:B:66:GLY:HA3	1:B:100:ARG:NH1	2.35	0.41
1:B:183:ILE:H	1:B:183:ILE:CD1	2.14	0.41
1:B:185:TYR:O	1:B:189:SER:OG	2.26	0.41
1:B:477:ARG:HD3	1:B:541:ALA:HA	2.02	0.41
1:B:551:PRO:HB2	1:B:552:PRO:CD	2.49	0.41
1:B:642:PRO:HD3	1:B:651:TRP:CH2	2.56	0.41
1:C:429:GLN:HG2	1:C:480:ALA:HB2	2.02	0.41
1:C:688:ARG:CZ	1:C:740:GLU:OE2	2.68	0.41
1:D:38:LEU:N	1:D:227:MET:CE	2.84	0.41
1:D:153:TYR:CD2	1:C:134:ASN:HB3	2.56	0.41
1:D:739:ARG:HG2	1:D:740:GLU:O	2.21	0.41
1:A:23:GLN:HA	1:A:90:LYS:O	2.21	0.41
1:A:86:GLN:HE21	1:A:173:ASN:ND2	2.18	0.41
1:A:255:THR:O	1:A:259:GLN:HG3	2.21	0.41
1:A:544:GLU:O	1:A:545:ARG:C	2.62	0.41
1:A:634:PHE:CD1	1:A:634:PHE:N	2.88	0.41
1:B:154:GLY:O	1:B:157:ARG:HB2	2.21	0.41
1:B:249:ILE:N	1:B:249:ILE:HD12	2.35	0.41
1:B:337:LYS:HE2	1:B:358:PHE:CE1	2.56	0.41
1:B:390:PHE:HD2	1:B:476:THR:OG1	2.02	0.41
1:B:599:ALA:O	1:B:758:LEU:HD23	2.21	0.41
1:C:212:LYS:C	1:C:213:THR:HG23	2.46	0.41
1:C:247:ASP:CG	1:C:248:ASP:H	2.28	0.41
1:C:414:ASP:HB3	1:C:419:ALA:HB1	2.03	0.41
1:C:641:ALA:N	1:C:667:ASN:OD1	2.51	0.41
1:C:671:LEU:HD11	1:C:691:PHE:HE1	1.85	0.41
1:C:760:TRP:CE2	1:C:764:THR:HG21	2.56	0.41
1:D:517:SER:C	1:D:519:ALA:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:SER:C	1:A:86:GLN:HG3	2.46	0.41
1:A:87:VAL:CG2	1:A:88:PRO:HD2	2.49	0.41
1:A:87:VAL:HG13	1:A:88:PRO:O	2.21	0.41
1:A:119:ALA:O	1:A:122:LEU:HB2	2.20	0.41
1:A:416:ASP:HB2	1:A:417:ILE:H	1.44	0.41
1:A:605:PRO:HG3	1:A:734:ALA:HB3	2.03	0.41
1:B:162:LEU:HD23	1:B:162:LEU:HA	1.61	0.41
1:B:312:ARG:HD3	1:B:315:TYR:CD2	2.55	0.41
1:B:596:LEU:HD13	1:B:669:THR:HA	2.02	0.41
1:B:628:ARG:HA	1:B:631:ASP:CB	2.41	0.41
1:C:172:ARG:HH11	1:C:172:ARG:HG3	1.84	0.41
1:D:66:GLY:HA2	1:A:322:ALA:HB1	2.03	0.41
1:D:355:LYS:HD2	1:D:359:ASP:OD2	2.21	0.41
1:D:391:GLN:HE21	1:D:391:GLN:HB3	1.62	0.41
1:D:482:HIS:ND1	1:D:494:ALA:HB2	2.36	0.41
1:D:740:GLU:HB3	1:D:741:GLU:H	1.68	0.41
1:A:17:PHE:CD1	1:A:307:VAL:HG21	2.56	0.41
1:A:228:ARG:HA	1:A:231:MET:HE3	2.03	0.41
1:A:330:LEU:HA	1:A:330:LEU:HD23	1.83	0.41
1:A:511:TRP:HH2	1:A:519:ALA:HB3	1.83	0.41
1:B:7:PHE:CD2	1:B:7:PHE:C	2.99	0.41
1:B:73:ASP:HB3	1:B:91:VAL:HG22	2.03	0.41
1:B:330:LEU:HD23	1:B:330:LEU:HA	1.75	0.41
1:B:618:SER:OG	1:B:619:GLY:N	2.54	0.41
1:B:720:ALA:HB1	1:B:723:ILE:HB	2.03	0.41
1:C:18:LEU:HA	1:C:18:LEU:HD23	1.72	0.41
1:C:86:GLN:NE2	1:C:172:ARG:HD3	2.36	0.41
1:C:207:PRO:C	1:C:208:ILE:HG22	2.46	0.41
1:C:349:TRP:CD1	1:C:349:TRP:O	2.74	0.41
1:C:523:GLY:HA2	1:C:526:ARG:NH2	2.36	0.41
1:C:630:ASN:O	1:C:632:GLU:N	2.54	0.41
1:C:639:HIS:HB3	1:C:641:ALA:O	2.21	0.41
1:C:665:ILE:H	1:C:665:ILE:HD13	1.86	0.41
1:D:337:LYS:NZ	1:D:362:GLU:CD	2.79	0.41
1:D:420:ARG:O	1:D:423:VAL:HB	2.20	0.41
1:D:563:GLN:O	1:D:566:SER:OG	2.39	0.41
1:A:31:GLN:NE2	1:A:95:ILE:O	2.54	0.41
1:A:168:ASP:OD1	1:A:180:ARG:N	2.38	0.41
1:B:44:LEU:HD22	1:B:44:LEU:HA	1.68	0.41
1:C:164:ARG:CG	1:C:164:ARG:NH1	2.83	0.41
1:C:600:SER:HA	1:C:603:SER:OG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:678:SER:OG	1:C:679:ALA:N	2.51	0.41
