



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:44 AM UTC

PDB ID : 2Y8I / pdb_00002y8i
Title : Structural basis for the allosteric interference of myosin function by mutants G680A and G680V of Dictyostelium myosin-2
Authors : Preller, M.; Bauer, S.; Adamek, N.; Fujita-Becker, S.; Fedorov, R.; Geeves, M.A.; Manstein, D.J.
Deposited on : 2011-02-07
Resolution : 3.13 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

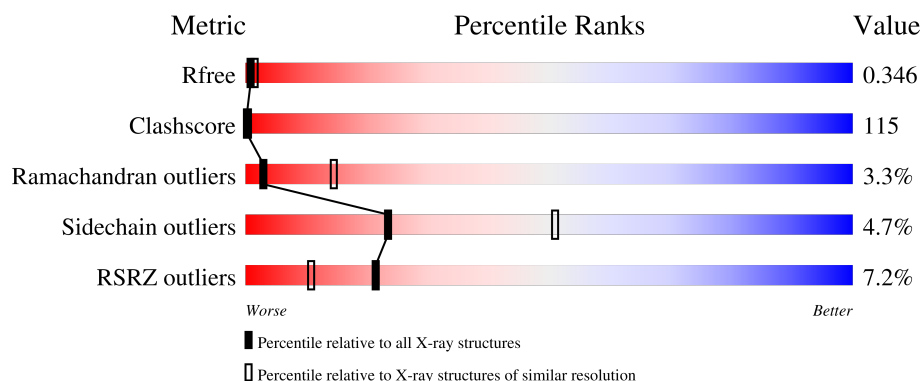
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	X	758	7% 16% 62% 21%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6376 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 MYOSIN-2 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	X	758	6090	3868	1053	1153	16	18	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	680	ALA	GLY	engineered mutation	UNP P08799

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	X	1	27	10	5	10	2	0	0

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

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

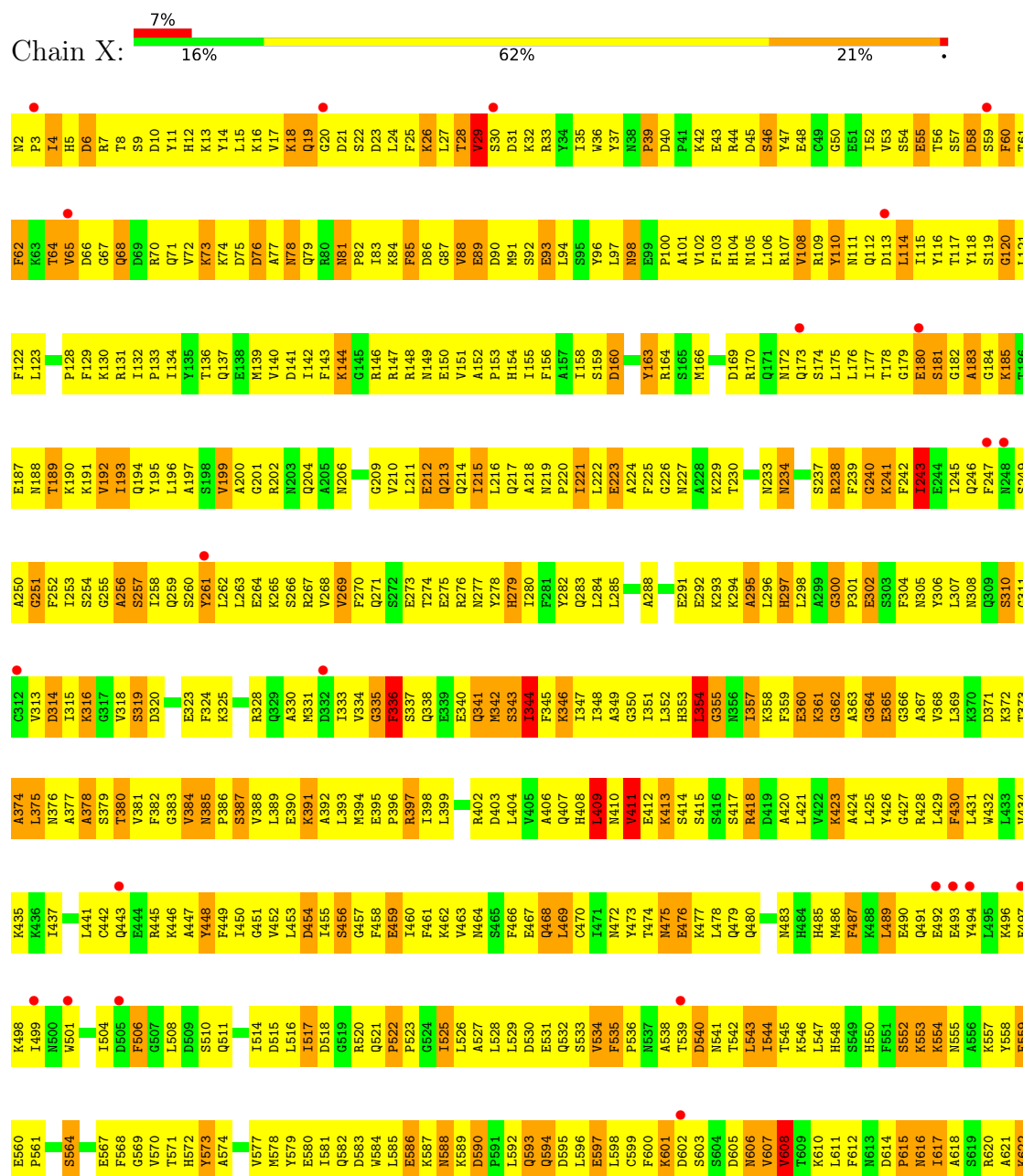
- Molecule 4 is water.

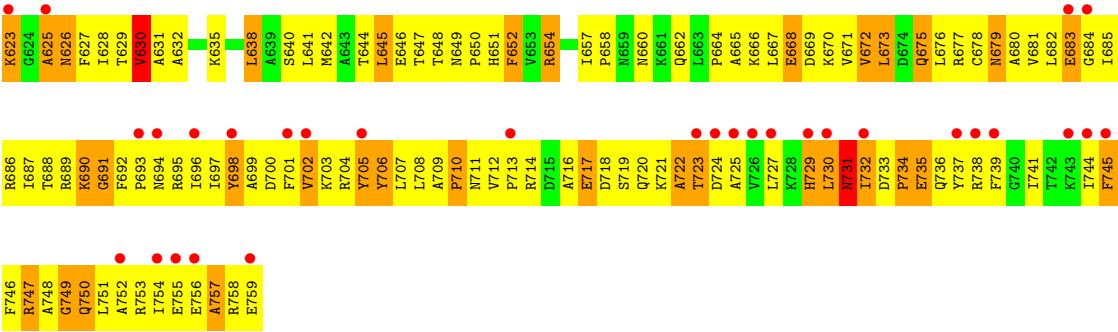
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	258	Total 258	O 258	0	0

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: MYOSIN-2 HEAVY CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	55.00Å 105.80Å 180.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.21 – 3.13 20.21 – 3.13	Depositor EDS
% Data completeness (in resolution range)	96.3 (20.21-3.13) 95.8 (20.21-3.13)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.16Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.245 , 0.337 0.315 , 0.346	Depositor DCC
R_{free} test set	942 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	6376	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	X	0.69	5/6210 (0.1%)	1.51	177/8379 (2.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	559	GLU	C-O	-5.79	1.17	1.23
1	X	375	LEU	CA-C	-5.78	1.44	1.52
1	X	654	ARG	C-O	-5.77	1.17	1.24
1	X	617	ILE	C-O	-5.59	1.18	1.23
1	X	221	ILE	C-O	-5.15	1.18	1.24

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	617	ILE	N-CA-C	22.36	130.01	111.90
1	X	594	GLN	N-CA-C	13.94	130.07	113.20
1	X	717	GLU	N-CA-C	12.28	124.75	111.36
1	X	28	THR	N-CA-C	-11.89	90.05	108.96
1	X	732	ILE	N-CA-C	11.71	123.99	107.37
1	X	29	VAL	N-CA-C	11.65	125.13	107.78
1	X	320	ASP	N-CA-C	-11.51	97.53	111.69
1	X	699	ALA	N-CA-C	-11.40	99.85	113.88
1	X	160	ASP	N-CA-C	-11.19	97.68	111.11
1	X	597	GLU	N-CA-C	-11.19	98.84	111.82
1	X	705	TYR	N-CA-C	10.70	133.59	110.80
1	X	78	ASN	N-CA-C	-10.70	93.86	109.59
1	X	469	LEU	N-CA-C	-10.61	99.44	112.38
1	X	607	VAL	CB-CA-C	-10.58	100.69	110.63
1	X	380	THR	N-CA-C	10.33	122.12	111.07
1	X	627	PHE	N-CA-C	10.26	125.40	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	343	SER	N-CA-C	9.95	123.37	111.33
1	X	199	VAL	N-CA-C	-9.79	100.33	111.00
1	X	85	PHE	N-CA-C	9.62	125.83	112.45
1	X	489	LEU	N-CA-C	-9.35	102.00	113.50
1	X	310	SER	N-CA-C	9.31	122.60	111.33
1	X	385	ASN	N-CA-C	9.28	125.82	109.58
1	X	723	THR	N-CA-C	-9.20	101.48	112.89
1	X	669	ASP	N-CA-C	-9.19	102.22	113.15
1	X	606	ASN	N-CA-C	-9.05	99.59	113.89
1	X	493	GLU	N-CA-C	-8.88	101.55	112.38
1	X	535	PHE	N-CA-C	-8.84	98.52	109.65
1	X	364	GLY	N-CA-C	-8.71	94.83	111.02
1	X	181	SER	N-CA-C	8.69	123.10	110.42
1	X	730	LEU	N-CA-C	-8.65	102.86	113.41
1	X	39	PRO	CB-CA-C	-8.44	97.64	111.56
1	X	423	LYS	N-CA-C	-8.41	102.11	111.28
1	X	164	ARG	N-CA-C	-8.39	102.14	111.28
1	X	534	VAL	CB-CA-C	-8.38	97.55	111.29
1	X	380	THR	CB-CA-C	-8.32	97.82	110.88
1	X	58	ASP	CB-CA-C	-8.28	96.51	109.34
1	X	413	LYS	N-CA-C	-8.22	102.69	112.89
1	X	731	ASN	N-CA-C	8.18	128.22	110.80
1	X	706	TYR	N-CA-CB	-8.09	97.84	111.27
1	X	193	ILE	N-CA-C	-8.06	102.40	110.62
1	X	192	VAL	CB-CA-C	-8.04	101.49	112.02
1	X	672	VAL	CB-CA-C	-7.98	101.59	112.04
1	X	698	TYR	CB-CA-C	-7.96	97.97	111.26
1	X	108	VAL	N-CA-C	7.95	118.01	110.30
1	X	543	LEU	N-CA-C	7.85	119.92	111.36
1	X	55	GLU	N-CA-C	-7.83	94.77	108.23
1	X	6	ASP	N-CA-C	-7.74	98.43	109.96
1	X	108	VAL	CB-CA-C	-7.72	102.16	111.81
1	X	660	ASN	N-CA-C	-7.69	103.46	112.92
1	X	251	GLY	N-CA-C	7.61	131.22	113.18
1	X	735	GLU	N-CA-C	-7.57	102.69	112.23
1	X	732	ILE	N-CA-CB	-7.47	103.83	111.90
1	X	76	ASP	N-CA-CB	-7.43	100.63	110.88
1	X	672	VAL	N-CA-C	7.42	119.08	110.62
1	X	588	ASN	N-CA-C	-7.40	103.22	111.28
1	X	564	SER	CB-CA-C	-7.33	98.85	109.84
1	X	750	GLN	N-CA-C	-7.31	96.65	108.41
1	X	169	ASP	N-CA-C	-7.26	105.34	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	365	GLU	N-CA-C	7.19	121.50	107.98
1	X	58	ASP	N-CA-C	7.19	122.61	113.55
1	X	434	VAL	N-CA-C	-7.19	105.63	111.81
1	X	384	VAL	CB-CA-C	-7.17	100.20	110.82
1	X	544	ILE	N-CA-C	-7.11	103.40	113.07
1	X	343	SER	CB-CA-C	-7.08	98.64	110.68
1	X	683	GLU	N-CA-C	7.06	125.84	110.80
1	X	456	SER	N-CA-C	7.01	119.97	109.25
1	X	240	GLY	N-CA-C	-6.97	100.93	111.10
1	X	749	GLY	N-CA-C	6.91	129.56	113.18
1	X	185	LYS	N-CA-C	-6.88	104.89	113.55
1	X	616	ASN	N-CA-C	-6.86	105.03	113.19
1	X	89	GLU	N-CA-C	6.85	119.33	111.11
1	X	686	ARG	N-CA-C	-6.85	103.60	112.23
1	X	234	ASN	N-CA-C	-6.84	106.13	114.75
1	X	683	GLU	CB-CA-C	-6.79	96.91	110.42
1	X	114	LEU	N-CA-C	-6.68	98.36	109.24
1	X	221	ILE	CB-CA-C	-6.67	103.30	112.04
1	X	630	VAL	CB-CA-C	-6.66	100.37	111.29
1	X	19	GLN	N-CA-C	-6.64	100.87	110.24
1	X	206	ASN	N-CA-C	6.64	120.27	110.30
1	X	528	LEU	N-CA-C	-6.62	104.68	112.89
1	X	553	LYS	N-CA-C	6.60	126.77	113.31
1	X	319	SER	N-CA-C	-6.56	98.50	108.67
1	X	120	GLY	N-CA-C	-6.55	97.66	113.18
1	X	314	ASP	N-CA-C	6.52	118.43	110.41
1	X	673	LEU	N-CA-C	-6.52	104.81	112.89
1	X	107	ARG	N-CA-C	-6.47	103.35	111.11
1	X	310	SER	CB-CA-C	-6.46	99.69	110.68
1	X	375	LEU	N-CA-C	-6.44	104.11	112.23
1	X	638	LEU	N-CA-C	6.43	117.98	110.97
1	X	71	GLN	N-CA-C	6.40	119.40	108.02
1	X	462	LYS	N-CA-C	6.38	118.03	111.14
1	X	342	MET	N-CA-C	-6.27	104.36	111.07
1	X	68	GLN	CB-CA-C	-6.24	99.16	112.63
1	X	734	PRO	CB-CA-C	-6.23	101.28	111.56
1	X	705	TYR	CB-CA-C	-6.22	98.05	110.42
1	X	32	LYS	N-CA-C	6.20	119.97	110.36
1	X	269	VAL	CB-CA-C	-6.16	104.03	111.85
1	X	630	VAL	N-CA-C	6.14	122.10	109.34
1	X	626	ASN	CB-CA-C	-6.10	99.58	112.82
1	X	59	SER	N-CA-CB	6.07	119.39	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	717	GLU	CB-CA-C	-6.07	100.53	110.85
1	X	622	LYS	N-CA-C	6.06	119.95	110.32
1	X	316	LYS	CB-CA-C	6.05	117.25	109.80
1	X	163	TYR	CB-CA-C	-6.04	100.64	110.79
1	X	260	SER	N-CA-C	-6.04	101.53	110.46
1	X	679	ASN	CB-CA-C	-6.03	99.34	109.65
1	X	163	TYR	N-CA-C	6.02	118.75	111.40
