



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:55 AM UTC

PDB ID : 1WAO / pdb_00001wao
Title : PP5 structure
Authors : Barford, D.
Deposited on : 2004-10-27
Resolution : 2.90 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

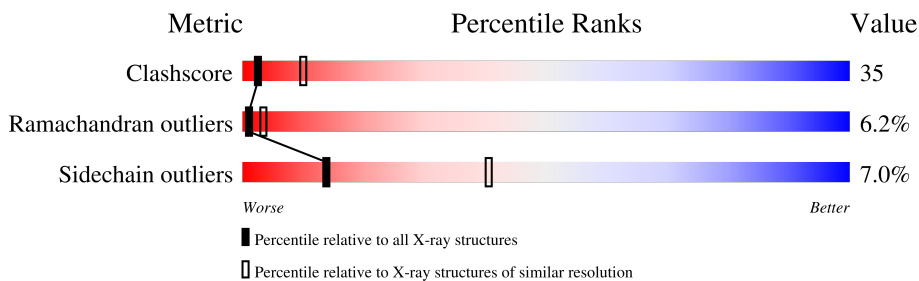
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	477	43% 43% 10% ..
1	2	477	50% 39% 8% ..
1	3	477	38% 51% 9% ..
1	4	477	48% 40% 10% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15082 atoms, of which 0 are hydrogens and 0 are deuteriums.

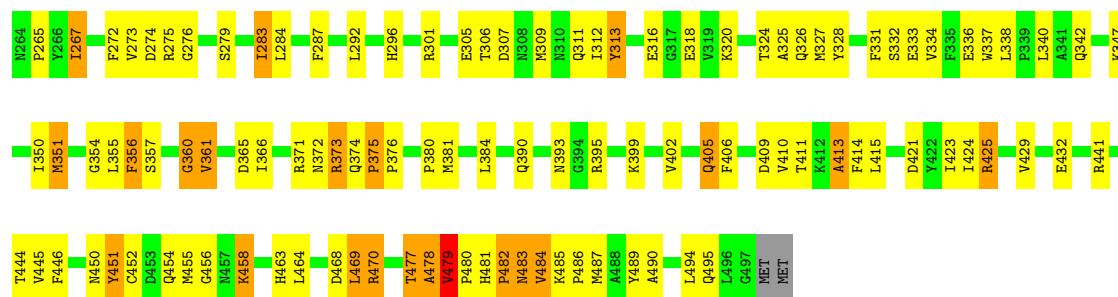
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SERINE/THREONINE PROTEIN PHOSPHATASE 5.

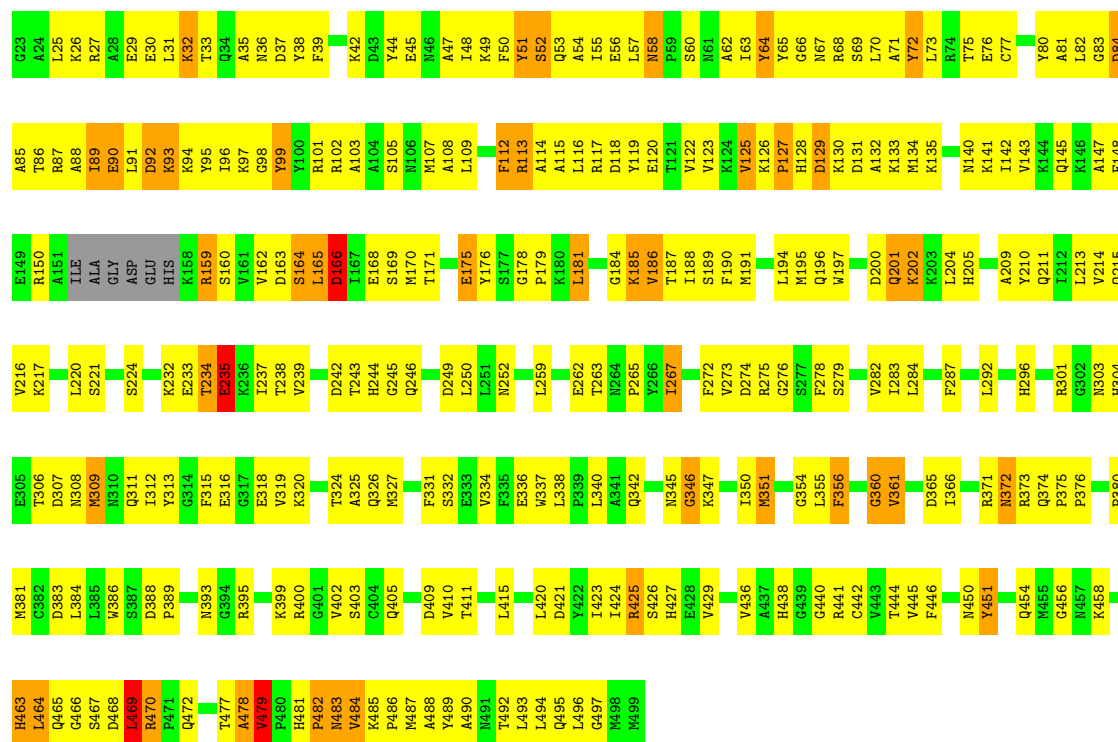
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	471	Total	C	N	O	S	0	0	0
			3781	2407	641	712	21			
1	2	469	Total	C	N	O	S	0	0	0
			3768	2399	639	710	20			
1	3	471	Total	C	N	O	S	0	0	0
			3778	2405	641	712	20			
1	4	466	Total	C	N	O	S	0	0	0
			3747	2386	635	706	20			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

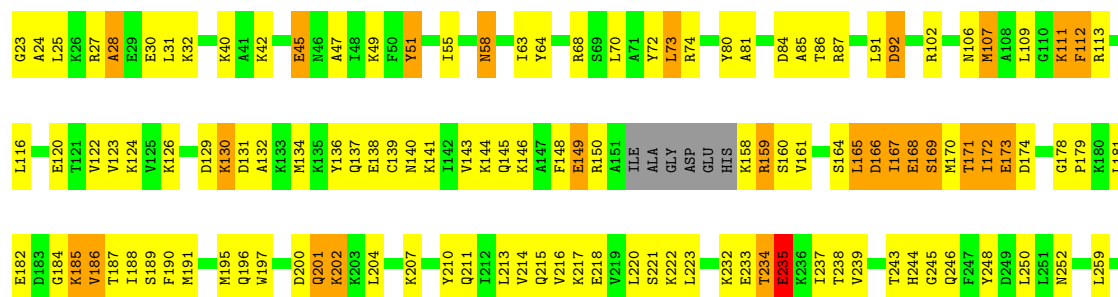
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1	2	Total	Mn	0	0
			2	2		
2	2	2	Total	Mn	0	0
			2	2		
2	3	2	Total	Mn	0	0
			2	2		
2	4	2	Total	Mn	0	0
			2	2		



- Molecule 1: SERINE/THREONINE PROTEIN PHOSPHATASE 5



- Molecule 1: SERINE/THREONINE PROTEIN PHOSPHATASE 5



T263	T264	P265	T266	I267	F272	R275	G276	S279	V282	I283	L284	T285	L286	F287	L292	L299	L300	R301	E305	T306	D307	N308	M309	M310	Q311	I312	Y313	E316	G317	E318	V319	K320	T324	A325	Q326	M327	Y328	F331	S332	E333	V334	F335	E336	W337	L338	F339	L340	A341	Q342		
C343	I344	N345	G346	K347	I350	M351	G354	L355	F356	G360	V361	D365	I366	I369	E370	R371	N372	R373	Q374	F375	P376	P380	M381	L384	Q390	N393	G394	R395	S396	K399	R400	G401	V402	Q405	D409	V410	T411	L415	L420	E336	D421	Y422	I423	I424	R425	S426					
H427	E428	V429	E432	R441	T444	V445	F446	N450	Y451	C452	D453	Q454	M455	G456	M457	K458	Y461	I462	H463	L464	Q465	G466	S467	D468	L469	R470	P471	Q472	T477	A478	V479	P480	H481	P482	M483	V484	K485	P486	M487	A488	Y489	A490	M491	T492	L493	L494	GLN	LEU	GLY	MET	MET

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.74Å 117.54Å 200.41Å 90.00° 93.79° 90.00°	Depositor
Resolution (Å)	33.78 – 2.90	Depositor
% Data completeness (in resolution range)	99.0 (33.78-2.90)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15082	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1	0.63	2/3864 (0.1%)	1.08	31/5211 (0.6%)
1	2	0.43	0/3850	0.96	17/5191 (0.3%)
1	3	0.41	0/3861	1.00	22/5208 (0.4%)
1	4	0.58	1/3830 (0.0%)	1.05	23/5166 (0.4%)
All	All	0.52	3/15405 (0.0%)	1.02	93/20776 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	498	MET	SD-CE	9.89	2.04	1.79
1	1	498	MET	CG-SD	5.57	1.94	1.80
1	4	107	MET	SD-CE	5.32	1.92	1.79

