



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:35 AM UTC

PDB ID : 2QZP / pdb_00002qzp
Title : Crystal structure of mutation of an acylptide hydrolase/esterase from Aeropyrum pernix K1
Authors : Zhang, H.F.; Zheng, B.S.; Rao, Z.
Deposited on : 2007-08-17
Resolution : 2.70 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

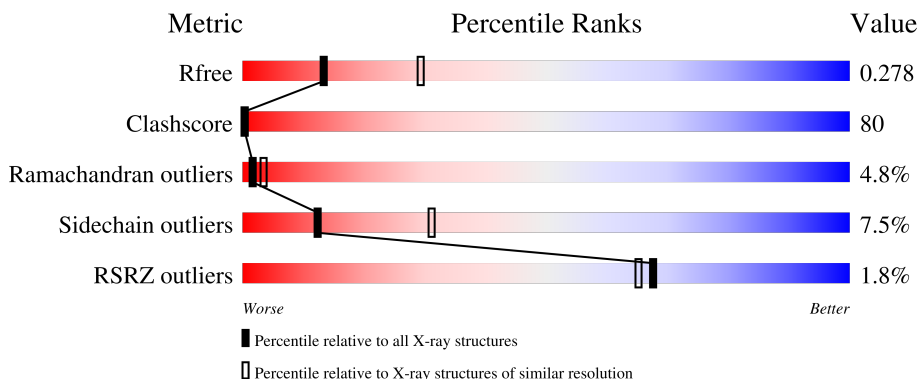
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	562	20% 67% 12% .
1	B	562	18% 67% 14% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8881 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 Acylamino-acid-releasing enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	560	Total	C	N	O	S	0	0	0
			4255	2685	750	808	12			
1	B	561	Total	C	N	O	S	0	0	0
			4260	2688	751	809	12			

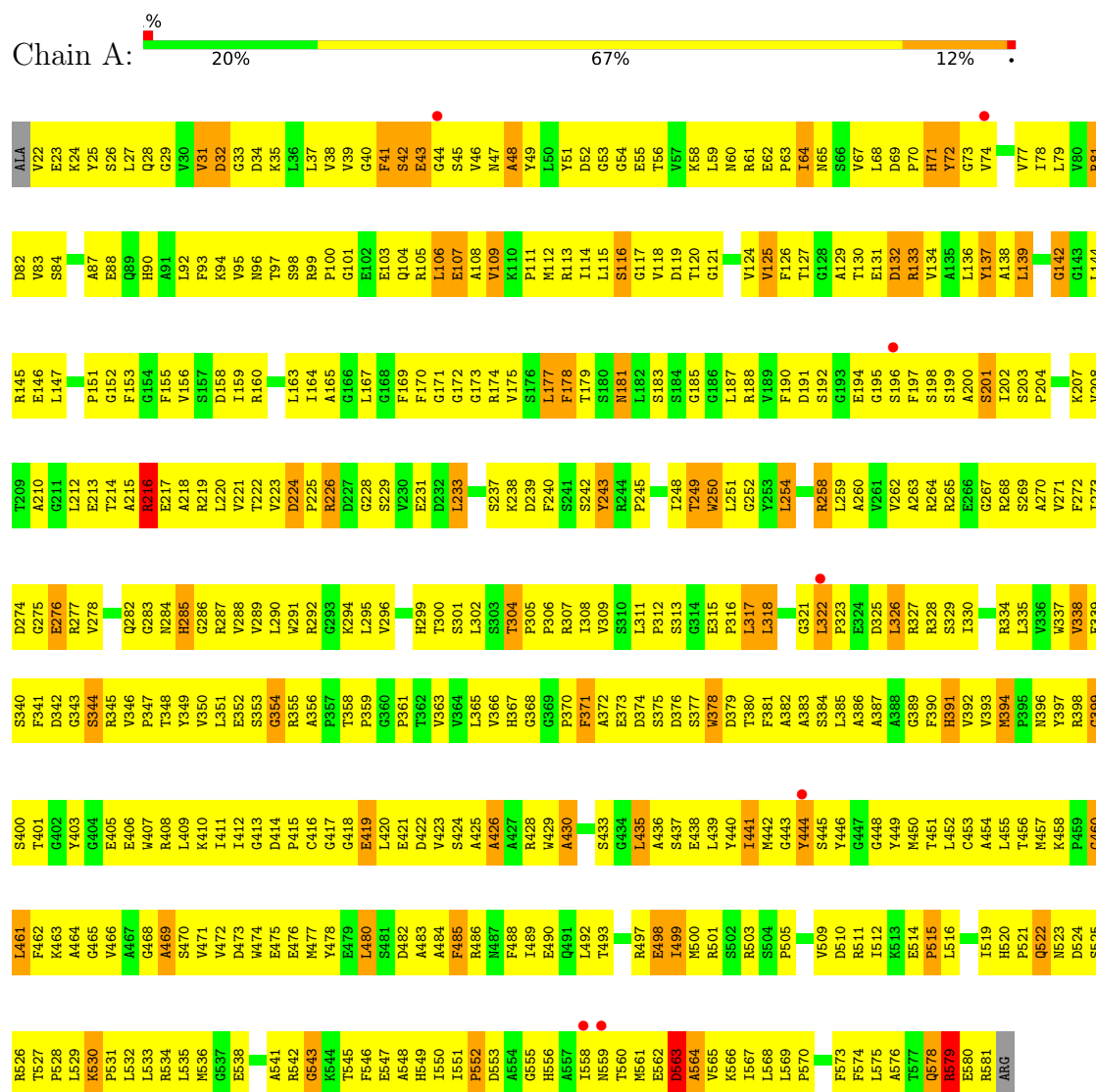
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	154	Total	O	0	0
			154	154		
2	B	212	Total	O	0	0
			212	212		

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: Acylamino-acid-releasing enzyme



• Molecule 1: Acylamino-acid-releasing enzyme



B581	A121	S84	E146	G276	V338	R398	P459	I519
ARG	S26	R85	L147	R277	E339	G399	G460	H520
	L27	G86	A148	V278	S340	S400	L461	P521
	Q28	A87	R149	E279	F341	T401	F462	N522
	Q29	E88	L150	A280	D342	G402	K463	N523
	V30	Q89	F153	P281	G343	Y403	A464	
	V31	H90	G154	Q282	S344	G404	G465	H526
	D32	A91	G155	G283	R345	E405	V466	T527
	D34	L92	F156	N284	V346	E406	A467	P528
	K35	F93	G33	H285	P347	G468	G469	L529
	K36	K94	S157	G286	T348	R408	A469	K530
	L37	V95	D158	R287	Y349	L409	S470	P531
	V38	N96	I159	V288	V350	K410	W471	L532
	V39	R99	A160	G226	L351	I411	W472	L533
	G40	P100	G161	S229	E352	D414	D473	H534
	F41	V39	D162	W291	S353	P415	W474	L535
	S42	G101	L163	R292	G354	E417	E475	N536
	E43	E102	I164	K294	R355	G418	E476	G537
	G44	Q103	G168	L233	A356	G419	W477	E538
	V46	Q104	F169	E234	P357	E418	Y478	L539
	N47	R105	F170	L235	P359	L420	E479	L540
	V48	E107	G171	P236	G360	E421	L480	A541
	A48	A108	G172	H299	T300	D422	D482	R542
	Y49	V109	G173	S301	L302	V423	A483	O543
	L50	K110	A174	L240	V363	S424	A484	K544
	Y51	P111	V175	S241	V364	A425	A485	T545
	D52	M12	S176	Y242	L365	A426	R486	F546
	G53	L114	L177	R244	P305	R427	N487	E547
	G54	F178	F178	P245	P306	R428	F488	A548
	E55	T179	T179	T246	R307	G368	W429	H549
	T56	S116	S180	K247	L308	G369	A430	L550
	V57	G117	N181	L248	V309	P370	R431	L551
	K58	D119	L182	T249	S310	F371	E432	P552
	L59	T120	G185	W250	L311	A372	S433	D553
	N60	G121	G186	L251	P312	E373	G434	A554
	R61	E122	L187	G252	S313	D374	L435	G494
	E62	A123	R188	Y253	G314	S375	A436	G495
	P63	V124	V199	L254	E315	D376	S437	S496
	I64	V125	G195	D256	P316	S377	E438	R497
	N65	F126	F196	G257	L318	W378	L439	E498
	S66	T127	F197	R258	E319	T380	I441	T499
	V67	T130	S198	L259	L322	F381	M442	R501
	L68	E131	A200	A260	P323	A382	G443	S502
	P70	D132	S199	V261	E324	A383	Y444	R503
	H71	R133	S201	A263	L325	S384	S445	S504
	Y72	V134	I202	R264	D326	L385	Y446	P505
	G73	A135	S203	R265	L326	A386	G447	I506
	V74	L136	P204	E266	R327	A387	G448	N507
	G75	Y137	G205	G267	S328	A388	Y449	H508
	R76	A138	M206	R268	S329	G389	M450	V509
	V77	L139	K207	S269	I330	F390	T451	D510
	L78	D140	V208	A270	A331	H391	L452	R511
	L79	G141	T209	V271	G332	V392	C453	I512
	V80	G142	A210	F272	S333	V393	A454	K513
	R81	G143	G211	L273	R334	M394	L455	E514
	D82	L144	D211	G275	L335	P395	T456	P515
	R83	R145	E213		V336	N396	M457	L516
					W337	Y397	K458	A517
								E580

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.12Å 102.18Å 163.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.11 – 2.70 48.11 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.0 (48.11-2.70) 92.0 (48.11-2.70)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.277 0.226 , 0.278	Depositor DCC
R_{free} test set	1393 reflections (3.96%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 87.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	8881	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.58	0/4346	1.15	37/5892 (0.6%)
1	B	0.56	0/4351	1.17	57/5899 (1.0%)
All	All	0.57	0/8697	1.16	94/11791 (0.8%)

There are no bond length outliers.

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	437	SER	N-CA-C	-11.39	97.78	112.93
1	A	564	ALA	N-CA-C	-9.88	99.35	111.40
1	B	327	ARG	N-CA-C	-9.43	101.20	112.89
1	A	399	GLY	N-CA-C	-9.41	103.28	114.48
1	B	564	ALA	N-CA-C	-8.76	101.56	113.30
1	A	304	THR	CA-C-N	8.44	125.73	119.66
1	A	304	THR	C-N-CA	8.44	125.73	119.66
1	B	477	MET	N-CA-C	-7.95	102.55	111.14
1	B	374	ASP	N-CA-C	-7.81	97.33	109.76
1	B	243	TYR	N-CA-C	-7.73	103.95	113.15
1	A	391	HIS	N-CA-C	-7.50	100.63	110.53
1	B	57	VAL	N-CA-C	7.37	118.73	108.12
1	B	486	ARG	N-CA-C	-7.35	103.20	111.07
1	B	490	GLU	N-CA-C	-7.33	103.29	111.28
1	B	326	LEU	N-CA-C	-7.32	103.82	112.89
1	B	69	ASP	CA-C-N	7.20	127.77	119.99
1	B	69	ASP	C-N-CA	7.20	127.77	119.99
1	A	317	LEU	N-CA-C	-7.12	102.55	112.45
1	B	392	VAL	N-CA-C	7.03	118.17	107.77
1	B	317	LEU	N-CA-C	-6.78	102.27	112.04
1	A	338	VAL	N-CA-C	6.63	118.23	109.21
1	B	91	ALA	N-CA-C	-6.62	99.88	110.14
1	B	414	ASP	CA-C-N	-6.60	112.97	119.90
1	B	414	ASP	C-N-CA	-6.60	112.97	119.90
1	B	504	SER	CA-C-N	6.51	127.98	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	504	SER	C-N-CA	6.51	127.98	119.84
1	A	243	TYR	N-CA-C	-6.51	104.22	111.71
1	B	244	ARG	CA-C-N	6.38	126.33	119.76
1	B	244	ARG	C-N-CA	6.38	126.33	119.76
1	B	394	MET	CA-C-N	6.32	126.65	119.83
1	B	394	MET	C-N-CA	6.32	126.65	119.83
1	B	458	LYS	CA-C-N	6.31	126.68	119.93
1	B	458	LYS	C-N-CA	6.31	126.68	119.93
1	B	209	THR	N-CA-C	-6.29	101.10	110.23
1	B	133	ARG	N-CA-C	6.28	118.07	108.52
1	B	315	GLU	CA-C-N	6.28	126.65	119.93
1	B	315	GLU	C-N-CA	6.28	126.65	119.93
1	B	309	VAL	N-CA-C	6.25	117.72	108.65
1	B	162	ASP	N-CA-C	-6.24	106.30	114.04
1	A	327	ARG	N-CA-C	-6.22	105.85	113.50
1	A	132	ASP	N-CA-C	6.18	120.08	112.54
1	B	382	ALA	N-CA-C	-6.07	104.36	110.97
1	A	133	ARG	N-CA-C	6.04	117.67	108.07
1	B	446	TYR	N-CA-C	-6.01	105.66	112.87
1	A	437	SER	N-CA-C	-5.98	105.81	113.23
1	A	485	PHE	N-CA-C	5.90	118.67	111.82
1	A	499	ILE	N-CA-C	-5.89	106.74	111.81
1	A	469	ALA	N-CA-C	-5.89	104.13	111.90
1	A	394	MET	CA-C-N	5.87	126.37	120.14
1	A	394	MET	C-N-CA	5.87	126.37	120.14
1	B	90	HIS	N-CA-C	5.87	119.65	110.32
1	B	155	PHE	N-CA-C	5.83	117.90	108.34
1	A	224	ASP	CA-C-N	5.81	125.94	119.32
1	A	224	ASP	C-N-CA	5.81	125.94	119.32
1	B	229	SER	N-CA-C	-5.76	102.77	110.55
1	B	224	ASP	CA-C-N	5.74	127.02	119.84
1	B	224	ASP	C-N-CA	5.74	127.02	119.84
1	B	426	ALA	N-CA-C	-5.73	105.96	113.12
1	A	448	GLY	N-CA-C	-5.65	105.54	112.77
1	B	215	ALA	N-CA-C	5.59	118.10	111.33
1	A	426	ALA	N-CA-C	-5.59	104.81	111.69
1	B	526	ARG	N-CA-C	-5.53	104.65	111.40
1	B	355	ARG	N-CA-C	-5.51	106.33	113.16
1	A	41	PHE	N-CA-C	-5.50	105.77	113.37
1	B	360	GLY	CA-C-N	5.47	126.68	119.84
1	B	360	GLY	C-N-CA	5.47	126.68	119.84
1	B	433	SER	N-CA-C	-5.47	106.52	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	ALA	N-CA-C	-5.43	102.84	110.50
1	A	226	ARG	N-CA-C	5.42	117.27	111.36
1	B	338	VAL	N-CA-C	5.38	116.53	109.21
1	A	242	SER	N-CA-C	-5.37	108.50	114.62
1	B	491	GLN	N-CA-C	5.36	117.20	111.36
1	A	326	LEU	N-CA-C	-5.34	106.72	113.18
1	A	155	PHE	N-CA-C	5.29	118.08	109.24
1	B	497	ARG	N-CA-C	5.27	118.04	111.24
1	B	567	ILE	N-CA-C	-5.27	107.69	112.96
1	B	134	VAL	N-CA-C	-5.26	100.87	108.87
1	A	378	TRP	N-CA-C	5.26	117.32	109.59
1	A	254	LEU	N-CA-C	-5.24	104.03	110.31
1	B	436	ALA	N-CA-C	5.20	117.72	109.24
1	A	107	GLU	N-CA-C	5.19	118.71	112.38
1	A	530	LYS	CA-C-N	5.19	124.81	119.56
1	A	530	LYS	C-N-CA	5.19	124.81	119.56
1	B	29	GLY	N-CA-C	5.19	117.60	111.63
1	B	421	GLU	N-CA-C	-5.18	105.07	111.40
1	B	506	ILE	N-CA-C	-5.17	106.52	112.98
1	B	62	GLU	N-CA-C	-5.13	102.81	110.20
1	A	258	ARG	N-CA-C	5.13	117.92	109.76
1	B	148	ALA	N-CA-C	5.11	116.29	108.42
1	A	282	GLN	N-CA-C	5.10	117.95	110.30
1	A	137	TYR	N-CA-C	5.09	118.36	110.17
1	A	578	GLN	N-CA-C	-5.06	105.41	111.03
1	B	173	GLY	N-CA-C	-5.04	108.37	115.32
1	A	125	VAL	N-CA-C	-5.01	101.44	109.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4255	0	4219	659	0
1	B	4260	0	4224	724	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	154	0	0	96	0
2	B	212	0	0	138	0
All	All	8881	0	8443	1365	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 80.