1:D:67:THR:H	1:D:100:ARG:HH12	1.69	0.40
1:D:396:LEU:HD13	1:D:397:THR:N	2.36	0.40
1:D:416:ASP:HB2	1:D:417:ILE:H	1.25	0.40
1:A:642:PRO:HD3	1:A:651:TRP:CE2	2.56	0.40
1:A:742:GLU:HG3	1:A:743:TRP:N	2.36	0.40
1:B:18:LEU:HB2	1:B:146:CYS:SG	2.61	0.40
1:B:404:ARG:HH11	1:B:404:ARG:HD2	1.72	0.40
1:B:488:GLU:OE1	1:B:489:THR:HG22	2.21	0.40
1:C:173:ASN:O	1:C:175:GLY:O	2.39	0.40
1:C:238:ALA:HB2	1:C:249:ILE:HD13	2.02	0.40
1:C:691:PHE:CD2	1:C:736:LEU:HD22	2.56	0.40
1:D:386:PRO:O	1:D:387:PHE:C	2.63	0.40
1:D:507:PHE:CD1	1:D:560:LEU:HD22	2.56	0.40
1:A:596:LEU:HD21	1:A:665:ILE:HG22	2.03	0.40
1:B:26:TYR:HD2	1:B:93:THR:HG22	1.85	0.40
1:D:26:TYR:CD1	1:D:163:ILE:HG22	2.55	0.40
1:D:417:ILE:C	1:D:419:ALA:H	2.29	0.40
1:D:437:PRO:HD3	1:D:479:PHE:CE2	2.57	0.40
1:D:496:GLN:CA	1:D:553:VAL:HG13	2.45	0.40
1:D:549:GLU:CG	1:D:550:VAL:HG23	2.49	0.40
1:D:596:LEU:HD13	1:D:669:THR:HA	2.03	0.40
1:A:469:ASP:O	1:A:470:ILE:C	2.63	0.40
1:A:475:LEU:HD21	1:A:504:CYS:SG	2.61	0.40
1:A:671:LEU:HD11	1:A:691:PHE:HE1	1.87	0.40
1:B:585:TYR:CD1	1:B:637:ILE:HG21	2.56	0.40
1:B:728:ARG:NE	1:B:728:ARG:HA	2.36	0.40
1:C:208:ILE:HG12	1:C:221:TYR:CE2	2.56	0.40
1:C:283:ASP:HA	1:C:287:THR:OG1	2.21	0.40
1:C:292:LEU:HD12	1:C:292:LEU:HA	1.84	0.40
1:C:349:TRP:O	1:C:350:GLN:CB	2.69	0.40
1:D:255:THR:O	1:D:256:ASP:C	2.65	0.40
1:D:320:PHE:HD1	1:D:320:PHE:O	2.05	0.40
1:D:584:VAL:HG13	1:D:591:LEU:HD13	2.04	0.40
1:A:549:GLU:O	1:A:550:VAL:HB	2.21	0.40
1:B:323:LEU:O	1:C:326:THR:HG21	2.22	0.40
1:B:331:THR:HG23	1:B:334:GLU:OE1	2.21	0.40
1:B:437:PRO:HG3	1:B:479:PHE:CE2	2.54	0.40
1:B:456:ALA:O	1:B:460:LEU:HG	2.21	0.40
1:B:734:ALA:O	1:B:738:GLN:HG3	2.22	0.40
1:C:151:MET:O	1:C:157:ARG:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:ARG:HA	1:C:231:MET:CE	2.47	0.40
1:C:320:PHE:C	1:C:320:PHE:CD1	2.98	0.40
1:C:404:ARG:HH11	1:C:404:ARG:HD2	1.73	0.40
1:C:565:ARG:O	1:C:566:SER:C	2.63	0.40
1:C:651:TRP:HE1	1:C:683:ALA:HA	1.83	0.40
1:C:706:LEU:HD12	1:C:714:LEU:HD23	2.04	0.40
1:D:161:ARG:O	1:D:162:LEU:O	2.40	0.40
1:D:686:LEU:HD21	1:D:712:GLN:HB3	2.04	0.40
1:A:65:LEU:HA	1:A:65:LEU:HD23	1.52	0.40
1:A:218:LEU:O	1:A:222:ARG:HG3	2.21	0.40
1:A:417:ILE:O	1:A:418:VAL:HB	2.22	0.40
1:A:447:CYS:HB2	1:A:494:ALA:HB1	2.03	0.40
1:A:760:TRP:HE3	1:A:761:ASP:OD1	2.03	0.40
1:B:507:PHE:CZ	1:B:511:TRP:CD1	3.09	0.40
1:B:597:LEU:HD22	1:B:623:THR:HB	2.04	0.40
1:C:84:ARG:O	1:C:85:SER:C	2.64	0.40
1:C:366:ASP:O	1:C:370:SER:HB2	2.21	0.40
1:C:482:HIS:HA	1:C:493:SER:CB	2.52	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]	1.94	0.26
1:D:84:ARG:N	1:C:211:ASP:OD2[4_457]	2.13	0.07
1:A:236:ARG:NH1	1:B:278:GLU:OE1[4_447]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	769/771 (100%)	613 (80%)	105 (14%)	51 (7%)	1 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	769/771 (100%)	605 (79%)	117 (15%)	47 (6%)	1	8
1	C	769/771 (100%)	612 (80%)	104 (14%)	53 (7%)	1	6
1	D	769/771 (100%)	609 (79%)	105 (14%)	55 (7%)	1	5
All	All	3076/3084 (100%)	2439 (79%)	431 (14%)	206 (7%)	1	7

