



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:24 PM UTC

PDB ID : 2C5X / pdb_00002c5x
Title : Differential Binding Of Inhibitors To Active And Inactive Cdk2 Provides Insights For Drug Design
Authors : Kontopidis, G.; McInnes, C.; Pandalaneni, S.R.; Mcnae, I.; Gibson, D.; Mezna, M.; Thomas, M.; Wood, G.; Wang, S.; Walkinshaw, M.D.; Fischer, P.M.
Deposited on : 2005-11-03
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
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

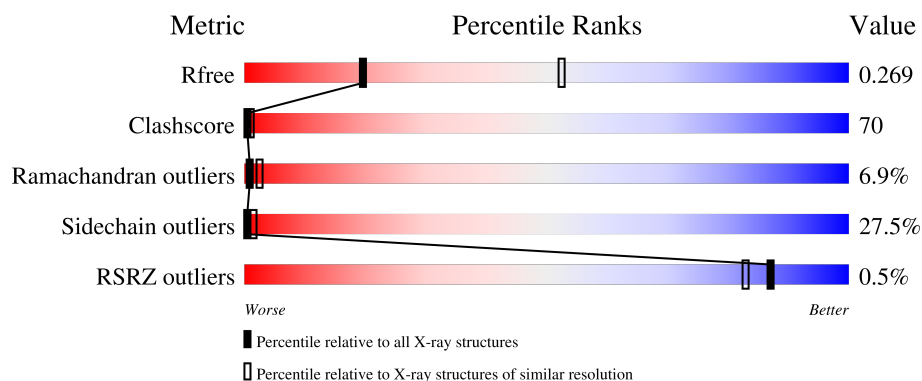
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	298	
1	C	298	
2	B	259	
2	D	259	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MTW	C	1297	-	-	X	-

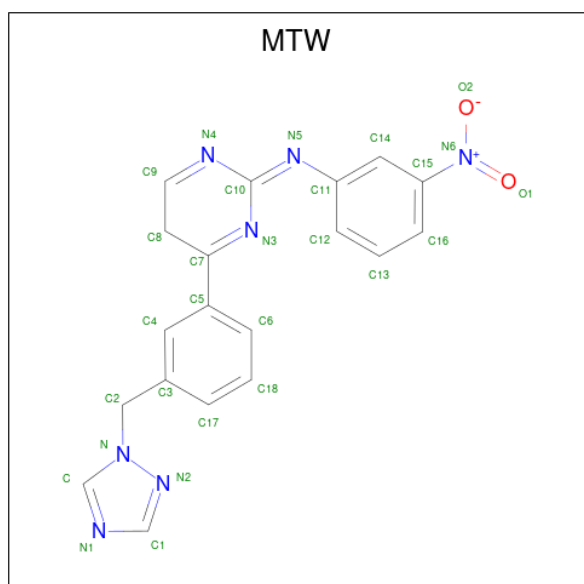
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total 2378	C 1547	N 403	O 420	S 8	0	0	0
1	C	296	Total 2388	C 1553	N 406	O 421	S 8	0	1	0

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total 2083	C 1350	N 339	O 383	S 11	0	0	0
2	D	258	Total 2092	C 1354	N 340	O 387	S 11	0	1	0

- Molecule 3 is HYDROXY(OXO)(3-{[(2Z)-4-[3-(1H-1,2,4-TRIAZOL-1-YLMETHYL)PHE
NYL]PYRIMIDIN-2(5H)-YLIDENE]AMINO}PHENYL)AMMONIUM (CCD ID: MTW)
(formula: C₁₉H₁₅N₇O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	19	7	2		
3	C	1	Total	C	N	O	0	0
			28	19	7	2		

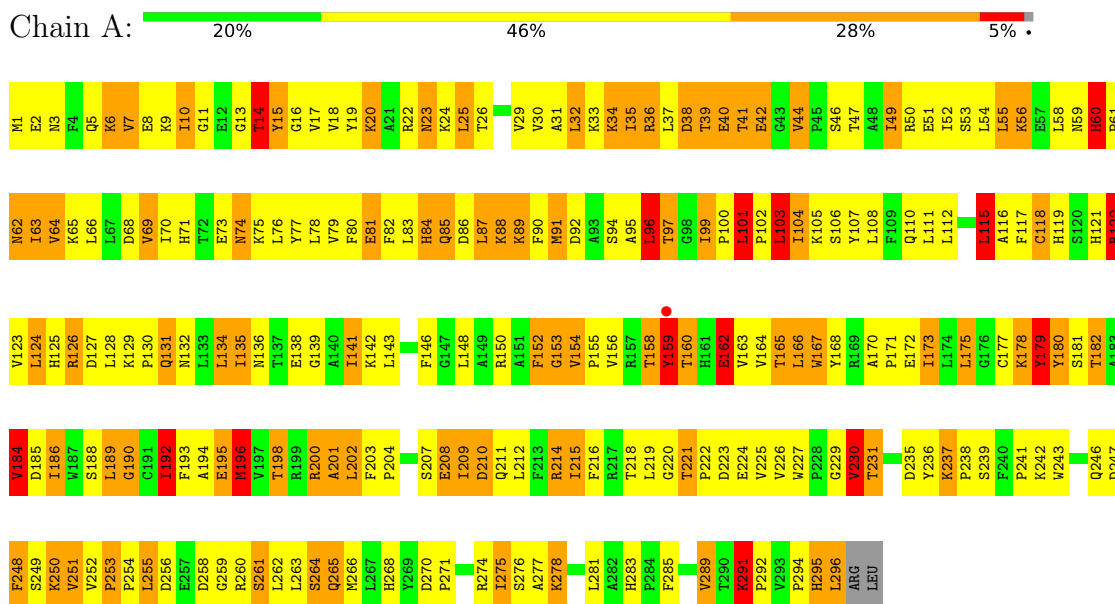
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		
4	B	17	Total	O	0	0
			17	17		
4	C	28	Total	O	0	0
			28	28		
4	D	17	Total	O	0	0
			17	17		

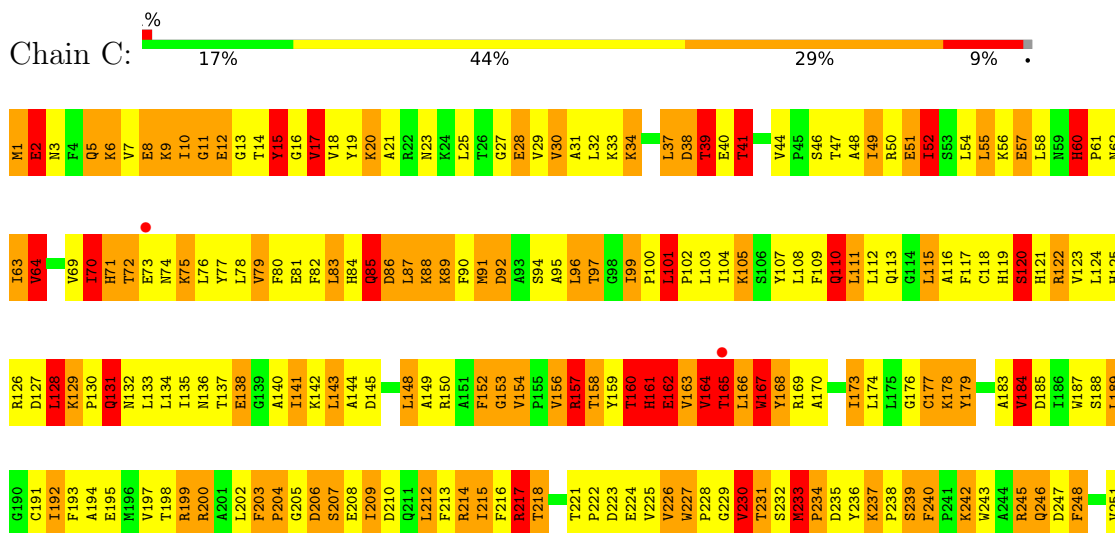
3 Residue-property plots

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: CELL DIVISION PROTEIN KINASE 2



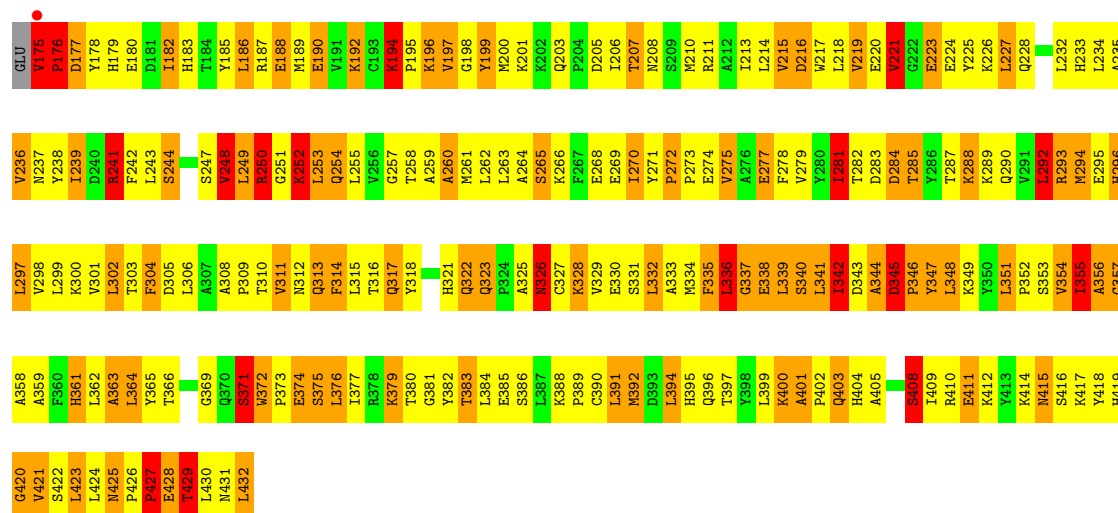
• Molecule 1: CELL DIVISION PROTEIN KINASE 2





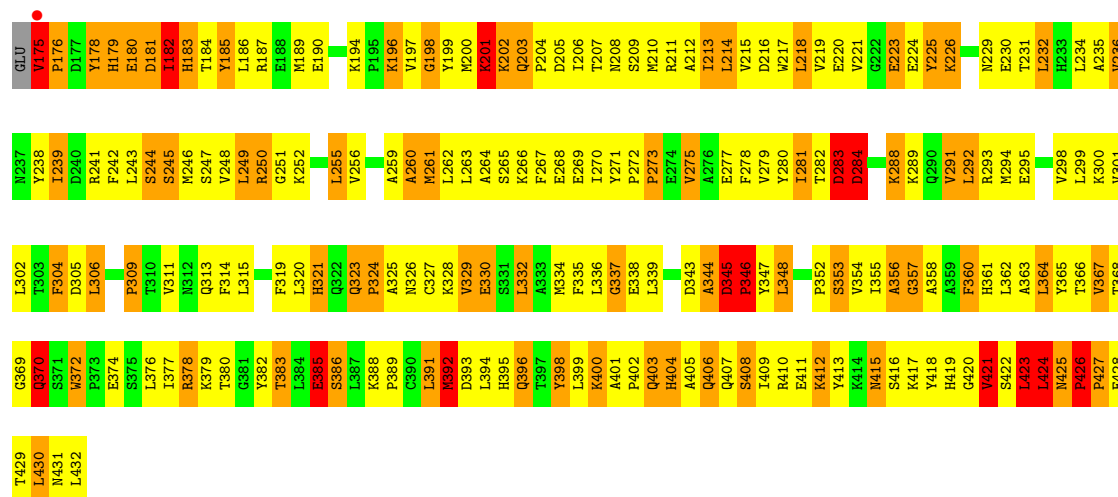
• Molecule 2: CYCLIN A2

Chain B: 14% 47% 31% 7%



• Molecule 2: CYCLIN A2

Chain D: 20% 48% 26% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.33Å 112.35Å 154.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.90) 98.7 (20.00-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.200 , 0.264 0.201 , 0.269	Depositor DCC
R_{free} test set	1197 reflections (4.11%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9085	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: MTW

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	0.86	0/2440	1.90	68/3313 (2.1%)
1	C	0.92	1/2451 (0.0%)	1.91	69/3328 (2.1%)
2	B	0.84	0/2133	1.80	55/2897 (1.9%)
2	D	0.87	0/2142	1.93	59/2908 (2.0%)
All	All	0.87	1/9166 (0.0%)	1.89	251/12446 (2.0%)

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	0	8
1	C	0	10
2	B	0	9
2	D	0	8
All	All	0	35

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	70	ILE	CA-CB	-5.88	1.46	1.55