All (1365) 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:B:497:ARG:HH11	1:B:497:ARG:HB2	0.94	1.11
1:A:552:PRO:HD3	1:B:547:GLU:HB2	1.30	1.11
1:A:346:VAL:HG21	1:A:422:ASP:HB3	1.32	1.09
1:B:334:ARG:HH21	1:B:350:VAL:HG11	1.03	1.09
1:A:547:GLU:HB3	1:B:552:PRO:HD3	1.18	1.07
1:B:92:LEU:HD12	1:B:109:VAL:HG21	1.34	1.03
1:B:90:HIS:HB2	1:B:114:ILE:HD13	1.42	1.00
1:A:530:LYS:HB3	1:A:531:PRO:HD3	1.41	1.00
1:B:376:ASP:HA	2:B:791:HOH:O	1.60	1.00
1:B:323:PRO:HB2	1:B:326:LEU:HB2	1.42	0.99
1:B:497:ARG:HB2	1:B:497:ARG:NH1	1.79	0.98
1:B:347:PRO:O	1:B:396:ASN:HB2	1.63	0.98
1:B:212:LEU:HD23	1:B:219:ARG:HH12	1.26	0.96
1:B:201:SER:HB3	2:B:767:HOH:O	1.65	0.96
1:A:558:ILE:HD12	1:A:563:ASP:HB3	1.45	0.95
1:B:322:LEU:HD12	1:B:323:PRO:HD2	1.49	0.94
1:B:567:ILE:HD12	1:B:568:LEU:N	1.82	0.94
1:B:497:ARG:HH11	1:B:497:ARG:CB	1.81	0.93
1:A:522:GLN:HA	1:A:529:LEU:HD22	1.45	0.93
1:A:471:VAL:HG12	2:A:657:HOH:O	1.68	0.92
1:A:558:ILE:HG23	1:A:563:ASP:HB2	1.51	0.92
1:B:212:LEU:HD23	1:B:219:ARG:NH1	1.85	0.91
1:A:529:LEU:HD11	1:A:550:ILE:HD12	1.51	0.90
1:B:530:LYS:HB3	1:B:531:PRO:HD3	1.51	0.90
1:B:42:SER:HA	1:B:561:MET:SD	2.12	0.90
1:B:88:GLU:HG2	1:B:113:ARG:NH1	1.85	0.90
1:B:363:VAL:HG22	1:B:440:TYR:HB2	1.52	0.89
1:A:449:TYR:HA	2:A:709:HOH:O	1.71	0.88
1:A:69:ASP:HB2	1:A:118:VAL:HG22	1.56	0.88
1:A:68:LEU:HD12	1:A:78:ILE:HG21	1.52	0.88
1:B:325:ASP:HA	1:B:328:ARG:HB2	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ASN:HD21	1:A:82:ASP:HB2	1.37	0.88
1:A:547:GLU:CB	1:B:552:PRO:HD3	2.03	0.88
1:B:334:ARG:NH2	1:B:350:VAL:HG11	1.87	0.88
1:B:509:VAL:HA	1:B:512:ILE:HD13	1.56	0.87
1:A:574:PHE:HA	2:A:602:HOH:O	1.74	0.87
1:A:127:THR:HB	2:A:677:HOH:O	1.73	0.87
1:B:208:VAL:HB	1:B:223:VAL:HB	1.56	0.87
1:B:528:PRO:HG3	2:B:756:HOH:O	1.75	0.86
1:B:284:ASN:HD22	1:B:376:ASP:C	1.83	0.86
1:A:545:THR:HB	2:A:613:HOH:O	1.73	0.86
1:A:457:MET:HB2	2:A:696:HOH:O	1.75	0.86
1:B:49:TYR:HA	1:B:57:VAL:O	1.74	0.86
1:B:505:PRO:HG2	2:B:731:HOH:O	1.76	0.86
1:B:520:HIS:HD2	1:B:521:PRO:HD2	1.40	0.86
1:B:539:LEU:HB2	2:B:678:HOH:O	1.75	0.86
1:A:515:PRO:HA	2:A:613:HOH:O	1.76	0.85
1:B:303:SER:O	1:B:304:THR:HG23	1.74	0.85
1:B:26:SER:HB3	1:B:39:VAL:HB	1.58	0.85
1:B:374:ASP:CG	1:B:394:MET:HB3	2.01	0.85
1:A:442:MET:HE3	1:A:444:TYR:HE1	1.40	0.85
1:A:569:LEU:HB3	1:A:570:PRO:HD3	1.57	0.85
1:A:412:ILE:HB	2:A:721:HOH:O	1.77	0.84
1:B:127:THR:HG23	1:B:156:VAL:HG23	1.59	0.84
1:B:278:VAL:HG11	1:B:295:LEU:HD12	1.56	0.84
1:A:215:ALA:HB1	1:A:406:GLU:HB2	1.57	0.84
1:A:558:ILE:HG22	1:A:560:THR:O	1.78	0.84
1:A:547:GLU:HB3	1:B:552:PRO:CD	2.07	0.84
1:A:273:ILE:O	1:A:276:GLU:HB2	1.77	0.83
1:B:561:MET:HA	2:B:589:HOH:O	1.76	0.83
1:B:338:VAL:HG11	1:B:425:ALA:O	1.78	0.83
1:B:484:ALA:HB3	2:B:604:HOH:O	1.79	0.83
1:A:194:GLU:HB2	1:A:212:LEU:HD21	1.60	0.83
1:A:548:ALA:HB3	1:B:550:ILE:HD13	1.58	0.83
1:B:463:LYS:HB2	2:B:658:HOH:O	1.77	0.82
1:B:458:LYS:HE3	2:B:778:HOH:O	1.79	0.82
1:A:116:SER:N	2:A:677:HOH:O	2.13	0.82
1:A:452:LEU:HD22	2:A:709:HOH:O	1.78	0.82
1:A:532:LEU:HD13	1:A:532:LEU:O	1.79	0.82
1:B:70:PRO:HB2	1:B:74:VAL:HG21	1.61	0.82
1:A:94:LYS:O	1:A:94:LYS:HG3	1.79	0.82
1:B:420:LEU:HD21	1:B:458:LYS:HD3	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:LEU:HG	2:B:600:HOH:O	1.79	0.81
1:A:177:LEU:HD21	1:A:208:VAL:HG11	1.62	0.81
1:A:138:ALA:HB2	1:A:147:LEU:HD21	1.63	0.81
1:A:458:LYS:HD3	1:A:461:LEU:HD13	1.63	0.80
1:B:102:GLU:HA	2:B:621:HOH:O	1.79	0.80
1:A:322:LEU:HD23	1:A:323:PRO:HD2	1.63	0.80
1:A:23:GLU:HA	2:A:730:HOH:O	1.80	0.80
1:B:158:ASP:O	1:B:159:ILE:HD13	1.80	0.80
1:B:406:GLU:HG2	1:B:410:LYS:HE2	1.64	0.80
1:A:545:THR:HG23	1:B:553:ASP:OD1	1.80	0.80
1:B:570:PRO:HD2	2:B:594:HOH:O	1.82	0.79
1:B:44:GLY:O	1:B:560:THR:HG22	1.83	0.79
1:B:78:ILE:HD13	1:B:124:VAL:HG13	1.63	0.79
1:A:38:VAL:HG12	1:A:39:VAL:N	1.97	0.79
1:B:281:PRO:O	1:B:285:HIS:HE1	1.66	0.78
1:A:238:LYS:HG2	2:A:614:HOH:O	1.84	0.78
1:B:376:ASP:HB2	2:B:616:HOH:O	1.82	0.78
1:A:558:ILE:HG23	1:A:563:ASP:CB	2.14	0.78
1:A:32:ASP:HB2	1:A:35:LYS:HB2	1.64	0.78
1:A:44:GLY:HA2	1:A:561:MET:H	1.49	0.78
1:B:353:SER:HB3	1:B:356:ALA:HB3	1.66	0.78
1:A:406:GLU:O	1:A:410:LYS:HG3	1.85	0.77
1:A:469:ALA:O	1:A:527:THR:HG21	1.84	0.77
1:B:522:GLN:HA	1:B:529:LEU:HD22	1.64	0.77
1:B:569:LEU:HB3	1:B:570:PRO:HD3	1.66	0.77
1:B:574:PHE:HA	2:B:784:HOH:O	1.84	0.77
1:A:83:VAL:HA	2:A:717:HOH:O	1.84	0.77
1:B:406:GLU:O	1:B:410:LYS:HG3	1.85	0.77
1:A:138:ALA:CB	1:A:147:LEU:HD21	2.13	0.77
1:A:562:GLU:O	1:A:564:ALA:N	2.17	0.77
1:B:268:ARG:HA	2:B:614:HOH:O	1.83	0.77
1:B:579:ARG:C	1:B:581:ARG:H	1.91	0.77
1:A:61:ARG:NH1	1:A:101:GLY:HA3	1.99	0.77
1:A:519:ILE:HA	1:A:549:HIS:HB2	1.66	0.77
1:A:523:ASN:ND2	1:A:553:ASP:HA	1.99	0.77
1:A:417:GLY:N	1:A:419:GLU:OE2	2.18	0.77
1:B:323:PRO:HG2	1:B:326:LEU:HD12	1.67	0.77
1:B:387:ALA:HB2	2:B:643:HOH:O	1.83	0.77
1:A:334:ARG:HH21	1:A:350:VAL:HG11	1.50	0.76
1:A:90:HIS:HD2	1:A:114:ILE:H	1.32	0.76
1:A:215:ALA:N	1:A:405:GLU:HB3	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:LEU:HD21	2:A:696:HOH:O	1.84	0.75
1:B:567:ILE:HD11	1:B:568:LEU:HD22	1.69	0.75
1:B:520:HIS:ND1	1:B:532:LEU:HG	2.01	0.75
1:A:552:PRO:CD	1:B:547:GLU:HB2	2.14	0.75
1:A:411:ILE:HD11	1:A:446:TYR:OH	1.87	0.74
1:A:442:MET:HE3	1:A:444:TYR:CE1	2.23	0.74
1:A:194:GLU:HB3	1:A:214:THR:CG2	2.16	0.74
1:B:139:LEU:HD13	1:B:144:LEU:HB2	1.69	0.74
1:B:542:ARG:HG3	1:B:542:ARG:HH11	1.49	0.74
1:A:428:ARG:HG3	2:A:622:HOH:O	1.87	0.74
1:B:480:LEU:HB2	2:B:756:HOH:O	1.88	0.74
1:A:534:ARG:O	1:A:538:GLU:HG2	1.88	0.74
1:A:309:VAL:HA	1:A:316:PRO:HA	1.68	0.73
1:B:59:LEU:O	1:B:95:VAL:HG11	1.87	0.73
1:A:311:LEU:HG	2:A:670:HOH:O	1.87	0.73
1:B:239:ASP:HB2	1:B:275:GLY:O	1.87	0.73
1:B:565:VAL:C	1:B:567:ILE:H	1.93	0.73
1:A:136:LEU:HD21	1:A:164:ILE:HG21	1.70	0.73
1:A:526:ARG:HH11	1:A:556:HIS:HD2	1.34	0.73
1:B:265:ARG:HB3	2:B:696:HOH:O	1.87	0.73
1:A:194:GLU:HB3	1:A:214:THR:HG21	1.70	0.73
1:A:163:LEU:C	1:A:164:ILE:HD12	2.13	0.73
1:B:428:ARG:HG2	2:B:592:HOH:O	1.88	0.73
1:B:445:SER:H	1:B:469:ALA:HB3	1.54	0.73
1:A:529:LEU:HD23	1:B:540:LEU:HD13	1.70	0.72
1:A:65:ASN:ND2	1:A:82:ASP:HB2	2.04	0.72
1:B:90:HIS:CB	1:B:114:ILE:HD13	2.20	0.72
1:B:477:MET:HG3	1:B:528:PRO:HD2	1.72	0.72
1:B:485:PHE:HA	1:B:488:PHE:HB3	1.72	0.72
1:B:503:ARG:O	1:B:505:PRO:HD3	1.89	0.72
1:B:133:ARG:HD3	1:B:149:ARG:HE	1.54	0.72
1:B:177:LEU:CD2	1:B:223:VAL:HG21	2.19	0.72
1:B:496:SER:HB3	2:B:619:HOH:O	1.89	0.72
1:A:251:LEU:HD13	1:A:259:LEU:HD11	1.71	0.71
1:B:71:HIS:O	1:B:74:VAL:HG13	1.89	0.71
1:B:519:ILE:HD13	2:B:594:HOH:O	1.90	0.71
1:A:271:VAL:HB	1:A:278:VAL:HB	1.71	0.71
1:A:419:GLU:HG3	2:A:643:HOH:O	1.90	0.71
1:B:95:VAL:HA	2:B:742:HOH:O	1.90	0.71
1:B:347:PRO:O	1:B:396:ASN:CB	2.38	0.71
1:B:573:PHE:HB2	2:B:653:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:MET:HE2	2:A:601:HOH:O	1.89	0.71
1:A:549:HIS:CE1	1:A:570:PRO:HB3	2.26	0.71
1:A:361:PRO:HA	1:A:438:GLU:CG	2.21	0.71
1:B:374:ASP:OD2	1:B:394:MET:HB3	1.90	0.71
1:B:381:PHE:CZ	1:B:567:ILE:HD13	2.25	0.71
1:B:417:GLY:O	1:B:421:GLU:HG2	1.89	0.71
1:A:350:VAL:O	1:A:351:LEU:HD23	1.89	0.71
1:B:364:VAL:HG22	2:B:775:HOH:O	1.91	0.71
1:B:472:VAL:HG12	1:B:506:ILE:HB	1.71	0.71
1:B:475:GLU:O	1:B:479:GLU:HG3	1.88	0.71
1:B:451:THR:CG2	1:B:467:ALA:HB2	2.21	0.71
1:B:577:THR:HB	2:B:784:HOH:O	1.89	0.71
1:B:160:ARG:HB3	1:B:202:ILE:HG21	1.74	0.70
1:A:338:VAL:O	1:A:345:ARG:HA	1.91	0.70
1:A:308:ILE:HB	1:A:318:LEU:HB2	1.73	0.70
1:B:45:SER:HA	1:B:560:THR:HA	1.72	0.70
1:A:71:HIS:O	1:A:74:VAL:HG23	1.91	0.70
1:A:363:VAL:HG12	2:A:693:HOH:O	1.92	0.70
1:A:284:ASN:ND2	1:A:377:SER:OG	2.25	0.70
1:A:309:VAL:HG12	1:A:316:PRO:HA	1.73	0.70
1:B:30:VAL:HG23	1:B:289:VAL:CG1	2.21	0.70
1:B:337:TRP:CG	1:B:345:ARG:HH21	2.09	0.70
1:B:356:ALA:HB2	1:B:389:GLY:O	1.92	0.70
1:B:362:THR:HG22	1:B:363:VAL:N	2.06	0.70
1:B:564:ALA:O	1:B:567:ILE:HD11	1.92	0.70
1:A:129:ALA:CB	1:A:134:VAL:HG22	2.21	0.70
1:B:164:ILE:HB	1:B:180:SER:HB3	1.74	0.70
1:B:373:GLU:OE2	1:B:396:ASN:HB3	1.91	0.70
1:B:331:ALA:HB3	1:B:352:GLU:HB3	1.73	0.69
1:A:335:LEU:HD12	1:A:348:THR:O	1.93	0.69
1:B:51:TYR:HE2	1:B:317:LEU:HB3	1.58	0.69
1:B:79:LEU:HD11	1:B:95:VAL:HG21	1.74	0.69
1:A:346:VAL:HG13	1:A:407:TRP:HZ2	1.58	0.69
1:A:90:HIS:HB2	1:A:114:ILE:HD13	1.75	0.69
1:A:441:ILE:HD13	1:A:442:MET:N	2.06	0.69
1:A:439:LEU:N	2:A:729:HOH:O	2.24	0.69
1:A:511:ARG:O	2:A:630:HOH:O	2.10	0.69
1:B:178:PHE:HB3	2:B:706:HOH:O	1.93	0.69
1:B:208:VAL:HG23	1:B:223:VAL:O	1.93	0.69
1:A:528:PRO:HD3	2:A:644:HOH:O	1.91	0.69
1:B:245:PRO:HA	2:B:696:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:GLU:O	1:B:327:ARG:HB3	1.92	0.69
1:A:130:THR:OG1	1:A:132:ASP:OD1	2.10	0.68
1:B:327:ARG:O	2:B:720:HOH:O	2.11	0.68
1:A:174:ARG:HE	1:A:409:LEU:HD11	1.59	0.68
1:B:35:LYS:HG2	1:B:52:ASP:OD1	1.93	0.68
1:A:200:ALA:HB3	2:A:639:HOH:O	1.92	0.68
1:A:214:THR:C	1:A:405:GLU:HB3	2.18	0.68
1:A:405:GLU:OE1	1:A:409:LEU:HG	1.93	0.68
1:A:164:ILE:HD13	1:A:181:ASN:C	2.18	0.68
1:A:474:TRP:HB2	1:A:500:MET:HB3	1.75	0.68
1:A:93:PHE:C	2:A:589:HOH:O	2.36	0.68
1:A:175:VAL:HG23	1:A:196:SER:HB3	1.76	0.68
1:A:525:SER:C	2:A:644:HOH:O	2.35	0.68
1:B:169:PHE:CZ	1:B:175:VAL:HG22	2.28	0.68
1:B:329:SER:HB2	1:B:387:ALA:HA	1.76	0.68
1:A:352:GLU:HA	1:A:391:HIS:ND1	2.09	0.68
1:A:361:PRO:HA	1:A:438:GLU:HG2	1.76	0.68
1:A:27:LEU:HD21	1:A:289:VAL:HG22	1.76	0.68
1:B:92:LEU:O	1:B:106:LEU:HD12	1.94	0.68
1:B:477:MET:HA	2:B:756:HOH:O	1.93	0.68
1:B:526:ARG:NH2	1:B:557:ALA:HB2	2.08	0.68
1:A:532:LEU:CD1	1:A:536:MET:HE3	2.24	0.67
1:B:218:ALA:HB1	1:B:248:ILE:HD11	1.76	0.67
1:B:526:ARG:HA	2:B:680:HOH:O	1.94	0.67
1:A:42:SER:HB2	2:A:649:HOH:O	1.94	0.67
1:B:222:THR:O	1:B:230:VAL:HG13	1.95	0.67
1:B:171:GLY:C	1:B:173:GLY:H	2.00	0.67
1:B:59:LEU:HD13	1:B:77:VAL:HG21	1.76	0.67
1:B:218:ALA:HB1	1:B:248:ILE:CD1	2.25	0.67
1:A:27:LEU:HD23	1:A:287:ARG:O	1.93	0.67
1:B:116:SER:C	2:B:596:HOH:O	2.38	0.67
1:A:368:GLY:HA2	2:A:686:HOH:O	1.95	0.67
1:B:295:LEU:O	1:B:311:LEU:HG	1.95	0.67
1:B:485:PHE:O	1:B:489:ILE:HG12	1.95	0.67
1:B:91:ALA:HB3	1:B:93:PHE:CZ	2.30	0.66
1:B:440:TYR:OH	1:B:463:LYS:HD3	1.94	0.66
1:B:221:VAL:HB	1:B:230:VAL:HG12	1.77	0.66
1:A:90:HIS:O	1:A:111:PRO:HA	1.96	0.66
1:A:386:ALA:HA	1:A:390:PHE:O	1.95	0.66
1:B:438:GLU:HA	2:B:714:HOH:O	1.95	0.66
1:B:449:TYR:HB2	2:B:685:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:GLU:HA	1:A:501:ARG:HD2	1.77	0.66
1:B:477:MET:HE2	1:B:489:ILE:HD11	1.77	0.66
1:B:559:ASN:O	1:B:560:THR:HG23	1.95	0.66
1:A:58:LYS:O	1:A:100:PRO:HB3	1.96	0.66
1:A:81:ARG:HB2	1:A:81:ARG:HH11	1.61	0.66
1:A:419:GLU:CD	1:A:420:LEU:H	2.03	0.66
1:A:423:VAL:HA	2:A:651:HOH:O	1.95	0.66
1:A:353:SER:O	1:A:356:ALA:N	2.29	0.66
1:A:529:LEU:HD11	1:A:550:ILE:CD1	2.25	0.66
1:B:159:ILE:HD12	1:B:164:ILE:HG23	1.78	0.66
1:A:322:LEU:HD23	1:A:323:PRO:CD	2.25	0.66
1:A:548:ALA:O	1:B:549:HIS:HA	1.95	0.66
1:A:551:ILE:HG23	1:A:552:PRO:HD2	1.77	0.66
1:B:574:PHE:O	1:B:577:THR:HB	1.96	0.66
1:A:480:LEU:HD21	1:A:530:LYS:HD2	1.78	0.66
1:A:567:ILE:HG13	1:A:567:ILE:O	1.95	0.66
1:B:424:SER:HB3	1:B:428:ARG:NH1	2.11	0.66
1:A:45:SER:HB2	1:A:63:PRO:HB3	1.76	0.65
1:A:125:VAL:HA	1:A:137:TYR:O	1.96	0.65
1:A:392:VAL:HG22	2:A:720:HOH:O	1.95	0.65
1:B:153:PHE:HE1	1:B:488:PHE:HB2	1.61	0.65
1:B:284:ASN:ND2	1:B:376:ASP:C	2.54	0.65
1:A:308:ILE:O	1:A:318:LEU:N	2.23	0.65
1:B:171:GLY:O	1:B:173:GLY:N	2.30	0.65
1:A:90:HIS:N	1:A:112:MET:O	2.21	0.65
1:A:536:MET:HE1	1:A:550:ILE:HD11	1.78	0.65
1:A:555:GLY:HA3	2:A:663:HOH:O	1.96	0.65
1:B:55:GLU:C	2:B:735:HOH:O	2.38	0.65
1:B:99:ARG:HB2	1:B:102:GLU:OE2	1.96	0.65
1:B:410:LYS:HG2	2:B:695:HOH:O	1.95	0.65
1:A:302:LEU:HD13	1:A:351:LEU:HD21	1.78	0.65
1:A:562:GLU:C	1:A:564:ALA:H	2.05	0.65
1:B:523:ASN:ND2	1:B:553:ASP:HA	2.11	0.65
1:A:579:ARG:NH1	1:A:579:ARG:HB2	2.12	0.65
1:B:103:GLU:HB2	2:B:687:HOH:O	1.97	0.65
1:B:458:LYS:HB3	1:B:461:LEU:HD22	1.79	0.65
1:B:532:LEU:O	1:B:536:MET:HG3	1.97	0.65
1:B:469:ALA:HB1	1:B:556:HIS:CE1	2.31	0.65
1:A:563:ASP:HA	1:A:566:LYS:CG	2.27	0.65
1:A:63:PRO:HA	2:A:595:HOH:O	1.97	0.65
1:B:278:VAL:HG11	1:B:295:LEU:CD1	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:GLY:CA	1:B:289:VAL:HG21	2.28	0.64
1:B:136:LEU:O	1:B:147:LEU:N	2.31	0.64
1:A:353:SER:O	1:A:355:ARG:N	2.30	0.64
1:B:100:PRO:O	1:B:102:GLU:HG3	1.96	0.64
1:B:133:ARG:HA	1:B:483:ALA:CB	2.27	0.64
1:B:137:TYR:HA	1:B:146:GLU:HA	1.80	0.64
1:B:362:THR:CG2	1:B:363:VAL:N	2.60	0.64
1:A:88:GLU:HG3	1:A:113:ARG:HH12	1.61	0.64
1:A:223:VAL:HA	1:A:229:SER:O	1.98	0.64
1:A:263:ALA:O	1:A:269:SER:HB2	1.97	0.64
1:A:325:ASP:HA	1:A:328:ARG:HB3	1.79	0.64
1:A:337:TRP:CZ3	1:A:347:PRO:HB3	2.33	0.64
1:B:69:ASP:O	1:B:118:VAL:HG13	1.97	0.64
1:B:201:SER:N	2:B:652:HOH:O	2.30	0.64
1:A:61:ARG:HH12	1:A:101:GLY:HA3	1.62	0.64
1:A:438:GLU:HB2	2:A:729:HOH:O	1.96	0.64
1:A:526:ARG:HD2	1:A:556:HIS:CD2	2.32	0.64
1:B:181:ASN:HB2	1:B:185:GLY:O	1.97	0.64
1:A:38:VAL:CG1	1:A:39:VAL:N	2.61	0.64
1:A:272:PHE:CE2	1:A:277:ARG:HD3	2.33	0.64
1:A:415:PRO:O	1:A:503:ARG:HD2	1.98	0.64
1:B:46:VAL:HG23	2:B:764:HOH:O	1.98	0.64
1:A:172:GLY:O	1:A:409:LEU:HD22	1.98	0.64
1:B:90:HIS:HB2	1:B:114:ILE:CD1	2.23	0.64
1:B:201:SER:CB	1:B:252:GLY:HA2	2.28	0.64
1:B:251:LEU:HG	2:B:652:HOH:O	1.97	0.64
1:B:361:PRO:HG3	1:B:438:GLU:CD	2.23	0.64
1:B:411:ILE:CD1	1:B:419:GLU:HG2	2.27	0.64
1:B:421:GLU:OE2	1:B:421:GLU:HA	1.96	0.64
1:A:129:ALA:HB2	1:A:134:VAL:HG22	1.80	0.64
1:A:200:ALA:CB	2:A:639:HOH:O	2.46	0.64
1:B:361:PRO:HA	1:B:438:GLU:HG2	1.80	0.64
1:B:373:GLU:OE1	1:B:396:ASN:ND2	2.31	0.64
1:A:370:PRO:O	1:A:372:ALA:N	2.29	0.63
1:A:511:ARG:HG2	2:A:630:HOH:O	1.98	0.63
1:B:137:TYR:CD2	1:B:146:GLU:HG3	2.32	0.63
1:B:565:VAL:C	1:B:567:ILE:N	2.56	0.63
1:A:493:THR:O	1:A:499:ILE:HD12	1.97	0.63
1:B:90:HIS:HD2	1:B:114:ILE:H	1.47	0.63
1:B:92:LEU:HD12	1:B:109:VAL:CG2	2.22	0.63
1:B:180:SER:HA	2:B:750:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:GLN:HG2	2:B:620:HOH:O	1.98	0.63
1:B:428:ARG:O	1:B:431:ARG:HB2	1.98	0.63
1:B:471:VAL:HG11	1:B:474:TRP:CH2	2.33	0.63
1:A:133:ARG:HA	1:A:483:ALA:CB	2.28	0.63
1:B:61:ARG:HB2	1:B:103:GLU:CD	2.24	0.63
1:B:411:ILE:HD11	1:B:446:TYR:OH	1.99	0.63
1:B:441:ILE:HG21	2:B:615:HOH:O	1.96	0.63
1:A:62:GLU:HB2	1:A:81:ARG:HH21	1.64	0.63
1:B:186:GLY:O	1:B:187:LEU:HB2	1.98	0.63
1:B:472:VAL:CG1	1:B:506:ILE:HB	2.29	0.63
1:B:542:ARG:HG3	1:B:542:ARG:NH1	2.14	0.63
1:B:61:ARG:HB2	1:B:103:GLU:OE1	1.99	0.62
1:B:278:VAL:HG13	1:B:312:PRO:HB3	1.80	0.62
1:B:340:SER:HB3	2:B:722:HOH:O	1.98	0.62
1:A:109:VAL:HG12	2:A:594:HOH:O	1.99	0.62
1:A:475:GLU:HB3	2:A:627:HOH:O	2.00	0.62
1:A:532:LEU:HD12	1:A:536:MET:HE3	1.80	0.62
1:B:99:ARG:NH2	1:B:102:GLU:HB3	2.13	0.62
1:B:264:ARG:O	1:B:264:ARG:HG3	1.97	0.62
1:B:78:ILE:HD13	1:B:124:VAL:CG1	2.30	0.62
1:A:523:ASN:HD21	1:A:553:ASP:HA	1.61	0.62
1:B:91:ALA:HB1	1:B:105:ARG:HE	1.65	0.62