All (206) 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	350	GLN
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	633	ALA
1	D	645	PRO
1	D	650	SER
1	D	682	ARG
1	D	727	ALA
1	A	4	LYS
1	A	36	TRP
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	350	GLN
1	A	353	GLU
1	A	444	VAL
1	A	551	PRO
1	A	552	PRO
1	A	565	ARG

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Mol	Chain	Res	Type
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	721	GLY
1	A	727	ALA
1	A	770	GLU
1	B	4	LYS
1	B	6	ILE
1	B	127	GLU
1	B	205	HIS
1	B	208	ILE
1	B	241	ALA
1	B	283	ASP
1	B	353	GLU
1	B	551	PRO
1	B	552	PRO
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	6	ILE
1	C	36	TRP
1	C	127	GLU
1	C	205	HIS
1	C	208	ILE
1	C	283	ASP
1	C	350	GLN
1	C	353	GLU
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

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Mol	Chain	Res	Type
1	C	727	ALA
1	C	770	GLU
1	D	6	ILE
1	D	211	ASP
1	D	241	ALA
1	D	417	ILE
1	D	444	VAL
1	D	450	ALA
1	D	467	GLY
1	D	587	HIS
1	D	631	ASP
1	D	685	HIS
1	D	695	SER
1	D	720	ALA
1	D	721	GLY
1	A	6	ILE
1	A	163	ILE
1	A	211	ASP
1	A	417	ILE
1	A	450	ALA
1	A	467	GLY
1	A	569	ILE
1	A	685	HIS
1	A	695	SER
1	A	718	SER
1	A	720	ALA
1	B	36	TRP
1	B	81	PRO
1	B	162	LEU
1	B	200	VAL
1	B	211	ASP
1	B	350	GLN
1	B	417	ILE
1	B	444	VAL
1	B	445	PRO
1	B	467	GLY
1	B	538	PRO
1	B	565	ARG
1	B	587	HIS
1	B	685	HIS
1	B	695	SER
1	B	721	GLY