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	35	ALA	N-CA-C	-10.71	102.41	114.62
1	1	356	PHE	N-CA-C	9.48	124.33	110.59
1	4	356	PHE	N-CA-C	8.94	123.69	110.46
1	3	356	PHE	N-CA-C	8.91	123.51	110.59
1	3	175	GLU	N-CA-C	-8.76	104.63	114.62
1	3	32	LYS	N-CA-C	-8.73	103.14	113.88
1	1	204	LEU	N-CA-C	-8.59	99.19	110.53
1	3	125	VAL	N-CA-C	-8.07	105.01	112.43
1	2	495	GLN	N-CA-C	-7.97	103.28	113.16
1	3	94	LYS	N-CA-C	-7.90	104.60	112.97
1	2	356	PHE	N-CA-C	7.68	121.82	110.46
1	1	30	GLU	N-CA-C	-7.50	103.93	113.23
1	2	327	MET	N-CA-C	-7.41	103.14	111.14
1	3	84	ASP	N-CA-C	-7.26	103.36	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	327	MET	N-CA-C	-7.12	102.94	111.69
1	1	458	LYS	N-CA-C	-7.09	101.39	110.53
1	3	327	MET	N-CA-C	-7.09	103.64	111.36
1	1	375	PRO	CA-C-N	6.82	126.73	119.85
1	1	375	PRO	C-N-CA	6.82	126.73	119.85
1	3	52	SER	N-CA-C	-6.77	103.61	112.41
1	2	313	TYR	N-CA-C	6.75	121.22	112.92
1	4	178	GLY	CA-C-N	6.60	128.09	119.84
1	4	178	GLY	C-N-CA	6.60	128.09	119.84
1	3	479	VAL	CA-C-N	6.59	126.57	119.78
1	3	479	VAL	C-N-CA	6.59	126.57	119.78
1	2	250	LEU	N-CA-C	-6.57	104.20	111.36
1	1	327	MET	N-CA-C	-6.53	104.24	111.36
1	3	108	ALA	N-CA-C	-6.42	104.28	111.28
1	4	316	GLU	N-CA-C	-6.42	104.21	111.07
1	1	178	GLY	CA-C-N	6.41	126.76	119.83
1	1	178	GLY	C-N-CA	6.41	126.76	119.83
1	4	283	ILE	N-CA-C	6.32	117.06	110.62
1	2	51	TYR	N-CA-C	-6.31	104.41	111.28
1	1	249	ASP	N-CA-C	-6.28	105.75	113.41
1	1	313	TYR	N-CA-C	6.25	120.94	112.88
1	1	234	THR	N-CA-C	-6.24	101.23	110.46
1	4	234	THR	N-CA-C	-6.18	101.32	110.46
1	1	174	ASP	N-CA-C	-6.17	105.02	112.54
1	3	458	LYS	N-CA-C	-6.17	102.57	110.53
1	1	283	ILE	N-CA-C	6.13	116.31	110.42
1	1	166	ASP	CB-CA-C	-6.12	108.90	117.23
1	1	305	GLU	N-CA-C	-6.04	104.50	112.72
1	4	458	LYS	N-CA-C	-5.99	102.80	110.53
1	4	130	LYS	N-CA-C	-5.95	102.66	110.33
1	4	313	TYR	N-CA-C	5.95	120.55	112.88
1	2	283	ILE	N-CA-C	5.92	116.66	110.62
1	3	89	ILE	N-CA-C	-5.92	107.52	113.20
1	2	234	THR	N-CA-C	-5.89	101.74	110.46
1	1	479	VAL	CA-C-N	5.87	125.82	119.78
1	1	479	VAL	C-N-CA	5.87	125.82	119.78
1	4	204	LEU	N-CA-C	-5.87	102.79	110.53
1	2	305	GLU	N-CA-C	-5.82	104.81	112.72
1	4	28	ALA	N-CA-C	-5.77	106.22	113.20
1	1	25	LEU	N-CA-C	-5.75	106.27	113.28
1	1	477	THR	N-CA-C	5.73	118.59	109.65
1	2	249	ASP	N-CA-C	-5.71	106.66	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	51	TYR	N-CA-C	-5.68	105.09	111.28
1	1	252	ASN	N-CA-C	-5.68	105.17	111.36
1	2	130	LYS	N-CA-C	-5.64	103.47	110.41
1	4	479	VAL	CA-C-N	5.62	125.57	119.78
1	4	479	VAL	C-N-CA	5.62	125.57	119.78
1	3	234	THR	N-CA-C	-5.61	102.16	110.46
1	2	477	THR	N-CA-C	5.58	118.36	109.65
1	3	204	LEU	N-CA-C	-5.58	103.16	110.53
1	2	458	LYS	N-CA-C	-5.54	102.31	110.52
1	1	26	LYS	N-CA-C	-5.54	104.75	112.45
1	3	316	GLU	N-CA-C	-5.53	104.94	110.97
1	3	90	GLU	N-CA-C	-5.53	106.59	113.55
1	4	109	LEU	N-CA-C	-5.49	106.35	113.16
1	4	461	TYR	N-CA-C	-5.48	100.74	109.23
1	1	316	GLU	N-CA-C	-5.44	105.25	111.07
1	1	480	PRO	N-CA-C	5.39	119.78	111.21
1	1	405	GLN	N-CA-C	-5.38	102.50	110.46
1	2	405	GLN	N-CA-C	-5.34	101.87	110.14
1	1	237	ILE	N-CA-C	-5.26	100.89	108.42
1	2	375	PRO	N-CA-C	5.26	116.21	110.58
1	3	250	LEU	N-CA-C	-5.24	105.65	111.36
1	3	93	LYS	N-CA-C	-5.21	106.92	113.28
1	4	405	GLN	N-CA-C	-5.21	102.06	110.14
1	3	488	ALA	N-CA-C	-5.20	106.89	113.18
1	1	196	GLN	N-CA-C	-5.17	105.54	111.07
1	3	25	LEU	N-CA-C	-5.12	106.98	113.18
1	3	249	ASP	N-CA-C	-5.12	107.21	113.50
1	1	51	TYR	N-CA-C	-5.09	105.91	111.82
1	4	250	LEU	N-CA-C	-5.09	105.81	111.36
1	4	399	LYS	N-CA-C	-5.08	106.34	112.54
1	4	480	PRO	N-CA-C	5.07	119.27	111.21
1	4	47	ALA	N-CA-C	-5.03	105.07	111.11
1	1	36	ASN	N-CA-C	-5.03	107.12	113.20
1	4	305	GLU	N-CA-C	-5.02	104.58	111.81
1	2	479	VAL	CA-C-N	5.02	124.95	119.78
1	2	479	VAL	C-N-CA	5.02	124.95	119.78
1	1	130	LYS	N-CA-C	-5.01	103.87	110.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3781	0	3714	270	0
1	2	3768	0	3702	221	0
1	3	3778	0	3707	308	0
1	4	3747	0	3681	236	0
2	1	2	0	0	0	0
2	2	2	0	0	0	0
2	3	2	0	0	0	0
2	4	2	0	0	0	0
All	All	15082	0	14804	1035	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (1035) 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)
1:1:498:MET:SD	1:1:498:MET:CE	2.04	1.46
1:1:165:LEU:HG	1:1:168:GLU:HB2	1.21	1.18
1:4:185:LYS:HE3	1:4:185:LYS:HA	1.36	1.05
1:1:166:ASP:HA	1:1:170:MET:HG3	1.38	1.00
1:1:187:THR:HG22	1:1:189:SER:H	1.27	0.98
1:1:232:LYS:H	1:1:232:LYS:HD3	1.30	0.96
1:1:165:LEU:HG	1:1:168:GLU:CB	1.96	0.95
1:3:350:ILE:HG22	1:3:424:ILE:HB	1.47	0.95
1:4:232:LYS:HD3	1:4:232:LYS:H	1.31	0.94
1:3:89:ILE:HD12	1:3:102:ARG:HD3	1.50	0.94
1:1:217:LYS:HB2	1:1:334:VAL:HG12	1.50	0.94
1:3:68:ARG:O	1:3:72:TYR:HB2	1.68	0.93
1:1:350:ILE:HG22	1:1:424:ILE:HB	1.49	0.93
1:1:487:MET:SD	1:1:498:MET:HE2	2.10	0.92
1:2:232:LYS:H	1:2:232:LYS:HD3	1.32	0.92
1:1:24:ALA:HB1	1:1:27:ARG:HB3	1.50	0.91
1:2:350:ILE:HG22	1:2:424:ILE:HB	1.53	0.90
1:3:232:LYS:H	1:3:232:LYS:HD3	1.34	0.90
1:4:217:LYS:HB2	1:4:334:VAL:HG12	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:116:LEU:HD22	1:3:143:VAL:HG21	1.53	0.89
1:1:171:THR:O	1:1:172:ILE:HB	1.73	0.88
1:4:23:GLY:C	1:4:25:LEU:H	1.79	0.88
1:3:217:LYS:HB2	1:3:334:VAL:HG12	1.55	0.88
1:2:171:THR:O	1:2:207:LYS:HD2	1.74	0.87
1:3:32:LYS:NZ	1:3:63:ILE:HG21	1.90	0.87
1:1:487:MET:CG	1:1:498:MET:HE2	2.05	0.87
1:3:165:LEU:O	1:3:166:ASP:HB2	1.75	0.86
1:3:267:ILE:HD13	1:3:350:ILE:HD11	1.58	0.85
1:2:165:LEU:HB3	1:2:168:GLU:HG2	1.58	0.85
1:4:146:LYS:HZ2	1:4:311:GLN:HE22	1.23	0.84
1:3:350:ILE:CG2	1:3:424:ILE:HB	2.07	0.84
1:4:146:LYS:NZ	1:4:311:GLN:HE22	1.75	0.84
1:1:267:ILE:HD13	1:1:350:ILE:HD11	1.59	0.84
1:3:31:LEU:HB2	1:3:54:ALA:HB2	1.59	0.84
1:1:166:ASP:CA	1:1:170:MET:HG3	2.07	0.83
1:2:307:ASP:H	1:2:374:GLN:HE22	1.21	0.83
1:3:80:TYR:CE1	1:3:399:LYS:HG2	2.14	0.83
1:4:201:GLN:HE21	1:4:201:GLN:N	1.76	0.83
1:4:350:ILE:HG22	1:4:424:ILE:HB	1.60	0.83
1:1:165:LEU:CG	1:1:168:GLU:HB2	2.06	0.83
1:3:450:ASN:HD22	1:3:456:GLY:H	1.26	0.83
1:2:165:LEU:HB2	1:2:169:SER:HB3	1.61	0.82
1:2:217:LYS:HB2	1:2:334:VAL:HG12	1.59	0.82
1:3:165:LEU:HB3	1:3:168:GLU:HB2	1.61	0.82
1:1:201:GLN:HE21	1:1:201:GLN:N	1.76	0.82
1:4:172:ILE:HG23	1:4:173:GLU:N	1.93	0.82
1:1:350:ILE:CG2	1:1:424:ILE:HB	2.09	0.82
1:3:267:ILE:CD1	1:3:350:ILE:HD11	2.11	0.80
1:3:145:GLN:HA	1:3:148:PHE:HB2	1.64	0.79
1:1:312:ILE:O	1:1:494:LEU:HD13	1.83	0.79
1:2:350:ILE:CG2	1:2:424:ILE:HB	2.11	0.79
1:2:450:ASN:HD22	1:2:456:GLY:H	1.30	0.79
1:2:172:ILE:HG12	1:2:173:GLU:H	1.49	0.78
1:2:167:ILE:HD13	1:2:211:GLN:HE21	1.49	0.78
1:1:126:LYS:HB3	1:1:129:ASP:HB2	1.66	0.78
1:2:187:THR:HG22	1:2:189:SER:H	1.48	0.78
1:3:181:LEU:HG	1:3:184:GLY:HA2	1.65	0.78
1:3:55:ILE:HD11	1:3:64:TYR:HB2	1.66	0.77
1:1:356:PHE:CE1	1:1:361:VAL:HG11	2.19	0.77
1:1:137:GLN:O	1:1:141:LYS:HG3	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:33:THR:O	1:3:37:ASP:HB2	1.84	0.77
1:1:80:TYR:CE1	1:1:399:LYS:HG2	2.20	0.76
1:2:169:SER:O	1:2:171:THR:HG23	1.85	0.76
1:2:137:GLN:O	1:2:141:LYS:HG3	1.85	0.76
1:2:356:PHE:CE1	1:2:361:VAL:HG11	2.20	0.76
1:3:96:ILE:HG13	1:3:126:LYS:HE3	1.67	0.76
1:4:137:GLN:O	1:4:141:LYS:HG3	1.85	0.76
1:4:126:LYS:HB3	1:4:129:ASP:HB2	1.66	0.76
1:4:351:MET:HE1	1:4:423:ILE:HD12	1.65	0.76
1:2:267:ILE:HD13	1:2:350:ILE:HD11	1.67	0.76
1:1:267:ILE:CD1	1:1:350:ILE:HD11	2.16	0.75
1:1:320:LYS:HE2	1:1:325:ALA:HB1	1.69	0.75
1:3:80:TYR:CE2	1:3:399:LYS:HA	2.21	0.75
1:3:32:LYS:HB2	1:3:64:TYR:CE2	2.22	0.75
1:4:283:ILE:HD11	1:4:287:PHE:CZ	2.22	0.75
1:3:373:ARG:HH12	1:3:376:PRO:HG3	1.52	0.74
1:4:172:ILE:HG23	1:4:173:GLU:H	1.52	0.74
1:4:167:ILE:CD1	1:4:211:GLN:HE21	2.00	0.74
1:2:267:ILE:CD1	1:2:350:ILE:HD11	2.17	0.74
1:2:45:GLU:O	1:2:49:LYS:HG2	1.88	0.74
1:3:83:GLY:HA2	1:3:86:THR:OG1	1.88	0.73
1:3:320:LYS:HG2	1:3:325:ALA:HA	1.71	0.73
1:2:126:LYS:HB3	1:2:129:ASP:HB2	1.70	0.73
1:3:373:ARG:NH1	1:3:376:PRO:HG3	2.04	0.73
1:4:267:ILE:HD13	1:4:350:ILE:HD11	1.69	0.73
1:2:167:ILE:CD1	1:2:211:GLN:HE21	2.03	0.72
1:3:356:PHE:CE1	1:3:361:VAL:HG11	2.23	0.72
1:2:145:GLN:O	1:2:149:GLU:HG3	1.88	0.72
1:1:320:LYS:HG2	1:1:325:ALA:HA	1.70	0.72
1:4:318:GLU:HA	1:4:489:TYR:CD2	2.24	0.72
1:3:307:ASP:H	1:3:374:GLN:HE22	1.37	0.72
1:1:36:ASN:HA	1:1:51:TYR:OH	1.90	0.72
1:4:45:GLU:O	1:4:49:LYS:HG2	1.89	0.72
1:1:450:ASN:HD22	1:1:456:GLY:H	1.38	0.71
1:4:483:ASN:O	1:4:484:VAL:HB	1.89	0.71
1:3:31:LEU:CB	1:3:54:ALA:HB2	2.20	0.71
1:3:35:ALA:HA	1:3:50:PHE:HB2	1.72	0.71
1:3:140:ASN:C	1:3:142:ILE:H	1.99	0.71
1:3:185:LYS:O	1:3:186:VAL:HB	1.90	0.71
1:1:307:ASP:O	1:1:311:GLN:HG2	1.91	0.71
1:3:31:LEU:HD13	1:3:53:GLN:C	2.15	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:320:LYS:HE2	1:3:325:ALA:HB1	1.72	0.71
1:2:106:ASN:OD1	1:2:111:LYS:HD3	1.91	0.70
1:3:97:LYS:O	1:3:101:ARG:HG3	1.92	0.70
1:3:307:ASP:OD2	1:3:332:SER:HB2	1.92	0.70
1:2:318:GLU:HA	1:2:489:TYR:CD2	2.26	0.70
1:3:301:ARG:NH1	1:3:336:GLU:HA	2.06	0.70
1:1:307:ASP:H	1:1:374:GLN:HE22	1.40	0.69
1:3:312:ILE:O	1:3:494:LEU:HD13	1.92	0.69
1:3:187:THR:HG22	1:3:189:SER:H	1.58	0.69
1:3:129:ASP:HB3	1:3:132:ALA:HB3	1.75	0.69
1:4:232:LYS:HD3	1:4:232:LYS:N	2.06	0.69
1:1:483:ASN:O	1:1:484:VAL:HB	1.92	0.69
1:2:24:ALA:HB1	1:2:27:ARG:HB2	1.73	0.69
1:2:483:ASN:O	1:2:484:VAL:HB	1.92	0.69
1:4:356:PHE:CE1	1:4:361:VAL:HG11	2.27	0.69
1:1:487:MET:HB2	1:1:498:MET:HE2	1.74	0.69
1:1:232:LYS:HD3	1:1:232:LYS:N	2.06	0.68
1:2:306:THR:HG23	1:2:374:GLN:NE2	2.08	0.68
1:3:44:TYR:O	1:3:48:ILE:HG13	1.94	0.68
1:4:450:ASN:HD22	1:4:456:GLY:H	1.40	0.68
1:2:112:PHE:HD2	1:2:113:ARG:HG3	1.58	0.68
1:3:131:ASP:HA	1:3:134:MET:HB2	1.75	0.68
1:4:350:ILE:CG2	1:4:424:ILE:HB	2.23	0.68
1:1:318:GLU:HA	1:1:489:TYR:CD2	2.29	0.68
1:3:340:LEU:HB3	1:3:384:LEU:HD23	1.76	0.68
1:3:201:GLN:N	1:3:201:GLN:HE21	1.92	0.68
