



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:24 PM UTC

PDB ID : 1EK1 / pdb_00001ek1
Title : CRYSTAL STRUCTURE OF MURINE SOLUBLE EPOXIDE HYDROLASE
COMPLEXED WITH CIU INHIBITOR
Authors : Argiriadi, M.A.; Morisseau, C.; Goodrow, M.H.; Dowdy, D.L.; Hammock,
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Deposited on : 2000-03-06
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

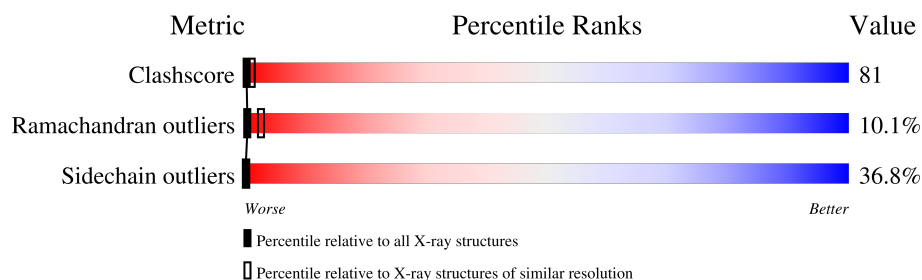
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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	A	554	
1	B	554	

2 Entry composition [i](#)

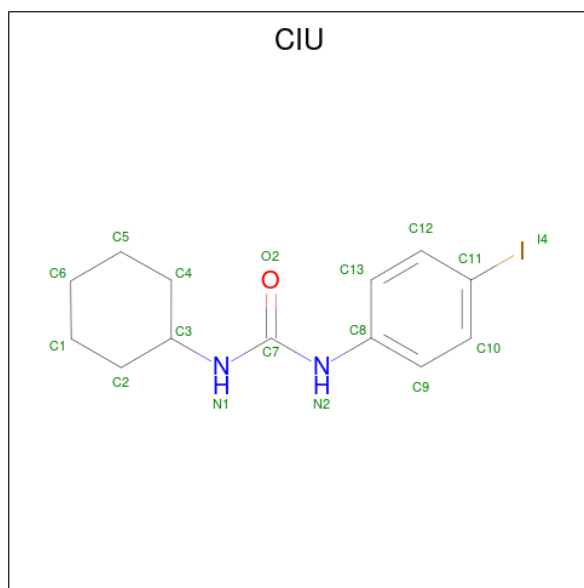
There are 3 unique types of molecules in this entry. The entry contains 8255 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 EPOXIDE HYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	61	0	0
			3901	2517	651	704	29			
1	B	541	Total	C	N	O	S	71	0	0
			4299	2766	719	783	31			

- Molecule 2 is N-CYCLOHEXYL-N'-(4-IODOPHENYL)UREA (CCD ID: CIU) (formula: C₁₃H₁₇IN₂O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	I	N	O	0	0
			17	13	1	2	1		
2	B	1	Total	C	I	N	O	0	0
			17	13	1	2	1		

- Molecule 3 is water.

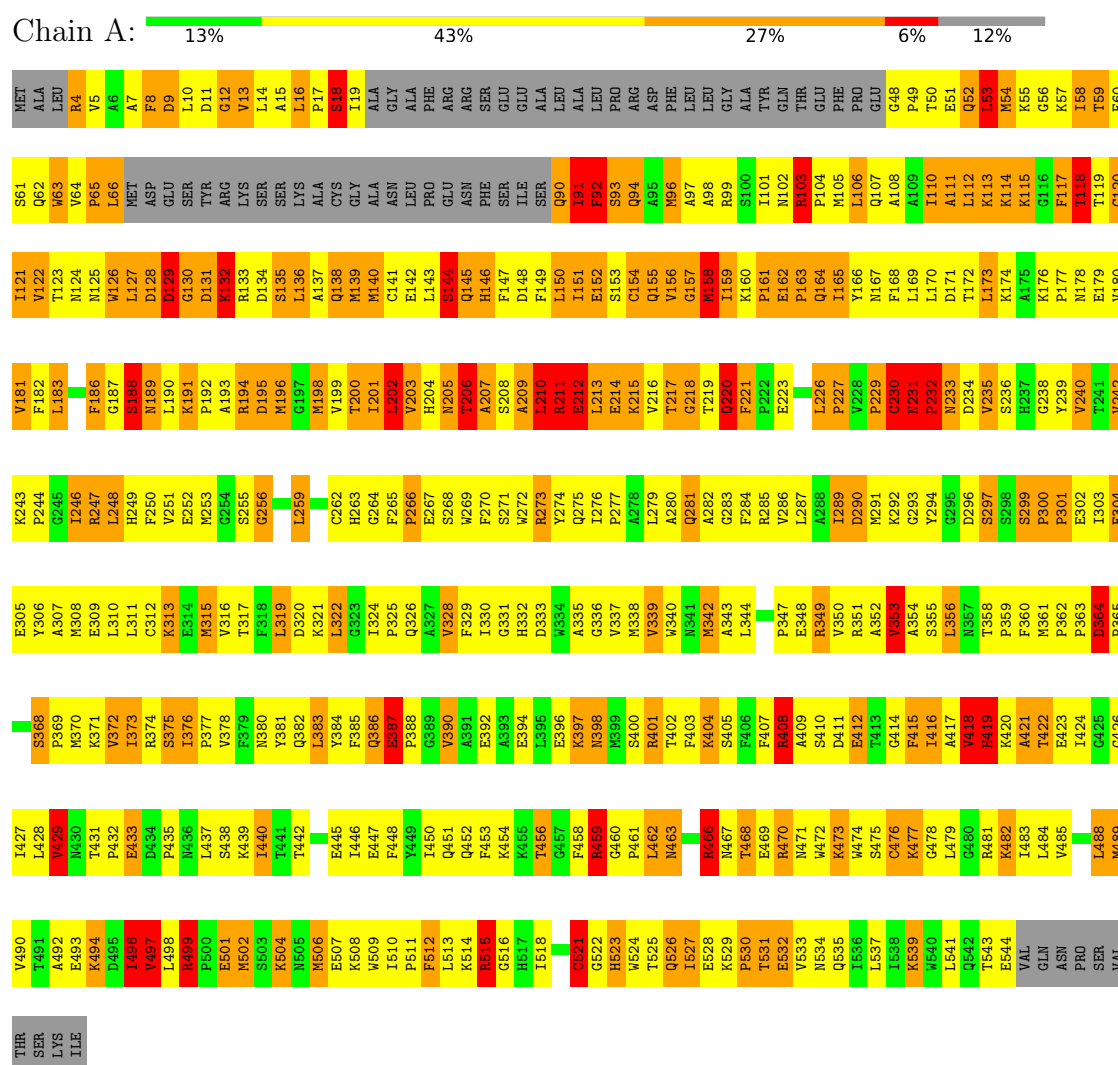
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total 4	O 4	0	0
3	B	17	Total 17	O 17	0	0

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. 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. 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.

Note EDS was not executed.

• Molecule 1: EPOXIDE HYDROLASE



• Molecule 1: EPOXIDE HYDROLASE





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	151.90Å 143.00Å 60.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.10)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.194 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8255	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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: CIU

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	0.92	2/4004 (0.0%)	1.45	70/5430 (1.3%)
1	B	0.90	2/4413 (0.0%)	1.47	84/5984 (1.4%)
All	All	0.91	4/8417 (0.0%)	1.46	154/11414 (1.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	MET	SD-CE	8.15	2.00	1.79
1	B	291	MET	SD-CE	5.91	1.94	1.79
1	B	105	MET	SD-CE	5.82	1.94	1.79
1	A	151	ILE	CA-CB	-5.55	1.47	1.54

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	SER	N-CA-C	-14.56	98.02	114.62
1	B	27	GLU	N-CA-C	-13.07	97.60	113.15
1	B	231	ASN	C-N-CD	-12.52	93.07	120.60
1	B	209	ALA	N-CA-C	-11.77	96.99	111.11
1	A	234	ASP	N-CA-C	-11.39	99.74	112.72
1	B	231	ASN	CA-C-N	11.24	153.97	127.00
1	B	231	ASN	C-N-CA	11.24	153.97	127.00
1	A	129	ASP	N-CA-C	-11.03	99.78	113.02
1	A	132	LYS	N-CA-C	-11.01	101.30	112.97
1	B	434	ASP	CA-C-N	10.34	132.76	119.84
1	B	434	ASP	C-N-CA	10.34	132.76	119.84
1	A	227	PRO	N-CA-C	-9.90	97.36	111.22
1	B	368	SER	CA-C-N	9.88	130.02	119.05
1	B	368	SER	C-N-CA	9.88	130.02	119.05
1	B	62	GLN	N-CA-C	-9.66	99.24	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	SER	CA-C-N	9.55	129.65	119.05
1	A	368	SER	C-N-CA	9.55	129.65	119.05
1	B	45	PHE	CA-C-N	9.39	130.75	120.13
1	B	45	PHE	C-N-CA	9.39	130.75	120.13
1	B	206	THR	N-CA-C	-9.30	99.67	113.61
1	A	226	LEU	CA-C-N	-9.13	111.44	120.21
1	A	226	LEU	C-N-CA	-9.13	111.44	120.21
1	B	508	LYS	N-CA-C	-8.54	101.48	112.23
1	B	118	THR	N-CA-C	-8.53	95.34	109.07
1	A	508	LYS	N-CA-C	-8.36	102.12	111.82
1	B	246	ILE	N-CA-C	8.20	119.96	107.99
1	A	392	GLU	N-CA-C	-8.07	102.17	110.97
1	A	53	LEU	N-CA-C	-8.07	103.33	113.01
1	B	145	GLN	N-CA-C	8.07	120.15	111.36
1	B	497	VAL	N-CA-C	-8.02	96.70	108.89
1	A	497	VAL	N-CA-C	-7.89	96.89	108.89
1	A	246	ILE	N-CA-C	7.89	119.50	107.99
1	B	9	ASP	N-CA-C	-7.86	100.16	110.53
1	B	114	LYS	N-CA-C	-7.75	102.77	111.14
1	A	387	GLU	CA-C-N	7.75	129.53	119.84
1	A	387	GLU	C-N-CA	7.75	129.53	119.84
1	A	131	ASP	N-CA-C	-7.74	104.36	113.88
1	B	387	GLU	CA-C-N	7.69	129.45	119.84
1	B	387	GLU	C-N-CA	7.69	129.45	119.84
1	A	433	GLU	N-CA-C	-7.67	104.06	113.50
1	A	49	PRO	N-CA-C	-7.66	103.53	114.18
1	A	231	ASN	N-CA-C	7.65	126.72	109.81
1	B	188	SER	N-CA-C	-7.63	103.85	113.01
1	A	342	MET	N-CA-C	-7.58	101.77	111.02
1	B	16	LEU	N-CA-C	7.58	114.81	108.07
1	B	267	GLU	N-CA-C	7.52	119.89	109.29
1	B	113	LYS	N-CA-C	-7.44	102.11	112.45
1	A	206	THR	N-CA-C	-7.38	102.87	113.21
1	A	114	LYS	N-CA-C	-7.36	103.26	111.28
1	B	342	MET	N-CA-C	-7.26	102.16	111.02
1	A	218	GLY	N-CA-C	-7.26	95.98	113.18
1	A	267	GLU	N-CA-C	7.24	119.49	109.29
1	B	525	THR	N-CA-C	7.11	118.72	110.97
1	B	186	PHE	N-CA-C	7.08	122.23	112.04
1	A	525	THR	N-CA-C	7.07	118.68	110.97
1	B	403	PHE	N-CA-C	6.97	118.96	111.36
1	A	403	PHE	N-CA-C	6.96	118.94	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	ASN	N-CA-C	6.95	125.18	109.81
1	B	392	GLU	N-CA-C	-6.93	103.42	110.97
1	B	196	MET	N-CA-C	-6.91	103.67	111.14
1	B	82	LEU	CA-C-N	6.88	128.43	119.84
1	B	82	LEU	C-N-CA	6.88	128.43	119.84
1	B	194	ARG	N-CA-C	-6.82	105.03	113.15
1	A	477	LYS	N-CA-C	-6.81	106.86	114.62
1	A	289	ILE	N-CA-C	6.78	118.91	109.55
1	A	521	CYS	N-CA-C	6.73	121.02	110.32
1	B	48	GLY	N-CA-C	6.72	126.06	112.34
1	B	87	SER	N-CA-C	6.62	117.31	108.38
1	A	220	GLN	N-CA-C	6.60	124.86	110.80
1	A	118	THR	N-CA-C	-6.59	98.16	108.90
1	B	477	LYS	N-CA-C	-6.53	107.17	114.62
1	B	523	HIS	N-CA-C	-6.50	105.17	113.23
1	A	120	CYS	N-CA-C	6.47	118.60	108.96
1	A	221	PHE	CA-C-N	6.46	127.91	119.84
1	A	221	PHE	C-N-CA	6.46	127.91	119.84
1	B	93	SER	N-CA-C	-6.45	105.52	113.19
1	A	353	VAL	CB-CA-C	-6.44	100.58	110.50
1	B	521	CYS	N-CA-C	6.41	120.49	110.17
1	B	408	ARG	N-CA-C	-6.41	99.56	109.24
1	B	117	PHE	N-CA-C	-6.38	100.11	109.18
1	B	289	ILE	N-CA-C	6.38	118.35	109.55
1	A	194	ARG	N-CA-C	-6.34	104.47	111.82
1	A	91	ILE	N-CA-C	6.33	122.51	109.34
1	A	158	MET	N-CA-C	6.25	118.91	108.73
1	B	133	ARG	N-CA-C	-6.21	104.40	112.23
1	A	103	ARG	N-CA-C	6.21	121.32	113.25
1	A	162	GLU	CA-C-N	6.15	127.53	119.84
1	A	162	GLU	C-N-CA	6.15	127.53	119.84
1	B	515	ARG	N-CA-C	6.11	119.49	109.72
1	B	427	ILE	CB-CA-C	-6.08	105.71	111.06
1	B	410	SER	N-CA-C	-6.07	105.68	114.12
1	B	353	VAL	CB-CA-C	-6.06	101.17	110.50
1	A	410	SER	N-CA-C	-5.99	105.79	114.12
1	A	364	ASP	CA-C-N	5.99	125.67	119.56
1	A	364	ASP	C-N-CA	5.99	125.67	119.56
1	A	515	ARG	N-CA-C	5.99	119.30	109.72
1	B	522	GLY	N-CA-C	-5.96	104.08	112.60
1	A	188	SER	N-CA-C	-5.96	105.86	113.01
1	B	364	ASP	CA-C-N	5.95	125.62	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	364	ASP	C-N-CA	5.95	125.62	119.56
1	A	408	ARG	N-CA-C	-5.93	100.28	109.24
1	A	419	HIS	N-CA-C	5.91	120.51	113.12
1	A	429	VAL	N-CA-C	5.91	121.63	109.34
1	A	54	MET	N-CA-C	-5.83	105.01	111.36
1	B	169	LEU	N-CA-C	-5.78	104.61	111.03
1	A	522	GLY	N-CA-C	-5.78	104.34	112.60
1	A	466	ARG	N-CA-C	5.76	123.07	110.80
1	B	173	LEU	N-CA-C	-5.72	98.61	110.80
1	B	466	ARG	N-CA-C	5.71	122.96	110.80
1	A	115	LYS	N-CA-C	5.63	118.18	111.71
1	B	40	ALA	CA-C-N	5.61	128.26	120.63
1	B	40	ALA	C-N-CA	5.61	128.26	120.63
1	A	523	HIS	N-CA-C	-5.61	106.27	113.23
1	A	209	ALA	N-CA-C	-5.58	105.57	112.38
1	B	269	TRP	N-CA-C	-5.57	105.30	111.71
1	B	70	SER	N-CA-C	-5.54	105.25	112.23
1	A	239	TYR	N-CA-C	5.50	119.63	109.24
1	B	66	LEU	N-CA-C	5.50	117.27	111.28
1	A	269	TRP	N-CA-C	-5.48	105.41	111.71
1	B	267	GLU	CB-CA-C	-5.46	107.58	114.40
1	A	267	GLU	CB-CA-C	-5.41	107.63	114.40
1	A	146	HIS	N-CA-C	5.36	119.81	113.16
1	A	496	ILE	N-CA-C	5.33	115.54	110.42
1	B	263	HIS	N-CA-C	5.31	116.94	110.41
1	A	460	GLY	CA-C-N	-5.30	113.17	119.05
1	A	460	GLY	C-N-CA	-5.30	113.17	119.05
1	A	499	ARG	CA-C-N	5.29	125.35	119.32
1	A	499	ARG	C-N-CA	5.29	125.35	119.32
1	B	222	PRO	CA-C-N	5.29	127.63	120.65
1	B	222	PRO	C-N-CA	5.29	127.63	120.65
1	A	161	PRO	N-CA-C	5.28	125.83	112.10
1	B	255	SER	N-CA-C	5.28	117.85	109.24
1	B	149	PHE	N-CA-C	5.28	118.17	109.72
1	A	351	ARG	N-CA-C	-5.27	105.12	112.45
1	B	129	ASP	N-CA-C	-5.27	106.72	112.72
1	A	186	PHE	N-CA-C	5.26	119.76	112.45
1	B	243	LYS	N-CA-C	-5.24	104.02	110.31
1	B	457	GLY	N-CA-C	-5.24	101.45	112.45
1	B	195	ASP	N-CA-C	-5.21	106.98	113.55
1	B	239	TYR	N-CA-C	5.21	119.08	109.24
1	A	232	PRO	N-CA-C	-5.20	98.58	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	ASN	N-CA-C	-5.20	105.62	111.28
1	B	468	THR	N-CA-C	5.17	117.33	111.02
1	B	467	ASN	N-CA-C	-5.14	104.46	111.56
1	B	419	HIS	N-CA-C	5.14	119.68	113.41
1	B	499	ARG	CA-C-N	5.12	125.15	119.32
1	B	499	ARG	C-N-CA	5.12	125.15	119.32
1	B	132	LYS	N-CA-C	-5.11	99.92	110.80
1	B	351	ARG	N-CA-C	-5.08	105.39	112.45
1	B	536	ILE	CB-CA-C	-5.07	105.21	111.70
1	B	460	GLY	CA-C-N	-5.03	113.47	119.05
1	B	460	GLY	C-N-CA	-5.03	113.47	119.05
1	B	258	ALA	N-CA-C	5.03	118.31	110.32
1	A	211	ARG	N-CA-C	-5.01	105.51	110.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3901	0	3890	625	0
1	B	4299	0	4270	720	0
2	A	17	0	17	2	0
2	B	17	0	17	6	0
3	A	4	0	0	0	0
3	B	17	0	0	5	0
All	All	8255	0	8194	1308	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 81.

