



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:47 AM UTC

PDB ID : 1SUQ / pdb_00001suq
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE (RT) IN
COMPLEX WITH JANSSEN-R185545
Authors : Das, K.; Arnold, E.
Deposited on : 2004-03-26
Resolution : 3.00 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

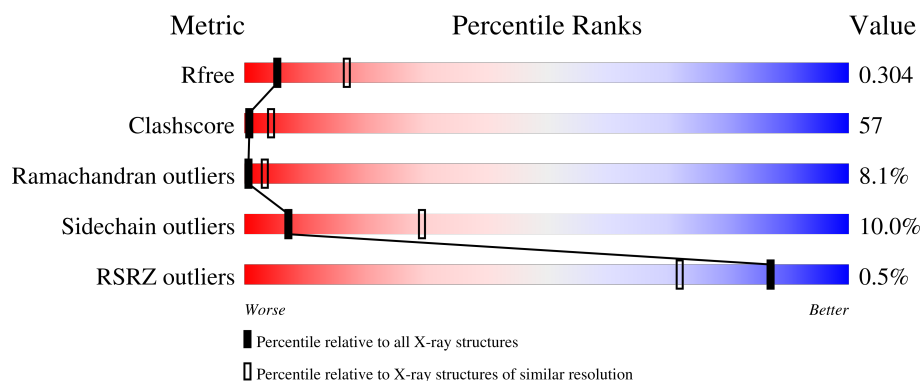
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

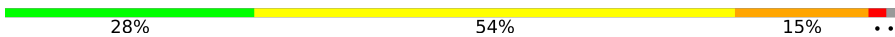
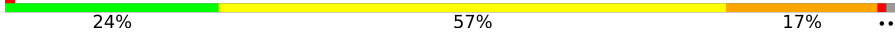
The reported resolution of this entry is 3.00 Å.

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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	560	 28% 54% 15% ..
2	B	430	 24% 57% 17% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8053 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 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	121	0	0
			4497	2912	748	830	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 2 is a protein called REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	60	0	0
			3526	2297	584	638	7			

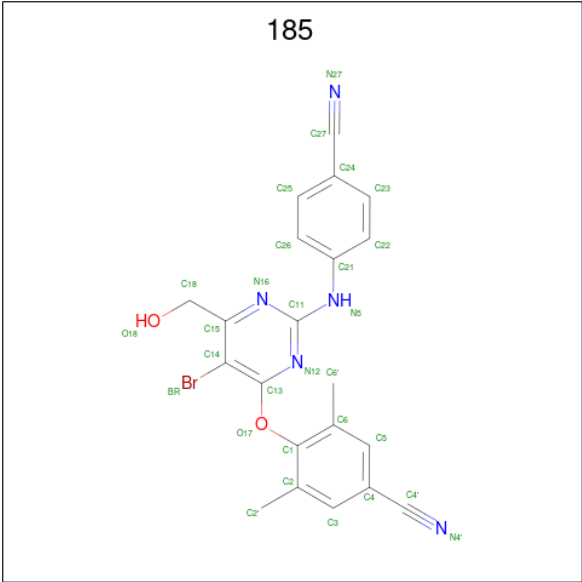
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is (6-[4-(AMINOMETHYL)-2,6-DIMETHYLPHENOXY]-2-{[4-(AMINOMETHYL)PHENYL]AMINO}-5-BROMOPYRIMIDIN-4-YL)METHANOL (CCD ID: 185) (formula: C₂₁H₁₆BrN₅O₂).

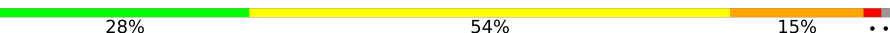


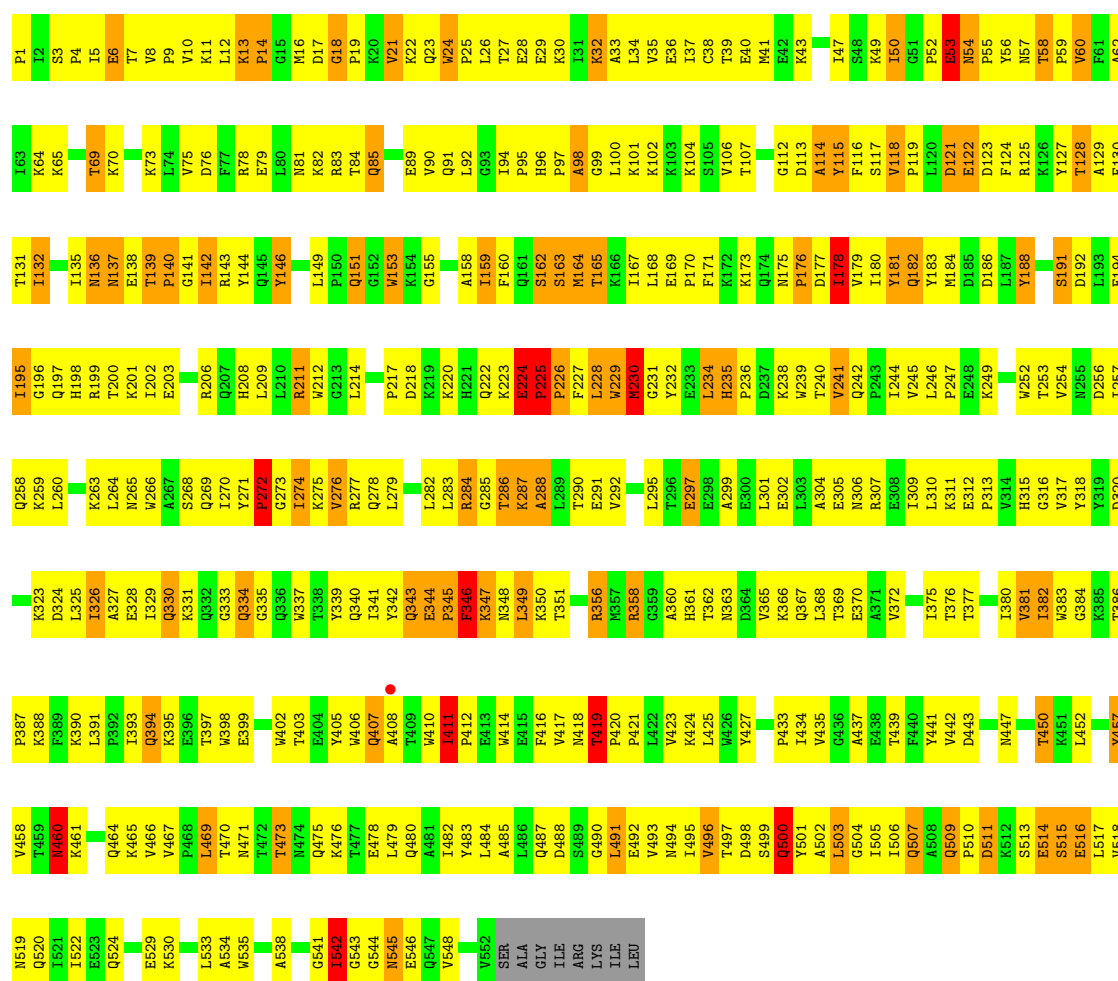
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	N	O		
4	A	1	29	1	21	5	2	0	0

3 Residue-property plots

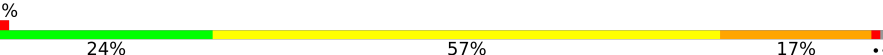
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain A: 



• Molecule 2: REVERSE TRANSCRIPTASE

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.11Å 69.47Å 104.26Å 90.00° 106.82° 90.00°	Depositor
Resolution (Å)	19.99 – 3.00 19.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.1 (19.99-3.00) 92.7 (19.99-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 3.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.262 , 0.325 0.251 , 0.304	Depositor DCC
R_{free} test set	1432 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	78.4	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8053	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 185

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	0.62	0/4615	1.24	63/6270 (1.0%)
2	B	0.71	0/3631	1.31	52/4936 (1.1%)
All	All	0.66	0/8246	1.27	115/11206 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
2	B	0	1
All	All	1	1

There are no bond length outliers.

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	270	ILE	N-CA-C	-13.31	99.03	111.67
1	A	224	GLU	CA-C-N	12.08	132.82	120.38
1	A	224	GLU	C-N-CA	12.08	132.82	120.38
2	B	89	GLU	N-CA-C	-12.04	98.57	113.38
1	A	225	PRO	CA-C-N	10.00	150.99	127.00
1	A	225	PRO	C-N-CA	10.00	150.99	127.00
1	A	225	PRO	C-N-CD	-9.69	99.29	120.60
2	B	401	TRP	N-CA-C	8.62	123.99	113.38
2	B	389	PHE	N-CA-C	8.59	122.39	109.25
2	B	246	LEU	N-CA-C	-8.56	98.88	110.36
1	A	225	PRO	N-CA-C	8.44	120.99	110.70
2	B	146	TYR	N-CA-C	8.42	120.76	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	245	VAL	N-CA-C	8.27	120.06	107.99
1	A	26	LEU	N-CA-C	8.24	123.08	107.75
2	B	94	ILE	CA-C-N	8.23	128.74	119.93
2	B	94	ILE	C-N-CA	8.23	128.74	119.93
2	B	96	HIS	CA-C-N	8.12	129.98	119.84
2	B	96	HIS	C-N-CA	8.12	129.98	119.84
2	B	235	HIS	CA-C-N	7.91	127.57	119.82
2	B	235	HIS	C-N-CA	7.91	127.57	119.82
1	A	271	TYR	CA-C-N	7.77	129.55	119.84
1	A	271	TYR	C-N-CA	7.77	129.55	119.84
1	A	344	GLU	CA-C-N	7.72	129.50	119.84
1	A	344	GLU	C-N-CA	7.72	129.50	119.84
2	B	267	ALA	N-CA-C	-7.65	101.95	111.75
2	B	172	LYS	N-CA-C	-7.64	103.84	113.01
2	B	7	THR	N-CA-C	7.55	120.92	110.35
2	B	143	ARG	N-CA-C	7.51	121.16	108.02
1	A	411	ILE	CA-C-N	7.33	129.00	119.84
1	A	411	ILE	C-N-CA	7.33	129.00	119.84
1	A	388	LYS	N-CA-C	-7.32	98.64	110.20
1	A	513	SER	N-CA-C	-7.20	97.57	108.52
2	B	117	SER	N-CA-C	-7.20	104.48	113.55
1	A	235	HIS	CA-C-N	7.17	128.81	119.84
1	A	235	HIS	C-N-CA	7.17	128.81	119.84
2	B	366	LYS	N-CA-C	-7.17	103.55	112.72
1	A	13	LYS	CA-C-N	7.14	128.76	119.84
1	A	13	LYS	C-N-CA	7.14	128.76	119.84
2	B	229	TRP	N-CA-C	7.06	120.48	109.96
1	A	343	GLN	N-CA-C	-6.96	105.40	114.04
1	A	132	ILE	N-CA-C	-6.95	100.74	107.76
1	A	118	VAL	CA-C-N	6.93	127.34	119.92
1	A	118	VAL	C-N-CA	6.93	127.34	119.92
1	A	460	ASN	N-CA-C	-6.81	103.86	111.28
1	A	151	GLN	N-CA-C	6.78	119.51	111.71
1	A	69	THR	N-CA-C	-6.71	105.22	113.41
1	A	358	ARG	N-CA-C	6.71	120.08	112.97
1	A	405	TYR	N-CA-C	6.57	120.01	110.42
2	B	362	THR	N-CA-C	6.56	120.22	109.72
2	B	391	LEU	N-CA-C	6.54	119.11	109.50
1	A	18	GLY	CA-C-N	6.46	126.22	119.76
1	A	18	GLY	C-N-CA	6.46	126.22	119.76
1	A	382	ILE	N-CA-C	6.45	116.61	110.74
2	B	346	PHE	N-CA-C	6.40	120.41	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	250	ASP	N-CA-C	-6.37	104.25	111.07
2	B	88	TRP	N-CA-C	-6.36	103.54	113.02
1	A	538	ALA	N-CA-C	6.31	124.23	110.80
1	A	178	ILE	N-CA-C	6.29	115.67	106.55
2	B	423	VAL	N-CA-C	6.29	117.04	110.62
1	A	349	LEU	N-CA-C	-6.26	105.29	113.12
2	B	378	GLU	N-CA-C	-6.24	104.39	111.07
2	B	186	ASP	N-CA-C	6.18	119.62	109.85
2	B	194	GLU	N-CA-C	-6.17	101.28	110.23
2	B	71	TRP	N-CA-C	6.17	118.87	110.35
1	A	24	TRP	N-CA-C	6.17	123.44	109.81
1	A	211	ARG	N-CA-C	-6.12	104.72	111.82
1	A	146	TYR	N-CA-C	6.12	118.87	110.24
2	B	295	LEU	N-CA-C	6.11	117.76	110.19
2	B	417	VAL	N-CA-C	6.09	117.45	106.61
2	B	204	GLU	N-CA-C	-6.08	104.72	111.71
1	A	278	GLN	N-CA-C	6.06	117.58	110.97
1	A	288	ALA	N-CA-C	6.05	119.37	110.30
1	A	507	GLN	N-CA-C	6.00	117.83	111.28
2	B	419	THR	N-CA-C	5.94	122.93	109.81
1	A	419	THR	CA-C-N	5.93	126.49	120.38
1	A	419	THR	C-N-CA	5.93	126.49	120.38
2	B	358	ARG	N-CA-C	5.90	118.52	108.02
2	B	417	VAL	CB-CA-C	-5.82	104.63	111.09
2	B	348	ASN	N-CA-C	5.75	117.43	109.15
1	A	284	ARG	N-CA-C	-5.75	104.39	111.75
1	A	149	LEU	CA-C-N	5.73	125.68	119.78
1	A	149	LEU	C-N-CA	5.73	125.68	119.78
2	B	246	LEU	CA-C-N	-5.65	112.78	119.84
2	B	246	LEU	C-N-CA	-5.65	112.78	119.84
2	B	343	GLN	N-CA-C	-5.65	107.03	114.04
1	A	511	ASP	N-CA-C	-5.57	105.30	111.71
1	A	191	SER	N-CA-C	5.54	116.67	108.86
1	A	361	HIS	N-CA-C	5.53	117.98	109.07
2	B	236	PRO	N-CA-C	5.51	121.09	113.98
2	B	59	PRO	N-CA-C	5.46	119.60	111.41
2	B	149	LEU	CA-C-N	-5.46	114.36	120.14
2	B	149	LEU	C-N-CA	-5.46	114.36	120.14
2	B	284	ARG	N-CA-C	-5.45	105.73	112.38
1	A	226	PRO	N-CA-C	5.41	126.16	112.10
1	A	32	LYS	N-CA-C	-5.37	105.07	111.03
1	A	234	LEU	N-CA-C	5.33	117.44	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	THR	CA-C-N	5.25	125.26	119.90
1	A	58	THR	C-N-CA	5.25	125.26	119.90
1	A	346	PHE	N-CA-C	5.25	117.13	108.48
2	B	248	GLU	N-CA-C	-5.24	99.97	108.41
1	A	500	GLN	N-CA-C	-5.20	106.19	112.54
1	A	488	ASP	N-CA-C	5.18	119.36	113.19
2	B	237	ASP	N-CA-C	-5.18	106.81	113.02
2	B	37	ILE	CB-CA-C	-5.16	105.28	112.04
1	A	381	VAL	CB-CA-C	-5.16	105.18	112.14
1	A	6	GLU	N-CA-C	-5.14	103.36	110.35
1	A	360	ALA	N-CA-C	5.13	118.99	112.12
1	A	548	VAL	N-CA-C	-5.13	107.83	112.96
2	B	307	ARG	N-CA-C	-5.13	105.81	111.71
1	A	242	GLN	N-CA-C	-5.12	103.14	109.64
2	B	249	LYS	N-CA-C	5.10	118.38	110.17
1	A	407	GLN	N-CA-C	-5.09	102.92	110.46
1	A	229	TRP	N-CA-C	-5.06	102.53	110.17
2	B	68	SER	N-CA-C	5.04	117.68	109.86
2	B	416	PHE	N-CA-C	5.02	117.93	109.95