1:A:45:SER:OG	1:A:47:ASN:ND2	2.30	0.62
1:B:523:ASN:HB2	1:B:554:ALA:O	1.99	0.62
1:A:58:LYS:HE2	1:A:60:ASN:O	1.99	0.62
1:B:68:LEU:O	1:B:70:PRO:HD3	2.00	0.62
1:B:345:ARG:HD2	2:B:684:HOH:O	2.00	0.62
1:B:539:LEU:HD13	1:B:546:PHE:CG	2.34	0.62
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.64	0.62
1:B:29:GLY:HA2	1:B:289:VAL:HG21	1.82	0.62
1:B:420:LEU:CD2	1:B:458:LYS:HD3	2.29	0.62
1:A:90:HIS:HB2	1:A:114:ILE:CD1	2.30	0.62
1:B:133:ARG:NH1	1:B:146:GLU:OE2	2.32	0.62
1:A:40:GLY:C	1:A:42:SER:H	2.07	0.61
1:A:45:SER:HB2	2:A:595:HOH:O	1.99	0.61
1:A:251:LEU:HD12	1:A:252:GLY:N	2.13	0.61
1:A:283:GLY:HA2	1:A:376:ASP:OD2	2.00	0.61
1:A:470:SER:O	1:A:527:THR:HB	2.00	0.61
1:B:115:LEU:HB2	1:B:127:THR:OG1	2.00	0.61
1:A:341:PHE:CD2	1:A:421:GLU:HB3	2.35	0.61
1:A:346:VAL:HG22	1:A:407:TRP:CH2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ILE:HG13	1:A:295:LEU:HD11	1.82	0.61
1:A:499:ILE:HD11	2:A:732:HOH:O	2.01	0.61
1:B:160:ARG:NH2	2:B:715:HOH:O	2.33	0.61
1:B:370:PRO:O	1:B:372:ALA:N	2.33	0.61
1:A:340:SER:HB2	1:A:344:SER:O	1.99	0.61
1:B:31:VAL:HG12	1:B:32:ASP:N	2.15	0.61
1:B:559:ASN:HB2	2:B:762:HOH:O	2.00	0.61
1:A:174:ARG:HH21	1:A:405:GLU:CD	2.08	0.61
1:A:342:ASP:CG	1:A:398:ARG:HH22	2.08	0.61
1:A:547:GLU:OE2	1:A:574:PHE:HB2	2.00	0.61
1:A:558:ILE:HG12	2:A:583:HOH:O	2.01	0.61
1:B:579:ARG:C	1:B:581:ARG:N	2.59	0.61
1:A:251:LEU:HD12	1:A:251:LEU:C	2.24	0.61
1:A:533:LEU:CD1	1:B:536:MET:HB3	2.30	0.61
1:B:323:PRO:CG	1:B:326:LEU:HD12	2.31	0.61
1:A:497:ARG:O	1:A:499:ILE:N	2.34	0.61
1:B:198:SER:HB3	1:B:213:GLU:CD	2.26	0.61
1:B:399:GLY:HA2	1:B:408:ARG:O	2.01	0.61
1:A:533:LEU:HD11	1:B:536:MET:HB3	1.81	0.61
1:B:45:SER:HB2	1:B:63:PRO:HB3	1.83	0.60
1:B:127:THR:HG23	1:B:156:VAL:CG2	2.29	0.60
1:B:347:PRO:HG2	1:B:396:ASN:HB2	1.83	0.60
1:B:282:GLN:HB3	2:B:700:HOH:O	1.99	0.60
1:B:567:ILE:CD1	1:B:568:LEU:HD22	2.32	0.60
1:A:264:ARG:NH2	1:A:373:GLU:OE2	2.33	0.60
1:B:26:SER:O	1:B:308:ILE:HD11	2.01	0.60
1:B:30:VAL:H	1:B:289:VAL:HG11	1.64	0.60
1:A:296:VAL:HG13	1:A:309:VAL:O	2.02	0.60
1:A:41:PHE:CE2	1:A:561:MET:HA	2.37	0.60
1:A:160:ARG:N	1:A:202:ILE:HD12	2.16	0.60
1:B:90:HIS:CD2	1:B:114:ILE:HD13	2.35	0.60
1:B:373:GLU:OE1	1:B:373:GLU:HA	1.99	0.60
1:A:178:PHE:CD1	1:A:178:PHE:C	2.80	0.60
1:A:533:LEU:HD21	1:B:536:MET:SD	2.42	0.60
1:A:41:PHE:CZ	1:A:561:MET:HA	2.35	0.60
1:A:309:VAL:HG12	1:A:316:PRO:CA	2.32	0.60
1:A:468:GLY:HA2	1:A:519:ILE:O	2.02	0.60
1:B:135:ALA:HB3	1:B:137:TYR:CZ	2.37	0.60
1:B:268:ARG:NH1	1:B:282:GLN:CD	2.60	0.60
1:B:517:ALA:HB2	1:B:574:PHE:CD1	2.37	0.60
1:B:530:LYS:HB3	1:B:531:PRO:CD	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ARG:HG3	2:A:694:HOH:O	2.01	0.60
1:A:532:LEU:HD13	1:A:532:LEU:C	2.26	0.60
1:B:330:ILE:HD12	2:B:720:HOH:O	2.02	0.60
1:A:385:LEU:HD13	2:A:720:HOH:O	2.00	0.60
1:A:541:ALA:C	1:A:543:GLY:H	2.09	0.59
1:B:361:PRO:O	1:B:390:PHE:HA	2.02	0.59
1:B:325:ASP:CA	1:B:328:ARG:HB2	2.30	0.59
1:B:410:LYS:HE3	2:B:786:HOH:O	2.02	0.59
1:A:171:GLY:O	1:A:174:ARG:HB2	2.02	0.59
1:A:510:ASP:CG	1:A:542:ARG:HE	2.10	0.59
1:B:175:VAL:HB	1:B:196:SER:HB3	1.84	0.59
1:B:451:THR:HG21	1:B:466:VAL:C	2.27	0.59
1:A:55:GLU:HA	2:A:604:HOH:O	2.03	0.59
1:A:267:GLY:HA2	1:A:375:SER:HB2	1.83	0.59
1:A:356:ALA:HB2	1:A:389:GLY:O	2.01	0.59
1:B:451:THR:HG21	1:B:467:ALA:HB2	1.85	0.59
1:A:558:ILE:CG2	1:A:560:THR:O	2.51	0.59
1:B:471:VAL:HG11	1:B:474:TRP:CZ3	2.37	0.59
1:A:37:LEU:HD23	1:A:70:PRO:HG3	1.85	0.59
1:A:480:LEU:HD21	1:A:530:LYS:CD	2.32	0.59
1:A:353:SER:O	1:A:354:GLY:C	2.45	0.59
1:A:530:LYS:CB	1:A:531:PRO:HD3	2.24	0.59
1:A:109:VAL:HG12	1:A:109:VAL:O	2.02	0.59
1:A:306:PRO:HD3	1:A:378:TRP:HB3	1.83	0.59
1:A:526:ARG:HH11	1:A:556:HIS:CD2	2.18	0.59
1:B:145:ARG:HG3	2:B:748:HOH:O	2.01	0.58
1:B:171:GLY:C	1:B:173:GLY:N	2.61	0.58
1:B:302:LEU:HD13	1:B:351:LEU:CD1	2.33	0.58
1:B:46:VAL:HB	1:B:64:ILE:O	2.03	0.58
1:B:60:ASN:CG	2:B:679:HOH:O	2.46	0.58
1:B:246:THR:HG22	1:B:264:ARG:O	2.03	0.58
1:B:251:LEU:CD1	1:B:259:LEU:HD11	2.33	0.58
1:B:456:THR:CG2	1:B:512:ILE:HD11	2.32	0.58
1:B:414:ASP:HA	1:B:503:ARG:HH12	1.66	0.58
1:B:210:ALA:HA	1:B:251:LEU:HD23	1.84	0.58
1:B:307:ARG:NH2	2:B:595:HOH:O	2.33	0.58
1:A:165:ALA:CB	2:A:653:HOH:O	2.51	0.58
1:A:455:LEU:HD23	2:A:682:HOH:O	2.03	0.58
1:A:465:GLY:O	1:A:516:LEU:HA	2.04	0.58
1:A:578:GLN:O	1:A:579:ARG:C	2.46	0.58
1:B:28:GLN:HG3	1:B:67:VAL:CG2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:TRP:HZ3	1:B:260:ALA:HB3	1.67	0.58
1:B:324:GLU:OE2	1:B:327:ARG:NH1	2.33	0.58
1:B:390:PHE:CE1	1:B:579:ARG:NH2	2.72	0.58
1:A:177:LEU:HB3	1:A:190:PHE:HB2	1.86	0.58
1:B:178:PHE:C	1:B:178:PHE:CD1	2.81	0.58
1:B:248:ILE:HD12	1:B:248:ILE:H	1.69	0.58
1:B:27:LEU:CD1	1:B:38:VAL:HG12	2.33	0.58
1:B:52:ASP:C	1:B:54:GLY:H	2.11	0.58
1:B:528:PRO:O	1:B:532:LEU:HD23	2.03	0.58
1:A:159:ILE:HG23	1:A:163:LEU:O	2.03	0.58
1:B:92:LEU:C	1:B:106:LEU:HD12	2.29	0.58
1:A:38:VAL:CG1	1:A:39:VAL:H	2.17	0.58
1:A:160:ARG:HD3	1:A:202:ILE:HG22	1.85	0.58
1:B:133:ARG:HA	1:B:483:ALA:HB2	1.85	0.58
1:B:497:ARG:O	1:B:500:MET:N	2.37	0.58
1:A:120:THR:HB	2:A:617:HOH:O	2.04	0.57
1:A:403:TYR:HD1	2:A:618:HOH:O	1.87	0.57
1:B:60:ASN:O	1:B:101:GLY:HA2	2.05	0.57
1:B:201:SER:HB2	1:B:252:GLY:HA2	1.86	0.57
1:A:217:GLU:HG2	1:A:245:PRO:O	2.05	0.57
1:B:295:LEU:HB2	1:B:311:LEU:HB2	1.85	0.57
1:B:343:GLY:N	2:B:722:HOH:O	2.37	0.57
1:A:44:GLY:HA2	1:A:561:MET:CB	2.34	0.57
1:A:51:TYR:CZ	1:A:53:GLY:HA2	2.39	0.57
1:A:497:ARG:C	1:A:499:ILE:H	2.13	0.57
1:B:266:GLU:HG2	1:B:337:TRP:HZ2	1.69	0.57
1:B:477:MET:HB3	2:B:642:HOH:O	2.05	0.57
1:B:477:MET:CE	1:B:489:ILE:HD11	2.34	0.57
1:B:326:LEU:HA	1:B:355:ARG:HH11	1.67	0.57
1:B:493:THR:O	1:B:494:GLY:C	2.47	0.57
1:A:187:LEU:HD12	1:A:188:ARG:H	1.68	0.57
1:A:412:ILE:HD13	1:A:492:LEU:HD12	1.86	0.57
1:A:475:GLU:HA	1:A:500:MET:HE2	1.86	0.57
1:B:233:LEU:HD23	1:B:234:GLU:N	2.20	0.57
1:A:38:VAL:HG12	1:A:39:VAL:H	1.65	0.57
1:A:187:LEU:HD12	1:A:188:ARG:N	2.20	0.57
1:A:267:GLY:HA2	1:A:375:SER:CB	2.34	0.57
1:A:372:ALA:O	1:A:401:THR:N	2.34	0.57
1:B:271:VAL:O	1:B:277:ARG:HA	2.03	0.57
1:B:47:ASN:HA	2:B:679:HOH:O	2.04	0.57
1:B:198:SER:HB3	1:B:213:GLU:OE2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:ILE:HB	1:B:554:ALA:HB2	1.87	0.57
1:A:323:PRO:HD2	1:A:326:LEU:HD12	1.86	0.57
1:A:569:LEU:HG	1:A:573:PHE:HE2	1.70	0.57
1:B:329:SER:HB3	1:B:355:ARG:HE	1.69	0.57
1:B:464:ALA:CB	1:B:578:GLN:HG3	2.35	0.57
1:A:169:PHE:HE2	1:A:371:PHE:CD1	2.22	0.57
1:A:449:TYR:HB2	1:A:471:VAL:HG23	1.86	0.57
1:A:113:ARG:NH2	1:A:525:SER:OG	2.38	0.56
1:A:446:TYR:HB3	2:A:686:HOH:O	2.05	0.56
1:B:68:LEU:HG	1:B:78:ILE:HB	1.87	0.56
1:A:419:GLU:O	1:A:423:VAL:HG23	2.06	0.56
1:A:473:ASP:N	2:A:657:HOH:O	2.38	0.56
1:A:526:ARG:HD2	1:A:556:HIS:CG	2.40	0.56
1:B:127:THR:HA	1:B:135:ALA:O	2.06	0.56
1:B:304:THR:O	1:B:378:TRP:HB2	2.06	0.56
1:A:363:VAL:HA	1:A:440:TYR:O	2.05	0.56
1:B:420:LEU:HD22	1:B:453:CYS:SG	2.46	0.56
1:A:305:PRO:HA	1:A:378:TRP:CG	2.41	0.56
1:A:429:TRP:CD1	1:A:433:SER:HB2	2.40	0.56
1:B:240:PHE:HE1	1:B:263:ALA:HB2	1.70	0.56
1:B:361:PRO:HA	1:B:438:GLU:CG	2.34	0.56
1:B:516:LEU:HD12	1:B:517:ALA:H	1.70	0.56
1:A:341:PHE:C	1:A:343:GLY:H	2.13	0.56
1:A:519:ILE:HG12	1:A:549:HIS:CD2	2.40	0.56
1:B:99:ARG:CZ	1:B:102:GLU:HB3	2.36	0.56
1:B:455:LEU:HD22	1:B:514:GLU:HB2	1.88	0.56
1:A:393:VAL:HG11	1:A:426:ALA:HB1	1.88	0.56
1:A:441:ILE:HB	1:A:462:PHE:CD1	2.41	0.56
1:A:486:ARG:HH11	1:A:486:ARG:HG3	1.71	0.56
1:B:90:HIS:O	1:B:111:PRO:HA	2.05	0.56
1:B:517:ALA:HB2	1:B:574:PHE:CE1	2.41	0.56
1:A:305:PRO:HD3	1:A:322:LEU:HD12	1.88	0.56
1:B:139:LEU:HD12	1:B:143:GLY:C	2.31	0.56
1:B:456:THR:HG23	1:B:512:ILE:HD11	1.87	0.56
1:A:46:VAL:N	2:A:595:HOH:O	2.38	0.56
1:A:106:LEU:HA	2:A:698:HOH:O	2.04	0.56
1:A:164:ILE:O	1:A:179:THR:HA	2.06	0.56
1:A:286:GLY:O	1:A:287:ARG:C	2.48	0.56
1:A:347:PRO:HG3	1:A:403:TYR:CD2	2.41	0.56
1:A:458:LYS:O	1:A:460:GLY:N	2.39	0.56
1:B:271:VAL:O	1:B:277:ARG:HD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:ALA:HB3	1:B:352:GLU:CB	2.36	0.56
1:A:550:ILE:O	1:B:547:GLU:HA	2.06	0.55
1:A:219:ARG:HG3	1:A:219:ARG:HH11	1.71	0.55
1:A:445:SER:HA	1:A:469:ALA:O	2.06	0.55
1:A:520:HIS:O	1:A:550:ILE:HA	2.06	0.55
1:B:350:VAL:HG21	1:B:429:TRP:CH2	2.41	0.55
1:B:453:CYS:HB2	2:B:731:HOH:O	2.07	0.55
1:A:92:LEU:O	1:A:106:LEU:HG	2.04	0.55
1:A:563:ASP:OD2	2:A:585:HOH:O	2.18	0.55
1:B:471:VAL:HG23	2:B:685:HOH:O	2.05	0.55
1:A:25:TYR:HB3	1:A:38:VAL:HG11	1.88	0.55
1:A:426:ALA:HB2	2:A:651:HOH:O	2.06	0.55
1:B:123:ALA:HA	1:B:139:LEU:O	2.06	0.55
1:B:326:LEU:HB3	2:B:794:HOH:O	2.05	0.55
1:B:455:LEU:CD2	1:B:514:GLU:HB2	2.37	0.55
1:A:399:GLY:O	1:A:408:ARG:HG3	2.06	0.55
1:A:478:TYR:HE1	1:A:486:ARG:O	1.90	0.55
1:A:499:ILE:HG23	1:A:503:ARG:HG3	1.89	0.55
1:B:51:TYR:CZ	1:B:53:GLY:HA2	2.42	0.55
1:B:476:GLU:HA	1:B:479:GLU:CD	2.31	0.55
1:A:379:ASP:OD1	1:A:381:PHE:N	2.38	0.55
1:A:474:TRP:CD1	1:A:500:MET:HA	2.42	0.55
1:B:59:LEU:HD22	2:B:727:HOH:O	2.07	0.55
1:B:255:PRO:O	1:B:257:GLY:N	2.39	0.55
1:B:496:SER:CB	2:B:619:HOH:O	2.52	0.55
1:A:579:ARG:HG2	1:A:580:GLU:HG3	1.88	0.55
1:B:169:PHE:CE2	1:B:175:VAL:HG22	2.40	0.55
1:B:246:THR:CG2	1:B:402:GLY:O	2.55	0.55
1:B:259:LEU:HD11	2:B:767:HOH:O	2.06	0.55
1:A:169:PHE:HE2	1:A:371:PHE:HD1	1.54	0.55
1:A:215:ALA:CB	1:A:406:GLU:HB2	2.35	0.55
1:A:418:GLY:O	1:A:421:GLU:HB2	2.07	0.55
1:A:550:ILE:HB	1:B:548:ALA:H	1.71	0.55
1:B:219:ARG:HG3	1:B:220:LEU:N	2.22	0.55
1:A:237:SER:HB3	1:A:276:GLU:N	2.21	0.55
1:B:373:GLU:HB3	2:B:739:HOH:O	2.05	0.55
1:A:173:GLY:O	1:A:408:ARG:NH1	2.38	0.55
1:A:449:TYR:HB2	1:A:471:VAL:CG2	2.36	0.55
1:A:472:VAL:HG21	1:A:535:LEU:HD13	1.88	0.55
1:A:159:ILE:HD12	1:A:164:ILE:HG13	1.89	0.54
1:A:269:SER:OG	1:A:285:HIS:CD2	2.60	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:ILE:HD13	1:A:441:ILE:C	2.31	0.54
1:A:563:ASP:HA	1:A:566:LYS:HB2	1.88	0.54
1:B:220:LEU:HG	1:B:240:PHE:CE2	2.43	0.54
1:B:250:TRP:CD2	1:B:287:ARG:HA	2.42	0.54
1:B:355:ARG:HG3	1:B:387:ALA:HA	1.88	0.54
1:B:406:GLU:HA	2:B:763:HOH:O	2.07	0.54
1:A:284:ASN:HB2	1:A:300:THR:HG23	1.89	0.54
1:A:519:ILE:HG22	1:A:567:ILE:HG22	1.89	0.54
1:B:90:HIS:CD2	1:B:114:ILE:H	2.25	0.54
1:B:357:PRO:O	1:B:360:GLY:HA3	2.07	0.54
1:B:359:PRO:HB3	1:B:434:GLY:O	2.07	0.54
1:B:458:LYS:O	1:B:461:LEU:HB2	2.07	0.54
1:A:322:LEU:HD22	1:A:323:PRO:O	2.07	0.54
1:B:35:LYS:HE2	1:B:52:ASP:OD2	2.07	0.54
1:B:411:ILE:HD12	1:B:419:GLU:HG2	1.87	0.54
1:A:307:ARG:HB2	1:A:318:LEU:O	2.08	0.54
1:A:346:VAL:HG13	1:A:407:TRP:CZ2	2.40	0.54
1:B:268:ARG:HH12	1:B:282:GLN:CD	2.15	0.54
1:A:220:LEU:HB3	1:A:233:LEU:HD12	1.89	0.54
1:A:549:HIS:HD1	1:B:549:HIS:CE1	2.25	0.54
1:B:91:ALA:HB1	1:B:105:ARG:NE	2.22	0.54
1:B:300:THR:O	1:B:301:SER:HB2	2.06	0.54
1:B:562:GLU:HG3	2:B:724:HOH:O	2.07	0.54
1:A:24:LYS:O	1:A:40:GLY:HA2	2.08	0.54
1:A:59:LEU:O	1:A:101:GLY:N	2.41	0.54
1:A:249:THR:HG22	1:A:250:TRP:HB3	1.88	0.54
1:A:175:VAL:HB	1:A:197:PHE:H	1.73	0.54
1:A:309:VAL:HG12	1:A:316:PRO:HB3	1.90	0.54
1:A:379:ASP:OD1	1:A:381:PHE:CD1	2.61	0.54
1:B:376:ASP:CB	2:B:616:HOH:O	2.46	0.54
1:B:397:TYR:HD1	1:B:419:GLU:HB3	1.71	0.54
1:A:105:ARG:O	1:A:107:GLU:N	2.40	0.54
1:A:172:GLY:C	1:A:174:ARG:N	2.63	0.54
1:B:245:PRO:HB2	1:B:263:ALA:HB1	1.90	0.54
1:B:323:PRO:CB	1:B:326:LEU:HD12	2.37	0.54
1:A:308:ILE:N	1:A:318:LEU:O	2.33	0.54
1:B:408:ARG:O	1:B:411:ILE:HG22	2.08	0.54
1:B:421:GLU:O	1:B:425:ALA:N	2.39	0.54
1:B:567:ILE:HD12	1:B:567:ILE:C	2.32	0.54
1:B:570:PRO:HA	2:B:653:HOH:O	2.07	0.54
1:A:468:GLY:C	1:A:470:SER:N	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ILE:HD11	1:B:182:LEU:HA	1.89	0.54
1:B:508:HIS:C	1:B:510:ASP:N	2.64	0.54
1:B:565:VAL:O	1:B:568:LEU:N	2.40	0.54
1:A:23:GLU:HG2	2:A:600:HOH:O	2.08	0.53
1:A:489:ILE:O	1:A:490:GLU:C	2.50	0.53
1:B:30:VAL:N	1:B:289:VAL:HG11	2.23	0.53
1:B:205:GLY:O	1:B:206:MET:HB2	2.08	0.53
1:A:258:ARG:HD2	1:A:273:ILE:CG2	2.38	0.53
1:B:177:LEU:HD22	1:B:223:VAL:HG21	1.89	0.53
1:B:490:GLU:O	1:B:495:GLY:N	2.27	0.53
1:B:522:GLN:HB3	1:B:551:ILE:O	2.07	0.53
1:B:536:MET:HE1	1:B:550:ILE:HD11	1.90	0.53
1:A:96:ASN:HD21	1:A:98:SER:HB2	1.73	0.53
1:A:175:VAL:CG2	1:A:196:SER:HB3	2.38	0.53
1:B:114:ILE:N	1:B:114:ILE:HD12	2.23	0.53
1:B:249:THR:N	1:B:262:VAL:O	2.42	0.53
1:B:543:GLY:O	1:B:544:LYS:C	2.50	0.53
1:A:37:LEU:HD12	1:A:49:TYR:O	2.08	0.53
1:A:292:ARG:O	1:A:294:LYS:HD2	2.08	0.53
1:A:334:ARG:NH2	1:A:350:VAL:HG11	2.22	0.53
1:A:579:ARG:HG2	1:A:580:GLU:N	2.22	0.53
1:A:46:VAL:O	1:A:64:ILE:HG12	2.09	0.53
1:A:115:LEU:O	1:A:116:SER:HB3	2.07	0.53
1:A:174:ARG:NH2	1:A:405:GLU:OE2	2.41	0.53
1:A:351:LEU:CD1	1:A:382:ALA:HB1	2.38	0.53
1:A:469:ALA:HA	1:A:520:HIS:CE1	2.44	0.53
1:B:195:GLY:HA3	1:B:213:GLU:O	2.08	0.53
1:A:22:VAL:HG21	1:A:323:PRO:HD3	1.90	0.53
1:A:274:ASP:C	1:A:276:GLU:H	2.17	0.53
1:A:442:MET:HG3	1:A:466:VAL:HB	1.89	0.53
1:A:456:THR:HG22	1:A:512:ILE:HG12	1.90	0.53
1:A:524:ASP:OD1	1:A:556:HIS:HB2	2.09	0.53
1:B:509:VAL:HA	1:B:512:ILE:CD1	2.35	0.53
1:A:58:LYS:HD3	2:A:736:HOH:O	2.08	0.53
1:A:62:GLU:HB2	1:A:81:ARG:NH2	2.23	0.53
1:A:115:LEU:HB2	2:A:677:HOH:O	2.08	0.53
1:A:379:ASP:OD1	1:A:381:PHE:HD1	1.92	0.53
1:B:423:VAL:HG21	1:B:450:MET:HG2	1.90	0.53
1:B:445:SER:C	1:B:447:GLY:N	2.66	0.53
1:A:194:GLU:HB3	1:A:214:THR:HG22	1.91	0.53
1:A:348:THR:HG21	1:A:393:VAL:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:VAL:CG1	1:B:32:ASP:N	2.71	0.53
1:B:42:SER:OG	1:B:43:GLU:N	2.42	0.53
1:A:151:PRO:HB2	1:A:170:PHE:CD2	2.44	0.53
1:A:169:PHE:CE2	1:A:371:PHE:HD1	2.27	0.53
1:A:328:ARG:HG2	1:A:328:ARG:NH1	2.23	0.52
1:A:350:VAL:HA	2:A:652:HOH:O	2.09	0.52
1:A:414:ASP:CG	1:A:414:ASP:O	2.51	0.52
1:A:84:SER:OG	1:A:87:ALA:HB3	2.10	0.52
1:A:125:VAL:HG13	1:A:137:TYR:O	2.09	0.52
1:B:325:ASP:C	1:B:328:ARG:H	2.17	0.52
1:A:497:ARG:C	1:A:499:ILE:N	2.67	0.52
1:B:133:ARG:HD2	1:B:146:GLU:OE2	2.09	0.52
1:B:539:LEU:HD13	1:B:546:PHE:CD1	2.44	0.52
1:A:106:LEU:HD11	2:A:589:HOH:O	2.09	0.52
1:A:551:ILE:N	1:A:551:ILE:HD12	2.25	0.52
1:B:209:THR:O	1:B:210:ALA:HB2	2.09	0.52
1:B:158:ASP:C	1:B:159:ILE:HD13	2.34	0.52
1:B:366:VAL:HG12	2:B:588:HOH:O	2.07	0.52
1:A:198:SER:HB3	1:A:213:GLU:OE2	2.09	0.52
1:A:392:VAL:HG12	1:A:393:VAL:N	2.25	0.52
1:A:441:ILE:HB	1:A:462:PHE:CE1	2.45	0.52
1:A:463:LYS:HB2	2:A:729:HOH:O	2.09	0.52
1:B:59:LEU:HA	1:B:100:PRO:HB3	1.90	0.52
1:B:242:SER:C	1:B:244:ARG:H	2.15	0.52
1:B:325:ASP:HA	1:B:328:ARG:NE	2.24	0.52
1:B:457:MET:C	1:B:459:PRO:HD2	2.34	0.52
1:A:132:ASP:O	1:A:133:ARG:HB3	2.09	0.52
1:A:354:GLY:C	1:A:356:ALA:H	2.18	0.52
1:A:415:PRO:HD3	1:A:492:LEU:O	2.08	0.52
1:B:246:THR:HG21	1:B:402:GLY:O	2.10	0.52
1:A:309:VAL:HG12	1:A:316:PRO:CB	2.39	0.52
1:A:353:SER:HB2	1:A:386:ALA:HA	1.92	0.52
1:B:501:ARG:O	1:B:507:ASN:OD1	2.27	0.52
1:A:304:THR:HG23	2:A:654:HOH:O	2.10	0.52
1:A:339:GLU:OE2	1:A:343:GLY:HA2	2.09	0.52
1:A:463:LYS:O	1:A:514:GLU:HB3	2.09	0.52