All (1308) 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:223:GLU:CD	1:B:223:GLU:H	1.53	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:GLY:HA2	1:A:299:SER:HB2	1.33	1.10
1:B:141:CYS:O	1:B:144:SER:HB3	1.52	1.10
1:B:61:SER:O	1:B:64:VAL:HG23	1.51	1.09
1:B:183:LEU:HD23	1:B:201:ILE:HD12	1.31	1.08
1:B:232:PRO:HD2	1:B:233:ASN:H	1.11	1.08
1:B:293:GLY:HA2	1:B:299:SER:HB2	1.28	1.07
1:B:49:PRO:HB2	1:B:67:MET:HG2	1.31	1.05
1:B:222:PRO:HG2	1:B:225:PRO:HG3	1.38	1.05
1:B:103:ARG:HB2	1:B:104:PRO:HD3	1.34	1.04
1:A:470:ARG:HA	1:A:473:LYS:HZ3	1.19	1.04
1:B:155:GLN:OE1	1:B:155:GLN:HA	1.50	1.04
1:B:5:VAL:HG23	1:B:118:THR:O	1.57	1.04
1:B:303:ILE:HD13	1:B:463:ASN:HD21	1.17	1.03
1:B:127:LEU:HD12	1:B:127:LEU:H	1.22	1.02
1:B:424:ILE:HD13	1:B:424:ILE:H	1.19	1.02
1:A:101:ILE:HG21	1:A:106:LEU:HD12	1.42	1.02
1:A:303:ILE:HD13	1:A:463:ASN:HD21	1.23	1.01
1:B:4:ARG:HH11	1:B:4:ARG:HB3	1.26	1.01
1:A:484:LEU:HD12	1:B:129:ASP:OD2	1.61	1.00
1:B:470:ARG:HA	1:B:473:LYS:HZ3	1.21	1.00
1:B:36:PHE:HE2	1:B:82:LEU:HD13	1.27	0.99
1:A:232:PRO:HD2	1:A:233:ASN:HD22	1.24	0.99
1:B:120:CYS:HB3	1:B:149:PHE:HB2	1.43	0.99
1:A:230:CYS:O	1:A:231:ASN:HB3	1.59	0.99
1:A:377:PRO:O	1:A:419:HIS:HB3	1.63	0.99
1:B:377:PRO:O	1:B:419:HIS:HB3	1.64	0.98
1:A:214:GLU:O	1:A:217:THR:HG23	1.64	0.97
1:A:529:LYS:HB3	1:A:532:GLU:HG3	1.46	0.97
1:B:25:ARG:HA	1:B:28:GLU:HG2	1.44	0.97
1:A:380:ASN:HB3	1:A:419:HIS:HA	1.48	0.95
1:B:380:ASN:HB3	1:B:419:HIS:HA	1.49	0.95
1:B:529:LYS:HB3	1:B:532:GLU:HG3	1.47	0.95
1:A:160:LYS:HB3	1:A:189:ASN:HD21	1.28	0.94
1:B:493:GLU:HG2	1:B:494:LYS:HG2	1.50	0.94
1:B:492:ALA:HB1	1:B:521:CYS:HB3	1.51	0.93
1:A:187:GLY:HA2	1:A:190:LEU:HD12	1.48	0.92
1:B:529:LYS:O	1:B:533:VAL:HG23	1.69	0.92
1:A:183:LEU:HB3	1:A:201:ILE:HB	1.51	0.92
1:A:496:ILE:HD12	1:A:496:ILE:H	1.33	0.92
1:A:13:VAL:HG22	1:A:203:VAL:HG11	1.49	0.92
1:B:434:ASP:H	1:B:435:PRO:HD3	1.34	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:ILE:H	1:B:496:ILE:HD12	1.33	0.92
1:A:205:ASN:H	1:A:205:ASN:HD22	1.01	0.91
1:B:139:MET:O	1:B:143:LEU:HG	1.70	0.91
1:B:160:LYS:HB3	1:B:189:ASN:HD21	1.35	0.90
1:A:529:LYS:O	1:A:533:VAL:HG23	1.71	0.90
1:A:493:GLU:HG2	1:A:494:LYS:HG2	1.51	0.90
1:B:232:PRO:CD	1:B:233:ASN:H	1.83	0.90
1:B:328:VAL:HG13	1:B:330:ILE:HD11	1.54	0.90
1:A:65:PRO:HG2	1:A:66:LEU:HD22	1.54	0.89
1:A:63:TRP:C	1:A:65:PRO:HD3	1.96	0.89
1:B:330:ILE:HG23	1:B:354:ALA:HB3	1.52	0.89
1:B:223:GLU:CD	1:B:223:GLU:N	2.27	0.89
1:B:489:MET:HB2	1:B:513:LEU:HD21	1.53	0.89
1:B:293:GLY:CA	1:B:299:SER:HB2	2.02	0.89
1:B:535:GLN:HB3	1:B:539:LYS:NZ	1.88	0.89
1:B:303:ILE:HA	1:B:463:ASN:ND2	1.88	0.89
1:B:434:ASP:H	1:B:435:PRO:CD	1.85	0.88
1:B:49:PRO:CB	1:B:67:MET:HG2	2.03	0.88
1:A:50:THR:OG1	1:A:66:LEU:HD11	1.73	0.88
1:A:159:ILE:O	1:A:165:ILE:HD11	1.71	0.88
1:A:303:ILE:HA	1:A:463:ASN:ND2	1.88	0.88
1:A:492:ALA:HB1	1:A:521:CYS:HB3	1.54	0.88
1:A:173:LEU:HD22	1:A:173:LEU:H	1.38	0.87
1:A:328:VAL:HG13	1:A:330:ILE:HD11	1.56	0.87
1:A:166:TYR:O	1:A:170:LEU:HD12	1.74	0.87
1:A:192:PRO:O	1:A:195:ASP:HB2	1.74	0.86
1:A:489:MET:HB2	1:A:513:LEU:HD21	1.56	0.86
1:B:122:VAL:HB	1:B:151:ILE:HD13	1.56	0.86
1:B:515:ARG:HH11	1:B:515:ARG:CG	1.88	0.86
1:A:535:GLN:HB3	1:A:539:LYS:NZ	1.91	0.85
1:B:328:VAL:CG1	1:B:330:ILE:HD11	2.05	0.85
1:A:330:ILE:HG23	1:A:354:ALA:HB3	1.56	0.85
1:B:16:LEU:HB2	1:B:17:PRO:HA	1.58	0.85
1:A:515:ARG:HH11	1:A:515:ARG:CG	1.89	0.85
1:A:348:GLU:HA	1:B:133:ARG:CG	2.06	0.85
1:A:8:PHE:HD2	1:A:183:LEU:HD11	1.40	0.85
1:B:232:PRO:HD2	1:B:233:ASN:N	1.90	0.85
1:B:329:PHE:O	1:B:330:ILE:HD13	1.77	0.84
1:B:293:GLY:HA2	1:B:299:SER:CB	2.07	0.84
1:B:212:GLU:C	1:B:214:GLU:H	1.83	0.84
1:B:49:PRO:HB2	1:B:67:MET:CG	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:LEU:HD22	1:B:126:TRP:HB2	1.60	0.84
1:B:187:GLY:HA2	1:B:190:LEU:HD12	1.60	0.83
1:A:293:GLY:CA	1:A:299:SER:HB2	2.06	0.83
1:A:155:GLN:HA	1:A:155:GLN:OE1	1.78	0.83
1:B:232:PRO:HD2	1:B:233:ASN:HD22	1.43	0.83
1:A:52:GLN:OE1	1:A:58:ILE:HD11	1.78	0.83
1:B:64:VAL:HB	1:B:65:PRO:HD3	1.60	0.83
1:B:75:SER:HB2	1:B:82:LEU:HB3	1.58	0.83
1:A:328:VAL:CG1	1:A:330:ILE:HD11	2.07	0.82
1:B:169:LEU:HD23	1:B:170:LEU:N	1.93	0.82
1:A:92:PHE:C	1:A:94:GLN:H	1.84	0.82
1:A:124:ASN:OD1	1:A:160:LYS:HB2	1.78	0.82
1:A:442:THR:OG1	1:A:445:GLU:HG3	1.78	0.82
1:B:13:VAL:HB	1:B:203:VAL:HG11	1.58	0.82
1:A:329:PHE:O	1:A:330:ILE:HD13	1.80	0.82
1:A:537:LEU:O	1:A:541:LEU:HD12	1.79	0.82
1:A:159:ILE:HD12	1:A:159:ILE:C	2.05	0.81
1:A:482:LYS:HB2	1:B:62:GLN:NE2	1.95	0.81
1:B:4:ARG:HH11	1:B:4:ARG:CB	1.93	0.81
1:B:26:SER:C	1:B:28:GLU:H	1.86	0.81
1:B:263:HIS:CD2	1:B:291:MET:HG2	2.15	0.81
1:A:380:ASN:CB	1:A:419:HIS:HA	2.09	0.81
1:B:404:LYS:O	1:B:408:ARG:HD2	1.81	0.81
1:A:106:LEU:O	1:A:106:LEU:HD23	1.80	0.81
1:A:4:ARG:HH21	1:A:179:GLU:HB3	1.45	0.81
1:B:442:THR:OG1	1:B:445:GLU:HG3	1.80	0.81
1:A:8:PHE:CD2	1:A:183:LEU:HD11	2.16	0.81
1:A:169:LEU:HD23	1:A:173:LEU:HD21	1.63	0.81
1:B:303:ILE:HD13	1:B:463:ASN:ND2	1.96	0.80
1:B:344:LEU:HD21	1:B:478:GLY:HA3	1.64	0.80
1:B:160:LYS:HD2	1:B:189:ASN:ND2	1.95	0.80
1:A:344:LEU:HD21	1:A:478:GLY:HA3	1.63	0.80
1:A:16:LEU:HB2	1:A:17:PRO:HA	1.63	0.79
1:A:499:ARG:O	1:A:502:MET:HG3	1.82	0.79
1:A:61:SER:HB2	1:B:484:LEU:HD13	1.64	0.79
1:B:199:VAL:HG21	3:B:1002:HOH:O	1.81	0.79
1:B:499:ARG:O	1:B:502:MET:HG3	1.83	0.79
1:B:49:PRO:HD2	1:B:67:MET:HE2	1.65	0.79
1:A:215:LYS:HG2	1:A:220:GLN:CB	2.12	0.78
1:A:301:PRO:HD2	1:A:302:GLU:H	1.48	0.78
1:B:36:PHE:CE2	1:B:82:LEU:HD13	2.15	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:ASN:CB	1:B:419:HIS:HA	2.11	0.78
1:A:137:ALA:HB1	1:B:325:PRO:O	1.83	0.78
1:A:62:GLN:O	1:A:62:GLN:HG3	1.83	0.78
1:B:73:LYS:O	1:B:77:ALA:HB3	1.83	0.78
1:A:240:VAL:HG21	1:A:322:LEU:HD12	1.65	0.78
1:A:122:VAL:HG22	1:A:122:VAL:O	1.83	0.78
1:B:347:PRO:HD2	1:B:348:GLU:OE1	1.84	0.78
1:B:515:ARG:HH11	1:B:515:ARG:HG3	1.48	0.77
1:A:483:ILE:HB	1:A:510:ILE:HG12	1.66	0.77
1:A:264:GLY:HA3	1:A:333:ASP:HB3	1.66	0.77
1:A:293:GLY:HA2	1:A:299:SER:CB	2.13	0.77
1:A:470:ARG:HA	1:A:473:LYS:NZ	2.00	0.77
1:A:470:ARG:CA	1:A:473:LYS:HZ3	1.98	0.77
1:B:112:LEU:HD23	1:B:117:PHE:CE1	2.20	0.77
1:B:158:MET:HG2	1:B:164:GLN:HB3	1.66	0.77
1:A:329:PHE:C	1:A:330:ILE:HD13	2.10	0.76
1:A:404:LYS:O	1:A:408:ARG:HD2	1.85	0.76
1:B:299:SER:OG	1:B:456:THR:HG22	1.85	0.76
1:B:127:LEU:HD12	1:B:127:LEU:N	2.01	0.76
1:B:226:LEU:HD12	1:B:226:LEU:H	1.49	0.76
1:B:301:PRO:HD2	1:B:302:GLU:H	1.51	0.76
1:A:16:LEU:HB2	1:A:17:PRO:CA	2.16	0.76
1:A:193:ALA:HB1	1:A:198:MET:SD	2.24	0.76
1:B:30:LEU:HB2	1:B:32:LEU:HD13	1.65	0.76
1:B:331:GLY:N	1:B:339:VAL:HG21	2.00	0.76
1:B:7:ALA:HB2	1:B:120:CYS:SG	2.25	0.76
1:B:329:PHE:C	1:B:330:ILE:HD13	2.10	0.76
1:B:424:ILE:HD13	1:B:424:ILE:N	2.00	0.76
1:B:470:ARG:HA	1:B:473:LYS:NZ	2.00	0.76
1:B:362:PRO:HG2	1:B:509:TRP:NE1	2.00	0.76
1:A:263:HIS:CD2	1:A:291:MET:HG2	2.21	0.76
1:B:372:VAL:HG22	1:B:373:ILE:HD13	1.67	0.76
1:B:483:ILE:HB	1:B:510:ILE:HG12	1.66	0.76
1:B:42:GLN:HB2	1:B:186:PHE:CE1	2.20	0.75
1:A:515:ARG:HH11	1:A:515:ARG:HG3	1.51	0.75
1:B:8:PHE:CD1	1:B:8:PHE:N	2.54	0.75
1:B:121:ILE:HG13	1:B:150:LEU:HD12	1.69	0.75
1:A:339:VAL:HG13	1:A:353:VAL:CG1	2.17	0.75
1:B:381:TYR:CZ	1:B:382:GLN:HG3	2.20	0.75
1:A:124:ASN:CG	1:A:160:LYS:HB2	2.12	0.75
1:B:535:GLN:HB3	1:B:539:LYS:HZ2	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ASN:CG	1:A:206:THR:H	1.93	0.74
1:B:264:GLY:HA3	1:B:333:ASP:HB3	1.67	0.74
1:A:62:GLN:OE1	1:B:481:ARG:HA	1.87	0.74
1:B:32:LEU:HD11	1:B:82:LEU:HD12	1.68	0.74
1:A:229:PRO:O	1:A:230:CYS:HB3	1.88	0.74
1:A:535:GLN:HB3	1:A:539:LYS:HZ2	1.50	0.74
1:B:183:LEU:CD2	1:B:201:ILE:HD12	2.16	0.74
1:B:320:ASP:OD1	1:B:349:ARG:NH2	2.20	0.74
1:B:339:VAL:HG13	1:B:353:VAL:CG1	2.17	0.74
1:A:5:VAL:HB	1:A:180:VAL:HG12	1.69	0.74
1:B:160:LYS:HD2	1:B:189:ASN:HD21	1.51	0.74
1:B:537:LEU:O	1:B:541:LEU:HD12	1.86	0.74
1:A:320:ASP:OD1	1:A:349:ARG:NH2	2.20	0.74
1:A:348:GLU:HA	1:B:133:ARG:HG2	1.70	0.74
1:B:28:GLU:OE1	1:B:28:GLU:HA	1.87	0.74
1:B:48:GLY:O	1:B:52:GLN:HG2	1.88	0.73
1:A:376:ILE:HD13	1:A:376:ILE:H	1.53	0.73
1:B:183:LEU:HB3	1:B:201:ILE:HB	1.68	0.73
1:A:303:ILE:HD13	1:A:463:ASN:ND2	2.01	0.73
1:B:39:GLY:O	1:B:43:THR:HG23	1.88	0.73
1:B:42:GLN:HB2	1:B:186:PHE:CZ	2.24	0.73
1:B:122:VAL:HB	1:B:151:ILE:CD1	2.18	0.73
1:A:372:VAL:HG22	1:A:373:ILE:HD13	1.69	0.73
1:B:25:ARG:HA	1:B:28:GLU:CG	2.18	0.73
1:B:303:ILE:HA	1:B:463:ASN:HD22	1.53	0.73
1:A:467:ASN:OD1	1:A:470:ARG:HD2	1.89	0.73
1:B:230:CYS:HB3	1:B:277:PRO:HD3	1.71	0.73
1:B:240:VAL:HG21	1:B:322:LEU:HD12	1.69	0.73
1:A:205:ASN:HD22	1:A:205:ASN:N	1.80	0.73
1:B:68:ASP:OD1	1:B:87:SER:HA	1.90	0.72
1:B:158:MET:HG2	1:B:164:GLN:CB	2.20	0.72
1:A:106:LEU:CD2	1:A:110:ILE:HD11	2.18	0.72
1:A:489:MET:HG3	1:A:506:MET:SD	2.29	0.72
1:A:270:PHE:HB2	1:A:448:PHE:HE2	1.54	0.72
1:B:11:ASP:OD1	1:B:99:ARG:NH1	2.21	0.72
1:B:340:TRP:CE2	1:B:355:SER:HB2	2.24	0.72
1:A:331:GLY:N	1:A:339:VAL:HG21	2.03	0.72
1:B:5:VAL:CG1	1:B:180:VAL:HG12	2.19	0.72
1:B:103:ARG:HB2	1:B:104:PRO:CD	2.16	0.72
1:B:270:PHE:HB2	1:B:448:PHE:HE2	1.53	0.72
1:A:169:LEU:O	1:A:173:LEU:HD22	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:PHE:HB2	1:B:14:LEU:HD13	1.70	0.72
1:B:535:GLN:O	1:B:539:LYS:HD3	1.90	0.72
1:A:193:ALA:O	1:A:198:MET:HG3	1.90	0.72
1:A:386:GLN:O	1:A:388:PRO:HD3	1.90	0.72
1:B:96:MET:SD	1:B:136:LEU:HD22	2.29	0.72
1:A:13:VAL:HG11	1:A:183:LEU:HD12	1.70	0.72
1:A:203:VAL:HG12	1:A:203:VAL:O	1.90	0.72
1:A:304:GLU:H	1:A:304:GLU:CD	1.97	0.72
1:A:8:PHE:HB3	1:A:183:LEU:HD11	1.72	0.72
1:B:230:CYS:H	1:B:277:PRO:CG	2.03	0.72
1:B:386:GLN:O	1:B:388:PRO:HD3	1.90	0.72
1:A:200:THR:C	1:A:201:ILE:HG12	2.14	0.71
1:A:92:PHE:C	1:A:94:GLN:N	2.45	0.71
1:A:339:VAL:O	1:A:342:MET:HB2	1.89	0.71
1:A:424:ILE:HD12	1:A:426:GLY:O	1.91	0.71
1:A:362:PRO:HG2	1:A:509:TRP:NE1	2.05	0.71
1:A:52:GLN:CB	1:A:55:LYS:HD2	2.20	0.71
1:A:376:ILE:HD13	1:A:376:ILE:N	2.04	0.71
1:B:489:MET:HG3	1:B:506:MET:SD	2.29	0.71
1:A:9:ASP:OD1	1:A:160:LYS:NZ	2.23	0.71
1:B:102:ASN:ND2	1:B:105:MET:HG2	2.05	0.71
1:B:304:GLU:CD	1:B:304:GLU:H	1.98	0.71
1:B:499:ARG:HB3	1:B:501:GLU:CD	2.14	0.71
1:B:204:HIS:O	1:B:205:ASN:CB	2.38	0.71
1:B:155:GLN:OE1	1:B:155:GLN:CA	2.35	0.71
1:A:10:LEU:O	1:A:12:GLY:N	2.23	0.71
1:A:347:PRO:HD2	1:A:348:GLU:OE1	1.91	0.70
1:A:499:ARG:HB3	1:A:501:GLU:CD	2.16	0.70
1:A:232:PRO:CD	1:A:233:ASN:HD22	2.03	0.70
1:A:303:ILE:HA	1:A:463:ASN:HD22	1.54	0.70
1:B:376:ILE:N	1:B:376:ILE:HD13	2.06	0.70
1:A:340:TRP:CE2	1:A:355:SER:HB2	2.27	0.70
1:B:183:LEU:HB2	1:B:203:VAL:CG2	2.22	0.70
1:B:340:TRP:CZ2	1:B:355:SER:HB2	2.26	0.70
1:A:458:PHE:O	1:A:461:PRO:HD2	1.91	0.70
1:A:535:GLN:O	1:A:539:LYS:HD3	1.91	0.70
1:B:14:LEU:HD21	1:B:147:PHE:CZ	2.27	0.70
1:B:496:ILE:H	1:B:496:ILE:CD1	2.00	0.70
1:A:122:VAL:O	1:A:122:VAL:CG2	2.39	0.70
1:B:343:ALA:HB2	1:B:353:VAL:HG21	1.73	0.70
1:A:230:CYS:O	1:A:230:CYS:SG	2.50	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:SER:OG	1:A:456:THR:HG22	1.91	0.69
1:A:160:LYS:HB3	1:A:189:ASN:ND2	2.07	0.69
1:B:376:ILE:HD13	1:B:376:ILE:H	1.57	0.69
1:B:470:ARG:CA	1:B:473:LYS:HZ3	2.01	0.69
1:A:50:THR:HA	1:A:63:TRP:HE1	1.56	0.69
1:B:208:SER:HA	1:B:211:ARG:HB2	1.74	0.69
1:A:381:TYR:CZ	1:A:382:GLN:HG3	2.27	0.69
1:B:8:PHE:O	1:B:121:ILE:HG22	1.90	0.69
1:B:211:ARG:HA	1:B:214:GLU:HG2	1.73	0.69
1:B:414:GLY:O	1:B:431:THR:HG23	1.92	0.69
1:B:416:ILE:HG23	1:B:427:ILE:HG22	1.74	0.69
1:A:343:ALA:HB2	1:A:353:VAL:HG21	1.74	0.69
1:A:216:VAL:O	1:A:217:THR:C	2.36	0.69
1:B:467:ASN:OD1	1:B:470:ARG:HD2	1.93	0.69
1:B:291:MET:HE1	1:B:315:MET:HE3	1.73	0.69
1:B:6:ALA:HB2	1:B:181:VAL:HG13	1.74	0.68
1:B:160:LYS:HB3	1:B:189:ASN:ND2	2.07	0.68
1:A:496:ILE:H	1:A:496:ILE:CD1	2.00	0.68
1:B:67:MET:HA	1:B:70:SER:HB3	1.75	0.68
1:A:176:LYS:HB3	1:A:178:ASN:ND2	2.08	0.68
1:A:426:GLY:O	1:A:429:VAL:HG23	1.93	0.68
1:B:158:MET:HB3	1:B:164:GLN:HB2	1.74	0.68
1:B:339:VAL:O	1:B:342:MET:HB2	1.92	0.68
1:A:529:LYS:HB3	1:A:532:GLU:CG	2.24	0.68
1:B:71:TYR:HE2	1:B:88:ILE:HD13	1.56	0.68
1:A:127:LEU:HG	1:A:154:CYS:SG	2.32	0.67
1:B:232:PRO:CD	1:B:233:ASN:N	2.48	0.67
1:A:263:HIS:NE2	1:A:291:MET:HB2	2.07	0.67
1:B:160:LYS:CB	1:B:189:ASN:HD21	2.08	0.67
1:B:231:ASN:OD1	1:B:270:PHE:HE1	1.78	0.67
1:B:483:ILE:HD12	1:B:510:ILE:HD11	1.76	0.67
1:A:8:PHE:HB3	1:A:183:LEU:CD1	2.24	0.67
1:B:43:THR:O	1:B:44:GLU:HB2	1.94	0.67
1:A:291:MET:HE1	1:A:315:MET:HE3	1.74	0.67
1:B:60:PHE:O	1:B:63:TRP:HB3	1.95	0.67
1:B:173:LEU:O	1:B:174:LYS:HD2	1.93	0.67
1:B:458:PHE:O	1:B:461:PRO:HD2	1.94	0.67
1:A:159:ILE:C	1:A:159:ILE:CD1	2.67	0.67
1:A:180:VAL:HG23	1:A:180:VAL:O	1.94	0.66
1:B:75:SER:OG	1:B:76:LYS:N	2.25	0.66
1:B:211:ARG:O	1:B:215:LYS:HD2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:VAL:HB	1:B:65:PRO:CD	2.22	0.66
1:A:115:LYS:HE3	1:A:219:THR:OG1	1.96	0.66
1:B:424:ILE:H	1:B:424:ILE:CD1	1.98	0.66
1:A:13:VAL:HG22	1:A:203:VAL:CG1	2.24	0.66
1:B:428:LEU:HA	1:B:431:THR:OG1	1.95	0.66
1:A:240:VAL:CG2	1:A:322:LEU:HD12	2.24	0.66
1:B:232:PRO:CD	1:B:233:ASN:HD22	2.08	0.66
1:A:101:ILE:HD13	1:A:106:LEU:HD12	1.77	0.66
1:A:101:ILE:HD11	1:A:142:GLU:HG2	1.78	0.66
1:B:203:VAL:HG12	1:B:203:VAL:O	1.94	0.66
1:A:190:LEU:CD2	1:A:200:THR:HG22	2.25	0.66
1:A:232:PRO:HD2	1:A:233:ASN:N	2.09	0.66
1:A:5:VAL:HG13	1:A:118:THR:O	1.96	0.66
1:A:16:LEU:HD21	1:A:206:THR:HG22	1.79	0.65
1:A:207:ALA:C	1:A:210:LEU:HB2	2.21	0.65
1:A:230:CYS:O	1:A:231:ASN:CB	2.36	0.65
1:A:490:VAL:HG22	1:A:516:GLY:HA3	1.77	0.65
1:B:458:PHE:O	1:B:462:LEU:HD12	1.95	0.65
1:A:227:PRO:HG2	1:A:274:TYR:HD1	1.60	0.65
1:A:326:GLN:NE2	1:B:134:ASP:HA	2.11	0.65
1:B:229:PRO:HA	1:B:273:ARG:O	1.96	0.65
1:A:133:ARG:HG2	1:B:348:GLU:HA	1.78	0.65
1:B:490:VAL:HG22	1:B:516:GLY:HA3	1.77	0.65
1:B:497:VAL:O	1:B:498:LEU:HB2	1.97	0.65
1:A:232:PRO:CD	1:A:233:ASN:N	2.56	0.65
1:A:340:TRP:CZ2	1:A:355:SER:HB2	2.31	0.65
1:A:159:ILE:O	1:A:159:ILE:HD12	1.97	0.65
1:A:291:MET:O	1:A:292:LYS:C	2.40	0.65
1:B:230:CYS:H	1:B:277:PRO:HG2	1.61	0.65
1:A:13:VAL:O	1:A:105:MET:HG2	1.96	0.65
1:A:348:GLU:HA	1:B:133:ARG:CD	2.25	0.65
1:B:5:VAL:HG13	1:B:180:VAL:HG12	1.78	0.65
1:B:119:THR:N	1:B:148:ASP:OD2	2.30	0.65
1:B:458:PHE:C	1:B:461:PRO:HD2	2.22	0.65