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	31	ILE	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	130	PHE	Sidechain

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	4497	0	4555	512	0
2	B	3526	0	3559	403	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	29	0	15	8	0
All	All	8053	0	8129	894	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 57.

All (894) 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:A:226:PRO:HG3	1:A:235:HIS:CE1	1.72	1.25
2:B:362:THR:HG22	2:B:367:GLN:HE21	1.16	1.11
1:A:224:GLU:HB3	1:A:225:PRO:HD2	1.21	1.10
2:B:314:VAL:HG22	2:B:315:HIS:H	1.16	1.10
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.27	1.09
1:A:228:LEU:HD13	1:A:228:LEU:O	1.50	1.08
1:A:287:LYS:HG3	1:A:288:ALA:H	1.13	1.08
2:B:422:LEU:HD12	2:B:425:LEU:HD12	1.34	1.07
2:B:206:ARG:HB3	2:B:206:ARG:NH1	1.75	1.01
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.37	1.00
1:A:224:GLU:HB3	1:A:225:PRO:CD	1.92	0.99
1:A:13:LYS:HB3	1:A:14:PRO:HD2	1.46	0.97
1:A:244:ILE:HD11	1:A:310:LEU:HD22	1.47	0.97
1:A:460:ASN:HD22	1:A:461:LYS:H	1.01	0.97
1:A:53:GLU:C	1:A:55:PRO:HD3	1.91	0.96
2:B:12:LEU:HD12	2:B:12:LEU:H	1.27	0.96
2:B:362:THR:CG2	2:B:367:GLN:HE21	1.78	0.96
2:B:222:GLN:HG2	2:B:223:LYS:H	1.28	0.96
1:A:337:TRP:HE1	1:A:367:GLN:HE21	0.98	0.95
1:A:545:ASN:HD22	1:A:545:ASN:H	1.15	0.94
1:A:545:ASN:HD22	1:A:545:ASN:N	1.66	0.92
2:B:5:ILE:HG12	2:B:119:PRO:HD2	1.51	0.92
1:A:406:TRP:HH2	2:B:418:ASN:HA	1.33	0.92
2:B:2:ILE:HG13	2:B:4:PRO:HD2	1.50	0.92
2:B:139:THR:HG22	2:B:140:PRO:HD2	1.50	0.92
1:A:318:TYR:HE1	4:A:600:185:H26	1.35	0.92
1:A:135:ILE:HG22	1:A:137:ASN:H	1.37	0.90
2:B:314:VAL:CG2	2:B:315:HIS:H	1.85	0.90
1:A:69:THR:HG23	1:A:70:LYS:HG3	1.55	0.89
1:A:287:LYS:CG	1:A:288:ALA:H	1.83	0.89
1:A:356:ARG:NH1	1:A:358:ARG:HB2	1.89	0.88
2:B:277:ARG:H	2:B:277:ARG:HD2	1.39	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ASN:HD22	1:A:461:LYS:N	1.71	0.88
1:A:460:ASN:ND2	1:A:461:LYS:H	1.71	0.88
2:B:314:VAL:HG22	2:B:315:HIS:N	1.86	0.88
2:B:206:ARG:HB3	2:B:206:ARG:HH11	1.38	0.86
2:B:5:ILE:HG13	2:B:6:GLU:N	1.87	0.86
1:A:27:THR:HG22	1:A:29:GLU:HG2	1.57	0.86
1:A:434:ILE:H	1:A:494:ASN:HD21	1.23	0.85
1:A:224:GLU:CB	1:A:225:PRO:CD	2.54	0.85
1:A:178:ILE:HG12	1:A:201:LYS:HG2	1.59	0.85
1:A:424:LYS:HD3	1:A:425:LEU:N	1.92	0.85
1:A:287:LYS:HG3	1:A:288:ALA:N	1.90	0.84
2:B:296:THR:OG1	2:B:299:ALA:HB2	1.76	0.84
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.57	0.84
2:B:7:THR:HB	2:B:121:ASP:HA	1.58	0.84
2:B:100:LEU:HD11	2:B:106:VAL:HG22	1.60	0.84
2:B:125:ARG:O	2:B:127:TYR:N	2.11	0.83
1:A:182:GLN:H	1:A:182:GLN:HE21	1.22	0.83
2:B:361:HIS:CD2	2:B:361:HIS:H	1.95	0.83
1:A:84:THR:HG22	1:A:124:PHE:HZ	1.43	0.83
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.60	0.83
1:A:317:VAL:HG22	1:A:318:TYR:H	1.44	0.83
2:B:362:THR:HG22	2:B:367:GLN:NE2	1.95	0.82
2:B:50:ILE:HG23	2:B:145:GLN:HG2	1.61	0.82
2:B:2:ILE:HG21	2:B:119:PRO:HG3	1.61	0.82
1:A:228:LEU:O	1:A:228:LEU:CD1	2.28	0.81
2:B:65:LYS:HA	2:B:72:ARG:HG3	1.60	0.81
1:A:362:THR:HG22	1:A:363:ASN:H	1.43	0.81
1:A:288:ALA:CB	1:A:291:GLU:HB2	2.09	0.81
1:A:382:ILE:HA	2:B:136:ASN:HD22	1.45	0.81
1:A:340:GLN:HA	1:A:351:THR:HA	1.62	0.81
1:A:270:ILE:O	1:A:272:PRO:HD3	1.81	0.81
2:B:31:ILE:O	2:B:35:VAL:HG23	1.81	0.80
2:B:195:ILE:HG23	2:B:196:GLY:H	1.45	0.80
2:B:274:ILE:HG23	2:B:306:ASN:CG	2.07	0.80
1:A:53:GLU:HG3	1:A:53:GLU:O	1.81	0.79
2:B:104:LYS:HA	2:B:237:ASP:OD2	1.83	0.79
1:A:33:ALA:O	1:A:36:GLU:HB2	1.83	0.79
1:A:224:GLU:HG2	1:A:225:PRO:HD3	1.65	0.78
2:B:195:ILE:HG12	2:B:199:ARG:HE	1.49	0.78
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.65	0.78
1:A:3:SER:HB3	1:A:212:TRP:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ILE:HB	1:A:139:THR:OG1	1.84	0.78
1:A:175:ASN:HB3	1:A:178:ILE:HD13	1.64	0.78
1:A:183:TYR:CD2	1:A:184:MET:HG3	2.18	0.78
2:B:13:LYS:O	2:B:16:MET:HB2	1.84	0.78
1:A:497:THR:HG22	1:A:498:ASP:N	1.97	0.78
1:A:337:TRP:HE1	1:A:367:GLN:NE2	1.79	0.78
1:A:19:PRO:O	1:A:56:TYR:HB3	1.84	0.78
2:B:393:ILE:HG21	2:B:398:TRP:HB2	1.65	0.78
1:A:503:LEU:CD2	1:A:535:TRP:HB2	2.15	0.77
1:A:136:ASN:C	1:A:138:GLU:H	1.91	0.77
1:A:57:ASN:ND2	1:A:58:THR:H	1.82	0.77
2:B:101:LYS:O	2:B:236:PRO:HB2	1.84	0.77
2:B:255:ASN:O	2:B:258:GLN:HB2	1.85	0.76
1:A:1:PRO:O	1:A:117:SER:HA	1.85	0.76
1:A:501:TYR:O	1:A:505:ILE:HG13	1.87	0.75
1:A:356:ARG:CZ	1:A:358:ARG:HD2	2.16	0.75
1:A:60:VAL:HG21	1:A:131:THR:O	1.87	0.75
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.20	0.75
1:A:178:ILE:N	1:A:178:ILE:HD12	2.02	0.75
2:B:257:ILE:O	2:B:261:VAL:HG23	1.86	0.75
1:A:545:ASN:H	1:A:545:ASN:ND2	1.83	0.75
2:B:361:HIS:H	2:B:361:HIS:HD2	1.34	0.74
2:B:27:THR:O	2:B:31:ILE:HD12	1.87	0.74
2:B:85:GLN:HG3	2:B:154:LYS:HB3	1.68	0.74
1:A:244:ILE:CD1	1:A:310:LEU:HD22	2.17	0.74
2:B:195:ILE:HG23	2:B:196:GLY:N	2.01	0.74
1:A:188:TYR:CD1	1:A:188:TYR:N	2.56	0.73
1:A:497:THR:HG22	1:A:499:SER:H	1.51	0.73
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.23	0.73
1:A:317:VAL:HG22	1:A:318:TYR:N	2.02	0.73
1:A:188:TYR:HD1	1:A:188:TYR:H	1.35	0.73
2:B:128:THR:OG1	2:B:146:TYR:HB2	1.88	0.73
1:A:417:VAL:O	1:A:419:THR:HG23	1.89	0.72
2:B:231:GLY:O	2:B:233:GLU:HG3	1.89	0.72
2:B:369:THR:O	2:B:373:GLN:HG3	1.88	0.72
1:A:181:TYR:HE2	1:A:183:TYR:HB2	1.54	0.72
2:B:118:VAL:HB	2:B:149:LEU:HG	1.71	0.72
1:A:542:ILE:HD13	1:A:543:GLY:H	1.53	0.72
2:B:223:LYS:O	2:B:225:PRO:HD3	1.88	0.72
1:A:288:ALA:HB1	1:A:291:GLU:HB2	1.70	0.72
1:A:427:TYR:OH	1:A:509:GLN:HA	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:THR:HG22	1:A:256:ASP:OD1	1.90	0.71
2:B:156:SER:N	2:B:157:PRO:HD2	2.04	0.71
2:B:114:ALA:HB2	2:B:214:LEU:HD22	1.72	0.71
1:A:500:GLN:H	1:A:500:GLN:HE21	1.38	0.71
1:A:132:ILE:HG22	1:A:142:ILE:O	1.91	0.71
1:A:181:TYR:C	1:A:181:TYR:CD2	2.69	0.71
2:B:222:GLN:HG2	2:B:223:LYS:N	2.05	0.70
2:B:274:ILE:HA	2:B:306:ASN:HD21	1.56	0.70
1:A:104:LYS:HG2	1:A:192:ASP:OD1	1.91	0.70
1:A:337:TRP:NE1	1:A:367:GLN:HE21	1.82	0.70
1:A:97:PRO:HA	1:A:100:LEU:HD12	1.73	0.70
2:B:365:VAL:HG12	2:B:365:VAL:O	1.92	0.70
2:B:253:THR:O	2:B:257:ILE:HG22	1.91	0.70
1:A:326:ILE:HD12	1:A:326:ILE:N	2.07	0.70
1:A:542:ILE:HD13	1:A:544:GLY:N	2.07	0.70
1:A:259:LYS:O	1:A:263:LYS:HG3	1.91	0.69
2:B:94:ILE:HG12	2:B:161:GLN:CD	2.16	0.69
1:A:317:VAL:HG12	1:A:348:ASN:O	1.93	0.69
1:A:5:ILE:HD11	1:A:167:ILE:HD11	1.75	0.69
2:B:5:ILE:HD13	2:B:118:VAL:HG13	1.74	0.69
2:B:252:TRP:O	2:B:292:VAL:HG13	1.92	0.69
1:A:7:THR:CG2	1:A:119:PRO:HB2	2.22	0.69
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.23	0.69
1:A:288:ALA:CB	1:A:291:GLU:CB	2.70	0.69
1:A:226:PRO:CG	1:A:235:HIS:CE1	2.66	0.68
1:A:325:LEU:HD21	1:A:383:TRP:CE3	2.28	0.68
1:A:301:LEU:O	1:A:305:GLU:HG3	1.93	0.68
1:A:458:VAL:HG22	1:A:464:GLN:CG	2.16	0.68
1:A:460:ASN:ND2	1:A:461:LYS:N	2.37	0.68
2:B:217:PRO:O	2:B:219:LYS:N	2.27	0.67
2:B:422:LEU:HD12	2:B:425:LEU:CD1	2.17	0.67
1:A:183:TYR:HE2	1:A:184:MET:SD	2.17	0.67
1:A:244:ILE:HD12	1:A:310:LEU:HD13	1.75	0.67
1:A:497:THR:CG2	1:A:498:ASP:N	2.57	0.67
1:A:542:ILE:CG1	1:A:543:GLY:H	2.06	0.67
1:A:112:GLY:C	1:A:114:ALA:H	2.00	0.67
1:A:465:LYS:HG3	1:A:466:VAL:N	2.09	0.67
1:A:478:GLU:OE2	1:A:497:THR:HG23	1.95	0.67
2:B:376:THR:HG21	2:B:410:TRP:CH2	2.30	0.66
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.30	0.66
1:A:318:TYR:CE1	4:A:600:185:H26	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:LEU:HD11	2:B:106:VAL:CG2	2.25	0.66
2:B:274:ILE:HA	2:B:306:ASN:ND2	2.10	0.66
2:B:350:LYS:HG2	2:B:351:THR:N	2.10	0.66
1:A:465:LYS:HG3	1:A:466:VAL:H	1.60	0.66
2:B:332:GLN:HB2	2:B:336:GLN:O	1.95	0.66
2:B:94:ILE:HG12	2:B:161:GLN:OE1	1.95	0.66
2:B:198:HIS:O	2:B:199:ARG:C	2.39	0.66
2:B:278:GLN:HG2	2:B:298:GLU:C	2.21	0.66
1:A:542:ILE:CD1	1:A:543:GLY:H	2.07	0.66
2:B:24:TRP:HE1	2:B:399:GLU:HG2	1.61	0.66
2:B:198:HIS:O	2:B:201:LYS:N	2.29	0.65
2:B:308:GLU:C	2:B:310:LEU:H	2.04	0.65
2:B:85:GLN:HG3	2:B:154:LYS:CB	2.26	0.65