1	X	20	GLY	N-CA-C	-5.99	103.43	112.89
1	X	270	PHE	CB-CA-C	5.97	119.98	109.89
1	X	476	GLU	N-CA-C	-5.91	106.20	113.41
1	X	325	LYS	N-CA-C	-5.89	104.55	110.97
1	X	81	ASN	CA-C-N	5.87	125.89	119.90
1	X	81	ASN	C-N-CA	5.87	125.89	119.90
1	X	336	PHE	N-CA-C	-5.87	101.22	109.96
1	X	387	SER	N-CA-C	5.84	117.64	111.28
1	X	668	GLU	CB-CA-C	5.84	118.56	110.16
1	X	64	THR	N-CA-C	5.82	117.80	110.24
1	X	62	PHE	N-CA-C	5.81	117.44	109.18
1	X	378	ALA	N-CA-C	-5.80	104.65	110.97
1	X	336	PHE	CB-CA-C	5.79	118.49	110.16
1	X	212	GLU	N-CA-C	5.76	117.55	111.28
1	X	387	SER	CB-CA-C	-5.74	101.26	110.79
1	X	645	LEU	N-CA-C	-5.73	106.92	114.31
1	X	374	ALA	N-CA-C	-5.72	105.03	112.23
1	X	110	TYR	N-CA-C	-5.67	105.19	111.71
1	X	39	PRO	N-CA-C	5.66	124.13	112.47
1	X	257	SER	N-CA-C	5.66	117.57	109.14
1	X	430	PHE	N-CA-C	-5.63	105.04	111.07
1	X	98	ASN	N-CA-C	-5.63	100.51	109.23
1	X	635	LYS	N-CA-C	5.61	118.12	111.33
1	X	6	ASP	CB-CA-C	5.61	118.24	110.16
1	X	354	LEU	CB-CA-C	5.60	121.56	110.42
1	X	675	GLN	N-CA-C	-5.58	106.31	113.23
1	X	627	PHE	N-CA-CB	-5.57	100.82	109.34
1	X	223	GLU	N-CA-C	5.54	120.04	113.12
1	X	212	GLU	CB-CA-C	-5.52	101.63	110.79
1	X	256	ALA	N-CA-C	5.51	115.12	107.73
1	X	418	ARG	N-CA-C	-5.50	105.29	111.28
1	X	180	GLU	N-CA-C	5.46	117.99	110.35
1	X	341	GLN	CB-CA-C	-5.41	99.88	110.11
1	X	722	ALA	N-CA-C	5.39	120.73	114.04
1	X	213	GLN	N-CA-C	-5.39	105.06	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	409	LEU	N-CA-C	-5.37	102.53	110.48
1	X	593	GLN	N-CA-C	-5.37	102.44	110.23
1	X	678	CYS	CB-CA-C	-5.37	100.88	110.70
1	X	417	SER	CB-CA-C	-5.35	101.76	110.85
1	X	608	VAL	N-CA-C	-5.35	105.17	111.00
1	X	459	GLU	N-CA-C	-5.34	100.99	109.59
1	X	355	GLY	N-CA-C	5.33	119.59	112.77
1	X	64	THR	CB-CA-C	-5.33	100.21	109.64
1	X	182	GLY	N-CA-C	-5.32	108.66	115.42
1	X	517	ILE	CB-CA-C	-5.32	103.49	112.16
1	X	652	PHE	N-CA-C	5.32	118.49	109.76
1	X	261	TYR	N-CA-C	-5.32	100.73	108.07
1	X	223	GLU	CB-CA-C	-5.31	100.79	109.56
1	X	18	LYS	N-CA-C	5.31	122.11	110.80
1	X	241	LYS	N-CA-C	5.27	117.27	108.99
1	X	666	LYS	N-CA-CB	-5.27	101.67	110.57
1	X	335	GLY	N-CA-C	-5.26	106.98	115.08
1	X	649	ASN	CA-C-N	-5.24	114.95	120.66
1	X	649	ASN	C-N-CA	-5.24	114.95	120.66
1	X	590	ASP	N-CA-C	5.22	121.36	109.81
1	X	522	PRO	CA-C-N	5.17	125.11	119.78
1	X	522	PRO	C-N-CA	5.17	125.11	119.78
1	X	360	GLU	CB-CA-C	-5.16	100.87	113.15
1	X	279	HIS	CB-CA-C	-5.14	100.18	110.42
1	X	437	ILE	CB-CA-C	-5.09	105.36	111.88
1	X	243	ILE	CB-CA-C	-5.08	104.01	110.98
1	X	366	GLY	N-CA-C	-5.08	101.15	113.18
1	X	346	LYS	N-CA-C	-5.07	106.20	112.38
1	X	362	GLY	N-CA-C	5.05	125.16	113.18
1	X	344	ILE	N-CA-C	-5.05	105.40	110.30
1	X	300	GLY	CA-C-N	5.03	126.12	119.84
1	X	300	GLY	C-N-CA	5.03	126.12	119.84
1	X	729	HIS	CB-CA-C	-5.02	102.68	109.16
1	X	475	ASN	N-CA-C	-5.02	107.13	113.20
1	X	552	SER	CB-CA-C	5.01	117.38	110.16

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	6090	0	6045	1393	3
2	X	27	0	12	5	0
3	X	1	0	0	0	0
4	X	258	0	0	234	2
All	All	6376	0	6057	1394	4

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 115.

All (1394) 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:X:27:LEU:HD12	1:X:28:THR:N	1.25	1.51
1:X:27:LEU:CD1	1:X:28:THR:H	1.26	1.48
1:X:35:ILE:CD1	1:X:77:ALA:HB1	1.42	1.47
1:X:35:ILE:HD11	1:X:77:ALA:CB	1.45	1.46
1:X:172:ASN:ND2	1:X:449:PHE:CD2	1.84	1.44
1:X:458:PHE:CE1	1:X:574:ALA:HB2	1.58	1.38
1:X:172:ASN:OD1	1:X:448:TYR:HA	1.23	1.35
1:X:85:PHE:O	1:X:88:VAL:HG13	1.26	1.31
1:X:432:TRP:CD1	1:X:610:LYS:NZ	2.00	1.28
1:X:222:LEU:C	4:X:2082:HOH:O	1.65	1.27
1:X:623:LYS:HB3	1:X:628:ILE:CD1	1.64	1.27
1:X:284:LEU:CD2	1:X:348:ILE:HD11	1.61	1.27
1:X:345:PHE:O	1:X:348:ILE:HG13	1.17	1.27
1:X:654:ARG:HG3	1:X:681:VAL:CG1	1.64	1.26
1:X:577:VAL:HG13	1:X:579:TYR:CE1	1.70	1.26
1:X:85:PHE:O	1:X:88:VAL:CG1	1.82	1.26
1:X:251:GLY:O	1:X:252:PHE:HD1	1.13	1.26
1:X:446:LYS:NZ	1:X:449:PHE:HB3	1.50	1.25
1:X:746:PHE:HB3	4:X:2248:HOH:O	1.35	1.25
1:X:544:ILE:HD13	1:X:581:ILE:CG1	1.66	1.25
1:X:172:ASN:ND2	1:X:449:PHE:HD2	1.24	1.24
1:X:117:THR:HG21	4:X:2046:HOH:O	1.26	1.24
1:X:247:PHE:CD1	1:X:253:ILE:HA	1.71	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:24:LEU:O	1:X:27:LEU:HD23	1.33	1.24
1:X:751:LEU:HA	4:X:2252:HOH:O	1.32	1.23
1:X:577:VAL:CG1	1:X:579:TYR:HE1	1.52	1.23
1:X:40:ASP:HB3	4:X:2022:HOH:O	1.07	1.22
1:X:449:PHE:CZ	1:X:648:THR:HG21	1.74	1.22
1:X:251:GLY:O	1:X:252:PHE:CD1	1.93	1.22
1:X:219:ASN:O	1:X:223:GLU:OE1	1.54	1.22
1:X:213:GLN:HB3	4:X:2078:HOH:O	1.34	1.21
1:X:357:ILE:CD1	1:X:375:LEU:HD12	1.70	1.21
1:X:458:PHE:CE1	1:X:574:ALA:CB	2.25	1.20
1:X:702:VAL:HG13	4:X:2233:HOH:O	1.38	1.19
1:X:610:LYS:HB2	4:X:2198:HOH:O	1.43	1.18
1:X:548:HIS:HA	4:X:2180:HOH:O	1.44	1.18
1:X:85:PHE:C	4:X:2039:HOH:O	1.84	1.17
1:X:736:GLN:O	1:X:747:ARG:HB2	1.41	1.17
1:X:458:PHE:HE1	1:X:574:ALA:CB	1.56	1.16
1:X:273:GLU:O	1:X:274:THR:HG22	1.45	1.16
1:X:432:TRP:HD1	1:X:610:LYS:NZ	1.39	1.15
1:X:147:ARG:HB2	1:X:150:GLU:HG2	1.18	1.15
1:X:703:LYS:C	4:X:2219:HOH:O	1.89	1.15
1:X:122:PHE:CD1	1:X:654:ARG:HG2	1.80	1.15
1:X:166:MET:HA	1:X:173:GLN:NE2	1.61	1.14
1:X:172:ASN:CG	1:X:449:PHE:CD2	2.26	1.14
1:X:593:GLN:O	4:X:2193:HOH:O	1.65	1.14
1:X:654:ARG:HG3	1:X:681:VAL:HG12	1.14	1.13
1:X:58:ASP:CA	4:X:2029:HOH:O	1.96	1.13
1:X:296:LEU:HD23	4:X:2104:HOH:O	1.49	1.13
1:X:432:TRP:CD1	1:X:610:LYS:HZ1	1.62	1.13
1:X:14:TYR:CZ	1:X:133:PRO:HG2	1.83	1.13
1:X:172:ASN:OD1	1:X:448:TYR:CA	1.96	1.13
1:X:385:ASN:HB3	1:X:388:VAL:HG22	1.31	1.12
1:X:725:ALA:HB1	4:X:2087:HOH:O	1.45	1.13
1:X:202:ARG:HB2	4:X:2077:HOH:O	1.47	1.12
1:X:296:LEU:HD12	1:X:296:LEU:O	1.45	1.12
1:X:733:ASP:OD1	1:X:734:PRO:HD2	1.46	1.12
1:X:692:PHE:CD1	4:X:2243:HOH:O	1.98	1.12
1:X:196:LEU:HD12	1:X:245:ILE:HD12	1.24	1.12
1:X:121:LEU:C	4:X:2048:HOH:O	1.92	1.11
1:X:723:THR:HG21	4:X:2234:HOH:O	1.46	1.11
1:X:747:ARG:HB3	4:X:2250:HOH:O	1.51	1.11
1:X:178:THR:HG22	4:X:2147:HOH:O	1.48	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:296:LEU:HB3	4:X:2104:HOH:O	1.48	1.11
1:X:679:ASN:ND2	4:X:2214:HOH:O	1.78	1.11
1:X:25:PHE:HZ	4:X:2254:HOH:O	1.31	1.10
1:X:702:VAL:O	1:X:706:TYR:CD2	2.04	1.10
1:X:357:ILE:HD11	1:X:375:LEU:HD12	1.32	1.09
1:X:621:ALA:O	1:X:628:ILE:HG12	1.52	1.09
1:X:238:ARG:HG2	1:X:278:TYR:HE1	0.95	1.09
1:X:343:SER:O	1:X:347:ILE:HG12	1.51	1.09
1:X:689:ARG:HG3	1:X:693:PRO:HD3	1.24	1.09
1:X:313:VAL:HG23	1:X:314:ASP:H	1.13	1.09
1:X:623:LYS:HB3	1:X:628:ILE:HD11	1.28	1.09
1:X:719:SER:HB3	1:X:723:THR:HB	1.24	1.08
1:X:606:ASN:HB2	4:X:2197:HOH:O	1.51	1.08
1:X:398:ILE:CD1	1:X:407:GLN:HE21	1.65	1.08
1:X:238:ARG:HG2	1:X:278:TYR:CE1	1.87	1.08
1:X:357:ILE:CD1	1:X:375:LEU:CD1	2.32	1.08
1:X:724:ASP:HB3	4:X:2235:HOH:O	1.50	1.08