1:A:350:VAL:O	1:B:133:ARG:NH1	2.31	0.64
1:B:204:HIS:O	1:B:205:ASN:HB2	1.97	0.64
1:A:126:TRP:NE1	1:A:128:ASP:OD1	2.20	0.64
1:B:86:PHE:CD1	1:B:87:SER:N	2.65	0.64
1:B:106:LEU:HD21	1:B:146:HIS:CD2	2.33	0.64
1:B:26:SER:C	1:B:28:GLU:N	2.54	0.64
1:B:240:VAL:CG2	1:B:322:LEU:HD12	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:ASP:N	1:B:435:PRO:CD	2.52	0.64
1:A:50:THR:CA	1:A:63:TRP:HE1	2.09	0.64
1:A:478:GLY:HA2	1:A:481:ARG:HG3	1.78	0.64
1:B:300:PRO:HG2	1:B:305:GLU:HG2	1.80	0.64
1:B:212:GLU:C	1:B:214:GLU:N	2.55	0.64
1:A:125:ASN:O	1:A:126:TRP:HB3	1.96	0.64
1:A:270:PHE:HB2	1:A:448:PHE:CE2	2.33	0.64
1:A:4:ARG:NH2	1:A:179:GLU:HB3	2.10	0.64
1:B:270:PHE:HB2	1:B:448:PHE:CE2	2.33	0.64
1:A:232:PRO:HD2	1:A:233:ASN:ND2	2.07	0.63
1:A:458:PHE:C	1:A:461:PRO:HD2	2.23	0.63
1:A:458:PHE:O	1:A:462:LEU:HD12	1.98	0.63
1:B:101:ILE:HD11	1:B:143:LEU:HD21	1.81	0.63
1:B:291:MET:O	1:B:292:LYS:C	2.41	0.63
1:A:131:ASP:C	1:A:133:ARG:H	2.05	0.63
1:A:497:VAL:O	1:A:498:LEU:HB2	1.97	0.63
1:B:303:ILE:CD1	1:B:463:ASN:HD21	2.01	0.63
1:B:386:GLN:NE2	1:B:468:THR:OG1	2.32	0.63
1:B:23:PHE:O	1:B:27:GLU:HG3	1.99	0.63
1:B:293:GLY:O	1:B:456:THR:HG21	1.99	0.63
1:A:380:ASN:O	1:A:383:LEU:N	2.27	0.63
1:A:242:VAL:HG12	1:A:317:THR:HB	1.80	0.62
1:A:386:GLN:NE2	1:A:468:THR:OG1	2.32	0.62
1:B:205:ASN:CG	1:B:206:THR:H	2.07	0.62
1:B:331:GLY:H	1:B:339:VAL:HG21	1.62	0.62
1:A:291:MET:HE3	1:A:291:MET:HA	1.82	0.62
1:B:176:LYS:HB3	1:B:178:ASN:ND2	2.15	0.62
1:A:193:ALA:CB	1:A:198:MET:SD	2.88	0.62
1:A:381:TYR:CE2	1:A:418:VAL:HG12	2.33	0.62
1:B:156:VAL:HG23	1:B:157:GLY:H	1.64	0.62
1:B:529:LYS:HB3	1:B:532:GLU:CG	2.24	0.62
1:B:159:ILE:O	1:B:165:ILE:HD11	1.98	0.62
1:B:524:TRP:O	1:B:528:GLU:HB3	1.99	0.62
1:A:300:PRO:HG2	1:A:305:GLU:HG2	1.81	0.62
1:B:16:LEU:CB	1:B:17:PRO:HA	2.26	0.62
1:A:191:LYS:CB	1:A:192:PRO:HD3	2.29	0.62
1:A:483:ILE:HD12	1:A:510:ILE:HD11	1.80	0.62
1:A:62:GLN:NE2	1:B:482:LYS:HB2	2.15	0.62
1:A:64:VAL:N	1:A:65:PRO:HD3	2.13	0.62
1:A:90:GLN:HG3	1:A:91:ILE:N	2.14	0.62
1:A:415:PHE:HD1	1:A:416:ILE:H	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ARG:CD	1:B:73:LYS:HZ3	2.13	0.61
1:B:263:HIS:NE2	1:B:291:MET:HB2	2.13	0.61
1:B:387:GLU:HB3	1:B:390:VAL:HG21	1.82	0.61
1:A:215:LYS:HG2	1:A:220:GLN:HB2	1.82	0.61
1:B:177:PRO:O	1:B:198:MET:HA	2.00	0.61
1:B:535:GLN:HB3	1:B:539:LYS:HZ3	1.61	0.61
1:A:156:VAL:O	1:A:158:MET:HG3	2.00	0.61
1:A:510:ILE:O	1:A:513:LEU:HB2	2.01	0.61
1:B:478:GLY:HA2	1:B:481:ARG:HG3	1.81	0.61
1:B:165:ILE:O	1:B:166:TYR:C	2.42	0.61
1:B:272:TRP:H	1:B:272:TRP:CD1	2.18	0.61
1:B:420:LYS:C	1:B:424:ILE:HD11	2.25	0.61
1:A:331:GLY:H	1:A:339:VAL:HG21	1.65	0.61
1:A:482:LYS:CB	1:B:62:GLN:NE2	2.63	0.61
1:A:489:MET:HE3	1:A:490:VAL:N	2.16	0.61
1:B:32:LEU:HD21	1:B:82:LEU:CD1	2.31	0.61
1:B:380:ASN:O	1:B:383:LEU:N	2.31	0.61
1:A:115:LYS:HZ1	1:A:218:GLY:HA3	1.64	0.61
1:A:121:ILE:HD11	1:A:147:PHE:CD1	2.36	0.61
1:A:190:LEU:HD23	1:A:200:THR:HG22	1.82	0.61
1:B:121:ILE:HG13	1:B:150:LEU:CD1	2.30	0.61
1:B:169:LEU:O	1:B:173:LEU:HD22	2.00	0.61
1:A:102:ASN:O	1:A:105:MET:HB3	2.01	0.61
1:A:231:ASN:HB2	1:A:232:PRO:HB3	1.82	0.61
1:B:32:LEU:HD23	1:B:37:LEU:HG	1.81	0.60
1:B:301:PRO:CD	1:B:302:GLU:H	2.13	0.60
1:A:535:GLN:HB3	1:A:539:LYS:HZ3	1.66	0.60
1:B:72:ARG:HH11	1:B:72:ARG:CB	2.14	0.60
1:B:426:GLY:HA3	1:B:429:VAL:CG2	2.31	0.60
1:B:50:THR:HG23	1:B:63:TRP:HZ2	1.66	0.60
1:A:128:ASP:O	1:A:133:ARG:HG3	2.01	0.60
1:A:428:LEU:O	1:A:431:THR:HB	2.01	0.60
1:B:415:PHE:HD1	1:B:416:ILE:H	1.49	0.60
1:A:289:ILE:CG2	1:A:290:ASP:N	2.64	0.60
1:A:293:GLY:O	1:A:456:THR:HG21	2.01	0.60
1:B:9:ASP:OD1	1:B:160:LYS:NZ	2.35	0.60
1:B:229:PRO:O	1:B:230:CYS:C	2.43	0.60
1:A:301:PRO:CD	1:A:302:GLU:H	2.13	0.60
1:B:25:ARG:C	1:B:28:GLU:HB2	2.27	0.60
1:B:211:ARG:HA	1:B:214:GLU:CG	2.31	0.60
1:B:477:LYS:C	1:B:479:LEU:H	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:TRP:H	1:A:272:TRP:CD1	2.16	0.60
1:A:405:SER:OG	1:A:431:THR:HG21	2.01	0.59
1:A:524:TRP:O	1:A:528:GLU:HB3	2.01	0.59
1:B:131:ASP:C	1:B:133:ARG:H	2.10	0.59
1:B:230:CYS:HB3	1:B:277:PRO:HG3	1.82	0.59
1:A:16:LEU:HA	1:A:17:PRO:C	2.28	0.59
1:B:134:ASP:OD1	1:B:135:SER:N	2.31	0.59
1:A:99:ARG:O	1:A:99:ARG:HG3	2.02	0.59
1:A:101:ILE:CD1	1:A:142:GLU:HG2	2.32	0.59
1:A:173:LEU:O	1:A:174:LYS:HB2	2.02	0.59
1:A:481:ARG:HG2	1:B:57:LYS:O	2.01	0.59
1:B:210:LEU:O	1:B:214:GLU:HB3	2.01	0.59
1:B:380:ASN:OD1	1:B:421:ALA:HB3	2.02	0.59
1:B:442:THR:H	1:B:445:GLU:HB2	1.68	0.59
1:A:442:THR:H	1:A:445:GLU:HB2	1.68	0.59
1:B:13:VAL:O	1:B:105:MET:HG3	2.02	0.59
1:B:281:GLN:O	1:B:282:ALA:C	2.43	0.59
1:A:289:ILE:HG22	1:A:290:ASP:N	2.15	0.59
1:A:453:PHE:HE2	1:A:461:PRO:HG2	1.68	0.59
1:B:242:VAL:HG12	1:B:317:THR:HB	1.84	0.59
1:B:7:ALA:HA	1:B:120:CYS:O	2.02	0.59
1:B:137:ALA:O	1:B:141:CYS:N	2.34	0.59
1:B:381:TYR:O	1:B:384:TYR:HB3	2.02	0.59
1:A:7:ALA:HB2	1:A:120:CYS:SG	2.42	0.59
1:A:50:THR:HG23	1:A:63:TRP:HZ2	1.68	0.59
1:A:210:LEU:O	1:A:214:GLU:CB	2.50	0.59
1:A:477:LYS:C	1:A:479:LEU:H	2.10	0.59
1:A:303:ILE:CD1	1:A:463:ASN:HD21	2.07	0.59
1:A:381:TYR:O	1:A:384:TYR:HB3	2.02	0.59
1:B:134:ASP:O	1:B:135:SER:C	2.45	0.59
1:A:4:ARG:HB3	1:A:179:GLU:HB2	1.84	0.59
1:A:381:TYR:CD2	1:A:418:VAL:HG12	2.38	0.59
1:A:488:LEU:HD13	1:A:490:VAL:HG23	1.84	0.59
1:A:138:GLN:HA	1:B:325:PRO:HB3	1.85	0.58
1:B:92:PHE:C	1:B:94:GLN:H	2.11	0.58
1:B:510:ILE:O	1:B:513:LEU:HB2	2.02	0.58
1:A:123:THR:HA	1:A:160:LYS:HE2	1.84	0.58
1:A:387:GLU:HB3	1:A:390:VAL:HG21	1.84	0.58
1:B:189:ASN:O	1:B:192:PRO:HD2	2.02	0.58
1:A:141:CYS:O	1:A:144:SER:HB3	2.03	0.58
1:A:293:GLY:C	1:A:299:SER:HB2	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:GLN:C	1:A:539:LYS:HD3	2.28	0.58
1:B:293:GLY:C	1:B:299:SER:HB2	2.28	0.58
1:A:4:ARG:NH2	1:A:179:GLU:CB	2.67	0.58
1:A:386:GLN:NE2	1:A:466:ARG:HA	2.19	0.58
1:A:16:LEU:CA	1:A:17:PRO:C	2.77	0.58
1:B:161:PRO:HB2	1:B:192:PRO:HG2	1.85	0.58
1:B:230:CYS:SG	1:B:276:ILE:HG21	2.44	0.58
1:B:535:GLN:C	1:B:539:LYS:HD3	2.28	0.58
1:A:134:ASP:O	1:A:138:GLN:HG3	2.04	0.58
1:A:168:PHE:C	1:A:168:PHE:CD2	2.82	0.58
1:A:242:VAL:CG1	1:A:317:THR:HB	2.34	0.58
1:B:269:TRP:HA	3:B:1016:HOH:O	2.03	0.57
1:A:144:SER:OG	1:A:145:GLN:N	2.36	0.57
1:B:255:SER:O	1:B:256:GLY:O	2.21	0.57
1:B:62:GLN:O	1:B:65:PRO:HD2	2.05	0.57
1:B:124:ASN:HA	1:B:153:SER:HB3	1.85	0.57
1:B:205:ASN:HB3	1:B:207:ALA:H	1.69	0.57
1:B:453:PHE:HE2	1:B:461:PRO:HG2	1.68	0.57
1:A:469:GLU:HG3	1:A:473:LYS:NZ	2.18	0.57
1:B:61:SER:C	1:B:64:VAL:HG23	2.28	0.57
1:B:214:GLU:HG3	1:B:215:LYS:N	2.19	0.57
1:A:139:MET:O	1:A:143:LEU:HD12	2.05	0.57
1:A:205:ASN:CG	1:A:206:THR:N	2.63	0.57
1:A:381:TYR:N	1:A:418:VAL:O	2.30	0.57
1:B:6:ALA:CB	1:B:181:VAL:HG13	2.35	0.57
1:B:72:ARG:O	1:B:72:ARG:HG2	2.05	0.57
1:A:270:PHE:O	1:A:273:ARG:HB3	2.05	0.57
1:B:24:ARG:HH21	1:B:35:ASP:N	2.03	0.57
1:B:243:LYS:HB3	1:B:246:ILE:HD13	1.87	0.57
1:B:291:MET:HE3	1:B:291:MET:HA	1.85	0.57
1:B:360:PHE:CB	1:B:506:MET:HE3	2.35	0.57
1:A:304:GLU:CD	1:A:304:GLU:N	2.62	0.57
1:B:94:GLN:HA	1:B:94:GLN:NE2	2.20	0.57
1:A:200:THR:O	1:A:201:ILE:HG12	2.05	0.56
1:B:222:PRO:CG	1:B:225:PRO:HG3	2.22	0.56
1:A:53:LEU:CD1	1:A:53:LEU:C	2.79	0.56
1:A:202:LEU:O	1:A:203:VAL:HB	2.04	0.56
1:B:13:VAL:CB	1:B:203:VAL:HG11	2.31	0.56
1:B:108:ALA:O	1:B:112:LEU:HD12	2.05	0.56
1:B:386:GLN:NE2	1:B:466:ARG:HA	2.20	0.56
1:A:64:VAL:O	1:A:64:VAL:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PRO:HG2	1:A:274:TYR:CD1	2.40	0.56
1:A:92:PHE:O	1:A:92:PHE:CD1	2.59	0.56
1:A:212:GLU:O	1:A:215:LYS:HB2	2.05	0.56
1:A:347:PRO:O	1:B:133:ARG:HD2	2.05	0.56
1:B:79:GLY:O	1:B:80:ALA:HB3	2.05	0.56
1:A:16:LEU:HA	1:A:17:PRO:O	2.06	0.56
1:A:53:LEU:C	1:A:53:LEU:HD13	2.30	0.56
1:A:187:GLY:CA	1:A:190:LEU:HD12	2.29	0.56
1:A:332:HIS:HB2	1:A:356:LEU:HB2	1.88	0.56
1:B:8:PHE:CE1	1:B:147:PHE:HE2	2.23	0.56
1:B:12:GLY:HA3	1:B:185:ASP:HB3	1.87	0.56
1:B:165:ILE:O	1:B:168:PHE:N	2.35	0.56
1:B:489:MET:HE3	1:B:490:VAL:N	2.20	0.56
1:A:513:LEU:HD23	1:A:514:LYS:O	2.05	0.56
1:A:50:THR:OG1	1:A:66:LEU:CD1	2.52	0.56
1:A:96:MET:O	1:A:99:ARG:HG2	2.06	0.56
1:A:122:VAL:HA	1:A:151:ILE:O	2.06	0.56
1:A:265:PHE:CD1	1:A:265:PHE:C	2.84	0.56
1:A:438:SER:C	1:A:440:ILE:H	2.14	0.56
1:B:30:LEU:O	1:B:31:ALA:C	2.48	0.56
1:B:115:LYS:HE3	1:B:219:THR:CG2	2.36	0.56
1:B:153:SER:HB2	1:B:159:ILE:HG22	1.87	0.56
1:B:360:PHE:HB2	1:B:506:MET:HE3	1.88	0.56
1:A:96:MET:SD	1:A:136:LEU:HD22	2.46	0.55
1:B:187:GLY:HA2	1:B:190:LEU:CD1	2.35	0.55
1:A:328:VAL:HG22	1:A:352:ALA:HB3	1.87	0.55
1:B:20:ALA:O	1:B:23:PHE:N	2.37	0.55
1:B:49:PRO:CD	1:B:67:MET:HE2	2.35	0.55
1:B:363:PRO:HB2	1:B:472:TRP:CD1	2.42	0.55
1:A:210:LEU:O	1:A:214:GLU:HB2	2.07	0.55
1:A:243:LYS:HB3	1:A:246:ILE:HD13	1.88	0.55
1:B:208:SER:O	1:B:209:ALA:C	2.49	0.55
1:B:463:ASN:HA	1:B:466:ARG:HG3	1.88	0.55
1:A:363:PRO:HB2	1:A:472:TRP:CD1	2.41	0.55
1:B:106:LEU:O	1:B:109:ALA:HB3	2.07	0.55
1:B:160:LYS:CD	1:B:189:ASN:HD21	2.19	0.55
1:B:230:CYS:HB3	1:B:277:PRO:CD	2.34	0.55
1:A:242:VAL:HG12	1:A:317:THR:CG2	2.37	0.55
1:A:90:GLN:CG	1:A:91:ILE:N	2.70	0.55
1:B:126:TRP:HD1	1:B:127:LEU:O	1.89	0.55
1:B:242:VAL:CG1	1:B:317:THR:HB	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LEU:O	1:A:282:ALA:HB3	2.07	0.55
1:B:328:VAL:HG22	1:B:352:ALA:HB3	1.89	0.55
1:B:407:PHE:HA	1:B:524:TRP:NE1	2.21	0.55
1:B:50:THR:HG23	1:B:63:TRP:CZ2	2.41	0.55
1:B:182:PHE:O	1:B:201:ILE:HG13	2.07	0.55
1:B:304:GLU:CD	1:B:304:GLU:N	2.64	0.55
1:A:303:ILE:HA	1:A:463:ASN:HD21	1.71	0.55
1:A:385:PHE:O	1:A:387:GLU:N	2.40	0.55
1:B:38:LEU:O	1:B:40:ALA:N	2.40	0.55
1:A:12:GLY:HA3	1:A:18:SER:OG	2.07	0.55
1:A:125:ASN:HD22	1:A:152:GLU:HB3	1.72	0.55
1:A:463:ASN:HA	1:A:466:ARG:HG3	1.87	0.55
1:A:511:PRO:C	1:A:512:PHE:CG	2.85	0.55
1:B:468:THR:HA	3:B:1005:HOH:O	2.07	0.55
1:A:512:PHE:O	1:A:513:LEU:C	2.49	0.54
1:B:279:LEU:O	1:B:282:ALA:HB3	2.07	0.54
1:B:333:ASP:OD2	1:B:523:HIS:NE2	2.36	0.54
1:A:281:GLN:O	1:A:282:ALA:C	2.49	0.54
1:A:385:PHE:O	1:A:386:GLN:C	2.49	0.54
1:A:482:LYS:HB2	1:B:62:GLN:HE22	1.72	0.54
1:B:206:THR:O	1:B:207:ALA:CB	2.55	0.54
1:B:265:PHE:CD1	1:B:265:PHE:C	2.85	0.54
1:A:155:GLN:C	1:A:157:GLY:H	2.15	0.54
1:B:242:VAL:HG12	1:B:317:THR:CG2	2.37	0.54
1:A:428:LEU:O	1:A:431:THR:CB	2.55	0.54
1:B:214:GLU:OE1	1:B:214:GLU:O	2.26	0.54
1:A:177:PRO:O	1:A:198:MET:HB3	2.07	0.54
1:A:202:LEU:O	1:A:203:VAL:CB	2.56	0.54
1:A:381:TYR:CE1	1:A:382:GLN:HG3	2.42	0.54
1:B:58:ILE:HG13	1:B:58:ILE:O	2.07	0.54
1:B:107:GLN:HG2	1:B:225:PRO:HG2	1.90	0.54
1:B:177:PRO:O	1:B:197:GLY:O	2.25	0.54
1:B:194:ARG:HB2	1:B:200:THR:HG21	1.88	0.54
1:B:215:LYS:O	1:B:219:THR:O	2.25	0.54
1:B:332:HIS:HB2	1:B:356:LEU:HB2	1.90	0.54
1:A:499:ARG:HB3	1:A:501:GLU:OE2	2.08	0.54
1:B:270:PHE:CD2	1:B:448:PHE:CD2	2.95	0.54
1:B:362:PRO:HG2	1:B:509:TRP:CE2	2.42	0.54
1:B:512:PHE:O	1:B:513:LEU:C	2.49	0.54
1:A:92:PHE:O	1:A:92:PHE:HD1	1.90	0.54
1:A:209:ALA:O	1:A:213:LEU:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:LEU:O	1:A:541:LEU:CD1	2.54	0.54
1:B:193:ALA:HB1	1:B:198:MET:HG3	1.90	0.54
1:B:205:ASN:OD1	1:B:207:ALA:O	2.26	0.54
1:B:272:TRP:O	1:B:274:TYR:N	2.41	0.54
1:B:286:VAL:C	1:B:287:LEU:HD12	2.32	0.54
1:A:53:LEU:HB3	1:A:58:ILE:HD12	1.90	0.54
1:A:101:ILE:HG22	1:A:102:ASN:N	2.23	0.54
1:B:182:PHE:C	1:B:183:LEU:HG	2.33	0.54
1:B:183:LEU:HD23	1:B:201:ILE:CD1	2.21	0.54
1:B:376:ILE:H	1:B:376:ILE:CD1	2.16	0.54
1:A:60:PHE:O	1:A:63:TRP:HB3	2.08	0.54
1:B:32:LEU:CD2	1:B:37:LEU:HG	2.38	0.54
1:B:438:SER:C	1:B:440:ILE:H	2.16	0.54
1:A:101:ILE:CG2	1:A:102:ASN:N	2.71	0.53
1:A:111:ALA:O	1:A:114:LYS:N	2.40	0.53
1:B:61:SER:OG	1:B:129:ASP:OD1	2.26	0.53
1:B:180:VAL:O	1:B:199:VAL:HG23	2.09	0.53
1:A:348:GLU:HA	1:B:133:ARG:HD2	1.90	0.53
1:A:360:PHE:CB	1:A:506:MET:HE3	2.38	0.53
1:B:50:THR:HA	1:B:63:TRP:HE1	1.74	0.53
1:B:183:LEU:HB2	1:B:203:VAL:HG23	1.90	0.53
1:B:325:PRO:HA	1:B:349:ARG:NH1	2.23	0.53
1:B:381:TYR:N	1:B:418:VAL:O	2.29	0.53
1:A:15:ALA:HB1	1:A:139:MET:HE1	1.89	0.53
1:A:117:PHE:CD1	1:A:117:PHE:N	2.75	0.53
1:A:122:VAL:HA	1:A:151:ILE:HB	1.91	0.53
1:A:433:GLU:HA	1:A:433:GLU:OE1	2.08	0.53
1:B:61:SER:O	1:B:65:PRO:HD2	2.09	0.53
1:A:13:VAL:HG22	1:A:203:VAL:HG21	1.90	0.53
1:A:263:HIS:O	1:A:335:ALA:HB2	2.09	0.53
1:A:286:VAL:C	1:A:287:LEU:HD12	2.33	0.53
1:B:173:LEU:O	1:B:174:LYS:HB2	2.08	0.53
1:B:173:LEU:HD22	1:B:173:LEU:H	1.73	0.53
1:B:381:TYR:CD2	1:B:418:VAL:HG12	2.44	0.53
1:A:92:PHE:O	1:A:94:GLN:N	2.42	0.53
1:A:205:ASN:H	1:A:205:ASN:ND2	1.83	0.53
1:A:255:SER:O	1:A:256:GLY:O	2.27	0.53
1:A:300:PRO:CG	1:A:305:GLU:HG2	2.39	0.53
1:A:401:ARG:O	1:A:402:THR:C	2.49	0.53
1:A:482:LYS:N	1:B:62:GLN:HE22	2.06	0.53
1:B:16:LEU:HD23	1:B:102:ASN:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ALA:O	1:A:112:LEU:HD12	2.08	0.53
1:A:125:ASN:N	1:A:153:SER:OG	2.42	0.53
1:A:272:TRP:O	1:A:274:TYR:N	2.41	0.53
1:B:124:ASN:HA	1:B:153:SER:CB	2.38	0.53
1:B:32:LEU:HD21	1:B:82:LEU:HD11	1.90	0.53
1:B:72:ARG:CD	1:B:73:LYS:NZ	2.72	0.53
1:B:232:PRO:HG2	1:B:233:ASN:ND2	2.24	0.53
1:B:488:LEU:HD13	1:B:490:VAL:HG23	1.90	0.53
1:B:499:ARG:HB3	1:B:501:GLU:OE2	2.07	0.53
1:A:515:ARG:HH11	1:A:515:ARG:HG2	1.70	0.53
1:B:381:TYR:CE2	1:B:418:VAL:HG12	2.44	0.53
1:B:513:LEU:HD23	1:B:514:LYS:O	2.09	0.53
1:B:515:ARG:HH11	1:B:515:ARG:HG2	1.71	0.53
1:B:523:HIS:CD2	2:B:1200:CIU:HC41	2.44	0.53
1:A:183:LEU:HA	1:A:201:ILE:O	2.09	0.53
1:B:40:ALA:HB2	1:B:71:TYR:OH	2.09	0.53
1:B:385:PHE:O	1:B:387:GLU:N	2.42	0.53
1:A:270:PHE:CD2	1:A:448:PHE:CD2	2.97	0.52
1:B:300:PRO:CG	1:B:305:GLU:HG2	2.39	0.52
1:A:52:GLN:CA	1:A:55:LYS:HD2	2.39	0.52
1:A:249:HIS:ND1	1:A:296:ASP:HB2	2.23	0.52
1:B:118:THR:CA	1:B:148:ASP:OD2	2.57	0.52
1:B:469:GLU:HG3	1:B:473:LYS:NZ	2.23	0.52
1:A:256:GLY:N	1:A:285:ARG:HB2	2.24	0.52
1:A:482:LYS:CB	1:B:62:GLN:HE22	2.21	0.52
1:B:475:SER:C	1:B:477:LYS:H	2.18	0.52
1:B:511:PRO:C	1:B:512:PHE:CG	2.87	0.52
1:A:162:GLU:O	1:A:164:GLN:N	2.42	0.52
1:A:360:PHE:HB2	1:A:506:MET:HE3	1.90	0.52
1:B:64:VAL:O	1:B:65:PRO:C	2.50	0.52
1:B:112:LEU:HB3	1:B:117:PHE:CD1	2.44	0.52
1:A:206:THR:O	1:A:207:ALA:HB2	2.09	0.52
1:B:20:ALA:O	1:B:22:ALA:N	2.43	0.52
1:B:156:VAL:HG23	1:B:157:GLY:N	2.24	0.52
1:B:191:LYS:HB3	1:B:192:PRO:HD3	1.92	0.52
1:A:213:LEU:O	1:A:216:VAL:HB	2.10	0.52