1:4:148:PHE:O	1:4:150:ARG:N	2.26	0.68
1:3:237:ILE:HA	1:3:265:PRO:HG2	1.76	0.67
1:4:139:CYS:O	1:4:143:VAL:HG23	1.93	0.67
1:1:172:ILE:HG23	1:1:173:GLU:N	2.07	0.67
1:1:487:MET:HB2	1:1:498:MET:CE	2.24	0.67
1:2:201:GLN:HE21	1:2:201:GLN:N	1.92	0.67
1:4:267:ILE:CD1	1:4:350:ILE:HD11	2.23	0.67
1:3:165:LEU:HB3	1:3:168:GLU:CB	2.25	0.67
1:3:425:ARG:O	1:3:444:THR:HA	1.94	0.67
1:2:140:ASN:OD1	1:2:144:LYS:HE2	1.95	0.67
1:3:118:ASP:O	1:3:122:VAL:HG23	1.94	0.67
1:2:139:CYS:O	1:2:143:VAL:HG23	1.94	0.67
1:4:429:VAL:HG22	1:4:446:PHE:CZ	2.30	0.67
1:1:373:ARG:NH1	1:1:376:PRO:HG3	2.10	0.67
1:2:429:VAL:HG22	1:2:446:PHE:CZ	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:232:LYS:HD3	1:3:232:LYS:N	2.09	0.67
1:1:234:THR:O	1:1:235:GLU:HB2	1.95	0.66
1:2:160:SER:HB3	1:2:333:GLU:OE2	1.95	0.66
1:4:351:MET:HE3	1:4:354:GLY:HA2	1.76	0.66
1:2:172:ILE:HG12	1:2:173:GLU:N	2.08	0.66
1:1:165:LEU:CD1	1:1:168:GLU:HG3	2.26	0.66
1:1:487:MET:CB	1:1:498:MET:HE2	2.25	0.66
1:3:147:ALA:HA	1:3:150:ARG:NH2	2.10	0.66
1:3:395:ARG:HG2	1:3:395:ARG:HH11	1.61	0.66
1:1:87:ARG:NH2	1:1:91:LEU:HD21	2.10	0.66
1:1:45:GLU:O	1:1:49:LYS:HG2	1.96	0.66
1:4:301:ARG:NH1	1:4:336:GLU:HA	2.10	0.66
1:2:29:GLU:OE2	1:2:32:LYS:HD3	1.95	0.66
1:2:148:PHE:O	1:2:150:ARG:N	2.29	0.66
1:3:45:GLU:O	1:3:49:LYS:HG2	1.96	0.66
1:3:96:ILE:HG13	1:3:126:LYS:CE	2.26	0.66
1:4:373:ARG:NH1	1:4:376:PRO:HG3	2.10	0.66
1:1:166:ASP:O	1:1:170:MET:HB2	1.96	0.65
1:3:185:LYS:HE3	1:3:185:LYS:HA	1.78	0.65
1:3:27:ARG:NH2	1:3:31:LEU:HD11	2.12	0.65
1:3:399:LYS:HG3	1:3:405:GLN:NE2	2.11	0.65
1:2:173:GLU:HG3	1:2:174:ASP:H	1.61	0.65
1:4:307:ASP:OD2	1:4:332:SER:HB2	1.97	0.65
1:3:105:SER:O	1:3:109:LEU:HG	1.97	0.65
1:4:244:HIS:O	1:4:276:GLY:HA3	1.96	0.65
1:4:306:THR:HG23	1:4:374:GLN:NE2	2.11	0.65
1:1:165:LEU:HG	1:1:168:GLU:CG	2.26	0.64
1:4:307:ASP:O	1:4:311:GLN:HG2	1.97	0.64
1:4:356:PHE:HZ	1:4:366:ILE:HD11	1.62	0.64
1:4:159:ARG:O	1:4:161:VAL:N	2.26	0.64
1:1:232:LYS:H	1:1:232:LYS:CD	2.07	0.64
1:2:232:LYS:HD3	1:2:232:LYS:N	2.08	0.64
1:2:373:ARG:NH1	1:2:376:PRO:HG3	2.12	0.64
1:3:140:ASN:O	1:3:142:ILE:N	2.30	0.64
1:1:85:ALA:HB1	1:1:102:ARG:HB2	1.80	0.64
1:1:58:ASN:C	1:1:58:ASN:HD22	2.04	0.64
1:1:171:THR:O	1:1:172:ILE:CB	2.46	0.64
1:2:275:ARG:HG3	1:2:275:ARG:HH11	1.63	0.64
1:3:44:TYR:HA	1:3:47:ALA:HB3	1.79	0.64
1:4:232:LYS:H	1:4:232:LYS:CD	2.07	0.64
1:3:165:LEU:HB3	1:3:168:GLU:HG2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:167:ILE:HD13	1:4:211:GLN:HE21	1.63	0.64
1:1:450:ASN:HD22	1:1:456:GLY:N	1.96	0.64
1:2:174:ASP:HB2	1:2:175:GLU:OE2	1.98	0.64
1:3:32:LYS:HZ2	1:3:63:ILE:HG21	1.59	0.64
1:4:68:ARG:HG2	1:4:72:TYR:CE1	2.34	0.63
1:1:139:CYS:O	1:1:143:VAL:HG23	1.99	0.63
1:1:165:LEU:HD23	1:1:169:SER:OG	1.98	0.63
1:2:252:ASN:CG	1:2:479:VAL:HG21	2.23	0.63
1:1:168:GLU:O	1:1:169:SER:C	2.41	0.63
1:1:200:ASP:C	1:1:201:GLN:HE21	2.07	0.63
1:1:275:ARG:HG3	1:1:275:ARG:HH11	1.63	0.63
1:4:159:ARG:O	1:4:161:VAL:HG23	1.98	0.63
1:3:232:LYS:H	1:3:232:LYS:CD	2.09	0.63
1:3:318:GLU:HA	1:3:489:TYR:CD2	2.34	0.63
1:3:483:ASN:O	1:3:484:VAL:HB	1.98	0.63
1:4:23:GLY:C	1:4:25:LEU:N	2.51	0.63
1:1:356:PHE:CZ	1:1:366:ILE:HD11	2.34	0.63
1:1:356:PHE:HZ	1:1:366:ILE:HD11	1.64	0.63
1:3:62:ALA:HB2	1:3:91:LEU:CB	2.28	0.63
1:4:85:ALA:HB1	1:4:102:ARG:HB2	1.81	0.63
1:3:210:TYR:O	1:3:214:VAL:HG23	1.98	0.63
1:3:450:ASN:HD22	1:3:456:GLY:N	1.95	0.63
1:4:234:THR:O	1:4:235:GLU:HB2	1.99	0.63
1:4:340:LEU:HD11	1:4:381:MET:HE3	1.79	0.63
1:1:29:GLU:HG3	1:1:32:LYS:HD3	1.80	0.62
1:2:210:TYR:O	1:2:214:VAL:HG23	1.99	0.62
1:3:340:LEU:HD11	1:3:381:MET:HE3	1.81	0.62
1:4:112:PHE:CD2	1:4:113:ARG:HG3	2.34	0.62
1:2:320:LYS:HG2	1:2:325:ALA:HA	1.81	0.62
1:1:486:PRO:HB2	1:1:498:MET:HE1	1.82	0.62
1:2:340:LEU:HD11	1:2:381:MET:HE3	1.81	0.62
1:4:491:ASN:OD1	1:4:493:LEU:HB2	1.99	0.62
1:3:62:ALA:HB2	1:3:91:LEU:HB2	1.81	0.62
1:2:232:LYS:H	1:2:232:LYS:CD	2.07	0.62
1:1:26:LYS:O	1:1:30:GLU:HG3	1.99	0.62
1:2:309:MET:HE3	1:2:313:TYR:CE2	2.35	0.62
1:2:338:LEU:O	1:2:371:ARG:HD3	2.00	0.62
1:3:429:VAL:HG22	1:3:446:PHE:CZ	2.35	0.62
1:4:275:ARG:HH11	1:4:275:ARG:HG3	1.65	0.62
1:3:88:ALA:HB1	1:3:95:TYR:CD2	2.34	0.62
1:3:129:ASP:HB3	1:3:132:ALA:CB	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:112:PHE:HD2	1:4:113:ARG:HG3	1.65	0.62
1:4:187:THR:HG22	1:4:189:SER:H	1.65	0.62
1:3:450:ASN:ND2	1:3:456:GLY:H	1.97	0.62
1:4:106:ASN:OD1	1:4:111:LYS:HD3	1.99	0.62
1:1:32:LYS:HD2	1:1:64:TYR:HE1	1.66	0.61
1:4:25:LEU:O	1:4:28:ALA:HB3	2.00	0.61
1:3:351:MET:HE1	1:3:423:ILE:HD12	1.81	0.61
1:4:171:THR:O	1:4:172:ILE:HG22	2.01	0.61
1:1:237:ILE:HA	1:1:265:PRO:HG2	1.82	0.61
1:1:32:LYS:HD2	1:1:64:TYR:CE1	2.35	0.61
1:3:27:ARG:HG2	1:3:57:LEU:HD13	1.82	0.61
1:2:234:THR:O	1:2:235:GLU:HB2	1.99	0.61
1:4:186:VAL:HG13	1:4:191:MET:HE3	1.83	0.61
1:4:373:ARG:HH12	1:4:376:PRO:HG3	1.64	0.61
1:2:80:TYR:CE1	1:2:399:LYS:HG2	2.36	0.61
1:3:234:THR:O	1:3:235:GLU:HB2	2.01	0.61
1:1:492:THR:O	1:1:496:LEU:HG	1.99	0.61
1:4:112:PHE:CD1	1:4:112:PHE:N	2.67	0.61
1:4:120:GLU:HB2	1:4:136:TYR:HE1	1.65	0.61
1:1:324:THR:C	1:1:326:GLN:H	2.09	0.61
1:1:356:PHE:CD1	1:1:361:VAL:HG11	2.35	0.61
1:4:170:MET:HA	1:4:170:MET:HE2	1.83	0.61
1:2:87:ARG:NH2	1:2:91:LEU:HD21	2.16	0.60
1:2:186:VAL:HG13	1:2:191:MET:HE3	1.81	0.60
1:1:233:GLU:OE1	1:1:233:GLU:HA	2.00	0.60
1:2:165:LEU:HD12	1:2:168:GLU:HG3	1.82	0.60
1:2:320:LYS:HE2	1:2:325:ALA:HB1	1.83	0.60
1:2:395:ARG:HG2	1:2:395:ARG:HH11	1.67	0.60
1:3:32:LYS:HZ1	1:3:63:ILE:HG21	1.64	0.60
1:1:112:PHE:HD2	1:1:113:ARG:HG3	1.67	0.60
1:1:373:ARG:HH12	1:1:376:PRO:HG3	1.66	0.60
1:2:85:ALA:HB1	1:2:102:ARG:HB2	1.82	0.60
1:2:307:ASP:OD2	1:2:332:SER:HB2	2.01	0.60
1:3:27:ARG:CZ	1:3:31:LEU:HD11	2.31	0.60
1:4:126:LYS:HB3	1:4:129:ASP:CB	2.31	0.60
1:3:275:ARG:HG3	1:3:275:ARG:HH11	1.65	0.60
1:3:409:ASP:OD1	1:3:410:VAL:HG23	2.02	0.60
1:4:134:MET:O	1:4:138:GLU:HB2	2.02	0.60
1:4:356:PHE:CZ	1:4:366:ILE:HD11	2.36	0.60
1:4:409:ASP:OD1	1:4:410:VAL:N	2.34	0.60
1:4:483:ASN:O	1:4:484:VAL:CB	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:126:LYS:HB3	1:1:129:ASP:CB	2.32	0.60
1:2:332:SER:O	1:2:336:GLU:HG3	2.00	0.60
1:1:190:PHE:CD2	1:1:191:MET:HE2	2.36	0.60
1:2:112:PHE:CD1	1:2:112:PHE:N	2.68	0.60
1:3:252:ASN:CG	1:3:479:VAL:HG21	2.27	0.60
1:1:142:ILE:CG2	1:1:146:LYS:HE3	2.32	0.60
1:1:181:LEU:HB3	1:1:184:GLY:HA2	1.84	0.60
1:2:450:ASN:HD22	1:2:456:GLY:N	1.99	0.60
1:3:39:PHE:CE1	1:3:71:ALA:HB2	2.37	0.60
1:4:320:LYS:HE2	1:4:325:ALA:HB1	1.84	0.60
1:2:58:ASN:C	1:2:58:ASN:HD22	2.10	0.60
1:3:186:VAL:HG13	1:3:191:MET:HE3	1.83	0.60
1:2:130:LYS:O	1:2:131:ASP:HB3	2.02	0.59
1:2:347:LYS:HD2	1:2:421:ASP:OD1	2.02	0.59
1:4:145:GLN:O	1:4:149:GLU:HG3	2.02	0.59
1:1:340:LEU:HD11	1:1:381:MET:HE3	1.83	0.59
1:1:409:ASP:OD1	1:1:410:VAL:N	2.34	0.59
1:2:112:PHE:CD2	1:2:113:ARG:HG3	2.35	0.59
1:2:331:PHE:O	1:2:334:VAL:HG22	2.02	0.59
1:1:483:ASN:O	1:1:484:VAL:CB	2.50	0.59
1:2:134:MET:O	1:2:138:GLU:HB2	2.02	0.59
1:2:237:ILE:HA	1:2:265:PRO:HG2	1.84	0.59
1:2:373:ARG:HH12	1:2:376:PRO:HG3	1.67	0.59
1:1:399:LYS:HG3	1:1:405:GLN:NE2	2.18	0.59
1:2:244:HIS:O	1:2:276:GLY:HA3	2.02	0.59
1:3:165:LEU:HB3	1:3:168:GLU:CG	2.32	0.59
1:4:307:ASP:H	1:4:374:GLN:HE22	1.49	0.59
1:1:201:GLN:N	1:1:201:GLN:NE2	2.50	0.59
1:1:351:MET:HE1	1:1:423:ILE:HD12	1.85	0.59
1:2:165:LEU:HB3	1:2:168:GLU:CG	2.30	0.59
1:4:201:GLN:N	1:4:201:GLN:NE2	2.49	0.59
1:1:409:ASP:OD1	1:1:410:VAL:HG23	2.03	0.59
1:2:415:LEU:HD11	1:2:441:ARG:HB3	1.83	0.59
1:2:26:LYS:O	1:2:30:GLU:HG3	2.02	0.59
1:4:393:ASN:HB3	1:4:409:ASP:OD2	2.02	0.59
1:3:86:THR:O	1:3:90:GLU:HG3	2.03	0.58
1:3:185:LYS:O	1:3:186:VAL:CB	2.51	0.58
1:3:307:ASP:O	1:3:311:GLN:HG2	2.02	0.58
1:1:73:LEU:HD22	1:1:81:ALA:HB1	1.85	0.58
1:3:313:TYR:HA	1:3:487:MET:HE3	1.84	0.58
1:1:165:LEU:HG	1:1:168:GLU:HG3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:309:MET:HE3	1:1:313:TYR:CE2	2.38	0.58
1:3:140:ASN:C	1:3:142:ILE:N	2.61	0.58
1:4:200:ASP:C	1:4:201:GLN:HE21	2.12	0.58
1:1:35:ALA:HB2	1:1:50:PHE:HB3	1.85	0.58
1:3:36:ASN:HB2	1:3:51:TYR:OH	2.02	0.58
1:3:356:PHE:CZ	1:3:366:ILE:HD11	2.39	0.58
1:4:172:ILE:CG2	1:4:173:GLU:N	2.64	0.58
1:4:221:SER:HA	1:4:337:TRP:CE3	2.38	0.58
1:4:338:LEU:O	1:4:371:ARG:HD3	2.03	0.58
1:1:130:LYS:O	1:1:131:ASP:HB3	2.04	0.58
1:1:145:GLN:HA	1:1:148:PHE:HB3	1.85	0.58
1:1:338:LEU:O	1:1:371:ARG:HD3	2.04	0.58
1:1:185:LYS:O	1:1:186:VAL:HB	2.04	0.58
1:3:415:LEU:HD11	1:3:441:ARG:HB3	1.86	0.58
1:2:307:ASP:O	1:2:311:GLN:HG2	2.04	0.58
1:1:221:SER:HA	1:1:337:TRP:CE3	2.39	0.57
1:3:165:LEU:H	1:3:165:LEU:HD22	1.68	0.57
1:1:106:ASN:OD1	1:1:111:LYS:HD3	2.03	0.57
1:1:201:GLN:O	1:1:202:LYS:HB2	2.04	0.57
1:2:172:ILE:HG23	1:2:173:GLU:N	2.19	0.57
1:4:493:LEU:O	1:4:494:LEU:HG	2.04	0.57
1:1:31:LEU:HB2	1:1:54:ALA:HB2	1.85	0.57
1:1:142:ILE:HG22	1:1:146:LYS:HE3	1.85	0.57
1:2:356:PHE:CZ	1:2:366:ILE:HD11	2.39	0.57
1:1:134:MET:O	1:1:138:GLU:HB2	2.03	0.57
1:2:181:LEU:HD11	1:2:185:LYS:H	1.68	0.57
1:4:165:LEU:HG	1:4:169:SER:HB2	1.87	0.57
1:2:126:LYS:HB3	1:2:129:ASP:CB	2.35	0.57
1:4:450:ASN:HD22	1:4:456:GLY:N	2.02	0.57
1:1:120:GLU:HB2	1:1:136:TYR:HE1	1.70	0.57
1:1:307:ASP:OD2	1:1:332:SER:HB2	2.04	0.57
1:2:351:MET:HE3	1:2:354:GLY:HA2	1.85	0.57
1:3:324:THR:C	1:3:326:GLN:H	2.13	0.57
1:3:465:GLN:O	1:3:469:LEU:HD13	2.04	0.57
1:4:58:ASN:HD22	1:4:58:ASN:C	2.13	0.57
1:1:33:THR:O	1:1:37:ASP:HB2	2.04	0.56
1:3:181:LEU:CG	1:3:184:GLY:HA2	2.35	0.56
1:3:356:PHE:HZ	1:3:366:ILE:HD11	1.70	0.56
1:4:166:ASP:O	1:4:168:GLU:N	2.38	0.56
1:1:150:ARG:HG3	1:1:151:ALA:H	1.70	0.56
1:2:483:ASN:O	1:2:484:VAL:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:120:GLU:HB2	1:4:136:TYR:CE1	2.39	0.56
1:4:159:ARG:C	1:4:161:VAL:H	2.11	0.56
1:4:190:PHE:CD2	1:4:191:MET:HE2	2.41	0.56
1:4:324:THR:C	1:4:326:GLN:H	2.12	0.56
1:1:399:LYS:HD2	1:1:405:GLN:HE22	1.70	0.56