1:X:486:MET:O	1:X:490:GLU:HG2	1.53	1.07
1:X:166:MET:CA	1:X:173:GLN:HE22	1.68	1.07
1:X:692:PHE:CG	4:X:2243:HOH:O	2.06	1.07
1:X:431:LEU:HD23	1:X:617:ILE:HG12	1.10	1.06
1:X:27:LEU:HD13	1:X:28:THR:HG23	1.36	1.06
1:X:594:GLN:HA	4:X:2193:HOH:O	1.56	1.06
1:X:84:LYS:NZ	1:X:704:ARG:HD2	1.71	1.05
1:X:695:ARG:HG2	1:X:745:PHE:HB3	1.31	1.05
1:X:14:TYR:CD2	4:X:2004:HOH:O	2.08	1.05
1:X:238:ARG:HG3	1:X:264:GLU:HB3	1.38	1.05
1:X:257:SER:HB3	4:X:2095:HOH:O	1.56	1.05
1:X:27:LEU:HB2	4:X:2016:HOH:O	1.57	1.04
1:X:689:ARG:HG3	1:X:693:PRO:CD	1.86	1.04
1:X:707:LEU:HD12	4:X:2221:HOH:O	1.56	1.04
1:X:296:LEU:HD11	1:X:298:LEU:CD1	1.88	1.03
1:X:130:LYS:HG3	1:X:132:ILE:HD11	1.37	1.03
1:X:172:ASN:CG	4:X:2067:HOH:O	1.99	1.03
1:X:424:ALA:O	1:X:428:ARG:HD2	1.57	1.03
1:X:544:ILE:CD1	1:X:581:ILE:HG13	1.88	1.03
1:X:296:LEU:HD11	1:X:298:LEU:HD11	1.39	1.03
1:X:27:LEU:HD13	4:X:2017:HOH:O	1.55	1.03
1:X:196:LEU:CD1	1:X:245:ILE:HD12	1.89	1.03
1:X:14:TYR:HD2	4:X:2004:HOH:O	1.38	1.02
1:X:431:LEU:CD2	1:X:617:ILE:HG12	1.90	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:577:VAL:CG1	1:X:579:TYR:CE1	2.34	1.02
1:X:692:PHE:CE1	4:X:2243:HOH:O	2.08	1.02
1:X:64:THR:O	1:X:67:GLY:N	1.91	1.01
1:X:736:GLN:O	1:X:747:ARG:CB	2.08	1.01
1:X:45:ASP:O	1:X:46:SER:HB2	1.59	1.01
1:X:229:LYS:HE2	1:X:234:ASN:ND2	1.75	1.01
1:X:276:ARG:HG3	1:X:282:TYR:CZ	1.94	1.01
1:X:284:LEU:CD2	1:X:348:ILE:CD1	2.39	1.01
1:X:337:SER:HA	4:X:2121:HOH:O	1.59	1.01
1:X:623:LYS:CB	1:X:628:ILE:HD11	1.90	1.01
1:X:706:TYR:CD2	4:X:2219:HOH:O	2.13	1.01
1:X:249:SER:HB2	4:X:2063:HOH:O	1.60	1.00
1:X:449:PHE:HZ	1:X:648:THR:CG2	1.74	1.00
1:X:628:ILE:HD13	4:X:2202:HOH:O	1.59	1.00
1:X:222:LEU:O	4:X:2082:HOH:O	1.55	1.00
1:X:257:SER:CB	4:X:2095:HOH:O	2.08	1.00
1:X:24:LEU:O	1:X:27:LEU:CD2	2.09	1.00
1:X:25:PHE:CZ	4:X:2254:HOH:O	2.09	1.00
1:X:449:PHE:HZ	1:X:648:THR:HG21	1.05	1.00
1:X:360:GLU:C	4:X:2127:HOH:O	2.03	1.00
1:X:431:LEU:HD23	1:X:617:ILE:CG1	1.92	1.00
1:X:238:ARG:NE	1:X:238:ARG:HA	1.76	0.99
1:X:432:TRP:CD1	1:X:610:LYS:HZ3	1.70	0.99
1:X:672:VAL:O	1:X:676:LEU:HD23	1.62	0.99
1:X:747:ARG:CB	4:X:2250:HOH:O	2.09	0.99
1:X:247:PHE:CE1	1:X:253:ILE:HG12	1.97	0.99
1:X:704:ARG:O	1:X:705:TYR:CD2	2.15	0.99
1:X:246:GLN:HG2	1:X:446:LYS:HE2	1.42	0.99
1:X:372:LYS:CA	4:X:2129:HOH:O	2.10	0.99
1:X:746:PHE:CD1	4:X:2250:HOH:O	2.15	0.99
1:X:14:TYR:HB2	4:X:2004:HOH:O	1.60	0.99
1:X:341:GLN:CG	4:X:2122:HOH:O	2.11	0.99
1:X:313:VAL:HG23	1:X:314:ASP:N	1.74	0.98
1:X:544:ILE:HD13	1:X:581:ILE:HG13	1.01	0.98
1:X:58:ASP:C	4:X:2029:HOH:O	2.04	0.98
1:X:706:TYR:CE2	4:X:2219:HOH:O	2.16	0.98
1:X:458:PHE:CZ	1:X:574:ALA:HB2	1.97	0.98
1:X:251:GLY:C	1:X:252:PHE:HD1	1.72	0.98
1:X:219:ASN:C	1:X:223:GLU:OE1	2.07	0.98
1:X:296:LEU:HD12	1:X:298:LEU:HG	1.42	0.97
1:X:398:ILE:HG12	1:X:407:GLN:NE2	1.79	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:577:VAL:HG13	1:X:579:TYR:HE1	0.84	0.97
1:X:118:TYR:HD2	1:X:148:ARG:HH21	1.05	0.97
1:X:284:LEU:HD23	1:X:348:ILE:HD11	1.45	0.97
1:X:345:PHE:O	1:X:348:ILE:CG1	2.12	0.97
1:X:702:VAL:HA	4:X:2233:HOH:O	1.63	0.97
1:X:166:MET:SD	1:X:448:TYR:HB3	2.05	0.96
1:X:623:LYS:HB3	1:X:628:ILE:HD12	1.47	0.96
1:X:446:LYS:HZ1	1:X:449:PHE:HB3	1.26	0.96
1:X:498:LYS:O	1:X:499:ILE:HG13	1.66	0.96
1:X:372:LYS:C	4:X:2129:HOH:O	2.06	0.96
1:X:398:ILE:HD13	1:X:407:GLN:HE21	1.27	0.96
1:X:590:ASP:OD1	1:X:590:ASP:O	1.84	0.96
1:X:706:TYR:CZ	1:X:714:ARG:HA	2.00	0.96
1:X:247:PHE:HD1	1:X:253:ILE:HA	1.29	0.95
1:X:398:ILE:CG1	1:X:407:GLN:NE2	2.29	0.95
1:X:146:ARG:HA	4:X:2055:HOH:O	1.66	0.95
1:X:87:GLY:N	1:X:105:ASN:OD1	2.00	0.95
1:X:118:TYR:HD2	1:X:148:ARG:NH2	1.65	0.95
1:X:172:ASN:CB	1:X:449:PHE:CE2	2.49	0.95
1:X:284:LEU:HD21	1:X:348:ILE:HD11	1.46	0.95
1:X:485:HIS:NE2	1:X:489:LEU:HD11	1.82	0.95
1:X:170:ARG:HA	1:X:448:TYR:HE2	1.30	0.95
1:X:746:PHE:CE1	4:X:2252:HOH:O	2.19	0.94
1:X:695:ARG:HG2	1:X:745:PHE:CB	1.97	0.94
1:X:747:ARG:HE	1:X:748:ALA:H	1.09	0.94
1:X:210:VAL:O	1:X:214:GLN:HG3	1.68	0.94
1:X:276:ARG:HD2	1:X:282:TYR:CG	2.02	0.94
1:X:84:LYS:HD3	1:X:755:GLU:OE2	1.66	0.93
1:X:498:LYS:C	1:X:499:ILE:HG13	1.94	0.93
1:X:397:ARG:HA	1:X:406:ALA:HA	1.48	0.93
1:X:296:LEU:CB	4:X:2104:HOH:O	2.08	0.93
1:X:172:ASN:CB	1:X:449:PHE:CD2	2.52	0.92
1:X:166:MET:HA	1:X:173:GLN:HE22	0.80	0.92
1:X:196:LEU:HD12	1:X:245:ILE:CD1	1.98	0.91
1:X:139:MET:HE2	1:X:139:MET:HA	1.51	0.91
1:X:753:ARG:H	1:X:753:ARG:HD2	1.33	0.91
1:X:238:ARG:CG	1:X:278:TYR:HE1	1.83	0.91
1:X:357:ILE:HD12	1:X:375:LEU:CD1	2.00	0.91
1:X:746:PHE:CB	4:X:2248:HOH:O	1.98	0.91
1:X:177:ILE:HD12	1:X:189:THR:OG1	1.69	0.91
1:X:180:GLU:O	1:X:183:ALA:CB	2.19	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:449:PHE:CZ	1:X:648:THR:CG2	2.48	0.90
1:X:57:SER:C	4:X:2029:HOH:O	2.14	0.90
1:X:361:LYS:HD2	1:X:361:LYS:O	1.70	0.90
1:X:672:VAL:O	1:X:676:LEU:CD2	2.20	0.90
1:X:738:ARG:HD2	4:X:2244:HOH:O	1.72	0.90
1:X:202:ARG:HH11	1:X:252:PHE:HB3	1.35	0.89
1:X:122:PHE:CD1	1:X:654:ARG:CG	2.56	0.89
1:X:284:LEU:HD23	1:X:348:ILE:CD1	2.01	0.89
1:X:733:ASP:OD1	1:X:734:PRO:CD	2.20	0.89
1:X:558:TYR:CE2	4:X:2180:HOH:O	2.25	0.89
1:X:605:ASP:HB3	1:X:608:VAL:HB	1.53	0.89
1:X:10:ASP:CG	4:X:2005:HOH:O	2.15	0.89
1:X:703:LYS:CA	4:X:2219:HOH:O	2.13	0.89
1:X:14:TYR:HE2	4:X:2005:HOH:O	1.55	0.89
1:X:35:ILE:HD13	1:X:77:ALA:HB1	1.54	0.89
1:X:172:ASN:OD1	1:X:449:PHE:N	2.06	0.89
1:X:457:GLY:C	4:X:2148:HOH:O	2.14	0.89
1:X:349:ALA:HA	1:X:352:LEU:HD23	1.53	0.89
1:X:213:GLN:NE2	1:X:333:ILE:HD12	1.88	0.88
1:X:170:ARG:NH2	4:X:2063:HOH:O	2.02	0.88
1:X:479:GLN:HE22	1:X:680:ALA:HB2	1.39	0.88
1:X:668:GLU:HB3	1:X:670:LYS:HG2	1.55	0.88
1:X:706:TYR:OH	1:X:714:ARG:CB	2.21	0.88
1:X:218:ALA:O	1:X:221:ILE:HB	1.73	0.88
1:X:296:LEU:CG	4:X:2104:HOH:O	2.20	0.88
1:X:123:LEU:HD22	1:X:158:ILE:HG12	1.54	0.88
1:X:242:PHE:HB3	1:X:259:GLN:HB3	1.53	0.88
1:X:110:TYR:CE2	1:X:667:LEU:HD13	2.09	0.88
1:X:384:VAL:HG12	1:X:385:ASN:N	1.89	0.88
1:X:410:ASN:ND2	1:X:413:LYS:CE	2.37	0.88
1:X:421:LEU:O	1:X:425:LEU:CD2	2.21	0.88
1:X:446:LYS:HZ2	1:X:449:PHE:HB3	1.36	0.87
1:X:692:PHE:CD2	4:X:2243:HOH:O	2.20	0.87
1:X:409:LEU:HD22	1:X:409:LEU:H	1.39	0.87
1:X:628:ILE:HG22	1:X:629:THR:H	1.40	0.87
1:X:580:GLU:HB3	1:X:582:GLN:OE1	1.73	0.87
1:X:692:PHE:CZ	4:X:2243:HOH:O	2.23	0.87
1:X:28:THR:HG23	4:X:2017:HOH:O	1.74	0.87
1:X:158:ILE:HG22	1:X:175:LEU:HD21	1.57	0.87
1:X:4:ILE:HD12	1:X:4:ILE:H	1.38	0.86
1:X:385:ASN:HB3	1:X:388:VAL:CG2	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:753:ARG:HD2	1:X:753:ARG:N	1.90	0.86
1:X:247:PHE:CE1	1:X:253:ILE:HA	2.10	0.86
1:X:385:ASN:ND2	1:X:388:VAL:HG13	1.89	0.86
1:X:410:ASN:OD1	1:X:412:GLU:HG2	1.75	0.86