1:A:407:PHE:HA	1:A:524:TRP:NE1	2.24	0.52
1:B:64:VAL:CB	1:B:65:PRO:CD	2.87	0.52
1:B:230:CYS:HB3	1:B:277:PRO:CG	2.39	0.52
1:B:270:PHE:CE1	1:B:273:ARG:HD3	2.45	0.52
1:B:458:PHE:HB3	1:B:462:LEU:CD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ASP:HB2	1:A:160:LYS:HZ3	1.74	0.52
1:A:94:GLN:O	1:A:97:ALA:N	2.43	0.52
1:A:136:LEU:HD12	1:A:140:MET:HG2	1.91	0.52
1:A:119:THR:OG1	1:A:147:PHE:HA	2.10	0.52
1:B:380:ASN:O	1:B:381:TYR:C	2.53	0.52
1:B:459:ARG:HH11	1:B:459:ARG:HG2	1.75	0.52
1:A:8:PHE:HE1	1:A:147:PHE:HE2	1.58	0.51
1:A:52:GLN:OE1	1:A:53:LEU:N	2.43	0.51
1:A:205:ASN:ND2	1:A:207:ALA:H	2.09	0.51
1:B:4:ARG:HD2	1:B:179:GLU:HB2	1.91	0.51
1:B:13:VAL:CG2	1:B:14:LEU:N	2.72	0.51
1:B:134:ASP:O	1:B:137:ALA:N	2.43	0.51
1:B:523:HIS:CD2	1:B:524:TRP:CZ3	2.98	0.51
1:B:54:MET:CB	1:B:159:ILE:HG21	2.39	0.51
1:B:263:HIS:O	1:B:335:ALA:HB2	2.10	0.51
1:B:401:ARG:O	1:B:402:THR:C	2.54	0.51
1:A:136:LEU:O	1:A:137:ALA:C	2.53	0.51
1:B:73:LYS:C	1:B:75:SER:H	2.19	0.51
1:B:247:ARG:HG2	1:B:248:LEU:N	2.26	0.51
1:A:17:PRO:HD2	1:A:99:ARG:HA	1.92	0.51
1:A:115:LYS:NZ	1:A:218:GLY:HA3	2.25	0.51
1:A:475:SER:C	1:A:477:LYS:H	2.18	0.51
1:B:42:GLN:HB2	1:B:186:PHE:HE1	1.72	0.51
1:B:72:ARG:HD3	1:B:73:LYS:NZ	2.25	0.51
1:B:303:ILE:HA	1:B:463:ASN:HD21	1.74	0.51
1:B:515:ARG:CG	1:B:515:ARG:NH1	2.59	0.51
1:A:380:ASN:O	1:A:381:TYR:C	2.53	0.51
1:B:13:VAL:HG22	1:B:14:LEU:N	2.25	0.51
1:B:86:PHE:CE1	1:B:87:SER:O	2.63	0.51
1:A:106:LEU:O	1:A:106:LEU:CD2	2.56	0.51
1:A:276:ILE:HG22	1:A:277:PRO:HD3	1.93	0.51
1:B:72:ARG:HB2	1:B:72:ARG:NH1	2.25	0.51
1:B:289:ILE:CG2	1:B:290:ASP:N	2.73	0.51
1:A:380:ASN:HB2	1:A:419:HIS:HA	1.93	0.51
1:A:459:ARG:HG2	1:A:459:ARG:HH11	1.75	0.51
1:B:162:GLU:HB3	1:B:164:GLN:HG2	1.92	0.51
1:B:303:ILE:CD1	1:B:463:ASN:ND2	2.68	0.51
1:A:113:LYS:NZ	1:A:146:HIS:HA	2.26	0.51
1:A:124:ASN:ND2	1:A:160:LYS:HB2	2.26	0.51
1:A:259:LEU:CD1	1:A:279:LEU:HD13	2.41	0.51
1:A:50:THR:HG23	1:A:63:TRP:CZ2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:PRO:HB2	1:A:301:PRO:CD	2.41	0.51
1:B:191:LYS:CB	1:B:192:PRO:HD3	2.40	0.51
1:B:299:SER:CB	1:B:456:THR:HG22	2.40	0.51
1:B:417:ALA:H	1:B:427:ILE:HG22	1.75	0.51
1:B:473:LYS:NZ	1:B:473:LYS:HB2	2.25	0.51
1:A:52:GLN:HA	1:A:55:LYS:HD2	1.92	0.51
1:B:72:ARG:HH11	1:B:72:ARG:HB2	1.75	0.51
1:A:90:GLN:HG3	1:A:91:ILE:H	1.75	0.50
1:A:299:SER:CB	1:A:456:THR:HG22	2.40	0.50
1:A:325:PRO:O	1:B:137:ALA:HB1	2.11	0.50
1:A:337:VAL:CG2	2:A:1100:CIU:H12	2.41	0.50
1:B:385:PHE:O	1:B:386:GLN:C	2.53	0.50
1:B:420:LYS:O	1:B:424:ILE:CD1	2.59	0.50
1:A:207:ALA:O	1:A:210:LEU:HB2	2.11	0.50
1:B:276:ILE:HG22	1:B:277:PRO:HD3	1.93	0.50
1:A:124:ASN:OD1	1:A:160:LYS:N	2.45	0.50
1:A:362:PRO:HG2	1:A:509:TRP:CE2	2.46	0.50
1:B:54:MET:HB2	1:B:159:ILE:HG21	1.92	0.50
1:A:117:PHE:N	1:A:117:PHE:HD1	2.10	0.50
1:A:291:MET:HE1	1:A:315:MET:CE	2.41	0.50
1:A:303:ILE:C	1:A:305:GLU:N	2.67	0.50
1:A:446:ILE:O	1:A:450:ILE:HG13	2.12	0.50
1:A:458:PHE:HB3	1:A:462:LEU:CD1	2.41	0.50
1:B:89:SER:OG	1:B:90:GLN:N	2.44	0.50
1:B:127:LEU:N	1:B:127:LEU:CD1	2.66	0.50
1:B:361:MET:HE1	2:B:1200:CIU:I4	2.81	0.50
1:A:5:VAL:O	1:A:180:VAL:HA	2.11	0.50
1:A:106:LEU:HD23	1:A:110:ILE:HD11	1.92	0.50
1:A:145:GLN:HE22	1:B:321:LYS:HD2	1.76	0.50
1:A:319:LEU:N	1:A:319:LEU:HD23	2.27	0.50
1:B:44:GLU:O	1:B:46:PRO:HD3	2.11	0.50
1:A:211:ARG:O	1:A:215:LYS:N	2.45	0.50
1:A:12:GLY:HA2	1:A:15:ALA:O	2.12	0.50
1:A:473:LYS:NZ	1:A:473:LYS:HB2	2.27	0.50
1:B:270:PHE:CD2	1:B:448:PHE:HD2	2.28	0.50
1:A:106:LEU:HD23	1:A:106:LEU:C	2.37	0.50
1:B:193:ALA:C	1:B:195:ASP:H	2.19	0.50
1:A:108:ALA:O	1:A:111:ALA:HB3	2.11	0.49
1:A:145:GLN:NE2	1:B:321:LYS:HD2	2.27	0.49
1:A:376:ILE:H	1:A:376:ILE:CD1	2.13	0.49
1:B:202:LEU:HD12	1:B:204:HIS:HB2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:LEU:O	1:B:212:GLU:N	2.45	0.49
1:B:289:ILE:HG22	1:B:290:ASP:N	2.26	0.49
1:A:106:LEU:CD2	1:A:106:LEU:C	2.86	0.49
1:A:307:ALA:O	1:A:311:LEU:HG	2.12	0.49
1:A:417:ALA:O	1:A:421:ALA:HB2	2.12	0.49
1:B:8:PHE:O	1:B:121:ILE:HA	2.11	0.49
1:B:91:ILE:O	1:B:91:ILE:CG1	2.61	0.49
1:B:212:GLU:O	1:B:214:GLU:N	2.44	0.49
1:A:190:LEU:HB3	1:A:200:THR:CG2	2.43	0.49
1:A:407:PHE:C	1:A:408:ARG:HG2	2.37	0.49
1:B:128:ASP:O	1:B:133:ARG:HG3	2.12	0.49
1:B:309:GLU:HA	1:B:474:TRP:CZ2	2.47	0.49
1:B:319:LEU:N	1:B:319:LEU:HD23	2.27	0.49
1:B:374:ARG:HG2	1:B:383:LEU:HD11	1.95	0.49
1:B:526:GLN:NE2	1:B:527:ILE:CD1	2.75	0.49
1:B:190:LEU:HD12	1:B:202:LEU:HD23	1.94	0.49
1:B:249:HIS:ND1	1:B:296:ASP:HB2	2.28	0.49
1:B:406:PHE:CD2	2:B:1200:CIU:HC12	2.47	0.49
1:A:180:VAL:O	1:A:180:VAL:CG2	2.61	0.49
1:B:86:PHE:CG	1:B:87:SER:N	2.81	0.49
1:B:136:LEU:O	1:B:136:LEU:HD12	2.13	0.49
1:B:160:LYS:HA	1:B:165:ILE:HD11	1.94	0.49
1:B:515:ARG:HG3	1:B:515:ARG:NH1	2.22	0.49
1:A:165:ILE:O	1:A:169:LEU:N	2.43	0.49
1:A:238:GLY:HA2	1:B:238:GLY:HA2	1.93	0.49
1:B:8:PHE:HA	1:B:183:LEU:HD12	1.93	0.49
1:B:126:TRP:HA	1:B:154:CYS:CB	2.43	0.49
1:A:173:LEU:HD22	1:A:173:LEU:N	2.18	0.49
1:A:215:LYS:HG2	1:A:220:GLN:CA	2.42	0.49
1:B:32:LEU:HD12	1:B:32:LEU:H	1.78	0.49
1:B:20:ALA:O	1:B:21:GLY:C	2.55	0.49
1:A:8:PHE:CB	1:A:183:LEU:HD11	2.43	0.49
1:A:247:ARG:HG2	1:A:248:LEU:N	2.28	0.49
1:A:302:GLU:HB3	1:A:304:GLU:OE1	2.11	0.49
1:B:92:PHE:C	1:B:94:GLN:N	2.67	0.49
1:B:210:LEU:C	1:B:212:GLU:H	2.20	0.49
1:B:381:TYR:CG	1:B:382:GLN:N	2.81	0.49
1:A:187:GLY:HA2	1:A:190:LEU:CD1	2.33	0.48
1:A:207:ALA:O	1:A:208:SER:HB3	2.12	0.48
1:A:242:VAL:HG12	1:A:317:THR:CB	2.43	0.48
1:A:440:ILE:HD12	1:A:440:ILE:HA	1.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:LEU:HD13	1:B:61:SER:HB2	1.93	0.48
1:B:41:TYR:CE1	1:B:54:MET:HE1	2.48	0.48
1:B:293:GLY:O	1:B:299:SER:HB2	2.13	0.48
1:B:408:ARG:O	1:B:524:TRP:HD1	1.95	0.48
1:A:10:LEU:C	1:A:12:GLY:N	2.70	0.48
1:A:272:TRP:C	1:A:274:TYR:H	2.21	0.48
1:A:326:GLN:NE2	1:B:134:ASP:CA	2.76	0.48
1:B:176:LYS:HB3	1:B:178:ASN:HD22	1.76	0.48
1:B:328:VAL:HG12	1:B:330:ILE:HD11	1.93	0.48
1:A:381:TYR:CG	1:A:382:GLN:N	2.81	0.48
1:B:5:VAL:HB	1:B:118:THR:OG1	2.13	0.48
1:B:103:ARG:CB	1:B:104:PRO:HD3	2.23	0.48
1:B:106:LEU:HD21	1:B:146:HIS:HD2	1.78	0.48
1:B:306:TYR:CD1	1:B:306:TYR:N	2.82	0.48
1:B:350:VAL:HG11	1:B:353:VAL:HG22	1.94	0.48
1:B:469:GLU:O	1:B:472:TRP:HB3	2.12	0.48
1:B:63:TRP:CG	1:B:63:TRP:O	2.67	0.48
1:B:93:SER:O	1:B:132:LYS:HG3	2.13	0.48
1:B:101:ILE:CD1	1:B:143:LEU:HD21	2.44	0.48
1:B:194:ARG:HB2	1:B:200:THR:CG2	2.43	0.48
1:B:272:TRP:C	1:B:274:TYR:H	2.21	0.48
1:B:385:PHE:HE1	1:B:427:ILE:HD11	1.78	0.48
1:A:63:TRP:O	1:A:63:TRP:CE3	2.66	0.48
1:A:270:PHE:CD2	1:A:448:PHE:HD2	2.32	0.48
1:B:256:GLY:N	1:B:285:ARG:HB2	2.28	0.48
1:A:182:PHE:CD1	1:A:183:LEU:N	2.81	0.48
1:A:211:ARG:HB2	1:A:215:LYS:NZ	2.27	0.48
1:A:270:PHE:CE1	1:A:273:ARG:HD3	2.49	0.48
1:A:333:ASP:OD2	1:A:523:HIS:NE2	2.36	0.48
1:A:380:ASN:HB3	1:A:418:VAL:O	2.14	0.48
1:B:340:TRP:CZ2	1:B:489:MET:HG2	2.49	0.48
1:B:446:ILE:O	1:B:450:ILE:HG13	2.14	0.48
1:A:102:ASN:ND2	1:A:105:MET:HB2	2.28	0.48
1:A:293:GLY:O	1:A:299:SER:HB2	2.14	0.48
1:A:459:ARG:HH11	1:A:459:ARG:CG	2.27	0.48
1:B:30:LEU:CB	1:B:32:LEU:HD13	2.38	0.48
1:B:131:ASP:C	1:B:133:ARG:N	2.68	0.48
1:A:13:VAL:HG22	1:A:203:VAL:CB	2.44	0.48
1:A:136:LEU:HD12	1:A:140:MET:CG	2.44	0.48
1:A:181:VAL:HG23	1:A:182:PHE:N	2.29	0.48
1:A:48:GLY:O	1:A:52:GLN:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:HIS:ND1	1:A:333:ASP:HB2	2.28	0.48
1:A:350:VAL:HG11	1:A:353:VAL:HG22	1.95	0.48
1:A:396:GLU:O	1:A:397:LYS:C	2.57	0.48
1:B:10:LEU:O	1:B:15:ALA:HB3	2.13	0.48
1:B:458:PHE:O	1:B:459:ARG:C	2.57	0.48
1:A:248:LEU:HA	1:A:297:SER:HB3	1.95	0.48
1:B:25:ARG:HA	1:B:28:GLU:HB2	1.94	0.48
1:B:259:LEU:CD1	1:B:279:LEU:HD13	2.43	0.48
1:A:214:GLU:OE1	1:A:217:THR:HG21	2.14	0.47
1:A:123:THR:HA	1:A:160:LYS:CE	2.44	0.47
1:B:38:LEU:HD22	1:B:42:GLN:HB3	1.95	0.47
1:B:149:PHE:CE2	1:B:173:LEU:HD13	2.50	0.47
1:B:302:GLU:HB3	1:B:304:GLU:OE1	2.14	0.47
1:B:340:TRP:NE1	1:B:355:SER:HB2	2.29	0.47
1:B:381:TYR:CE1	1:B:382:GLN:HG3	2.49	0.47
1:A:140:MET:HE3	1:A:140:MET:HA	1.96	0.47
1:A:195:ASP:O	1:A:196:MET:C	2.58	0.47
1:A:271:SER:C	1:A:273:ARG:H	2.23	0.47
1:B:126:TRP:CD1	1:B:126:TRP:C	2.92	0.47
1:B:305:GLU:HB3	1:B:306:TYR:CD1	2.49	0.47
1:B:416:ILE:HG23	1:B:417:ALA:N	2.29	0.47
1:A:58:ILE:HG22	1:A:62:GLN:CD	2.40	0.47
1:A:291:MET:HA	1:A:291:MET:CE	2.45	0.47
1:A:340:TRP:NE1	1:A:355:SER:HB2	2.28	0.47
1:B:74:SER:O	1:B:75:SER:O	2.32	0.47
1:B:115:LYS:HE3	1:B:219:THR:HG23	1.96	0.47
1:B:178:ASN:CG	1:B:179:GLU:N	2.73	0.47
1:B:231:ASN:OD1	1:B:270:PHE:CE1	2.62	0.47
1:A:301:PRO:CD	1:A:302:GLU:N	2.78	0.47
1:B:76:LYS:HA	1:B:80:ALA:O	2.14	0.47
1:B:158:MET:CB	1:B:164:GLN:HB2	2.43	0.47
1:B:219:THR:HB	1:B:220:GLN:H	1.32	0.47
1:B:223:GLU:N	1:B:223:GLU:OE2	2.46	0.47
1:B:499:ARG:CB	1:B:501:GLU:OE2	2.63	0.47
1:A:122:VAL:HG11	1:A:169:LEU:HD11	1.96	0.47
1:A:132:LYS:O	1:A:135:SER:HB2	2.14	0.47
1:A:252:GLU:HG2	3:B:1013:HOH:O	2.13	0.47
1:B:16:LEU:O	1:B:100:SER:N	2.45	0.47
1:B:202:LEU:CD1	1:B:204:HIS:CD2	2.97	0.47
1:B:300:PRO:HB2	1:B:301:PRO:CD	2.45	0.47
1:B:428:LEU:CD1	1:B:428:LEU:N	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:PRO:O	1:A:198:MET:CB	2.63	0.47
1:A:469:GLU:O	1:A:472:TRP:HB3	2.15	0.47
1:A:501:GLU:O	1:A:504:LYS:HG2	2.15	0.47
1:B:229:PRO:HB3	1:B:274:TYR:CD1	2.49	0.47
1:B:270:PHE:O	1:B:273:ARG:HB3	2.14	0.47
1:A:361:MET:HB2	1:A:361:MET:HE3	1.71	0.47
1:B:28:GLU:C	1:B:30:LEU:N	2.72	0.47
1:A:103:ARG:H	1:A:103:ARG:HG2	1.19	0.47
1:A:303:ILE:O	1:A:304:GLU:C	2.58	0.47
1:A:347:PRO:O	1:B:133:ARG:CD	2.63	0.47
1:B:490:VAL:HA	1:B:516:GLY:O	2.15	0.47
1:A:416:ILE:HG23	1:A:417:ALA:N	2.30	0.46
1:A:50:THR:HA	1:A:63:TRP:NE1	2.26	0.46
1:A:52:GLN:HB3	1:A:55:LYS:HD2	1.96	0.46
1:A:92:PHE:C	1:A:92:PHE:CD1	2.93	0.46
1:A:163:PRO:HA	1:A:166:TYR:CD1	2.50	0.46
1:A:511:PRO:O	1:A:512:PHE:CG	2.69	0.46
1:B:8:PHE:HD1	1:B:120:CYS:O	1.99	0.46
1:B:168:PHE:C	1:B:168:PHE:CD2	2.92	0.46
1:A:53:LEU:HA	1:A:58:ILE:HG13	1.98	0.46
1:A:103:ARG:N	1:A:104:PRO:HD2	2.31	0.46
1:A:128:ASP:C	1:A:130:GLY:H	2.23	0.46
1:A:340:TRP:CZ2	1:A:489:MET:HG2	2.50	0.46
1:A:408:ARG:O	1:A:524:TRP:HD1	1.99	0.46
1:A:523:HIS:CD2	1:A:524:TRP:CZ3	3.02	0.46
1:B:16:LEU:CB	1:B:17:PRO:CA	2.92	0.46
1:B:177:PRO:C	1:B:197:GLY:O	2.58	0.46
1:B:193:ALA:HA	1:B:196:MET:HG3	1.96	0.46
1:B:407:PHE:C	1:B:408:ARG:HG2	2.39	0.46
1:A:101:ILE:HD13	1:A:106:LEU:CD1	2.44	0.46
1:A:123:THR:CA	1:A:160:LYS:HE2	2.45	0.46
1:A:137:ALA:O	1:A:140:MET:HB2	2.16	0.46
1:B:28:GLU:O	1:B:30:LEU:N	2.48	0.46
1:B:124:ASN:HA	1:B:153:SER:OG	2.15	0.46
1:B:232:PRO:CG	1:B:233:ASN:HD22	2.29	0.46
1:B:380:ASN:HB3	1:B:418:VAL:O	2.15	0.46
1:A:259:LEU:HD11	1:A:279:LEU:HD13	1.97	0.46
1:A:489:MET:HE3	1:A:490:VAL:H	1.78	0.46
1:A:515:ARG:CG	1:A:515:ARG:NH1	2.60	0.46
1:B:271:SER:C	1:B:273:ARG:H	2.23	0.46
1:B:434:ASP:N	1:B:435:PRO:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:THR:HG23	1:B:445:GLU:OE1	2.15	0.46
1:B:459:ARG:HH11	1:B:459:ARG:CG	2.28	0.46
1:A:53:LEU:CD1	1:A:54:MET:N	2.78	0.46
1:A:180:VAL:HG23	1:A:198:MET:CE	2.46	0.46
1:A:400:SER:O	1:A:404:LYS:HG2	2.16	0.46
1:A:489:MET:CE	1:A:490:VAL:N	2.78	0.46
1:B:119:THR:H	1:B:148:ASP:CG	2.24	0.46
1:A:294:TYR:CZ	1:A:461:PRO:HB3	2.51	0.46
1:A:499:ARG:CB	1:A:501:GLU:OE2	2.63	0.46
1:B:10:LEU:HD12	1:B:15:ALA:HB2	1.98	0.46
1:B:242:VAL:HG12	1:B:317:THR:CB	2.46	0.46
1:B:396:GLU:O	1:B:397:LYS:C	2.58	0.46
1:B:431:THR:O	1:B:432:PRO:C	2.59	0.46
1:A:262:CYS:C	1:A:272:TRP:HZ2	2.24	0.46
1:B:25:ARG:HA	1:B:28:GLU:CB	2.46	0.46
1:B:48:GLY:HA3	1:B:49:PRO:HD3	1.71	0.46
1:B:248:LEU:HA	1:B:297:SER:HB3	1.98	0.46
1:A:374:ARG:HG2	1:A:383:LEU:HD11	1.97	0.46
1:A:450:ILE:O	1:A:454:LYS:HG2	2.16	0.46
1:A:529:LYS:HA	1:A:529:LYS:HD3	1.74	0.46
1:B:161:PRO:CB	1:B:192:PRO:HG2	2.46	0.46
1:A:305:GLU:HB3	1:A:306:TYR:CD1	2.51	0.46
1:A:416:ILE:CG2	1:A:417:ALA:N	2.79	0.46
1:B:10:LEU:CD1	1:B:15:ALA:HB2	2.46	0.46
1:B:332:HIS:ND1	1:B:333:ASP:HB2	2.31	0.46
1:B:416:ILE:HG23	1:B:427:ILE:CG2	2.45	0.46
1:A:205:ASN:CG	1:A:207:ALA:H	2.23	0.45
1:A:272:TRP:C	1:A:274:TYR:N	2.73	0.45
1:B:77:ALA:O	1:B:78:CYS:HB2	2.16	0.45
1:B:214:GLU:O	1:B:215:LYS:C	2.58	0.45
1:B:294:TYR:CZ	1:B:461:PRO:HB3	2.51	0.45
1:B:408:ARG:HH21	1:B:412:GLU:HG2	1.81	0.45
1:A:126:TRP:CD1	1:A:126:TRP:C	2.94	0.45
1:A:368:SER:HB3	1:A:371:LYS:CG	2.46	0.45
1:A:513:LEU:HD23	1:A:513:LEU:C	2.41	0.45
1:B:303:ILE:C	1:B:305:GLU:N	2.70	0.45
1:B:378:VAL:HG22	1:B:418:VAL:HG11	1.98	0.45
1:A:129:ASP:OD2	1:B:484:LEU:HD12	2.16	0.45
1:A:134:ASP:O	1:A:135:SER:C	2.59	0.45
1:A:303:ILE:CD1	1:A:463:ASN:ND2	2.74	0.45
1:A:458:PHE:O	1:A:459:ARG:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:LEU:CD1	1:B:129:ASP:OD2	2.50	0.45
1:B:14:LEU:HD22	1:B:121:ILE:HG21	1.98	0.45
1:B:364:ASP:OD1	1:B:364:ASP:N	2.50	0.45
1:B:400:SER:O	1:B:404:LYS:HG2	2.17	0.45
1:A:60:PHE:CE1	1:A:92:PHE:CZ	3.04	0.45
1:A:442:THR:HG23	1:A:445:GLU:OE1	2.16	0.45
1:A:490:VAL:HA	1:A:516:GLY:O	2.17	0.45
1:B:28:GLU:C	1:B:30:LEU:H	2.24	0.45
1:B:416:ILE:CG2	1:B:417:ALA:N	2.79	0.45
1:A:7:ALA:O	1:A:182:PHE:HA	2.16	0.45
1:A:309:GLU:HA	1:A:474:TRP:CZ2	2.51	0.45
1:A:512:PHE:N	1:A:512:PHE:CD1	2.85	0.45
1:B:178:ASN:C	1:B:180:VAL:H	2.25	0.45
1:B:291:MET:HE1	1:B:315:MET:CE	2.43	0.45
1:B:419:HIS:ND1	1:B:419:HIS:N	2.64	0.45
1:B:537:LEU:O	1:B:541:LEU:CD1	2.60	0.45
1:A:530:PRO:O	1:A:531:THR:C	2.59	0.45
1:B:134:ASP:C	1:B:136:LEU:N	2.75	0.45
1:A:369:PRO:O	1:A:372:VAL:HG13	2.17	0.45
1:A:526:GLN:NE2	1:A:527:ILE:CD1	2.80	0.45
1:B:119:THR:HB	1:B:147:PHE:CD2	2.52	0.45
1:B:187:GLY:C	1:B:189:ASN:H	2.24	0.45
1:B:307:ALA:O	1:B:311:LEU:HG	2.16	0.45
1:B:380:ASN:HB2	1:B:419:HIS:HA	1.96	0.45
1:B:476:CYS:HA	1:B:479:LEU:CD1	2.46	0.45
1:B:511:PRO:O	1:B:512:PHE:CG	2.70	0.45
1:A:207:ALA:HA	1:A:210:LEU:HB2	1.98	0.45
1:B:42:GLN:CB	1:B:186:PHE:CE1	2.97	0.45
1:B:270:PHE:CZ	1:B:273:ARG:HD3	2.52	0.45
1:B:526:GLN:HE22	1:B:527:ILE:HD11	1.81	0.45
1:A:168:PHE:CE2	1:A:172:THR:OG1	2.69	0.45
1:A:279:LEU:HD23	1:A:279:LEU:HA	1.79	0.45
1:A:306:TYR:CD1	1:A:306:TYR:N	2.85	0.45
1:B:50:THR:HA	1:B:63:TRP:NE1	2.30	0.45
1:B:132:LYS:HD3	1:B:132:LYS:H	1.81	0.45
1:B:272:TRP:C	1:B:274:TYR:N	2.73	0.45
1:A:4:ARG:HH21	1:A:179:GLU:CB	2.19	0.45
1:A:209:ALA:HA	1:A:212:GLU:HB2	1.99	0.45