2:B:350:LYS:HG2	2:B:351:THR:H	1.62	0.65
1:A:3:SER:OG	1:A:5:ILE:HG13	1.96	0.65
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.25	0.65
2:B:257:ILE:HG12	2:B:283:LEU:HD11	1.78	0.65
1:A:21:VAL:O	1:A:57:ASN:HB3	1.97	0.65
1:A:424:LYS:HD3	1:A:425:LEU:H	1.62	0.65
1:A:131:THR:OG1	1:A:143:ARG:HG3	1.96	0.65
1:A:55:PRO:HB2	1:A:143:ARG:CZ	2.27	0.64
2:B:278:GLN:O	2:B:281:LYS:HG2	1.97	0.64
1:A:98:ALA:CB	1:A:350:LYS:HB2	2.27	0.64
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.32	0.64
1:A:245:VAL:O	1:A:247:PRO:HD3	1.98	0.64
1:A:279:LEU:HD23	1:A:299:ALA:HB1	1.80	0.64
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.78	0.64
1:A:244:ILE:CD1	1:A:310:LEU:HD13	2.27	0.64
2:B:371:ALA:O	2:B:375:ILE:HG13	1.97	0.64
1:A:342:TYR:HA	1:A:349:LEU:HB2	1.80	0.64
1:A:478:GLU:HG2	1:A:499:SER:HB3	1.80	0.64
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.32	0.64
2:B:395:LYS:HG2	2:B:399:GLU:OE1	1.97	0.64
1:A:518:VAL:O	1:A:522:ILE:HG13	1.97	0.63
2:B:195:ILE:CG1	2:B:199:ARG:HE	2.11	0.63
2:B:361:HIS:CD2	2:B:361:HIS:N	2.66	0.63
1:A:341:ILE:HG21	1:A:383:TRP:CH2	2.34	0.63
1:A:494:ASN:HB3	2:B:289:LEU:HD12	1.80	0.63
1:A:276:VAL:HG12	1:A:276:VAL:O	1.98	0.63
1:A:328:GLU:HG2	1:A:390:LYS:CB	2.28	0.63
2:B:249:LYS:HB2	2:B:252:TRP:CZ3	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:TRP:C	2:B:268:SER:N	2.52	0.63
1:A:188:TYR:N	1:A:188:TYR:HD1	1.95	0.63
1:A:492:GLU:OE1	1:A:530:LYS:HD2	1.99	0.63
1:A:514:GLU:OE1	1:A:514:GLU:HA	1.98	0.63
1:A:95:PRO:HG3	1:A:181:TYR:CE1	2.34	0.62
1:A:497:THR:HG22	1:A:499:SER:N	2.13	0.62
1:A:543:GLY:HA3	2:B:284:ARG:HH11	1.64	0.62
1:A:64:LYS:O	1:A:64:LYS:HG3	1.99	0.62
1:A:173:LYS:O	1:A:176:PRO:HD3	1.99	0.62
1:A:195:ILE:O	1:A:199:ARG:HG3	2.00	0.62
1:A:341:ILE:O	1:A:349:LEU:HB3	2.00	0.62
1:A:362:THR:HG22	1:A:363:ASN:N	2.13	0.62
2:B:7:THR:CB	2:B:121:ASP:HA	2.28	0.62
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.32	0.62
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.34	0.62
2:B:131:THR:OG1	2:B:143:ARG:HG2	1.99	0.62
1:A:258:GLN:HE21	1:A:283:LEU:HD21	1.63	0.62
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.82	0.62
2:B:210:LEU:C	2:B:212:TRP:H	2.07	0.61
2:B:44:GLU:OE1	2:B:46:LYS:HE3	2.00	0.61
2:B:115:TYR:OH	2:B:184:MET:O	2.17	0.61
2:B:308:GLU:C	2:B:310:LEU:N	2.57	0.61
1:A:90:VAL:HG12	1:A:91:GLN:N	2.15	0.61
2:B:278:GLN:HE21	2:B:296:THR:CB	2.13	0.61
1:A:30:LYS:HD3	1:A:62:ALA:HB3	1.81	0.61
1:A:50:ILE:HD11	1:A:55:PRO:HG3	1.83	0.61
2:B:78:ARG:HD3	2:B:412:PRO:O	2.00	0.61
2:B:16:MET:HE3	2:B:16:MET:HA	1.83	0.61
2:B:287:LYS:HB3	2:B:287:LYS:HZ2	1.65	0.61
1:A:420:PRO:HA	1:A:421:PRO:O	2.01	0.61
2:B:5:ILE:CG1	2:B:6:GLU:N	2.54	0.61
1:A:136:ASN:C	1:A:138:GLU:N	2.59	0.61
2:B:50:ILE:HG13	2:B:143:ARG:HB3	1.82	0.61
1:A:95:PRO:HG2	1:A:229:TRP:CH2	2.35	0.61
1:A:288:ALA:HB3	1:A:291:GLU:HB3	1.83	0.60
1:A:460:ASN:HD21	1:A:461:LYS:HD3	1.66	0.60
2:B:5:ILE:CG1	2:B:6:GLU:H	2.14	0.60
1:A:408:ALA:O	2:B:393:ILE:HG13	2.01	0.60
1:A:287:LYS:CG	1:A:288:ALA:N	2.55	0.60
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.36	0.60
1:A:138:GLU:OE1	1:A:138:GLU:HA	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASN:N	1:A:55:PRO:HD3	2.16	0.60
1:A:224:GLU:CG	1:A:225:PRO:HD3	2.31	0.60
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.17	0.60
1:A:543:GLY:CA	2:B:284:ARG:HH11	2.15	0.59
1:A:183:TYR:HD2	1:A:184:MET:HG3	1.64	0.59
1:A:342:TYR:CD1	1:A:342:TYR:C	2.80	0.59
2:B:56:TYR:O	2:B:143:ARG:NH2	2.35	0.59
2:B:357:MET:HB3	2:B:361:HIS:CE1	2.37	0.59
1:A:220:LYS:HB3	1:A:222:GLN:HE22	1.68	0.59
2:B:100:LEU:O	2:B:100:LEU:HD12	2.02	0.59
1:A:194:GLU:O	1:A:196:GLY:N	2.35	0.59
2:B:277:ARG:HA	2:B:280:SER:OG	2.02	0.59
2:B:305:GLU:O	2:B:308:GLU:HB3	2.03	0.59
1:A:433:PRO:HB3	2:B:255:ASN:HD22	1.68	0.59
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.38	0.59
1:A:491:LEU:O	1:A:529:GLU:HB3	2.02	0.59
1:A:478:GLU:HG2	1:A:499:SER:CB	2.33	0.59
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.37	0.59
1:A:115:TYR:OH	1:A:151:GLN:HG3	2.03	0.59
1:A:326:ILE:CD1	1:A:343:GLN:HA	2.33	0.59
2:B:363:ASN:HD21	2:B:366:LYS:HB2	1.67	0.59
1:A:457:TYR:C	1:A:457:TYR:CD2	2.81	0.59
2:B:308:GLU:O	2:B:310:LEU:N	2.35	0.58
1:A:181:TYR:OH	1:A:183:TYR:HD1	1.85	0.58
1:A:182:GLN:HE21	1:A:182:GLN:N	1.99	0.58
2:B:168:LEU:C	2:B:170:PRO:HD2	2.28	0.58
2:B:267:ALA:HA	2:B:426:TRP:CZ2	2.38	0.58
2:B:339:TYR:C	2:B:340:GLN:OE1	2.47	0.58
1:A:178:ILE:CG1	1:A:201:LYS:HG2	2.32	0.58
1:A:112:GLY:C	1:A:114:ALA:N	2.55	0.58
2:B:298:GLU:HB3	2:B:301:LEU:HD13	1.86	0.58
1:A:224:GLU:O	1:A:226:PRO:O	2.21	0.58
2:B:265:ASN:O	2:B:268:SER:HB3	2.03	0.58
2:B:266:TRP:CZ3	2:B:346:PHE:CE2	2.91	0.58
2:B:267:ALA:HA	2:B:426:TRP:CH2	2.39	0.58
1:A:457:TYR:C	1:A:457:TYR:HD2	2.12	0.58
1:A:510:PRO:O	1:A:522:ILE:HD13	2.04	0.58
2:B:266:TRP:O	2:B:267:ALA:C	2.46	0.58
1:A:53:GLU:H	1:A:55:PRO:HD3	1.68	0.58
1:A:408:ALA:HB1	2:B:364:ASP:CB	2.33	0.58
1:A:417:VAL:HG12	1:A:419:THR:CG2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:SER:OG	1:A:198:HIS:ND1	2.36	0.57
2:B:12:LEU:HD12	2:B:12:LEU:N	2.10	0.57
2:B:27:THR:HG22	2:B:29:GLU:H	1.70	0.57
2:B:278:GLN:HG3	2:B:296:THR:OG1	2.03	0.57
2:B:419:THR:H	2:B:420:PRO:HD3	1.68	0.57
2:B:100:LEU:CD1	2:B:106:VAL:HG22	2.33	0.57
2:B:232:TYR:CE1	2:B:234:LEU:HD21	2.40	0.57
1:A:229:TRP:HB2	1:A:234:LEU:HD12	1.87	0.57
1:A:460:ASN:HD22	1:A:460:ASN:N	2.03	0.57
1:A:509:GLN:N	1:A:510:PRO:HD3	2.20	0.57
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.87	0.57
2:B:363:ASN:C	2:B:363:ASN:HD22	2.10	0.57
1:A:202:ILE:O	1:A:206:ARG:HB2	2.04	0.57
1:A:277:ARG:HD2	1:A:334:GLN:HB3	1.85	0.57
2:B:34:LEU:HD21	2:B:61:PHE:O	2.04	0.57
2:B:335:GLY:O	2:B:355:ALA:HA	2.05	0.57
1:A:417:VAL:O	1:A:417:VAL:HG12	2.05	0.57
2:B:84:THR:O	2:B:86:ASP:N	2.38	0.57
1:A:22:LYS:HG2	1:A:24:TRP:CZ2	2.40	0.57
1:A:178:ILE:HG12	1:A:201:LYS:CG	2.31	0.57
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.70	0.56
1:A:164:MET:O	1:A:167:ILE:N	2.33	0.56
2:B:183:TYR:O	2:B:184:MET:HB2	2.05	0.56
1:A:307:ARG:O	1:A:311:LYS:HB2	2.05	0.56
1:A:447:ASN:CG	1:A:450:THR:HG23	2.29	0.56
2:B:369:THR:HG22	2:B:373:GLN:HE21	1.70	0.56
1:A:124:PHE:CE2	1:A:153:TRP:CZ2	2.94	0.56
1:A:407:GLN:HG2	2:B:392:PRO:O	2.06	0.56
1:A:162:SER:O	1:A:163:SER:C	2.47	0.56
1:A:200:THR:O	1:A:203:GLU:N	2.39	0.56
2:B:91:GLN:O	2:B:92:LEU:HD23	2.05	0.56
2:B:210:LEU:HA	2:B:214:LEU:O	2.04	0.56
1:A:35:VAL:O	1:A:39:THR:HG23	2.04	0.56
1:A:241:VAL:CG1	1:A:266:TRP:HE1	2.18	0.56
2:B:75:VAL:HG11	2:B:77:PHE:CE2	2.40	0.56
2:B:325:LEU:HD12	2:B:385:LYS:HG3	1.87	0.56
1:A:33:ALA:HA	1:A:36:GLU:OE1	2.05	0.56
2:B:303:LEU:O	2:B:307:ARG:HB2	2.06	0.56
1:A:97:PRO:HA	1:A:100:LEU:CD1	2.35	0.56
2:B:50:ILE:CG1	2:B:143:ARG:HB3	2.36	0.56
2:B:314:VAL:HG13	2:B:317:VAL:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:376:THR:HG22	2:B:380:ILE:HD11	1.87	0.56
2:B:376:THR:O	2:B:380:ILE:HG13	2.06	0.56
1:A:288:ALA:HB3	1:A:291:GLU:CB	2.35	0.56
2:B:419:THR:O	2:B:420:PRO:C	2.49	0.56
1:A:125:ARG:HG2	1:A:146:TYR:O	2.06	0.55
1:A:183:TYR:CE2	1:A:184:MET:SD	2.99	0.55
1:A:238:LYS:HA	1:A:316:GLY:O	2.07	0.55
2:B:4:PRO:HG3	2:B:117:SER:O	2.07	0.55
2:B:275:LYS:HB2	2:B:302:GLU:OE1	2.06	0.55
1:A:96:HIS:CD2	1:A:98:ALA:HB3	2.41	0.55
2:B:53:GLU:O	2:B:55:PRO:HD3	2.06	0.55
2:B:125:ARG:O	2:B:126:LYS:C	2.50	0.55
2:B:261:VAL:HG21	2:B:283:LEU:HD12	1.87	0.55
1:A:96:HIS:HE1	1:A:269:GLN:NE2	2.05	0.55
2:B:139:THR:CG2	2:B:140:PRO:HD2	2.30	0.55
2:B:366:LYS:O	2:B:370:GLU:HG3	2.07	0.55
1:A:69:THR:CG2	1:A:70:LYS:HE2	2.37	0.55
1:A:226:PRO:HG3	1:A:235:HIS:NE2	2.18	0.55
1:A:232:TYR:HE2	1:A:269:GLN:HE22	1.51	0.55
1:A:317:VAL:CG2	1:A:318:TYR:H	2.17	0.55
2:B:125:ARG:HD3	2:B:147:ASN:HA	1.89	0.55
2:B:206:ARG:HB3	2:B:206:ARG:CZ	2.33	0.55
1:A:84:THR:HG22	1:A:124:PHE:CZ	2.33	0.55
2:B:271:TYR:HD2	2:B:274:ILE:HD11	1.71	0.55
1:A:95:PRO:O	1:A:229:TRP:HH2	1.88	0.55
1:A:247:PRO:O	1:A:252:TRP:HH2	1.90	0.55
1:A:402:TRP:HE3	1:A:402:TRP:O	1.89	0.55
2:B:178:ILE:HD11	2:B:201:LYS:HG2	1.88	0.55