1:3:221:SER:HA	1:3:337:TRP:CE3	2.41	0.56
1:3:356:PHE:CD1	1:3:361:VAL:HG11	2.41	0.56
1:3:393:ASN:HB3	1:3:409:ASP:OD2	2.05	0.56
1:1:244:HIS:O	1:1:276:GLY:HA3	2.05	0.56
1:1:331:PHE:O	1:1:334:VAL:HG22	2.06	0.56
1:1:393:ASN:HB3	1:1:409:ASP:OD2	2.05	0.56
1:3:39:PHE:HE1	1:3:71:ALA:HB2	1.71	0.56
1:4:415:LEU:HD11	1:4:441:ARG:HB3	1.86	0.56
1:2:173:GLU:HB3	1:2:176:TYR:HB3	1.87	0.56
1:3:42:LYS:HD3	1:3:454:GLN:O	2.06	0.56
1:3:91:LEU:O	1:3:92:ASP:HB2	2.06	0.56
1:1:51:TYR:O	1:1:55:ILE:HG12	2.05	0.55
1:1:465:GLN:O	1:1:469:LEU:HD13	2.05	0.55
1:1:169:SER:O	1:1:170:MET:C	2.49	0.55
1:2:129:ASP:OD2	1:2:132:ALA:HB2	2.06	0.55
1:2:169:SER:O	1:2:171:THR:N	2.39	0.55
1:3:145:GLN:C	1:3:147:ALA:H	2.14	0.55
1:3:187:THR:HG22	1:3:188:ILE:N	2.22	0.55
1:3:332:SER:O	1:3:336:GLU:HG3	2.06	0.55
1:1:58:ASN:C	1:1:58:ASN:ND2	2.64	0.55
1:3:87:ARG:NE	1:3:91:LEU:HD11	2.22	0.55
1:4:181:LEU:HD11	1:4:186:VAL:N	2.21	0.55
1:1:187:THR:HG22	1:1:188:ILE:N	2.20	0.55
1:1:145:GLN:O	1:1:148:PHE:HB3	2.07	0.55
1:2:120:GLU:HB2	1:2:136:TYR:HE1	1.70	0.55
1:2:356:PHE:CZ	1:2:384:LEU:HD13	2.41	0.55
1:2:393:ASN:HB3	1:2:409:ASP:OD2	2.07	0.55
1:4:130:LYS:O	1:4:131:ASP:HB3	2.07	0.55
1:1:112:PHE:CD1	1:1:112:PHE:N	2.68	0.55
1:2:356:PHE:CD1	1:2:361:VAL:HG11	2.41	0.55
1:3:39:PHE:HZ	1:3:70:LEU:HG	1.71	0.55
1:3:188:ILE:HG12	1:3:292:LEU:HD21	1.88	0.55
1:1:112:PHE:CD2	1:1:113:ARG:HG3	2.41	0.55
1:1:140:ASN:OD1	1:1:144:LYS:HE2	2.06	0.55
1:3:69:SER:O	1:3:73:LEU:HB2	2.07	0.55
1:3:113:ARG:O	1:3:116:LEU:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:320:LYS:HG2	1:4:325:ALA:HA	1.87	0.55
1:4:421:ASP:N	1:4:421:ASP:OD1	2.40	0.55
1:1:429:VAL:HG22	1:1:446:PHE:CZ	2.42	0.54
1:3:87:ARG:HE	1:3:91:LEU:HD11	1.72	0.54
1:4:129:ASP:OD2	1:4:132:ALA:HB2	2.07	0.54
1:4:232:LYS:HE2	1:4:235:GLU:HB2	1.89	0.54
1:1:129:ASP:OD2	1:1:132:ALA:HB2	2.07	0.54
1:4:351:MET:CE	1:4:354:GLY:HA2	2.37	0.54
1:2:185:LYS:O	1:2:186:VAL:HG23	2.06	0.54
1:2:191:MET:O	1:2:195:MET:HG3	2.06	0.54
1:3:483:ASN:O	1:3:484:VAL:CB	2.56	0.54
1:3:69:SER:CB	1:3:85:ALA:HB2	2.37	0.54
1:3:233:GLU:OE1	1:3:233:GLU:HA	2.07	0.54
1:1:450:ASN:ND2	1:1:456:GLY:HA2	2.23	0.54
1:4:191:MET:O	1:4:195:MET:HG3	2.07	0.54
1:4:234:THR:O	1:4:235:GLU:CB	2.56	0.54
1:3:80:TYR:CZ	1:3:399:LYS:HA	2.43	0.54
1:1:34:GLN:O	1:1:34:GLN:HG2	2.07	0.54
1:2:351:MET:HE1	1:2:423:ILE:HD12	1.89	0.54
1:3:273:VAL:O	1:3:274:ASP:HB2	2.07	0.54
1:4:351:MET:HE3	1:4:354:GLY:CA	2.37	0.54
1:2:307:ASP:N	1:2:374:GLN:HE22	2.00	0.54
1:3:93:LYS:C	1:3:95:TYR:H	2.15	0.54
1:2:351:MET:CE	1:2:354:GLY:HA2	2.38	0.54
1:4:309:MET:HE3	1:4:313:TYR:CE2	2.43	0.54
1:3:60:SER:C	1:3:91:LEU:HD13	2.33	0.53
1:3:96:ILE:HG13	1:3:126:LYS:NZ	2.23	0.53
1:3:485:LYS:HB3	1:3:486:PRO:HD2	1.90	0.53
1:4:432:GLU:OE1	1:4:458:LYS:NZ	2.39	0.53
1:1:195:MET:HE1	1:1:259:LEU:CD2	2.37	0.53
1:2:336:GLU:O	1:2:371:ARG:HG2	2.08	0.53
1:3:309:MET:HE3	1:3:313:TYR:CE2	2.43	0.53
1:4:331:PHE:O	1:4:334:VAL:HG22	2.08	0.53
1:1:190:PHE:HD2	1:1:191:MET:HE2	1.72	0.53
1:4:168:GLU:O	1:4:170:MET:N	2.40	0.53
1:1:347:LYS:HD2	1:1:421:ASP:OD1	2.07	0.53
1:2:68:ARG:HG2	1:2:72:TYR:CE1	2.44	0.53
1:3:361:VAL:HA	1:3:365:ASP:OD1	2.09	0.53
1:4:140:ASN:OD1	1:4:144:LYS:HE2	2.07	0.53
1:2:87:ARG:CZ	1:2:91:LEU:HD21	2.39	0.53
1:2:399:LYS:HG3	1:2:405:GLN:NE2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:360:GLY:O	1:3:361:VAL:O	2.27	0.53
1:3:399:LYS:HG3	1:3:405:GLN:HE22	1.72	0.53
1:4:346:GLY:O	1:4:420:LEU:HD23	2.08	0.53
1:1:145:GLN:O	1:1:148:PHE:N	2.41	0.53
1:1:487:MET:SD	1:1:498:MET:HG2	2.48	0.53
1:2:73:LEU:HD22	1:2:81:ALA:HB1	1.89	0.53
1:3:112:PHE:N	1:3:112:PHE:CD1	2.76	0.53
1:4:485:LYS:HB3	1:4:486:PRO:HD2	1.90	0.53
1:2:301:ARG:NH1	1:2:336:GLU:HA	2.24	0.53
1:3:123:VAL:HG21	1:3:133:LYS:HG2	1.91	0.53
1:3:128:HIS:HA	1:3:133:LYS:HE2	1.89	0.53
1:4:220:LEU:HD13	1:4:338:LEU:HD23	1.91	0.53
1:1:145:GLN:O	1:1:146:LYS:C	2.51	0.53
1:1:361:VAL:HA	1:1:365:ASP:OD1	2.09	0.53
1:4:201:GLN:O	1:4:202:LYS:HB2	2.08	0.53
1:2:307:ASP:H	1:2:374:GLN:NE2	1.98	0.53
1:3:88:ALA:HB1	1:3:95:TYR:CE2	2.44	0.53
1:4:400:ARG:NE	1:4:427:HIS:NE2	2.57	0.53
1:1:356:PHE:CD1	1:1:356:PHE:N	2.76	0.53
1:1:477:THR:HG23	1:1:478:ALA:N	2.24	0.53
1:3:179:PRO:HG2	1:3:194:LEU:HA	1.89	0.53
1:4:491:ASN:CG	1:4:493:LEU:HD12	2.34	0.53
1:2:239:VAL:HA	1:2:267:ILE:HG23	1.90	0.52
1:3:395:ARG:HH11	1:3:395:ARG:CG	2.20	0.52
1:3:400:ARG:NE	1:3:427:HIS:NE2	2.58	0.52
1:1:351:MET:HE3	1:1:354:GLY:HA2	1.91	0.52
1:2:200:ASP:C	1:2:201:GLN:HE21	2.17	0.52
1:2:283:ILE:HD11	1:2:287:PHE:CZ	2.43	0.52
1:2:409:ASP:OD1	1:2:410:VAL:N	2.42	0.52
1:1:283:ILE:HD11	1:1:287:PHE:CZ	2.44	0.52
1:2:312:ILE:HG23	1:2:494:LEU:CD1	2.38	0.52
1:2:356:PHE:HZ	1:2:366:ILE:HD11	1.72	0.52
1:1:351:MET:HE3	1:1:354:GLY:C	2.34	0.52
1:3:27:ARG:HE	1:3:57:LEU:HD12	1.73	0.52
1:3:89:ILE:O	1:3:93:LYS:HG2	2.09	0.52
1:3:200:ASP:C	1:3:201:GLN:HE21	2.18	0.52
1:3:239:VAL:HA	1:3:267:ILE:HG23	1.91	0.52
1:3:306:THR:HG23	1:3:374:GLN:NE2	2.25	0.52
1:4:158:LYS:O	1:4:159:ARG:CB	2.58	0.52
1:4:232:LYS:O	1:4:466:GLY:HA3	2.09	0.52
1:4:390:GLN:HE22	1:4:396:SER:CB	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:213:LEU:HD21	1:2:331:PHE:CE1	2.44	0.52
1:3:54:ALA:O	1:3:58:ASN:HB3	2.10	0.52
1:3:130:LYS:O	1:3:131:ASP:HB3	2.10	0.52
1:1:234:THR:O	1:1:235:GLU:CB	2.55	0.52
1:3:150:ARG:HG2	1:3:150:ARG:HH11	1.75	0.52
1:4:200:ASP:O	1:4:202:LYS:HG3	2.10	0.52
1:1:188:ILE:HG12	1:1:292:LEU:HD21	1.91	0.52
1:2:159:ARG:O	1:2:161:VAL:N	2.41	0.52
1:2:232:LYS:HE2	1:2:235:GLU:HB2	1.92	0.52
1:2:324:THR:C	1:2:326:GLN:H	2.17	0.52
1:3:162:VAL:HG12	1:3:162:VAL:O	2.10	0.52
1:4:233:GLU:HA	1:4:233:GLU:OE1	2.09	0.52
1:1:232:LYS:HE2	1:1:235:GLU:HB2	1.92	0.52
1:1:486:PRO:C	1:1:498:MET:HE1	2.35	0.52
1:2:233:GLU:HA	1:2:233:GLU:OE1	2.09	0.52
1:3:232:LYS:HE2	1:3:235:GLU:HB2	1.91	0.52
1:3:350:ILE:HG22	1:3:424:ILE:CB	2.31	0.52
1:2:58:ASN:C	1:2:58:ASN:ND2	2.67	0.51
1:2:190:PHE:CD2	1:2:191:MET:HE2	2.45	0.51
1:3:72:TYR:HB3	1:3:81:ALA:HB2	1.92	0.51
1:3:244:HIS:O	1:3:276:GLY:HA3	2.10	0.51
1:4:116:LEU:HD22	1:4:143:VAL:HG21	1.92	0.51
1:1:150:ARG:O	1:1:151:ALA:HB3	2.10	0.51
1:2:221:SER:HA	1:2:337:TRP:CE3	2.45	0.51
1:3:176:TYR:CE2	1:3:205:HIS:HB2	2.46	0.51
1:1:29:GLU:O	1:1:29:GLU:HG2	2.10	0.51
1:2:167:ILE:HD13	1:2:211:GLN:NE2	2.23	0.51
1:3:315:PHE:O	1:3:319:VAL:HG23	2.10	0.51
1:3:338:LEU:O	1:3:371:ARG:HD3	2.10	0.51
1:3:409:ASP:OD1	1:3:410:VAL:N	2.43	0.51
1:4:181:LEU:HG	1:4:184:GLY:HA2	1.91	0.51
1:4:409:ASP:OD1	1:4:410:VAL:HG23	2.10	0.51
1:1:165:LEU:HB3	1:1:169:SER:HB2	1.93	0.51
1:3:72:TYR:O	1:3:77:CYS:HB2	2.10	0.51
1:3:347:LYS:HD2	1:3:421:ASP:OD1	2.11	0.51
1:3:400:ARG:CZ	1:3:427:HIS:NE2	2.74	0.51
1:4:238:THR:O	1:4:267:ILE:HG22	2.11	0.51
1:3:87:ARG:O	1:3:87:ARG:HG3	2.11	0.51
1:1:235:GLU:N	1:1:235:GLU:CD	2.68	0.51
1:2:44:TYR:O	1:2:48:ILE:HG13	2.11	0.51
1:3:245:GLY:O	1:3:278:PHE:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:267:ILE:HD11	1:3:350:ILE:HD11	1.91	0.51
1:4:148:PHE:CD1	1:4:149:GLU:N	2.78	0.51
1:3:64:TYR:C	1:3:66:GLY:H	2.18	0.51
1:4:168:GLU:C	1:4:170:MET:H	2.19	0.51
1:4:237:ILE:HA	1:4:265:PRO:HG2	1.93	0.51
1:1:27:ARG:HA	1:1:30:GLU:OE1	2.10	0.50
1:1:235:GLU:OE1	1:1:235:GLU:HA	2.10	0.50
1:1:468:ASP:OD2	1:1:470:ARG:HB2	2.12	0.50
1:4:165:LEU:HD12	1:4:169:SER:N	2.27	0.50
1:4:415:LEU:HD12	1:4:441:ARG:HD2	1.93	0.50
1:2:176:TYR:CZ	1:2:205:HIS:HB2	2.46	0.50
1:2:234:THR:O	1:2:235:GLU:CB	2.58	0.50
1:3:331:PHE:O	1:3:334:VAL:HG22	2.11	0.50
1:3:57:LEU:O	1:3:58:ASN:HB2	2.11	0.50
1:3:72:TYR:CE1	1:3:80:TYR:HB3	2.47	0.50
1:3:123:VAL:CG2	1:3:133:LYS:HG2	2.41	0.50
1:4:187:THR:HG22	1:4:188:ILE:N	2.26	0.50
1:4:399:LYS:HG3	1:4:405:GLN:NE2	2.26	0.50
1:1:399:LYS:HG3	1:1:405:GLN:HE22	1.76	0.50
1:3:262:GLU:HA	1:3:296:HIS:CG	2.47	0.50
1:4:415:LEU:CD1	1:4:441:ARG:HB3	2.41	0.50
1:1:393:ASN:CB	1:1:409:ASP:OD2	2.59	0.50
1:4:27:ARG:O	1:4:31:LEU:HD12	2.12	0.50
1:1:450:ASN:O	1:1:451:TYR:C	2.55	0.50
1:2:187:THR:HG22	1:2:188:ILE:N	2.26	0.50
1:3:89:ILE:O	1:3:89:ILE:HG22	2.11	0.50
1:3:96:ILE:HD11	1:3:125:VAL:HG11	1.93	0.50
1:2:450:ASN:ND2	1:2:456:GLY:H	2.02	0.50
1:3:103:ALA:C	1:3:105:SER:N	2.69	0.50
1:4:166:ASP:OD1	1:4:210:TYR:HB3	2.11	0.50
1:3:72:TYR:HH	1:3:80:TYR:HD1	1.59	0.50
1:1:320:LYS:HE2	1:1:325:ALA:CB	2.41	0.49
1:2:24:ALA:O	1:2:27:ARG:HB3	2.12	0.49
1:3:283:ILE:HD11	1:3:287:PHE:CZ	2.47	0.49
1:4:58:ASN:C	1:4:58:ASN:ND2	2.68	0.49
1:4:91:LEU:O	1:4:92:ASP:HB2	2.11	0.49
1:1:186:VAL:HG13	1:1:191:MET:HE3	1.94	0.49
1:2:182:GLU:O	1:2:184:GLY:N	2.43	0.49
1:2:201:GLN:N	1:2:201:GLN:NE2	2.58	0.49
1:3:83:GLY:O	1:3:86:THR:HB	2.12	0.49
1:3:346:GLY:O	1:3:420:LEU:HD23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:393:ASN:CB	1:4:409:ASP:OD2	2.60	0.49
1:3:32:LYS:O	1:3:36:ASN:HB3	2.13	0.49
1:3:64:TYR:N	1:3:64:TYR:CD1	2.79	0.49
1:3:125:VAL:HG13	1:3:126:LYS:HG3	1.94	0.49
1:4:450:ASN:ND2	1:4:456:GLY:HA2	2.27	0.49
1:1:32:LYS:O	1:1:32:LYS:HG2	2.13	0.49
1:1:161:VAL:C	1:1:163:ASP:N	2.67	0.49
1:2:313:TYR:HA	1:2:487:MET:HE3	1.94	0.49
1:4:489:TYR:CD1	1:4:489:TYR:N	2.80	0.49
1:2:415:LEU:CD1	1:2:441:ARG:HB3	2.42	0.49
1:1:242:ASP:OD1	1:1:426:SER:HB3	2.12	0.49
1:1:415:LEU:HD12	1:1:441:ARG:HD2	1.95	0.49
1:3:320:LYS:HE2	1:3:325:ALA:CB	2.42	0.49
1:3:356:PHE:CD1	1:3:356:PHE:N	2.79	0.49
1:4:148:PHE:CD1	1:4:148:PHE:C	2.90	0.49
1:2:267:ILE:HD11	1:2:350:ILE:HD11	1.93	0.49
1:2:360:GLY:O	1:2:361:VAL:O	2.30	0.49
1:3:113:ARG:C	1:3:117:ARG:HG3	2.37	0.49
1:3:492:THR:HG22	1:3:495:GLN:OE1	2.12	0.49
1:1:355:LEU:CD1	1:1:411:THR:HA	2.43	0.49
1:2:172:ILE:HG23	1:2:173:GLU:H	1.77	0.49
1:3:450:ASN:O	1:3:451:TYR:C	2.56	0.49
1:3:468:ASP:C	1:3:470:ARG:H	2.21	0.49
1:2:340:LEU:HB3	1:2:384:LEU:HD23	1.95	0.49
1:2:409:ASP:OD1	1:2:410:VAL:HG23	2.12	0.49
1:2:445:VAL:O	1:2:445:VAL:HG13	2.13	0.49
1:3:351:MET:HE3	1:3:354:GLY:C	2.37	0.49