1:A:336:GLY:HA2	1:A:339:VAL:HB	1.98	0.45
1:A:470:ARG:CA	1:A:473:LYS:NZ	2.71	0.45
1:A:483:ILE:C	1:A:484:LEU:HG	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ASP:O	1:B:13:VAL:HG22	2.17	0.45
1:B:27:GLU:HG2	1:B:37:LEU:HB2	1.99	0.45
1:B:229:PRO:CA	1:B:273:ARG:O	2.63	0.45
1:B:232:PRO:HG2	1:B:233:ASN:HD22	1.81	0.45
1:A:202:LEU:O	1:A:203:VAL:HG23	2.17	0.44
1:A:271:SER:HA	1:A:273:ARG:NH1	2.32	0.44
1:A:470:ARG:N	1:A:473:LYS:NZ	2.65	0.44
1:B:73:LYS:HA	1:B:73:LYS:HD3	1.65	0.44
1:B:173:LEU:O	1:B:174:LYS:CB	2.64	0.44
1:B:206:THR:O	1:B:207:ALA:HB3	2.17	0.44
1:A:58:ILE:HA	1:A:62:GLN:OE1	2.17	0.44
1:A:131:ASP:C	1:A:133:ARG:N	2.74	0.44
1:A:231:ASN:HB2	1:A:232:PRO:CB	2.46	0.44
1:A:312:CYS:SG	1:A:338:MET:HG3	2.57	0.44
1:A:515:ARG:HG3	1:A:515:ARG:NH1	2.25	0.44
1:A:177:PRO:O	1:A:198:MET:HA	2.17	0.44
1:B:24:ARG:O	1:B:27:GLU:HB2	2.18	0.44
1:B:150:LEU:HD12	1:B:150:LEU:HA	1.84	0.44
1:A:124:ASN:HA	1:A:153:SER:OG	2.18	0.44
1:A:173:LEU:H	1:A:173:LEU:CD2	2.20	0.44
1:A:215:LYS:HG2	1:A:220:GLN:HB3	1.99	0.44
1:A:339:VAL:HG13	1:A:353:VAL:HG13	1.97	0.44
1:A:469:GLU:C	1:A:473:LYS:NZ	2.75	0.44
1:B:82:LEU:HA	1:B:83:PRO:HD2	1.72	0.44
1:B:183:LEU:CB	1:B:203:VAL:HG23	2.47	0.44
1:B:208:SER:C	1:B:210:LEU:N	2.72	0.44
1:B:301:PRO:CD	1:B:302:GLU:N	2.78	0.44
1:B:404:LYS:HG3	1:B:435:PRO:HB2	1.99	0.44
1:B:202:LEU:HD11	1:B:204:HIS:CD2	2.52	0.44
1:B:293:GLY:HA2	1:B:299:SER:HA	2.00	0.44
1:B:428:LEU:N	1:B:428:LEU:HD13	2.32	0.44
1:B:523:HIS:HD2	1:B:524:TRP:CH2	2.36	0.44
1:A:476:CYS:HA	1:A:479:LEU:CD1	2.48	0.44
1:B:72:ARG:CG	1:B:73:LYS:HZ3	2.30	0.44
1:B:122:VAL:CB	1:B:151:ILE:CD1	2.94	0.44
1:B:265:PHE:HA	1:B:266:PRO:HA	1.80	0.44
1:B:336:GLY:HA2	1:B:339:VAL:HB	1.99	0.44
1:B:532:GLU:O	1:B:533:VAL:C	2.61	0.44
1:A:171:ASP:O	1:A:174:LYS:HG3	2.17	0.44
1:A:404:LYS:HG3	1:A:435:PRO:HB2	1.99	0.44
1:A:488:LEU:HD22	1:A:489:MET:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LYS:O	1:B:75:SER:N	2.51	0.44
1:A:305:GLU:O	1:A:310:LEU:HD23	2.18	0.44
1:A:372:VAL:O	1:A:376:ILE:HD11	2.18	0.44
1:A:380:ASN:OD1	1:A:422:THR:N	2.50	0.44
1:A:438:SER:C	1:A:440:ILE:N	2.75	0.44
1:B:91:ILE:O	1:B:91:ILE:HG12	2.17	0.44
1:B:160:LYS:CG	1:B:189:ASN:HD21	2.31	0.44
1:B:216:VAL:HG12	1:B:217:THR:N	2.32	0.44
1:B:530:PRO:O	1:B:531:THR:C	2.59	0.44
1:A:226:LEU:C	1:A:227:PRO:O	2.57	0.44
1:A:364:ASP:HA	1:A:365:PRO:HD2	1.84	0.44
1:B:5:VAL:O	1:B:180:VAL:HA	2.17	0.44
1:B:101:ILE:CG2	1:B:102:ASN:N	2.80	0.44
1:B:202:LEU:O	1:B:204:HIS:N	2.45	0.44
1:B:215:LYS:O	1:B:216:VAL:C	2.60	0.44
1:A:93:SER:O	1:A:132:LYS:HB2	2.17	0.43
1:A:159:ILE:HD13	1:A:160:LYS:C	2.42	0.43
1:B:32:LEU:CD2	1:B:36:PHE:HD2	2.31	0.43
1:B:306:TYR:HD2	1:B:464:TRP:CD1	2.36	0.43
1:A:143:LEU:O	1:A:144:SER:C	2.61	0.43
1:A:236:SER:HB2	1:B:322:LEU:HG	1.99	0.43
1:B:132:LYS:H	1:B:132:LYS:CD	2.31	0.43
1:B:158:MET:HG2	1:B:164:GLN:HB2	1.96	0.43
1:A:156:VAL:O	1:A:158:MET:N	2.51	0.43
1:A:205:ASN:OD1	1:A:208:SER:HB2	2.19	0.43
1:A:250:PHE:CD2	1:A:250:PHE:C	2.96	0.43
1:A:398:ASN:OD1	1:A:400:SER:HB3	2.18	0.43
1:A:404:LYS:HG2	1:A:404:LYS:H	1.37	0.43
1:B:291:MET:HA	1:B:291:MET:CE	2.49	0.43
1:B:440:ILE:HD12	1:B:440:ILE:HA	1.70	0.43
1:B:488:LEU:HD22	1:B:489:MET:N	2.33	0.43
1:A:102:ASN:ND2	1:A:105:MET:CB	2.81	0.43
1:A:135:SER:O	1:A:139:MET:HB3	2.18	0.43
1:A:138:GLN:O	1:A:139:MET:C	2.60	0.43
1:A:207:ALA:CA	1:A:210:LEU:HB2	2.49	0.43
1:A:308:MET:O	1:A:309:GLU:C	2.61	0.43
1:B:142:GLU:HG3	1:B:281:GLN:OE1	2.18	0.43
1:A:124:ASN:OD1	1:A:160:LYS:CB	2.58	0.43
1:A:162:GLU:C	1:A:164:GLN:H	2.26	0.43
1:A:265:PHE:HA	1:A:266:PRO:HA	1.81	0.43
1:A:368:SER:HB3	1:A:371:LYS:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ASP:O	1:B:136:LEU:N	2.51	0.43
1:B:375:SER:O	1:B:376:ILE:C	2.61	0.43
1:A:53:LEU:HD12	1:A:54:MET:N	2.32	0.43
1:A:59:THR:OG1	1:A:60:PHE:N	2.51	0.43
1:A:122:VAL:O	1:A:160:LYS:HE2	2.19	0.43
1:A:160:LYS:HA	1:A:161:PRO:HA	1.83	0.43
1:A:270:PHE:CZ	1:A:273:ARG:HD3	2.53	0.43
1:A:364:ASP:OD1	1:A:364:ASP:N	2.50	0.43
1:A:534:ASN:O	1:A:535:GLN:C	2.61	0.43
1:B:16:LEU:HA	1:B:17:PRO:C	2.44	0.43
1:B:61:SER:HA	1:B:64:VAL:CG2	2.48	0.43
1:B:190:LEU:O	1:B:191:LYS:C	2.61	0.43
1:B:271:SER:HA	1:B:273:ARG:NH1	2.34	0.43
1:B:414:GLY:O	1:B:415:PHE:O	2.35	0.43
1:B:501:GLU:H	1:B:501:GLU:HG3	1.42	0.43
1:B:537:LEU:HD23	1:B:537:LEU:HA	1.74	0.43
1:A:181:VAL:HB	1:A:199:VAL:HB	2.01	0.43
1:B:246:ILE:HD12	1:B:246:ILE:N	2.34	0.43
1:A:149:PHE:CD2	1:A:173:LEU:HD12	2.54	0.43
1:A:159:ILE:O	1:A:165:ILE:CD1	2.55	0.43
1:A:190:LEU:HD22	1:A:200:THR:HG22	1.98	0.43
1:A:313:LYS:O	1:A:316:VAL:HB	2.18	0.43
1:A:337:VAL:HG21	2:A:1100:CIU:H12	2.01	0.43
1:A:481:ARG:HA	1:B:62:GLN:OE1	2.18	0.43
1:A:501:GLU:H	1:A:501:GLU:HG3	1.42	0.43
1:B:32:LEU:HD23	1:B:36:PHE:HD2	1.84	0.43
1:B:50:THR:CA	1:B:63:TRP:HE1	2.31	0.43
1:B:281:GLN:C	1:B:283:GLY:N	2.73	0.43
1:B:501:GLU:O	1:B:504:LYS:HG2	2.19	0.43
1:A:170:LEU:HD21	1:A:177:PRO:HA	2.00	0.43
1:A:263:HIS:NE2	1:A:291:MET:CB	2.79	0.43
1:A:280:ALA:HA	1:A:284:PHE:O	2.18	0.43
1:A:533:VAL:O	1:A:537:LEU:HB2	2.19	0.43
1:B:162:GLU:HA	1:B:163:PRO:HD2	1.81	0.43
1:B:183:LEU:CB	1:B:203:VAL:CG2	2.96	0.43
1:B:361:MET:HE3	1:B:361:MET:HB2	1.74	0.43
1:B:424:ILE:HB	1:B:429:VAL:HG11	2.01	0.43
1:A:178:ASN:OD1	1:A:179:GLU:N	2.52	0.43
1:A:263:HIS:CD2	1:A:291:MET:H	2.37	0.43
1:A:459:ARG:CG	1:A:459:ARG:NH1	2.82	0.43
1:B:187:GLY:O	1:B:190:LEU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:LYS:O	1:B:316:VAL:HB	2.19	0.43
1:B:368:SER:HB3	1:B:371:LYS:CG	2.49	0.43
1:A:13:VAL:CG2	1:A:203:VAL:HG21	2.49	0.42
1:A:16:LEU:CB	1:A:17:PRO:C	2.92	0.42
1:A:52:GLN:OE1	1:A:52:GLN:C	2.62	0.42
1:A:220:GLN:NE2	1:A:220:GLN:C	2.77	0.42
1:A:300:PRO:CB	1:A:301:PRO:CD	2.97	0.42
1:B:6:ALA:HB2	1:B:181:VAL:CG1	2.45	0.42
1:B:477:LYS:C	1:B:479:LEU:N	2.77	0.42
1:A:250:PHE:CD2	1:A:251:VAL:N	2.87	0.42
1:A:414:GLY:O	1:A:415:PHE:O	2.36	0.42
1:B:293:GLY:HA2	1:B:299:SER:CA	2.48	0.42
1:B:322:LEU:HD23	3:B:1013:HOH:O	2.19	0.42
1:A:97:ALA:O	1:A:99:ARG:N	2.52	0.42
1:A:375:SER:O	1:A:376:ILE:C	2.60	0.42
1:A:408:ARG:HH21	1:A:412:GLU:HG2	1.83	0.42
1:A:440:ILE:HG23	1:A:440:ILE:O	2.19	0.42
1:A:470:ARG:O	1:A:471:ASN:C	2.62	0.42
1:A:511:PRO:HB2	1:A:512:PHE:CE1	2.54	0.42
1:B:88:ILE:C	1:B:91:ILE:HG23	2.44	0.42
1:B:276:ILE:HB	1:B:277:PRO:HD3	2.00	0.42
1:B:280:ALA:HA	1:B:284:PHE:O	2.19	0.42
1:B:438:SER:C	1:B:440:ILE:N	2.76	0.42
1:A:97:ALA:HB2	1:A:132:LYS:HG2	2.01	0.42
1:A:160:LYS:CB	1:A:189:ASN:HD21	2.13	0.42
1:B:63:TRP:NE1	1:B:67:MET:HG3	2.34	0.42
1:B:139:MET:HE2	1:B:139:MET:HB2	1.81	0.42
1:B:159:ILE:C	1:B:165:ILE:HD11	2.45	0.42
1:B:325:PRO:O	1:B:326:GLN:HG3	2.20	0.42
1:B:534:ASN:O	1:B:535:GLN:C	2.62	0.42
1:A:277:PRO:O	1:A:280:ALA:HB3	2.19	0.42
1:A:294:TYR:CE2	1:A:461:PRO:HB3	2.55	0.42
1:B:53:LEU:HD23	1:B:53:LEU:HA	1.82	0.42
1:B:440:ILE:HG23	1:B:440:ILE:O	2.20	0.42
1:B:470:ARG:CA	1:B:473:LYS:NZ	2.72	0.42
1:A:211:ARG:HB2	1:A:215:LYS:HZ3	1.85	0.42
1:A:276:ILE:HG22	1:A:277:PRO:CD	2.49	0.42
1:A:325:PRO:O	1:A:326:GLN:HG3	2.20	0.42
1:B:19:ILE:HD13	1:B:19:ILE:HA	1.77	0.42
1:B:75:SER:C	1:B:77:ALA:N	2.77	0.42
1:B:169:LEU:HG	1:B:173:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:VAL:HG13	1:B:353:VAL:HG13	1.98	0.42
1:A:138:GLN:CA	1:B:325:PRO:HB3	2.49	0.42
1:A:158:MET:HE1	1:A:168:PHE:CD1	2.54	0.42
1:A:513:LEU:CD2	1:A:514:LYS:O	2.67	0.42
1:B:54:MET:HB3	1:B:159:ILE:CG2	2.49	0.42
1:B:122:VAL:CA	1:B:151:ILE:HD12	2.50	0.42
1:B:202:LEU:C	1:B:204:HIS:H	2.25	0.42
1:B:248:LEU:HA	1:B:248:LEU:HD13	1.93	0.42
1:B:262:CYS:C	1:B:272:TRP:HZ2	2.28	0.42
1:B:276:ILE:HG22	1:B:277:PRO:CD	2.49	0.42
1:B:309:GLU:HA	1:B:474:TRP:CE2	2.55	0.42
1:B:529:LYS:HA	1:B:529:LYS:HD3	1.70	0.42
1:A:55:LYS:HG3	1:A:159:ILE:HG23	2.02	0.42
1:A:128:ASP:O	1:A:133:ARG:CG	2.67	0.42
1:A:422:THR:H	1:A:422:THR:HG1	1.41	0.42
1:B:42:GLN:HB2	1:B:186:PHE:HZ	1.80	0.42
1:B:163:PRO:HA	1:B:166:TYR:HD1	1.84	0.42
1:A:186:PHE:C	1:A:188:SER:H	2.28	0.42
1:A:378:VAL:HG22	1:A:418:VAL:HG11	2.01	0.42
1:B:61:SER:O	1:B:62:GLN:C	2.62	0.42
1:B:96:MET:HE2	1:B:96:MET:HB3	1.94	0.42
1:B:337:VAL:O	1:B:341:ASN:ND2	2.52	0.42
1:B:378:VAL:HA	1:B:419:HIS:CD2	2.55	0.42
1:B:406:PHE:HD2	2:B:1200:CIU:HC12	1.85	0.42
1:B:469:GLU:HG3	1:B:473:LYS:HZ1	1.85	0.42
1:A:233:ASN:C	1:A:235:VAL:H	2.25	0.42
1:B:8:PHE:CE1	1:B:147:PHE:CE2	3.06	0.42
1:B:43:THR:O	1:B:44:GLU:CB	2.66	0.42
1:B:118:THR:HA	1:B:148:ASP:OD2	2.18	0.42
1:B:167:ASN:ND2	1:B:196:MET:HE1	2.34	0.42
1:B:183:LEU:HB2	1:B:203:VAL:HG21	2.00	0.42
1:B:329:PHE:HB3	1:B:339:VAL:HG22	2.02	0.42
1:B:386:GLN:HE22	1:B:468:THR:HG1	1.67	0.42
1:A:229:PRO:HB2	1:A:230:CYS:H	1.69	0.41
1:A:246:ILE:N	1:A:246:ILE:HD12	2.35	0.41
1:B:72:ARG:O	1:B:75:SER:HB3	2.20	0.41
1:B:103:ARG:H	1:B:103:ARG:HG2	1.54	0.41
1:B:358:THR:HA	1:B:359:PRO:HD3	1.83	0.41
1:A:65:PRO:O	1:A:66:LEU:C	2.62	0.41
1:A:121:ILE:HB	1:A:150:LEU:CD1	2.51	0.41
1:A:380:ASN:C	1:A:382:GLN:N	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:LYS:C	1:A:424:ILE:HG12	2.45	0.41
1:B:33:PRO:O	1:B:34:ARG:C	2.64	0.41
1:B:190:LEU:CD1	1:B:202:LEU:HD23	2.50	0.41
1:B:399:MET:SD	1:B:454:LYS:HE3	2.60	0.41
1:A:191:LYS:HB3	1:A:192:PRO:HD3	2.02	0.41
1:A:360:PHE:O	1:A:362:PRO:HD3	2.19	0.41
1:B:132:LYS:CD	1:B:132:LYS:N	2.84	0.41
1:B:284:PHE:CD1	1:B:284:PHE:N	2.89	0.41
1:B:301:PRO:HD2	1:B:302:GLU:CD	2.45	0.41
1:B:433:GLU:C	1:B:434:ASP:OD2	2.63	0.41
1:B:489:MET:HE3	1:B:490:VAL:H	1.84	0.41
1:B:243:LYS:CB	1:B:246:ILE:HD13	2.50	0.41
1:B:250:PHE:CD2	1:B:251:VAL:N	2.88	0.41
1:B:326:GLN:HG2	1:B:348:GLU:O	2.21	0.41
1:A:138:GLN:C	1:A:140:MET:N	2.78	0.41
1:A:190:LEU:HB3	1:A:200:THR:HG21	2.02	0.41
1:A:386:GLN:NE2	1:A:468:THR:HG1	2.17	0.41
1:B:96:MET:C	1:B:98:ALA:N	2.76	0.41
1:B:160:LYS:HA	1:B:165:ILE:CD1	2.49	0.41
1:B:187:GLY:HA2	1:B:190:LEU:HB2	2.02	0.41
1:B:233:ASN:N	1:B:233:ASN:HD22	2.19	0.41
1:B:360:PHE:O	1:B:362:PRO:HD3	2.20	0.41
1:B:427:ILE:HB	1:B:428:LEU:HD13	2.02	0.41
1:B:459:ARG:CG	1:B:459:ARG:NH1	2.83	0.41
1:B:489:MET:CE	1:B:490:VAL:N	2.82	0.41
1:A:54:MET:O	1:A:154:CYS:CA	2.69	0.41
1:A:220:GLN:NE2	1:A:220:GLN:O	2.54	0.41
1:A:396:GLU:O	1:A:398:ASN:N	2.53	0.41
1:B:259:LEU:HD11	1:B:279:LEU:HD13	2.03	0.41
1:B:406:PHE:HE2	2:B:1200:CIU:HC11	1.85	0.41
1:A:54:MET:O	1:A:154:CYS:HA	2.21	0.41
1:A:58:ILE:HG22	1:A:62:GLN:OE1	2.20	0.41
1:A:97:ALA:C	1:A:99:ARG:H	2.28	0.41
1:A:321:LYS:HE3	1:B:234:ASP:HB2	2.03	0.41
1:A:394:GLU:OE1	1:A:427:ILE:HG22	2.21	0.41
1:A:467:ASN:O	1:A:471:ASN:CG	2.64	0.41
1:A:532:GLU:H	1:A:532:GLU:HG2	1.56	0.41
1:B:42:GLN:CB	1:B:186:PHE:HE1	2.32	0.41
1:B:73:LYS:C	1:B:75:SER:N	2.78	0.41
1:B:308:MET:O	1:B:309:GLU:C	2.63	0.41
1:B:380:ASN:C	1:B:382:GLN:N	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:GLU:C	1:B:473:LYS:NZ	2.79	0.41
1:A:149:PHE:HD2	1:A:173:LEU:HD12	1.86	0.41
1:A:210:LEU:O	1:A:214:GLU:HB3	2.19	0.41
1:B:4:ARG:HH11	1:B:4:ARG:CG	2.30	0.41
1:B:105:MET:O	1:B:106:LEU:C	2.64	0.41
1:B:259:LEU:HB3	1:B:328:VAL:HB	2.01	0.41
1:B:340:TRP:HZ2	1:B:489:MET:HG2	1.85	0.41
1:B:470:ARG:N	1:B:473:LYS:NZ	2.68	0.41
1:B:513:LEU:C	1:B:513:LEU:HD23	2.45	0.41
1:A:58:ILE:HG22	1:A:62:GLN:HG3	2.03	0.41
1:A:62:GLN:HE22	1:B:482:LYS:N	2.19	0.41
1:A:208:SER:C	1:A:210:LEU:N	2.78	0.41
1:A:208:SER:OG	1:A:209:ALA:N	2.52	0.41
1:A:231:ASN:HB2	1:A:232:PRO:CA	2.51	0.41
1:A:276:ILE:CB	1:A:277:PRO:HD3	2.51	0.41
1:A:281:GLN:C	1:A:283:GLY:N	2.77	0.41
1:A:293:GLY:HA2	1:A:299:SER:HA	2.03	0.41
1:A:322:LEU:HG	1:B:236:SER:HB2	2.02	0.41
1:A:329:PHE:HB3	1:A:339:VAL:HG22	2.03	0.41
1:A:340:TRP:HZ2	1:A:489:MET:HG2	1.85	0.41
1:A:475:SER:C	1:A:477:LYS:N	2.79	0.41
1:B:112:LEU:CD2	1:B:117:PHE:CE1	3.00	0.41
1:B:159:ILE:O	1:B:162:GLU:HB2	2.21	0.41
1:B:272:TRP:HA	1:B:275:GLN:OE1	2.21	0.41
1:B:420:LYS:O	1:B:424:ILE:HD11	2.20	0.41
1:B:483:ILE:C	1:B:484:LEU:HG	2.44	0.41
1:A:64:VAL:N	1:A:65:PRO:CD	2.83	0.41
1:A:112:LEU:HA	1:A:115:LYS:HB3	2.03	0.41
1:A:191:LYS:CB	1:A:192:PRO:CD	2.97	0.41
1:B:276:ILE:CB	1:B:277:PRO:HD3	2.50	0.41
1:B:294:TYR:CE2	1:B:461:PRO:HB3	2.55	0.41
1:B:395:LEU:HD23	1:B:428:LEU:HD21	2.03	0.41
1:B:404:LYS:HG2	1:B:404:LYS:H	1.35	0.41
1:A:7:ALA:N	1:A:181:VAL:O	2.51	0.40
1:A:94:GLN:O	1:A:97:ALA:HB3	2.21	0.40
1:B:122:VAL:O	1:B:122:VAL:HG22	2.20	0.40
1:B:149:PHE:CD2	1:B:173:LEU:HD13	2.56	0.40
1:B:173:LEU:HB2	1:B:174:LYS:H	1.64	0.40
1:B:187:GLY:C	1:B:189:ASN:N	2.75	0.40
1:B:203:VAL:O	1:B:203:VAL:CG1	2.65	0.40
1:B:372:VAL:O	1:B:376:ILE:HD11	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:SER:O	1:B:408:ARG:CG	2.68	0.40
1:B:479:LEU:HD23	1:B:479:LEU:HA	1.82	0.40
1:A:137:ALA:CB	1:B:325:PRO:O	2.61	0.40
1:A:141:CYS:C	1:A:144:SER:HB3	2.46	0.40
1:B:4:ARG:CG	1:B:4:ARG:NH1	2.85	0.40
1:B:250:PHE:CD2	1:B:250:PHE:C	2.99	0.40
1:B:303:ILE:O	1:B:304:GLU:C	2.64	0.40
1:B:431:THR:O	1:B:432:PRO:O	2.40	0.40
1:A:4:ARG:NH2	1:A:179:GLU:HB2	2.36	0.40
1:A:10:LEU:C	1:A:12:GLY:H	2.29	0.40
1:A:187:GLY:C	1:A:189:ASN:H	2.25	0.40
1:A:358:THR:HA	1:A:359:PRO:HD3	1.82	0.40
1:B:41:TYR:OH	1:B:126:TRP:HZ3	2.04	0.40
1:B:129:ASP:OD1	1:B:129:ASP:N	2.52	0.40
1:B:398:ASN:OD1	1:B:400:SER:HB3	2.21	0.40
1:B:524:TRP:CZ2	2:B:1200:CIU:HC62	2.56	0.40
1:A:17:PRO:O	1:A:18:SER:O	2.39	0.40
1:A:56:GLY:HA2	1:A:127:LEU:HD11	2.03	0.40
1:A:91:ILE:O	1:A:91:ILE:HG22	2.20	0.40
1:A:138:GLN:HG2	1:B:325:PRO:CG	2.52	0.40
1:A:158:MET:HE1	1:A:168:PHE:HD1	1.85	0.40
1:A:405:SER:O	1:A:408:ARG:CG	2.69	0.40
1:B:8:PHE:CB	1:B:14:LEU:HD13	2.47	0.40
1:B:59:THR:OG1	1:B:60:PHE:N	2.52	0.40
1:B:125:ASN:C	1:B:154:CYS:HB3	2.47	0.40
1:B:228:VAL:O	1:B:277:PRO:HG2	2.22	0.40
1:B:276:ILE:CG2	1:B:277:PRO:HD3	2.52	0.40
1:B:325:PRO:HA	1:B:349:ARG:HH12	1.86	0.40
1:B:364:ASP:HB2	1:B:367:VAL:CG2	2.52	0.40
1:A:90:GLN:CD	1:A:90:GLN:C	2.90	0.40
1:A:276:ILE:HB	1:A:277:PRO:HD3	2.03	0.40
1:A:284:PHE:CD1	1:A:284:PHE:N	2.89	0.40
1:A:326:GLN:HG2	1:A:348:GLU:O	2.21	0.40
1:A:339:VAL:CG1	1:A:353:VAL:CG1	2.95	0.40
1:B:249:HIS:CG	1:B:250:PHE:N	2.89	0.40
1:B:305:GLU:O	1:B:310:LEU:HD23	2.22	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	A	484/554 (87%)	345 (71%)	90 (19%)	49 (10%)	0	3
1	B	539/554 (97%)	384 (71%)	101 (19%)	54 (10%)	0	3
All	All	1023/1108 (92%)	729 (71%)	191 (19%)	103 (10%)	0	3