All (251) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	175	VAL	CA-C-N	-18.92	96.19	119.84
2	D	175	VAL	C-N-CA	-18.92	96.19	119.84
1	C	166	LEU	N-CA-C	-12.74	95.99	112.93
1	C	99	ILE	CB-CA-C	-11.71	100.05	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	18	VAL	CB-CA-C	-11.54	98.89	111.59
1	A	63	ILE	N-CA-C	10.78	123.43	107.80
1	A	60	HIS	CA-C-N	10.78	130.52	119.64
1	A	60	HIS	C-N-CA	10.78	130.52	119.64
1	A	14	THR	N-CA-C	-10.42	88.61	110.80
2	D	180	GLU	N-CA-C	10.40	122.63	111.09
2	D	345	ASP	CA-C-N	10.36	132.79	119.84
2	D	345	ASP	C-N-CA	10.36	132.79	119.84
1	A	101	LEU	CA-C-N	10.33	130.11	118.85
1	A	101	LEU	C-N-CA	10.33	130.11	118.85
1	A	261	SER	N-CA-C	-9.78	100.61	111.07
2	B	216	ASP	N-CA-C	-9.30	99.95	111.11
2	B	241	ARG	N-CA-C	-9.29	101.16	111.28
2	B	188	GLU	N-CA-C	-9.27	100.35	112.68
1	C	101	LEU	CA-C-N	9.23	130.18	119.47
1	C	101	LEU	C-N-CA	9.23	130.18	119.47
1	A	159	TYR	CA-C-N	-9.19	107.05	120.28
1	A	159	TYR	C-N-CA	-9.19	107.05	120.28
1	C	131	GLN	N-CA-C	-8.86	101.54	111.82
1	A	138	GLU	N-CA-C	8.78	123.60	113.15
1	A	283	HIS	CA-C-N	8.63	130.62	119.84
1	A	283	HIS	C-N-CA	8.63	130.62	119.84
1	C	204	PRO	CA-C-N	-8.52	116.30	122.18
1	C	204	PRO	C-N-CA	-8.52	116.30	122.18
1	C	237	LYS	CA-C-N	-8.49	110.98	119.56
1	C	237	LYS	C-N-CA	-8.49	110.98	119.56
1	A	192	ILE	N-CA-C	-8.42	102.61	110.53
2	B	342	ILE	N-CA-C	8.37	122.66	111.44
1	C	56	LYS	N-CA-C	-8.30	103.06	113.02
1	C	64	VAL	CB-CA-C	-8.29	97.69	111.29
2	B	252	LYS	N-CA-C	8.21	122.55	112.54
2	D	353	SER	N-CA-C	-8.16	102.59	112.54
2	B	293	ARG	N-CA-C	-8.15	102.36	111.82
2	D	242	PHE	N-CA-C	-8.13	102.49	111.36
2	D	372	TRP	CA-C-N	8.05	127.98	119.85
2	D	372	TRP	C-N-CA	8.05	127.98	119.85
2	D	292	LEU	N-CA-C	-8.03	102.12	112.23
1	A	44	VAL	CB-CA-C	-7.99	103.51	110.94
2	B	363	ALA	N-CA-C	-7.98	101.36	112.45
2	B	372	TRP	CA-C-N	7.97	128.03	119.90
2	B	372	TRP	C-N-CA	7.97	128.03	119.90
2	B	270	ILE	CB-CA-C	-7.95	101.63	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	LYS	CA-C-N	-7.89	115.01	122.66
1	A	6	LYS	C-N-CA	-7.89	115.01	122.66
1	C	183	ALA	N-CA-C	7.89	119.51	111.07
2	B	330	GLU	N-CA-C	-7.86	102.67	111.07
1	C	17	VAL	N-CA-C	7.82	125.60	109.34
1	C	197	VAL	N-CA-C	7.81	117.87	110.53
1	C	293	VAL	CA-C-N	7.75	127.77	119.78
1	C	293	VAL	C-N-CA	7.75	127.77	119.78
1	C	217	ARG	N-CA-C	-7.68	103.91	113.20
2	B	317	GLN	N-CA-C	-7.60	102.93	111.14
2	D	370	GLN	N-CA-C	7.53	121.52	109.86
2	B	270	ILE	N-CA-C	-7.49	103.56	110.82
2	D	423	LEU	N-CA-C	-7.45	103.18	112.72
2	D	218	LEU	N-CA-C	-7.43	102.55	111.69
1	C	51	GLU	N-CA-C	-7.38	103.23	111.28
2	B	221	VAL	CB-CA-C	-7.36	101.30	112.05
1	C	203	PHE	CA-C-N	7.34	129.02	119.84
1	C	203	PHE	C-N-CA	7.34	129.02	119.84
1	A	122	ARG	N-CA-C	-7.27	102.17	111.92
1	A	160	THR	N-CA-CB	7.26	121.41	110.22
2	B	394	LEU	N-CA-C	-7.24	103.47	111.36
2	B	345	ASP	CA-C-N	7.24	128.88	119.84
2	B	345	ASP	C-N-CA	7.24	128.88	119.84
2	D	279	VAL	CB-CA-C	-7.19	102.60	112.02
2	D	260	ALA	N-CA-C	-7.15	103.42	111.07
2	B	311	VAL	N-CA-C	-7.14	103.56	110.42
1	A	24	LYS	N-CA-C	-7.14	104.03	112.89
1	A	214	ARG	N-CA-C	-7.06	103.67	111.36
2	B	308	ALA	CA-C-N	7.01	127.40	119.83
2	B	308	ALA	C-N-CA	7.01	127.40	119.83
1	A	180	TYR	N-CA-C	-7.00	99.56	110.42
1	C	124	LEU	CB-CA-C	-7.00	97.67	109.50
2	D	255	LEU	N-CA-C	-7.00	103.08	111.69
1	A	41	THR	N-CA-C	7.00	120.27	111.24
1	C	221	THR	CA-C-N	6.97	127.01	119.90
1	C	221	THR	C-N-CA	6.97	127.01	119.90
2	B	248	VAL	CB-CA-C	-6.96	99.88	111.29
1	A	215	ILE	N-CA-C	-6.96	103.74	110.42
1	C	92	ASP	N-CA-C	-6.89	103.85	111.36
2	D	306	LEU	CA-C-N	-6.89	111.23	122.26
2	D	306	LEU	C-N-CA	-6.89	111.23	122.26
2	D	256	VAL	N-CA-C	-6.86	103.62	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	270	ASP	CA-C-N	6.86	126.48	119.56
1	C	270	ASP	C-N-CA	6.86	126.48	119.56
1	A	237	LYS	CA-C-N	-6.84	112.75	119.87
1	A	237	LYS	C-N-CA	-6.84	112.75	119.87
1	A	118	CYS	N-CA-C	-6.84	103.75	111.07
2	D	426	PRO	CA-C-N	6.84	127.23	119.92
2	D	426	PRO	C-N-CA	6.84	127.23	119.92
1	A	210	ASP	N-CA-C	-6.81	103.88	111.71
1	A	249	SER	N-CA-C	-6.80	105.10	113.19
1	C	191	CYS	N-CA-C	-6.78	103.92	111.71
1	A	221	THR	CB-CA-C	-6.77	98.82	109.52
2	D	425	ASN	CB-CA-C	-6.76	99.65	109.38
2	D	309	PRO	CB-CA-C	-6.74	102.77	111.46
2	D	273	PRO	CB-CA-C	-6.73	103.01	111.56
2	B	175	VAL	CA-C-N	-6.72	111.43	119.84
2	B	175	VAL	C-N-CA	-6.72	111.43	119.84
1	A	238	PRO	N-CA-C	-6.68	105.81	114.03
2	D	194	LYS	CA-C-N	6.63	127.54	120.11
2	D	194	LYS	C-N-CA	6.63	127.54	120.11
2	D	356	ALA	N-CA-C	6.61	118.17	110.97
1	C	280	ALA	N-CA-C	-6.59	104.72	112.89
1	C	160	THR	CA-C-N	-6.56	113.18	122.63
1	C	160	THR	C-N-CA	-6.56	113.18	122.63
2	D	201	LYS	N-CA-C	6.56	118.43	111.28
2	B	332	LEU	N-CA-C	-6.56	104.13	111.28
1	C	70	ILE	N-CA-C	6.54	118.92	108.85
2	B	232	LEU	N-CA-C	6.53	118.94	111.11
1	C	270	ASP	N-CA-CB	6.47	121.89	110.37
1	C	213	PHE	N-CA-C	-6.43	103.78	111.69
1	C	60	HIS	CA-C-N	6.42	126.91	119.47
1	C	60	HIS	C-N-CA	6.42	126.91	119.47
2	D	185	TYR	N-CA-C	-6.41	103.80	111.69
2	D	295	GLU	N-CA-C	-6.41	104.30	111.28
1	A	81	GLU	CA-C-N	-6.40	113.96	122.99
1	A	81	GLU	C-N-CA	-6.40	113.96	122.99
2	D	283	ASP	CB-CA-C	-6.37	103.66	111.82
1	C	161	HIS	N-CA-C	-6.37	102.68	111.28
2	B	219	VAL	CB-CA-C	-6.37	100.85	111.29
1	A	29	VAL	N-CA-C	6.36	117.86	109.21
1	C	138	GLU	N-CA-C	-6.36	105.28	113.16
1	C	69	VAL	CA-C-N	-6.35	112.00	122.67
1	C	69	VAL	C-N-CA	-6.35	112.00	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	GLN	N-CA-C	6.29	119.07	111.40
1	C	253	PRO	CA-C-N	-6.27	114.44	120.83
1	C	253	PRO	C-N-CA	-6.27	114.44	120.83
1	A	116	ALA	N-CA-C	-6.23	104.57	111.36
1	C	112	LEU	N-CA-C	-6.21	104.59	111.36
2	D	250	ARG	NE-CZ-NH1	-6.19	115.31	121.50
2	D	367	VAL	N-CA-C	6.19	116.83	110.82
1	A	179	TYR	N-CA-C	6.17	118.44	109.07
1	C	233	MET	O-C-N	-6.15	111.50	121.59
2	B	186	LEU	N-CA-C	-6.14	103.89	111.33
2	B	361	HIS	CA-C-N	-6.14	111.44	120.28
2	B	361	HIS	C-N-CA	-6.14	111.44	120.28
1	A	268	HIS	N-CA-C	-6.12	102.03	110.35
1	C	110	GLN	N-CA-C	6.12	123.83	110.80
1	A	49	ILE	CB-CA-C	-6.11	103.89	112.14
2	D	279	VAL	N-CA-C	6.10	116.26	110.53
1	A	124	LEU	CB-CA-C	-6.09	98.42	109.38
2	D	398	TYR	N-CA-C	-6.05	104.38	110.97
2	B	347	TYR	N-CA-C	6.04	119.91	112.54
1	A	195	GLU	N-CA-C	-6.04	103.45	111.24
2	D	236	VAL	CB-CA-C	-6.04	103.89	112.22
2	D	327	CYS	CB-CA-C	-6.03	101.37	110.90
1	A	40	GLU	CB-CA-C	6.02	120.82	110.23
2	D	271	TYR	CA-C-N	-6.01	114.18	120.38
2	D	271	TYR	C-N-CA	-6.01	114.18	120.38
1	A	6	LYS	N-CA-C	-5.99	100.98	109.96
1	C	165	THR	N-CA-CB	5.97	120.92	111.43
1	A	175	LEU	N-CA-C	-5.96	105.31	113.30
1	A	178	LYS	N-CA-C	-5.95	105.93	112.72
2	B	376	LEU	N-CA-C	-5.94	104.19	112.45
1	A	198	THR	N-CA-C	-5.93	104.57	112.94
1	C	152	PHE	N-CA-C	5.91	120.07	112.26
2	D	225	TYR	N-CA-C	-5.90	105.39	113.30
1	C	167	TRP	CA-CB-CG	-5.89	102.40	113.60
1	A	115	LEU	N-CA-C	-5.84	104.92	111.28
1	C	85	GLN	N-CA-C	5.82	117.10	107.73
1	A	186	ILE	N-CA-C	5.81	116.55	110.62
2	D	291	VAL	CB-CA-C	-5.79	104.32	112.14
2	D	203	GLN	CA-C-O	5.78	123.05	119.29
2	B	275	VAL	CB-CA-C	-5.77	101.82	111.29
1	A	85	GLN	N-CA-C	5.76	115.89	108.34
1	C	128	LEU	CB-CA-C	5.76	118.06	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	351	LEU	N-CA-C	5.73	116.92	109.64
1	A	66	LEU	N-CA-C	-5.72	99.20	108.52
2	D	360	PHE	N-CA-C	-5.72	104.68	111.03
1	A	135	ILE	CB-CA-C	-5.70	102.69	110.90
2	B	309	PRO	CB-CA-C	-5.68	104.48	111.64
2	B	292	LEU	N-CA-C	5.67	117.91	111.11
1	A	152	PHE	N-CA-C	5.66	119.77	112.41
2	B	335	PHE	N-CA-C	-5.66	104.32	111.11
2	B	277	GLU	N-CA-C	-5.65	105.02	111.07
2	D	178	TYR	N-CA-C	-5.65	105.33	114.09
2	D	393	ASP	N-CA-C	-5.65	105.12	111.28
2	D	372	TRP	N-CA-C	-5.65	101.69	109.71
1	C	79	VAL	N-CA-C	5.63	116.24	107.28
2	D	277	GLU	N-CA-C	-5.63	105.23	111.71
2	B	371	SER	N-CA-C	5.63	116.80	108.86
1	A	32	LEU	CB-CG-CD1	-5.60	93.90	110.70
1	A	182	THR	CB-CA-C	5.58	121.52	110.42
1	A	295	HIS	CB-CA-C	-5.58	103.75	112.12
2	D	175	VAL	C-N-CD	5.55	147.76	125.00
2	D	427	PRO	CB-CA-C	-5.52	104.00	111.12
1	C	2	GLU	CA-C-N	-5.47	114.07	122.60
1	C	2	GLU	C-N-CA	-5.47	114.07	122.60
2	B	381	GLY	CA-C-N	-5.46	114.39	122.41
2	B	381	GLY	C-N-CA	-5.46	114.39	122.41
1	C	52	ILE	N-CA-CB	5.46	116.57	110.62
2	D	247	SER	N-CA-C	-5.41	101.84	109.96
2	B	215	VAL	CB-CA-C	-5.40	104.94	112.02
2	D	272	PRO	CA-C-N	5.40	125.41	119.90
2	D	272	PRO	C-N-CA	5.40	125.41	119.90
2	D	365	TYR	N-CA-C	-5.39	105.57	111.82
1	A	25	LEU	N-CA-C	5.37	119.91	112.45
1	C	168	TYR	N-CA-C	5.37	118.63	112.57
1	C	78	LEU	CA-C-N	-5.35	115.96	123.13
1	C	78	LEU	C-N-CA	-5.35	115.96	123.13
2	D	330	GLU	N-CA-C	5.34	117.53	111.02
2	B	408	SER	CA-C-N	-5.33	113.11	120.74
2	B	408	SER	C-N-CA	-5.33	113.11	120.74
2	B	314	PHE	N-CA-C	5.33	116.78	110.97
2	B	411	GLU	N-CA-C	-5.33	104.93	111.75
1	C	118	CYS	CA-C-O	5.31	126.18	120.55
1	C	60	HIS	N-CA-C	5.31	121.54	109.81
1	C	57	GLU	N-CA-C	-5.30	107.18	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	281	ILE	CB-CA-C	-5.29	102.61	111.29
1	A	99	ILE	CA-C-N	5.28	126.44	119.84
1	A	99	ILE	C-N-CA	5.28	126.44	119.84
2	B	281	ILE	CA-C-N	-5.27	114.29	122.67
2	B	281	ILE	C-N-CA	-5.27	114.29	122.67
2	B	176	PRO	N-CA-C	5.25	123.29	112.47
2	B	316	THR	CA-C-N	-5.25	113.30	120.44
2	B	316	THR	C-N-CA	-5.25	113.30	120.44
1	A	281	LEU	N-CA-C	-5.25	105.67	111.71
1	C	157	ARG	N-CA-C	5.25	117.10	110.33
1	A	103	LEU	N-CA-C	-5.24	105.65	111.36
2	D	243	LEU	N-CA-C	-5.24	106.84	113.18
2	D	182	ILE	N-CA-C	-5.24	104.65	110.62
1	A	173	ILE	CB-CG1-CD1	-5.22	102.84	113.80
2	B	186	LEU	CA-CB-CG	-5.22	98.03	116.30
1	A	146	PHE	CA-C-N	-5.22	113.59	120.22
1	A	146	PHE	C-N-CA	-5.22	113.59	120.22
1	A	276	SER	CB-CA-C	-5.20	100.72	109.83
1	A	87	LEU	N-CA-C	-5.20	105.69	111.36
1	C	177	CYS	CA-CB-SG	-5.20	102.44	114.40
1	C	179	TYR	N-CA-C	5.16	117.65	109.50
1	A	47	THR	CB-CA-C	-5.14	102.78	110.90
2	B	194	LYS	CA-C-N	5.13	126.47	120.98
2	B	194	LYS	C-N-CA	5.13	126.47	120.98
1	C	107	TYR	N-CA-CB	-5.12	102.57	110.20
2	B	236	VAL	CB-CA-C	-5.12	105.23	112.14
1	C	143	LEU	N-CA-C	-5.12	102.28	109.96
1	C	212	LEU	N-CA-C	-5.08	105.86	111.71
1	C	222	PRO	CB-CA-C	-5.08	105.11	111.56
2	D	280	TYR	N-CA-C	5.06	117.18	111.11
1	C	246	GLN	N-CA-C	5.06	117.66	109.06
2	B	260	ALA	N-CA-C	-5.05	105.68	111.14
1	A	184	VAL	N-CA-C	5.05	116.38	110.62
1	A	283	HIS	N-CA-C	5.04	116.23	109.83
1	A	41	THR	CB-CA-C	5.02	119.14	110.86
1	C	218	THR	N-CA-C	5.01	119.02	111.96
2	D	232	LEU	CB-CG-CD1	-5.01	95.68	110.70

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	GLY	Peptide
1	A	13	GLY	Peptide
1	A	166	LEU	Peptide
1	A	19	TYR	Peptide
1	A	295	HIS	Peptide
1	A	59	ASN	Peptide
1	A	62	ASN	Peptide
1	A	91	MET	Peptide
2	B	270	ILE	Peptide
2	B	272	PRO	Peptide
2	B	336	LEU	Peptide
2	B	340	SER	Peptide
2	B	344	ALA	Peptide
2	B	345	ASP	Peptide
2	B	423	LEU	Peptide
2	B	427	PRO	Peptide
2	B	429	THR	Peptide
1	C	11	GLY	Peptide
1	C	15	TYR	Peptide
1	C	161	HIS	Peptide
1	C	164	VAL	Peptide
1	C	165	THR	Peptide
1	C	206	ASP	Peptide
1	C	233	MET	Mainchain
1	C	64	VAL	Mainchain
1	C	70	ILE	Peptide
1	C	8	GLU	Peptide
2	D	198	GLY	Peptide
2	D	283	ASP	Peptide
2	D	324	PRO	Peptide
2	D	344	ALA	Peptide
2	D	345	ASP	Peptide
2	D	346	PRO	Peptide
2	D	369	GLY	Peptide
2	D	423	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2378	0	2426	331	0
1	C	2388	0	2432	390	1
2	B	2083	0	2107	301	1
2	D	2092	0	2110	270	0
3	A	28	0	15	6	0
3	C	28	0	15	13	0
4	A	26	0	0	10	0
4	B	17	0	0	8	0
4	C	28	0	0	18	0
4	D	17	0	0	7	0
All	All	9085	0	9105	1270	1

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 70.