1:X:558:TYR:HE2	4:X:2180:HOH:O	1.56	0.86
1:X:421:LEU:O	1:X:425:LEU:HD23	1.76	0.86
1:X:255:GLY:HA3	1:X:441:LEU:O	1.76	0.85
1:X:14:TYR:CE1	1:X:133:PRO:HG2	2.09	0.85
1:X:213:GLN:O	4:X:2079:HOH:O	1.94	0.85
1:X:217:GLN:HG3	4:X:2079:HOH:O	1.76	0.85
1:X:276:ARG:HD2	1:X:282:TYR:CD2	2.10	0.85
1:X:695:ARG:NH2	4:X:2218:HOH:O	2.09	0.85
1:X:211:LEU:CD2	1:X:254:SER:O	2.25	0.85
1:X:117:THR:CG2	4:X:2046:HOH:O	1.97	0.85
1:X:180:GLU:O	1:X:183:ALA:HB3	1.76	0.85
1:X:725:ALA:CB	4:X:2087:HOH:O	2.12	0.85
1:X:654:ARG:CG	1:X:681:VAL:CG1	2.51	0.85
1:X:746:PHE:HE1	4:X:2252:HOH:O	1.53	0.85
1:X:27:LEU:HD12	1:X:28:THR:CA	2.06	0.85
1:X:175:LEU:HD23	1:X:651:HIS:HB2	1.59	0.85
1:X:455:ILE:CG2	4:X:2147:HOH:O	2.25	0.85
1:X:147:ARG:CB	1:X:150:GLU:HG2	2.03	0.85
1:X:82:PRO:HG3	1:X:756:GLU:OE2	1.76	0.84
1:X:172:ASN:OD1	1:X:448:TYR:C	2.19	0.84
1:X:343:SER:O	1:X:347:ILE:CG1	2.23	0.84
1:X:719:SER:HA	1:X:722:ALA:HB3	1.58	0.84
1:X:313:VAL:CG2	1:X:314:ASP:H	1.90	0.84
1:X:279:HIS:O	1:X:283:GLN:HG3	1.77	0.84
1:X:748:ALA:O	4:X:2251:HOH:O	1.95	0.84
1:X:736:GLN:O	1:X:747:ARG:HD2	1.76	0.84
1:X:24:LEU:HD12	1:X:26:LYS:HD2	1.58	0.84
1:X:747:ARG:NE	1:X:748:ALA:H	1.76	0.84
1:X:692:PHE:CE2	4:X:2243:HOH:O	2.28	0.84
1:X:361:LYS:HG3	1:X:411:VAL:HG11	1.60	0.84
1:X:388:VAL:HA	1:X:391:LYS:HB3	1.59	0.84
1:X:265:LYS:O	1:X:268:VAL:HG12	1.77	0.83
1:X:398:ILE:HD13	1:X:407:GLN:NE2	1.94	0.83
1:X:35:ILE:CD1	1:X:77:ALA:CB	2.24	0.83
1:X:174:SER:CB	4:X:2207:HOH:O	2.27	0.83
1:X:514:ILE:O	1:X:518:ASP:OD1	1.96	0.83
1:X:706:TYR:OH	1:X:714:ARG:HB2	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:526:LEU:HD22	1:X:631:ALA:HB1	1.60	0.83
1:X:695:ARG:HG2	1:X:745:PHE:CG	2.13	0.83
1:X:212:GLU:O	1:X:216:LEU:HG	1.79	0.82
1:X:732:ILE:HD12	1:X:732:ILE:H	1.44	0.82
1:X:122:PHE:HD1	1:X:654:ARG:HG2	1.43	0.82
1:X:166:MET:SD	1:X:448:TYR:CB	2.66	0.82
1:X:640:SER:O	1:X:644:THR:OG1	1.96	0.82
1:X:254:SER:HB2	1:X:443:GLN:OE1	1.78	0.82
1:X:345:PHE:HA	1:X:348:ILE:HG12	1.59	0.82
1:X:431:LEU:CD2	1:X:617:ILE:CG1	2.53	0.82
1:X:357:ILE:HD11	1:X:375:LEU:CD1	2.02	0.82
1:X:215:ILE:HG12	1:X:441:LEU:HD13	1.60	0.82
1:X:626:ASN:C	4:X:2201:HOH:O	2.23	0.82
1:X:398:ILE:CG1	1:X:407:GLN:HE21	1.92	0.82
1:X:605:ASP:CB	1:X:608:VAL:HB	2.10	0.82
1:X:747:ARG:HE	1:X:748:ALA:N	1.77	0.82
1:X:702:VAL:O	1:X:706:TYR:HD2	1.64	0.81
1:X:58:ASP:N	4:X:2029:HOH:O	2.06	0.81
1:X:195:TYR:CE2	1:X:199:VAL:HG11	2.16	0.81
1:X:172:ASN:ND2	1:X:449:PHE:CE2	2.37	0.81
1:X:628:ILE:HG22	1:X:629:THR:N	1.95	0.81
1:X:130:LYS:CG	1:X:132:ILE:HD11	2.10	0.81
1:X:213:GLN:HB2	4:X:2079:HOH:O	1.80	0.81
1:X:263:LEU:HD21	1:X:430:PHE:CD2	2.16	0.80
1:X:118:TYR:HE1	1:X:153:PRO:HA	1.43	0.80
1:X:132:ILE:CD1	4:X:2050:HOH:O	2.28	0.80
1:X:736:GLN:O	1:X:747:ARG:CD	2.29	0.80
1:X:56:THR:HG22	1:X:57:SER:N	1.94	0.80
1:X:357:ILE:CG1	1:X:375:LEU:HD12	2.11	0.80
1:X:396:PRO:HG2	1:X:398:ILE:HD11	1.62	0.80
1:X:357:ILE:HD12	1:X:375:LEU:HD11	1.64	0.80
1:X:654:ARG:CG	1:X:681:VAL:HG12	2.06	0.80
1:X:141:ASP:OD2	4:X:2053:HOH:O	2.00	0.80
1:X:520:ARG:O	1:X:523:PRO:HG3	1.82	0.80
1:X:689:ARG:HG3	1:X:693:PRO:CG	2.11	0.79
1:X:662:GLN:CG	4:X:2208:HOH:O	2.29	0.79
1:X:458:PHE:CE2	4:X:2215:HOH:O	2.34	0.79
1:X:262:LEU:HD12	1:X:262:LEU:O	1.81	0.79
1:X:296:LEU:CD1	1:X:298:LEU:HG	2.12	0.79
1:X:385:ASN:CB	1:X:388:VAL:HG22	2.12	0.79
1:X:273:GLU:O	1:X:274:THR:CG2	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:84:LYS:CE	1:X:704:ARG:HD2	2.12	0.79
1:X:184:GLY:HA2	2:X:1001:ADP:PA	2.23	0.79
1:X:98:ASN:O	1:X:102:VAL:HG23	1.83	0.78
1:X:410:ASN:ND2	1:X:413:LYS:HE3	1.99	0.78
1:X:172:ASN:CB	4:X:2067:HOH:O	2.28	0.78
1:X:136:THR:O	1:X:139:MET:HB2	1.82	0.78
1:X:361:LYS:O	1:X:361:LYS:CD	2.30	0.78
1:X:276:ARG:CG	1:X:282:TYR:CZ	2.66	0.78
1:X:380:THR:O	4:X:2132:HOH:O	2.01	0.78
1:X:28:THR:CG2	4:X:2017:HOH:O	2.28	0.78
1:X:122:PHE:CE1	1:X:654:ARG:HG2	2.19	0.77
1:X:593:GLN:C	4:X:2193:HOH:O	2.17	0.77
1:X:29:VAL:O	1:X:29:VAL:HG12	1.83	0.77
1:X:35:ILE:HD11	1:X:77:ALA:HB1	0.78	0.77
1:X:132:ILE:HD12	4:X:2050:HOH:O	1.82	0.77
1:X:695:ARG:CG	1:X:745:PHE:HB3	2.11	0.77
1:X:504:ILE:HA	4:X:2166:HOH:O	1.83	0.77
1:X:172:ASN:HB3	1:X:449:PHE:CD2	2.19	0.77
1:X:14:TYR:CZ	1:X:133:PRO:CG	2.68	0.77
1:X:361:LYS:HB3	1:X:367:ALA:HA	1.66	0.77
1:X:239:PHE:HD1	1:X:240:GLY:O	1.68	0.77
1:X:432:TRP:HD1	1:X:610:LYS:HZ3	1.13	0.76
1:X:288:ALA:HB1	1:X:292:GLU:CD	2.10	0.76
1:X:172:ASN:HB2	1:X:449:PHE:CE2	2.18	0.76
1:X:19:GLN:HB2	4:X:2003:HOH:O	1.83	0.76
1:X:428:ARG:HB3	1:X:611:LEU:HD22	1.66	0.76
1:X:24:LEU:CD1	1:X:26:LYS:HD2	2.15	0.76
1:X:26:LYS:O	1:X:26:LYS:CG	2.30	0.76
1:X:45:ASP:O	1:X:46:SER:CB	2.34	0.76
1:X:702:VAL:CG1	4:X:2233:HOH:O	2.08	0.76
1:X:594:GLN:O	1:X:594:GLN:HG3	1.85	0.76
1:X:689:ARG:CG	1:X:693:PRO:HD3	2.13	0.76
1:X:296:LEU:O	1:X:296:LEU:CD1	2.30	0.76
1:X:368:VAL:O	1:X:369:LEU:HD23	1.85	0.76
1:X:447:ALA:O	1:X:448:TYR:O	2.04	0.76
1:X:118:TYR:CD2	1:X:148:ARG:NE	2.53	0.75
1:X:158:ILE:CG2	1:X:175:LEU:HD21	2.16	0.75
1:X:247:PHE:CD1	1:X:253:ILE:CA	2.63	0.75
1:X:620:ARG:HD2	1:X:628:ILE:O	1.85	0.75
1:X:428:ARG:CB	1:X:611:LEU:HD13	2.16	0.75
1:X:377:ALA:O	1:X:380:THR:HB	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:147:ARG:H	1:X:150:GLU:HG3	1.52	0.75
1:X:82:PRO:HA	1:X:756:GLU:OE1	1.86	0.74
1:X:337:SER:OG	1:X:340:GLU:HB2	1.87	0.74
1:X:147:ARG:H	1:X:150:GLU:CG	1.99	0.74
1:X:577:VAL:HG11	1:X:579:TYR:CE1	2.22	0.74
1:X:600:PHE:HB3	1:X:612:PHE:CD2	2.22	0.74
1:X:296:LEU:CD2	4:X:2104:HOH:O	2.12	0.74
1:X:331:MET:HG2	1:X:336:PHE:HD2	1.51	0.74
1:X:296:LEU:CD1	1:X:298:LEU:CD1	2.64	0.74
1:X:446:LYS:HZ1	1:X:449:PHE:CB	1.99	0.74
1:X:211:LEU:HD21	1:X:254:SER:O	1.86	0.74
1:X:108:VAL:O	1:X:111:ASN:HB2	1.87	0.74
1:X:727:LEU:HD23	1:X:737:TYR:OH	1.86	0.74
1:X:84:LYS:HZ1	1:X:704:ARG:HD2	1.52	0.74
1:X:304:PHE:CE2	1:X:352:LEU:HB3	2.23	0.74
1:X:341:GLN:HG3	4:X:2122:HOH:O	1.78	0.74
1:X:385:ASN:O	1:X:389:LEU:HB2	1.88	0.74
1:X:398:ILE:HD13	1:X:407:GLN:CG	2.18	0.74
1:X:455:ILE:HG23	4:X:2147:HOH:O	1.84	0.74
1:X:458:PHE:CE1	1:X:574:ALA:HB3	2.22	0.73
1:X:706:TYR:OH	1:X:714:ARG:HA	1.87	0.73
1:X:682:LEU:O	1:X:685:ILE:HG22	1.87	0.73
1:X:274:THR:HG22	4:X:2098:HOH:O	1.87	0.73
1:X:276:ARG:CG	1:X:282:TYR:CE1	2.71	0.73
1:X:213:GLN:CB	4:X:2078:HOH:O	2.06	0.73
1:X:275:GLU:N	4:X:2099:HOH:O	2.22	0.73
1:X:732:ILE:CG2	1:X:737:TYR:CD2	2.71	0.73
1:X:395:GLU:HA	1:X:407:GLN:O	1.89	0.73
1:X:426:TYR:CZ	4:X:2139:HOH:O	2.41	0.73
1:X:458:PHE:HE1	1:X:574:ALA:HB2	1.10	0.73
1:X:735:GLU:HA	1:X:738:ARG:HH22	1.54	0.73
1:X:110:TYR:HE2	1:X:667:LEU:HD13	1.52	0.73
1:X:276:ARG:HD2	1:X:282:TYR:CD1	2.24	0.73
1:X:230:THR:HA	1:X:275:GLU:HG2	1.69	0.73
1:X:385:ASN:OD1	1:X:385:ASN:C	2.30	0.73