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	18	SER
1	A	63	TRP
1	A	65	PRO
1	A	91	ILE
1	A	144	SER
1	A	203	VAL
1	A	207	ALA
1	A	212	GLU
1	A	217	THR
1	A	229	PRO
1	A	230	CYS
1	A	256	GLY
1	A	415	PHE
1	A	466	ARG
1	B	18	SER
1	B	32	LEU
1	B	44	GLU
1	B	59	THR
1	B	75	SER
1	B	78	CYS
1	B	89	SER
1	B	174	LYS
1	B	205	ASN
1	B	207	ALA

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Mol	Chain	Res	Type
1	B	211	ARG
1	B	225	PRO
1	B	232	PRO
1	B	256	GLY
1	B	415	PHE
1	B	421	ALA
1	B	434	ASP
1	B	435	PRO
1	B	466	ARG
1	A	98	ALA
1	A	126	TRP
1	A	130	GLY
1	A	156	VAL
1	A	163	PRO
1	A	210	LEU
1	A	273	ARG
1	A	301	PRO
1	A	386	GLN
1	A	397	LYS
1	A	421	ALA
1	A	543	THR
1	B	21	GLY
1	B	39	GLY
1	B	63	TRP
1	B	74	SER
1	B	203	VAL
1	B	213	LEU
1	B	216	VAL
1	B	219	THR
1	B	273	ARG
1	B	386	GLN
1	B	397	LYS
1	B	543	THR
1	A	111	ALA
1	A	157	GLY
1	A	164	GLN
1	A	202	LEU
1	A	244	PRO
1	A	409	ALA
1	B	29	ALA
1	B	73	LYS
1	B	179	GLU