2:B:278:GLN:HA	2:B:281:LYS:HE3	1.89	0.55
1:A:94:ILE:HG12	1:A:183:TYR:HE1	1.72	0.55
2:B:254:VAL:O	2:B:258:GLN:HG3	2.06	0.55
1:A:17:ASP:OD2	1:A:56:TYR:HE2	1.90	0.54
1:A:34:LEU:HB3	1:A:132:ILE:HD12	1.88	0.54
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.72	0.54
1:A:365:VAL:O	1:A:368:LEU:HB3	2.07	0.54
2:B:195:ILE:CG2	2:B:196:GLY:H	2.16	0.54
1:A:460:ASN:ND2	1:A:461:LYS:HD3	2.22	0.54
2:B:77:PHE:CD1	2:B:80:LEU:HD23	2.42	0.54
1:A:356:ARG:HE	1:A:370:GLU:CD	2.15	0.54
1:A:79:GLU:HG3	1:A:83:ARG:HH12	1.72	0.54
1:A:96:HIS:CE1	1:A:350:LYS:HE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:GLN:OE1	1:A:340:GLN:NE2	2.39	0.54
1:A:377:THR:O	1:A:381:VAL:HG23	2.08	0.54
2:B:359:GLY:O	2:B:361:HIS:N	2.41	0.54
2:B:369:THR:HG23	2:B:406:TRP:HE3	1.73	0.54
1:A:467:VAL:HG23	1:A:484:LEU:HD21	1.90	0.54
1:A:390:LYS:O	1:A:391:LEU:HD23	2.07	0.54
1:A:424:LYS:CD	1:A:425:LEU:H	2.20	0.54
2:B:376:THR:O	2:B:379:SER:HB3	2.07	0.54
1:A:198:HIS:O	1:A:202:ILE:HG12	2.08	0.54
1:A:208:HIS:HA	1:A:211:ARG:NH1	2.22	0.54
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.43	0.54
2:B:129:ALA:HA	2:B:145:GLN:HA	1.89	0.54
2:B:282:LEU:HG	2:B:293:ILE:HD12	1.90	0.54
2:B:103:LYS:HD2	2:B:191:SER:CA	2.39	0.53
2:B:195:ILE:CD1	2:B:199:ARG:HE	2.22	0.53
1:A:95:PRO:HG3	1:A:181:TYR:HE1	1.73	0.53
2:B:332:GLN:HA	2:B:332:GLN:OE1	2.09	0.53
1:A:155:GLY:O	1:A:159:ILE:HG13	2.08	0.53
2:B:131:THR:OG1	2:B:143:ARG:NH1	2.41	0.53
2:B:341:ILE:HD11	2:B:375:ILE:HG23	1.90	0.53
1:A:228:LEU:HD12	1:A:228:LEU:H	1.74	0.53
1:A:465:LYS:CG	1:A:466:VAL:N	2.71	0.53
1:A:181:TYR:C	1:A:181:TYR:HD2	2.17	0.53
1:A:434:ILE:HB	1:A:494:ASN:OD1	2.08	0.53
2:B:202:ILE:O	2:B:205:LEU:HB3	2.08	0.53
2:B:279:LEU:C	2:B:281:LYS:H	2.17	0.53
1:A:81:ASN:C	1:A:83:ARG:H	2.17	0.53
1:A:106:VAL:HG12	1:A:107:THR:N	2.24	0.53
1:A:135:ILE:HG22	1:A:137:ASN:N	2.15	0.53
1:A:139:THR:HG22	1:A:140:PRO:HD2	1.90	0.53
1:A:178:ILE:N	1:A:178:ILE:CD1	2.70	0.53
1:A:223:LYS:HE2	1:A:228:LEU:HG	1.89	0.53
1:A:254:VAL:O	1:A:257:ILE:HG22	2.08	0.53
1:A:331:LYS:HB2	1:A:337:TRP:CZ3	2.44	0.53
1:A:496:VAL:HG22	1:A:534:ALA:HB3	1.91	0.53
2:B:21:VAL:O	2:B:57:ASN:ND2	2.41	0.53
1:A:114:ALA:O	1:A:116:PHE:N	2.42	0.53
1:A:239:TRP:O	1:A:240:THR:HB	2.08	0.53
2:B:363:ASN:C	2:B:363:ASN:ND2	2.67	0.53
2:B:300:GLU:OE1	2:B:300:GLU:HA	2.10	0.52
2:B:326:ILE:O	2:B:341:ILE:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:THR:O	1:A:290:THR:HG22	2.08	0.52
1:A:312:GLU:O	1:A:312:GLU:HG2	2.09	0.52
1:A:442:VAL:CG1	1:A:485:ALA:HB2	2.38	0.52
2:B:164:MET:O	2:B:167:ILE:N	2.42	0.52
1:A:49:LYS:HA	1:A:143:ARG:O	2.10	0.52
2:B:107:THR:HA	2:B:232:TYR:O	2.09	0.52
2:B:266:TRP:CZ3	2:B:269:GLN:HB2	2.44	0.52
1:A:382:ILE:CA	2:B:136:ASN:HD22	2.20	0.52
2:B:219:LYS:O	2:B:221:HIS:N	2.43	0.52
1:A:277:ARG:HD2	1:A:334:GLN:CB	2.40	0.52
2:B:72:ARG:NH2	2:B:409:THR:HG22	2.25	0.52
2:B:111:VAL:O	2:B:113:ASP:N	2.43	0.52
2:B:341:ILE:HD11	2:B:375:ILE:CG2	2.38	0.52
1:A:38:CYS:HB3	1:A:144:TYR:CE2	2.44	0.52
1:A:479:LEU:O	1:A:482:ILE:N	2.43	0.52
2:B:195:ILE:O	2:B:196:GLY:C	2.53	0.52
1:A:54:ASN:N	1:A:55:PRO:CD	2.73	0.52
1:A:317:VAL:CG2	1:A:318:TYR:N	2.73	0.52
1:A:324:ASP:O	1:A:343:GLN:HG2	2.10	0.52
1:A:333:GLY:C	1:A:335:GLY:H	2.18	0.52
1:A:398:TRP:CZ2	1:A:411:ILE:HG12	2.45	0.52
1:A:417:VAL:HG12	1:A:419:THR:HG23	1.92	0.52
1:A:10:VAL:HG12	1:A:11:LYS:N	2.24	0.52
1:A:232:TYR:OH	1:A:269:GLN:NE2	2.43	0.52
2:B:125:ARG:C	2:B:127:TYR:N	2.68	0.52
2:B:252:TRP:HA	2:B:252:TRP:CE3	2.45	0.52
2:B:255:ASN:OD1	2:B:259:LYS:HE3	2.10	0.52
2:B:337:TRP:NE1	2:B:367:GLN:HB3	2.24	0.51
1:A:5:ILE:CD1	1:A:167:ILE:HD11	2.40	0.51
1:A:188:TYR:HD2	4:A:600:185:C4'	2.23	0.51
1:A:318:TYR:HE1	4:A:600:185:C26	2.17	0.51
1:A:406:TRP:CZ3	1:A:407:GLN:HG3	2.46	0.51
2:B:17:ASP:O	2:B:18:GLY:O	2.28	0.51
2:B:96:HIS:HE1	2:B:381:VAL:O	1.92	0.51
2:B:149:LEU:N	2:B:149:LEU:HD23	2.24	0.51
2:B:296:THR:H	2:B:299:ALA:HB3	1.75	0.51
2:B:354:TYR:OH	2:B:370:GLU:OE1	2.27	0.51
1:A:382:ILE:HG23	2:B:136:ASN:ND2	2.24	0.51
2:B:99:GLY:O	2:B:102:LYS:HB2	2.10	0.51
1:A:206:ARG:HH22	1:A:217:PRO:C	2.18	0.51
1:A:158:ALA:C	1:A:160:PHE:N	2.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:LYS:HD3	1:A:425:LEU:C	2.36	0.51
2:B:266:TRP:HZ3	2:B:346:PHE:CE2	2.29	0.51
2:B:419:THR:H	2:B:420:PRO:CD	2.24	0.51
1:A:341:ILE:O	1:A:349:LEU:CB	2.59	0.51
1:A:496:VAL:CG2	1:A:534:ALA:HB3	2.41	0.51
2:B:130:PHE:CE2	2:B:144:TYR:HB2	2.46	0.51
1:A:241:VAL:HG13	1:A:266:TRP:HE1	1.76	0.51
2:B:30:LYS:HD2	2:B:62:ALA:HB3	1.91	0.51
2:B:194:GLU:O	2:B:195:ILE:C	2.53	0.51
2:B:198:HIS:O	2:B:200:THR:N	2.44	0.51
2:B:252:TRP:HA	2:B:252:TRP:HE3	1.75	0.51
2:B:277:ARG:HA	2:B:280:SER:HG	1.75	0.51
2:B:357:MET:CB	2:B:361:HIS:CE1	2.93	0.51
1:A:276:VAL:O	1:A:276:VAL:CG1	2.58	0.51
1:A:424:LYS:CD	1:A:425:LEU:N	2.70	0.51
1:A:460:ASN:ND2	1:A:461:LYS:CD	2.74	0.50
2:B:278:GLN:HE21	2:B:296:THR:HB	1.75	0.50
2:B:278:GLN:NE2	2:B:296:THR:OG1	2.43	0.50
2:B:364:ASP:C	2:B:366:LYS:H	2.19	0.50
1:A:323:LYS:NZ	1:A:344:GLU:OE2	2.41	0.50
1:A:288:ALA:HB1	1:A:291:GLU:CB	2.35	0.50
1:A:542:ILE:CG1	1:A:543:GLY:N	2.75	0.50
2:B:4:PRO:CG	2:B:117:SER:O	2.60	0.50
2:B:314:VAL:HG13	2:B:317:VAL:CG2	2.42	0.50
2:B:271:TYR:CE2	2:B:310:LEU:HA	2.47	0.50
1:A:34:LEU:HB2	1:A:132:ILE:HD11	1.92	0.50
1:A:95:PRO:HG2	1:A:229:TRP:HH2	1.76	0.50
1:A:132:ILE:HG23	1:A:132:ILE:O	2.12	0.50
2:B:301:LEU:O	2:B:305:GLU:HB3	2.11	0.50
1:A:325:LEU:HD23	1:A:387:PRO:HB3	1.93	0.50
1:A:503:LEU:O	1:A:504:GLY:C	2.54	0.50
2:B:124:PHE:O	2:B:125:ARG:C	2.54	0.50
1:A:59:PRO:O	1:A:75:VAL:HG13	2.11	0.49
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.46	0.49
1:A:136:ASN:OD1	1:A:136:ASN:N	2.37	0.49
1:A:182:GLN:H	1:A:182:GLN:NE2	2.00	0.49
1:A:362:THR:CG2	1:A:363:ASN:H	2.21	0.49
1:A:490:GLY:C	1:A:492:GLU:H	2.20	0.49
1:A:515:SER:O	1:A:517:LEU:N	2.44	0.49
2:B:85:GLN:NE2	2:B:89:GLU:HB2	2.27	0.49
2:B:203:GLU:HG3	2:B:207:GLN:HE22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:O	1:A:41:MET:HB2	2.12	0.49
1:A:84:THR:CG2	1:A:124:PHE:HZ	2.20	0.49
1:A:286:THR:O	1:A:286:THR:HG22	2.13	0.49
2:B:262:GLY:O	2:B:263:LYS:C	2.54	0.49
2:B:304:ALA:HA	2:B:307:ARG:HB2	1.93	0.49
2:B:346:PHE:N	2:B:346:PHE:CD1	2.80	0.49
1:A:22:LYS:O	1:A:23:GLN:CD	2.55	0.49
1:A:283:LEU:C	1:A:285:GLY:N	2.68	0.49
1:A:326:ILE:HB	1:A:342:TYR:CE1	2.47	0.49
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.48	0.49
2:B:5:ILE:HD13	2:B:118:VAL:CG1	2.40	0.49
2:B:195:ILE:CD1	2:B:199:ARG:NE	2.75	0.49
2:B:2:ILE:HG13	2:B:4:PRO:CD	2.33	0.49
2:B:94:ILE:HA	2:B:161:GLN:OE1	2.13	0.49
2:B:319:TYR:CE2	2:B:321:PRO:HG3	2.48	0.49
2:B:253:THR:HG22	2:B:292:VAL:HG22	1.93	0.49
1:A:442:VAL:HG13	1:A:485:ALA:HB2	1.95	0.49
2:B:370:GLU:O	2:B:371:ALA:C	2.54	0.49
2:B:382:ILE:HG22	2:B:383:TRP:CD2	2.48	0.49
1:A:96:HIS:HD2	1:A:98:ALA:HB3	1.77	0.49
1:A:115:TYR:CE2	1:A:151:GLN:HA	2.48	0.49
1:A:260:LEU:HD21	1:A:279:LEU:HD13	1.95	0.49
2:B:296:THR:H	2:B:299:ALA:CB	2.25	0.48
2:B:153:TRP:C	2:B:155:GLY:H	2.20	0.48
2:B:416:PHE:CD2	2:B:416:PHE:N	2.80	0.48
1:A:102:LYS:HG3	1:A:102:LYS:O	2.13	0.48
1:A:460:ASN:ND2	1:A:460:ASN:N	2.60	0.48
4:A:600:185:H22	4:A:600:185:N12	2.29	0.48
2:B:7:THR:CG2	2:B:121:ASP:HA	2.43	0.48
2:B:115:TYR:C	2:B:117:SER:H	2.21	0.48
2:B:276:VAL:O	2:B:279:LEU:N	2.33	0.48
1:A:158:ALA:C	1:A:160:PHE:H	2.21	0.48
1:A:171:PHE:HB2	1:A:208:HIS:CD2	2.48	0.48
1:A:208:HIS:CE1	1:A:212:TRP:HE1	2.31	0.48
1:A:484:LEU:O	1:A:485:ALA:C	2.55	0.48
2:B:308:GLU:O	2:B:311:LYS:N	2.45	0.48
2:B:379:SER:OG	2:B:387:PRO:HD3	2.14	0.48
1:A:236:PRO:HA	4:A:600:185:H25	1.94	0.48
1:A:284:ARG:HG3	1:A:285:GLY:N	2.29	0.48
1:A:325:LEU:C	1:A:326:ILE:HD12	2.39	0.48
2:B:305:GLU:HG3	2:B:306:ASN:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:GLU:O	1:A:54:ASN:HB3	2.13	0.48
1:A:90:VAL:HG12	1:A:91:GLN:H	1.79	0.48
1:A:329:ILE:HD12	1:A:391:LEU:HD22	1.95	0.48
1:A:341:ILE:HG21	1:A:383:TRP:CZ3	2.49	0.48
2:B:31:ILE:HG22	2:B:35:VAL:CG2	2.43	0.48
1:A:273:GLY:O	1:A:274:ILE:C	2.54	0.48