1:X:27:LEU:CD1	4:X:2017:HOH:O	2.22	0.72
1:X:177:ILE:HG22	1:X:185:LYS:HG2	1.70	0.72
1:X:344:ILE:HG22	1:X:345:PHE:N	2.04	0.72
1:X:250:ALA:HB3	4:X:2094:HOH:O	1.89	0.72
1:X:265:LYS:HE2	1:X:423:LYS:HB3	1.71	0.72
1:X:213:GLN:C	4:X:2079:HOH:O	2.31	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:559:GLU:O	1:X:559:GLU:OE1	2.08	0.72
1:X:98:ASN:OD1	1:X:100:PRO:HG2	1.88	0.72
1:X:133:PRO:C	4:X:2051:HOH:O	2.30	0.72
1:X:115:ILE:HG21	1:X:128:PRO:HG3	1.71	0.72
1:X:120:GLY:O	1:X:148:ARG:NH2	2.23	0.72
1:X:172:ASN:HB3	1:X:449:PHE:CE2	2.25	0.72
1:X:498:LYS:O	1:X:499:ILE:CG1	2.37	0.72
1:X:525:ILE:O	1:X:529:LEU:HB2	1.89	0.72
1:X:345:PHE:C	1:X:348:ILE:HG13	2.10	0.72
1:X:548:HIS:ND1	1:X:560:GLU:HG3	2.05	0.72
1:X:35:ILE:HG13	1:X:79:GLN:HA	1.70	0.72
1:X:737:TYR:CD1	1:X:739:PHE:CE1	2.78	0.72
1:X:296:LEU:O	1:X:297:HIS:O	2.07	0.71
1:X:359:PHE:O	4:X:2127:HOH:O	2.08	0.71
1:X:546:LYS:NZ	1:X:550:HIS:HE1	1.89	0.71
1:X:731:ASN:CG	1:X:731:ASN:O	2.33	0.71
1:X:146:ARG:HH11	1:X:151:VAL:HG11	1.54	0.71
1:X:211:LEU:HD22	1:X:254:SER:O	1.90	0.71
1:X:424:ALA:O	1:X:428:ARG:CD	2.37	0.71
1:X:623:LYS:CB	1:X:628:ILE:CD1	2.53	0.71
1:X:175:LEU:HD23	1:X:651:HIS:CB	2.20	0.71
1:X:446:LYS:NZ	1:X:449:PHE:CB	2.43	0.71
1:X:250:ALA:CB	4:X:2094:HOH:O	2.37	0.71
1:X:398:ILE:HD13	1:X:407:GLN:HG3	1.71	0.71
1:X:529:LEU:HD22	1:X:588:ASN:HD22	1.55	0.71
1:X:131:ARG:O	1:X:132:ILE:HD13	1.91	0.71
1:X:296:LEU:O	1:X:297:HIS:C	2.32	0.71
1:X:410:ASN:HD21	1:X:413:LYS:HE2	1.56	0.71
1:X:541:ASN:O	1:X:545:THR:OG1	2.04	0.71
1:X:367:ALA:HB2	1:X:411:VAL:HA	1.72	0.71
1:X:706:TYR:OH	1:X:714:ARG:CA	2.38	0.71
1:X:458:PHE:CZ	4:X:2215:HOH:O	2.44	0.70
1:X:305:ASN:HA	1:X:308:ASN:OD1	1.90	0.70
1:X:398:ILE:CD1	1:X:407:GLN:NE2	2.41	0.70
1:X:27:LEU:CD1	1:X:28:THR:HG23	2.17	0.70
1:X:485:HIS:NE2	1:X:489:LEU:CD1	2.55	0.70
1:X:118:TYR:HD1	1:X:153:PRO:HB3	1.57	0.70
1:X:331:MET:HE1	1:X:345:PHE:CZ	2.26	0.70
1:X:458:PHE:N	4:X:2148:HOH:O	2.23	0.70
1:X:581:ILE:HG22	1:X:581:ILE:O	1.90	0.70
1:X:331:MET:O	1:X:336:PHE:HB2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:56:THR:HG22	1:X:57:SER:H	1.55	0.70
1:X:104:HIS:O	1:X:108:VAL:HG23	1.89	0.70
1:X:707:LEU:O	4:X:2221:HOH:O	2.09	0.70
1:X:732:ILE:CG2	1:X:737:TYR:HD2	2.04	0.70
1:X:753:ARG:H	1:X:753:ARG:CD	2.04	0.70
1:X:184:GLY:HA2	2:X:1001:ADP:O3A	1.91	0.70
1:X:85:PHE:CA	4:X:2039:HOH:O	2.31	0.70
1:X:487:PHE:CZ	1:X:506:PHE:HB2	2.26	0.70
1:X:123:LEU:HD22	1:X:158:ILE:CG1	2.22	0.69
1:X:621:ALA:O	1:X:628:ILE:CG1	2.35	0.69
1:X:76:ASP:CB	4:X:2032:HOH:O	2.38	0.69
1:X:118:TYR:CE2	1:X:148:ARG:NE	2.60	0.69
1:X:625:ALA:O	1:X:626:ASN:OD1	2.10	0.69
1:X:249:SER:O	4:X:2063:HOH:O	2.11	0.69
1:X:54:SER:N	1:X:61:THR:OG1	2.25	0.69
1:X:410:ASN:CG	1:X:412:GLU:HG2	2.16	0.69
1:X:142:ILE:HG22	1:X:143:PHE:N	2.07	0.69
1:X:687:ILE:O	1:X:690:LYS:HB2	1.93	0.69
1:X:703:LYS:HA	4:X:2219:HOH:O	1.84	0.69
1:X:202:ARG:NH1	1:X:252:PHE:HB3	2.08	0.69
1:X:229:LYS:HE2	1:X:234:ASN:HD21	1.58	0.69
1:X:445:ARG:O	1:X:445:ARG:HG3	1.92	0.69
1:X:681:VAL:HG23	1:X:682:LEU:N	2.08	0.69
1:X:212:GLU:O	1:X:216:LEU:CG	2.40	0.69
1:X:241:LYS:HA	1:X:259:GLN:O	1.91	0.69
1:X:623:LYS:N	1:X:628:ILE:HD11	2.07	0.69
1:X:595:ASP:OD1	1:X:598:LEU:HD23	1.93	0.69
1:X:217:GLN:O	1:X:330:ALA:HB1	1.93	0.68
1:X:732:ILE:HG22	1:X:737:TYR:CD2	2.28	0.68
1:X:118:TYR:CD2	1:X:148:ARG:NH2	2.56	0.68
1:X:187:GLU:CB	4:X:2068:HOH:O	2.40	0.68
1:X:473:TYR:O	1:X:477:LYS:HG2	1.93	0.68
1:X:6:ASP:O	1:X:12:HIS:NE2	2.26	0.68
1:X:160:ASP:O	1:X:163:TYR:HB3	1.92	0.68
1:X:196:LEU:CD1	1:X:245:ILE:CD1	2.64	0.68
1:X:594:GLN:O	1:X:594:GLN:CG	2.41	0.68
1:X:747:ARG:HG3	1:X:749:GLY:H	1.59	0.68
1:X:142:ILE:C	1:X:144:LYS:H	2.02	0.68
1:X:428:ARG:HB2	1:X:611:LEU:HD13	1.74	0.68
1:X:144:LYS:HE3	1:X:199:VAL:HG12	1.74	0.68
1:X:251:GLY:C	1:X:252:PHE:CD1	2.61	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:359:PHE:CE1	1:X:415:SER:HA	2.29	0.68
1:X:342:MET:SD	1:X:346:LYS:HB2	2.34	0.68
1:X:628:ILE:CG2	1:X:629:THR:H	2.07	0.68
1:X:121:LEU:CB	4:X:2048:HOH:O	2.41	0.68
1:X:341:GLN:O	1:X:345:PHE:CD2	2.47	0.68
1:X:91:MET:HA	4:X:2041:HOH:O	1.94	0.67
1:X:131:ARG:NH1	1:X:132:ILE:O	2.26	0.67
1:X:319:SER:HA	4:X:2116:HOH:O	1.93	0.67
1:X:464:ASN:HD22	1:X:577:VAL:CG2	2.07	0.67
1:X:654:ARG:HG3	1:X:681:VAL:HG13	1.74	0.67
1:X:255:GLY:CA	1:X:441:LEU:O	2.42	0.67
1:X:271:GLN:HB3	1:X:275:GLU:O	1.94	0.67
1:X:64:THR:O	1:X:66:ASP:N	2.27	0.67
1:X:275:GLU:C	4:X:2099:HOH:O	2.35	0.67
1:X:593:GLN:O	1:X:596:LEU:HD12	1.93	0.67
1:X:341:GLN:HG2	4:X:2122:HOH:O	1.84	0.67
1:X:681:VAL:HG23	1:X:682:LEU:H	1.59	0.67
1:X:90:ASP:C	4:X:2041:HOH:O	2.36	0.67
1:X:504:ILE:N	4:X:2169:HOH:O	2.26	0.67
1:X:564:SER:HB3	4:X:2186:HOH:O	1.94	0.67
1:X:455:ILE:HG22	4:X:2147:HOH:O	1.89	0.67
1:X:53:VAL:HB	1:X:61:THR:HB	1.76	0.67
1:X:185:LYS:NZ	2:X:1001:ADP:O2B	2.28	0.67
1:X:668:GLU:CD	1:X:670:LYS:HE2	2.19	0.67
1:X:84:LYS:HZ2	1:X:704:ARG:HD2	1.58	0.67
1:X:225:PHE:HD1	1:X:280:ILE:HG21	1.59	0.67
1:X:319:SER:O	1:X:323:GLU:HB2	1.94	0.67
1:X:178:THR:CG2	4:X:2147:HOH:O	2.22	0.67
1:X:27:LEU:CD1	1:X:28:THR:N	2.09	0.66
1:X:175:LEU:C	1:X:176:LEU:HD12	2.18	0.66
1:X:257:SER:O	1:X:258:ILE:HG13	1.94	0.66
1:X:641:LEU:O	1:X:644:THR:HB	1.94	0.66
1:X:410:ASN:HD21	1:X:413:LYS:CE	2.08	0.66
1:X:30:SER:C	1:X:31:ASP:OD1	2.37	0.66
1:X:26:LYS:O	1:X:26:LYS:HG2	1.95	0.66
1:X:193:ILE:O	1:X:196:LEU:HB2	1.96	0.66
1:X:672:VAL:HA	1:X:675:GLN:HE21	1.59	0.66
1:X:479:GLN:NE2	1:X:680:ALA:HB2	2.10	0.66
1:X:48:GLU:HG2	1:X:65:VAL:HG21	1.77	0.66
1:X:27:LEU:HD13	1:X:28:THR:CG2	2.21	0.66
1:X:360:GLU:O	4:X:2127:HOH:O	2.06	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:88:VAL:HG23	4:X:2041:HOH:O	1.96	0.66
1:X:662:GLN:HG2	4:X:2208:HOH:O	1.90	0.66
1:X:689:ARG:HB2	1:X:693:PRO:HB3	1.78	0.66
1:X:56:THR:CG2	1:X:57:SER:N	2.59	0.65
1:X:476:GLU:OE2	1:X:510:SER:HB2	1.96	0.65
1:X:72:VAL:HG11	1:X:77:ALA:HB2	1.78	0.65
1:X:242:PHE:HD1	1:X:453:LEU:HB2	1.60	0.65
1:X:315:ILE:HB	4:X:2114:HOH:O	1.95	0.65
1:X:719:SER:CB	1:X:723:THR:HB	2.15	0.65
1:X:82:PRO:HB3	1:X:756:GLU:CD	2.22	0.65
1:X:230:THR:HG22	1:X:275:GLU:OE1	1.95	0.65
1:X:420:ALA:CB	1:X:592:LEU:HD13	2.27	0.65
1:X:546:LYS:HZ3	1:X:550:HIS:HE1	1.42	0.65
1:X:371:ASP:O	4:X:2129:HOH:O	2.14	0.65
1:X:409:LEU:HD22	1:X:409:LEU:N	2.11	0.65
1:X:103:PHE:CZ	1:X:667:LEU:HD23	2.32	0.65
1:X:82:PRO:HB3	1:X:756:GLU:OE1	1.97	0.65
1:X:174:SER:HB3	4:X:2207:HOH:O	1.93	0.65
1:X:594:GLN:OE1	1:X:597:GLU:HB2	1.97	0.65
1:X:122:PHE:CE1	1:X:654:ARG:CG	2.79	0.65
1:X:180:GLU:O	1:X:183:ALA:HB2	1.95	0.65
1:X:390:GLU:HA	1:X:393:LEU:HB2	1.78	0.65
1:X:54:SER:HB2	1:X:61:THR:HG21	1.80	0.64
1:X:87:GLY:HA2	1:X:109:ARG:HG3	1.78	0.64