1:1:301:ARG:NH1	1:1:336:GLU:HA	2.27	0.49
1:2:351:MET:HE3	1:2:354:GLY:C	2.38	0.49
1:4:232:LYS:HE2	1:4:235:GLU:CB	2.43	0.49
1:1:87:ARG:CZ	1:1:91:LEU:HD21	2.43	0.48
1:1:165:LEU:CG	1:1:168:GLU:HG3	2.42	0.48
1:3:351:MET:CE	1:3:354:GLY:HA2	2.42	0.48
1:2:48:ILE:HD13	1:2:72:TYR:CE2	2.48	0.48
1:2:485:LYS:HB3	1:2:486:PRO:HD2	1.95	0.48
1:3:35:ALA:HB2	1:3:50:PHE:HB3	1.94	0.48
1:1:400:ARG:CZ	1:1:427:HIS:NE2	2.76	0.48
1:3:35:ALA:CA	1:3:50:PHE:HB2	2.42	0.48
1:1:450:ASN:HD22	1:1:456:GLY:CA	2.26	0.48
1:3:415:LEU:HD12	1:3:441:ARG:HD2	1.96	0.48
1:4:23:GLY:O	1:4:25:LEU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:283:ILE:HG23	1:4:284:LEU:N	2.28	0.48
1:1:38:TYR:HD1	1:1:46:ASN:HB3	1.78	0.48
1:1:274:ASP:O	1:1:276:GLY:N	2.42	0.48
1:1:400:ARG:NE	1:1:427:HIS:NE2	2.62	0.48
1:3:181:LEU:HD23	1:3:211:GLN:OE1	2.14	0.48
1:3:213:LEU:HD21	1:3:331:PHE:CE1	2.48	0.48
1:2:167:ILE:O	1:2:207:LYS:HE3	2.14	0.48
1:2:195:MET:HE1	1:2:259:LEU:HD22	1.95	0.48
1:2:478:ALA:O	1:2:479:VAL:HB	2.13	0.48
1:3:112:PHE:HB2	1:3:143:VAL:HG13	1.96	0.48
1:3:165:LEU:CB	1:3:168:GLU:HB2	2.37	0.48
1:4:371:ARG:O	1:4:373:ARG:N	2.47	0.48
1:4:450:ASN:HD22	1:4:456:GLY:HA2	1.77	0.48
1:1:120:GLU:HB2	1:1:136:TYR:CE1	2.49	0.48
1:2:181:LEU:HD12	1:2:182:GLU:N	2.28	0.48
1:1:332:SER:O	1:1:336:GLU:HG3	2.13	0.48
1:1:486:PRO:CB	1:1:498:MET:HE1	2.42	0.48
1:3:29:GLU:HA	1:3:64:TYR:OH	2.14	0.48
1:4:87:ARG:NH2	1:4:91:LEU:HD21	2.29	0.48
1:2:468:ASP:C	1:2:470:ARG:H	2.22	0.48
1:3:95:TYR:CD2	1:3:98:GLY:HA3	2.49	0.48
1:1:283:ILE:HG23	1:1:284:LEU:N	2.29	0.47
1:2:148:PHE:C	1:2:148:PHE:CD1	2.91	0.47
1:4:158:LYS:O	1:4:158:LYS:HG3	2.13	0.47
1:4:361:VAL:HA	1:4:365:ASP:OD1	2.14	0.47
1:1:44:TYR:O	1:1:48:ILE:HG13	2.14	0.47
1:1:196:GLN:O	1:1:197:TRP:C	2.57	0.47
1:2:395:ARG:HH11	1:2:395:ARG:CG	2.27	0.47
1:4:166:ASP:O	1:4:167:ILE:C	2.57	0.47
1:4:207:LYS:O	1:4:211:GLN:HG3	2.14	0.47
1:2:181:LEU:HD11	1:2:185:LYS:N	2.28	0.47
1:3:45:GLU:C	1:3:47:ALA:H	2.21	0.47
1:3:81:ALA:HA	1:3:84:ASP:HB3	1.97	0.47
1:3:127:PRO:O	1:3:129:ASP:N	2.45	0.47
1:4:112:PHE:H	1:4:112:PHE:HD1	1.55	0.47
1:4:450:ASN:HD22	1:4:456:GLY:CA	2.27	0.47
1:1:35:ALA:HB2	1:1:50:PHE:CB	2.44	0.47
1:1:279:SER:O	1:1:283:ILE:HG22	2.14	0.47
1:1:351:MET:CE	1:1:354:GLY:HA2	2.45	0.47
1:1:399:LYS:CD	1:1:405:GLN:HE22	2.27	0.47
1:2:306:THR:HG23	1:2:374:GLN:HE22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:120:GLU:O	1:3:123:VAL:HG12	2.13	0.47
1:4:395:ARG:HH11	1:4:395:ARG:HG2	1.79	0.47
1:1:107:MET:O	1:1:110:GLY:N	2.43	0.47
1:1:167:ILE:HD11	1:1:211:GLN:HE21	1.79	0.47
1:2:351:MET:HE3	1:2:354:GLY:CA	2.45	0.47
1:3:42:LYS:HG2	1:3:44:TYR:OH	2.15	0.47
1:3:234:THR:O	1:3:235:GLU:CB	2.62	0.47
1:3:415:LEU:CD1	1:3:441:ARG:HB3	2.43	0.47
1:4:73:LEU:HD22	1:4:81:ALA:HB1	1.97	0.47
1:4:351:MET:HE3	1:4:354:GLY:C	2.40	0.47
1:1:29:GLU:HG3	1:1:32:LYS:HB3	1.97	0.47
1:1:324:THR:C	1:1:326:GLN:N	2.70	0.47
1:2:146:LYS:HE2	1:2:311:GLN:OE1	2.13	0.47
1:1:38:TYR:HB3	1:1:43:ASP:HB3	1.95	0.47
1:1:182:GLU:O	1:1:182:GLU:HG2	2.14	0.47
1:2:224:SER:C	1:2:371:ARG:NH2	2.73	0.47
1:4:136:TYR:CE2	1:4:140:ASN:ND2	2.82	0.47
1:4:313:TYR:HA	1:4:487:MET:HE3	1.97	0.47
1:4:429:VAL:HG22	1:4:446:PHE:CE2	2.49	0.47
1:4:432:GLU:OE1	1:4:432:GLU:HA	2.15	0.47
1:2:273:VAL:O	1:2:274:ASP:HB2	2.13	0.47
1:4:306:THR:HG23	1:4:374:GLN:HE22	1.77	0.47
1:1:345:ASN:C	1:1:347:LYS:H	2.23	0.47
1:1:371:ARG:O	1:1:373:ARG:N	2.48	0.47
1:2:355:LEU:CD1	1:2:411:THR:HA	2.44	0.47
1:3:44:TYR:O	1:3:47:ALA:HB3	2.15	0.47
1:3:66:GLY:O	1:3:69:SER:N	2.44	0.47
1:4:493:LEU:C	1:4:494:LEU:HG	2.40	0.47
1:3:185:LYS:HE3	1:3:185:LYS:CA	2.44	0.46
1:3:345:ASN:C	1:3:347:LYS:H	2.22	0.46
1:1:232:LYS:HE2	1:1:235:GLU:CB	2.45	0.46
1:3:31:LEU:HB2	1:3:54:ALA:CB	2.40	0.46
1:3:35:ALA:HB2	1:3:50:PHE:CB	2.45	0.46
1:3:168:GLU:O	1:3:170:MET:N	2.48	0.46
1:3:463:HIS:HB2	1:3:472:GLN:HB2	1.97	0.46
1:4:146:LYS:NZ	1:4:311:GLN:NE2	2.55	0.46
1:4:450:ASN:ND2	1:4:456:GLY:H	2.10	0.46
1:4:464:LEU:HD12	1:4:464:LEU:HA	1.80	0.46
1:1:187:THR:CG2	1:1:188:ILE:N	2.78	0.46
1:1:346:GLY:O	1:1:420:LEU:HD23	2.15	0.46
1:2:120:GLU:HB2	1:2:136:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:232:LYS:O	1:3:466:GLY:HA3	2.15	0.46
1:3:116:LEU:HD22	1:3:143:VAL:CG2	2.37	0.46
1:3:383:ASP:HA	1:3:403:SER:OG	2.15	0.46
1:1:403:SER:OG	1:1:404:CYS:N	2.43	0.46
1:3:116:LEU:CD2	1:3:143:VAL:HG21	2.35	0.46
1:4:171:THR:O	1:4:172:ILE:CB	2.63	0.46
1:4:267:ILE:HD12	1:4:342:GLN:CD	2.41	0.46
1:3:393:ASN:CB	1:3:409:ASP:OD2	2.64	0.46
1:4:80:TYR:CE1	1:4:399:LYS:HG2	2.50	0.46
1:4:131:ASP:O	1:4:134:MET:N	2.48	0.46
1:4:275:ARG:HG3	1:4:275:ARG:NH1	2.31	0.46
1:1:356:PHE:CZ	1:1:384:LEU:HD13	2.51	0.46
1:2:165:LEU:O	1:2:168:GLU:OE2	2.34	0.46
1:2:267:ILE:HD12	1:2:342:GLN:CD	2.40	0.46
1:3:336:GLU:O	1:3:371:ARG:HG2	2.16	0.46
1:4:210:TYR:O	1:4:214:VAL:HG23	2.16	0.46
1:4:356:PHE:CD1	1:4:356:PHE:N	2.83	0.46
1:4:400:ARG:CZ	1:4:427:HIS:NE2	2.79	0.46
1:4:468:ASP:OD2	1:4:470:ARG:HB2	2.16	0.46
1:1:161:VAL:C	1:1:163:ASP:H	2.22	0.46
1:1:351:MET:HE3	1:1:354:GLY:CA	2.45	0.46
1:1:412:LYS:HE2	1:1:416:GLU:OE1	2.16	0.46
1:2:275:ARG:HG3	1:2:275:ARG:NH1	2.30	0.46
1:3:375:PRO:HA	1:3:376:PRO:HD3	1.82	0.46
1:3:436:VAL:CG1	1:3:440:GLY:HA2	2.46	0.46
1:4:211:GLN:O	1:4:215:GLN:HG3	2.15	0.46
1:4:239:VAL:HA	1:4:267:ILE:HG23	1.97	0.46
1:4:355:LEU:CD1	1:4:411:THR:HA	2.46	0.46
1:3:112:PHE:O	1:3:113:ARG:C	2.59	0.46
1:3:267:ILE:HD12	1:3:342:GLN:CD	2.41	0.46
1:3:324:THR:C	1:3:326:GLN:N	2.72	0.46
1:4:201:GLN:O	1:4:202:LYS:CB	2.64	0.46
1:3:60:SER:HA	1:3:87:ARG:HH21	1.80	0.46
1:3:60:SER:O	1:3:91:LEU:HD22	2.16	0.46
1:3:64:TYR:C	1:3:66:GLY:N	2.74	0.46
1:3:176:TYR:CE1	1:3:178:GLY:HA3	2.52	0.46
1:4:356:PHE:CD1	1:4:361:VAL:HG11	2.51	0.46
1:4:452:CYS:C	1:4:454:GLN:N	2.74	0.46
1:1:191:MET:O	1:1:195:MET:HG3	2.15	0.45
1:1:450:ASN:HD22	1:1:456:GLY:HA2	1.79	0.45
1:3:179:PRO:HB2	1:3:190:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:425:ARG:HD3	1:3:425:ARG:C	2.41	0.45
1:4:136:TYR:O	1:4:140:ASN:HB2	2.16	0.45
1:4:345:ASN:C	1:4:347:LYS:H	2.24	0.45
1:1:85:ALA:O	1:1:89:ILE:HG13	2.16	0.45
1:3:181:LEU:CD2	1:3:184:GLY:HA2	2.44	0.45
1:3:304:HIS:C	1:3:306:THR:H	2.24	0.45
1:4:336:GLU:O	1:4:371:ARG:HG2	2.17	0.45
1:3:371:ARG:O	1:3:373:ARG:N	2.50	0.45
1:1:29:GLU:HG3	1:1:32:LYS:CD	2.46	0.45
1:2:96:ILE:HG13	1:2:126:LYS:HE3	1.97	0.45
1:3:112:PHE:HB2	1:3:113:ARG:H	1.53	0.45
1:3:168:GLU:C	1:3:170:MET:H	2.24	0.45
1:4:245:GLY:HA2	1:4:282:VAL:HG21	1.99	0.45
1:4:324:THR:C	1:4:326:GLN:N	2.74	0.45
1:2:131:ASP:O	1:2:134:MET:N	2.50	0.45
1:4:195:MET:HE1	1:4:259:LEU:HD22	1.99	0.45
1:1:138:GLU:HB3	1:1:493:LEU:HD11	1.99	0.45
1:1:388:ASP:OD1	1:1:427:HIS:HD2	1.99	0.45
1:1:492:THR:HG22	1:1:495:GLN:OE1	2.17	0.45
1:2:279:SER:O	1:2:283:ILE:HG22	2.16	0.45
1:3:26:LYS:O	1:3:30:GLU:HG3	2.16	0.45
1:3:89:ILE:HD11	1:3:99:TYR:HA	1.99	0.45
1:4:64:TYR:N	1:4:64:TYR:HD1	2.15	0.45
1:3:42:LYS:HA	1:3:44:TYR:CZ	2.51	0.45
1:3:283:ILE:HG23	1:3:284:LEU:N	2.32	0.45
1:3:307:ASP:N	1:3:374:GLN:HE22	2.10	0.45
1:1:201:GLN:O	1:1:202:LYS:CB	2.62	0.45
1:1:292:LEU:HD23	1:1:293:TYR:CE2	2.51	0.45
1:2:188:ILE:HG12	1:2:292:LEU:HD21	1.98	0.45
1:3:445:VAL:O	1:3:445:VAL:HG13	2.17	0.45
1:4:64:TYR:N	1:4:64:TYR:CD1	2.83	0.45
1:4:336:GLU:HB3	1:4:372:ASN:HA	1.98	0.45
1:1:96:ILE:HG13	1:1:126:LYS:HE3	1.99	0.45
1:1:130:LYS:H	1:1:130:LYS:HG3	1.59	0.45
1:2:160:SER:C	1:2:162:VAL:N	2.74	0.45
1:3:66:GLY:O	1:3:67:ASN:C	2.60	0.45
1:3:73:LEU:HD13	1:3:81:ALA:HB3	1.99	0.45
1:2:262:GLU:HA	1:2:296:HIS:CG	2.52	0.45
1:3:115:ALA:O	1:3:119:TYR:CD2	2.71	0.45
1:3:274:ASP:C	1:3:276:GLY:H	2.25	0.45
1:3:481:HIS:O	1:3:482:PRO:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:232:LYS:O	1:4:233:GLU:C	2.58	0.45
1:1:218:GLU:OE2	1:1:222:LYS:NZ	2.50	0.44
1:2:172:ILE:HD11	1:2:180:LYS:NZ	2.32	0.44
1:2:213:LEU:O	1:2:216:VAL:HG12	2.17	0.44
1:2:356:PHE:CD1	1:2:356:PHE:N	2.84	0.44
1:3:201:GLN:N	1:3:201:GLN:NE2	2.63	0.44
1:3:468:ASP:OD2	1:3:470:ARG:HB2	2.17	0.44
1:4:213:LEU:HD21	1:4:331:PHE:CE1	2.52	0.44
1:1:463:HIS:HB2	1:1:472:GLN:HB2	1.99	0.44
1:2:207:LYS:O	1:2:211:GLN:HG3	2.17	0.44
1:3:191:MET:O	1:3:195:MET:HG3	2.18	0.44
1:4:481:HIS:O	1:4:482:PRO:O	2.35	0.44
1:1:245:GLY:O	1:1:278:PHE:HB2	2.18	0.44
1:1:273:VAL:O	1:1:274:ASP:HB2	2.17	0.44
1:2:70:LEU:HB2	1:2:101:ARG:HE	1.83	0.44
1:2:194:LEU:HD11	1:2:198:TYR:CZ	2.52	0.44
1:2:316:GLU:HA	1:2:328:TYR:CD1	2.52	0.44
1:2:415:LEU:HD12	1:2:441:ARG:HD2	1.99	0.44
1:3:122:VAL:O	1:3:122:VAL:HG12	2.16	0.44
1:3:438:HIS:C	1:3:440:GLY:H	2.25	0.44
1:4:166:ASP:HB3	1:4:167:ILE:H	1.67	0.44
1:4:181:LEU:HD11	1:4:186:VAL:H	1.82	0.44
1:1:136:TYR:O	1:1:140:ASN:HB2	2.17	0.44
1:1:306:THR:HG23	1:1:374:GLN:NE2	2.33	0.44
1:2:51:TYR:O	1:2:55:ILE:HG12	2.18	0.44
1:2:399:LYS:HD2	1:2:405:GLN:HE22	1.81	0.44
1:2:481:HIS:HB2	1:2:482:PRO:HD2	1.98	0.44
1:3:267:ILE:HD13	1:3:350:ILE:CD1	2.40	0.44
1:1:165:LEU:HD11	1:1:168:GLU:HG3	1.98	0.44
1:2:32:LYS:O	1:2:36:ASN:HB2	2.17	0.44
1:3:44:TYR:HA	1:3:47:ALA:CB	2.47	0.44
1:3:107:MET:SD	1:3:493:LEU:HD13	2.58	0.44
1:4:307:ASP:N	1:4:374:GLN:HE22	2.14	0.44
1:1:166:ASP:O	1:1:167:ILE:C	2.60	0.44
1:1:278:PHE:CZ	1:1:482:PRO:HG2	2.53	0.44
1:3:107:MET:HG3	1:3:115:ALA:HB1	2.00	0.44
1:3:147:ALA:HA	1:3:150:ARG:HH22	1.80	0.44
1:3:220:LEU:HB3	1:3:337:TRP:O	2.18	0.44
1:3:336:GLU:HB3	1:3:372:ASN:HA	2.00	0.44
1:4:171:THR:O	1:4:172:ILE:CG2	2.65	0.44
1:4:181:LEU:CG	1:4:184:GLY:HA2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:304:HIS:C	1:1:306:THR:H	2.26	0.44
1:1:468:ASP:C	1:1:470:ARG:H	2.25	0.44
1:1:487:MET:HG3	1:1:498:MET:HE2	1.96	0.44
1:2:49:LYS:HA	1:2:49:LYS:HD3	1.78	0.44
1:3:44:TYR:CA	1:3:47:ALA:HB3	2.47	0.44
1:3:96:ILE:HG13	1:3:126:LYS:HZ1	1.82	0.44
1:4:181:LEU:HD11	1:4:186:VAL:CA	2.48	0.44
1:4:182:GLU:C	1:4:184:GLY:N	2.76	0.44
1:1:120:GLU:O	1:1:123:VAL:HG12	2.18	0.44