All (1270) 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:60:HIS:CD2	1:A:61:PRO:HD2	1.21	1.61
1:A:60:HIS:CD2	1:A:61:PRO:CD	1.91	1.50
1:C:164:VAL:HB	4:C:2013:HOH:O	1.27	1.33
1:A:121:HIS:O	1:A:122:ARG:HG3	1.25	1.33
1:C:83:LEU:O	3:C:1297:MTW:H12	1.26	1.33
2:B:206:ILE:HA	2:B:210:MET:CE	1.61	1.31
2:B:282:THR:O	2:B:285:THR:HG22	1.27	1.31
2:B:175:VAL:O	2:B:177:ASP:N	1.64	1.27
1:C:95:ALA:O	1:C:96:LEU:HG	1.41	1.20
2:B:239:ILE:HD11	2:B:257:GLY:HA2	1.25	1.19
1:C:122:ARG:CG	1:C:122:ARG:HH21	1.56	1.19
2:B:327:CYS:HB3	4:B:2011:HOH:O	1.42	1.19
2:B:430:LEU:HB3	2:B:432:LEU:HD22	1.26	1.17
1:A:294:PRO:HB2	1:A:296:LEU:CD1	1.72	1.17
2:B:282:THR:O	2:B:285:THR:CG2	1.94	1.16
1:C:248:PHE:CE2	1:C:263:LEU:HD23	1.80	1.15
1:A:56:LYS:O	1:A:56:LYS:NZ	1.80	1.14
1:A:294:PRO:HB2	1:A:296:LEU:HD13	1.30	1.14
1:C:162:GLU:OE1	1:C:164:VAL:HG13	1.46	1.13
3:C:1297:MTW:H	3:C:1297:MTW:O1	1.49	1.12
1:A:71:HIS:CD2	2:B:296:HIS:CE1	2.38	1.11
1:A:178:LYS:HG2	1:A:179:TYR:CE2	1.86	1.10
2:D:345:ASP:OD2	2:D:346:PRO:HD3	1.48	1.10
2:D:218:LEU:HD22	2:D:261:MET:HE2	1.25	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:VAL:HG13	1:A:163:VAL:O	1.44	1.08
1:A:42:GLU:OE2	1:A:42:GLU:HA	1.47	1.07
2:D:345:ASP:OD2	2:D:346:PRO:CD	2.03	1.06
2:B:223:GLU:OE2	2:B:412:LYS:HG3	1.52	1.06
2:D:323:GLN:O	2:D:323:GLN:HG2	1.53	1.06
2:B:206:ILE:CA	2:B:210:MET:HE1	1.86	1.06
1:A:71:HIS:NE2	2:B:296:HIS:ND1	2.04	1.05
1:A:164:VAL:O	1:A:165:THR:HG22	1.57	1.05
1:C:230:VAL:O	1:C:232:SER:N	1.90	1.05
1:A:60:HIS:HD2	1:A:61:PRO:N	1.56	1.04
1:C:60:HIS:CD2	1:C:62:ASN:H	1.75	1.04
1:C:162:GLU:OE2	1:C:163:VAL:N	1.90	1.04
1:A:166:LEU:HB3	1:A:167:TRP:HD1	1.19	1.03
1:A:34:LYS:HG3	1:A:77:TYR:HE2	1.24	1.02
1:A:34:LYS:HG3	1:A:77:TYR:CE2	1.93	1.02
1:C:12:GLU:HB3	1:C:17:VAL:HG12	1.40	1.01
1:C:60:HIS:HD2	1:C:62:ASN:H	1.06	1.01
2:B:395:HIS:CE1	2:B:399:LEU:HD11	1.94	1.01
2:D:196:LYS:HG3	4:D:2003:HOH:O	1.61	1.01
2:B:207:THR:CG2	2:B:210:MET:HE2	1.90	1.00
1:A:121:HIS:C	1:A:122:ARG:HG3	1.83	1.00
2:B:207:THR:HG22	2:B:210:MET:CE	1.92	1.00
1:C:91:MET:HE2	1:C:195:GLU:HG2	1.41	1.00
1:C:60:HIS:CG	1:C:61:PRO:HD2	1.95	1.00
1:A:294:PRO:CB	1:A:296:LEU:CD1	2.41	0.99
1:A:60:HIS:CD2	1:A:61:PRO:N	2.31	0.99
2:D:404:HIS:CD2	2:D:406:GLN:H	1.79	0.98
2:B:425:ASN:HB2	4:B:2017:HOH:O	1.64	0.98
2:B:206:ILE:CA	2:B:210:MET:CE	2.40	0.98
1:C:32:LEU:CD2	1:C:79:VAL:HG22	1.95	0.97
2:D:401:ALA:HB1	2:D:410:ARG:HD2	1.46	0.97
1:A:241:PRO:HG2	1:A:243:TRP:CZ3	2.00	0.97
1:A:164:VAL:O	1:A:165:THR:CG2	2.13	0.96
2:B:373:PRO:HG2	2:B:376:LEU:HD12	1.48	0.96
1:A:164:VAL:O	1:A:165:THR:CB	2.13	0.96
1:C:40:GLU:O	2:D:288:LYS:NZ	1.96	0.96
2:B:263:LEU:HD21	2:B:295:GLU:HG3	1.48	0.96
1:C:122:ARG:HH21	1:C:122:ARG:HG3	1.28	0.95
1:C:160:THR:C	1:C:161:HIS:CD2	2.45	0.95
1:A:60:HIS:NE2	1:A:61:PRO:HD2	1.81	0.95
2:B:199:TYR:CD1	2:B:199:TYR:C	2.45	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:PRO:CB	1:A:296:LEU:HD13	1.98	0.94
1:A:178:LYS:CG	1:A:179:TYR:CE2	2.49	0.94
1:C:101:LEU:CD2	1:C:101:LEU:H	1.80	0.94
1:A:241:PRO:HG2	1:A:243:TRP:CH2	2.03	0.94
2:D:385:GLU:HA	2:D:385:GLU:OE1	1.65	0.94
1:A:95:ALA:O	1:A:96:LEU:HB3	1.67	0.93
2:B:207:THR:HG22	2:B:210:MET:HE2	0.97	0.93
1:C:75:LYS:HB3	4:C:2003:HOH:O	1.67	0.93
1:C:200:ARG:HH11	1:C:200:ARG:CG	1.81	0.93
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.48	0.93
1:C:15:TYR:CD1	1:C:15:TYR:N	2.37	0.93
1:C:122:ARG:HH21	1:C:122:ARG:HG2	1.31	0.93
1:A:139:GLY:HA2	4:A:2014:HOH:O	1.67	0.93
2:B:199:TYR:CD1	2:B:200:MET:N	2.38	0.92
1:C:200:ARG:HH11	1:C:200:ARG:HG2	1.34	0.92
1:A:14:THR:O	1:A:16:GLY:N	2.01	0.92
1:A:60:HIS:CG	1:A:61:PRO:CD	2.52	0.91
2:D:336:LEU:HD13	2:D:362:LEU:HD23	1.51	0.91
1:A:1:MET:HE3	1:A:77:TYR:CG	2.05	0.91
1:C:39:THR:O	1:C:39:THR:CG2	2.18	0.91
1:A:163:VAL:O	1:A:163:VAL:CG1	2.19	0.91
1:A:97:THR:HB	4:A:2011:HOH:O	1.69	0.90
1:C:14:THR:HB	1:C:15:TYR:CE1	2.06	0.90
1:C:101:LEU:CD2	1:C:101:LEU:N	2.33	0.89
2:D:335:PHE:HB2	2:D:413:TYR:CD2	2.07	0.89
2:B:395:HIS:CG	2:B:430:LEU:HD21	2.08	0.89
1:A:96:LEU:HB3	4:A:2009:HOH:O	1.73	0.88
1:A:170:ALA:HB3	1:A:173:ILE:HD12	1.55	0.88
1:C:122:ARG:HG2	1:C:122:ARG:NH2	1.87	0.88
2:B:206:ILE:HA	2:B:210:MET:HE1	0.91	0.88
1:C:39:THR:O	1:C:39:THR:HG23	1.71	0.88
1:C:32:LEU:HD23	1:C:79:VAL:HG22	1.52	0.88
1:C:101:LEU:N	1:C:101:LEU:HD22	1.87	0.88
1:A:294:PRO:HB2	1:A:296:LEU:HD12	1.55	0.88
3:A:1297:MTW:N3	3:A:1297:MTW:H14	1.88	0.87
2:D:214:LEU:O	2:D:214:LEU:HD12	1.74	0.87
2:B:217:TRP:HZ2	2:B:281:ILE:HD12	1.39	0.87
1:A:1:MET:HE2	1:A:70:ILE:HD12	1.53	0.86
1:C:85:GLN:HG3	1:C:86:ASP:N	1.88	0.86
1:A:166:LEU:HB3	1:A:167:TRP:CD1	2.09	0.86
1:C:125:HIS:CG	1:C:128:LEU:HD21	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:214:LEU:HD12	2:D:214:LEU:C	1.98	0.85
2:B:430:LEU:HB3	2:B:432:LEU:CD2	2.06	0.85
3:C:1297:MTW:O1	3:C:1297:MTW:C	2.24	0.85
2:D:262:LEU:HD11	2:D:266:LYS:HE3	1.58	0.84
2:D:379:LYS:HG3	4:D:2002:HOH:O	1.76	0.84
1:A:23:ASN:C	1:A:23:ASN:OD1	2.20	0.84
1:C:101:LEU:H	1:C:101:LEU:HD23	1.41	0.84
1:C:115:LEU:HD12	1:C:189:LEU:CD2	2.08	0.84
2:B:415:ASN:OD1	2:B:417:LYS:N	2.10	0.84
1:C:135:ILE:CG2	1:C:141:ILE:HD12	2.08	0.84
1:A:38:ASP:OD2	1:A:41:THR:HB	1.78	0.83
1:C:159:TYR:CD2	1:C:162:GLU:HG2	2.13	0.83
2:D:415:ASN:OD1	2:D:417:LYS:N	2.11	0.83
2:B:207:THR:H	2:B:210:MET:HE3	1.44	0.83
2:B:239:ILE:CD1	2:B:257:GLY:HA2	2.09	0.83
1:C:70:ILE:N	1:C:77:TYR:O	2.11	0.83
1:A:236:TYR:CD1	1:A:237:LYS:N	2.47	0.83
2:B:223:GLU:HA	2:B:223:GLU:OE1	1.77	0.82
1:C:233:MET:O	1:C:234:PRO:C	2.23	0.81
2:B:190:GLU:OE1	2:B:352:PRO:HD2	1.80	0.81
2:B:194:LYS:HG2	2:B:195:PRO:HD2	1.61	0.81
1:C:60:HIS:CD2	1:C:60:HIS:C	2.59	0.81
1:C:159:TYR:O	1:C:161:HIS:N	2.14	0.81
1:C:162:GLU:CD	1:C:163:VAL:C	2.48	0.81
2:B:233:HIS:CD2	4:B:2010:HOH:O	2.34	0.81
2:D:223:GLU:OE1	2:D:223:GLU:HA	1.79	0.81
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.63	0.81
2:D:218:LEU:CD2	2:D:261:MET:HE2	2.10	0.80
2:B:419:HIS:O	2:B:421:VAL:N	2.14	0.80
1:A:60:HIS:HD2	1:A:61:PRO:CD	1.66	0.80
1:A:159:TYR:HD1	1:A:159:TYR:N	1.76	0.80
2:D:217:TRP:CH2	2:D:281:ILE:HD12	2.16	0.80
1:C:248:PHE:CZ	1:C:263:LEU:HD23	2.16	0.80
2:B:199:TYR:C	2:B:199:TYR:HD1	1.89	0.80
2:B:353:SER:O	2:B:356:ALA:HB3	1.82	0.80
1:C:115:LEU:HD12	1:C:189:LEU:HD22	1.64	0.80
2:B:252:LYS:HG3	1:C:25:LEU:O	1.82	0.79
1:A:154:VAL:HG13	1:A:155:PRO:HD2	1.62	0.79
2:B:401:ALA:HB3	2:B:402:PRO:HD3	1.61	0.79
1:C:111:LEU:HD23	1:C:143:LEU:HD23	1.64	0.79
1:C:162:GLU:OE2	1:C:163:VAL:C	2.25	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ASP:HB2	1:C:210:ASP:OD2	1.82	0.79
2:B:211:ARG:O	2:B:215:VAL:HG23	1.83	0.79
1:C:128:LEU:HD23	1:C:128:LEU:N	1.97	0.79
1:A:139:GLY:CA	4:A:2014:HOH:O	2.25	0.79
1:A:115:LEU:HD13	1:A:119:HIS:CE1	2.18	0.79
2:B:217:TRP:CZ2	2:B:281:ILE:HD12	2.17	0.79
2:B:331:SER:HB2	2:B:421:VAL:HG11	1.64	0.79
1:C:156:VAL:HG12	1:C:156:VAL:O	1.81	0.79
2:D:431:ASN:O	2:D:432:LEU:HD23	1.83	0.79
1:A:83:LEU:HD21	1:A:142:LYS:HD2	1.63	0.79
1:C:122:ARG:CG	1:C:122:ARG:NH2	2.27	0.79
2:B:273:PRO:HB2	2:B:278:PHE:CE2	2.18	0.79
1:C:86:ASP:C	1:C:86:ASP:OD1	2.25	0.78
1:C:159:TYR:C	1:C:161:HIS:H	1.91	0.78
2:D:404:HIS:CD2	2:D:406:GLN:N	2.50	0.78
1:A:42:GLU:OE2	1:A:42:GLU:CA	2.28	0.78
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.08	0.78
1:A:81:GLU:O	3:A:1297:MTW:H9	1.84	0.78
1:C:95:ALA:O	1:C:96:LEU:CG	2.29	0.78
1:C:83:LEU:O	3:C:1297:MTW:C12	2.22	0.78
1:C:115:LEU:CD1	1:C:189:LEU:HD22	2.12	0.78
1:A:159:TYR:N	1:A:159:TYR:CD1	2.49	0.78
1:A:62:ASN:ND2	1:A:110:GLN:HB3	1.99	0.78
2:D:389:PRO:O	2:D:392:MET:HB2	1.82	0.78
2:D:207:THR:HG23	2:D:210:MET:H	1.48	0.78
2:D:305:ASP:C	2:D:306:LEU:HD23	2.09	0.78
1:A:178:LYS:HG2	1:A:179:TYR:HE2	1.48	0.77
2:D:323:GLN:O	2:D:323:GLN:CG	2.32	0.77
1:A:164:VAL:O	1:A:165:THR:HB	1.83	0.77
1:A:178:LYS:HG2	1:A:179:TYR:CD2	2.20	0.77
1:C:74:ASN:OD1	1:C:75:LYS:HD3	1.85	0.77
1:A:38:ASP:C	1:A:38:ASP:OD1	2.26	0.76
2:B:207:THR:N	2:B:210:MET:CE	2.47	0.76
1:A:121:HIS:O	1:A:123:VAL:HG23	1.85	0.76
1:C:12:GLU:HB3	1:C:17:VAL:CG1	2.15	0.76
1:C:226:VAL:HG13	1:C:226:VAL:O	1.86	0.76
2:B:321:HIS:CE1	2:B:379:LYS:HE2	2.21	0.76
2:B:430:LEU:CB	2:B:432:LEU:HD22	2.13	0.75
1:C:165:THR:O	4:C:2012:HOH:O	2.04	0.75
2:D:218:LEU:HD22	2:D:261:MET:CE	2.12	0.75
2:B:282:THR:HB	2:B:285:THR:HG23	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:VAL:HG12	1:C:30:VAL:N	2.01	0.75
2:B:345:ASP:CB	2:B:346:PRO:CD	2.64	0.75
1:C:88:LYS:HD2	1:C:92:ASP:OD2	1.86	0.75
2:B:205:ASP:OD2	2:B:250:ARG:HG2	1.87	0.75
2:B:219:VAL:HG21	2:B:409:ILE:HG13	1.68	0.75
1:C:122:ARG:HG3	1:C:122:ARG:O	1.85	0.75
1:C:10:ILE:HD13	1:C:20:LYS:HB3	1.68	0.74
1:C:166:LEU:O	1:C:168:TYR:N	2.20	0.74
2:D:345:ASP:OD2	2:D:346:PRO:HD2	1.83	0.74
2:B:178:TYR:O	2:B:179:HIS:C	2.27	0.74
1:C:111:LEU:HD23	1:C:143:LEU:CD2	2.18	0.74
1:C:159:TYR:HD2	1:C:162:GLU:CB	2.00	0.74
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.21	0.74
2:D:419:HIS:O	4:D:2015:HOH:O	2.04	0.74
2:B:268:GLU:OE1	2:B:268:GLU:HA	1.88	0.74
1:C:51:GLU:O	1:C:55:LEU:HB2	1.87	0.74
1:C:200:ARG:HH11	1:C:200:ARG:CB	2.00	0.74
1:A:71:HIS:NE2	2:B:296:HIS:CE1	2.49	0.74
1:C:137:THR:HG23	4:C:2010:HOH:O	1.86	0.74
2:D:319:PHE:CE2	2:D:330:GLU:HG2	2.22	0.74
1:C:31:ALA:HB3	1:C:80:PHE:HB2	1.70	0.74
2:D:238:TYR:OH	2:D:306:LEU:HB3	1.88	0.74
1:A:38:ASP:OD1	1:A:38:ASP:O	2.06	0.74
2:B:342:ILE:HD11	2:B:409:ILE:HD12	1.69	0.74
2:B:388:LYS:N	2:B:389:PRO:HD2	2.02	0.74
2:B:293:ARG:HB3	1:C:25:LEU:HD11	1.70	0.74
1:A:87:LEU:O	1:A:91:MET:HG3	1.87	0.73
2:B:384:LEU:HD12	2:B:384:LEU:O	1.88	0.73
1:C:159:TYR:HD2	1:C:162:GLU:HB3	1.53	0.73
1:A:170:ALA:HB3	1:A:173:ILE:CD1	2.18	0.73
1:A:181:SER:HB3	4:A:2016:HOH:O	1.89	0.73
2:D:236:VAL:HA	2:D:239:ILE:HG13	1.70	0.73
1:C:159:TYR:HD2	1:C:162:GLU:HG2	1.51	0.73
1:A:60:HIS:CD2	1:A:62:ASN:H	2.07	0.73
1:A:121:HIS:C	1:A:122:ARG:CG	2.60	0.73
1:A:156:VAL:HG12	1:A:180:TYR:HD1	1.53	0.73
1:A:14:THR:O	1:A:15:TYR:C	2.31	0.72
1:A:222:PRO:HA	4:A:2018:HOH:O	1.88	0.72
1:C:162:GLU:CD	1:C:163:VAL:N	2.47	0.72
1:A:227:TRP:O	1:A:230:VAL:HG22	1.88	0.72
2:B:354:VAL:O	2:B:355:ILE:C	2.30	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:407:GLN:O	2:D:409:ILE:N	2.21	0.72
1:A:227:TRP:CD2	1:A:230:VAL:HG13	2.23	0.72
2:B:255:LEU:HG	2:B:294:MET:HG3	1.72	0.72
2:B:331:SER:CB	2:B:421:VAL:HG11	2.20	0.72
2:D:321:HIS:N	2:D:321:HIS:CD2	2.56	0.72
1:A:105:LYS:HE3	1:A:285:PHE:CZ	2.25	0.72
1:C:165:THR:C	4:C:2012:HOH:O	2.32	0.72
2:D:336:LEU:HD13	2:D:362:LEU:CD2	2.18	0.72
1:A:154:VAL:HG13	1:A:155:PRO:CD	2.20	0.72
1:A:115:LEU:HD11	1:A:185:ASP:HB3	1.71	0.72
2:B:233:HIS:HD2	4:B:2010:HOH:O	1.68	0.72
2:B:415:ASN:OD1	2:B:415:ASN:C	2.32	0.72
2:D:335:PHE:HD1	2:D:413:TYR:CG	2.08	0.72
1:A:224:GLU:OE2	1:A:231:THR:OG1	2.07	0.71
2:B:207:THR:H	2:B:210:MET:CE	2.02	0.71
3:C:1297:MTW:N3	3:C:1297:MTW:H14	2.05	0.71
2:B:175:VAL:O	2:B:176:PRO:C	2.33	0.71
1:A:1:MET:HE3	1:A:77:TYR:CB	2.21	0.71
2:D:415:ASN:OD1	2:D:415:ASN:C	2.34	0.71
1:A:96:LEU:CD2	4:A:2009:HOH:O	2.38	0.71
1:C:1:MET:HE2	1:C:70:ILE:HD13	1.73	0.71
1:C:127:ASP:OD2	1:C:129:LYS:HE2	1.89	0.71
1:A:69:VAL:HG13	1:A:78:LEU:HD23	1.72	0.71
1:C:48:ALA:O	1:C:52:ILE:HD12	1.90	0.71
1:C:167:TRP:NE1	1:C:205:GLY:H	1.88	0.71
2:B:364:LEU:O	2:B:365:TYR:C	2.34	0.71
1:A:89:LYS:O	1:A:90:PHE:C	2.33	0.70
2:B:182:ILE:HG22	2:B:183:HIS:N	2.05	0.70
1:A:190:GLY:N	1:A:266:MET:HE2	2.05	0.70
1:C:212:LEU:HD22	1:C:216:PHE:CZ	2.26	0.70
1:A:277:ALA:O	1:A:278:LYS:C	2.33	0.70
1:A:156:VAL:HG12	1:A:180:TYR:CD1	2.26	0.70
2:B:206:ILE:CA	2:B:210:MET:HE3	2.19	0.70
2:D:343:ASP:HB3	2:D:345:ASP:OD2	1.90	0.70
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.72	0.70
2:D:338:GLU:O	2:D:339:LEU:C	2.35	0.70
1:C:200:ARG:CB	1:C:200:ARG:NH1	2.55	0.70
1:C:60:HIS:HD2	1:C:62:ASN:N	1.86	0.70
2:D:315:LEU:HD23	2:D:356:ALA:HB1	1.73	0.70
2:B:400:LYS:O	2:B:401:ALA:C	2.33	0.69
1:C:12:GLU:CB	1:C:17:VAL:HG12	2.20	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:HIS:CG	1:C:61:PRO:CD	2.74	0.69
1:C:127:ASP:OD2	1:C:129:LYS:CE	2.40	0.69
1:C:260:ARG:O	1:C:264:SER:OG	2.09	0.69
1:A:202:LEU:HD13	1:A:203:PHE:CE2	2.27	0.69
1:A:247:ASP:O	1:A:250:LYS:HB2	1.93	0.69
1:C:200:ARG:CG	1:C:200:ARG:NH1	2.52	0.69
1:C:245:ARG:HG3	1:C:245:ARG:NH1	2.07	0.69
1:A:50:ARG:O	1:A:51:GLU:C	2.33	0.69
1:A:222:PRO:CA	4:A:2018:HOH:O	2.40	0.69
2:B:338:GLU:O	2:B:341:LEU:HB2	1.92	0.69
2:B:225:TYR:HE1	2:B:281:ILE:HG21	1.57	0.69
1:C:60:HIS:CD2	1:C:61:PRO:HD2	2.28	0.69
1:C:160:THR:O	1:C:161:HIS:CB	2.39	0.69
2:D:378:ARG:HB3	2:D:378:ARG:HH11	1.57	0.69
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.28	0.69
1:C:70:ILE:CG2	1:C:71:HIS:N	2.56	0.69
2:D:306:LEU:HD23	2:D:306:LEU:N	2.06	0.69
1:A:38:ASP:OD1	1:A:41:THR:N	2.21	0.69
2:B:271:TYR:HB2	2:B:272:PRO:HD2	1.75	0.68
2:B:345:ASP:HB3	2:B:346:PRO:HD3	1.74	0.68
1:C:259:GLY:HA2	1:C:285:PHE:CD1	2.28	0.68
2:D:319:PHE:CD2	2:D:330:GLU:HG2	2.28	0.68
1:A:34:LYS:CG	1:A:77:TYR:CE2	2.75	0.68
2:B:208:ASN:HB3	2:B:345:ASP:OD1	1.93	0.68
1:A:95:ALA:O	1:A:96:LEU:CB	2.39	0.68
1:C:166:LEU:O	1:C:169:ARG:N	2.26	0.68
1:C:159:TYR:CD2	1:C:162:GLU:HB3	2.29	0.68
2:B:395:HIS:CD2	2:B:430:LEU:HD21	2.28	0.68
1:C:72:THR:OG1	1:C:75:LYS:HG2	1.93	0.68
1:C:159:TYR:HD2	1:C:162:GLU:CG	2.06	0.68
1:C:94:SER:O	1:C:97:THR:HG23	1.93	0.68
2:B:207:THR:N	2:B:210:MET:HE3	2.08	0.68
2:B:336:LEU:O	2:B:339:LEU:HB2	1.94	0.68
2:D:214:LEU:O	2:D:217:TRP:HB3	1.94	0.68
2:D:335:PHE:CD1	2:D:413:TYR:CG	2.82	0.68
1:C:85:GLN:HA	3:C:1297:MTW:H13	1.76	0.68
2:D:357:GLY:O	2:D:358:ALA:C	2.37	0.67
1:A:227:TRP:CE3	1:A:230:VAL:CG1	2.76	0.67
1:C:60:HIS:CD2	1:C:61:PRO:N	2.62	0.67
2:D:362:LEU:O	2:D:362:LEU:HG	1.95	0.67
2:B:182:ILE:O	2:B:183:HIS:C	2.36	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ILE:HB	1:A:77:TYR:HB2	1.76	0.67
1:A:209:ILE:O	1:A:209:ILE:HG13	1.95	0.67
1:C:60:HIS:CD2	1:C:61:PRO:CD	2.78	0.67
2:B:345:ASP:HB2	2:B:346:PRO:HD2	1.75	0.67
1:C:12:GLU:OE2	1:C:12:GLU:N	2.24	0.67
1:A:294:PRO:CG	1:A:296:LEU:HD13	2.24	0.66
2:B:419:HIS:C	2:B:421:VAL:H	2.04	0.66
1:C:152:PHE:C	1:C:154:VAL:N	2.51	0.66
2:D:282:THR:O	2:D:283:ASP:HB2	1.93	0.66
1:A:56:LYS:HZ2	1:A:56:LYS:C	1.95	0.66
2:B:203:GLN:HB3	2:B:206:ILE:HG12	1.76	0.66
2:B:415:ASN:OD1	2:B:416:SER:N	2.28	0.66
1:C:101:LEU:HB2	1:C:102:PRO:HD3	1.76	0.66
2:B:297:LEU:HD12	2:B:297:LEU:O	1.95	0.66
1:C:162:GLU:OE2	1:C:163:VAL:CA	2.44	0.66
2:D:329:VAL:HG23	2:D:367:VAL:HB	1.75	0.66
1:C:162:GLU:OE2	1:C:163:VAL:O	2.14	0.66
1:C:165:THR:O	4:C:2013:HOH:O	2.13	0.66
2:D:229:ASN:HD22	2:D:334:MET:CE	2.09	0.66
2:B:189:MET:O	2:B:192:LYS:N	2.28	0.66
2:B:197:VAL:HG23	2:B:198:GLY:N	2.10	0.66
1:A:166:LEU:CB	1:A:167:TRP:HD1	2.01	0.66
1:A:175:LEU:HA	1:A:235:ASP:HB2	1.77	0.66
1:C:91:MET:CE	1:C:195:GLU:HG2	2.22	0.66
1:C:145:ASP:OD2	1:C:145:ASP:C	2.36	0.66
1:C:160:THR:O	1:C:161:HIS:HB2	1.96	0.66
1:A:101:LEU:CB	1:A:102:PRO:HD3	2.26	0.65
1:A:170:ALA:HB1	1:A:172:GLU:OE2	1.95	0.65
1:A:170:ALA:HB1	1:A:172:GLU:CD	2.21	0.65
2:D:400:LYS:O	2:D:401:ALA:C	2.38	0.65
1:A:129:LYS:HD2	1:A:131:GLN:HG3	1.77	0.65
2:B:314:PHE:CE2	2:B:353:SER:HB3	2.32	0.65
1:C:6:LYS:HE3	4:C:2001:HOH:O	1.97	0.65
1:C:61:PRO:O	1:C:142:LYS:HE2	1.97	0.65
1:C:101:LEU:N	1:C:102:PRO:HD2	2.10	0.65
1:A:96:LEU:HD22	4:A:2009:HOH:O	1.94	0.65
1:C:85:GLN:NE2	1:C:89:LYS:HB3	2.11	0.65
1:C:268[B]:HIS:C	1:C:269:TYR:O	2.26	0.65
2:D:392:MET:HE2	2:D:392:MET:HA	1.79	0.65
2:D:215:VAL:O	2:D:219:VAL:HG23	1.95	0.65
1:A:1:MET:HG2	1:A:70:ILE:CD1	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ILE:O	1:C:76:LEU:HD12	1.97	0.65
1:C:131:GLN:NE2	1:C:131:GLN:N	2.44	0.65
2:B:344:ALA:CB	2:B:348:LEU:HD22	2.25	0.65
1:C:159:TYR:C	1:C:161:HIS:N	2.46	0.65
2:D:335:PHE:CD1	2:D:413:TYR:CB	2.80	0.65
1:C:64:VAL:HG22	1:C:143:LEU:O	1.97	0.64
1:C:121:HIS:O	1:C:122:ARG:CG	2.45	0.64
1:A:99:ILE:HD12	1:A:196:MET:HG2	1.80	0.64
1:C:85:GLN:HA	3:C:1297:MTW:C13	2.28	0.64
1:A:115:LEU:HD13	1:A:119:HIS:HE1	1.60	0.64
2:B:395:HIS:ND1	2:B:430:LEU:HD21	2.12	0.64
1:C:158:THR:HB	1:C:178:LYS:O	1.98	0.64
1:C:160:THR:C	1:C:161:HIS:HD2	2.00	0.64
1:C:130:PRO:HB2	1:C:131:GLN:NE2	2.11	0.64
1:A:100:PRO:C	1:A:102:PRO:HD2	2.22	0.64
1:A:100:PRO:C	1:A:102:PRO:CD	2.71	0.64
1:A:91:MET:HE3	1:A:196:MET:HG3	1.79	0.64
2:B:418:TYR:O	2:B:421:VAL:HG22	1.98	0.64
2:B:400:LYS:O	2:B:402:PRO:N	2.30	0.64
2:D:217:TRP:HH2	2:D:281:ILE:HD12	1.62	0.64
1:A:178:LYS:C	1:A:179:TYR:CD2	2.76	0.63
1:C:119:HIS:O	1:C:122:ARG:N	2.27	0.63
1:A:202:LEU:HD22	1:A:202:LEU:O	1.97	0.63
1:A:252:VAL:O	1:A:253:PRO:C	2.41	0.63
2:B:343:ASP:HB3	2:B:345:ASP:HB2	1.80	0.63
2:B:249:LEU:C	2:B:251:GLY:N	2.54	0.63
2:D:413:TYR:HB3	2:D:422:SER:HB3	1.79	0.63
2:B:332:LEU:HD23	2:B:363:ALA:HA	1.80	0.63
1:C:166:LEU:O	1:C:167:TRP:C	2.39	0.63
2:D:404:HIS:HD2	2:D:406:GLN:N	1.96	0.63
2:B:315:LEU:O	2:B:318:TYR:HB2	1.99	0.63
1:C:70:ILE:CG2	1:C:71:HIS:H	2.11	0.63
1:A:166:LEU:O	1:A:168:TYR:N	2.32	0.63
2:B:241:ARG:O	2:B:244:SER:HB2	1.99	0.63
2:D:230:GLU:O	2:D:231:THR:C	2.40	0.63
2:D:417:LYS:HD2	2:D:418:TYR:CE2	2.33	0.63
1:C:11:GLY:O	1:C:17:VAL:HB	1.99	0.62
2:B:315:LEU:O	2:B:318:TYR:N	2.32	0.62
1:C:170:ALA:HB3	1:C:173:ILE:HD13	1.82	0.62
1:A:294:PRO:HG2	1:A:296:LEU:HD13	1.82	0.62
1:C:268[B]:HIS:O	1:C:269:TYR:O	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLY:C	4:A:2014:HOH:O	2.42	0.62
2:B:214:LEU:HD22	2:B:253:LEU:HG	1.79	0.62
2:B:216:ASP:CG	2:B:408:SER:HB2	2.24	0.62
1:C:17:VAL:CG2	1:C:17:VAL:O	2.47	0.62
1:C:200:ARG:NH1	1:C:200:ARG:HB3	2.15	0.62
2:D:336:LEU:CD1	2:D:362:LEU:HD23	2.26	0.62
1:A:1:MET:HE3	1:A:77:TYR:HB3	1.82	0.62
1:A:56:LYS:HA	1:A:56:LYS:HZ3	1.64	0.62
1:A:135:ILE:HD12	1:A:296:LEU:HD11	1.82	0.62
2:B:395:HIS:CE1	2:B:430:LEU:CD2	2.83	0.62
1:C:159:TYR:HB3	1:C:162:GLU:H	1.65	0.62
2:D:202:LYS:NZ	2:D:202:LYS:HB3	2.15	0.62
2:B:410:ARG:O	2:B:411:GLU:C	2.40	0.62
1:C:160:THR:C	1:C:161:HIS:CG	2.72	0.62
1:C:176:GLY:HA2	4:C:2014:HOH:O	1.99	0.62
2:B:326:ASN:C	2:B:326:ASN:OD1	2.40	0.62
1:C:159:TYR:CD1	2:D:270:ILE:HD12	2.35	0.62
2:D:282:THR:O	2:D:283:ASP:CB	2.48	0.62
2:D:415:ASN:OD1	2:D:417:LYS:HG2	1.99	0.62
1:A:108:LEU:O	1:A:112:LEU:HD12	1.99	0.61
1:A:203:PHE:CE1	1:A:215:ILE:HA	2.34	0.61
1:C:83:LEU:HD21	1:C:142:LYS:HD2	1.81	0.61
2:B:395:HIS:CE1	2:B:430:LEU:HD21	2.35	0.61
1:A:172:GLU:HG2	1:A:173:ILE:N	2.15	0.61
2:B:365:TYR:HE2	2:B:430:LEU:HA	1.65	0.61
1:A:10:ILE:HD13	1:A:20:LYS:N	2.15	0.61
1:A:200:ARG:O	1:A:201:ALA:C	2.43	0.61
2:B:254:GLN:OE1	2:B:282:THR:HG22	2.00	0.61
2:B:345:ASP:HB2	2:B:346:PRO:CD	2.29	0.61
1:C:293:VAL:CG2	1:C:293:VAL:O	2.45	0.61
2:D:418:TYR:O	2:D:420:GLY:N	2.33	0.61
1:C:245:ARG:HG2	1:C:246:GLN:N	2.12	0.61
1:C:236:TYR:CG	1:C:237:LYS:N	2.69	0.61
2:D:178:TYR:C	2:D:178:TYR:CD2	2.79	0.61
2:B:361:HIS:C	2:B:361:HIS:CD2	2.79	0.61
2:D:255:LEU:HD23	2:D:294:MET:HE2	1.83	0.61
1:A:178:LYS:HG3	1:A:179:TYR:CE2	2.36	0.61
2:B:420:GLY:O	2:B:421:VAL:C	2.43	0.61
1:C:245:ARG:HH11	1:C:245:ARG:CG	2.14	0.61
1:A:202:LEU:O	1:A:202:LEU:CD2	2.49	0.60
2:B:277:GLU:OE1	2:B:277:GLU:HA	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ILE:HG22	1:C:71:HIS:N	2.15	0.60
2:D:345:ASP:CG	2:D:346:PRO:HD3	2.22	0.60
2:D:392:MET:HE2	2:D:392:MET:CA	2.31	0.60
1:A:100:PRO:O	1:A:101:LEU:C	2.41	0.60
1:A:108:LEU:HG	1:A:112:LEU:HD12	1.84	0.60
1:A:150:ARG:NH1	2:B:268:GLU:O	2.35	0.60
2:B:278:PHE:O	2:B:281:ILE:HG13	2.01	0.60
1:C:29:VAL:CG1	1:C:30:VAL:N	2.65	0.60
2:D:392:MET:HA	2:D:392:MET:CE	2.30	0.60
2:D:418:TYR:O	2:D:419:HIS:C	2.41	0.60
3:C:1297:MTW:O2	3:C:1297:MTW:N1	2.34	0.60
1:A:1:MET:CE	1:A:70:ILE:HD12	2.30	0.60
1:C:29:VAL:C	1:C:30:VAL:HG13	2.25	0.60
2:D:175:VAL:O	2:D:175:VAL:CG1	2.49	0.60
2:D:248:VAL:HG12	2:D:249:LEU:O	2.01	0.60
2:D:335:PHE:CE2	2:D:339:LEU:HD11	2.36	0.60
2:D:421:VAL:HA	2:D:424:LEU:HD22	1.84	0.60
2:B:225:TYR:CE1	2:B:281:ILE:HG21	2.36	0.60
1:C:29:VAL:C	1:C:30:VAL:CG1	2.75	0.60
2:D:405:ALA:HB1	2:D:406:GLN:HE22	1.66	0.60
1:A:1:MET:HE1	1:A:32:LEU:HD22	1.82	0.60
2:B:357:GLY:O	2:B:358:ALA:C	2.45	0.60
2:B:404:HIS:HD2	2:B:405:ALA:N	1.99	0.60
1:C:1:MET:CE	1:C:70:ILE:HD13	2.31	0.60
1:C:227:TRP:O	1:C:228:PRO:C	2.44	0.60
2:D:332:LEU:HD12	2:D:332:LEU:O	2.02	0.60
2:D:248:VAL:HG12	2:D:249:LEU:N	2.17	0.60
2:D:415:ASN:CG	2:D:417:LYS:HG2	2.26	0.60
2:D:420:GLY:O	2:D:422:SER:N	2.35	0.60
1:A:23:ASN:OD1	1:A:25:LEU:N	2.34	0.60
2:B:219:VAL:HG12	2:B:220:GLU:N	2.11	0.60
2:D:372:TRP:NE1	2:D:382:TYR:O	2.26	0.60
1:A:1:MET:HG2	1:A:70:ILE:HD13	1.83	0.60
2:B:252:LYS:HD3	2:B:252:LYS:N	2.17	0.60
1:C:166:LEU:CD2	1:C:169:ARG:CZ	2.79	0.60
1:A:122:ARG:HB3	2:B:182:ILE:HG12	1.84	0.59
1:C:34:LYS:CG	1:C:34:LYS:O	2.48	0.59
1:C:63:ILE:O	1:C:64:VAL:C	2.45	0.59
1:C:101:LEU:O	1:C:104:ILE:N	2.35	0.59
2:D:235:ALA:O	2:D:239:ILE:HG12	2.02	0.59
1:C:110:GLN:O	1:C:111:LEU:C	2.45	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:LYS:O	1:C:130:PRO:C	2.45	0.59
2:D:216:ASP:CG	2:D:406:GLN:HB3	2.28	0.59
2:D:377:ILE:HG13	2:D:382:TYR:O	2.01	0.59
2:B:216:ASP:OD1	2:B:408:SER:HB2	2.03	0.59
2:B:259:ALA:HB2	2:B:294:MET:HB3	1.83	0.59
2:B:268:GLU:OE1	2:B:268:GLU:CA	2.47	0.59
1:C:70:ILE:HG23	1:C:71:HIS:H	1.68	0.59
1:C:204:PRO:O	1:C:214:ARG:HD3	2.03	0.59
1:A:108:LEU:HG	1:A:112:LEU:CD1	2.33	0.59
2:B:211:ARG:HG2	2:B:211:ARG:HH11	1.67	0.59
1:C:91:MET:HE2	1:C:195:GLU:CG	2.27	0.59
2:D:211:ARG:O	2:D:212:ALA:C	2.44	0.59
2:B:332:LEU:HB3	2:B:363:ALA:HB1	1.85	0.59
1:C:246:GLN:O	1:C:247:ASP:C	2.45	0.59
1:C:252:VAL:N	1:C:253:PRO:CD	2.66	0.59
1:A:86:ASP:OD1	1:A:89:LYS:N	2.36	0.59
2:B:233:HIS:HB3	4:B:2010:HOH:O	2.01	0.59
2:D:354:VAL:O	2:D:355:ILE:C	2.45	0.59
1:C:206:ASP:CB	1:C:210:ASP:OD2	2.50	0.59
1:A:60:HIS:HD2	1:A:62:ASN:H	1.50	0.58
2:B:371:SER:O	2:B:373:PRO:HD3	2.04	0.58
2:B:317:GLN:O	2:B:318:TYR:C	2.44	0.58
1:C:126:ARG:NH1	1:C:159:TYR:CZ	2.71	0.58
1:C:152:PHE:O	1:C:153:GLY:C	2.46	0.58
2:B:218:LEU:HD22	2:B:261:MET:SD	2.43	0.58
1:C:30:VAL:HG23	1:C:31:ALA:N	2.19	0.58
1:A:195:GLU:O	1:A:196:MET:C	2.45	0.58
3:A:1297:MTW:N3	3:A:1297:MTW:C14	2.58	0.58
1:C:34:LYS:O	1:C:34:LYS:HG3	2.02	0.58
1:C:289:VAL:C	1:C:290:THR:HG23	2.28	0.58
2:D:415:ASN:OD1	2:D:417:LYS:CG	2.51	0.58
1:A:253:PRO:HB2	1:A:254:PRO:HD3	1.86	0.58
1:C:125:HIS:ND1	1:C:128:LEU:CD2	2.67	0.58
1:C:144:ALA:O	1:C:145:ASP:HB3	2.03	0.58
1:C:200:ARG:HH11	1:C:200:ARG:HB3	1.67	0.58
1:A:15:TYR:O	1:A:35:ILE:HG23	2.04	0.58
2:B:206:ILE:HB	2:B:210:MET:HE3	1.84	0.58
2:B:258:THR:O	2:B:259:ALA:C	2.45	0.58
1:C:89:LYS:NZ	4:C:2006:HOH:O	2.25	0.58
2:D:241:ARG:HA	2:D:244:SER:HB2	1.86	0.58
1:C:245:ARG:HG3	1:C:245:ARG:HH11	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:321:HIS:N	2:D:321:HIS:HD2	2.01	0.58
1:A:88:LYS:HG3	1:A:89:LYS:N	2.17	0.57
1:A:164:VAL:C	1:A:165:THR:HG22	2.27	0.57
1:C:54:LEU:HD13	1:C:123:VAL:HG13	1.86	0.57
1:C:96:LEU:C	1:C:96:LEU:HD12	2.29	0.57
1:C:214:ARG:HG2	1:C:214:ARG:HH11	1.69	0.57
1:A:190:GLY:CA	1:A:266:MET:HE2	2.33	0.57
2:B:249:LEU:O	2:B:251:GLY:N	2.37	0.57
1:C:167:TRP:CD1	1:C:205:GLY:H	2.21	0.57
2:D:294:MET:O	2:D:298:VAL:HG23	2.04	0.57
2:B:400:LYS:C	2:B:402:PRO:CD	2.78	0.57
1:C:12:GLU:HA	1:C:17:VAL:CA	2.34	0.57
1:C:84:HIS:HD2	1:C:296:LEU:HG	1.69	0.57
1:C:202:LEU:O	1:C:203:PHE:CD1	2.58	0.57
1:A:23:ASN:OD1	1:A:23:ASN:O	2.22	0.57
2:B:247:SER:OG	1:C:28:GLU:OE2	2.22	0.57
1:C:230:VAL:C	1:C:232:SER:H	2.12	0.57
1:A:107:TYR:CD1	1:A:141:ILE:HG21	2.40	0.57
1:A:236:TYR:CD1	1:A:236:TYR:C	2.81	0.57
2:B:337:GLY:O	2:B:338:GLU:C	2.46	0.57
2:B:346:PRO:O	2:B:349:LYS:HB2	2.03	0.57
1:C:214:ARG:HH11	1:C:214:ARG:CG	2.17	0.57
2:B:249:LEU:C	2:B:251:GLY:H	2.13	0.57
1:C:23:ASN:O	1:C:27:GLY:N	2.38	0.57
1:C:167:TRP:CD1	1:C:167:TRP:N	2.71	0.57
2:B:249:LEU:O	2:B:250:ARG:C	2.44	0.56
2:B:383:THR:HG1	2:B:386:SER:H	1.53	0.56
1:C:184:VAL:CG2	1:C:185:ASP:N	2.68	0.56
1:C:108:LEU:HD22	1:C:193:PHE:CG	2.39	0.56
2:D:250:ARG:O	2:D:251:GLY:C	2.48	0.56
1:A:31:ALA:HB3	3:A:1297:MTW:C9	2.36	0.56
1:A:105:LYS:CE	1:A:285:PHE:CZ	2.88	0.56
1:A:216:PHE:CE1	1:A:222:PRO:HD3	2.40	0.56
1:C:5:GLN:HG3	1:C:5:GLN:O	2.05	0.56
1:C:173:ILE:CD1	1:C:173:ILE:N	2.68	0.56
1:C:173:ILE:N	1:C:173:ILE:HD12	2.19	0.56
1:C:178:LYS:HD3	1:C:179:TYR:CE2	2.40	0.56
2:D:326:ASN:C	2:D:326:ASN:OD1	2.47	0.56
1:A:60:HIS:CD2	1:A:60:HIS:C	2.83	0.56
2:D:235:ALA:O	2:D:239:ILE:CG1	2.53	0.56
2:B:410:ARG:C	2:B:412:LYS:N	2.62	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ARG:HG2	1:C:157:ARG:HH11	1.69	0.56
2:D:314:PHE:O	2:D:315:LEU:C	2.48	0.56
1:C:167:TRP:CD1	1:C:167:TRP:H	2.24	0.56
1:A:266:MET:O	1:A:274:ARG:HD3	2.05	0.56
1:C:214:ARG:CG	1:C:214:ARG:NH1	2.69	0.56
2:D:268:GLU:HG3	2:D:268:GLU:O	2.06	0.56
2:D:299:LEU:HD22	2:D:304:PHE:CE1	2.41	0.56
1:A:104:ILE:HG22	1:A:105:LYS:N	2.21	0.56
1:A:128:LEU:HB2	1:A:188:SER:CB	2.36	0.56
1:A:214:ARG:O	1:A:215:ILE:C	2.48	0.56
1:C:200:ARG:HG2	1:C:200:ARG:NH1	2.12	0.56
2:D:383:THR:OG1	2:D:385:GLU:HB3	2.06	0.56
2:B:328:LYS:O	2:B:329:VAL:C	2.49	0.56
1:C:115:LEU:CD1	1:C:189:LEU:CD2	2.79	0.56
1:C:160:THR:O	1:C:161:HIS:CD2	2.59	0.56
2:D:223:GLU:OE1	2:D:223:GLU:CA	2.53	0.56
2:B:264:ALA:O	2:B:265:SER:C	2.48	0.55
2:D:407:GLN:O	2:D:408:SER:C	2.48	0.55
1:A:56:LYS:NZ	1:A:56:LYS:C	2.58	0.55
1:A:60:HIS:CG	1:A:61:PRO:HD3	2.41	0.55
1:A:229:GLY:O	1:A:230:VAL:C	2.49	0.55
2:D:372:TRP:CD1	2:D:377:ILE:HD11	2.40	0.55
1:A:128:LEU:HB2	1:A:188:SER:HB2	1.87	0.55
1:A:129:LYS:O	1:A:131:GLN:N	2.40	0.55
2:B:282:THR:HB	2:B:285:THR:CG2	2.35	0.55
2:B:396:GLN:O	2:B:397:THR:C	2.49	0.55
1:C:84:HIS:O	3:C:1297:MTW:H13	2.06	0.55
1:C:215:ILE:O	1:C:218:THR:N	2.30	0.55
2:D:391:LEU:O	2:D:392:MET:C	2.49	0.55
2:D:395:HIS:CE1	2:D:430:LEU:HG	2.41	0.55
2:D:415:ASN:ND2	2:D:417:LYS:HG2	2.21	0.55
1:A:103:LEU:HA	1:A:292:PRO:HG2	1.88	0.55
1:A:153:GLY:HA3	2:B:313:GLN:HG2	1.88	0.55
2:D:178:TYR:HA	2:D:181[B]:ASP:OD2	2.05	0.55
1:A:154:VAL:CG1	1:A:155:PRO:N	2.68	0.55
1:C:256:ASP:O	1:C:260:ARG:HG3	2.06	0.55
2:D:263:LEU:O	2:D:264:ALA:C	2.45	0.55
1:A:129:LYS:HA	1:A:192:ILE:HD11	1.87	0.55
1:C:100:PRO:O	1:C:101:LEU:C	2.46	0.55
2:B:389:PRO:HG2	2:B:390:CYS:H	1.70	0.55
2:D:202:LYS:HB3	2:D:202:LYS:HZ2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:406:GLN:N	2:D:406:GLN:CD	2.65	0.55
2:B:251:GLY:C	2:B:252:LYS:HD3	2.32	0.55
1:C:113:GLN:HA	1:C:281:LEU:HD11	1.88	0.55
1:A:71:HIS:CE1	2:B:296:HIS:HD1	2.25	0.55
1:C:17:VAL:O	1:C:17:VAL:HG23	2.07	0.55
1:C:14:THR:HB	1:C:15:TYR:CD1	2.41	0.55
1:C:121:HIS:O	1:C:122:ARG:HG2	2.05	0.55
1:C:129:LYS:HE2	4:C:2009:HOH:O	2.07	0.55
2:D:217:TRP:CZ2	2:D:281:ILE:HD12	2.42	0.55
2:D:338:GLU:OE1	2:D:413:TYR:HE1	1.90	0.55
1:C:105:LYS:HB2	1:C:285:PHE:CE2	2.42	0.54
2:D:347:TYR:OH	2:D:394:LEU:HA	2.07	0.54
2:B:283:ASP:O	2:B:284:ASP:C	2.49	0.54
2:D:207:THR:HG22	2:D:210:MET:SD	2.47	0.54
1:A:39:THR:O	2:B:289:LYS:HE2	2.08	0.54
1:A:62:ASN:HD22	1:A:110:GLN:HB3	1.71	0.54
1:A:68:ASP:O	1:A:79:VAL:HG23	2.07	0.54
1:A:83:LEU:HD23	1:A:136:ASN:HB3	1.88	0.54
2:D:404:HIS:HD2	2:D:406:GLN:O	1.90	0.54
1:A:223:ASP:OD1	1:A:225:VAL:HB	2.07	0.54
1:C:38:ASP:C	1:C:40:GLU:H	2.13	0.54
2:D:383:THR:HG23	2:D:386:SER:OG	2.07	0.54
1:A:101:LEU:N	1:A:102:PRO:CD	2.71	0.54
1:A:129:LYS:O	1:A:130:PRO:C	2.50	0.54
1:A:159:TYR:O	1:A:160:THR:C	2.43	0.54
1:A:248:PHE:CE2	1:A:264:SER:CB	2.91	0.54
2:B:419:HIS:C	2:B:421:VAL:N	2.64	0.54
1:C:32:LEU:HD22	1:C:79:VAL:HG22	1.86	0.54
1:C:252:VAL:O	1:C:252:VAL:HG23	2.07	0.54
1:A:91:MET:HE3	1:A:196:MET:CG	2.38	0.54
1:A:158:THR:OG1	1:A:178:LYS:HA	2.08	0.54
2:B:384:LEU:O	2:B:384:LEU:CD1	2.54	0.54
1:C:40:GLU:O	1:C:41:THR:O	2.26	0.54
1:C:84:HIS:CD2	1:C:296:LEU:HG	2.42	0.54
1:C:282:ALA:HB1	4:C:2028:HOH:O	2.08	0.54