1:X:226:GLY:HA3	1:X:239:PHE:HE2	1.62	0.64
1:X:261:TYR:HD1	4:X:2097:HOH:O	1.79	0.64
1:X:56:THR:CG2	1:X:57:SER:H	2.10	0.64
1:X:118:TYR:CE1	1:X:153:PRO:HA	2.30	0.64
1:X:166:MET:CA	1:X:173:GLN:NE2	2.40	0.64
1:X:497:GLU:O	1:X:498:LYS:HB3	1.97	0.64
1:X:19:GLN:CB	4:X:2003:HOH:O	2.41	0.64
1:X:154:HIS:CE1	1:X:155:ILE:HG22	2.33	0.64
1:X:361:LYS:HG3	1:X:411:VAL:CG1	2.27	0.64
1:X:384:VAL:CG1	1:X:385:ASN:N	2.60	0.64
1:X:174:SER:N	4:X:2207:HOH:O	2.30	0.64
1:X:174:SER:O	1:X:651:HIS:N	2.29	0.64
1:X:226:GLY:O	1:X:238:ARG:HB2	1.97	0.64
1:X:229:LYS:HG3	1:X:234:ASN:HA	1.78	0.64
1:X:293:LYS:HA	1:X:298:LEU:HB2	1.79	0.64
1:X:703:LYS:HA	4:X:2224:HOH:O	1.97	0.64
1:X:747:ARG:HG3	1:X:749:GLY:N	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:662:GLN:HG3	4:X:2208:HOH:O	1.96	0.64
1:X:380:THR:C	4:X:2132:HOH:O	2.40	0.64
1:X:657:ILE:HG12	1:X:658:PRO:HD2	1.79	0.64
1:X:130:LYS:HG3	1:X:132:ILE:CD1	2.22	0.64
1:X:202:ARG:HH11	1:X:252:PHE:CB	2.10	0.64
1:X:331:MET:HG2	1:X:336:PHE:CD2	2.31	0.64
1:X:373:THR:O	1:X:376:ASN:HB2	1.98	0.64
1:X:548:HIS:CE1	1:X:560:GLU:HG3	2.33	0.64
1:X:388:VAL:O	1:X:392:ALA:N	2.28	0.63
1:X:710:PRO:HG3	4:X:2221:HOH:O	1.97	0.63
1:X:371:ASP:C	4:X:2129:HOH:O	2.40	0.63
1:X:744:ILE:C	1:X:745:PHE:CD1	2.76	0.63
1:X:7:ARG:HA	1:X:12:HIS:CE1	2.33	0.63
1:X:420:ALA:HB3	1:X:592:LEU:HD13	1.81	0.63
1:X:564:SER:CB	4:X:2186:HOH:O	2.46	0.63
1:X:694:ASN:HD22	1:X:751:LEU:HD13	1.63	0.63
1:X:746:PHE:N	4:X:2248:HOH:O	2.31	0.63
1:X:58:ASP:OD1	1:X:73:LYS:HG3	1.98	0.63
1:X:137:GLN:O	1:X:140:VAL:HB	1.99	0.63
1:X:238:ARG:HG3	1:X:264:GLU:CB	2.22	0.63
1:X:695:ARG:HG2	1:X:745:PHE:CD1	2.33	0.63
1:X:47:TYR:HE1	1:X:673:LEU:CD2	2.12	0.63
1:X:139:MET:HA	1:X:139:MET:CE	2.28	0.63
1:X:385:ASN:OD1	1:X:386:PRO:N	2.32	0.63
1:X:479:GLN:HE22	1:X:680:ALA:CB	2.11	0.63
1:X:360:GLU:CA	4:X:2127:HOH:O	2.43	0.63
1:X:703:LYS:HA	1:X:706:TYR:HE2	1.64	0.63
1:X:732:ILE:HG21	1:X:737:TYR:CD2	2.34	0.63
1:X:296:LEU:CD1	1:X:298:LEU:CG	2.76	0.63
1:X:385:ASN:OD1	1:X:387:SER:N	2.32	0.63
1:X:121:LEU:HB3	4:X:2048:HOH:O	1.98	0.62
1:X:256:ALA:O	1:X:442:CYS:HB2	1.99	0.62
1:X:37:TYR:O	1:X:48:GLU:N	2.32	0.62
1:X:172:ASN:ND2	4:X:2067:HOH:O	2.22	0.62
1:X:723:THR:CG2	4:X:2234:HOH:O	2.21	0.62
1:X:706:TYR:CZ	1:X:714:ARG:CA	2.79	0.62
1:X:734:PRO:HD3	4:X:2241:HOH:O	1.98	0.62
1:X:144:LYS:HB2	1:X:144:LYS:NZ	2.12	0.62
1:X:249:SER:CB	4:X:2063:HOH:O	2.33	0.62
1:X:361:LYS:HD2	1:X:361:LYS:N	2.14	0.62
1:X:514:ILE:O	1:X:518:ASP:CG	2.42	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:62:PHE:HB2	1:X:70:ARG:O	2.00	0.62
1:X:97:LEU:HD13	1:X:689:ARG:HD2	1.81	0.62
1:X:225:PHE:CD1	1:X:280:ILE:HG21	2.35	0.62
1:X:338:GLN:NE2	4:X:2123:HOH:O	2.31	0.62
1:X:357:ILE:HG13	1:X:375:LEU:HD12	1.80	0.62
1:X:526:LEU:HD22	1:X:631:ALA:CB	2.28	0.62
1:X:735:GLU:HA	1:X:738:ARG:NH2	2.14	0.62
1:X:14:TYR:CE1	1:X:133:PRO:CG	2.82	0.62
1:X:85:PHE:O	1:X:88:VAL:HG12	1.90	0.62
1:X:431:LEU:HD21	1:X:617:ILE:HG13	1.81	0.62
1:X:457:GLY:HA2	1:X:475:ASN:OD1	1.99	0.62
1:X:685:ILE:HG21	4:X:2047:HOH:O	2.00	0.62
1:X:119:SER:O	1:X:120:GLY:C	2.42	0.61
1:X:459:GLU:HB3	1:X:461:PHE:CZ	2.35	0.61
1:X:628:ILE:CG2	1:X:629:THR:N	2.63	0.61
1:X:668:GLU:C	1:X:670:LYS:H	2.08	0.61
1:X:689:ARG:CD	1:X:693:PRO:HG3	2.30	0.61
1:X:337:SER:N	1:X:340:GLU:OE1	2.30	0.61
1:X:708:LEU:O	1:X:708:LEU:HD23	2.00	0.61
1:X:238:ARG:NE	1:X:238:ARG:CA	2.59	0.61
1:X:331:MET:HE1	1:X:345:PHE:HZ	1.64	0.61
1:X:664:PRO:O	1:X:665:ALA:HB3	2.01	0.61
1:X:357:ILE:CD1	1:X:374:ALA:HB3	2.29	0.61
1:X:243:ILE:HG23	1:X:257:SER:O	2.01	0.61
1:X:3:PRO:O	1:X:6:ASP:O	2.19	0.61
1:X:27:LEU:HD12	1:X:28:THR:H	0.48	0.61
1:X:35:ILE:HG13	1:X:78:ASN:O	2.00	0.61
1:X:238:ARG:HE	1:X:264:GLU:HB2	1.65	0.61
1:X:247:PHE:CZ	1:X:253:ILE:HG12	2.34	0.61
1:X:732:ILE:HD12	1:X:732:ILE:N	2.14	0.61
1:X:8:THR:HG23	1:X:9:SER:N	2.16	0.61
1:X:19:GLN:HG3	4:X:2003:HOH:O	1.99	0.61
1:X:91:MET:N	4:X:2041:HOH:O	2.33	0.61
1:X:247:PHE:CE1	1:X:253:ILE:CG1	2.81	0.61
1:X:180:GLU:OE1	1:X:675:GLN:HG2	2.00	0.61
1:X:172:ASN:HB3	1:X:449:PHE:CG	2.36	0.60
1:X:82:PRO:CA	1:X:756:GLU:OE1	2.49	0.60
1:X:409:LEU:N	1:X:409:LEU:HD13	2.15	0.60
1:X:698:TYR:CG	1:X:698:TYR:O	2.52	0.60
1:X:590:ASP:OD1	1:X:590:ASP:C	2.42	0.60
1:X:706:TYR:CE1	1:X:713:PRO:C	2.79	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:64:THR:C	1:X:66:ASP:N	2.58	0.60
1:X:241:LYS:HG2	1:X:454:ASP:OD1	2.01	0.60
1:X:586:GLU:HG3	1:X:586:GLU:O	2.02	0.60
1:X:606:ASN:CB	4:X:2197:HOH:O	2.25	0.60
1:X:736:GLN:C	1:X:747:ARG:HD2	2.26	0.60
1:X:711:ASN:ND2	1:X:729:HIS:CG	2.70	0.60
1:X:540:ASP:HB3	1:X:581:ILE:HG22	1.82	0.60
1:X:672:VAL:HA	1:X:675:GLN:NE2	2.17	0.60
1:X:691:GLY:O	1:X:748:ALA:HB2	2.01	0.60
1:X:730:LEU:HD13	1:X:754:ILE:HG21	1.83	0.60
1:X:213:GLN:CB	4:X:2079:HOH:O	2.45	0.60
1:X:739:PHE:CD2	1:X:744:ILE:HD11	2.36	0.60
1:X:670:LYS:HG3	1:X:671:VAL:HG23	1.84	0.60
1:X:134:ILE:C	1:X:139:MET:HG3	2.26	0.60
1:X:410:ASN:CG	1:X:413:LYS:HE3	2.26	0.60
1:X:238:ARG:HA	1:X:238:ARG:HE	1.62	0.60
1:X:704:ARG:O	1:X:705:TYR:CG	2.53	0.60
1:X:275:GLU:CA	4:X:2099:HOH:O	2.50	0.59
1:X:487:PHE:CE2	1:X:506:PHE:HB2	2.37	0.59
1:X:539:THR:O	1:X:540:ASP:C	2.44	0.59
1:X:29:VAL:O	1:X:29:VAL:CG1	2.40	0.59
1:X:567:GLU:OE1	1:X:578:MET:HE3	2.02	0.59
1:X:35:ILE:HD11	1:X:77:ALA:HB3	1.69	0.59
1:X:330:ALA:O	1:X:334:VAL:HG22	2.02	0.59
1:X:458:PHE:O	1:X:458:PHE:CD1	2.55	0.59
1:X:159:SER:O	1:X:160:ASP:C	2.45	0.59
1:X:44:ARG:CB	4:X:2023:HOH:O	2.50	0.59
1:X:269:VAL:HG12	1:X:306:TYR:CZ	2.38	0.59
1:X:432:TRP:NE1	1:X:610:LYS:NZ	2.48	0.59
1:X:15:LEU:HD13	1:X:143:PHE:HZ	1.67	0.59
1:X:331:MET:C	1:X:336:PHE:HB2	2.28	0.59
1:X:538:ALA:HB1	1:X:542:THR:HG21	1.84	0.59
1:X:170:ARG:HA	1:X:448:TYR:CE2	2.23	0.59
1:X:249:SER:CA	4:X:2063:HOH:O	2.49	0.59
1:X:396:PRO:O	1:X:398:ILE:HD12	2.03	0.59
1:X:706:TYR:HD1	1:X:712:VAL:O	1.85	0.59
1:X:390:GLU:HG2	1:X:394:MET:HG2	1.83	0.59
1:X:410:ASN:OD1	1:X:412:GLU:CG	2.49	0.59
1:X:657:ILE:CG1	1:X:658:PRO:HD2	2.33	0.59
1:X:586:GLU:OE1	4:X:2192:HOH:O	2.17	0.58
1:X:158:ILE:CG2	1:X:175:LEU:CD2	2.81	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:720:GLN:HE22	1:X:741:ILE:HG13	1.67	0.58
1:X:54:SER:H	1:X:61:THR:HG1	1.50	0.58
1:X:276:ARG:HG2	1:X:282:TYR:CE1	2.39	0.58
1:X:432:TRP:HE1	1:X:610:LYS:HE2	1.68	0.58
1:X:195:TYR:O	1:X:199:VAL:HG22	2.03	0.58
1:X:477:LYS:CD	1:X:514:ILE:HD12	2.32	0.58
1:X:24:LEU:HD12	1:X:26:LYS:CD	2.31	0.58
1:X:337:SER:O	4:X:2122:HOH:O	2.16	0.58
1:X:667:LEU:HD11	1:X:672:VAL:HG21	1.85	0.58
1:X:727:LEU:HD21	1:X:739:PHE:HE2	1.68	0.58
1:X:477:LYS:HD3	1:X:514:ILE:HD12	1.86	0.58
1:X:711:ASN:HD21	1:X:729:HIS:CG	2.22	0.58
1:X:118:TYR:CD1	1:X:153:PRO:HB3	2.39	0.58
1:X:428:ARG:HH12	1:X:618:ALA:HB2	1.69	0.58