1:1:194:LEU:HD11	1:1:198:TYR:CZ	2.53	0.44
1:1:232:LYS:O	1:1:466:GLY:HA3	2.18	0.44
1:1:316:GLU:HA	1:1:328:TYR:CD1	2.53	0.44
1:2:312:ILE:CG2	1:2:494:LEU:HD13	2.48	0.44
1:3:50:PHE:HA	1:3:53:GLN:NE2	2.32	0.44
1:3:159:ARG:O	1:3:160:SER:HB3	2.18	0.44
1:3:395:ARG:CG	1:3:395:ARG:NH1	2.78	0.44
1:4:218:GLU:OE2	1:4:222:LYS:NZ	2.51	0.44
1:3:88:ALA:HB1	1:3:95:TYR:HD2	1.82	0.43
1:4:51:TYR:O	1:4:55:ILE:HG12	2.18	0.43
1:4:399:LYS:HG3	1:4:405:GLN:HE22	1.83	0.43
1:4:426:SER:O	1:4:428:GLU:N	2.50	0.43
1:1:33:THR:HA	1:1:36:ASN:HB3	1.99	0.43
1:1:213:LEU:HD21	1:1:331:PHE:CE1	2.53	0.43
1:2:142:ILE:HG22	1:2:146:LYS:HE3	1.99	0.43
1:2:150:ARG:HA	1:2:150:ARG:NE	2.33	0.43
1:2:218:GLU:OE2	1:2:222:LYS:NZ	2.51	0.43
1:2:390:GLN:N	1:2:406:PHE:O	2.51	0.43
1:3:127:PRO:HB2	1:3:128:HIS:H	1.66	0.43
1:3:468:ASP:OD1	1:3:470:ARG:NH1	2.51	0.43
1:1:91:LEU:O	1:1:92:ASP:HB2	2.17	0.43
1:1:360:GLY:O	1:1:361:VAL:O	2.37	0.43
1:4:286:LEU:HB3	1:4:299:LEU:HD21	2.00	0.43
1:4:332:SER:O	1:4:336:GLU:HG3	2.19	0.43
1:1:464:LEU:HA	1:1:464:LEU:HD12	1.74	0.43
1:1:486:PRO:O	1:1:498:MET:CE	2.67	0.43
1:2:357:SER:O	1:2:395:ARG:NH2	2.51	0.43
1:3:242:ASP:OD1	1:3:426:SER:HB3	2.19	0.43
1:3:275:ARG:NH1	1:3:451:TYR:OH	2.51	0.43
1:1:195:MET:HE1	1:1:259:LEU:HD21	2.00	0.43
1:1:468:ASP:OD1	1:1:470:ARG:NH1	2.52	0.43
1:2:200:ASP:O	1:2:202:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:249:ASP:OD1	1:2:478:ALA:O	2.36	0.43
1:3:487:MET:O	1:3:495:GLN:NE2	2.50	0.43
1:4:185:LYS:O	1:4:186:VAL:HB	2.19	0.43
1:1:165:LEU:HD12	1:1:165:LEU:HA	1.80	0.43
1:1:185:LYS:O	1:1:186:VAL:CB	2.67	0.43
1:2:109:LEU:HD12	1:2:111:LYS:HD2	2.01	0.43
1:2:375:PRO:HA	1:2:376:PRO:HD3	1.81	0.43
1:4:179:PRO:HD3	1:4:197:TRP:CD2	2.54	0.43
1:1:32:LYS:O	1:1:36:ASN:HB2	2.18	0.43
1:1:307:ASP:N	1:1:374:GLN:HE22	2.11	0.43
1:1:489:TYR:O	1:1:490:ALA:HB3	2.17	0.43
1:2:450:ASN:O	1:2:451:TYR:C	2.60	0.43
1:4:181:LEU:CD2	1:4:184:GLY:HA2	2.48	0.43
1:1:38:TYR:N	1:1:38:TYR:CD2	2.87	0.43
1:1:167:ILE:CD1	1:1:211:GLN:HE21	2.31	0.43
1:1:267:ILE:HD12	1:1:342:GLN:CD	2.44	0.43
1:3:72:TYR:HD2	1:3:72:TYR:HA	1.77	0.43
1:3:209:ALA:O	1:3:213:LEU:HG	2.18	0.43
1:3:233:GLU:O	1:3:467:SER:N	2.51	0.43
1:4:425:ARG:O	1:4:444:THR:HA	2.19	0.43
1:1:313:TYR:HA	1:1:487:MET:HE3	2.00	0.43
1:1:485:LYS:HB3	1:1:486:PRO:HD2	2.01	0.43
1:1:494:LEU:O	1:1:497:GLY:N	2.44	0.43
1:2:112:PHE:H	1:2:112:PHE:HD1	1.59	0.43
1:2:173:GLU:HG2	1:2:176:TYR:HB2	2.00	0.43
1:2:188:ILE:O	1:2:192:LYS:HG3	2.19	0.43
1:2:451:TYR:HD1	1:2:455:MET:HE3	1.84	0.43
1:3:389:PRO:HD3	1:3:425:ARG:CZ	2.49	0.43
1:4:366:ILE:O	1:4:369:ILE:HG13	2.19	0.43
1:4:468:ASP:C	1:4:470:ARG:H	2.27	0.43
1:1:233:GLU:O	1:1:467:SER:N	2.52	0.43
1:1:320:LYS:HG2	1:1:325:ALA:CA	2.45	0.43
1:1:64:TYR:N	1:1:64:TYR:CD1	2.87	0.42
1:2:432:GLU:OE1	1:2:458:LYS:NZ	2.52	0.42
1:2:468:ASP:OD1	1:2:470:ARG:NH1	2.52	0.42
1:3:238:THR:O	1:3:267:ILE:HG22	2.19	0.42
1:3:389:PRO:HB3	1:3:442:CYS:SG	2.59	0.42
1:4:159:ARG:C	1:4:161:VAL:N	2.75	0.42
1:4:188:ILE:HG12	1:4:292:LEU:HD21	1.99	0.42
1:4:252:ASN:CG	1:4:479:VAL:HG21	2.44	0.42
1:1:391:PRO:HG2	1:1:392:GLN:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:312:ILE:HG23	1:2:494:LEU:HD11	2.01	0.42
1:4:166:ASP:HA	1:4:170:MET:HG3	2.01	0.42
1:4:181:LEU:HD23	1:4:184:GLY:HA2	2.00	0.42
1:2:361:VAL:HA	1:2:365:ASP:OD1	2.19	0.42
1:3:31:LEU:HD13	1:3:53:GLN:HB3	2.01	0.42
1:3:45:GLU:C	1:3:47:ALA:N	2.78	0.42
1:4:27:ARG:HA	1:4:30:GLU:HG3	2.01	0.42
1:1:49:LYS:HA	1:1:49:LYS:HD3	1.82	0.42
1:2:373:ARG:HD2	1:2:374:GLN:O	2.18	0.42
1:4:167:ILE:HD13	1:4:211:GLN:NE2	2.31	0.42
1:2:220:LEU:HD13	1:2:338:LEU:HD23	2.01	0.42
1:2:479:VAL:HA	1:2:480:PRO:HD2	1.90	0.42
1:4:356:PHE:CZ	1:4:361:VAL:HG11	2.55	0.42
1:4:489:TYR:O	1:4:490:ALA:HB3	2.18	0.42
1:1:323:TYR:CD2	1:1:327:MET:HE3	2.55	0.42
1:1:481:HIS:O	1:1:482:PRO:O	2.37	0.42
1:1:498:MET:CE	1:1:498:MET:CG	2.98	0.42
1:2:432:GLU:OE1	1:2:432:GLU:HA	2.20	0.42
1:3:274:ASP:O	1:3:276:GLY:N	2.42	0.42
1:3:388:ASP:OD1	1:3:427:HIS:HD2	2.02	0.42
1:4:356:PHE:CZ	1:4:384:LEU:HD13	2.54	0.42
1:1:55:ILE:CD1	1:1:64:TYR:HB3	2.50	0.42
1:1:64:TYR:N	1:1:64:TYR:HD1	2.17	0.42
1:1:74:ARG:HG3	1:1:74:ARG:HH11	1.84	0.42
1:2:373:ARG:CZ	1:2:376:PRO:HG3	2.50	0.42
1:3:275:ARG:HG3	1:3:275:ARG:NH1	2.31	0.42
1:3:351:MET:SD	1:3:351:MET:N	2.92	0.42
1:3:389:PRO:CD	1:3:425:ARG:CZ	2.98	0.42
1:3:489:TYR:CD1	1:3:489:TYR:N	2.87	0.42
1:1:33:THR:O	1:1:37:ASP:CB	2.67	0.42
1:1:489:TYR:N	1:1:489:TYR:CD1	2.88	0.42
1:3:244:HIS:CD2	1:3:451:TYR:HE2	2.38	0.42
1:3:279:SER:O	1:3:283:ILE:HG22	2.20	0.42
1:4:40:LYS:C	1:4:42:LYS:H	2.27	0.42
1:4:185:LYS:HE3	1:4:185:LYS:CA	2.23	0.42
1:1:40:LYS:C	1:1:42:LYS:H	2.28	0.42
1:1:165:LEU:CD2	1:1:168:GLU:HB2	2.50	0.42
1:1:181:LEU:O	1:1:183:ASP:N	2.52	0.42
1:1:211:GLN:O	1:1:215:GLN:HG3	2.20	0.42
1:2:248:TYR:O	1:2:479:VAL:HG11	2.20	0.42
1:2:275:ARG:NH1	1:2:451:TYR:OH	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:312:ILE:O	1:2:494:LEU:HD13	2.20	0.42
1:2:395:ARG:CG	1:2:395:ARG:NH1	2.83	0.42
1:3:184:GLY:O	1:3:215:GLN:NE2	2.53	0.42
1:1:421:ASP:OD1	1:1:421:ASP:N	2.53	0.42
1:3:464:LEU:HD12	1:3:464:LEU:HA	1.75	0.42
1:4:70:LEU:O	1:4:73:LEU:HB2	2.20	0.42
1:4:168:GLU:HB3	1:4:169:SER:H	1.44	0.42
1:4:248:TYR:CE1	1:4:482:PRO:HD2	2.55	0.42
1:4:279:SER:O	1:4:283:ILE:HG22	2.19	0.42
1:2:393:ASN:CB	1:2:409:ASP:OD2	2.68	0.41
1:3:87:ARG:NH2	1:3:91:LEU:HD21	2.35	0.41
1:3:135:LYS:CE	1:3:496:LEU:HD12	2.50	0.41
1:3:411:THR:O	1:3:415:LEU:HG	2.20	0.41
1:4:42:LYS:HD3	1:4:454:GLN:O	2.20	0.41
1:4:399:LYS:HD2	1:4:405:GLN:HE22	1.85	0.41
1:4:453:ASP:OD1	1:4:481:HIS:HE1	2.03	0.41
1:1:181:LEU:HD23	1:1:184:GLY:HA2	2.02	0.41
1:1:479:VAL:HA	1:1:480:PRO:HD2	1.88	0.41
1:2:489:TYR:N	1:2:489:TYR:CD1	2.87	0.41
1:3:75:THR:O	1:3:76:GLU:HB2	2.20	0.41
1:4:72:TYR:HE1	1:4:84:ASP:OD2	2.03	0.41
1:1:390:GLN:N	1:1:406:PHE:O	2.53	0.41
1:1:481:HIS:C	1:1:482:PRO:O	2.60	0.41
1:2:64:TYR:N	1:2:64:TYR:CD1	2.88	0.41
1:2:168:GLU:CD	1:2:168:GLU:H	2.28	0.41
1:2:181:LEU:CD1	1:2:186:VAL:N	2.84	0.41
1:2:413:ALA:O	1:2:414:PHE:C	2.63	0.41
1:3:31:LEU:HD13	1:3:53:GLN:CB	2.49	0.41
1:3:65:TYR:CD2	1:3:87:ARG:HG2	2.55	0.41
1:3:73:LEU:HD12	1:3:73:LEU:HA	1.91	0.41
1:1:280:VAL:HG23	1:1:318:GLU:OE2	2.20	0.41
1:1:362:THR:O	1:1:365:ASP:HB2	2.20	0.41
1:1:487:MET:O	1:1:495:GLN:HG2	2.21	0.41
1:2:165:LEU:O	1:2:166:ASP:HB2	2.20	0.41
1:2:168:GLU:O	1:2:169:SER:C	2.64	0.41
1:2:312:ILE:HG23	1:2:494:LEU:HD13	2.01	0.41
1:3:38:TYR:HE2	1:3:50:PHE:CZ	2.38	0.41
1:3:355:LEU:CD1	1:3:411:THR:HA	2.50	0.41
1:4:166:ASP:HA	1:4:170:MET:CG	2.49	0.41
1:4:463:HIS:HB2	1:4:472:GLN:HB2	2.02	0.41
1:1:445:VAL:O	1:1:445:VAL:HG13	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:70:LEU:HB2	1:2:101:ARG:NE	2.34	0.41
1:2:283:ILE:HG23	1:2:284:LEU:N	2.35	0.41
1:3:163:ASP:CG	1:3:164:SER:N	2.77	0.41
1:3:232:LYS:O	1:3:233:GLU:C	2.61	0.41
1:4:217:LYS:HB2	1:4:334:VAL:CG1	2.37	0.41
1:1:160:SER:HB3	1:1:333:GLU:OE2	2.21	0.41
1:2:106:ASN:O	1:2:111:LYS:HG3	2.20	0.41
1:2:162:VAL:HG12	1:2:162:VAL:O	2.20	0.41
1:2:452:CYS:C	1:2:454:GLN:N	2.76	0.41
1:3:303:ASN:HB2	1:3:386:TRP:CE2	2.55	0.41
1:1:275:ARG:HG3	1:1:275:ARG:NH1	2.31	0.41
1:2:216:VAL:O	1:2:220:LEU:HG	2.20	0.41
1:3:31:LEU:HD13	1:3:54:ALA:N	2.36	0.41
1:3:190:PHE:CD2	1:3:191:MET:HE2	2.56	0.41
1:3:351:MET:HE2	1:3:354:GLY:HA2	2.01	0.41
1:4:347:LYS:HD2	1:4:421:ASP:OD1	2.20	0.41
1:4:373:ARG:CZ	1:4:376:PRO:HG3	2.50	0.41
1:1:217:LYS:NZ	1:1:333:GLU:OE1	2.51	0.41
1:1:436:VAL:CG1	1:1:440:GLY:HA2	2.51	0.41
1:2:136:TYR:CE2	1:2:140:ASN:ND2	2.89	0.41
1:2:181:LEU:HD23	1:2:211:GLN:CD	2.46	0.41
1:2:425:ARG:O	1:2:444:THR:HA	2.21	0.41
1:3:481:HIS:HB2	1:3:482:PRO:HD2	2.02	0.41
1:4:74:ARG:HA	1:4:74:ARG:HD3	1.93	0.41
1:4:415:LEU:HD23	1:4:415:LEU:HA	1.93	0.41
1:1:29:GLU:OE2	1:1:32:LYS:HD3	2.21	0.41
1:1:112:PHE:H	1:1:112:PHE:HD1	1.55	0.41
1:2:136:TYR:O	1:2:140:ASN:HB2	2.21	0.41
1:2:181:LEU:HD23	1:2:211:GLN:OE1	2.21	0.41
1:2:181:LEU:HD13	1:2:186:VAL:N	2.36	0.41
1:3:128:HIS:HA	1:3:133:LYS:CE	2.51	0.41
1:3:195:MET:HE1	1:3:259:LEU:HD22	2.02	0.41
1:3:197:TRP:CH2	1:3:202:LYS:HD3	2.56	0.41
1:3:478:ALA:O	1:3:479:VAL:HB	2.19	0.41
1:4:63:ILE:O	1:4:64:TYR:C	2.63	0.41
1:4:123:VAL:O	1:4:123:VAL:HG22	2.21	0.41
1:4:220:LEU:CD1	1:4:338:LEU:HD23	2.50	0.41
1:1:68:ARG:HG2	1:1:72:TYR:CE1	2.56	0.41
1:1:493:LEU:HD23	1:1:493:LEU:HA	1.91	0.41
1:3:181:LEU:HG	1:3:184:GLY:CA	2.44	0.41
1:4:267:ILE:HD11	1:4:350:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:122:VAL:C	1:4:124:LYS:N	2.79	0.40
1:4:130:LYS:O	1:4:132:ALA:N	2.48	0.40
1:4:223:LEU:O	1:4:371:ARG:NH2	2.36	0.40
1:4:343:CYS:SG	1:4:346:GLY:HA2	2.62	0.40
1:1:112:PHE:HB3	1:1:146:LYS:HD2	2.02	0.40
1:1:163:ASP:O	1:1:164:SER:C	2.63	0.40
1:1:188:ILE:O	1:1:192:LYS:HG3	2.21	0.40
1:1:375:PRO:HA	1:1:376:PRO:HD3	1.74	0.40
1:1:452:CYS:C	1:1:454:GLN:N	2.77	0.40
1:2:232:LYS:HE2	1:2:235:GLU:CB	2.51	0.40
1:3:87:ARG:O	1:3:91:LEU:HD12	2.20	0.40
1:1:338:LEU:C	1:1:371:ARG:HD3	2.46	0.40
1:1:357:SER:O	1:1:395:ARG:NH2	2.55	0.40
1:2:232:LYS:O	1:2:233:GLU:C	2.63	0.40
1:2:357:SER:O	1:2:395:ARG:CZ	2.70	0.40
1:3:52:SER:O	1:3:56:GLU:HB2	2.22	0.40
1:3:58:ASN:C	1:3:58:ASN:HD22	2.28	0.40
1:3:96:ILE:HD11	1:3:125:VAL:CG1	2.52	0.40
1:3:245:GLY:HA2	1:3:282:VAL:HG21	2.03	0.40
1:3:306:THR:HG22	1:3:308:ASN:H	1.86	0.40
1:3:345:ASN:O	1:3:347:LYS:N	2.54	0.40
1:4:122:VAL:C	1:4:124:LYS:H	2.29	0.40
1:1:315:PHE:O	1:1:319:VAL:HG23	2.22	0.40
1:1:429:VAL:HG21	1:1:451:TYR:CD1	2.57	0.40
1:2:371:ARG:O	1:2:373:ARG:N	2.53	0.40
1:3:44:TYR:C	1:3:47:ALA:HB3	2.46	0.40
1:3:80:TYR:CD2	1:3:399:LYS:HA	2.57	0.40
1:4:173:GLU:HB3	1:4:174:ASP:H	1.48	0.40
1:1:432:GLU:O	1:1:475:GLN:NE2	2.44	0.40
1:3:224:SER:C	1:3:371:ARG:NH2	2.80	0.40
1:4:316:GLU:HA	1:4:328:TYR:CD1	2.57	0.40
1:4:479:VAL:HA	1:4:480:PRO:HD2	1.87	0.40