2:D:420:GLY:C	2:D:422:SER:H	2.15	0.54
2:B:322:GLN:OE1	2:B:325:ALA:HA	2.07	0.54
1:A:84:HIS:N	1:A:84:HIS:CD2	2.76	0.54
1:C:122:ARG:HG3	1:C:122:ARG:NH2	2.08	0.54
1:C:125:HIS:ND1	1:C:128:LEU:HD23	2.23	0.54
1:C:236:TYR:CD1	1:C:237:LYS:N	2.76	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:212:ALA:O	2:D:213:ILE:C	2.49	0.54
2:D:321:HIS:CE1	2:D:379:LYS:HD3	2.43	0.54
1:A:103:LEU:O	1:A:106:SER:HB3	2.07	0.54
1:C:230:VAL:O	1:C:231:THR:C	2.47	0.54
2:B:409:ILE:O	2:B:412:LYS:HB3	2.08	0.53
2:D:335:PHE:CZ	2:D:339:LEU:HD11	2.44	0.53
2:D:368:THR:OG1	2:D:370:GLN:HG3	2.09	0.53
2:B:197:VAL:CG2	2:B:198:GLY:N	2.70	0.53
1:C:162:GLU:OE1	1:C:164:VAL:N	2.41	0.53
2:D:335:PHE:HB2	2:D:413:TYR:CE2	2.44	0.53
1:C:162:GLU:OE1	1:C:163:VAL:C	2.51	0.53
1:A:2:GLU:HG3	1:C:73:GLU:OE1	2.08	0.53
1:A:294:PRO:CB	1:A:296:LEU:HD12	2.23	0.53
2:B:185:TYR:O	2:B:186:LEU:C	2.51	0.53
2:B:321:HIS:CE1	2:B:379:LYS:CE	2.91	0.53
2:D:209:SER:O	2:D:212:ALA:HB3	2.08	0.53
2:D:249:LEU:N	2:D:249:LEU:CD1	2.69	0.53
2:B:220:GLU:O	2:B:221:VAL:C	2.50	0.53
1:C:12:GLU:HA	1:C:17:VAL:HA	1.89	0.53
2:D:220:GLU:HG3	2:D:408:SER:OG	2.08	0.53
2:B:216:ASP:OD1	2:B:408:SER:CB	2.56	0.53
2:B:391:LEU:O	2:B:392:MET:C	2.49	0.53
2:D:190:GLU:N	2:D:309:PRO:HG3	2.24	0.53
2:D:198:GLY:HA3	4:D:2003:HOH:O	2.08	0.53
1:A:84:HIS:CD2	1:A:84:HIS:H	2.27	0.53
2:B:188:GLU:HB2	4:B:2003:HOH:O	2.08	0.53
1:C:224:GLU:OE2	1:C:231:THR:OG1	2.26	0.53
2:D:284:ASP:OD1	2:D:284:ASP:N	2.42	0.53
1:A:207:SER:O	1:A:208:GLU:C	2.52	0.53
1:C:11:GLY:O	1:C:17:VAL:HA	2.09	0.53
1:C:29:VAL:O	1:C:30:VAL:CG1	2.57	0.53
1:C:131:GLN:NE2	1:C:131:GLN:H	2.06	0.53
1:C:178:LYS:HG2	1:C:179:TYR:CD2	2.44	0.53
1:A:23:ASN:OD1	1:A:26:THR:N	2.35	0.53
1:A:38:ASP:O	1:A:38:ASP:CG	2.49	0.53
1:A:248:PHE:HA	1:A:251:VAL:HG23	1.90	0.53
1:C:212:LEU:HD22	1:C:216:PHE:CE1	2.44	0.53
1:C:87:LEU:HD22	1:C:87:LEU:O	2.09	0.53
1:C:130:PRO:HB2	1:C:131:GLN:HE21	1.74	0.53
1:C:245:ARG:NH1	1:C:245:ARG:CG	2.70	0.53
2:D:216:ASP:O	2:D:217:TRP:C	2.52	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:VAL:O	1:A:8:GLU:HB3	2.09	0.52
1:C:164:VAL:HG23	4:C:2012:HOH:O	2.09	0.52
1:A:241:PRO:CG	1:A:243:TRP:CH2	2.88	0.52
1:C:125:HIS:CE1	1:C:128:LEU:HD23	2.44	0.52
1:C:189:LEU:HB3	1:C:266:MET:CE	2.39	0.52
2:D:198:GLY:O	2:D:201:LYS:HG2	2.09	0.52
2:D:335:PHE:CD1	2:D:413:TYR:HB2	2.44	0.52
1:A:56:LYS:HZ3	1:A:56:LYS:CA	2.23	0.52
2:B:206:ILE:C	2:B:210:MET:CE	2.82	0.52
1:C:245:ARG:CG	1:C:246:GLN:N	2.69	0.52
2:D:183:HIS:ND1	2:D:183:HIS:C	2.67	0.52
2:D:407:GLN:O	2:D:410:ARG:N	2.42	0.52
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.92	0.52
1:A:64:VAL:O	1:A:64:VAL:CG1	2.56	0.52
2:B:206:ILE:CB	2:B:210:MET:HE3	2.40	0.52
2:B:321:HIS:CD2	2:B:321:HIS:N	2.77	0.52
2:B:404:HIS:CD2	2:B:405:ALA:N	2.77	0.52
1:C:9:LYS:N	1:C:19:TYR:CD2	2.78	0.52
2:D:398:TYR:O	2:D:399:LEU:C	2.52	0.52
1:C:166:LEU:C	1:C:168:TYR:N	2.68	0.52
2:D:392:MET:HE2	2:D:392:MET:N	2.24	0.52
2:B:194:LYS:HG2	2:B:195:PRO:CD	2.36	0.52
2:B:271:TYR:CB	2:B:272:PRO:HD2	2.39	0.52
2:B:374:GLU:HA	2:B:377:ILE:HD12	1.92	0.52
1:C:29:VAL:O	1:C:30:VAL:HG12	2.09	0.52
1:C:177:CYS:HB3	1:C:233:MET:CE	2.40	0.52
2:B:321:HIS:HE1	2:B:379:LYS:HE2	1.74	0.51
2:B:410:ARG:O	2:B:412:LYS:N	2.43	0.51
2:D:198:GLY:N	4:D:2003:HOH:O	2.32	0.51
2:D:262:LEU:CD1	2:D:266:LYS:HE3	2.36	0.51
2:D:283:ASP:O	2:D:284:ASP:C	2.53	0.51
2:D:320:LEU:HB2	2:D:321:HIS:HD2	1.75	0.51
1:A:38:ASP:OD2	1:A:41:THR:CB	2.53	0.51
2:B:218:LEU:O	2:B:219:VAL:C	2.54	0.51
2:B:260:ALA:O	2:B:261:MET:C	2.53	0.51
1:C:195:GLU:O	1:C:199:ARG:N	2.44	0.51
2:D:230:GLU:HG3	2:D:234:LEU:HD12	1.91	0.51
2:B:346:PRO:HG2	2:B:347:TYR:CD2	2.45	0.51
2:D:358:ALA:HB1	2:D:391:LEU:HD13	1.92	0.51
2:B:425:ASN:C	2:B:426:PRO:O	2.53	0.51
1:C:46:SER:O	1:C:47:THR:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:THR:HB	4:B:2010:HOH:O	2.10	0.51
1:C:125:HIS:CG	1:C:128:LEU:CD2	2.90	0.51
2:D:178:TYR:C	2:D:178:TYR:HD2	2.16	0.51
2:D:275:VAL:HG21	2:D:292:LEU:HD11	1.93	0.51
1:A:252:VAL:N	1:A:253:PRO:HD3	2.26	0.51
1:C:64:VAL:HG22	1:C:144:ALA:HB2	1.93	0.51
1:C:184:VAL:HG23	1:C:185:ASP:N	2.26	0.51
1:C:259:GLY:CA	1:C:285:PHE:CD1	2.93	0.51
1:A:134:LEU:HD23	1:A:134:LEU:N	2.24	0.51
1:A:166:LEU:C	1:A:168:TYR:H	2.19	0.51
2:B:354:VAL:O	2:B:356:ALA:N	2.44	0.51
1:C:20:LYS:HB2	1:C:82:PHE:CE2	2.46	0.51
2:D:420:GLY:C	2:D:422:SER:N	2.69	0.51
1:C:117:PHE:CE2	1:C:121:HIS:CE1	2.98	0.51
1:C:255:LEU:O	1:C:260:ARG:NH1	2.44	0.51
1:C:84:HIS:HB2	4:C:2010:HOH:O	2.10	0.51
2:D:229:ASN:ND2	2:D:334:MET:CE	2.74	0.51
1:A:2:GLU:CG	1:C:73:GLU:OE1	2.59	0.51
2:B:386:SER:O	2:B:389:PRO:HD2	2.10	0.51
1:C:39:THR:O	1:C:39:THR:HG22	2.09	0.51
2:D:378:ARG:HH11	2:D:378:ARG:CB	2.22	0.51
1:A:101:LEU:N	1:A:102:PRO:HD3	2.25	0.50
2:B:351:LEU:HD22	2:B:352:PRO:CD	2.41	0.50
1:C:7:VAL:HB	1:C:20:LYS:HG3	1.93	0.50
1:C:83:LEU:HD22	1:C:134:LEU:HB2	1.93	0.50
1:C:96:LEU:HG	1:C:97:THR:HG22	1.91	0.50
1:A:55:LEU:HD23	1:A:80:PHE:HE2	1.76	0.50
1:A:105:LYS:CE	1:A:285:PHE:CE2	2.94	0.50
1:A:153:GLY:CA	2:B:313:GLN:HG2	2.41	0.50
1:A:193:PHE:O	1:A:194:ALA:C	2.52	0.50
2:D:383:THR:HG1	2:D:386:SER:H	1.57	0.50
1:C:289:VAL:HG22	1:C:290:THR:N	2.27	0.50
2:D:262:LEU:HD11	2:D:266:LYS:CE	2.34	0.50
1:A:270:ASP:O	1:A:271:PRO:C	2.54	0.50
2:B:214:LEU:HD12	2:B:217:TRP:HE3	1.75	0.50
1:C:50:ARG:O	1:C:51:GLU:C	2.52	0.50
1:C:289:VAL:C	1:C:290:THR:CG2	2.84	0.50
1:C:293:VAL:O	1:C:293:VAL:HG23	2.09	0.50
1:A:216:PHE:O	1:A:220:GLY:HA2	2.10	0.50
2:B:215:VAL:O	2:B:216:ASP:C	2.54	0.50
2:B:217:TRP:CZ2	2:B:281:ILE:CD1	2.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:PHE:CD1	1:C:216:PHE:N	2.77	0.50
2:D:395:HIS:ND1	2:D:430:LEU:HG	2.26	0.50
2:B:351:LEU:O	2:B:352:PRO:C	2.53	0.50
1:C:38:ASP:O	1:C:40:GLU:N	2.32	0.50
2:D:401:ALA:HB3	2:D:402:PRO:HD3	1.92	0.50
2:B:199:TYR:CD1	2:B:200:MET:CA	2.95	0.50
2:B:332:LEU:O	2:B:335:PHE:HB3	2.11	0.50
2:B:401:ALA:HB3	2:B:402:PRO:CD	2.38	0.50
1:C:23:ASN:O	1:C:27:GLY:HA2	2.12	0.50
2:B:347:TYR:OH	2:B:397:THR:OG1	2.25	0.50
1:C:44:VAL:HG12	1:C:49:ILE:HG12	1.94	0.50
1:C:188:SER:O	1:C:192:ILE:HG13	2.12	0.50
2:D:229:ASN:HD22	2:D:334:MET:HE1	1.77	0.50
2:D:234:LEU:O	2:D:235:ALA:C	2.54	0.50
1:A:25:LEU:O	2:D:252:LYS:HD2	2.12	0.50
1:C:85:GLN:HE22	1:C:89:LYS:HB3	1.75	0.50
1:C:283:HIS:CE1	1:C:284:PRO:HD2	2.47	0.50
1:C:60:HIS:HD2	1:C:60:HIS:C	2.16	0.49
1:C:251:VAL:O	1:C:252:VAL:HG13	2.12	0.49
2:D:206:ILE:HA	2:D:210:MET:SD	2.52	0.49
2:D:300:LYS:O	2:D:301:VAL:C	2.52	0.49
1:A:105:LYS:HB2	1:A:285:PHE:CE2	2.48	0.49
1:A:190:GLY:HA2	1:A:266:MET:HE2	1.93	0.49
2:B:221:VAL:HG22	2:B:281:ILE:HD13	1.94	0.49
2:B:388:LYS:N	2:B:389:PRO:CD	2.73	0.49
2:B:403:GLN:O	2:B:404:HIS:C	2.53	0.49
1:C:11:GLY:O	1:C:17:VAL:CA	2.60	0.49
1:C:217:ARG:HB3	1:C:243:TRP:CZ3	2.46	0.49
1:A:1:MET:HE1	1:A:32:LEU:CD2	2.41	0.49
1:A:38:ASP:CG	1:A:41:THR:H	2.13	0.49
1:A:129:LYS:O	1:A:132:ASN:N	2.29	0.49
1:A:1:MET:HG2	1:A:70:ILE:HD12	1.93	0.49
2:B:262:LEU:O	2:B:263:LEU:C	2.55	0.49
2:D:321:HIS:CD2	2:D:321:HIS:H	2.29	0.49
2:D:383:THR:O	2:D:386:SER:HB2	2.11	0.49
2:B:216:ASP:O	2:B:219:VAL:HB	2.13	0.49
2:B:239:ILE:HG22	2:B:243:LEU:HD12	1.93	0.49
1:C:20:LYS:NZ	1:C:82:PHE:CZ	2.80	0.49
1:C:204:PRO:HD2	1:C:214:ARG:HH11	1.76	0.49
1:C:296:LEU:C	1:C:296:LEU:HD12	2.38	0.49
2:D:418:TYR:O	2:D:421:VAL:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:LEU:O	2:B:190:GLU:HB3	2.13	0.49
2:B:420:GLY:O	2:B:422:SER:N	2.45	0.49
1:A:111:LEU:HD21	1:A:141:ILE:HG12	1.94	0.49
2:B:351:LEU:HD22	2:B:352:PRO:HD3	1.95	0.49
1:C:288:ASP:OD1	1:C:288:ASP:N	2.45	0.49
2:D:403:GLN:HE21	2:D:403:GLN:HB2	1.38	0.49
2:D:425:ASN:O	2:D:426:PRO:C	2.53	0.49
2:B:302:LEU:O	2:B:303:THR:C	2.55	0.49
2:B:338:GLU:O	2:B:340:SER:N	2.45	0.49
2:D:178:TYR:O	2:D:179:HIS:C	2.55	0.49
2:D:190:GLU:HA	2:D:309:PRO:HG3	1.95	0.49
2:D:388:LYS:HG3	2:D:392:MET:HE3	1.95	0.49
1:A:92:ASP:C	1:A:94:SER:H	2.20	0.49
1:C:162:GLU:OE1	1:C:164:VAL:CG1	2.39	0.49
1:C:226:VAL:O	1:C:227:TRP:HB2	2.13	0.49
2:D:190:GLU:OE1	2:D:352:PRO:HD2	2.12	0.49
1:A:178:LYS:CG	1:A:179:TYR:HE2	2.12	0.48
1:A:259:GLY:HA2	1:A:285:PHE:CD1	2.47	0.48
2:B:235:ALA:O	2:B:238:TYR:HB2	2.12	0.48
2:B:342:ILE:HD11	2:B:409:ILE:CD1	2.41	0.48
2:B:361:HIS:O	2:B:362:LEU:C	2.49	0.48
1:C:84:HIS:C	3:C:1297:MTW:H13	2.38	0.48
2:D:198:GLY:CA	4:D:2003:HOH:O	2.61	0.48
2:D:388:LYS:O	2:D:391:LEU:N	2.46	0.48
1:A:33:LYS:NZ	3:A:1297:MTW:H17	2.28	0.48
2:B:430:LEU:CB	2:B:432:LEU:CD2	2.82	0.48
1:C:11:GLY:O	1:C:17:VAL:CB	2.61	0.48
1:C:95:ALA:C	1:C:97:THR:H	2.21	0.48
1:C:99:ILE:CG2	1:C:104:ILE:HG13	2.43	0.48
1:A:190:GLY:N	1:A:266:MET:CE	2.76	0.48
1:C:223:ASP:HB3	4:C:2021:HOH:O	2.12	0.48
2:D:298:VAL:CG1	2:D:302:LEU:HD12	2.44	0.48
2:D:396:GLN:O	2:D:399:LEU:HB2	2.13	0.48
2:D:421:VAL:O	2:D:424:LEU:HB2	2.13	0.48
1:A:291:LYS:H	1:A:292:PRO:HD3	1.78	0.48
2:B:196:LYS:O	2:B:197:VAL:C	2.57	0.48
2:B:252:LYS:O	2:B:255:LEU:HB3	2.14	0.48
2:B:302:LEU:O	2:B:305:ASP:HB2	2.13	0.48
2:D:338:GLU:OE1	2:D:413:TYR:CE1	2.67	0.48
2:D:362:LEU:HB2	2:D:391:LEU:HD11	1.94	0.48
1:A:128:LEU:HD23	1:A:128:LEU:HA	1.58	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LYS:O	1:A:179:TYR:CD2	2.67	0.48
2:B:347:TYR:OH	2:B:394:LEU:HA	2.12	0.48
1:A:107:TYR:CD1	1:A:141:ILE:CG2	2.96	0.48
2:B:298:VAL:O	2:B:299:LEU:C	2.56	0.48
1:C:153:GLY:HA3	2:D:313:GLN:HG2	1.96	0.48
2:D:220:GLU:O	2:D:221:VAL:C	2.56	0.48
2:D:399:LEU:HD23	2:D:399:LEU:HA	1.52	0.48
2:B:196:LYS:HD2	2:B:196:LYS:HA	1.43	0.48
1:C:231:THR:HA	1:C:236:TYR:CE1	2.48	0.48
2:D:329:VAL:HG11	2:D:364:LEU:HD13	1.96	0.48
1:A:91:MET:HE3	1:A:196:MET:HA	1.95	0.48
1:A:121:HIS:O	1:A:122:ARG:CG	2.22	0.48
1:C:15:TYR:H	1:C:15:TYR:HD1	1.44	0.48
1:A:237:LYS:HB3	1:A:239:SER:HB3	1.96	0.48
2:B:395:HIS:ND1	2:B:430:LEU:CD2	2.76	0.48
2:D:214:LEU:C	2:D:214:LEU:CD1	2.68	0.48
2:D:372:TRP:CD1	2:D:377:ILE:CD1	2.97	0.48
2:B:225:TYR:O	2:B:227:LEU:HD23	2.13	0.48
2:B:242:PHE:C	2:B:244:SER:N	2.70	0.48
2:B:425:ASN:O	2:B:426:PRO:O	2.31	0.48
1:C:116:ALA:O	1:C:120:SER:HB3	2.14	0.48
1:A:5:GLN:NE2	1:A:6:LYS:O	2.47	0.47
1:C:7:VAL:HG23	1:C:21:ALA:HA	1.96	0.47
1:C:125:HIS:CE1	1:C:128:LEU:CD2	2.97	0.47
1:C:135:ILE:HG23	1:C:141:ILE:HD12	1.93	0.47
2:D:224:GLU:HG3	2:D:224:GLU:O	2.14	0.47
2:D:298:VAL:HG12	2:D:302:LEU:HD12	1.96	0.47
1:A:190:GLY:O	1:A:193:PHE:HB3	2.15	0.47
1:A:193:PHE:CZ	1:A:255:LEU:HD21	2.49	0.47
2:B:186:LEU:HB3	2:B:314:PHE:CZ	2.49	0.47
1:C:6:LYS:CE	4:C:2001:HOH:O	2.60	0.47
1:C:159:TYR:CE1	2:D:270:ILE:HD12	2.49	0.47
2:D:210:MET:O	2:D:213:ILE:HB	2.14	0.47
2:D:264:ALA:O	2:D:267:PHE:N	2.46	0.47
1:A:46:SER:O	1:A:50:ARG:HD2	2.14	0.47
1:A:178:LYS:HE3	1:A:179:TYR:OH	2.13	0.47
1:A:219:LEU:N	1:A:219:LEU:HD23	2.22	0.47
2:D:248:VAL:CG1	2:D:249:LEU:N	2.77	0.47
1:A:52:ILE:O	1:A:56:LYS:HB2	2.15	0.47
2:B:268:GLU:O	2:B:268:GLU:HG3	2.14	0.47
2:D:176:PRO:HB2	2:D:178:TYR:CE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LEU:HA	1:A:55:LEU:HD12	1.61	0.47
2:B:252:LYS:HD2	2:B:252:LYS:HA	1.43	0.47
2:B:345:ASP:CB	2:B:346:PRO:HD3	2.33	0.47
2:B:425:ASN:O	2:B:426:PRO:C	2.57	0.47
1:C:1:MET:CE	1:C:70:ILE:CD1	2.91	0.47
1:C:177:CYS:HB3	1:C:233:MET:HE1	1.96	0.47
1:A:105:LYS:HE3	1:A:285:PHE:CE2	2.50	0.47
2:B:274:GLU:O	2:B:275:VAL:C	2.57	0.47
1:C:99:ILE:HG23	1:C:103:LEU:HD23	1.97	0.47
1:C:252:VAL:N	1:C:253:PRO:HD3	2.29	0.47
2:D:339:LEU:HD23	2:D:339:LEU:HA	1.76	0.47
2:D:430:LEU:O	2:D:431:ASN:CB	2.62	0.47
1:A:49:ILE:HG23	2:B:306:LEU:CD1	2.45	0.47
1:A:122:ARG:HA	2:B:182:ILE:HD11	1.96	0.47
1:A:294:PRO:CG	1:A:296:LEU:CD1	2.87	0.47
2:B:254:GLN:HE21	2:B:254:GLN:HB2	1.56	0.47
1:C:90:PHE:O	1:C:94:SER:HB2	2.15	0.47
1:C:129:LYS:HA	1:C:192:ILE:HD11	1.96	0.47
1:C:230:VAL:C	1:C:232:SER:N	2.61	0.47
1:C:269:TYR:O	1:C:270:ASP:C	2.56	0.47
2:D:190:GLU:CA	2:D:309:PRO:HG3	2.44	0.47
2:D:208:ASN:HD22	2:D:344:ALA:HB3	1.79	0.47
2:B:214:LEU:O	2:B:217:TRP:HB3	2.15	0.47
2:B:236:VAL:HG21	2:B:341:LEU:HD22	1.97	0.47
1:C:198:THR:C	1:C:199:ARG:CG	2.87	0.47
1:C:238:PRO:C	1:C:240:PHE:H	2.22	0.47
1:A:178:LYS:O	1:A:179:TYR:CG	2.68	0.47
1:C:70:ILE:O	1:C:77:TYR:N	2.44	0.47
1:C:258:ASP:HB3	1:C:285:PHE:HA	1.95	0.47
2:D:235:ALA:O	2:D:238:TYR:HB2	2.15	0.47
2:D:255:LEU:CD2	2:D:294:MET:HE2	2.44	0.47
2:D:357:GLY:O	2:D:360:PHE:N	2.48	0.47
1:A:211:GLN:O	1:A:215:ILE:HG13	2.14	0.47
2:B:207:THR:N	2:B:210:MET:HE2	2.23	0.47
2:B:211:ARG:HG2	2:B:211:ARG:NH1	2.30	0.47
2:B:248:VAL:O	2:B:248:VAL:HG12	2.08	0.47
1:C:129:LYS:O	1:C:132:ASN:N	2.47	0.47
1:C:284:PRO:HB3	1:C:287:GLN:OE1	2.14	0.47
2:D:267:PHE:C	2:D:267:PHE:CD2	2.93	0.47
2:D:329:VAL:CG2	2:D:367:VAL:HB	2.44	0.47
2:D:175:VAL:O	2:D:175:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:238:TYR:HH	2:D:306:LEU:HB3	1.80	0.46
2:B:419:HIS:O	2:B:420:GLY:C	2.57	0.46
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.51	0.46
2:B:304:PHE:N	2:B:304:PHE:CD2	2.84	0.46
1:A:56:LYS:NZ	1:A:56:LYS:CA	2.79	0.46
1:A:193:PHE:CD1	1:A:193:PHE:C	2.90	0.46
2:B:343:ASP:HB3	2:B:345:ASP:CB	2.43	0.46
1:C:167:TRP:HE1	1:C:205:GLY:H	1.60	0.46
2:D:202:LYS:NZ	2:D:202:LYS:CB	2.78	0.46
1:A:20:LYS:HB2	1:A:20:LYS:HE2	1.85	0.46
1:A:108:LEU:HA	1:A:108:LEU:HD12	1.69	0.46
2:B:221:VAL:CG2	2:B:281:ILE:HD13	2.46	0.46
2:B:257:GLY:O	2:B:260:ALA:N	2.49	0.46
2:B:385:GLU:O	2:B:386:SER:C	2.58	0.46
1:C:108:LEU:HG	1:C:286:PHE:HZ	1.81	0.46
2:D:334:MET:O	2:D:338:GLU:HG3	2.16	0.46
2:D:376:LEU:O	2:D:380:THR:HG23	2.16	0.46
1:A:71:HIS:CD2	2:B:296:HIS:HE1	2.21	0.46
1:A:88:LYS:NZ	1:A:92:ASP:OD2	2.49	0.46
1:A:99:ILE:O	1:A:104:ILE:HD12	2.15	0.46
1:A:128:LEU:O	1:A:129:LYS:HB3	2.16	0.46
1:A:236:TYR:HD1	1:A:237:LYS:N	2.11	0.46
1:C:159:TYR:CE1	2:D:270:ILE:CD1	2.98	0.46
1:C:198:THR:C	1:C:199:ARG:HG2	2.39	0.46
1:C:277:ALA:N	4:C:2027:HOH:O	2.33	0.46
2:D:396:GLN:NE2	2:D:396:GLN:HA	2.30	0.46
1:A:190:GLY:H	1:A:266:MET:HE2	1.79	0.46
1:C:136:ASN:OD1	1:C:136:ASN:C	2.58	0.46
1:C:233:MET:O	1:C:235:ASP:N	2.49	0.46
1:C:291:LYS:HG3	4:C:2007:HOH:O	2.14	0.46
2:D:319:PHE:CZ	2:D:330:GLU:HA	2.51	0.46
1:A:54:LEU:N	1:A:54:LEU:HD23	2.29	0.46
1:A:60:HIS:HD2	1:A:62:ASN:N	2.14	0.46
2:B:287:THR:O	2:B:290:GLN:N	2.48	0.46
1:C:149:ALA:C	1:C:150:ARG:HG2	2.41	0.46
1:C:187:TRP:CD1	1:C:187:TRP:C	2.94	0.46
2:B:372:TRP:HA	2:B:373:PRO:HD2	1.77	0.46
2:B:395:HIS:ND1	2:B:399:LEU:HD11	2.30	0.46
2:B:414:LYS:HE2	2:B:423:LEU:HD21	1.98	0.46
2:D:405:ALA:HB1	2:D:406:GLN:NE2	2.31	0.46
1:A:294:PRO:HG2	1:A:296:LEU:CD1	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:HIS:ND1	1:C:125:HIS:C	2.74	0.45
1:A:166:LEU:C	1:A:168:TYR:N	2.74	0.45
2:B:214:LEU:CD1	2:B:217:TRP:HE3	2.29	0.45
2:B:314:PHE:O	2:B:315:LEU:C	2.59	0.45
1:C:110:GLN:O	1:C:113:GLN:N	2.50	0.45
1:C:111:LEU:HD22	1:C:133:LEU:HD13	1.98	0.45
2:D:209:SER:O	2:D:210:MET:C	2.58	0.45
2:B:221:VAL:O	2:B:221:VAL:CG1	2.61	0.45
1:C:121:HIS:O	1:C:123:VAL:HG23	2.16	0.45
2:B:277:GLU:O	2:B:278:PHE:C	2.57	0.45
1:C:178:LYS:CG	1:C:179:TYR:CD2	3.00	0.45
1:A:125:HIS:HE1	1:A:127:ASP:HB3	1.81	0.45
1:C:125:HIS:CD2	1:C:128:LEU:HD21	2.52	0.45
1:C:167:TRP:N	1:C:167:TRP:HD1	2.13	0.45
2:D:332:LEU:HD12	2:D:332:LEU:C	2.42	0.45
2:D:370:GLN:HA	4:D:2011:HOH:O	2.16	0.45
1:A:105:LYS:HE2	1:A:285:PHE:CE2	2.52	0.45
2:B:234:LEU:O	2:B:237:ASN:HB3	2.16	0.45
1:C:283:HIS:ND1	1:C:284:PRO:HD2	2.32	0.45
2:D:332:LEU:HB3	2:D:363:ALA:HB1	1.98	0.45
2:D:403:GLN:O	2:D:404:HIS:C	2.60	0.45
1:A:262:LEU:O	1:A:263:LEU:C	2.58	0.45
2:B:311:VAL:O	2:B:312:ASN:C	2.57	0.45
2:D:430:LEU:O	2:D:431:ASN:HB3	2.17	0.45
1:A:126:ARG:NH2	1:A:148:LEU:HD22	2.32	0.45
1:A:152:PHE:C	1:A:154:VAL:N	2.73	0.45
2:B:322:GLN:HB3	2:B:325:ALA:HA	1.99	0.45
2:B:331:SER:HB2	2:B:421:VAL:CG1	2.43	0.45
2:D:181[B]:ASP:O	2:D:184:THR:N	2.50	0.45
2:D:336:LEU:O	2:D:337:GLY:C	2.59	0.45
2:D:362:LEU:O	2:D:362:LEU:CG	2.63	0.45
1:A:71:HIS:HE2	2:B:296:HIS:CG	2.34	0.45
1:A:219:LEU:HD23	1:A:219:LEU:HA	1.49	0.45
2:B:361:HIS:HB2	2:B:372:TRP:HB2	1.99	0.45
1:C:23:ASN:O	1:C:27:GLY:CA	2.65	0.45
1:C:131:GLN:N	1:C:131:GLN:HE21	2.15	0.45
1:C:136:ASN:ND2	1:C:140:ALA:HB3	2.32	0.45
2:D:335:PHE:HD1	2:D:413:TYR:CD1	2.35	0.45
1:A:154:VAL:CG1	1:A:155:PRO:CD	2.93	0.44
1:A:255:LEU:HD12	1:A:255:LEU:HA	1.47	0.44
1:A:291:LYS:N	1:A:292:PRO:CD	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:PHE:C	2:B:244:SER:H	2.23	0.44
1:C:58:LEU:HA	1:C:58:LEU:HD23	1.37	0.44
2:D:182:ILE:HD13	2:D:182:ILE:HG21	1.71	0.44
1:A:223:ASP:O	1:A:230:VAL:HG21	2.16	0.44
1:A:2:GLU:HG2	1:C:73:GLU:HG3	2.00	0.44
1:A:60:HIS:HA	1:A:61:PRO:HD3	1.62	0.44
1:C:165:THR:N	4:C:2013:HOH:O	2.46	0.44
1:C:166:LEU:CD2	1:C:169:ARG:NH2	2.81	0.44
2:D:187:ARG:HD2	2:D:190:GLU:OE2	2.17	0.44
2:D:269:GLU:O	2:D:270:ILE:C	2.57	0.44
2:D:356:ALA:O	2:D:357:GLY:C	2.61	0.44
1:A:37:LEU:HD12	1:A:37:LEU:HA	1.83	0.44
1:A:73:GLU:HG3	1:C:2:GLU:OE1	2.17	0.44
1:A:210:ASP:O	1:A:214:ARG:HG3	2.17	0.44
1:A:256:ASP:OD1	1:A:256:ASP:C	2.60	0.44
1:A:291:LYS:N	1:A:292:PRO:HD3	2.32	0.44
2:B:297:LEU:HD12	2:B:297:LEU:C	2.42	0.44
2:B:401:ALA:N	2:B:402:PRO:CD	2.80	0.44
1:C:152:PHE:N	1:C:152:PHE:CD1	2.84	0.44
2:D:215:VAL:O	2:D:218:LEU:HB2	2.16	0.44
1:A:91:MET:HE1	1:A:196:MET:N	2.33	0.44
1:A:189:LEU:HA	1:A:189:LEU:HD12	1.48	0.44
2:B:186:LEU:HA	2:B:186:LEU:HD23	1.41	0.44
2:B:361:HIS:CD2	2:B:361:HIS:O	2.70	0.44
1:A:54:LEU:O	1:A:55:LEU:C	2.60	0.44
1:A:189:LEU:O	1:A:190:GLY:C	2.61	0.44
2:B:292:LEU:HA	2:B:292:LEU:HD12	1.56	0.44
2:B:402:PRO:HB3	2:B:410:ARG:NH1	2.32	0.44
2:D:203:GLN:HA	2:D:204:PRO:HD3	1.77	0.44
2:D:298:VAL:O	2:D:299:LEU:C	2.61	0.44
1:A:85:GLN:HG2	1:A:86:ASP:H	1.83	0.44
1:A:90:PHE:CZ	1:A:294:PRO:HB3	2.53	0.44
2:B:365:TYR:O	2:B:366:THR:C	2.60	0.44
2:B:374:GLU:O	2:B:375:SER:C	2.61	0.44
2:D:320:LEU:HB2	2:D:321:HIS:CD2	2.52	0.44
2:D:415:ASN:OD1	2:D:416:SER:N	2.50	0.44
2:D:417:LYS:HD2	2:D:418:TYR:HE2	1.80	0.44
1:A:251:VAL:C	1:A:253:PRO:HD3	2.43	0.44
1:A:252:VAL:N	1:A:253:PRO:CD	2.80	0.44
2:B:182:ILE:O	2:B:185:TYR:N	2.51	0.44
1:C:85:GLN:CA	3:C:1297:MTW:H13	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:GLY:HA2	1:C:285:PHE:CE1	2.53	0.44
2:D:320:LEU:HA	2:D:320:LEU:HD23	1.36	0.44
1:A:107:TYR:HD1	1:A:141:ILE:HG21	1.82	0.44
1:A:126:ARG:HE	1:A:126:ARG:HB2	1.55	0.44
2:B:275:VAL:O	2:B:278:PHE:HB2	2.17	0.44
1:C:167:TRP:NE1	1:C:205:GLY:N	2.61	0.44
1:A:275:ILE:HD13	1:A:275:ILE:HG21	1.70	0.43
1:A:289:VAL:O	1:A:289:VAL:CG1	2.64	0.43
2:B:356:ALA:O	2:B:359:ALA:HB3	2.18	0.43
2:D:223:GLU:CD	2:D:412:LYS:HD2	2.42	0.43
2:D:366:THR:OG1	2:D:427:PRO:CG	2.66	0.43
1:A:101:LEU:CB	1:A:102:PRO:CD	2.96	0.43
2:B:178:TYR:O	2:B:180:GLU:N	2.51	0.43
2:B:348:LEU:HA	2:B:348:LEU:HD12	1.12	0.43
2:B:351:LEU:HA	2:B:351:LEU:HD23	1.57	0.43
1:C:80:PHE:CB	3:C:1297:MTW:H9	2.48	0.43
1:C:95:ALA:O	1:C:97:THR:N	2.46	0.43
1:C:101:LEU:N	1:C:102:PRO:CD	2.77	0.43
1:A:171:PRO:O	1:A:172:GLU:C	2.61	0.43
2:B:216:ASP:OD2	2:B:408:SER:HB2	2.17	0.43
2:B:228:GLN:N	2:B:269:GLU:OE2	2.33	0.43
2:B:416:SER:C	2:B:418:TYR:N	2.76	0.43
1:C:37:LEU:HD23	1:C:37:LEU:HA	1.80	0.43
1:A:3:ASN:CG	1:A:25:LEU:HD12	2.43	0.43
1:A:192:ILE:O	1:A:195:GLU:N	2.51	0.43
1:A:212:LEU:HA	1:A:212:LEU:HD23	1.19	0.43
2:B:210:MET:O	2:B:213:ILE:HB	2.18	0.43
2:B:338:GLU:O	2:B:339:LEU:C	2.61	0.43
2:B:391:LEU:HD13	2:B:391:LEU:HA	1.81	0.43
2:B:253:LEU:O	2:B:254:GLN:C	2.56	0.43
1:C:203:PHE:N	1:C:204:PRO:HD3	2.32	0.43
2:D:175:VAL:O	2:D:176:PRO:C	2.47	0.43
2:D:385:GLU:OE1	2:D:385:GLU:CA	2.42	0.43
1:A:248:PHE:C	1:A:250:LYS:N	2.71	0.43
1:C:55:LEU:C	1:C:57:GLU:H	2.27	0.43
1:C:174:LEU:HD23	1:C:174:LEU:HA	1.89	0.43
2:D:186:LEU:HD22	2:D:309:PRO:HB3	2.00	0.43
2:D:249:LEU:HD12	2:D:249:LEU:HA	1.53	0.43
2:D:394:LEU:HA	2:D:394:LEU:HD12	1.55	0.43
1:A:223:ASP:OD1	1:A:226:VAL:N	2.35	0.43
2:D:238:TYR:N	2:D:238:TYR:CD1	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:417:LYS:O	2:B:417:LYS:HG2	2.19	0.43
2:B:420:GLY:O	2:B:423:LEU:HB2	2.19	0.43
1:C:81:GLU:HG3	1:C:83:LEU:HD12	2.01	0.43
1:C:111:LEU:CD2	1:C:133:LEU:HD13	2.48	0.43
1:C:252:VAL:C	1:C:254:PRO:HD2	2.43	0.43
1:C:275:ILE:CG1	1:C:276:SER:N	2.82	0.43
2:D:229:ASN:ND2	2:D:334:MET:HE3	2.33	0.43
2:B:343:ASP:CB	2:B:345:ASP:HB2	2.49	0.43
1:C:158:THR:HB	1:C:178:LYS:C	2.44	0.43
1:C:248:PHE:HE2	1:C:263:LEU:HD23	1.64	0.43
1:C:275:ILE:HG13	1:C:276:SER:H	1.84	0.43
1:A:261:SER:O	1:A:265:GLN:HG3	2.19	0.43
2:B:344:ALA:HB1	2:B:348:LEU:CD2	2.42	0.43
1:C:100:PRO:C	1:C:102:PRO:HD2	2.44	0.43
1:C:105:LYS:HE2	1:C:285:PHE:O	2.19	0.43
1:C:204:PRO:HD2	1:C:214:ARG:NH1	2.33	0.43
1:A:101:LEU:HB2	1:A:102:PRO:HD3	1.98	0.42
1:A:248:PHE:O	1:A:251:VAL:HG23	2.19	0.42
2:B:300:LYS:O	2:B:300:LYS:HG2	2.18	0.42
2:B:389:PRO:HG2	2:B:390:CYS:N	2.34	0.42
1:C:115:LEU:HD22	1:C:119:HIS:CE1	2.54	0.42
2:D:205:ASP:CG	2:D:250:ARG:HE	2.26	0.42
1:C:6:LYS:HA	1:C:21:ALA:CB	2.49	0.42
1:C:162:GLU:CD	1:C:163:VAL:O	2.58	0.42
2:D:186:LEU:HA	2:D:186:LEU:HD23	1.63	0.42
2:D:321:HIS:HE1	2:D:379:LYS:HD3	1.85	0.42
2:D:417:LYS:CD	2:D:418:TYR:CE2	3.02	0.42
1:A:159:TYR:HB2	1:A:162:GLU:HA	2.01	0.42
2:B:242:PHE:O	2:B:243:LEU:C	2.59	0.42
2:D:323:GLN:HA	2:D:324:PRO:HA	1.71	0.42
1:A:1:MET:HG3	1:A:77:TYR:CD1	2.53	0.42
1:A:3:ASN:OD1	1:A:25:LEU:CD1	2.67	0.42
1:A:203:PHE:N	1:A:204:PRO:HD3	2.35	0.42
2:D:205:ASP:OD2	2:D:250:ARG:HG2	2.18	0.42
2:D:345:ASP:CB	2:D:346:PRO:HD3	2.50	0.42
1:A:131:GLN:H	1:A:131:GLN:HG2	1.32	0.42
1:A:195:GLU:O	1:A:198:THR:N	2.51	0.42
2:B:288:LYS:HE2	2:B:288:LYS:HB3	1.61	0.42
2:B:299:LEU:HA	2:B:299:LEU:HD23	1.71	0.42
1:C:54:LEU:HD12	1:C:149:ALA:CB	2.49	0.42
1:C:95:ALA:C	1:C:97:THR:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:PRO:CG	1:C:296:LEU:HD22	2.49	0.42
2:D:235:ALA:O	2:D:239:ILE:HG13	2.19	0.42
2:D:249:LEU:N	2:D:249:LEU:HD13	2.33	0.42
2:D:372:TRP:CZ3	2:D:376:LEU:HD13	2.54	0.42
1:A:86:ASP:OD1	1:A:86:ASP:C	2.62	0.42
1:A:263:LEU:HD12	1:A:263:LEU:HA	1.55	0.42
1:A:289:VAL:O	1:A:289:VAL:HG13	2.18	0.42
2:B:332:LEU:HD12	2:B:332:LEU:HA	1.33	0.42
1:C:161:HIS:CD2	1:C:161:HIS:N	2.77	0.42
3:C:1297:MTW:N3	3:C:1297:MTW:C14	2.69	0.42
2:D:395:HIS:O	2:D:396:GLN:C	2.63	0.42
2:D:418:TYR:C	2:D:420:GLY:N	2.74	0.42
1:A:33:LYS:HZ1	3:A:1297:MTW:H17	1.85	0.42
1:A:253:PRO:N	1:A:254:PRO:CD	2.83	0.42
2:B:199:TYR:CD1	2:B:200:MET:HA	2.55	0.42
2:B:420:GLY:C	2:B:422:SER:N	2.77	0.42
1:C:108:LEU:HD22	1:C:193:PHE:CD2	2.54	0.42
1:C:296:LEU:C	1:C:296:LEU:CD1	2.93	0.42
2:D:268:GLU:O	2:D:268:GLU:CG	2.68	0.42
1:A:63:ILE:O	1:A:64:VAL:C	2.62	0.42
2:B:233:HIS:CB	4:B:2010:HOH:O	2.65	0.42
2:B:310:THR:H	2:B:313:GLN:NE2	2.18	0.42
1:C:152:PHE:C	1:C:154:VAL:H	2.28	0.42
1:C:163:VAL:O	1:C:163:VAL:CG1	2.67	0.42
2:D:275:VAL:O	2:D:278:PHE:N	2.52	0.42
2:D:358:ALA:CB	2:D:391:LEU:HD13	2.49	0.42
1:A:105:LYS:HE3	1:A:105:LYS:HB2	1.65	0.42
1:A:164:VAL:C	1:A:165:THR:CG2	2.89	0.42
1:A:184:VAL:O	1:A:185:ASP:C	2.62	0.42
1:C:38:ASP:C	1:C:40:GLU:N	2.76	0.42
1:C:51:GLU:O	1:C:52:ILE:C	2.60	0.42
1:C:101:LEU:HB2	1:C:102:PRO:CD	2.48	0.42
1:C:160:THR:O	1:C:161:HIS:CG	2.73	0.42
1:C:207:SER:OG	1:C:209:ILE:HG22	2.20	0.42
1:A:10:ILE:HD11	1:A:18:VAL:HG12	2.02	0.42
1:A:35:ILE:HG21	1:A:35:ILE:HD12	1.72	0.42
1:A:90:PHE:O	1:A:94:SER:HB2	2.20	0.42
1:A:125:HIS:CE1	1:A:127:ASP:HB3	2.55	0.42
1:A:181:SER:O	1:A:182:THR:C	2.63	0.42
2:B:296:HIS:CD2	2:B:296:HIS:C	2.96	0.42
2:B:380:THR:OG1	2:B:382:TYR:N	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:410:ARG:C	2:B:412:LYS:H	2.28	0.42
1:C:12:GLU:HA	1:C:17:VAL:HG12	2.02	0.42
1:C:55:LEU:HD12	1:C:55:LEU:HA	1.94	0.42
1:C:64:VAL:CG2	1:C:144:ALA:HA	2.50	0.42
1:A:37:LEU:HB3	1:A:74:ASN:O	2.20	0.41
2:B:185:TYR:C	2:B:187:ARG:N	2.75	0.41
2:B:277:GLU:OE1	2:B:277:GLU:CA	2.68	0.41
2:B:321:HIS:NE2	2:B:379:LYS:HE2	2.33	0.41
1:C:148:LEU:HD23	1:C:148:LEU:HA	1.74	0.41
2:D:245:SER:OG	2:D:246:MET:HG2	2.20	0.41
2:D:347:TYR:O	2:D:348:LEU:C	2.60	0.41
1:A:117:PHE:O	1:A:118:CYS:C	2.61	0.41
2:B:207:THR:HG23	2:B:210:MET:H	1.84	0.41
1:C:34:LYS:HE3	1:C:77:TYR:HE2	1.85	0.41
1:C:105:LYS:HB2	1:C:285:PHE:HE2	1.85	0.41
1:C:125:HIS:ND1	1:C:125:HIS:O	2.53	0.41
2:D:180:GLU:O	2:D:184:THR:N	2.34	0.41
2:D:213:ILE:O	2:D:214:LEU:C	2.64	0.41
2:D:360:PHE:O	2:D:361:HIS:C	2.62	0.41
1:A:91:MET:CE	1:A:196:MET:HA	2.51	0.41
1:A:143:LEU:HA	1:A:143:LEU:HD23	1.47	0.41
1:C:268[B]:HIS:O	1:C:269:TYR:C	2.64	0.41
1:A:20:LYS:HD3	1:A:82:PHE:CZ	2.55	0.41
1:A:56:LYS:O	1:A:56:LYS:CE	2.64	0.41
1:A:99:ILE:HA	1:A:100:PRO:HD2	1.62	0.41
1:A:105:LYS:HB2	1:A:285:PHE:CZ	2.55	0.41
1:A:125:HIS:ND1	1:A:125:HIS:C	2.77	0.41
2:B:333:ALA:O	2:B:334:MET:C	2.63	0.41
2:B:339:LEU:HA	2:B:339:LEU:HD23	1.21	0.41
1:C:62:ASN:HD21	1:C:110:GLN:HG2	1.86	0.41
2:D:180:GLU:O	2:D:181[B]:ASP:C	2.63	0.41
2:D:181[A]:ASP:O	2:D:185:TYR:N	2.52	0.41
2:D:401:ALA:CB	2:D:410:ARG:HD2	2.34	0.41
1:A:3:ASN:OD1	1:A:25:LEU:HD11	2.19	0.41
1:A:91:MET:CE	1:A:196:MET:N	2.83	0.41
1:A:179:TYR:CD2	1:A:179:TYR:N	2.89	0.41
1:A:248:PHE:HB3	1:A:260:ARG:HD2	2.02	0.41
1:C:101:LEU:CB	1:C:102:PRO:CD	2.98	0.41
2:D:410:ARG:O	2:D:411:GLU:C	2.62	0.41
2:B:416:SER:C	2:B:418:TYR:H	2.27	0.41
1:C:212:LEU:HA	1:C:212:LEU:HD23	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:LEU:HD23	1:C:281:LEU:HA	1.91	0.41
2:D:329:VAL:HG12	2:D:330:GLU:N	2.29	0.41
1:C:88:LYS:C	1:C:88:LYS:HD3	2.45	0.41
1:C:284:PRO:O	1:C:285:PHE:C	2.64	0.41
1:A:168:TYR:OH	1:A:195:GLU:OE1	2.20	0.41
2:B:395:HIS:CE1	2:B:430:LEU:HD23	2.55	0.41
2:B:428:GLU:HG2	2:B:429:THR:HG22	2.02	0.41
1:C:240:PHE:HD1	1:C:240:PHE:HA	1.76	0.41
1:C:278:LYS:O	1:C:281:LEU:HB2	2.21	0.41
2:D:407:GLN:C	2:D:409:ILE:N	2.78	0.41
2:B:289:LYS:HB2	2:B:289:LYS:HE3	1.67	0.41
2:B:371:SER:OG	2:B:372:TRP:N	2.54	0.41
1:C:51:GLU:HG3	1:C:55:LEU:HD22	2.03	0.41
1:C:109:PHE:HB3	1:C:110:GLN:H	1.66	0.41
2:D:181[B]:ASP:O	2:D:182:ILE:C	2.64	0.41
2:D:259:ALA:O	2:D:260:ALA:C	2.63	0.41
2:D:314:PHE:CD2	2:D:353:SER:HA	2.55	0.41
2:D:335:PHE:CE2	2:D:339:LEU:CD1	3.03	0.41
2:D:335:PHE:HE1	2:D:410:ARG:HA	1.85	0.41
1:A:58:LEU:N	1:A:58:LEU:HD23	2.35	0.41
1:A:92:ASP:O	1:A:94:SER:N	2.53	0.41
1:C:189:LEU:HA	1:C:189:LEU:HD12	0.96	0.41
1:C:194:ALA:HB3	1:C:202:LEU:HD22	2.03	0.41
2:D:225:TYR:O	2:D:226:LYS:HB2	2.20	0.41
1:A:259:GLY:CA	1:A:285:PHE:CD1	3.04	0.40
2:B:226:LYS:HB2	2:B:226:LYS:HE2	1.79	0.40
2:B:332:LEU:HD23	2:B:363:ALA:CA	2.49	0.40
2:B:341:LEU:HD23	2:B:341:LEU:HA	1.78	0.40
1:A:86:ASP:OD2	1:A:89:LYS:HD3	2.21	0.40
1:A:105:LYS:HG2	1:A:289:VAL:HG23	2.04	0.40
1:A:216:PHE:O	1:A:220:GLY:CA	2.69	0.40
2:B:323:GLN:CD	2:B:323:GLN:N	2.79	0.40
1:C:64:VAL:CG2	1:C:144:ALA:CB	2.99	0.40
1:A:106:SER:O	1:A:110:GLN:HG3	2.20	0.40
2:B:273:PRO:HB2	2:B:278:PHE:HE2	1.80	0.40
2:B:331:SER:HB3	2:B:421:VAL:HG11	1.97	0.40
1:C:10:ILE:HD13	1:C:20:LYS:CB	2.44	0.40
1:C:160:THR:O	1:C:161:HIS:C	2.63	0.40
2:D:335:PHE:HB2	2:D:413:TYR:CG	2.53	0.40
2:D:335:PHE:O	2:D:336:LEU:C	2.61	0.40
1:A:44:VAL:O	2:B:266:LYS:NZ	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:MET:HE2	1:C:25:LEU:HB3	2.03	0.40
1:C:229:GLY:O	1:C:230:VAL:O	2.39	0.40
1:C:242:LYS:HA	1:C:242:LYS:HD3	1.87	0.40
2:D:218:LEU:HA	2:D:218:LEU:HD23	1.85	0.40
2:D:291:VAL:O	2:D:291:VAL:HG12	2.20	0.40
2:D:388:LYS:HD3	2:D:432:LEU:HB3	2.04	0.40
2:D:415:ASN:HD21	2:D:417:LYS:HG2	1.87	0.40
1:A:141:ILE:O	1:A:141:ILE:HG23	2.22	0.40
1:A:202:LEU:CD2	1:A:202:LEU:C	2.94	0.40
1:A:221:THR:CG2	1:A:222:PRO:HD2	2.51	0.40
2:B:268:GLU:O	2:B:268:GLU:CG	2.69	0.40
1:C:13:GLY:O	1:C:16:GLY:HA3	2.21	0.40
1:C:88:LYS:HD3	1:C:88:LYS:O	2.22	0.40
1:C:248:PHE:HE2	1:C:263:LEU:HB3	1.86	0.40
2:D:241:ARG:O	2:D:244:SER:HB2	2.22	0.40
2:D:255:LEU:HG	2:D:294:MET:HG2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:431:ASN:ND2	1:C:210:ASP:OD1[2_664]	1.73	0.47