1:X:263:LEU:HB2	1:X:265:LYS:HG3	1.86	0.58
1:X:585:LEU:HD11	4:X:2175:HOH:O	2.04	0.57
1:X:384:VAL:HG12	1:X:385:ASN:H	1.68	0.57
1:X:474:THR:CG2	1:X:478:LEU:HD11	2.34	0.57
1:X:570:VAL:HG12	1:X:571:THR:N	2.19	0.57
1:X:170:ARG:CA	1:X:448:TYR:HE2	2.13	0.57
1:X:247:PHE:CE1	1:X:253:ILE:CA	2.84	0.57
1:X:292:GLU:O	1:X:296:LEU:HG	2.04	0.57
1:X:701:PHE:HA	1:X:704:ARG:HB3	1.85	0.57
1:X:27:LEU:CD1	1:X:28:THR:OG1	2.53	0.57
1:X:530:ASP:CG	1:X:629:THR:HG1	2.12	0.57
1:X:617:ILE:O	1:X:617:ILE:CG2	2.49	0.57
1:X:268:VAL:HG13	1:X:269:VAL:HG13	1.86	0.57
1:X:580:GLU:O	1:X:581:ILE:HD13	2.04	0.57
1:X:82:PRO:CB	1:X:756:GLU:OE1	2.51	0.57
1:X:241:LYS:O	1:X:453:LEU:HD12	2.05	0.57
1:X:623:LYS:CA	1:X:628:ILE:HD11	2.33	0.57
1:X:737:TYR:O	1:X:738:ARG:HD3	2.05	0.57
1:X:118:TYR:CD2	1:X:148:ARG:CZ	2.88	0.57
1:X:266:SER:CA	1:X:423:LYS:HE2	2.35	0.57
1:X:550:HIS:O	1:X:554:LYS:HE3	2.05	0.57
1:X:732:ILE:HG22	1:X:737:TYR:HD2	1.67	0.57
1:X:342:MET:SD	1:X:346:LYS:HD3	2.44	0.57
1:X:410:ASN:OD1	1:X:410:ASN:C	2.46	0.57
1:X:583:ASP:O	1:X:587:LYS:HG2	2.04	0.57
1:X:110:TYR:HA	1:X:114:LEU:O	2.05	0.57
1:X:468:GLN:C	1:X:470:CYS:N	2.54	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:102:VAL:O	1:X:106:LEU:CD2	2.53	0.56
1:X:209:GLY:HA2	4:X:2072:HOH:O	2.05	0.56
1:X:474:THR:O	1:X:478:LEU:HG	2.05	0.56
1:X:571:THR:OG1	4:X:2187:HOH:O	2.18	0.56
1:X:739:PHE:CG	1:X:744:ILE:HD11	2.39	0.56
1:X:27:LEU:CG	1:X:28:THR:H	2.03	0.56
1:X:58:ASP:HA	1:X:74:LYS:HB2	1.86	0.56
1:X:657:ILE:HG22	1:X:675:GLN:NE2	2.20	0.56
1:X:727:LEU:HD21	1:X:739:PHE:CE2	2.40	0.56
1:X:35:ILE:HD11	1:X:77:ALA:CA	2.30	0.56
1:X:149:ASN:OD1	1:X:150:GLU:N	2.38	0.56
1:X:242:PHE:CD1	1:X:453:LEU:HB2	2.39	0.56
1:X:668:GLU:OE1	1:X:670:LYS:HE3	2.05	0.56
1:X:732:ILE:H	1:X:732:ILE:CD1	2.16	0.56
1:X:746:PHE:C	4:X:2250:HOH:O	2.47	0.56
1:X:431:LEU:HD21	1:X:617:ILE:CG1	2.33	0.56
1:X:546:LYS:C	1:X:548:HIS:H	2.12	0.56
1:X:723:THR:CB	4:X:2234:HOH:O	2.53	0.56
1:X:154:HIS:ND1	1:X:155:ILE:N	2.53	0.56
1:X:353:HIS:C	1:X:355:GLY:N	2.58	0.56
1:X:331:MET:CG	1:X:336:PHE:HD2	2.19	0.56
1:X:345:PHE:HA	1:X:348:ILE:CG1	2.33	0.56
1:X:682:LEU:O	1:X:685:ILE:CG2	2.53	0.56
1:X:747:ARG:NE	1:X:748:ALA:N	2.45	0.56
1:X:691:GLY:O	1:X:692:PHE:CG	2.59	0.56
1:X:87:GLY:HA2	1:X:109:ARG:CG	2.35	0.56
1:X:178:THR:HA	1:X:185:LYS:HD3	1.88	0.56
1:X:247:PHE:HE1	1:X:253:ILE:HG23	1.70	0.56
1:X:584:TRP:HD1	4:X:2190:HOH:O	1.88	0.56
1:X:285:LEU:HD13	1:X:301:PRO:HB3	1.88	0.56
1:X:426:TYR:CE1	4:X:2139:HOH:O	2.59	0.56
1:X:426:TYR:HB2	4:X:2140:HOH:O	2.05	0.56
1:X:62:PHE:CE1	1:X:72:VAL:HG12	2.40	0.55
1:X:72:VAL:HG22	1:X:73:LYS:N	2.21	0.55
1:X:72:VAL:CG1	1:X:77:ALA:HB2	2.35	0.55
1:X:691:GLY:C	1:X:692:PHE:CD1	2.84	0.55
1:X:354:LEU:O	1:X:418:ARG:NH1	2.39	0.55
1:X:709:ALA:O	1:X:711:ASN:N	2.39	0.55
1:X:735:GLU:C	1:X:738:ARG:HH12	2.13	0.55
1:X:4:ILE:H	1:X:4:ILE:CD1	2.14	0.55
1:X:170:ARG:NH2	4:X:2065:HOH:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:227:ASN:OD1	1:X:237:SER:HA	2.06	0.55
1:X:266:SER:HA	1:X:423:LYS:HE2	1.88	0.55
1:X:670:LYS:HG3	1:X:671:VAL:N	2.22	0.55
1:X:61:THR:C	1:X:62:PHE:HD1	2.15	0.55
1:X:91:MET:HG2	1:X:118:TYR:O	2.06	0.55
1:X:212:GLU:HG2	4:X:2077:HOH:O	2.06	0.55
1:X:377:ALA:HA	1:X:380:THR:HB	1.87	0.55
1:X:30:SER:O	1:X:31:ASP:OD1	2.25	0.55
1:X:540:ASP:O	1:X:543:LEU:N	2.40	0.55
1:X:737:TYR:CB	1:X:747:ARG:H	2.19	0.55
1:X:40:ASP:C	1:X:42:LYS:H	2.15	0.55
1:X:82:PRO:HG3	1:X:756:GLU:CD	2.31	0.55
1:X:118:TYR:HD2	1:X:148:ARG:CZ	2.20	0.55
1:X:238:ARG:CG	1:X:278:TYR:CE1	2.69	0.55
1:X:657:ILE:HG22	1:X:675:GLN:CD	2.32	0.55
1:X:681:VAL:CG2	1:X:682:LEU:H	2.19	0.55
1:X:617:ILE:O	1:X:617:ILE:HG23	2.07	0.55
1:X:44:ARG:HB2	4:X:2023:HOH:O	2.07	0.55
1:X:194:GLN:O	1:X:197:ALA:HB3	2.07	0.55
1:X:296:LEU:O	1:X:298:LEU:HG	2.06	0.55
1:X:390:GLU:HG2	1:X:394:MET:CG	2.36	0.55
1:X:592:LEU:HD11	1:X:596:LEU:HD13	1.88	0.55
1:X:311:GLY:HA2	4:X:2109:HOH:O	2.07	0.55
1:X:91:MET:CA	4:X:2041:HOH:O	2.55	0.54
1:X:458:PHE:CB	1:X:472:ASN:HD22	2.19	0.54
1:X:570:VAL:HG12	1:X:571:THR:H	1.70	0.54
1:X:739:PHE:CE2	1:X:744:ILE:HD11	2.41	0.54
1:X:276:ARG:HD2	1:X:282:TYR:CE2	2.40	0.54
1:X:17:VAL:O	1:X:18:LYS:HB3	2.06	0.54
1:X:6:ASP:O	1:X:12:HIS:CE1	2.61	0.54
1:X:213:GLN:CA	4:X:2079:HOH:O	2.56	0.54
1:X:247:PHE:O	1:X:447:ALA:HB3	2.07	0.54
1:X:361:LYS:CB	1:X:367:ALA:HA	2.35	0.54
1:X:372:LYS:HA	4:X:2129:HOH:O	1.88	0.54
1:X:279:HIS:O	1:X:283:GLN:CG	2.52	0.54
1:X:459:GLU:HG2	1:X:461:PHE:HE1	1.73	0.54
1:X:703:LYS:HA	1:X:706:TYR:CE2	2.42	0.54
1:X:705:TYR:CE2	1:X:755:GLU:HA	2.43	0.54
1:X:10:ASP:HB3	1:X:14:TYR:CD2	2.42	0.54
1:X:142:ILE:HG23	1:X:146:ARG:NH1	2.22	0.54
1:X:315:ILE:O	1:X:316:LYS:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:498:LYS:O	1:X:498:LYS:HG3	2.08	0.54
1:X:546:LYS:C	1:X:548:HIS:N	2.66	0.54
1:X:702:VAL:HG22	1:X:723:THR:OG1	2.08	0.54
1:X:222:LEU:CB	4:X:2082:HOH:O	2.54	0.54
1:X:238:ARG:HB3	1:X:264:GLU:H	1.72	0.54
1:X:428:ARG:HB3	1:X:611:LEU:HD13	1.87	0.54
1:X:501:TRP:CH2	1:X:738:ARG:HG3	2.43	0.54
1:X:534:VAL:O	1:X:536:PRO:HD3	2.07	0.54
1:X:561:PRO:HG2	1:X:564:SER:O	2.08	0.54
1:X:581:ILE:O	1:X:581:ILE:CG2	2.55	0.54
1:X:361:LYS:CD	1:X:361:LYS:C	2.78	0.54
1:X:734:PRO:O	1:X:738:ARG:NH1	2.41	0.54
1:X:480:GLN:O	1:X:483:ASN:HB2	2.08	0.53
1:X:607:VAL:HG12	1:X:607:VAL:O	2.08	0.53
1:X:700:ASP:O	1:X:703:LYS:HG2	2.08	0.53
1:X:296:LEU:HD12	1:X:298:LEU:CG	2.27	0.53
1:X:533:SER:O	1:X:589:LYS:HD2	2.08	0.53
1:X:588:ASN:OD1	1:X:629:THR:HB	2.08	0.53
1:X:48:GLU:HG2	1:X:65:VAL:CG2	2.38	0.53
1:X:48:GLU:CG	1:X:65:VAL:HG21	2.37	0.53
1:X:173:GLN:C	4:X:2207:HOH:O	2.50	0.53
1:X:33:ARG:CZ	1:X:753:ARG:NH1	2.71	0.53
1:X:154:HIS:CE1	1:X:155:ILE:CG2	2.91	0.53
1:X:530:ASP:CG	1:X:588:ASN:HD21	2.16	0.53
1:X:539:THR:O	1:X:542:THR:HG22	2.07	0.53
1:X:10:ASP:HB3	1:X:14:TYR:CE2	2.43	0.53
1:X:684:GLY:C	1:X:687:ILE:HG22	2.34	0.53
1:X:543:LEU:O	1:X:547:LEU:HG	2.08	0.53
1:X:692:PHE:HD2	1:X:748:ALA:N	2.06	0.53
1:X:746:PHE:CE1	4:X:2250:HOH:O	2.49	0.53
1:X:27:LEU:HD12	1:X:28:THR:CB	2.39	0.53
1:X:58:ASP:HA	4:X:2029:HOH:O	1.85	0.53
1:X:106:LEU:HD23	1:X:106:LEU:H	1.73	0.53
1:X:130:LYS:CD	1:X:132:ILE:HD11	2.38	0.53
1:X:155:ILE:HG23	1:X:156:PHE:N	2.23	0.53
1:X:246:GLN:O	1:X:254:SER:N	2.37	0.53
1:X:596:LEU:HA	1:X:599:CYS:SG	2.49	0.53
1:X:736:GLN:CA	1:X:747:ARG:HD2	2.39	0.53
1:X:73:LYS:HG2	1:X:74:LYS:N	2.23	0.53
1:X:620:ARG:NH1	1:X:629:THR:HA	2.24	0.53
1:X:668:GLU:OE1	1:X:670:LYS:CE	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:398:ILE:HG12	1:X:407:GLN:HE22	1.70	0.53
1:X:739:PHE:CG	1:X:744:ILE:CD1	2.91	0.53
1:X:82:PRO:CB	1:X:756:GLU:CD	2.82	0.53
1:X:131:ARG:C	1:X:132:ILE:HD13	2.34	0.53