1:A:339:TYR:HE2	1:A:341:ILE:HD11	1.77	0.48
2:B:257:ILE:HG23	2:B:283:LEU:HD21	1.95	0.48
2:B:315:HIS:C	2:B:317:VAL:HG22	2.39	0.48
1:A:81:ASN:O	1:A:83:ARG:N	2.47	0.48
1:A:473:THR:HG23	1:A:476:LYS:H	1.77	0.48
2:B:364:ASP:O	2:B:366:LYS:N	2.47	0.48
1:A:57:ASN:ND2	1:A:58:THR:N	2.58	0.48
1:A:98:ALA:HB2	1:A:350:LYS:HB2	1.94	0.48
1:A:482:ILE:HD12	1:A:502:ALA:HB1	1.95	0.48
1:A:95:PRO:CD	1:A:181:TYR:HE1	2.27	0.47
1:A:170:PRO:HG2	1:A:171:PHE:H	1.79	0.47
1:A:503:LEU:HD12	1:A:533:LEU:HD13	1.96	0.47
1:A:514:GLU:O	1:A:516:GLU:N	2.47	0.47
2:B:114:ALA:CB	2:B:214:LEU:HD22	2.43	0.47
2:B:342:TYR:CD1	2:B:342:TYR:C	2.92	0.47
1:A:96:HIS:CD2	1:A:98:ALA:H	2.32	0.47
1:A:41:MET:HG2	1:A:47:ILE:HG23	1.95	0.47
1:A:282:LEU:HD11	1:A:299:ALA:HB2	1.95	0.47
2:B:13:LYS:O	2:B:16:MET:CB	2.58	0.47
2:B:18:GLY:HA3	2:B:56:TYR:CE1	2.49	0.47
2:B:195:ILE:O	2:B:198:HIS:N	2.48	0.47
2:B:222:GLN:CG	2:B:223:LYS:H	2.15	0.47
2:B:314:VAL:CG1	2:B:317:VAL:HG11	2.43	0.47
2:B:376:THR:CG2	2:B:410:TRP:CH2	2.97	0.47
1:A:57:ASN:HD22	1:A:58:THR:H	1.58	0.47
1:A:434:ILE:HG21	1:A:492:GLU:OE2	2.15	0.47
2:B:31:ILE:C	2:B:35:VAL:HG23	2.38	0.47
2:B:164:MET:O	2:B:165:THR:C	2.56	0.47
2:B:326:ILE:HB	2:B:342:TYR:CE1	2.50	0.47
1:A:8:VAL:O	1:A:10:VAL:HG23	2.15	0.47
1:A:244:ILE:HD11	1:A:310:LEU:CD2	2.31	0.47
2:B:207:GLN:HE21	2:B:207:GLN:HB2	1.52	0.47
1:A:81:ASN:C	1:A:83:ARG:N	2.72	0.47
1:A:264:LEU:CD1	1:A:279:LEU:HD12	2.44	0.47
1:A:320:ASP:OD2	1:A:323:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:GLY:O	1:A:542:ILE:O	2.31	0.47
1:A:542:ILE:HG12	1:A:543:GLY:H	1.80	0.47
2:B:50:ILE:HD13	2:B:129:ALA:HB1	1.97	0.47
2:B:178:ILE:HG23	2:B:190:GLY:O	2.15	0.47
1:A:17:ASP:O	1:A:83:ARG:HD3	2.15	0.47
1:A:208:HIS:HE1	1:A:212:TRP:HE1	1.61	0.47
1:A:339:TYR:CG	1:A:375:ILE:HD11	2.50	0.47
1:A:344:GLU:HA	1:A:345:PRO:HD3	1.65	0.47
2:B:178:ILE:CG2	2:B:189:VAL:HG12	2.44	0.47
1:A:100:LEU:O	1:A:318:TYR:HB3	2.15	0.47
1:A:235:HIS:HB2	1:A:238:LYS:HG3	1.97	0.47
2:B:76:ASP:C	2:B:78:ARG:H	2.23	0.47
2:B:161:GLN:O	2:B:162:SER:C	2.58	0.47
2:B:278:GLN:CD	2:B:298:GLU:H	2.22	0.47
2:B:329:ILE:HD11	2:B:375:ILE:HD12	1.96	0.47
1:A:98:ALA:HB1	1:A:350:LYS:HB2	1.95	0.47
1:A:241:VAL:CG1	1:A:266:TRP:NE1	2.78	0.47
1:A:279:LEU:CD2	1:A:299:ALA:HB1	2.45	0.47
1:A:309:ILE:O	1:A:312:GLU:CD	2.58	0.47
1:A:326:ILE:CD1	1:A:342:TYR:O	2.63	0.47
1:A:342:TYR:C	1:A:342:TYR:HD1	2.22	0.47
1:A:529:GLU:C	1:A:530:LYS:HG3	2.40	0.47
2:B:148:VAL:O	2:B:149:LEU:C	2.57	0.47
2:B:373:GLN:HE22	2:B:406:TRP:HA	1.80	0.47
1:A:11:LYS:O	1:A:85:GLN:HG2	2.15	0.46
1:A:91:GLN:O	1:A:92:LEU:C	2.57	0.46
1:A:102:LYS:HA	1:A:318:TYR:HD1	1.81	0.46
1:A:160:PHE:C	1:A:162:SER:N	2.72	0.46
1:A:497:THR:CG2	1:A:498:ASP:H	2.26	0.46
2:B:48:SER:O	2:B:144:TYR:HA	2.14	0.46
2:B:145:GLN:O	2:B:145:GLN:HG3	2.15	0.46
1:A:55:PRO:HB2	1:A:143:ARG:NH2	2.30	0.46
2:B:23:GLN:HG3	2:B:24:TRP:O	2.15	0.46
2:B:120:LEU:O	2:B:121:ASP:C	2.58	0.46
2:B:362:THR:HG21	2:B:367:GLN:HG3	1.97	0.46
1:A:27:THR:CG2	1:A:29:GLU:HG2	2.37	0.46
1:A:229:TRP:O	1:A:231:GLY:N	2.49	0.46
1:A:326:ILE:N	1:A:326:ILE:CD1	2.77	0.46
1:A:328:GLU:HG2	1:A:390:LYS:HB3	1.97	0.46
1:A:542:ILE:O	2:B:284:ARG:HD2	2.16	0.46
2:B:332:GLN:HE21	2:B:338:THR:CG2	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:362:THR:OG1	2:B:366:LYS:NZ	2.48	0.46
1:A:34:LEU:HD12	1:A:132:ILE:HG13	1.97	0.46
1:A:101:LYS:HB3	4:A:600:185:H181	1.98	0.46
1:A:158:ALA:O	1:A:160:PHE:N	2.48	0.46
1:A:247:PRO:O	1:A:252:TRP:CH2	2.69	0.46
1:A:306:ASN:HA	1:A:309:ILE:HD12	1.98	0.46
1:A:519:ASN:O	1:A:520:GLN:C	2.57	0.46
2:B:197:GLN:O	2:B:198:HIS:C	2.58	0.46
2:B:266:TRP:C	2:B:268:SER:H	2.22	0.46
2:B:277:ARG:H	2:B:277:ARG:CD	2.11	0.46
2:B:332:GLN:CG	2:B:338:THR:HG23	2.45	0.46
1:A:328:GLU:CG	1:A:390:LYS:HB2	2.44	0.46
1:A:416:PHE:CD1	1:A:417:VAL:N	2.84	0.46
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.98	0.46
2:B:326:ILE:HB	2:B:342:TYR:CD1	2.51	0.46
1:A:328:GLU:O	1:A:339:TYR:HB2	2.15	0.46
1:A:420:PRO:HA	1:A:421:PRO:C	2.39	0.46
1:A:443:ASP:OD2	1:A:545:ASN:HB3	2.16	0.46
2:B:76:ASP:O	2:B:76:ASP:CG	2.58	0.46
2:B:315:HIS:C	2:B:317:VAL:N	2.72	0.46
1:A:78:ARG:CG	1:A:79:GLU:N	2.78	0.46
1:A:97:PRO:HG2	1:A:232:TYR:CG	2.51	0.46
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.50	0.46
1:A:135:ILE:HG22	1:A:137:ASN:CB	2.45	0.46
1:A:186:ASP:HB2	1:A:188:TYR:HE1	1.80	0.46
1:A:442:VAL:O	1:A:443:ASP:HB2	2.16	0.46
2:B:80:LEU:HD11	2:B:124:PHE:HZ	1.81	0.46
2:B:120:LEU:HD21	2:B:124:PHE:HD2	1.81	0.46
1:A:34:LEU:HB2	1:A:132:ILE:CD1	2.46	0.46
1:A:406:TRP:CZ3	2:B:420:PRO:HD2	2.51	0.46
1:A:33:ALA:O	1:A:37:ILE:HG12	2.16	0.46
1:A:101:LYS:H	4:A:600:185:H181	1.81	0.46
1:A:339:TYR:CD1	1:A:375:ILE:HD11	2.51	0.46
2:B:171:PHE:C	2:B:173:LYS:N	2.73	0.46
2:B:179:VAL:HG23	2:B:179:VAL:O	2.15	0.46
2:B:109:LEU:O	2:B:186:ASP:HB3	2.16	0.45
2:B:259:LYS:O	2:B:262:GLY:N	2.46	0.45
1:A:163:SER:O	1:A:167:ILE:HG13	2.15	0.45
1:A:376:THR:O	1:A:380:ILE:HG13	2.17	0.45
2:B:187:LEU:HD12	2:B:187:LEU:HA	1.82	0.45
2:B:395:LYS:CG	2:B:399:GLU:OE1	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ASP:HB2	1:A:188:TYR:CE1	2.51	0.45
1:A:356:ARG:NE	1:A:358:ARG:HD2	2.31	0.45
2:B:80:LEU:HD11	2:B:124:PHE:CZ	2.51	0.45
2:B:197:GLN:O	2:B:200:THR:HB	2.17	0.45
2:B:279:LEU:C	2:B:281:LYS:N	2.72	0.45
1:A:315:HIS:CD2	1:A:347:LYS:HD3	2.51	0.45
1:A:393:ILE:HD12	1:A:423:VAL:CG1	2.47	0.45
1:A:121:ASP:O	1:A:122:GLU:C	2.58	0.45
1:A:497:THR:CG2	1:A:499:SER:H	2.24	0.45
2:B:53:GLU:OE1	2:B:53:GLU:N	2.44	0.45
2:B:261:VAL:HG21	2:B:283:LEU:CD1	2.47	0.45
2:B:388:LYS:NZ	2:B:415:GLU:OE1	2.41	0.45
2:B:10:VAL:HA	2:B:88:TRP:CZ2	2.51	0.45
2:B:60:VAL:HG13	2:B:130:PHE:HB2	1.99	0.45
2:B:85:GLN:O	2:B:89:GLU:N	2.50	0.45
2:B:363:ASN:HD22	2:B:363:ASN:H	1.63	0.45
2:B:302:GLU:HA	2:B:305:GLU:HB3	1.99	0.45
1:A:56:TYR:N	1:A:56:TYR:CD1	2.84	0.45
1:A:168:LEU:O	1:A:169:GLU:C	2.59	0.45
1:A:439:THR:CG2	1:A:441:TYR:CE1	3.00	0.45
1:A:183:TYR:O	1:A:184:MET:HB2	2.17	0.45
1:A:252:TRP:O	1:A:292:VAL:HG13	2.17	0.45
1:A:326:ILE:HD13	1:A:343:GLN:HA	1.98	0.45
1:A:501:TYR:CD1	1:A:505:ILE:HD11	2.52	0.45
2:B:58:THR:HA	2:B:59:PRO:HD3	1.87	0.45
2:B:245:VAL:HG12	2:B:246:LEU:O	2.17	0.45
2:B:332:GLN:HB2	2:B:336:GLN:C	2.42	0.45
1:A:3:SER:HB2	1:A:4:PRO:HD2	1.98	0.44
1:A:34:LEU:CB	1:A:132:ILE:HD12	2.47	0.44
1:A:183:TYR:CD2	1:A:183:TYR:C	2.95	0.44
1:A:235:HIS:HB2	1:A:238:LYS:CG	2.48	0.44
2:B:10:VAL:HA	2:B:88:TRP:HZ2	1.83	0.44
2:B:203:GLU:HG3	2:B:207:GLN:NE2	2.32	0.44
2:B:203:GLU:HA	2:B:206:ARG:HG3	1.99	0.44
2:B:319:TYR:O	2:B:321:PRO:HD3	2.18	0.44
1:A:241:VAL:HG11	1:A:266:TRP:CD1	2.51	0.44
1:A:356:ARG:HH11	1:A:356:ARG:CG	2.31	0.44
2:B:326:ILE:CG2	2:B:342:TYR:CE1	3.01	0.44
2:B:332:GLN:HG2	2:B:338:THR:HG23	1.99	0.44
1:A:13:LYS:CB	1:A:14:PRO:HD2	2.17	0.44
2:B:103:LYS:HD2	2:B:191:SER:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:ARG:C	2:B:127:TYR:H	2.25	0.44
2:B:151:GLN:HB3	2:B:185:ASP:OD2	2.16	0.44
2:B:168:LEU:CD1	2:B:180:ILE:HG21	2.47	0.44
1:A:125:ARG:O	1:A:128:THR:OG1	2.31	0.44
1:A:470:THR:O	1:A:471:ASN:HB3	2.17	0.44
1:A:542:ILE:HD13	1:A:543:GLY:N	2.27	0.44
2:B:171:PHE:C	2:B:171:PHE:CD1	2.95	0.44
1:A:435:VAL:HG22	2:B:290:THR:CG2	2.47	0.44
1:A:136:ASN:O	1:A:138:GLU:N	2.51	0.44
1:A:335:GLY:HA2	1:A:367:GLN:HE22	1.82	0.44
1:A:395:LYS:C	1:A:397:THR:H	2.26	0.44
1:A:487:GLN:HA	1:A:524:GLN:OE1	2.18	0.44
2:B:349:LEU:HB3	2:B:383:TRP:HZ2	1.83	0.44
1:A:96:HIS:CE1	1:A:269:GLN:NE2	2.86	0.44
1:A:117:SER:HB2	1:A:214:LEU:HD23	2.00	0.44
2:B:96:HIS:CE1	2:B:381:VAL:O	2.70	0.44
2:B:419:THR:N	2:B:420:PRO:CD	2.80	0.44
1:A:411:ILE:HA	1:A:412:PRO:HD3	1.70	0.44
1:A:411:ILE:HD12	1:A:414:TRP:CD1	2.52	0.44
2:B:153:TRP:O	2:B:155:GLY:N	2.39	0.44
2:B:255:ASN:O	2:B:258:GLN:N	2.50	0.44
1:A:39:THR:O	1:A:43:LYS:HB2	2.18	0.44
1:A:483:TYR:O	1:A:487:GLN:HG3	2.17	0.44
1:A:30:LYS:C	1:A:32:LYS:N	2.74	0.43
1:A:395:LYS:C	1:A:397:THR:N	2.74	0.43
1:A:503:LEU:HG	1:A:507:GLN:NE2	2.33	0.43
2:B:111:VAL:C	2:B:113:ASP:N	2.76	0.43