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	294/298 (99%)	226 (77%)	51 (17%)	17 (6%)	1	4
1	C	295/298 (99%)	231 (78%)	44 (15%)	20 (7%)	1	2
2	B	256/259 (99%)	188 (73%)	45 (18%)	23 (9%)	0	1
2	D	257/259 (99%)	205 (80%)	35 (14%)	17 (7%)	1	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1102/1114 (99%)	850 (77%)	175 (16%)	77 (7%)	1 2

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	TYR
1	A	36	ARG
1	A	165	THR
1	A	230	VAL
2	B	176	PRO
2	B	304	PHE
2	B	345	ASP
2	B	420	GLY
2	B	421	VAL
2	B	424	LEU
1	C	17	VAL
1	C	30	VAL
1	C	39	THR
1	C	41	THR
1	C	110	GLN
1	C	120	SER
1	C	160	THR
1	C	215	ILE
1	C	230	VAL
1	C	231	THR
1	C	269	TYR
2	D	284	ASP
2	D	304	PHE
2	D	337	GLY
2	D	424	LEU
1	A	153	GLY
1	A	190	GLY
2	B	284	ASP
2	B	337	GLY
2	B	339	LEU
2	B	341	LEU
2	B	346	PRO
2	B	355	ILE
2	B	357	GLY
2	B	369	GLY
1	C	167	TRP
2	D	181[A]	ASP