1:A:530:LYS:HB3	1:A:531:PRO:CD	2.28	0.52
1:B:159:ILE:CD1	1:B:164:ILE:HG23	2.39	0.52
1:B:472:VAL:HG23	1:B:532:LEU:HD22	1.92	0.52
1:B:564:ALA:HB2	2:B:729:HOH:O	2.10	0.52
1:A:468:GLY:O	1:A:469:ALA:C	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:THR:HG22	1:B:265:ARG:HA	1.91	0.52
1:B:489:ILE:HG21	1:B:500:MET:HE3	1.91	0.52
1:A:202:ILE:HG13	2:A:653:HOH:O	2.09	0.51
1:B:37:LEU:HD23	1:B:70:PRO:HG3	1.91	0.51
1:B:145:ARG:HD3	2:B:664:HOH:O	2.09	0.51
1:B:281:PRO:HG3	2:B:595:HOH:O	2.09	0.51
1:A:129:ALA:HB1	1:A:134:VAL:HG22	1.91	0.51
1:A:133:ARG:HD2	2:A:609:HOH:O	2.10	0.51
1:A:497:ARG:O	1:A:500:MET:N	2.43	0.51
1:A:471:VAL:HG11	1:A:474:TRP:CZ3	2.46	0.51
1:B:397:TYR:CD1	1:B:419:GLU:HB3	2.45	0.51
1:B:495:GLY:O	1:B:496:SER:C	2.54	0.51
1:B:497:ARG:N	2:B:648:HOH:O	2.42	0.51
1:A:482:ASP:OD1	1:A:485:PHE:HD1	1.93	0.51
1:B:141:GLY:C	1:B:143:GLY:H	2.18	0.51
1:A:181:ASN:HB3	1:A:185:GLY:H	1.75	0.51
1:A:299:HIS:CG	1:A:300:THR:N	2.77	0.51
1:B:72:TYR:CE2	1:B:289:VAL:HG13	2.46	0.51
1:B:136:LEU:O	1:B:147:LEU:HB2	2.10	0.51
1:B:463:LYS:O	2:B:689:HOH:O	2.19	0.51
1:B:579:ARG:O	1:B:581:ARG:N	2.43	0.51
1:A:87:ALA:HA	1:A:523:ASN:O	2.11	0.51
1:A:284:ASN:ND2	1:A:376:ASP:O	2.43	0.51
1:A:305:PRO:O	1:A:306:PRO:C	2.52	0.51
1:B:78:ILE:HD11	1:B:124:VAL:HG22	1.93	0.51
1:B:411:ILE:HD12	1:B:419:GLU:CG	2.41	0.51
1:B:487:ASN:O	1:B:491:GLN:HG3	2.10	0.51
1:A:27:LEU:HB3	2:A:605:HOH:O	2.10	0.51
1:B:225:PRO:HB2	2:B:738:HOH:O	2.11	0.51
1:A:399:GLY:HA2	1:A:408:ARG:O	2.10	0.51
1:A:350:VAL:HG12	1:A:351:LEU:N	2.26	0.51
1:B:344:SER:N	2:B:722:HOH:O	2.43	0.51
1:A:63:PRO:HB3	2:A:595:HOH:O	2.11	0.51
1:A:81:ARG:O	1:A:90:HIS:HA	2.11	0.51
1:A:174:ARG:HH21	1:A:405:GLU:CG	2.23	0.51
1:A:385:LEU:HB3	2:A:720:HOH:O	2.11	0.51
1:A:474:TRP:CB	1:A:500:MET:HB3	2.40	0.51
1:B:349:TYR:HB3	1:B:394:MET:HE3	1.93	0.51
1:B:362:THR:CG2	1:B:363:VAL:H	2.23	0.51
1:B:401:THR:HG22	1:B:408:ARG:CD	2.41	0.51
1:A:172:GLY:C	1:A:174:ARG:H	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ASP:OD1	1:B:84:SER:OG	2.22	0.50
1:B:379:ASP:O	1:B:380:THR:C	2.53	0.50
1:A:371:PHE:N	1:A:371:PHE:CD2	2.78	0.50
1:B:139:LEU:HD12	1:B:143:GLY:O	2.11	0.50
1:B:430:ALA:O	1:B:436:ALA:N	2.38	0.50
1:A:202:ILE:CG1	2:A:653:HOH:O	2.58	0.50
1:A:415:PRO:O	1:A:416:CYS:HB3	2.11	0.50
1:A:472:VAL:HG21	1:A:535:LEU:HD22	1.93	0.50
1:A:551:ILE:CG2	1:A:552:PRO:HD2	2.41	0.50
1:B:451:THR:O	2:B:615:HOH:O	2.18	0.50
1:B:482:ASP:HB2	2:B:604:HOH:O	2.12	0.50
1:A:29:GLY:O	1:A:37:LEU:HB3	2.11	0.50
1:A:207:LYS:HE2	1:A:224:ASP:HB2	1.93	0.50
1:A:569:LEU:O	1:A:573:PHE:CD2	2.65	0.50
1:B:109:VAL:CG2	1:B:139:LEU:HD22	2.41	0.50
1:B:235:LEU:HD13	1:B:274:ASP:C	2.37	0.50
1:B:314:GLY:HA3	2:B:595:HOH:O	2.09	0.50
1:B:353:SER:HB3	1:B:356:ALA:CB	2.38	0.50
1:A:160:ARG:NH1	1:A:203:SER:HA	2.27	0.50
1:A:268:ARG:HA	1:A:283:GLY:O	2.11	0.50
1:A:400:SER:C	2:A:618:HOH:O	2.53	0.50
1:B:76:ARG:NH2	2:B:725:HOH:O	2.32	0.50
1:B:362:THR:OG1	1:B:391:HIS:HB2	2.11	0.50
1:B:35:LYS:HB2	1:B:50:LEU:HD22	1.93	0.50
1:B:56:THR:N	2:B:735:HOH:O	2.43	0.50
1:B:81:ARG:HB3	1:B:93:PHE:CE1	2.47	0.50
1:B:393:VAL:HB	2:B:775:HOH:O	2.11	0.50
1:B:476:GLU:O	1:B:480:LEU:HG	2.12	0.50
1:A:365:LEU:HB2	2:A:693:HOH:O	2.12	0.50
1:A:399:GLY:N	1:A:407:TRP:O	2.45	0.50
1:B:35:LYS:CG	1:B:52:ASP:OD1	2.60	0.50
1:B:250:TRP:CZ3	1:B:260:ALA:HB3	2.46	0.50
1:B:255:PRO:C	1:B:257:GLY:H	2.19	0.50
1:B:371:PHE:CE2	1:B:408:ARG:NH1	2.79	0.50
1:A:249:THR:HG22	1:A:250:TRP:N	2.25	0.50
1:A:294:LYS:O	1:A:296:VAL:HG23	2.12	0.50
1:A:366:VAL:HG12	1:A:367:HIS:O	2.12	0.50
1:B:34:ASP:O	1:B:35:LYS:HG2	2.10	0.50
1:B:445:SER:C	1:B:447:GLY:H	2.19	0.50
1:B:455:LEU:CD1	1:B:516:LEU:HD13	2.42	0.50
1:A:94:LYS:HB3	1:A:106:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:GLY:HA2	1:A:493:THR:HA	1.93	0.50
1:A:308:ILE:O	1:A:317:LEU:N	2.44	0.49
1:A:536:MET:CE	1:A:550:ILE:HD11	2.41	0.49
1:B:522:GLN:HE21	1:B:523:ASN:CG	2.19	0.49
1:A:202:ILE:HG22	1:A:203:SER:N	2.26	0.49
1:A:529:LEU:CD1	1:A:550:ILE:HD12	2.33	0.49
1:B:431:ARG:HG3	1:B:431:ARG:HH11	1.77	0.49
1:A:60:ASN:ND2	1:A:62:GLU:O	2.37	0.49
1:A:240:PHE:HD1	1:A:272:PHE:CD1	2.31	0.49
1:B:251:LEU:HD11	1:B:259:LEU:HD11	1.93	0.49
1:A:71:HIS:HB2	1:A:119:ASP:O	2.11	0.49
1:A:522:GLN:HG2	1:A:552:PRO:HA	1.94	0.49
1:B:49:TYR:CA	1:B:57:VAL:O	2.54	0.49
1:B:405:GLU:HG3	1:B:409:LEU:HG	1.95	0.49
1:B:451:THR:HG21	1:B:466:VAL:O	2.12	0.49
1:A:68:LEU:HB2	1:A:78:ILE:HB	1.94	0.49
1:A:408:ARG:O	1:A:411:ILE:HG22	2.13	0.49
1:A:417:GLY:H	1:A:419:GLU:CD	2.19	0.49
1:B:153:PHE:CE1	1:B:488:PHE:HB2	2.45	0.49
1:B:311:LEU:HB3	1:B:312:PRO:HA	1.95	0.49
1:B:486:ARG:O	1:B:490:GLU:HG3	2.12	0.49
1:A:44:GLY:HA2	1:A:561:MET:N	2.22	0.49
1:B:243:TYR:CZ	1:B:270:ALA:HB2	2.47	0.49
1:B:431:ARG:HG3	1:B:431:ARG:NH1	2.28	0.49
1:A:160:ARG:HH22	1:A:204:PRO:HG3	1.78	0.49
1:A:309:VAL:HA	1:A:317:LEU:H	1.77	0.49
1:B:365:LEU:HD23	1:B:394:MET:HG2	1.94	0.49
1:A:142:GLY:HA3	2:A:636:HOH:O	2.11	0.49
1:A:416:CYS:SG	1:A:416:CYS:O	2.70	0.49
1:B:90:HIS:CG	1:B:114:ILE:HD13	2.46	0.49
1:B:376:ASP:C	2:B:600:HOH:O	2.55	0.49
1:A:174:ARG:NE	1:A:409:LEU:HD11	2.25	0.49
1:B:36:LEU:HD11	1:B:296:VAL:HG11	1.94	0.49
1:B:209:THR:HG23	1:B:233:LEU:HD12	1.95	0.49
1:A:124:VAL:N	1:A:139:LEU:O	2.38	0.49
1:A:224:ASP:OD1	1:A:225:PRO:HD2	2.12	0.49
1:A:475:GLU:OE1	1:A:497:ARG:HG3	2.13	0.49
1:B:65:ASN:HD21	1:B:82:ASP:HB2	1.77	0.49
1:B:280:ALA:CB	1:B:285:HIS:CE1	2.96	0.49
1:B:506:ILE:CD1	1:B:535:LEU:HA	2.43	0.49
1:B:522:GLN:HG3	1:B:523:ASN:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:VAL:HG11	1:A:121:GLY:CA	2.43	0.48
1:A:240:PHE:CE1	1:A:245:PRO:HG3	2.47	0.48
1:A:305:PRO:HD2	2:A:654:HOH:O	2.11	0.48
1:A:379:ASP:OD1	1:A:379:ASP:C	2.56	0.48
1:B:71:HIS:HA	2:B:666:HOH:O	2.13	0.48
1:B:411:ILE:HD13	1:B:419:GLU:HG2	1.94	0.48
1:A:194:GLU:CB	1:A:212:LEU:HD21	2.38	0.48
1:A:277:ARG:HD2	1:A:278:VAL:H	1.77	0.48
1:B:239:ASP:HA	1:B:242:SER:OG	2.13	0.48
1:A:341:PHE:CG	1:A:342:ASP:N	2.82	0.48
1:A:579:ARG:NH1	1:A:579:ARG:CB	2.75	0.48
1:B:379:ASP:HB3	1:B:382:ALA:CB	2.43	0.48
1:B:459:PRO:HG3	2:B:605:HOH:O	2.13	0.48
1:B:516:LEU:HD21	1:B:518:LEU:HD21	1.94	0.48
1:A:136:LEU:HD11	1:A:156:VAL:HG22	1.96	0.48
1:A:194:GLU:OE2	1:A:219:ARG:NH2	2.47	0.48
1:B:68:LEU:HD12	1:B:78:ILE:CD1	2.43	0.48
1:B:243:TYR:O	1:B:244:ARG:C	2.56	0.48
1:B:453:CYS:N	2:B:731:HOH:O	2.46	0.48
1:A:374:ASP:CG	1:A:394:MET:HB3	2.39	0.48
1:A:563:ASP:HA	1:A:566:LYS:CB	2.43	0.48
1:B:40:GLY:HA3	1:B:49:TYR:HE1	1.79	0.48
1:B:272:PHE:CE2	1:B:277:ARG:HB2	2.48	0.48
1:A:40:GLY:C	1:A:42:SER:N	2.72	0.48
1:A:361:PRO:HB3	1:A:438:GLU:OE2	2.14	0.48
1:A:384:SER:O	1:A:387:ALA:HB3	2.13	0.48
1:B:68:LEU:HD12	1:B:124:VAL:HG13	1.95	0.48
1:B:210:ALA:O	1:B:211:GLY:C	2.55	0.48
1:A:26:SER:OG	1:A:28:GLN:NE2	2.46	0.48
1:A:130:THR:O	1:A:131:GLU:C	2.56	0.48
1:A:192:SER:HB3	1:A:195:GLY:O	2.13	0.48
1:A:258:ARG:HB3	1:A:273:ILE:HG23	1.96	0.48
1:A:264:ARG:NE	1:A:373:GLU:OE2	2.45	0.48
1:A:374:ASP:N	1:A:396:ASN:OD1	2.35	0.48
1:B:376:ASP:HA	2:B:600:HOH:O	2.12	0.48
1:A:129:ALA:CB	1:A:484:ALA:HB2	2.43	0.48
1:A:330:ILE:HD12	1:A:330:ILE:N	2.29	0.48
1:A:452:LEU:HB3	1:A:505:PRO:HG2	1.95	0.48
1:A:549:HIS:ND1	1:A:570:PRO:HB3	2.29	0.48
1:B:28:GLN:HG3	1:B:67:VAL:HG21	1.96	0.48
1:B:449:TYR:N	2:B:685:HOH:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:ILE:HD13	1:B:567:ILE:O	2.13	0.48
1:A:173:GLY:O	1:A:408:ARG:NH2	2.47	0.48
1:A:174:ARG:NH2	1:A:195:GLY:HA2	2.29	0.48
1:A:222:THR:HB	1:A:231:GLU:CG	2.43	0.48
1:A:553:ASP:OD1	1:B:545:THR:CG2	2.61	0.48
1:B:331:ALA:HB3	1:B:352:GLU:C	2.38	0.48
1:B:365:LEU:HD11	1:B:381:PHE:HB3	1.96	0.48
1:B:367:HIS:CE1	1:B:400:SER:OG	2.67	0.48
1:B:442:MET:HG3	1:B:466:VAL:CG1	2.44	0.48
1:B:468:GLY:HA2	1:B:519:ILE:O	2.13	0.48
1:B:38:VAL:CG1	1:B:308:ILE:HD13	2.44	0.48
1:B:282:GLN:NE2	2:B:660:HOH:O	2.46	0.48
1:B:294:LYS:HG2	2:B:705:HOH:O	2.13	0.48
1:B:411:ILE:HG12	1:B:492:LEU:HD11	1.95	0.48
1:B:458:LYS:N	1:B:459:PRO:CD	2.77	0.48
1:B:568:LEU:O	1:B:572:VAL:HG23	2.14	0.48
1:A:90:HIS:HD2	1:A:114:ILE:N	2.08	0.47
1:A:415:PRO:HG3	1:A:493:THR:HG22	1.95	0.47
1:A:460:GLY:O	1:A:461:LEU:C	2.57	0.47
1:A:474:TRP:HD1	1:A:500:MET:HA	1.79	0.47
1:A:569:LEU:HB3	1:A:570:PRO:CD	2.36	0.47
1:B:333:SER:HA	1:B:350:VAL:O	2.14	0.47
1:B:520:HIS:CB	2:B:744:HOH:O	2.62	0.47
1:A:214:THR:C	1:A:216:ARG:N	2.70	0.47
1:A:372:ALA:O	1:A:373:GLU:HB3	2.14	0.47
1:A:521:PRO:CB	1:A:555:GLY:O	2.62	0.47
1:B:406:GLU:HG2	1:B:410:LYS:CE	2.41	0.47
1:B:451:THR:HA	2:B:615:HOH:O	2.14	0.47
1:A:98:SER:C	1:A:100:PRO:HD3	2.39	0.47
1:B:27:LEU:HD12	1:B:38:VAL:HG12	1.94	0.47
1:B:73:GLY:O	1:B:74:VAL:C	2.57	0.47
1:B:322:LEU:O	1:B:323:PRO:O	2.33	0.47
1:B:475:GLU:O	1:B:478:TYR:HB3	2.14	0.47
1:A:224:ASP:O	1:A:228:GLY:HA2	2.14	0.47
1:A:515:PRO:CA	2:A:613:HOH:O	2.47	0.47
1:B:212:LEU:CD2	1:B:219:ARG:HH12	2.12	0.47
1:B:550:ILE:N	1:B:550:ILE:HD12	2.29	0.47
1:A:309:VAL:CA	1:A:316:PRO:HA	2.41	0.47
1:B:70:PRO:HA	1:B:119:ASP:HB3	1.97	0.47
1:B:248:ILE:HD12	1:B:248:ILE:N	2.28	0.47
1:B:504:SER:O	1:B:506:ILE:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:HIS:CE1	2:B:618:HOH:O	2.67	0.47
1:B:551:ILE:HB	1:B:554:ALA:CB	2.43	0.47
1:B:385:LEU:O	1:B:390:PHE:N	2.45	0.47
1:B:477:MET:HA	1:B:528:PRO:HG3	1.96	0.47
1:A:104:GLN:NE2	2:A:699:HOH:O	2.47	0.47
1:A:219:ARG:HH12	1:A:221:VAL:CG1	2.27	0.47
1:A:254:LEU:HD11	1:A:295:LEU:HD21	1.96	0.47
1:A:312:PRO:O	1:A:313:SER:C	2.58	0.47
1:A:358:THR:HA	1:A:359:PRO:C	2.39	0.47
1:A:430:ALA:HB1	1:A:436:ALA:HB2	1.97	0.47
1:B:112:MET:HB2	1:B:130:THR:HG22	1.97	0.47
1:B:250:TRP:CE3	1:B:287:ARG:HA	2.50	0.47
1:B:309:VAL:HG12	1:B:316:PRO:CA	2.45	0.47
1:B:477:MET:CA	2:B:756:HOH:O	2.58	0.47
1:B:480:LEU:CB	2:B:756:HOH:O	2.52	0.47
1:A:258:ARG:HD2	1:A:273:ILE:HG21	1.97	0.47
1:A:346:VAL:HG22	1:A:407:TRP:CZ2	2.50	0.47
1:A:367:HIS:HE1	1:A:396:ASN:HA	1.80	0.47
1:B:476:GLU:CG	1:B:531:PRO:HG3	2.45	0.47
1:B:495:GLY:O	1:B:496:SER:O	2.33	0.47
1:A:237:SER:O	1:A:275:GLY:HA3	2.14	0.47
1:A:267:GLY:CA	1:A:375:SER:HB2	2.45	0.47
1:A:452:LEU:HB2	2:A:709:HOH:O	2.14	0.47
1:B:445:SER:HA	1:B:469:ALA:O	2.15	0.47
1:B:472:VAL:HG23	2:B:683:HOH:O	2.14	0.47
1:A:62:GLU:HB2	1:A:81:ARG:HE	1.80	0.47
1:A:519:ILE:CG2	1:A:567:ILE:HG22	2.44	0.47
1:B:47:ASN:HB2	2:B:656:HOH:O	2.15	0.47
1:B:89:GLN:HA	1:B:112:MET:O	2.15	0.47
1:B:280:ALA:HB3	1:B:285:HIS:CE1	2.50	0.47
1:B:367:HIS:HD2	1:B:368:GLY:O	1.98	0.47
1:B:441:ILE:HD13	2:B:615:HOH:O	2.15	0.47
1:A:151:PRO:HD2	1:A:170:PHE:CZ	2.49	0.46
1:A:366:VAL:HG13	1:A:397:TYR:CE2	2.50	0.46
1:B:52:ASP:C	1:B:54:GLY:N	2.74	0.46
1:B:322:LEU:O	1:B:323:PRO:C	2.59	0.46
1:B:428:ARG:O	1:B:429:TRP:C	2.58	0.46
1:B:431:ARG:HA	1:B:436:ALA:HB3	1.98	0.46
1:A:45:SER:CB	2:A:595:HOH:O	2.59	0.46
1:A:160:ARG:NH2	1:A:204:PRO:HG3	2.30	0.46
1:B:133:ARG:HD2	2:B:608:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:HG	1:A:376:ASP:OD1	2.15	0.46
1:A:532:LEU:O	1:A:536:MET:HG3	2.15	0.46
1:B:332:GLY:H	1:B:352:GLU:HB2	1.80	0.46
1:B:520:HIS:CD2	1:B:521:PRO:HD2	2.32	0.46
1:A:88:GLU:HG3	1:A:113:ARG:NH1	2.29	0.46
1:A:270:ALA:HB3	2:A:588:HOH:O	2.15	0.46
1:A:399:GLY:CA	1:A:408:ARG:HA	2.46	0.46
1:B:41:PHE:HZ	1:B:558:ILE:HG22	1.80	0.46
1:B:71:HIS:O	1:B:72:TYR:C	2.58	0.46
1:B:134:VAL:HB	1:B:150:LEU:HB2	1.97	0.46
1:B:178:PHE:HB2	1:B:187:LEU:HD11	1.96	0.46
1:B:251:LEU:HD12	1:B:259:LEU:HD11	1.97	0.46
1:B:458:LYS:O	1:B:461:LEU:CB	2.63	0.46
1:A:486:ARG:HG3	1:A:486:ARG:NH1	2.29	0.46
1:A:510:ASP:HB2	2:A:607:HOH:O	2.16	0.46
1:B:160:ARG:HD2	1:B:202:ILE:CG2	2.46	0.46
1:B:504:SER:C	1:B:506:ILE:H	2.24	0.46
1:A:93:PHE:HA	1:A:104:GLN:O	2.16	0.46
1:A:272:PHE:HD2	1:A:277:ARG:HA	1.80	0.46
1:A:370:PRO:C	1:A:372:ALA:H	2.21	0.46
1:A:398:ARG:HD3	1:A:410:LYS:HB3	1.97	0.46
1:B:51:TYR:CE2	1:B:53:GLY:HA2	2.51	0.46
1:B:88:GLU:HG2	1:B:113:ARG:HH12	1.74	0.46
1:B:323:PRO:HG2	1:B:326:LEU:CD1	2.43	0.46
1:A:138:ALA:HB2	1:A:147:LEU:CD2	2.38	0.46
1:A:222:THR:HG22	1:A:222:THR:O	2.16	0.46
1:A:240:PHE:CZ	1:A:245:PRO:HG3	2.51	0.46
1:A:265:ARG:HD3	2:A:598:HOH:O	2.15	0.46
1:A:579:ARG:CB	1:A:579:ARG:HH11	2.28	0.46
1:B:125:VAL:HA	1:B:138:ALA:HA	1.96	0.46
1:A:277:ARG:HD2	1:A:278:VAL:N	2.31	0.46
1:A:444:TYR:O	1:A:445:SER:HB3	2.16	0.46
1:B:51:TYR:CE2	1:B:317:LEU:HB3	2.43	0.46
1:B:448:GLY:HA3	1:B:470:SER:HB3	1.97	0.46
1:B:464:ALA:HB2	1:B:578:GLN:HG3	1.98	0.46
1:B:577:THR:CB	2:B:784:HOH:O	2.57	0.46
1:A:152:GLY:O	1:A:153:PHE:C	2.57	0.46
1:A:574:PHE:O	1:A:578:GLN:HG2	2.15	0.46
1:B:30:VAL:CG2	1:B:290:LEU:O	2.64	0.46
1:B:75:GLY:O	1:B:96:ASN:OD1	2.34	0.46
1:B:347:PRO:HG2	1:B:396:ASN:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:LYS:HB3	1:B:461:LEU:CD2	2.45	0.46
1:B:476:GLU:CD	1:B:531:PRO:HG3	2.41	0.46
1:A:95:VAL:CG2	1:A:103:GLU:HG2	2.45	0.45
1:A:451:THR:HG21	1:A:466:VAL:C	2.42	0.45
1:B:48:ALA:O	1:B:58:LYS:HA	2.17	0.45
1:B:251:LEU:HD11	1:B:259:LEU:HD21	1.98	0.45
1:B:279:GLU:HB2	1:B:312:PRO:O	2.15	0.45
1:B:334:ARG:NH2	1:B:429:TRP:HH2	2.14	0.45
1:A:47:ASN:HB3	1:A:60:ASN:OD1	2.17	0.45
1:A:178:PHE:CD1	1:A:178:PHE:O	2.70	0.45
1:A:420:LEU:HD11	1:A:454:ALA:HA	1.97	0.45
1:A:558:ILE:HD12	1:A:563:ASP:CB	2.31	0.45
1:B:178:PHE:HD2	2:B:706:HOH:O	1.99	0.45
1:B:307:ARG:HB2	1:B:319:GLU:CB	2.46	0.45
1:A:446:TYR:O	1:A:449:TYR:HB3	2.15	0.45
1:B:326:LEU:HD23	1:B:355:ARG:NH1	2.31	0.45
1:A:129:ALA:HA	1:A:134:VAL:HA	1.99	0.45
1:A:413:GLY:H	1:A:492:LEU:C	2.24	0.45
1:B:178:PHE:C	1:B:178:PHE:HD1	2.24	0.45
1:B:327:ARG:NH2	2:B:651:HOH:O	2.48	0.45
1:B:482:ASP:O	1:B:486:ARG:HG3	2.17	0.45
1:A:475:GLU:HG2	1:A:500:MET:HB2	1.98	0.45
1:B:27:LEU:HD13	1:B:38:VAL:HG12	1.98	0.45
1:B:61:ARG:N	1:B:103:GLU:OE2	2.50	0.45
1:B:91:ALA:CB	1:B:105:ARG:NE	2.79	0.45
1:B:92:LEU:CD1	1:B:109:VAL:HG11	2.46	0.45
1:B:95:VAL:HG13	2:B:742:HOH:O	2.15	0.45
1:B:551:ILE:HD11	1:B:567:ILE:HG22	1.98	0.45
1:A:44:GLY:CA	1:A:561:MET:H	2.24	0.45
1:A:160:ARG:HD3	1:A:202:ILE:CG2	2.46	0.45
1:A:346:VAL:HG22	1:A:407:TRP:HH2	1.81	0.45
1:A:463:LYS:CB	2:A:729:HOH:O	2.63	0.45
1:A:579:ARG:HB2	1:A:579:ARG:CZ	2.46	0.45
1:B:164:ILE:O	1:B:179:THR:HA	2.16	0.45
1:B:233:LEU:HD22	1:B:235:LEU:HG	1.99	0.45
1:B:444:TYR:HA	1:B:468:GLY:O	2.17	0.45
1:A:34:ASP:O	1:A:291:TRP:NE1	2.50	0.45
1:A:251:LEU:HA	1:A:260:ALA:O	2.17	0.45
1:A:440:TYR:HE2	1:A:578:GLN:HB3	1.82	0.45
1:B:219:ARG:HD2	1:B:232:ASP:OD1	2.16	0.45
1:B:424:SER:CB	2:B:778:HOH:O	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LEU:HD12	1:A:78:ILE:CG2	2.35	0.45
1:A:239:ASP:O	1:A:243:TYR:N	2.48	0.45
1:A:370:PRO:HG3	1:A:411:ILE:HD13	1.99	0.45
1:A:421:GLU:OE2	1:A:458:LYS:CE	2.65	0.45
1:A:475:GLU:HA	1:A:500:MET:CE	2.47	0.45
1:A:547:GLU:HB2	1:B:550:ILE:O	2.17	0.45
1:B:29:GLY:HA3	1:B:289:VAL:HG21	1.99	0.45
1:B:398:ARG:NH2	1:B:407:TRP:HZ3	2.13	0.45
1:B:411:ILE:CG1	1:B:492:LEU:HD11	2.46	0.45
1:B:479:GLU:HG2	2:B:617:HOH:O	2.16	0.45