2:B:156:SER:N	2:B:157:PRO:CD	2.76	0.43
2:B:191:SER:OG	2:B:198:HIS:ND1	2.31	0.43
2:B:195:ILE:HD11	2:B:199:ARG:CZ	2.47	0.43
1:A:10:VAL:CG1	1:A:11:LYS:N	2.81	0.43
1:A:178:ILE:HD11	1:A:201:LYS:NZ	2.33	0.43
1:A:232:TYR:HE2	1:A:269:GLN:NE2	2.15	0.43
1:A:367:GLN:O	1:A:368:LEU:C	2.59	0.43
1:A:384:GLY:O	2:B:27:THR:HG23	2.18	0.43
1:A:452:LEU:HD22	1:A:470:THR:HG22	2.00	0.43
2:B:90:VAL:HG12	2:B:91:GLN:N	2.32	0.43
2:B:266:TRP:O	2:B:268:SER:N	2.52	0.43
2:B:331:LYS:HA	2:B:337:TRP:CE3	2.53	0.43
1:A:5:ILE:HG22	1:A:6:GLU:O	2.17	0.43
1:A:285:GLY:O	1:A:287:LYS:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:LYS:HG3	2:B:14:PRO:HD2	2.00	0.43
2:B:125:ARG:HD3	2:B:147:ASN:OD1	2.18	0.43
1:A:162:SER:HB2	2:B:52:PRO:CG	2.48	0.43
1:A:279:LEU:HG	1:A:302:GLU:OE1	2.18	0.43
2:B:43:LYS:C	2:B:45:GLY:H	2.26	0.43
2:B:362:THR:CG2	2:B:363:ASN:N	2.81	0.43
2:B:363:ASN:ND2	2:B:363:ASN:H	2.17	0.43
2:B:363:ASN:ND2	2:B:363:ASN:O	2.49	0.43
2:B:393:ILE:CG2	2:B:398:TRP:HB2	2.41	0.43
1:A:50:ILE:CD1	1:A:55:PRO:HG3	2.48	0.43
1:A:112:GLY:O	1:A:114:ALA:N	2.52	0.43
1:A:356:ARG:NH2	1:A:358:ARG:HD2	2.34	0.43
1:A:394:GLN:O	1:A:395:LYS:C	2.61	0.43
2:B:22:LYS:HG2	2:B:23:GLN:N	2.34	0.43
2:B:417:VAL:HG23	2:B:417:VAL:O	2.19	0.43
1:A:95:PRO:CG	1:A:181:TYR:HE1	2.32	0.43
1:A:229:TRP:O	1:A:230:MET:C	2.60	0.43
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.99	0.43
1:A:493:VAL:HG22	1:A:494:ASN:N	2.32	0.43
1:A:17:ASP:O	1:A:83:ARG:CD	2.67	0.43
1:A:406:TRP:HH2	2:B:418:ASN:CA	2.18	0.43
2:B:205:LEU:O	2:B:206:ARG:C	2.61	0.43
2:B:295:LEU:HD23	2:B:295:LEU:H	1.83	0.43
1:A:73:LYS:NZ	1:A:130:PHE:CE2	2.83	0.43
2:B:306:ASN:HA	2:B:309:ILE:HG22	2.00	0.43
1:A:34:LEU:C	1:A:36:GLU:N	2.74	0.43
1:A:162:SER:O	1:A:164:MET:N	2.52	0.43
1:A:226:PRO:HG3	1:A:235:HIS:HE1	1.62	0.43
1:A:232:TYR:CE2	1:A:269:GLN:NE2	2.78	0.43
2:B:46:LYS:HD3	2:B:116:PHE:CD1	2.54	0.43
2:B:76:ASP:O	2:B:78:ARG:N	2.49	0.43
2:B:157:PRO:HG2	2:B:158:ALA:H	1.83	0.43
2:B:314:VAL:HG13	2:B:317:VAL:HG11	2.00	0.43
2:B:330:GLN:CD	2:B:330:GLN:N	2.76	0.43
2:B:377:THR:O	2:B:378:GLU:C	2.59	0.43
1:A:249:LYS:HB2	1:A:249:LYS:NZ	2.34	0.42
1:A:469:LEU:HD21	1:A:480:GLN:HG2	2.01	0.42
1:A:490:GLY:C	1:A:492:GLU:N	2.75	0.42
1:A:495:ILE:HB	1:A:533:LEU:HD23	2.01	0.42
2:B:85:GLN:HE21	2:B:89:GLU:HB2	1.84	0.42
1:A:180:ILE:HG22	1:A:181:TYR:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:GLY:O	1:A:492:GLU:N	2.52	0.42
2:B:249:LYS:HB2	2:B:252:TRP:CE3	2.54	0.42
1:A:56:TYR:O	1:A:129:ALA:HB3	2.18	0.42
1:A:57:ASN:HD22	1:A:58:THR:N	2.15	0.42
1:A:418:ASN:O	1:A:419:THR:HG22	2.18	0.42
2:B:393:ILE:HG22	2:B:416:PHE:HD1	1.84	0.42
1:A:197:GLN:O	1:A:200:THR:HB	2.20	0.42
1:A:323:LYS:HB2	1:A:343:GLN:NE2	2.35	0.42
1:A:410:TRP:O	1:A:410:TRP:CG	2.70	0.42
1:A:496:VAL:O	1:A:496:VAL:HG12	2.19	0.42
2:B:248:GLU:HA	2:B:307:ARG:HH22	1.84	0.42
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.77	0.42
1:A:398:TRP:CE2	1:A:411:ILE:HG12	2.54	0.42
1:A:424:LYS:CG	1:A:425:LEU:H	2.33	0.42
2:B:27:THR:C	2:B:31:ILE:HD12	2.44	0.42
2:B:325:LEU:HD12	2:B:385:LYS:CG	2.50	0.42
1:A:35:VAL:O	1:A:35:VAL:HG12	2.19	0.42
1:A:90:VAL:CG1	1:A:91:GLN:N	2.81	0.42
1:A:97:PRO:O	1:A:99:GLY:N	2.52	0.42
1:A:121:ASP:O	1:A:123:ASP:N	2.52	0.42
1:A:220:LYS:CB	1:A:222:GLN:HE22	2.32	0.42
1:A:478:GLU:HG2	1:A:499:SER:OG	2.19	0.42
2:B:50:ILE:CD1	2:B:129:ALA:HB1	2.49	0.42
1:A:27:THR:O	1:A:28:GLU:C	2.62	0.42
1:A:153:TRP:HZ3	1:A:159:ILE:HD12	1.84	0.42
1:A:331:LYS:HB2	1:A:337:TRP:CH2	2.55	0.42
1:A:399:GLU:HA	1:A:402:TRP:NE1	2.33	0.42
2:B:19:PRO:HG3	2:B:80:LEU:HB2	2.00	0.42
2:B:278:GLN:NE2	2:B:296:THR:HB	2.35	0.42
2:B:358:ARG:O	2:B:361:HIS:NE2	2.53	0.42
2:B:394:GLN:O	2:B:395:LYS:C	2.62	0.42
1:A:201:LYS:HD3	1:A:201:LYS:HA	1.87	0.42
1:A:246:LEU:CD1	1:A:310:LEU:HD12	2.49	0.42
1:A:254:VAL:HA	1:A:257:ILE:HG22	2.01	0.42
1:A:326:ILE:HG22	1:A:327:ALA:N	2.35	0.42
1:A:340:GLN:CB	1:A:351:THR:HG22	2.49	0.42
2:B:96:HIS:HA	2:B:97:PRO:HD2	1.60	0.42
2:B:363:ASN:HD22	2:B:363:ASN:N	2.17	0.42
2:B:414:TRP:CD1	2:B:414:TRP:C	2.98	0.42
1:A:325:LEU:HD23	1:A:387:PRO:HD3	2.01	0.42
1:A:418:ASN:C	1:A:419:THR:CG2	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:THR:HG1	2:B:299:ALA:HB2	1.78	0.42
2:B:342:TYR:C	2:B:342:TYR:HD1	2.27	0.42
2:B:370:GLU:C	2:B:372:VAL:N	2.75	0.42
2:B:395:LYS:NZ	2:B:399:GLU:OE1	2.52	0.42
1:A:130:PHE:CD1	1:A:130:PHE:C	2.97	0.42
1:A:245:VAL:O	1:A:245:VAL:HG12	2.19	0.42
1:A:419:THR:O	1:A:419:THR:OG1	2.37	0.42
2:B:3:SER:HB2	2:B:4:PRO:CD	2.49	0.42
2:B:27:THR:HG22	2:B:28:GLU:N	2.35	0.42
2:B:224:GLU:O	2:B:226:PRO:HD3	2.20	0.42
2:B:323:LYS:NZ	2:B:344:GLU:OE1	2.51	0.42
2:B:393:ILE:HG22	2:B:416:PHE:CD1	2.55	0.42
2:B:395:LYS:NZ	2:B:399:GLU:OE2	2.52	0.42
1:A:139:THR:O	1:A:141:GLY:N	2.53	0.41
1:A:164:MET:O	1:A:165:THR:C	2.63	0.41
1:A:200:THR:O	1:A:201:LYS:C	2.63	0.41
1:A:402:TRP:O	1:A:402:TRP:CE3	2.72	0.41
1:A:407:GLN:OE1	2:B:393:ILE:C	2.63	0.41
1:A:515:SER:O	1:A:516:GLU:C	2.62	0.41
2:B:130:PHE:CZ	2:B:144:TYR:CB	3.01	0.41
2:B:282:LEU:HD12	2:B:282:LEU:HA	1.83	0.41
1:A:240:THR:HB	1:A:315:HIS:HA	2.02	0.41
1:A:326:ILE:O	1:A:341:ILE:HG23	2.20	0.41
1:A:339:TYR:CE2	1:A:341:ILE:HD11	2.55	0.41
2:B:30:LYS:O	2:B:31:ILE:C	2.63	0.41
2:B:266:TRP:O	2:B:266:TRP:CE3	2.73	0.41
2:B:283:LEU:C	2:B:285:GLY:N	2.78	0.41
1:A:266:TRP:O	1:A:269:GLN:HG3	2.19	0.41
2:B:171:PHE:C	2:B:173:LYS:H	2.28	0.41
1:A:95:PRO:O	1:A:229:TRP:CH2	2.71	0.41
1:A:503:LEU:HG	1:A:507:GLN:HE21	1.86	0.41
2:B:103:LYS:HG3	2:B:190:GLY:HA3	2.02	0.41
2:B:404:GLU:HB3	2:B:405:TYR:CE1	2.55	0.41
1:A:168:LEU:C	1:A:170:PRO:HD2	2.45	0.41
2:B:369:THR:HG22	2:B:373:GLN:NE2	2.35	0.41
2:B:382:ILE:HB	2:B:383:TRP:CE3	2.56	0.41
1:A:24:TRP:N	1:A:25:PRO:CD	2.83	0.41
1:A:53:GLU:N	1:A:55:PRO:HD3	2.32	0.41
1:A:162:SER:HB2	2:B:52:PRO:HG3	2.03	0.41
1:A:178:ILE:HD12	1:A:178:ILE:H	1.83	0.41
1:A:275:LYS:C	1:A:276:VAL:HG23	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ILE:O	1:A:393:ILE:HG23	2.20	0.41
2:B:3:SER:HB2	2:B:4:PRO:HD3	2.02	0.41
1:A:434:ILE:HG21	1:A:437:ALA:HB2	2.03	0.41
1:A:515:SER:O	1:A:518:VAL:N	2.53	0.41
1:A:265:ASN:O	1:A:268:SER:N	2.49	0.41
2:B:85:GLN:CD	2:B:85:GLN:C	2.88	0.41
2:B:184:MET:HE2	2:B:184:MET:HB3	1.57	0.41
1:A:106:VAL:HG12	1:A:107:THR:H	1.85	0.41
1:A:209:LEU:O	1:A:212:TRP:N	2.50	0.41
1:A:509:GLN:N	1:A:510:PRO:CD	2.84	0.41
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.55	0.41
2:B:123:ASP:O	2:B:126:LYS:HG2	2.20	0.41
2:B:195:ILE:HD13	2:B:199:ARG:HH21	1.85	0.41
2:B:210:LEU:C	2:B:212:TRP:N	2.72	0.41
2:B:319:TYR:CD2	2:B:383:TRP:HD1	2.39	0.41
2:B:326:ILE:HG21	2:B:342:TYR:CE1	2.56	0.41
2:B:365:VAL:O	2:B:365:VAL:CG1	2.63	0.41
2:B:380:ILE:O	2:B:384:GLY:HA2	2.21	0.41
1:A:386:THR:HA	1:A:387:PRO:HD2	1.94	0.41
1:A:533:LEU:HD23	1:A:533:LEU:HA	1.82	0.41
2:B:2:ILE:O	2:B:3:SER:C	2.64	0.41
2:B:306:ASN:HA	2:B:306:ASN:HD22	1.74	0.41
1:A:304:ALA:C	1:A:306:ASN:N	2.78	0.40
1:A:344:GLU:O	1:A:346:PHE:N	2.54	0.40
2:B:44:GLU:CD	2:B:46:LYS:HE3	2.47	0.40
2:B:60:VAL:HG12	2:B:75:VAL:HG22	2.03	0.40
2:B:278:GLN:NE2	2:B:296:THR:CB	2.84	0.40
2:B:331:LYS:NZ	2:B:364:ASP:OD1	2.53	0.40
2:B:369:THR:HG23	2:B:406:TRP:CE3	2.56	0.40
1:A:177:ASP:HB3	1:A:178:ILE:HD12	2.03	0.40
1:A:457:TYR:HD2	1:A:457:TYR:O	2.05	0.40
2:B:46:LYS:HZ3	2:B:116:PHE:HD1	1.67	0.40
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.56	0.40
2:B:236:PRO:C	2:B:238:LYS:H	2.30	0.40
1:A:476:LYS:HD3	1:A:517:LEU:CD2	2.52	0.40
2:B:410:TRP:CE3	2:B:410:TRP:O	2.74	0.40
1:A:8:VAL:O	1:A:9:PRO:C	2.65	0.40
1:A:32:LYS:O	1:A:33:ALA:C	2.64	0.40
1:A:366:LYS:O	1:A:369:THR:HB	2.22	0.40
2:B:149:LEU:HD23	2:B:149:LEU:H	1.87	0.40
2:B:223:LYS:HD3	2:B:223:LYS:HA	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:279:LEU:HD23	2:B:279:LEU:HA	1.96	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	550/560 (98%)	400 (73%)	110 (20%)	40 (7%)	1	4
2	B	425/430 (99%)	319 (75%)	67 (16%)	39 (9%)	0	2
All	All	975/990 (98%)	719 (74%)	177 (18%)	79 (8%)	1	3