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Mol	Chain	Res	Type
2	D	181[B]	ASP
2	D	386	SER
2	D	408	SER
2	D	421	VAL
1	A	96	LEU
1	A	196	MET
1	A	201	ALA
1	A	291	LYS
2	B	326	ASN
2	B	356	ALA
1	C	239	SER
2	D	176	PRO
2	D	325	ALA
2	D	385	GLU
2	D	404	HIS
1	A	14	THR
1	A	162	GLU
1	A	278	LYS
2	B	250	ARG
2	B	336	LEU
2	B	354	VAL
1	C	227	TRP
2	D	346	PRO
1	A	101	LEU
1	A	167	TRP
2	B	364	LEU
2	B	401	ALA
1	C	164	VAL
2	D	392	MET
1	A	60	HIS
1	A	88	LYS
2	B	427	PRO
1	C	162	GLU
1	C	234	PRO
2	D	357	GLY
1	C	153	GLY
1	C	270	ASP
2	D	426	PRO
2	B	197	VAL
1	C	184	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/263 (99%)	191 (73%)	70 (27%)	0	1
1	C	262/263 (100%)	176 (67%)	86 (33%)	0	1
2	B	232/233 (100%)	173 (75%)	59 (25%)	0	2
2	D	233/233 (100%)	176 (76%)	57 (24%)	1	2
All	All	988/992 (100%)	716 (72%)	272 (28%)	0	1