1:B:520:HIS:HD2	1:B:521:PRO:CD	2.21	0.45
1:B:520:HIS:HB2	2:B:744:HOH:O	2.17	0.45
1:A:125:VAL:O	1:A:126:PHE:HB3	2.16	0.45
1:A:262:VAL:O	1:A:262:VAL:HG12	2.17	0.45
1:A:263:ALA:O	1:A:269:SER:CB	2.65	0.45
1:A:335:LEU:HD13	1:A:349:TYR:CE1	2.51	0.45
1:B:226:ARG:NE	2:B:769:HOH:O	2.49	0.45
1:B:476:GLU:HA	1:B:479:GLU:CG	2.47	0.45
1:B:476:GLU:HA	1:B:479:GLU:HG3	1.99	0.45
1:B:565:VAL:O	1:B:567:ILE:N	2.50	0.45
1:B:569:LEU:CB	1:B:570:PRO:HD3	2.42	0.45
1:A:179:THR:H	1:A:187:LEU:CD1	2.30	0.45
1:A:353:SER:C	1:A:355:ARG:N	2.74	0.45
1:B:415:PRO:O	1:B:503:ARG:HG3	2.17	0.45
1:B:448:GLY:HA3	1:B:470:SER:HA	1.99	0.45
1:B:508:HIS:C	1:B:510:ASP:H	2.25	0.45
1:A:163:LEU:HB3	1:A:202:ILE:HD13	1.98	0.44
1:B:38:VAL:HG11	1:B:308:ILE:HD13	1.99	0.44
1:B:156:VAL:HG23	2:B:596:HOH:O	2.16	0.44
1:B:497:ARG:O	1:B:498:GLU:C	2.60	0.44
1:A:25:TYR:HB3	1:A:38:VAL:CG1	2.46	0.44
1:A:284:ASN:ND2	1:A:376:ASP:C	2.75	0.44
1:A:499:ILE:C	1:A:501:ARG:N	2.76	0.44
1:B:330:ILE:HG23	1:B:351:LEU:HD21	1.99	0.44
1:B:364:VAL:HA	1:B:393:VAL:O	2.17	0.44
1:A:224:ASP:HA	1:A:225:PRO:HD3	1.83	0.44
1:A:520:HIS:N	1:A:549:HIS:O	2.35	0.44
1:B:255:PRO:C	1:B:257:GLY:N	2.76	0.44
1:B:340:SER:CA	2:B:722:HOH:O	2.65	0.44
1:B:551:ILE:HG23	1:B:566:LYS:HD3	1.98	0.44
1:A:109:VAL:HA	2:A:728:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:GLU:HG2	1:A:218:ALA:H	1.82	0.44
1:A:393:VAL:HG22	2:A:652:HOH:O	2.16	0.44
1:A:424:SER:HB3	1:A:461:LEU:HD21	1.99	0.44
1:B:40:GLY:N	1:B:47:ASN:O	2.32	0.44
1:B:221:VAL:HG12	1:B:232:ASP:HA	2.00	0.44
1:B:401:THR:HG22	1:B:408:ARG:HD3	1.97	0.44
1:B:571:ALA:HA	2:B:723:HOH:O	2.16	0.44
1:A:304:THR:HA	1:A:305:PRO:HD3	1.82	0.44
1:A:488:PHE:HZ	2:A:672:HOH:O	2.00	0.44
1:A:509:VAL:O	1:A:509:VAL:HG12	2.17	0.44
1:B:226:ARG:HG3	1:B:226:ARG:HH11	1.82	0.44
1:B:240:PHE:CE1	1:B:263:ALA:HB2	2.52	0.44
1:B:340:SER:N	2:B:722:HOH:O	2.43	0.44
1:B:538:GLU:O	1:B:539:LEU:C	2.60	0.44
1:A:31:VAL:HB	1:A:74:VAL:O	2.16	0.44
1:A:219:ARG:NH1	1:A:221:VAL:HG12	2.33	0.44
1:A:367:HIS:HD2	1:A:372:ALA:HB3	1.81	0.44
1:A:499:ILE:O	1:A:503:ARG:HB2	2.17	0.44
1:A:576:ALA:O	1:A:579:ARG:HB3	2.18	0.44
1:B:135:ALA:HB2	2:B:608:HOH:O	2.17	0.44
1:B:239:ASP:HA	1:B:242:SER:HG	1.82	0.44
1:B:456:THR:HG22	1:B:512:ILE:CD1	2.47	0.44
1:A:428:ARG:O	1:A:429:TRP:C	2.61	0.44
1:A:451:THR:O	1:A:455:LEU:HG	2.18	0.44
1:B:59:LEU:HB3	2:B:727:HOH:O	2.17	0.44
1:B:100:PRO:C	1:B:102:GLU:N	2.75	0.44
1:B:301:SER:HA	1:B:376:ASP:O	2.18	0.44
1:B:371:PHE:HD2	1:B:408:ARG:HH11	1.61	0.44
1:A:51:TYR:CE2	1:A:53:GLY:HA2	2.53	0.44
1:A:499:ILE:C	1:A:501:ARG:H	2.25	0.44
1:B:465:GLY:O	1:B:516:LEU:HD12	2.18	0.44
1:B:549:HIS:CE1	2:B:686:HOH:O	2.70	0.44
1:A:72:TYR:OH	1:A:289:VAL:HG12	2.18	0.44
1:A:117:GLY:HA2	1:A:126:PHE:HA	2.00	0.44
1:A:430:ALA:HB3	1:A:439:LEU:HD11	2.00	0.44
1:A:440:TYR:HD2	1:A:464:ALA:HB3	1.82	0.44
1:B:523:ASN:ND2	1:B:553:ASP:CA	2.81	0.44
1:A:61:ARG:NH1	1:A:101:GLY:CA	2.74	0.43
1:A:174:ARG:NH2	1:A:405:GLU:HG2	2.33	0.43
1:A:195:GLY:HA3	1:A:213:GLU:O	2.18	0.43
1:A:309:VAL:HB	1:A:315:GLU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ILE:CD1	2:A:732:HOH:O	2.63	0.43
1:A:503:ARG:HA	2:A:601:HOH:O	2.17	0.43
1:B:48:ALA:N	2:B:679:HOH:O	2.50	0.43
1:B:118:VAL:HG21	1:B:159:ILE:HG12	1.99	0.43
1:B:264:ARG:HA	1:B:269:SER:HA	2.00	0.43
1:A:22:VAL:HG12	1:A:23:GLU:N	2.32	0.43
1:A:62:GLU:CB	1:A:81:ARG:HH21	2.31	0.43
1:B:86:GLY:CA	1:B:555:GLY:HA3	2.48	0.43
1:B:169:PHE:CZ	1:B:175:VAL:CG2	2.99	0.43
1:B:170:PHE:HD1	1:B:189:VAL:HG11	1.83	0.43
1:B:251:LEU:CD2	2:B:652:HOH:O	2.66	0.43
1:B:405:GLU:O	1:B:406:GLU:C	2.59	0.43
1:A:79:LEU:HD11	1:A:95:VAL:HG21	1.99	0.43
1:A:165:ALA:HB2	2:A:653:HOH:O	2.16	0.43
1:A:338:VAL:HG11	1:A:425:ALA:C	2.44	0.43
1:A:438:GLU:HG3	1:A:440:TYR:HE1	1.83	0.43
1:A:532:LEU:CD1	1:A:532:LEU:C	2.91	0.43
1:A:565:VAL:O	1:A:569:LEU:HB2	2.18	0.43
1:B:198:SER:HB2	1:B:248:ILE:O	2.18	0.43
1:B:209:THR:CA	1:B:222:THR:HG22	2.48	0.43
1:B:270:ALA:HB1	1:B:277:ARG:CZ	2.48	0.43
1:B:431:ARG:NH2	2:B:714:HOH:O	2.47	0.43
1:B:457:MET:C	1:B:459:PRO:CD	2.91	0.43
1:B:472:VAL:CG2	1:B:532:LEU:HD22	2.48	0.43
1:B:487:ASN:HA	1:B:490:GLU:OE1	2.17	0.43
1:B:580:GLU:O	1:B:581:ARG:HB2	2.18	0.43
1:A:164:ILE:HD13	1:A:181:ASN:CA	2.47	0.43
1:A:248:ILE:N	1:A:248:ILE:HD12	2.33	0.43
1:A:469:ALA:HB1	1:A:556:HIS:CE1	2.54	0.43
1:A:469:ALA:HB1	1:A:556:HIS:ND1	2.32	0.43
1:A:546:PHE:C	1:B:552:PRO:HB3	2.43	0.43
1:B:224:ASP:HB3	1:B:227:ASP:OD1	2.18	0.43
1:B:487:ASN:O	1:B:487:ASN:OD1	2.37	0.43
1:A:277:ARG:NH1	1:A:277:ARG:HG2	2.33	0.43
1:A:366:VAL:HG11	1:A:450:MET:HG3	2.00	0.43
1:A:578:GLN:O	1:A:581:ARG:N	2.52	0.43
1:B:42:SER:HA	1:B:561:MET:CE	2.48	0.43
1:B:79:LEU:HD11	1:B:95:VAL:CG2	2.45	0.43
1:B:207:LYS:HG2	1:B:222:THR:HB	1.99	0.43
1:B:371:PHE:HA	1:B:399:GLY:O	2.19	0.43
1:B:414:ASP:OD2	1:B:418:GLY:N	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:THR:HA	2:B:629:HOH:O	2.18	0.43
1:A:33:GLY:H	1:A:73:GLY:HA2	1.83	0.43
1:A:74:VAL:HG11	1:A:121:GLY:HA3	2.00	0.43
1:A:146:GLU:CD	2:A:609:HOH:O	2.61	0.43
1:A:421:GLU:O	1:A:424:SER:HB2	2.19	0.43
1:A:509:VAL:O	1:A:509:VAL:CG1	2.66	0.43
1:B:472:VAL:HG21	1:B:532:LEU:HA	2.01	0.43
1:B:472:VAL:O	1:B:505:PRO:HD2	2.18	0.43
1:B:473:ASP:OD1	1:B:475:GLU:N	2.49	0.43
1:B:494:GLY:O	1:B:496:SER:N	2.51	0.43
1:B:522:GLN:HB3	1:B:550:ILE:HG22	1.99	0.43
1:B:523:ASN:HD21	1:B:553:ASP:HA	1.82	0.43
1:A:106:LEU:CD2	2:A:698:HOH:O	2.66	0.43
1:A:178:PHE:HB2	1:A:187:LEU:HD11	2.01	0.43
1:B:240:PHE:O	1:B:245:PRO:CD	2.67	0.43
1:B:419:GLU:O	1:B:423:VAL:HG23	2.19	0.43
1:B:427:ALA:O	1:B:428:ARG:C	2.60	0.43
1:B:508:HIS:O	1:B:509:VAL:C	2.62	0.43
1:A:77:VAL:HG23	1:A:97:THR:CG2	2.49	0.43
1:A:197:PHE:HD2	1:A:210:ALA:HB1	1.84	0.43
1:A:381:PHE:O	1:A:385:LEU:HB2	2.18	0.43
1:A:475:GLU:CA	1:A:500:MET:HE2	2.49	0.43
1:B:137:TYR:CD1	1:B:137:TYR:N	2.86	0.43
1:B:209:THR:OG1	1:B:253:TYR:OH	2.32	0.43
1:B:246:THR:CG2	1:B:265:ARG:HA	2.49	0.43
1:B:299:HIS:CG	1:B:300:THR:N	2.86	0.43
1:B:300:THR:O	1:B:301:SER:CB	2.67	0.43
1:B:377:SER:N	2:B:600:HOH:O	2.51	0.43
1:B:520:HIS:CE1	1:B:529:LEU:HA	2.54	0.43
1:B:30:VAL:HG23	1:B:289:VAL:HG12	1.99	0.43
1:A:71:HIS:HB2	1:A:120:THR:HA	2.01	0.43
1:A:78:ILE:HG23	2:A:589:HOH:O	2.19	0.43
1:A:167:LEU:CD2	1:A:197:PHE:HB2	2.49	0.43
1:B:59:LEU:CD1	1:B:77:VAL:HG21	2.46	0.43
1:B:205:GLY:O	1:B:206:MET:CB	2.67	0.43
1:B:334:ARG:NH2	1:B:429:TRP:CH2	2.87	0.43
1:B:489:ILE:HG13	2:B:642:HOH:O	2.18	0.43
1:A:138:ALA:HB3	1:A:147:LEU:HD21	1.98	0.42
1:A:167:LEU:HD11	1:A:199:SER:HA	2.01	0.42
1:A:188:ARG:HG3	1:A:188:ARG:HH11	1.84	0.42
1:A:350:VAL:HG22	2:A:652:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:VAL:HG21	1:B:37:LEU:HD22	2.00	0.42
1:B:203:SER:O	1:B:206:MET:N	2.46	0.42
1:B:324:GLU:OE1	1:B:324:GLU:HA	2.19	0.42
1:A:32:ASP:CB	1:A:35:LYS:HD2	2.49	0.42
1:A:120:THR:HG22	1:A:120:THR:O	2.19	0.42
1:B:26:SER:OG	1:B:28:GLN:NE2	2.51	0.42
1:B:50:LEU:CD1	1:B:59:LEU:HD21	2.48	0.42
1:B:218:ALA:HB1	1:B:248:ILE:HD12	1.97	0.42
1:B:401:THR:HG22	1:B:408:ARG:HD2	2.01	0.42
1:B:526:ARG:HH21	1:B:557:ALA:HB2	1.81	0.42
1:A:203:SER:CB	1:A:204:PRO:CD	2.97	0.42
1:A:288:VAL:CG1	1:A:295:LEU:HD22	2.49	0.42
1:A:351:LEU:HD12	1:A:382:ALA:HB1	2.00	0.42
1:B:84:SER:HB3	1:B:89:GLN:HB2	2.01	0.42
1:B:100:PRO:C	1:B:102:GLU:H	2.27	0.42
1:B:428:ARG:O	1:B:431:ARG:N	2.49	0.42
1:B:450:MET:HA	1:B:453:CYS:HB3	2.01	0.42
1:A:203:SER:HB2	1:A:204:PRO:CD	2.49	0.42
1:A:342:ASP:N	1:A:342:ASP:OD1	2.50	0.42
1:A:440:TYR:HE2	1:A:578:GLN:CB	2.32	0.42
1:B:330:ILE:HB	2:B:720:HOH:O	2.19	0.42
1:B:536:MET:HA	2:B:678:HOH:O	2.19	0.42
1:A:35:LYS:HG2	1:A:52:ASP:OD2	2.20	0.42
1:A:96:ASN:HD22	1:A:99:ARG:HG3	1.84	0.42
1:B:123:ALA:CB	1:B:182:LEU:HD11	2.50	0.42
1:B:359:PRO:O	1:B:437:SER:HB3	2.19	0.42
1:B:574:PHE:CB	2:B:723:HOH:O	2.67	0.42
1:A:158:ASP:HB2	1:A:201:SER:HA	2.02	0.42
1:A:170:PHE:HB2	2:A:662:HOH:O	2.20	0.42
1:B:70:PRO:HB2	1:B:74:VAL:CG2	2.41	0.42
1:B:501:ARG:NH1	2:B:749:HOH:O	2.52	0.42
1:A:29:GLY:HA2	1:A:289:VAL:HG11	2.02	0.42
1:A:48:ALA:HB2	1:A:67:VAL:HG21	2.01	0.42
1:A:359:PRO:HA	1:A:435:LEU:HA	2.02	0.42
1:A:393:VAL:CG1	1:A:426:ALA:HB1	2.49	0.42
1:A:476:GLU:CD	1:A:531:PRO:HG3	2.45	0.42
1:A:542:ARG:O	1:A:543:GLY:C	2.62	0.42
1:A:579:ARG:CG	1:A:580:GLU:N	2.82	0.42
1:B:476:GLU:OE1	1:B:531:PRO:HA	2.20	0.42
1:A:371:PHE:CE1	1:A:408:ARG:NH1	2.88	0.42
1:B:392:VAL:HG12	1:B:394:MET:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:GLY:O	1:B:421:GLU:HB2	2.19	0.42
1:B:429:TRP:C	1:B:431:ARG:N	2.75	0.42
1:B:530:LYS:O	1:B:531:PRO:C	2.61	0.42
1:A:44:GLY:HA2	1:A:561:MET:HB3	2.01	0.42
1:A:84:SER:CB	1:A:87:ALA:HB3	2.50	0.42
1:A:315:GLU:OE1	1:A:315:GLU:HA	2.18	0.42
1:A:370:PRO:C	1:A:372:ALA:N	2.78	0.42
1:A:443:GLY:C	1:A:444:TYR:CD1	2.98	0.42
1:A:469:ALA:HB1	1:A:556:HIS:HD1	1.85	0.42
1:B:79:LEU:N	1:B:93:PHE:O	2.43	0.42
1:B:209:THR:HA	1:B:222:THR:HG22	2.02	0.42
1:B:305:PRO:HA	1:B:306:PRO:HD3	1.92	0.42
1:B:443:GLY:HA2	2:B:601:HOH:O	2.19	0.42
1:A:212:LEU:HG	1:A:214:THR:HG23	2.01	0.42
1:A:367:HIS:N	2:A:584:HOH:O	2.53	0.42
1:B:76:ARG:HA	1:B:96:ASN:HA	2.01	0.42
1:B:133:ARG:NE	1:B:149:ARG:HH21	2.18	0.42
1:A:46:VAL:C	2:A:595:HOH:O	2.63	0.41
1:A:92:LEU:HB3	1:A:106:LEU:HD12	2.02	0.41
1:B:59:LEU:C	1:B:95:VAL:HG11	2.45	0.41
1:B:168:GLY:HA3	2:B:706:HOH:O	2.20	0.41
1:B:240:PHE:HD1	1:B:272:PHE:CD1	2.37	0.41
1:B:569:LEU:HD12	1:B:569:LEU:HA	1.83	0.41
1:A:264:ARG:HA	1:A:269:SER:HA	2.02	0.41
1:B:176:SER:HA	2:B:746:HOH:O	2.19	0.41
1:B:302:LEU:HD13	1:B:351:LEU:HD13	2.02	0.41
1:B:315:GLU:HA	1:B:316:PRO:HD2	1.75	0.41
1:B:520:HIS:HA	1:B:521:PRO:HD3	1.81	0.41
1:A:296:VAL:HA	2:A:670:HOH:O	2.20	0.41
1:B:201:SER:HB3	2:B:652:HOH:O	2.20	0.41
1:B:227:ASP:OD1	1:B:227:ASP:N	2.42	0.41
1:B:264:ARG:HH11	1:B:264:ARG:HG2	1.85	0.41
1:B:300:THR:OG1	1:B:301:SER:N	2.53	0.41
1:B:419:GLU:OE2	1:B:420:LEU:N	2.45	0.41
1:A:250:TRP:CE3	1:A:250:TRP:C	2.98	0.41
1:A:373:GLU:HB2	1:A:396:ASN:OD1	2.20	0.41
1:B:457:MET:O	1:B:459:PRO:HD2	2.20	0.41
1:A:169:PHE:CE2	1:A:371:PHE:CD1	3.04	0.41
1:A:219:ARG:NH1	1:A:221:VAL:CG1	2.84	0.41
1:B:86:GLY:O	1:B:555:GLY:HA3	2.21	0.41
1:B:133:ARG:HE	1:B:133:ARG:HB3	1.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:TRP:O	1:B:292:ARG:HB2	2.19	0.41
1:B:309:VAL:HA	1:B:316:PRO:HA	2.02	0.41
1:B:397:TYR:CB	1:B:422:ASP:HB2	2.49	0.41
1:B:567:ILE:HD12	1:B:568:LEU:CA	2.47	0.41
1:B:569:LEU:HB3	1:B:570:PRO:CD	2.43	0.41
1:A:108:ALA:O	1:A:144:LEU:HB2	2.21	0.41
1:A:198:SER:CB	1:A:213:GLU:OE2	2.68	0.41
1:A:421:GLU:O	1:A:425:ALA:N	2.53	0.41
1:A:476:GLU:C	1:A:478:TYR:N	2.74	0.41
1:B:30:VAL:H	1:B:289:VAL:CG1	2.33	0.41
1:B:31:VAL:HG22	1:B:74:VAL:CG2	2.51	0.41
1:B:325:ASP:O	1:B:328:ARG:HB2	2.21	0.41
1:B:456:THR:HG22	1:B:512:ILE:HD11	2.00	0.41
1:B:504:SER:C	1:B:506:ILE:N	2.79	0.41
1:A:25:TYR:HA	1:A:39:VAL:O	2.20	0.41
1:A:71:HIS:O	1:A:72:TYR:C	2.64	0.41
1:A:226:ARG:HA	1:A:226:ARG:HD3	1.93	0.41
1:A:569:LEU:H	1:A:570:PRO:CD	2.33	0.41
1:B:78:ILE:CD1	1:B:124:VAL:HG22	2.50	0.41
1:B:328:ARG:NH1	2:B:682:HOH:O	2.54	0.41
1:B:444:TYR:OH	1:B:521:PRO:HG2	2.21	0.41
1:A:26:SER:HA	2:A:725:HOH:O	2.21	0.41
1:A:349:TYR:HB3	1:A:394:MET:HE3	2.03	0.41
1:A:367:HIS:CE1	1:A:396:ASN:HA	2.56	0.41
1:A:393:VAL:HA	2:A:652:HOH:O	2.21	0.41
1:A:551:ILE:HD13	1:A:567:ILE:HG22	2.03	0.41
1:A:562:GLU:C	1:A:564:ALA:N	2.68	0.41
1:B:125:VAL:HG13	1:B:137:TYR:O	2.20	0.41
1:B:263:ALA:O	1:B:269:SER:HA	2.21	0.41
1:B:514:GLU:HA	1:B:515:PRO:HD3	1.90	0.41
1:A:158:ASP:CB	1:A:201:SER:HA	2.50	0.41
1:A:190:PHE:CD1	1:A:190:PHE:N	2.88	0.41
1:A:194:GLU:CB	1:A:214:THR:HG22	2.51	0.41
1:A:224:ASP:O	1:A:228:GLY:N	2.53	0.41
1:A:322:LEU:HB2	2:A:697:HOH:O	2.21	0.41
1:A:329:SER:HB2	1:A:387:ALA:HA	2.02	0.41
1:A:398:ARG:HB2	1:A:410:LYS:HB2	2.03	0.41
1:A:562:GLU:O	1:A:565:VAL:N	2.52	0.41
1:B:29:GLY:HA2	1:B:289:VAL:HG11	2.03	0.41
1:B:31:VAL:CG1	1:B:32:ASP:H	2.34	0.41
1:B:145:ARG:NH1	2:B:624:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:PHE:HA	1:B:276:GLU:O	2.21	0.41
1:B:491:GLN:NE2	2:B:747:HOH:O	2.53	0.41
1:B:522:GLN:NE2	2:B:663:HOH:O	2.53	0.41
1:B:522:GLN:OE1	1:B:552:PRO:HA	2.21	0.41
1:A:59:LEU:O	1:A:101:GLY:HA2	2.20	0.41
1:A:119:ASP:OD1	1:A:120:THR:N	2.55	0.41
1:A:270:ALA:HB1	1:A:277:ARG:NE	2.36	0.41
1:A:309:VAL:CG1	1:A:316:PRO:HA	2.46	0.41
1:B:77:VAL:O	1:B:94:LYS:HA	2.20	0.41
1:B:156:VAL:CG1	1:B:159:ILE:HD11	2.51	0.41
1:B:280:ALA:HB1	1:B:285:HIS:CE1	2.56	0.41
1:B:357:PRO:O	1:B:360:GLY:CA	2.69	0.41
1:B:511:ARG:NH1	2:B:605:HOH:O	2.37	0.41
1:B:520:HIS:O	1:B:550:ILE:HA	2.21	0.41
1:B:534:ARG:HD3	1:B:534:ARG:HA	1.80	0.41
1:B:538:GLU:O	1:B:541:ALA:N	2.54	0.41
1:A:136:LEU:CD1	1:A:156:VAL:HG22	2.51	0.40
1:A:520:HIS:HA	1:A:521:PRO:HD3	1.80	0.40
1:A:521:PRO:HG2	1:A:555:GLY:O	2.21	0.40
1:B:93:PHE:CD1	1:B:93:PHE:N	2.89	0.40
1:B:364:VAL:CG1	1:B:395:PRO:HD3	2.51	0.40
1:B:453:CYS:CB	2:B:731:HOH:O	2.66	0.40
1:A:95:VAL:O	1:A:95:VAL:HG12	2.22	0.40
1:A:163:LEU:HD23	1:A:202:ILE:HD13	2.03	0.40
1:A:249:THR:HB	1:A:262:VAL:O	2.21	0.40
1:A:383:ALA:O	1:A:384:SER:C	2.65	0.40
1:B:95:VAL:HB	2:B:727:HOH:O	2.20	0.40
1:B:199:SER:OG	1:B:251:LEU:HB3	2.22	0.40
1:B:210:ALA:HA	1:B:251:LEU:CD2	2.51	0.40
1:B:278:VAL:CG1	1:B:312:PRO:HB3	2.49	0.40
1:B:397:TYR:HB2	1:B:422:ASP:HB2	2.03	0.40
1:B:440:TYR:CZ	1:B:463:LYS:HD3	2.56	0.40
1:B:567:ILE:HA	2:B:594:HOH:O	2.21	0.40
1:A:117:GLY:HA3	1:A:126:PHE:CB	2.51	0.40
1:A:147:LEU:HD22	2:A:695:HOH:O	2.21	0.40
1:A:219:ARG:HG3	1:A:219:ARG:NH1	2.36	0.40
1:A:428:ARG:CG	2:A:622:HOH:O	2.58	0.40
1:A:497:ARG:HD3	1:A:501:ARG:HE	1.85	0.40
1:B:371:PHE:CD2	1:B:408:ARG:NH1	2.79	0.40
1:B:379:ASP:HB3	1:B:382:ALA:HB3	2.03	0.40
1:B:398:ARG:HG2	1:B:419:GLU:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:TRP:O	1:B:431:ARG:N	2.54	0.40
1:A:23:GLU:H	1:A:23:GLU:HG3	1.69	0.40
1:A:107:GLU:C	1:A:109:VAL:H	2.29	0.40
1:A:188:ARG:HH11	1:A:188:ARG:CG	2.35	0.40
1:A:420:LEU:O	1:A:424:SER:N	2.54	0.40
1:A:477:MET:HE3	1:A:489:ILE:HD11	2.04	0.40
1:B:60:ASN:O	1:B:61:ARG:HG2	2.21	0.40
1:B:432:GLU:HG3	2:B:759:HOH:O	2.21	0.40
1:B:444:TYR:O	1:B:447:GLY:N	2.50	0.40
1:A:98:SER:O	1:A:100:PRO:HD3	2.21	0.40
1:A:305:PRO:CD	1:A:322:LEU:HD12	2.50	0.40
1:A:444:TYR:CD1	1:A:444:TYR:N	2.90	0.40
1:A:575:LEU:HD23	1:A:575:LEU:HA	1.93	0.40
1:B:131:GLU:OE2	1:B:131:GLU:O	2.40	0.40
1:B:133:ARG:CD	2:B:608:HOH:O	2.70	0.40
1:B:266:GLU:HA	1:B:403:TYR:CE2	2.57	0.40
1:B:281:PRO:HB2	1:B:299:HIS:CE1	2.57	0.40
1:B:334:ARG:HD2	2:B:661:HOH:O	2.22	0.40
1:B:340:SER:C	2:B:722:HOH:O	2.64	0.40
1:B:385:LEU:HD11	1:B:442:MET:CE	2.51	0.40
1:B:520:HIS:O	1:B:550:ILE:HG23	2.21	0.40
1:B:521:PRO:HA	1:B:554:ALA:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	558/562 (99%)	445 (80%)	90 (16%)	23 (4%)	2 5
1	B	559/562 (100%)	432 (77%)	96 (17%)	31 (6%)	1 2
All	All	1117/1124 (99%)	877 (78%)	186 (17%)	54 (5%)	2 3