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Mol	Chain	Res	Type
1	C	81	PRO
1	C	211	ASP
1	C	241	ALA
1	C	417	ILE
1	C	444	VAL
1	C	445	PRO
1	C	450	ALA
1	C	467	GLY
1	C	565	ARG
1	C	587	HIS
1	C	685	HIS
1	C	721	GLY
1	D	162	LEU
1	D	164	ARG
1	D	416	ASP
1	D	445	PRO
1	D	569	ILE
1	D	718	SER
1	D	770	GLU
1	A	162	LEU
1	A	445	PRO
1	A	538	PRO
1	A	587	HIS
1	B	450	ALA
1	B	569	ILE
1	B	631	ASP
1	B	718	SER
1	B	720	ALA
1	C	200	VAL
1	C	248	ASP
1	C	449	ASP
1	C	538	PRO
1	C	695	SER
1	C	720	ALA
1	D	81	PRO
1	D	620	LEU
1	A	81	PRO
1	A	566	SER
1	B	164	ARG
1	B	727	ALA
1	C	162	LEU
1	C	164	ARG

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Mol	Chain	Res	Type
1	C	281	GLU
1	C	392	ASP
1	C	448	ASP
1	C	569	ILE
1	C	620	LEU
1	D	466	GLY
1	D	519	ALA
1	D	736	LEU
1	A	166	TYR
1	A	248	ASP
1	A	392	ASP
1	A	519	ALA
1	A	537	MET
1	A	550	VAL
1	A	648	ASN
1	A	673	ALA
1	B	620	LEU
1	C	537	MET
1	C	632	GLU
1	C	648	ASN
1	C	718	SER
1	D	126	ASP
1	D	414	ASP
1	D	550	VAL
1	D	648	ASN
1	D	728	ARG
1	A	620	LEU
1	A	736	LEU
1	B	163	ILE
1	B	166	TYR
1	B	168	ASP
1	B	414	ASP
1	B	550	VAL
1	C	247	ASP
1	C	550	VAL
1	D	160	PRO
1	B	568	GLY
1	C	163	ILE
1	C	466	GLY
1	C	568	GLY
1	D	418	VAL
1	D	537	MET

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Mol	Chain	Res	Type
1	D	163	ILE
1	A	568	GLY
1	D	640	VAL
1	D	672	PRO
1	B	160	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	651/651 (100%)	561 (86%)	90 (14%)	3	14
1	B	651/651 (100%)	563 (86%)	88 (14%)	4	15
1	C	651/651 (100%)	547 (84%)	104 (16%)	2	10
1	D	651/651 (100%)	559 (86%)	92 (14%)	3	13
All	All	2604/2604 (100%)	2230 (86%)	374 (14%)	3	13

All (374) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3	THR
1	D	7	PHE
1	D	12	LEU
1	D	14	VAL
1	D	32	ARG
1	D	44	LEU
1	D	52	LEU
1	D	57	GLU
1	D	59	GLU
1	D	62	ILE
1	D	65	LEU
1	D	68	VAL
1	D	75	ASN
1	D	86	GLN
1	D	87	VAL
1	D	91	VAL

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Mol	Chain	Res	Type
1	D	99	GLN
1	D	104	LEU
1	D	105	LEU
1	D	106	LEU
1	D	109	THR
1	D	110	VAL
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	208	ILE
1	D	216	VAL
1	D	227	MET
1	D	243	VAL
1	D	249	ILE
1	D	251	LEU
1	D	262	ASN
1	D	275	SER
1	D	279	GLN
1	D	280	LEU
1	D	283	ASP
1	D	287	THR
1	D	292	LEU
1	D	305	VAL
1	D	323	LEU
1	D	328	GLN
1	D	339	ARG
1	D	342	LYS
1	D	348	GLU
1	D	349	TRP
1	D	350	GLN
1	D	365	LEU
1	D	378	THR