All (272) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	9	LYS
1	A	10	ILE
1	A	14	THR
1	A	17	VAL
1	A	20	LYS
1	A	22	ARG
1	A	23	ASN
1	A	30	VAL
1	A	34	LYS
1	A	35	ILE
1	A	36	ARG
1	A	38	ASP
1	A	39	THR
1	A	40	GLU
1	A	42	GLU
1	A	53	SER
1	A	55	LEU
1	A	56	LYS
1	A	64	VAL
1	A	65	LYS
1	A	69	VAL
1	A	74	ASN
1	A	75	LYS

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Mol	Chain	Res	Type
1	A	76	LEU
1	A	84	HIS
1	A	89	LYS
1	A	96	LEU
1	A	97	THR
1	A	101	LEU
1	A	103	LEU
1	A	104	ILE
1	A	115	LEU
1	A	122	ARG
1	A	124	LEU
1	A	126	ARG
1	A	131	GLN
1	A	134	LEU
1	A	141	ILE
1	A	154	VAL
1	A	158	THR
1	A	159	TYR
1	A	162	GLU
1	A	177	CYS
1	A	179	TYR
1	A	184	VAL
1	A	186	ILE
1	A	189	LEU
1	A	192	ILE
1	A	196	MET
1	A	200	ARG
1	A	202	LEU
1	A	208	GLU
1	A	209	ILE
1	A	218	THR
1	A	230	VAL
1	A	231	THR
1	A	242	LYS
1	A	246	GLN
1	A	248	PHE
1	A	250	LYS
1	A	251	VAL
1	A	253	PRO
1	A	255	LEU
1	A	258	ASP
1	A	264	SER

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Mol	Chain	Res	Type
1	A	275	ILE
1	A	289	VAL
1	A	291	LYS
1	A	296	LEU
2	B	175	VAL
2	B	177	ASP
2	B	182	ILE
2	B	190	GLU
2	B	192	LYS
2	B	194	LYS
2	B	196	LYS
2	B	199	TYR
2	B	201	LYS
2	B	207	THR
2	B	221	VAL
2	B	223	GLU
2	B	224	GLU
2	B	227	LEU
2	B	239	ILE
2	B	241	ARG
2	B	244	SER
2	B	248	VAL
2	B	249	LEU
2	B	250	ARG
2	B	252	LYS
2	B	253	LEU
2	B	254	GLN
2	B	265	SER
2	B	279	VAL
2	B	281	ILE
2	B	285	THR
2	B	288	LYS
2	B	292	LEU
2	B	294	MET
2	B	296	HIS
2	B	297	LEU
2	B	301	VAL
2	B	302	LEU
2	B	313	GLN
2	B	322	GLN
2	B	323	GLN
2	B	326	ASN