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Mol	Chain	Res	Type
1	B	244	PRO
1	B	301	PRO
1	B	409	ALA
1	B	459	ARG
1	A	12	GLY
1	A	92	PHE
1	A	231	ASN
1	A	232	PRO
1	A	459	ARG
1	B	34	ARG
1	A	195	ASP
1	A	423	GLU
1	A	476	CYS
1	B	20	ALA
1	B	90	GLN
1	B	229	PRO
1	B	423	GLU
1	B	432	PRO
1	B	534	ASN
1	A	145	GLN
1	A	506	MET
1	A	530	PRO
1	B	111	ALA
1	B	418	VAL
1	B	530	PRO
1	A	300	PRO
1	A	390	VAL
1	A	432	PRO
1	B	165	ILE
1	B	300	PRO
1	B	390	VAL
1	A	418	VAL
1	B	103	ARG
1	B	197	GLY
1	A	266	PRO
1	B	266	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/480 (89%)	274 (64%)	153 (36%)	0	0
1	B	468/480 (98%)	292 (62%)	176 (38%)	0	0
All	All	895/960 (93%)	566 (63%)	329 (37%)	0	0

All (329) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	8	PHE
1	A	9	ASP
1	A	13	VAL
1	A	14	LEU
1	A	16	LEU
1	A	18	SER
1	A	19	ILE
1	A	51	GLU
1	A	52	GLN
1	A	53	LEU
1	A	57	LYS
1	A	58	ILE
1	A	59	THR
1	A	66	LEU
1	A	90	GLN
1	A	92	PHE
1	A	93	SER
1	A	94	GLN
1	A	96	MET
1	A	103	ARG
1	A	106	LEU
1	A	107	GLN
1	A	110	ILE
1	A	112	LEU
1	A	113	LYS
1	A	117	PHE
1	A	118	THR
1	A	121	ILE
1	A	122	VAL
1	A	127	LEU
1	A	128	ASP
1	A	129	ASP