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Mol	Chain	Res	Type
1	D	383	VAL
1	D	384	LEU
1	D	391	GLN
1	D	394	THR
1	D	396	LEU
1	D	400	LEU
1	D	408	ARG
1	D	414	ASP
1	D	444	VAL
1	D	452	LEU
1	D	470	ILE
1	D	489	THR
1	D	511	TRP
1	D	514	SER
1	D	537	MET
1	D	542	ARG
1	D	545	ARG
1	D	569	ILE
1	D	591	LEU
1	D	593	ARG
1	D	594	LEU
1	D	618	SER
1	D	634	PHE
1	D	636	THR
1	D	654	ASP
1	D	665	ILE
1	D	682	ARG
1	D	692	ARG
1	D	705	THR
1	D	728	ARG
1	D	730	LEU
1	D	744	THR
1	D	754	ARG
1	D	764	THR
1	A	1	MET
1	A	3	THR
1	A	14	VAL
1	A	32	ARG
1	A	44	LEU
1	A	45	LEU
1	A	48	VAL
1	A	52	LEU

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Mol	Chain	Res	Type
1	A	57	GLU
1	A	62	ILE
1	A	63	CYS
1	A	64	PHE
1	A	65	LEU
1	A	68	VAL
1	A	75	ASN
1	A	86	GLN
1	A	91	VAL
1	A	98	GLN
1	A	99	GLN
1	A	104	LEU
1	A	105	LEU
1	A	109	THR
1	A	110	VAL
1	A	130	VAL
1	A	140	THR
1	A	144	SER
1	A	151	MET
1	A	157	ARG
1	A	163	ILE
1	A	167	TYR
1	A	172	ARG
1	A	176	GLU
1	A	183	ILE
1	A	198	ASP
1	A	208	ILE
1	A	216	VAL
1	A	227	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	305	VAL
1	A	323	LEU
1	A	328	GLN
1	A	348	GLU

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Mol	Chain	Res	Type
1	A	349	TRP
1	A	365	LEU
1	A	383	VAL
1	A	385	LEU
1	A	391	GLN
1	A	400	LEU
1	A	429	GLN
1	A	444	VAL
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	512	ARG
1	A	514	SER
1	A	542	ARG
1	A	545	ARG
1	A	547	LEU
1	A	566	SER
1	A	569	ILE
1	A	591	LEU
1	A	592	THR
1	A	594	LEU
1	A	609	THR
1	A	618	SER
1	A	623	THR
1	A	652	ASN
1	A	654	ASP
1	A	661	LEU
1	A	665	ILE
1	A	667	ASN
1	A	682	ARG
1	A	692	ARG
1	A	728	ARG
1	A	730	LEU
1	A	744	THR
1	A	758	LEU
1	A	764	THR
1	A	769	PHE
1	B	1	MET
1	B	3	THR

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Mol	Chain	Res	Type
1	B	7	PHE
1	B	14	VAL
1	B	44	LEU
1	B	45	LEU
1	B	52	LEU
1	B	53	ASP
1	B	62	ILE
1	B	64	PHE
1	B	65	LEU
1	B	68	VAL
1	B	86	GLN
1	B	87	VAL
1	B	91	VAL
1	B	98	GLN
1	B	99	GLN
1	B	101	MET
1	B	104	LEU
1	B	105	LEU
1	B	109	THR
1	B	110	VAL
1	B	130	VAL
1	B	157	ARG
1	B	163	ILE
1	B	167	TYR
1	B	176	GLU
1	B	183	ILE
1	B	198	ASP
1	B	200	VAL
1	B	208	ILE
1	B	213	THR
1	B	216	VAL
1	B	221	TYR
1	B	243	VAL
1	B	249	ILE
1	B	251	LEU
1	B	262	ASN
1	B	279	GLN
1	B	280	LEU
1	B	283	ASP
1	B	287	THR
1	B	292	LEU
1	B	305	VAL

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Mol	Chain	Res	Type
1	B	312	ARG
1	B	323	LEU
1	B	328	GLN
1	B	342	LYS
1	B	348	GLU
1	B	349	TRP
1	B	350	GLN
1	B	354	SER
1	B	383	VAL
1	B	384	LEU
1	B	391	GLN
1	B	394	THR
1	B	396	LEU
1	B	400	LEU
1	B	414	ASP
1	B	421	ARG
1	B	429	GLN
1	B	444	VAL
1	B	452	LEU
1	B	470	ILE
1	B	486	SER
1	B	489	THR
1	B	511	TRP
1	B	514	SER
1	B	542	ARG
1	B	543	PHE
1	B	545	ARG
1	B	546	ASP
1	B	547	LEU
1	B	566	SER
1	B	569	ILE
1	B	591	LEU
1	B	593	ARG
1	B	594	LEU
1	B	636	THR
1	B	654	ASP
1	B	665	ILE
1	B	682	ARG
1	B	692	ARG
1	B	705	THR
1	B	728	ARG
1	B	744	THR