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Mol	Chain	Res	Type
2	B	328	LYS
2	B	338	GLU
2	B	342	ILE
2	B	348	LEU
2	B	355	ILE
2	B	371	SER
2	B	374	GLU
2	B	375	SER
2	B	379	LYS
2	B	383	THR
2	B	391	LEU
2	B	392	MET
2	B	400	LYS
2	B	403	GLN
2	B	408	SER
2	B	415	ASN
2	B	425	ASN
2	B	427	PRO
2	B	428	GLU
2	B	429	THR
2	B	432	LEU
1	C	1	MET
1	C	2	GLU
1	C	3	ASN
1	C	5	GLN
1	C	6	LYS
1	C	8	GLU
1	C	9	LYS
1	C	10	ILE
1	C	12	GLU
1	C	15	TYR
1	C	17	VAL
1	C	20	LYS
1	C	28	GLU
1	C	33	LYS
1	C	34	LYS
1	C	37	LEU
1	C	38	ASP
1	C	39	THR
1	C	41	THR
1	C	49	ILE
1	C	52	ILE

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Mol	Chain	Res	Type
1	C	55	LEU
1	C	60	HIS
1	C	63	ILE
1	C	64	VAL
1	C	71	HIS
1	C	72	THR
1	C	75	LYS
1	C	83	LEU
1	C	85	GLN
1	C	86	ASP
1	C	87	LEU
1	C	88	LYS
1	C	89	LYS
1	C	91	MET
1	C	96	LEU
1	C	97	THR
1	C	101	LEU
1	C	105	LYS
1	C	111	LEU
1	C	115	LEU
1	C	120	SER
1	C	122	ARG
1	C	128	LEU
1	C	129	LYS
1	C	131	GLN
1	C	138	GLU
1	C	141	ILE
1	C	148	LEU
1	C	154	VAL
1	C	156	VAL
1	C	157	ARG
1	C	158	THR
1	C	160	THR
1	C	162	GLU
1	C	163	VAL
1	C	165	THR
1	C	173	ILE
1	C	178	LYS
1	C	184	VAL
1	C	189	LEU
1	C	192	ILE
1	C	199	ARG

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Mol	Chain	Res	Type
1	C	200	ARG
1	C	207	SER
1	C	208	GLU
1	C	209	ILE
1	C	214	ARG
1	C	217	ARG
1	C	225	VAL
1	C	226	VAL
1	C	230	VAL
1	C	239	SER
1	C	240	PHE
1	C	242	LYS
1	C	245	ARG
1	C	248	PHE
1	C	264	SER
1	C	267	LEU
1	C	268[A]	HIS
1	C	268[B]	HIS
1	C	278	LYS
1	C	287	GLN
1	C	291	LYS
1	C	293	VAL
1	C	296	LEU
2	D	175	VAL
2	D	179	HIS
2	D	182	ILE
2	D	183	HIS
2	D	189	MET
2	D	196	LYS
2	D	197	VAL
2	D	199	TYR
2	D	200	MET
2	D	201	LYS
2	D	202	LYS
2	D	213	ILE
2	D	214	LEU
2	D	223	GLU
2	D	226	LYS
2	D	232	LEU
2	D	239	ILE
2	D	244	SER
2	D	245	SER

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Mol	Chain	Res	Type
2	D	249	LEU
2	D	261	MET
2	D	265	SER
2	D	273	PRO
2	D	275	VAL
2	D	283	ASP
2	D	284	ASP
2	D	288	LYS
2	D	289	LYS
2	D	293	ARG
2	D	311	VAL
2	D	321	HIS
2	D	323	GLN
2	D	328	LYS
2	D	329	VAL
2	D	332	LEU
2	D	345	ASP
2	D	348	LEU
2	D	364	LEU
2	D	370	GLN
2	D	374	GLU
2	D	378	ARG
2	D	383	THR
2	D	385	GLU
2	D	391	LEU
2	D	392	MET
2	D	396	GLN
2	D	400	LYS
2	D	403	GLN
2	D	406	GLN
2	D	412	LYS
2	D	415	ASN
2	D	421	VAL
2	D	423	LEU
2	D	424	LEU
2	D	428	GLU
2	D	429	THR
2	D	430	LEU

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	60	HIS
1	A	74	ASN
1	A	84	HIS
1	A	85	GLN
1	A	113	GLN
2	B	208	ASN
2	B	313	GLN
2	B	323	GLN
2	B	403	GLN
2	B	404	HIS
2	B	406	GLN
2	B	431	ASN
1	C	3	ASN
1	C	59	ASN
1	C	60	HIS
1	C	84	HIS
1	C	131	GLN
1	C	161	HIS
1	C	211	GLN
2	D	208	ASN
2	D	233	HIS
2	D	321	HIS
2	D	396	GLN
2	D	403	GLN
2	D	404	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	MTW	C	1297	-	28,31,31	3.00	6 (21%)	33,42,42	2.19	15 (45%)
3	MTW	A	1297	-	28,31,31	3.14	6 (21%)	33,42,42	1.95	9 (27%)

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
3	MTW	C	1297	-	-	5/14/26/26	0/3/4/4
3	MTW	A	1297	-	-	3/14/26/26	0/3/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1297	MTW	O1-N6	12.87	1.45	1.22
3	C	1297	MTW	O1-N6	11.51	1.42	1.22
3	A	1297	MTW	N-N2	-6.39	1.23	1.36
3	C	1297	MTW	N-N2	-5.95	1.24	1.36
3	C	1297	MTW	C15-N6	-5.32	1.32	1.45
3	C	1297	MTW	C11-N5	-4.91	1.34	1.42
3	A	1297	MTW	C11-N5	-4.50	1.34	1.42
3	A	1297	MTW	C5-C7	-4.44	1.39	1.47
3	A	1297	MTW	C15-N6	-4.28	1.35	1.45
3	C	1297	MTW	C5-C7	-3.23	1.41	1.47
3	C	1297	MTW	C2-C3	2.53	1.56	1.51
3	A	1297	MTW	C9-N4	2.10	1.33	1.28

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1297	MTW	C5-C7-N3	4.80	124.41	118.11
3	A	1297	MTW	C7-N3-C10	4.07	121.68	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1297	MTW	C6-C5-C4	-4.06	114.55	119.25
3	A	1297	MTW	C15-C14-C11	3.72	121.30	118.50
3	C	1297	MTW	C1-N2-N	3.56	110.84	102.60
3	A	1297	MTW	C14-C15-N6	3.52	121.77	118.74
3	C	1297	MTW	C7-N3-C10	3.47	120.99	117.06
3	A	1297	MTW	O1-N6-C15	3.18	123.20	118.82
3	A	1297	MTW	C-N-N2	3.13	113.71	109.39
3	C	1297	MTW	C5-C4-C3	2.99	124.71	120.86
3	A	1297	MTW	C6-C5-C7	-2.92	117.38	120.84
3	A	1297	MTW	N-C-N1	-2.92	104.38	110.42
3	C	1297	MTW	N2-C1-N1	-2.88	106.69	114.90
3	C	1297	MTW	C11-N5-C10	2.65	126.86	120.70
3	C	1297	MTW	C18-C17-C3	-2.63	116.92	120.61
3	C	1297	MTW	C4-C5-C7	2.56	125.75	120.61
3	C	1297	MTW	C16-C15-C14	2.49	123.32	120.11
3	C	1297	MTW	C3-C2-N	2.48	116.62	112.14
3	C	1297	MTW	C2-N-N2	2.40	125.37	121.04
3	A	1297	MTW	N2-C1-N1	-2.30	108.33	114.90
3	A	1297	MTW	C9-N4-C10	2.28	119.83	115.90
3	C	1297	MTW	C6-C18-C17	2.28	123.18	120.24
3	C	1297	MTW	C2-C3-C17	-2.08	116.92	120.75
3	C	1297	MTW	C13-C12-C11	2.07	122.45	119.75

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1297	MTW	N4-C10-N5-C11
3	C	1297	MTW	N4-C10-N5-C11
3	C	1297	MTW	C14-C15-N6-O1
3	C	1297	MTW	C16-C15-N6-O1
3	A	1297	MTW	C14-C11-N5-C10
3	C	1297	MTW	C14-C11-N5-C10
3	A	1297	MTW	C12-C11-N5-C10
3	C	1297	MTW	C12-C11-N5-C10

There are no ring outliers.

2 monomers are involved in 19 short contacts:

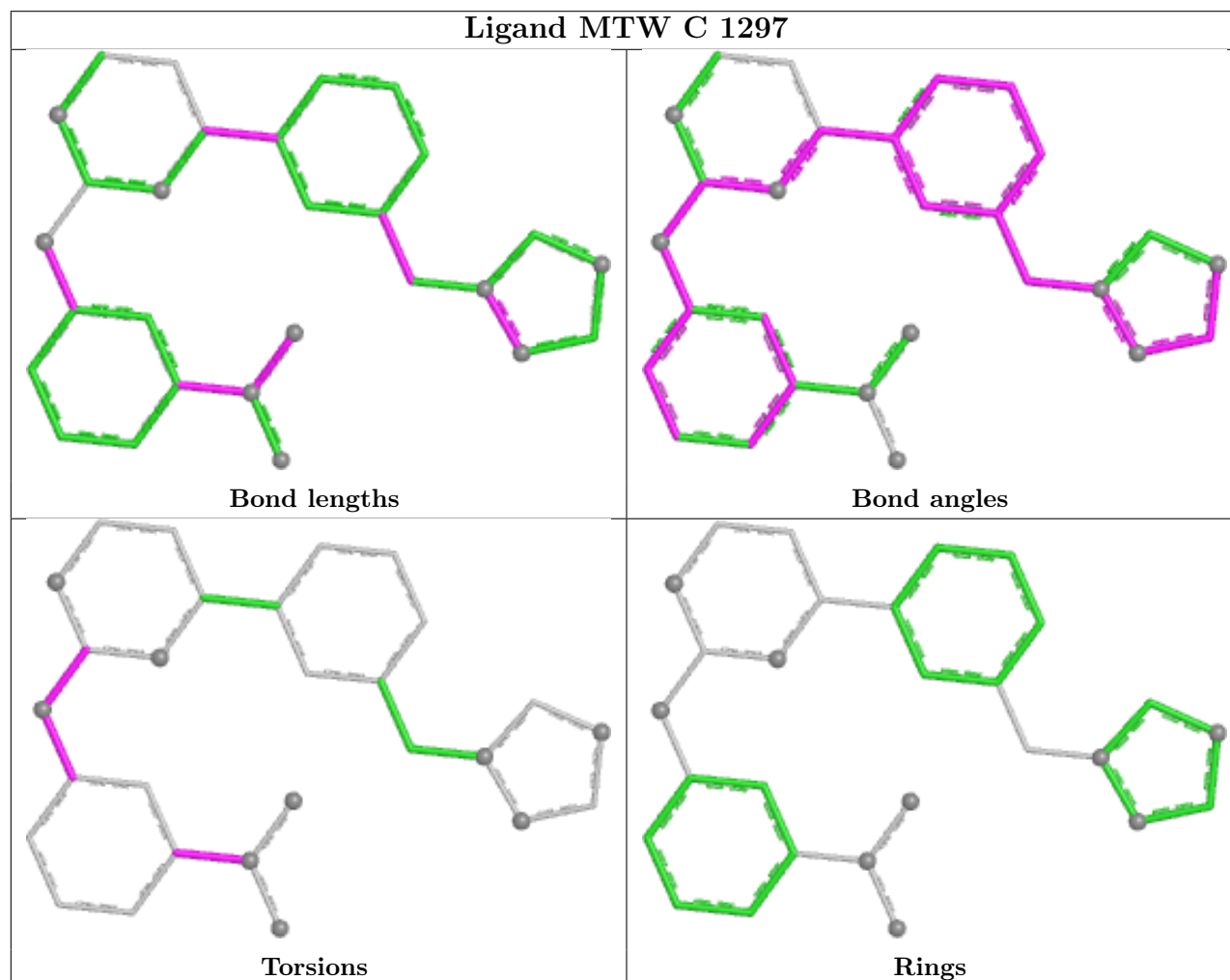
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1297	MTW	13	0

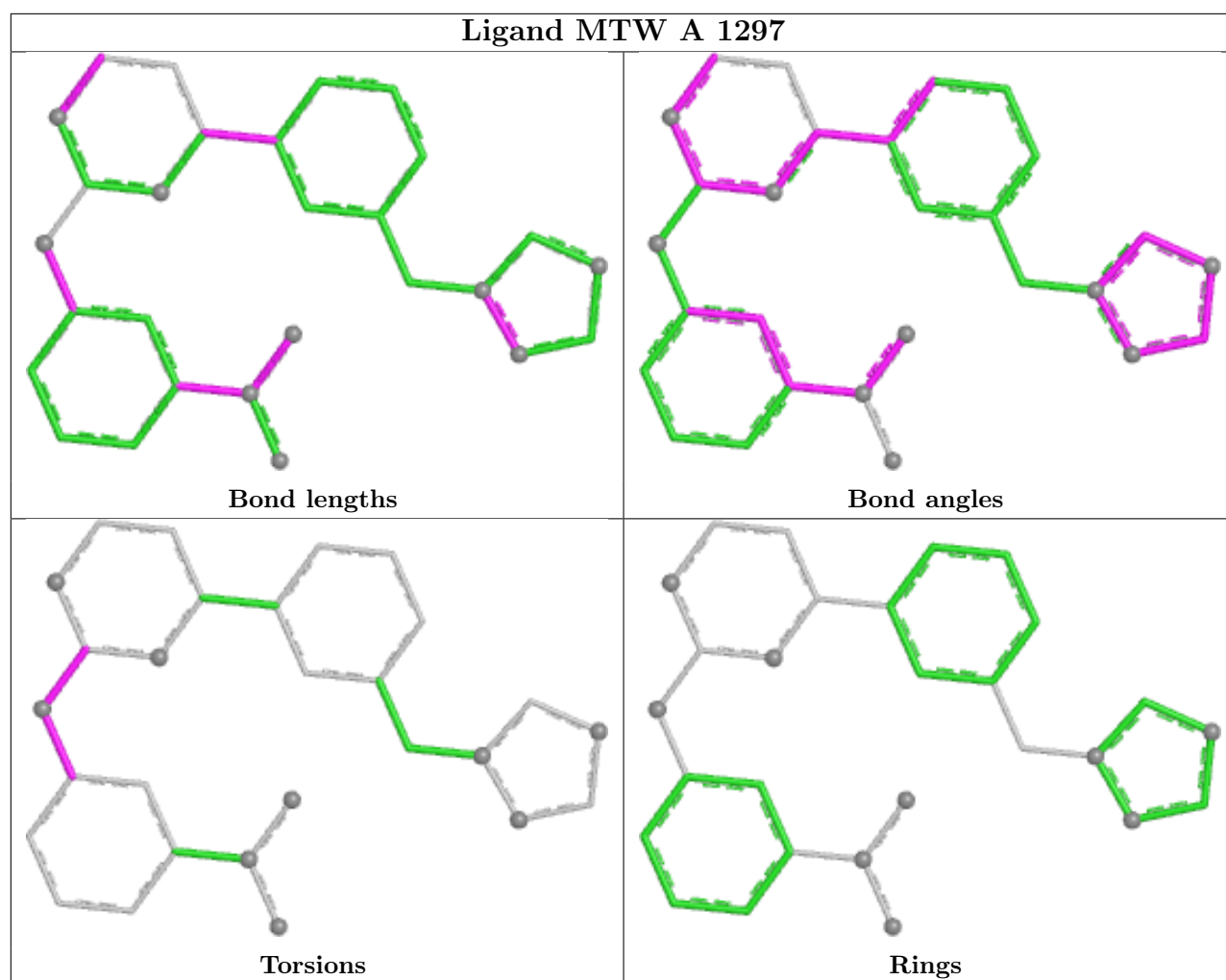
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1297	MTW	6	0

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	296/298 (99%)	-0.56	1 (0%) 90 87	12, 32, 66, 93	1 (0%)
1	C	296/298 (99%)	-0.50	2 (0%) 84 79	11, 32, 69, 95	1 (0%)
2	B	258/259 (99%)	-0.60	1 (0%) 88 85	6, 33, 60, 85	0
2	D	258/259 (99%)	-0.56	1 (0%) 88 85	8, 33, 59, 86	1 (0%)
All	All	1108/1114 (99%)	-0.55	5 (0%) 87 83	6, 32, 63, 95	3 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	175	VAL	3.2
1	C	73	GLU	2.3
2	D	175	VAL	2.3
1	A	159	TYR	2.2
1	C	165	THR	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,

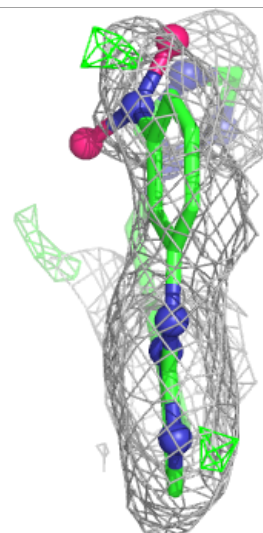
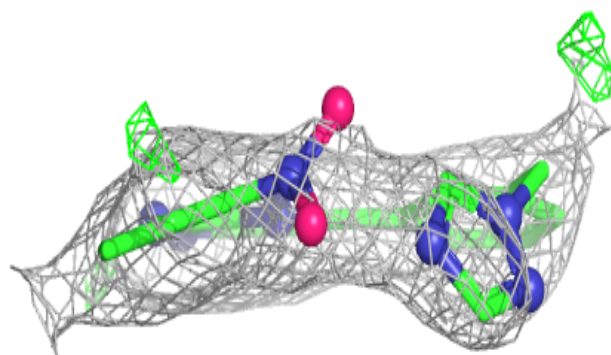
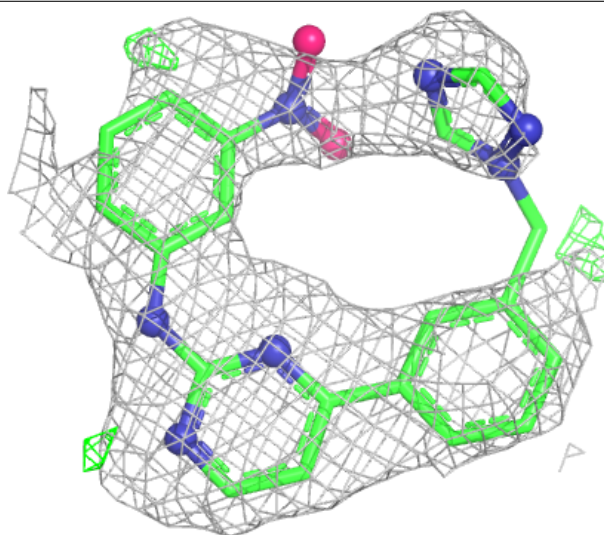
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MTW	C	1297	28/28	0.86	0.15	40,79,105,116	0
3	MTW	A	1297	28/28	0.91	0.10	27,65,91,94	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.

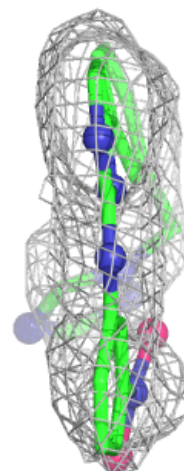
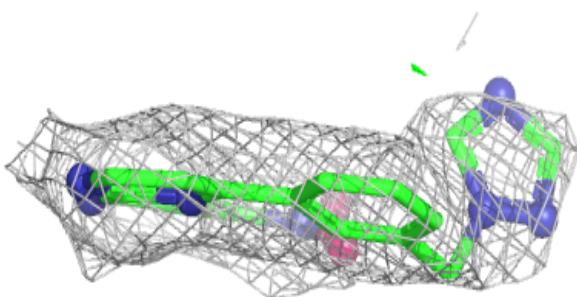
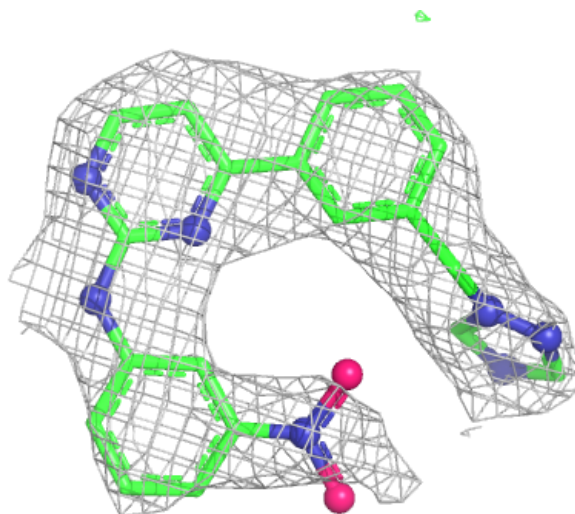
Electron density around MTW C 1297:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MTW A 1297:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.