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Mol	Chain	Res	Type
1	A	132	LYS
1	A	135	SER
1	A	136	LEU
1	A	138	GLN
1	A	139	MET
1	A	144	SER
1	A	148	ASP
1	A	150	LEU
1	A	152	GLU
1	A	154	CYS
1	A	155	GLN
1	A	158	MET
1	A	159	ILE
1	A	165	ILE
1	A	173	LEU
1	A	181	VAL
1	A	183	LEU
1	A	188	SER
1	A	189	ASN
1	A	191	LYS
1	A	194	ARG
1	A	196	MET
1	A	198	MET
1	A	200	THR
1	A	201	ILE
1	A	202	LEU
1	A	204	HIS
1	A	205	ASN
1	A	206	THR
1	A	210	LEU
1	A	211	ARG
1	A	212	GLU
1	A	213	LEU
1	A	214	GLU
1	A	215	LYS
1	A	220	GLN
1	A	221	PHE
1	A	223	GLU
1	A	230	CYS
1	A	231	ASN
1	A	233	ASN
1	A	235	VAL

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Mol	Chain	Res	Type
1	A	240	VAL
1	A	242	VAL
1	A	247	ARG
1	A	248	LEU
1	A	253	MET
1	A	259	LEU
1	A	268	SER
1	A	275	GLN
1	A	281	GLN
1	A	290	ASP
1	A	297	SER
1	A	299	SER
1	A	304	GLU
1	A	313	LYS
1	A	315	MET
1	A	319	LEU
1	A	322	LEU
1	A	324	ILE
1	A	328	VAL
1	A	339	VAL
1	A	349	ARG
1	A	353	VAL
1	A	356	LEU
1	A	364	ASP
1	A	370	MET
1	A	372	VAL
1	A	373	ILE
1	A	375	SER
1	A	376	ILE
1	A	383	LEU
1	A	387	GLU
1	A	398	ASN
1	A	401	ARG
1	A	404	LYS
1	A	408	ARG
1	A	411	ASP
1	A	412	GLU
1	A	416	ILE
1	A	418	VAL
1	A	419	HIS
1	A	422	THR
1	A	429	VAL

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Mol	Chain	Res	Type
1	A	437	LEU
1	A	439	LYS
1	A	440	ILE
1	A	447	GLU
1	A	451	GLN
1	A	452	GLN
1	A	456	THR
1	A	459	ARG
1	A	462	LEU
1	A	463	ASN
1	A	466	ARG
1	A	468	THR
1	A	470	ARG
1	A	473	LYS
1	A	482	LYS
1	A	485	VAL
1	A	488	LEU
1	A	489	MET
1	A	494	LYS
1	A	496	ILE
1	A	497	VAL
1	A	499	ARG
1	A	501	GLU
1	A	502	MET
1	A	504	LYS
1	A	507	GLU
1	A	512	PHE
1	A	515	ARG
1	A	518	ILE
1	A	521	CYS
1	A	526	GLN
1	A	527	ILE
1	A	531	THR
1	A	532	GLU
1	A	539	LYS
1	A	544	GLU
1	B	4	ARG
1	B	8	PHE
1	B	10	LEU
1	B	13	VAL
1	B	14	LEU
1	B	16	LEU

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Mol	Chain	Res	Type
1	B	19	ILE
1	B	24	ARG
1	B	28	GLU
1	B	34	ARG
1	B	38	LEU
1	B	41	TYR
1	B	43	THR
1	B	44	GLU
1	B	47	GLU
1	B	50	THR
1	B	51	GLU
1	B	53	LEU
1	B	57	LYS
1	B	59	THR
1	B	60	PHE
1	B	61	SER
1	B	62	GLN
1	B	64	VAL
1	B	66	LEU
1	B	67	MET
1	B	69	GLU
1	B	70	SER
1	B	72	ARG
1	B	73	LYS
1	B	74	SER
1	B	75	SER
1	B	76	LYS
1	B	84	GLU
1	B	85	ASN
1	B	88	ILE
1	B	90	GLN
1	B	91	ILE
1	B	96	MET
1	B	101	ILE
1	B	103	ARG
1	B	106	LEU
1	B	107	GLN
1	B	110	ILE
1	B	113	LYS
1	B	118	THR
1	B	119	THR
1	B	120	CYS

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Mol	Chain	Res	Type
1	B	121	ILE
1	B	122	VAL
1	B	127	LEU
1	B	129	ASP
1	B	132	LYS
1	B	133	ARG
1	B	136	LEU
1	B	139	MET
1	B	144	SER
1	B	148	ASP
1	B	151	ILE
1	B	152	GLU
1	B	155	GLN
1	B	158	MET
1	B	159	ILE
1	B	165	ILE
1	B	167	ASN
1	B	169	LEU
1	B	170	LEU
1	B	173	LEU
1	B	181	VAL
1	B	183	LEU
1	B	189	ASN
1	B	191	LYS
1	B	195	ASP
1	B	198	MET
1	B	199	VAL
1	B	201	ILE
1	B	202	LEU
1	B	204	HIS
1	B	206	THR
1	B	208	SER
1	B	210	LEU
1	B	212	GLU
1	B	213	LEU
1	B	214	GLU
1	B	215	LYS
1	B	217	THR
1	B	219	THR
1	B	220	GLN
1	B	223	GLU
1	B	226	LEU

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Mol	Chain	Res	Type
1	B	228	VAL
1	B	235	VAL
1	B	240	VAL
1	B	242	VAL
1	B	247	ARG
1	B	248	LEU
1	B	253	MET
1	B	259	LEU
1	B	268	SER
1	B	275	GLN
1	B	281	GLN
1	B	290	ASP
1	B	297	SER
1	B	299	SER
1	B	304	GLU
1	B	306	TYR
1	B	313	LYS
1	B	315	MET
1	B	319	LEU
1	B	322	LEU
1	B	324	ILE
1	B	328	VAL
1	B	339	VAL
1	B	349	ARG
1	B	353	VAL
1	B	356	LEU
1	B	357	ASN
1	B	364	ASP
1	B	370	MET
1	B	372	VAL
1	B	373	ILE
1	B	375	SER
1	B	376	ILE
1	B	383	LEU
1	B	387	GLU
1	B	398	ASN
1	B	401	ARG
1	B	404	LYS
1	B	408	ARG
1	B	411	ASP
1	B	412	GLU
1	B	416	ILE

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Mol	Chain	Res	Type
1	B	418	VAL
1	B	419	HIS
1	B	423	GLU
1	B	424	ILE
1	B	427	ILE
1	B	428	LEU
1	B	431	THR
1	B	433	GLU
1	B	437	LEU
1	B	439	LYS
1	B	440	ILE
1	B	447	GLU
1	B	451	GLN
1	B	452	GLN
1	B	455	LYS
1	B	456	THR
1	B	459	ARG
1	B	462	LEU
1	B	463	ASN
1	B	466	ARG
1	B	468	THR
1	B	470	ARG
1	B	473	LYS
1	B	485	VAL
1	B	488	LEU
1	B	489	MET
1	B	494	LYS
1	B	496	ILE
1	B	497	VAL
1	B	499	ARG
1	B	501	GLU
1	B	502	MET
1	B	504	LYS
1	B	507	GLU
1	B	512	PHE
1	B	515	ARG
1	B	521	CYS
1	B	526	GLN
1	B	527	ILE
1	B	529	LYS
1	B	531	THR
1	B	532	GLU

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Mol	Chain	Res	Type
1	B	539	LYS
1	B	544	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	125	ASN
1	A	189	ASN
1	A	220	GLN
1	A	231	ASN
1	A	233	ASN
1	A	281	GLN
1	A	326	GLN
1	A	386	GLN
1	A	451	GLN
1	A	463	ASN
1	A	526	GLN
1	B	102	ASN
1	B	146	HIS
1	B	167	ASN
1	B	178	ASN
1	B	189	ASN
1	B	204	HIS
1	B	205	ASN
1	B	233	ASN
1	B	386	GLN
1	B	430	ASN
1	B	451	GLN
1	B	463	ASN
1	B	526	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CIU	B	1200	-	18,18,18	2.84	10 (55%)	23,23,23	1.99	4 (17%)
2	CIU	A	1100	-	18,18,18	2.84	10 (55%)	23,23,23	1.99	4 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIU	B	1200	-	-	0/8/16/16	0/2/2/2
2	CIU	A	1100	-	-	0/8/16/16	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1200	CIU	C11-I4	6.54	2.27	2.10
2	A	1100	CIU	C11-I4	6.51	2.27	2.10
2	B	1200	CIU	C4-C3	4.04	1.61	1.52
2	B	1200	CIU	C12-C11	4.03	1.47	1.38
2	A	1100	CIU	C12-C11	4.02	1.47	1.38
2	A	1100	CIU	C4-C3	4.02	1.61	1.52
2	B	1200	CIU	C2-C3	3.56	1.60	1.52
2	A	1100	CIU	C2-C3	3.54	1.60	1.52
2	A	1100	CIU	C13-C8	2.91	1.44	1.39
2	B	1200	CIU	C13-C8	2.91	1.44	1.39
2	B	1200	CIU	C6-C5	2.83	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1100	CIU	C6-C5	2.82	1.62	1.51
2	A	1100	CIU	C6-C1	2.65	1.61	1.51
2	B	1200	CIU	C6-C1	2.63	1.61	1.51
2	A	1100	CIU	C5-C4	2.60	1.59	1.53
2	B	1200	CIU	C5-C4	2.60	1.59	1.53
2	A	1100	CIU	C10-C11	2.55	1.44	1.38
2	B	1200	CIU	C10-C11	2.52	1.44	1.38
2	B	1200	CIU	C13-C12	2.01	1.42	1.38
2	A	1100	CIU	C13-C12	2.00	1.42	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1200	CIU	N2-C7-N1	5.44	121.25	113.77
2	A	1100	CIU	N2-C7-N1	5.43	121.24	113.77
2	B	1200	CIU	C8-N2-C7	4.56	135.92	126.61
2	A	1100	CIU	C8-N2-C7	4.55	135.89	126.61
2	A	1100	CIU	O2-C7-N1	-3.90	114.34	122.67
2	B	1200	CIU	O2-C7-N1	-3.89	114.38	122.67
2	A	1100	CIU	C3-N1-C7	2.95	129.27	122.92
2	B	1200	CIU	C3-N1-C7	2.94	129.24	122.92

There are no chirality outliers.

There are no torsion outliers.

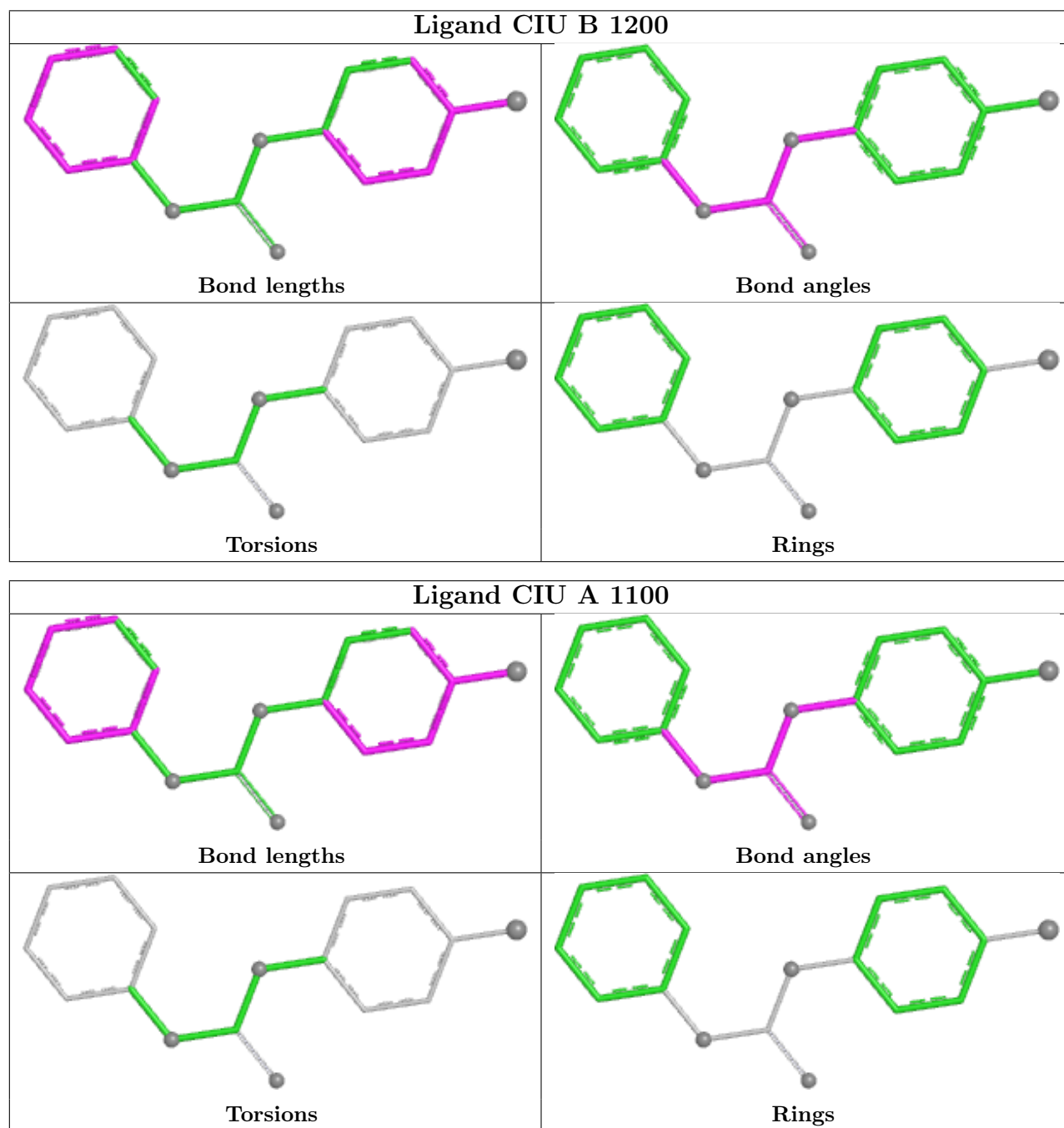
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1200	CIU	6	0
2	A	1100	CIU	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

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.