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Mol	Chain	Res	Type
1	B	764	THR
1	B	769	PHE
1	C	1	MET
1	C	3	THR
1	C	14	VAL
1	C	38	LEU
1	C	44	LEU
1	C	45	LEU
1	C	52	LEU
1	C	57	GLU
1	C	62	ILE
1	C	64	PHE
1	C	65	LEU
1	C	68	VAL
1	C	75	ASN
1	C	86	GLN
1	C	87	VAL
1	C	91	VAL
1	C	99	GLN
1	C	105	LEU
1	C	106	LEU
1	C	109	THR
1	C	110	VAL
1	C	127	GLU
1	C	129	SER
1	C	130	VAL
1	C	140	THR
1	C	144	SER
1	C	157	ARG
1	C	163	ILE
1	C	164	ARG
1	C	165	SER
1	C	167	TYR
1	C	172	ARG
1	C	176	GLU
1	C	183	ILE
1	C	200	VAL
1	C	206	VAL
1	C	213	THR
1	C	216	VAL
1	C	243	VAL
1	C	249	ILE

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Mol	Chain	Res	Type
1	C	251	LEU
1	C	255	THR
1	C	262	ASN
1	C	275	SER
1	C	279	GLN
1	C	280	LEU
1	C	282	ASP
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	328	GLN
1	C	337	LYS
1	C	342	LYS
1	C	348	GLU
1	C	349	TRP
1	C	350	GLN
1	C	356	LEU
1	C	365	LEU
1	C	374	ASP
1	C	383	VAL
1	C	384	LEU
1	C	391	GLN
1	C	394	THR
1	C	396	LEU
1	C	398	LYS
1	C	399	ARG
1	C	400	LEU
1	C	408	ARG
1	C	410	VAL
1	C	417	ILE
1	C	429	GLN
1	C	444	VAL
1	C	448	ASP
1	C	452	LEU
1	C	458	ILE
1	C	468	HIS
1	C	470	ILE
1	C	489	THR
1	C	511	TRP

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Mol	Chain	Res	Type
1	C	514	SER
1	C	542	ARG
1	C	545	ARG
1	C	546	ASP
1	C	547	LEU
1	C	569	ILE
1	C	591	LEU
1	C	592	THR
1	C	594	LEU
1	C	618	SER
1	C	623	THR
1	C	634	PHE
1	C	636	THR
1	C	652	ASN
1	C	654	ASP
1	C	665	ILE
1	C	682	ARG
1	C	692	ARG
1	C	728	ARG
1	C	736	LEU
1	C	744	THR
1	C	764	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	16	GLN
1	D	50	HIS
1	D	145	ASN
1	D	205	HIS
1	D	601	GLN
1	D	663	ASN
1	A	16	GLN
1	A	75	ASN
1	A	98	GLN
1	A	173	ASN
1	A	279	GLN
1	A	328	GLN
1	A	377	GLN
1	A	401	ASN
1	A	557	GLN
1	A	630	ASN

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Mol	Chain	Res	Type
1	A	667	ASN
1	B	16	GLN
1	B	54	GLN
1	B	223	HIS
1	B	279	GLN
1	B	301	HIS
1	B	496	GLN
1	B	531	HIS
1	B	586	GLN
1	C	75	ASN
1	C	145	ASN
1	C	279	GLN
1	C	324	ASN
1	C	391	GLN
1	C	455	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.37	1 (0%) 92 92	84, 138, 228, 331	0
1	B	771/771 (100%)	-0.31	5 (0%) 85 75	74, 180, 334, 405	0
1	C	771/771 (100%)	-0.42	4 (0%) 87 78	57, 129, 243, 347	0
1	D	771/771 (100%)	-0.43	3 (0%) 88 81	67, 143, 228, 341	0
All	All	3084/3084 (100%)	-0.38	13 (0%) 88 81	57, 142, 295, 405	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	594	LEU	4.0
1	B	458	ILE	3.1
1	C	714	LEU	2.7
1	D	623	THR	2.3
1	B	595	LEU	2.3
1	D	729	TYR	2.3
1	C	215	GLY	2.2
1	A	346	LEU	2.2
1	B	763	LEU	2.2
1	C	727	ALA	2.2
1	B	707	ALA	2.2
1	C	600	SER	2.1
1	D	621	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.