There are no symmetry-related clashes.

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	1	467/477 (98%)	390 (84%)	50 (11%)	27 (6%)	1	4
1	2	463/477 (97%)	387 (84%)	48 (10%)	28 (6%)	1	4
1	3	467/477 (98%)	358 (77%)	77 (16%)	32 (7%)	1	2
1	4	462/477 (97%)	385 (83%)	49 (11%)	28 (6%)	1	4
All	All	1859/1908 (97%)	1520 (82%)	224 (12%)	115 (6%)	1	3

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	168	GLU
1	1	169	SER
1	1	172	ILE
1	1	361	VAL
1	1	372	ASN
1	1	451	TYR
1	1	478	ALA
1	2	149	GLU
1	2	168	GLU
1	2	170	MET
1	2	361	VAL
1	2	372	ASN
1	2	451	TYR
1	2	478	ALA
1	3	58	ASN
1	3	127	PRO
1	3	165	LEU
1	3	166	ASP
1	3	169	SER
1	3	181	LEU
1	3	361	VAL
1	3	372	ASN
1	3	451	TYR
1	3	478	ALA
1	4	149	GLU
1	4	160	SER
1	4	167	ILE
1	4	168	GLU

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Mol	Chain	Res	Type
1	4	169	SER
1	4	171	THR
1	4	172	ILE
1	4	361	VAL
1	4	372	ASN
1	4	451	TYR
1	4	478	ALA
1	1	182	GLU
1	1	186	VAL
1	1	235	GLU
1	1	360	GLY
1	1	483	ASN
1	2	169	SER
1	2	202	LYS
1	2	360	GLY
1	2	484	VAL
1	3	92	ASP
1	3	141	LYS
1	3	186	VAL
1	3	202	LYS
1	3	360	GLY
1	3	484	VAL
1	4	164	SER
1	4	235	GLU
1	4	427	HIS
1	4	484	VAL
1	1	92	ASP
1	1	159	ARG
1	1	160	SER
1	1	170	MET
1	1	380	PRO
1	1	427	HIS
1	1	479	VAL
1	1	490	ALA
1	2	160	SER
1	2	163	ASP
1	2	235	GLU
1	2	380	PRO
1	2	483	ASN
1	2	490	ALA
1	3	82	LEU
1	3	159	ARG