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	72	TYR
1	A	563	ASP
1	B	206	MET
1	B	232	ASP
1	B	371	PHE
1	B	496	SER
1	A	106	LEU
1	A	321	GLY
1	A	354	GLY
1	A	371	PHE
1	A	498	GLU
1	A	543	GLY
1	A	568	LEU
1	B	45	SER
1	B	60	ASN
1	B	107	GLU
1	B	172	GLY
1	B	187	LEU
1	B	210	ALA
1	B	211	GLY
1	B	256	ASP
1	B	580	GLU
1	A	42	SER
1	A	216	ARG
1	B	323	PRO
1	B	498	GLU
1	B	505	PRO
1	B	522	GLN
1	B	544	LYS
1	A	116	SER
1	B	61	ARG
1	B	74	VAL
1	B	121	GLY
1	B	122	GLU
1	B	380	THR
1	B	430	ALA
1	B	560	THR
1	B	562	GLU
1	A	31	VAL
1	A	32	ASP
1	A	276	GLU

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Mol	Chain	Res	Type
1	A	579	ARG
1	B	292	ARG
1	A	430	ALA
1	B	301	SER
1	B	417	GLY
1	A	54	GLY
1	A	64	ILE
1	A	142	GLY
1	A	460	GLY
1	A	515	PRO
1	B	306	PRO
1	B	472	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	448/449 (100%)	412 (92%)	36 (8%)	11	28
1	B	448/449 (100%)	417 (93%)	31 (7%)	14	34
All	All	896/898 (100%)	829 (92%)	67 (8%)	12	31