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	MET
1	A	54	ASN
1	A	114	ALA
1	A	122	GLU
1	A	195	ILE
1	A	297	GLU
1	A	542	ILE
2	B	18	GLY
2	B	85	GLN
2	B	116	PHE
2	B	126	LYS
2	B	218	ASP
2	B	220	LYS
2	B	231	GLY
2	B	288	ALA
2	B	360	ALA
2	B	365	VAL

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Mol	Chain	Res	Type
2	B	419	THR
1	A	14	PRO
1	A	115	TYR
1	A	121	ASP
1	A	225	PRO
1	A	345	PRO
1	A	516	GLU
2	B	5	ILE
2	B	77	PHE
2	B	112	GLY
2	B	154	LYS
2	B	198	HIS
2	B	277	ARG
2	B	420	PRO
2	B	421	PRO
1	A	82	LYS
1	A	140	PRO
1	A	164	MET
1	A	272	PRO
1	A	287	LYS
1	A	334	GLN
1	A	491	LEU
1	A	515	SER
2	B	137	ASN
2	B	162	SER
2	B	223	LYS
2	B	297	GLU
2	B	309	ILE
2	B	426	TRP
1	A	18	GLY
1	A	65	LYS
1	A	98	ALA
1	A	137	ASN
1	A	162	SER
1	A	230	MET
1	A	286	THR
2	B	65	LYS
2	B	169	GLU
2	B	199	ARG
2	B	294	PRO
2	B	314	VAL
2	B	395	LYS