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Mol	Chain	Res	Type
1	3	235	GLU
1	3	380	PRO
1	3	469	LEU
1	3	482	PRO
1	3	483	ASN
1	3	490	ALA
1	3	497	GLY
1	4	92	ASP
1	4	159	ARG
1	4	360	GLY
1	4	380	PRO
1	4	482	PRO
1	4	490	ALA
1	1	112	PHE
1	1	484	VAL
1	2	469	LEU
1	2	479	VAL
1	2	482	PRO
1	3	113	ARG
1	3	346	GLY
1	3	479	VAL
1	4	166	ASP
1	4	479	VAL
1	4	483	ASN
1	1	202	LYS
1	1	413	ALA
1	1	469	LEU
1	1	482	PRO
1	2	112	PHE
1	2	172	ILE
1	2	184	GLY
1	2	373	ARG
1	2	413	ALA
1	3	114	ALA
1	3	164	SER
1	3	171	THR
1	4	186	VAL
1	4	202	LYS
1	2	176	TYR
1	2	267	ILE
1	4	24	ALA
1	2	162	VAL

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Mol	Chain	Res	Type
1	3	267	ILE
1	4	346	GLY
1	1	346	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	407/413 (98%)	373 (92%)	34 (8%)	10	31
1	2	406/413 (98%)	382 (94%)	24 (6%)	18	48
1	3	406/413 (98%)	380 (94%)	26 (6%)	16	44
1	4	404/413 (98%)	374 (93%)	30 (7%)	13	38
All	All	1623/1652 (98%)	1509 (93%)	114 (7%)	14	40

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	45	GLU
1	1	58	ASN
1	1	73	LEU
1	1	86	THR
1	1	107	MET
1	1	111	LYS
1	1	112	PHE
1	1	118	ASP
1	1	168	GLU
1	1	170	MET
1	1	172	ILE
1	1	181	LEU
1	1	189	SER
1	1	196	GLN
1	1	201	GLN
1	1	216	VAL
1	1	235	GLU
1	1	243	THR

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Mol	Chain	Res	Type
1	1	246	GLN
1	1	263	THR
1	1	309	MET
1	1	332	SER
1	1	350	ILE
1	1	351	MET
1	1	402	VAL
1	1	425	ARG
1	1	450	ASN
1	1	463	HIS
1	1	464	LEU
1	1	469	LEU
1	1	470	ARG
1	1	477	THR
1	1	479	VAL
1	1	498	MET
1	2	36	ASN
1	2	45	GLU
1	2	73	LEU
1	2	86	THR
1	2	107	MET
1	2	111	LYS
1	2	112	PHE
1	2	118	ASP
1	2	168	GLU
1	2	196	GLN
1	2	201	GLN
1	2	235	GLU
1	2	243	THR
1	2	246	GLN
1	2	263	THR
1	2	272	PHE
1	2	351	MET
1	2	402	VAL
1	2	425	ARG
1	2	463	HIS
1	2	464	LEU
1	2	469	LEU
1	2	470	ARG
1	2	477	THR
1	3	51	TYR
1	3	64	TYR

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Mol	Chain	Res	Type
1	3	72	TYR
1	3	99	TYR
1	3	112	PHE
1	3	129	ASP
1	3	166	ASP
1	3	175	GLU
1	3	185	LYS
1	3	196	GLN
1	3	201	GLN
1	3	216	VAL
1	3	235	GLU
1	3	243	THR
1	3	246	GLN
1	3	263	THR
1	3	272	PHE
1	3	309	MET
1	3	351	MET
1	3	402	VAL
1	3	425	ARG
1	3	463	HIS
1	3	464	LEU
1	3	469	LEU
1	3	470	ARG
1	3	477	THR
1	4	32	LYS
1	4	45	GLU
1	4	58	ASN
1	4	73	LEU
1	4	86	THR
1	4	107	MET
1	4	111	LYS
1	4	112	PHE
1	4	165	LEU
1	4	173	GLU
1	4	185	LYS
1	4	196	GLN
1	4	201	GLN
1	4	216	VAL
1	4	235	GLU
1	4	243	THR
1	4	246	GLN
1	4	263	THR

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Mol	Chain	Res	Type
1	4	272	PHE
1	4	309	MET
1	4	350	ILE
1	4	351	MET
1	4	361	VAL
1	4	402	VAL
1	4	425	ARG
1	4	463	HIS
1	4	464	LEU
1	4	469	LEU
1	4	470	ARG
1	4	477	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	36	ASN
1	1	58	ASN
1	1	137	GLN
1	1	201	GLN
1	1	211	GLN
1	1	296	HIS
1	1	310	ASN
1	1	374	GLN
1	1	393	ASN
1	1	405	GLN
1	1	419	ASN
1	1	450	ASN
1	1	481	HIS
1	2	34	GLN
1	2	58	ASN
1	2	67	ASN
1	2	137	GLN
1	2	196	GLN
1	2	201	GLN
1	2	211	GLN
1	2	296	HIS
1	2	298	HIS
1	2	310	ASN
1	2	374	GLN
1	2	390	GLN
1	2	393	ASN

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Mol	Chain	Res	Type
1	2	405	GLN
1	2	419	ASN
1	2	450	ASN
1	3	46	ASN
1	3	53	GLN
1	3	67	ASN
1	3	137	GLN
1	3	196	GLN
1	3	201	GLN
1	3	296	HIS
1	3	298	HIS
1	3	310	ASN
1	3	374	GLN
1	3	390	GLN
1	3	405	GLN
1	3	450	ASN
1	3	481	HIS
1	4	34	GLN
1	4	53	GLN
1	4	58	ASN
1	4	137	GLN
1	4	196	GLN
1	4	201	GLN
1	4	211	GLN
1	4	296	HIS
1	4	298	HIS
1	4	310	ASN
1	4	311	GLN
1	4	374	GLN
1	4	390	GLN
1	4	393	ASN
1	4	405	GLN
1	4	450	ASN
1	4	481	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	185:LYS	C	186:VAL	N	2.86

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.