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	56	THR
1	A	71	HIS
1	A	81	ARG
1	A	109	VAL
1	A	139	LEU
1	A	145	ARG
1	A	177	LEU
1	A	178	PHE
1	A	181	ASN
1	A	183	SER

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Mol	Chain	Res	Type
1	A	191	ASP
1	A	201	SER
1	A	216	ARG
1	A	233	LEU
1	A	249	THR
1	A	250	TRP
1	A	285	HIS
1	A	290	LEU
1	A	301	SER
1	A	318	LEU
1	A	322	LEU
1	A	344	SER
1	A	380	THR
1	A	419	GLU
1	A	435	LEU
1	A	441	ILE
1	A	444	TYR
1	A	453	CYS
1	A	461	LEU
1	A	480	LEU
1	A	522	GLN
1	A	552	PRO
1	A	559	ASN
1	A	563	ASP
1	A	579	ARG
1	B	56	THR
1	B	83	VAL
1	B	99	ARG
1	B	114	ILE
1	B	133	ARG
1	B	134	VAL
1	B	137	TYR
1	B	162	ASP
1	B	198	SER
1	B	204	PRO
1	B	219	ARG
1	B	222	THR
1	B	236	PRO
1	B	271	VAL
1	B	304	THR
1	B	315	GLU
1	B	322	LEU