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Mol	Chain	Res	Type
1	A	53	GLU
1	A	153	TRP
1	A	165	THR
1	A	372	VAL
1	A	503	LEU
2	B	184	MET
2	B	268	SER
2	B	280	SER
2	B	404	GLU
1	A	163	SER
1	A	274	ILE
2	B	195	ILE
2	B	196	GLY
1	A	159	ILE
1	A	176	PRO
1	A	224	GLU
1	A	276	VAL
2	B	225	PRO
2	B	359	GLY
1	A	52	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	493/500 (99%)	442 (90%)	51 (10%)	7	28
2	B	388/392 (99%)	351 (90%)	37 (10%)	8	31
All	All	881/892 (99%)	793 (90%)	88 (10%)	7	29

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	40	GLU
1	A	50	ILE

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Mol	Chain	Res	Type
1	A	53	GLU
1	A	60	VAL
1	A	76	ASP
1	A	85	GLN
1	A	89	GLU
1	A	113	ASP
1	A	128	THR
1	A	136	ASN
1	A	139	THR
1	A	142	ILE
1	A	178	ILE
1	A	179	VAL
1	A	181	TYR
1	A	182	GLN
1	A	188	TYR
1	A	218	ASP
1	A	224	GLU
1	A	225	PRO
1	A	228	LEU
1	A	230	MET
1	A	241	VAL
1	A	272	PRO
1	A	295	LEU
1	A	297	GLU
1	A	313	PRO
1	A	326	ILE
1	A	330	GLN
1	A	346	PHE
1	A	347	LYS
1	A	356	ARG
1	A	394	GLN
1	A	403	THR
1	A	411	ILE
1	A	419	THR
1	A	450	THR
1	A	457	TYR
1	A	460	ASN
1	A	469	LEU
1	A	473	THR
1	A	496	VAL
1	A	500	GLN
1	A	506	ILE

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Mol	Chain	Res	Type
1	A	509	GLN
1	A	511	ASP
1	A	514	GLU
1	A	542	ILE
1	A	545	ASN
1	A	546	GLU
2	B	12	LEU
2	B	16	MET
2	B	42	GLU
2	B	69	THR
2	B	91	GLN
2	B	113	ASP
2	B	135	ILE
2	B	136	ASN
2	B	139	THR
2	B	149	LEU
2	B	162	SER
2	B	169	GLU
2	B	177	ASP
2	B	186	ASP
2	B	189	VAL
2	B	206	ARG
2	B	207	GLN
2	B	212	TRP
2	B	215	THR
2	B	230	MET
2	B	239	TRP
2	B	252	TRP
2	B	266	TRP
2	B	269	GLN
2	B	271	TYR
2	B	277	ARG
2	B	317	VAL
2	B	318	TYR
2	B	330	GLN
2	B	361	HIS
2	B	363	ASN
2	B	374	LYS
2	B	386	THR
2	B	399	GLU
2	B	403	THR
2	B	418	ASN

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Mol	Chain	Res	Type
2	B	419	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	147	ASN
1	A	151	GLN
1	A	182	GLN
1	A	222	GLN
1	A	258	GLN
1	A	269	GLN
1	A	315	HIS
1	A	332	GLN
1	A	334	GLN
1	A	367	GLN
1	A	373	GLN
1	A	460	ASN
1	A	475	GLN
1	A	487	GLN
1	A	494	ASN
1	A	500	GLN
1	A	507	GLN
1	A	509	GLN
1	A	519	ASN
2	B	136	ASN
2	B	174	GLN
2	B	175	ASN
2	B	182	GLN
2	B	207	GLN
2	B	255	ASN
2	B	258	GLN
2	B	278	GLN
2	B	315	HIS
2	B	363	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
4	185	A	600	-	30,31,31	1.73	5 (16%)	39,43,43	1.72	6 (15%)

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
4	185	A	600	-	-	2/14/14/14	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	185	BR-C14	-3.69	1.80	1.89
4	A	600	185	C22-C21	3.68	1.45	1.39
4	A	600	185	C13-N12	3.49	1.37	1.32
4	A	600	185	O18-C18	-3.25	1.27	1.41
4	A	600	185	C23-C22	3.10	1.43	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	185	O18-C18-C15	4.90	123.60	112.14
4	A	600	185	N16-C11-N12	-4.55	118.80	126.26
4	A	600	185	C14-C13-N12	-3.96	119.52	123.78
4	A	600	185	C11-N12-C13	3.61	121.60	115.38
4	A	600	185	BR-C14-C13	-2.99	117.36	121.55
4	A	600	185	C1-O17-C13	-2.05	114.71	116.84

There are no chirality outliers.

All (2) torsion outliers are listed below:

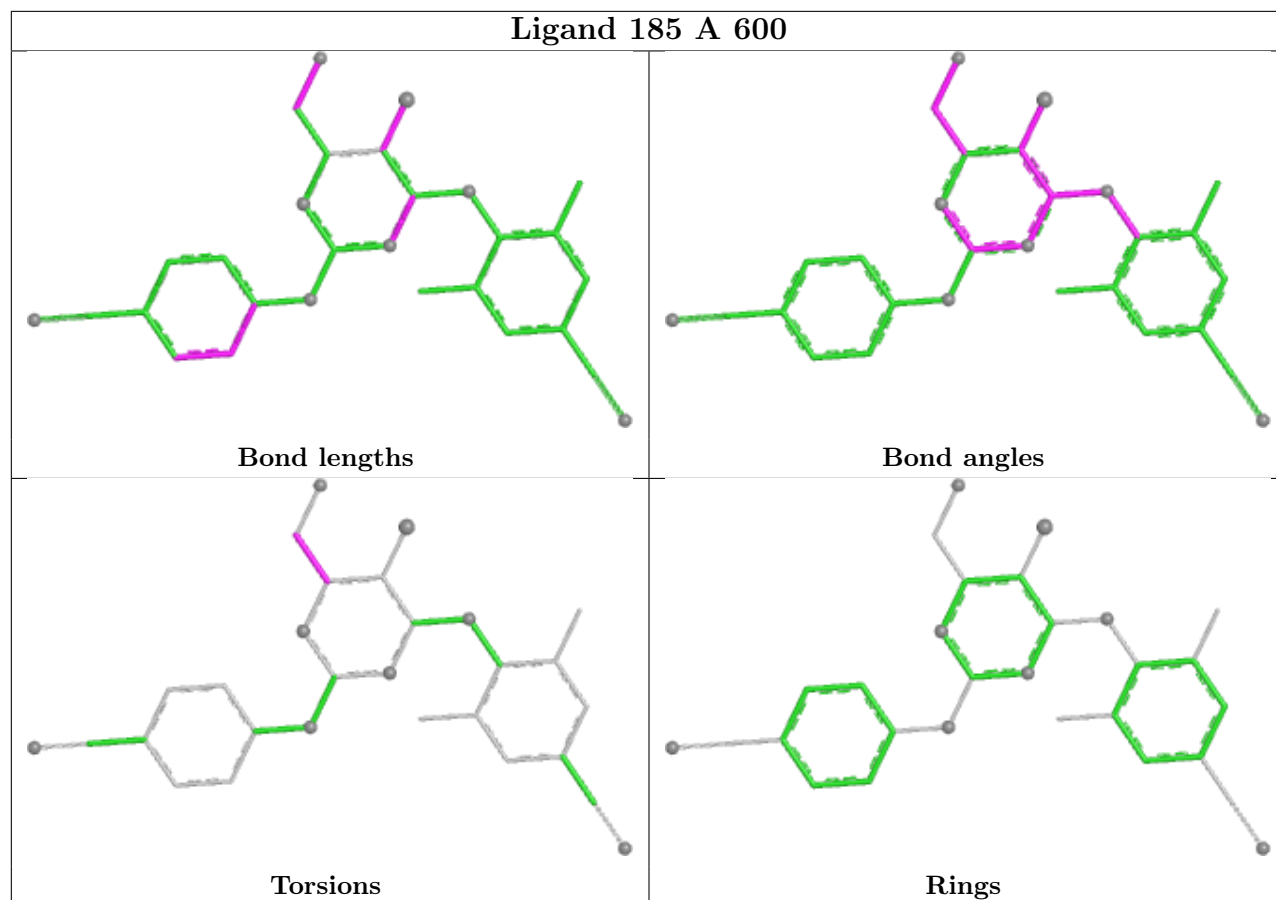
Mol	Chain	Res	Type	Atoms
4	A	600	185	N16-C15-C18-O18
4	A	600	185	C14-C15-C18-O18

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	185	8	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 [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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	545/560 (97%)	-0.28	1 (0%) 91 83	38, 90, 112, 121	18 (3%)
2	B	427/430 (99%)	-0.38	4 (0%) 81 61	22, 72, 114, 121	15 (3%)
All	All	972/990 (98%)	-0.32	5 (0%) 87 72	22, 84, 113, 121	33 (3%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	5	ILE	3.8
1	A	408	ALA	2.4
2	B	2	ILE	2.2
2	B	4	PRO	2.2
2	B	295	LEU	2.1

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](#)

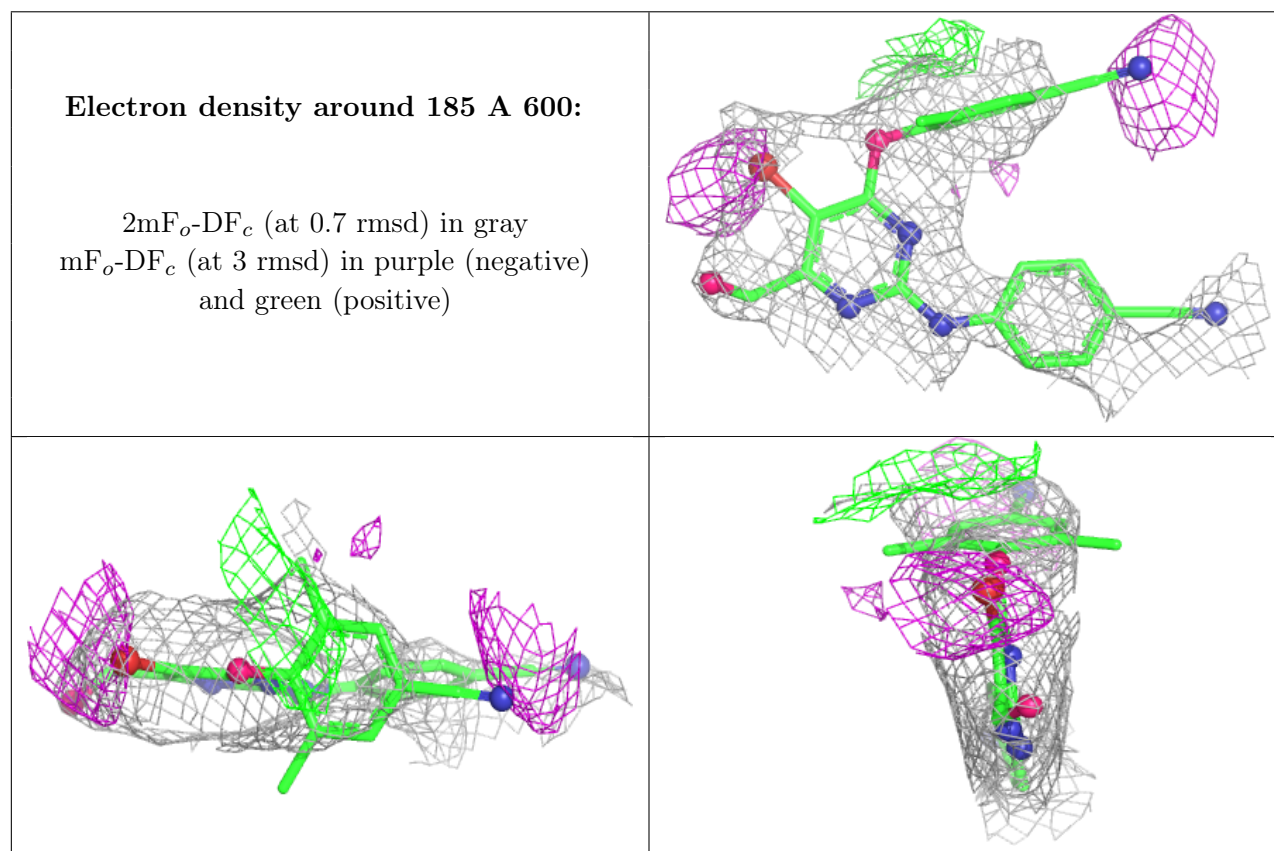
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	185	A	600	29/29	0.88	0.15	80,94,97,119	0
3	MG	A	601	1/1	0.92	0.06	86,86,86,86	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.