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Mol	Chain	Res	Type
1	B	327	ARG
1	B	336	VAL
1	B	341	PHE
1	B	358	THR
1	B	384	SER
1	B	411	ILE
1	B	419	GLU
1	B	445	SER
1	B	456	THR
1	B	482	ASP
1	B	497	ARG
1	B	522	GLN
1	B	560	THR
1	B	568	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	90	HIS
1	A	96	ASN
1	A	104	GLN
1	A	284	ASN
1	A	285	HIS
1	A	578	GLN
1	B	28	GLN
1	B	65	ASN
1	B	90	HIS
1	B	96	ASN
1	B	104	GLN
1	B	282	GLN
1	B	284	ASN
1	B	367	HIS
1	B	396	ASN
1	B	491	GLN
1	B	507	ASN
1	B	520	HIS
1	B	522	GLN
1	B	523	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	560/562 (99%)	0.20	7 (1%) 75 73	7, 26, 44, 73	0
1	B	561/562 (99%)	0.45	13 (2%) 61 58	9, 32, 51, 71	0
All	All	1121/1124 (99%)	0.33	20 (1%) 67 65	7, 28, 49, 73	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	558	ILE	4.4
1	B	262	VAL	4.3
1	B	467	ALA	3.2
1	A	44	GLY	3.1
1	B	295	LEU	2.9
1	B	560	THR	2.5
1	B	558	ILE	2.5
1	B	67	VAL	2.4
1	A	322	LEU	2.3
1	B	218	ALA	2.3
1	A	444	TYR	2.2
1	B	235	LEU	2.2
1	B	285	HIS	2.2
1	B	41	PHE	2.2
1	B	225	PRO	2.1
1	B	40	GLY	2.1
1	A	559	ASN	2.1
1	B	360	GLY	2.1
1	A	74	VAL	2.1
1	A	196	SER	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.