1:X:172:ASN:HB2	4:X:2067:HOH:O	2.02	0.53
1:X:369:LEU:HD12	1:X:390:GLU:OE1	2.09	0.53
1:X:486:MET:O	1:X:490:GLU:CG	2.43	0.53
1:X:573:TYR:OH	1:X:683:GLU:HG2	2.09	0.53
1:X:625:ALA:C	1:X:626:ASN:OD1	2.52	0.53
1:X:284:LEU:HD22	1:X:348:ILE:CD1	2.36	0.52
1:X:756:GLU:O	1:X:757:ALA:HB2	2.08	0.52
1:X:27:LEU:CD1	1:X:28:THR:CB	2.86	0.52
1:X:53:VAL:HB	1:X:61:THR:CB	2.38	0.52
1:X:122:PHE:CE1	1:X:654:ARG:NE	2.76	0.52
1:X:758:ARG:NE	4:X:2019:HOH:O	2.43	0.52
1:X:375:LEU:C	1:X:377:ALA:H	2.17	0.52
1:X:397:ARG:HA	1:X:406:ALA:CA	2.31	0.52
1:X:596:LEU:HA	1:X:599:CYS:HG	1.73	0.52
1:X:26:LYS:O	1:X:26:LYS:HG3	2.09	0.52
1:X:120:GLY:HA3	4:X:2049:HOH:O	2.09	0.52
1:X:172:ASN:HD22	1:X:449:PHE:HE2	1.47	0.52
1:X:176:LEU:N	1:X:651:HIS:O	2.39	0.52
1:X:202:ARG:HD3	1:X:252:PHE:HB3	1.89	0.52
1:X:458:PHE:CB	1:X:472:ASN:ND2	2.72	0.52
1:X:530:ASP:OD1	1:X:588:ASN:ND2	2.42	0.52
1:X:90:ASP:O	1:X:93:GLU:HG3	2.10	0.52
1:X:263:LEU:HD21	1:X:430:PHE:CE2	2.44	0.52
1:X:492:GLU:C	1:X:494:TYR:N	2.63	0.52
1:X:603:SER:OG	1:X:608:VAL:HG11	2.09	0.52
1:X:628:ILE:HG22	1:X:632:ALA:HB3	1.91	0.52
1:X:700:ASP:O	1:X:704:ARG:N	2.43	0.52
1:X:18:LYS:O	1:X:19:GLN:C	2.53	0.52
1:X:202:ARG:NH1	1:X:252:PHE:CB	2.71	0.52
1:X:324:PHE:HE2	1:X:328:ARG:HH21	1.54	0.52
1:X:681:VAL:CG2	1:X:682:LEU:N	2.72	0.52
1:X:712:VAL:HG13	1:X:713:PRO:HD2	1.91	0.52
1:X:694:ASN:HD22	1:X:751:LEU:CD1	2.22	0.52
1:X:293:LYS:CA	1:X:298:LEU:HB2	2.39	0.52
1:X:410:ASN:O	1:X:412:GLU:N	2.43	0.52
1:X:732:ILE:HG21	1:X:737:TYR:HD2	1.68	0.52
1:X:736:GLN:O	1:X:747:ARG:CG	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:377:ALA:HA	1:X:380:THR:CB	2.39	0.52
1:X:428:ARG:NH1	1:X:618:ALA:HB2	2.25	0.52
1:X:534:VAL:O	1:X:534:VAL:HG12	2.09	0.52
1:X:88:VAL:CG2	4:X:2041:HOH:O	2.56	0.52
1:X:116:TYR:HE2	1:X:134:ILE:CD1	2.23	0.52
1:X:468:GLN:C	1:X:470:CYS:H	2.17	0.52
1:X:595:ASP:HA	1:X:598:LEU:CB	2.40	0.52
1:X:712:VAL:CG2	1:X:725:ALA:HB3	2.40	0.52
1:X:759:GLU:OXT	1:X:759:GLU:HG2	2.10	0.52
1:X:110:TYR:CD2	1:X:667:LEU:HD13	2.43	0.51
1:X:224:ALA:O	1:X:280:ILE:N	2.42	0.51
1:X:304:PHE:CD2	1:X:352:LEU:HB3	2.43	0.51
1:X:544:ILE:O	1:X:548:HIS:CD2	2.63	0.51
1:X:142:ILE:C	1:X:144:LYS:N	2.63	0.51
1:X:181:SER:C	1:X:183:ALA:H	2.16	0.51
1:X:288:ALA:CB	1:X:292:GLU:OE2	2.59	0.51
1:X:388:VAL:O	1:X:389:LEU:C	2.53	0.51
1:X:147:ARG:O	1:X:150:GLU:HB2	2.10	0.51
1:X:219:ASN:O	1:X:220:PRO:C	2.53	0.51
1:X:552:SER:HB2	4:X:2180:HOH:O	2.10	0.51
1:X:103:PHE:HA	1:X:106:LEU:HD21	1.91	0.51
1:X:213:GLN:HA	1:X:216:LEU:HB2	1.92	0.51
1:X:464:ASN:ND2	1:X:577:VAL:CG2	2.72	0.51
1:X:732:ILE:CG2	1:X:737:TYR:CE2	2.93	0.51
1:X:64:THR:O	1:X:65:VAL:C	2.53	0.51
1:X:142:ILE:O	1:X:144:LYS:N	2.43	0.51
1:X:233:ASN:CG	1:X:234:ASN:H	2.17	0.51
1:X:361:LYS:CG	1:X:411:VAL:HG11	2.35	0.51
1:X:446:LYS:HG2	1:X:447:ALA:N	2.25	0.51
1:X:644:THR:HG22	1:X:644:THR:O	2.11	0.51
1:X:14:TYR:OH	1:X:133:PRO:CG	2.58	0.51
1:X:368:VAL:C	1:X:369:LEU:HD23	2.36	0.51
1:X:483:ASN:HB3	1:X:508:LEU:HD21	1.93	0.51
1:X:689:ARG:CB	1:X:693:PRO:HB3	2.41	0.51
1:X:739:PHE:CD1	1:X:744:ILE:HD11	2.45	0.51
1:X:21:ASP:CG	4:X:2011:HOH:O	2.52	0.51
1:X:172:ASN:CG	1:X:449:PHE:N	2.69	0.51
1:X:233:ASN:OD1	1:X:234:ASN:N	2.36	0.51
1:X:383:GLY:HA2	4:X:2132:HOH:O	2.09	0.51
1:X:353:HIS:O	1:X:354:LEU:C	2.53	0.51
1:X:620:ARG:NH2	1:X:630:VAL:HG23	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:706:TYR:CD1	1:X:712:VAL:O	2.61	0.51
1:X:735:GLU:CA	1:X:738:ARG:HH12	2.23	0.51
1:X:737:TYR:HA	1:X:747:ARG:HA	1.93	0.51
1:X:605:ASP:OD1	1:X:608:VAL:N	2.44	0.51
1:X:719:SER:O	1:X:723:THR:HG22	2.10	0.51
1:X:4:ILE:HD12	1:X:4:ILE:N	2.16	0.51
1:X:37:TYR:OH	1:X:48:GLU:OE1	2.25	0.51
1:X:284:LEU:HD23	1:X:348:ILE:HD13	1.92	0.51
1:X:485:HIS:CD2	1:X:489:LEU:CD1	2.94	0.51
1:X:600:PHE:C	1:X:602:ASP:N	2.69	0.51
1:X:662:GLN:N	4:X:2208:HOH:O	2.43	0.51
1:X:706:TYR:OH	1:X:714:ARG:CG	2.58	0.51
1:X:10:ASP:O	1:X:13:LYS:HG2	2.11	0.50
1:X:703:LYS:CA	4:X:2224:HOH:O	2.56	0.50
1:X:172:ASN:HB3	1:X:449:PHE:CZ	2.45	0.50
1:X:347:ILE:HD12	1:X:608:VAL:CG2	2.42	0.50
1:X:630:VAL:O	1:X:630:VAL:CG1	2.53	0.50
1:X:18:LYS:O	1:X:18:LYS:HG3	2.10	0.50
1:X:133:PRO:CA	4:X:2051:HOH:O	2.59	0.50
1:X:219:ASN:C	1:X:221:ILE:N	2.68	0.50
1:X:16:LYS:C	1:X:18:LYS:H	2.18	0.50
1:X:89:GLU:O	1:X:118:TYR:O	2.29	0.50
1:X:409:LEU:HD23	1:X:414:SER:CB	2.42	0.50
1:X:445:ARG:O	1:X:445:ARG:CG	2.58	0.50
1:X:467:GLU:O	1:X:470:CYS:HB2	2.12	0.50
1:X:577:VAL:HG11	1:X:579:TYR:CZ	2.46	0.50
1:X:19:GLN:CG	4:X:2003:HOH:O	2.58	0.50
1:X:64:THR:C	1:X:66:ASP:H	2.19	0.50
1:X:266:SER:N	1:X:423:LYS:HE2	2.27	0.50
1:X:614:ASP:O	1:X:616:ASN:N	2.44	0.50
1:X:79:GLN:HB2	4:X:2036:HOH:O	2.10	0.50
1:X:202:ARG:HG2	1:X:253:ILE:HB	1.94	0.50
1:X:515:ASP:O	1:X:516:LEU:C	2.52	0.50
1:X:572:HIS:C	1:X:574:ALA:H	2.19	0.50
1:X:97:LEU:HD12	1:X:689:ARG:NH1	2.26	0.50
1:X:732:ILE:HG22	1:X:737:TYR:CE2	2.47	0.50
1:X:246:GLN:CG	1:X:446:LYS:HE2	2.27	0.50
1:X:450:ILE:HG22	1:X:450:ILE:O	2.12	0.50
1:X:47:TYR:CE1	1:X:673:LEU:CD2	2.94	0.50
1:X:199:VAL:HG23	1:X:200:ALA:N	2.25	0.50
1:X:399:LEU:HD12	1:X:403:ASP:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:458:PHE:HB3	1:X:472:ASN:HD22	1.77	0.50
1:X:702:VAL:O	1:X:706:TYR:CE2	2.61	0.50
1:X:731:ASN:O	1:X:731:ASN:ND2	2.44	0.50
1:X:224:ALA:O	1:X:280:ILE:HB	2.11	0.49
1:X:269:VAL:HG12	1:X:306:TYR:CE1	2.47	0.49
1:X:594:GLN:O	1:X:594:GLN:OE1	2.30	0.49
1:X:735:GLU:HA	1:X:738:ARG:HH12	1.76	0.49
1:X:288:ALA:CB	1:X:292:GLU:CD	2.84	0.49
1:X:377:ALA:O	1:X:381:VAL:N	2.41	0.49
1:X:385:ASN:CG	1:X:388:VAL:HG13	2.37	0.49
1:X:409:LEU:H	1:X:409:LEU:CD2	2.09	0.49
1:X:526:LEU:O	1:X:530:ASP:HB2	2.11	0.49
1:X:27:LEU:CD1	1:X:28:THR:CG2	2.88	0.49
1:X:141:ASP:HA	1:X:144:LYS:NZ	2.26	0.49
1:X:189:THR:O	1:X:193:ILE:HG12	2.12	0.49
1:X:458:PHE:HB2	1:X:472:ASN:ND2	2.27	0.49
1:X:73:LYS:HG2	1:X:74:LYS:H	1.77	0.49
1:X:247:PHE:HE1	1:X:253:ILE:HG12	1.70	0.49
1:X:459:GLU:HG2	1:X:461:PHE:CE1	2.48	0.49
1:X:166:MET:CG	1:X:448:TYR:CD2	2.96	0.49
1:X:485:HIS:CD2	1:X:489:LEU:HD12	2.47	0.49
1:X:2:ASN:HB3	1:X:4:ILE:HD13	1.94	0.49
1:X:139:MET:O	1:X:140:VAL:C	2.55	0.49
1:X:691:GLY:C	1:X:692:PHE:CG	2.91	0.49
1:X:739:PHE:CZ	1:X:744:ILE:HD11	2.48	0.49
1:X:173:GLN:HB2	1:X:450:ILE:HD13	1.95	0.49
1:X:353:HIS:O	1:X:355:GLY:N	2.46	0.49
1:X:361:LYS:HG2	1:X:411:VAL:HG21	1.95	0.49
1:X:409:LEU:H	1:X:409:LEU:HD13	1.78	0.49
1:X:561:PRO:HD3	1:X:568:PHE:HA	1.94	0.49
1:X:336:PHE:HD1	1:X:340:GLU:CD	2.20	0.48
1:X:696:ILE:HG13	1:X:698:TYR:H	1.78	0.48
1:X:713:PRO:HG2	1:X:716:ALA:HB2	1.94	0.48
1:X:172:ASN:O	1:X:648:THR:HB	2.13	0.48
1:X:397:ARG:HD2	1:X:404:LEU:HG	1.94	0.48
1:X:584:TRP:CD1	4:X:2190:HOH:O	2.65	0.48
1:X:642:MET:C	1:X:644:THR:H	2.20	0.48
1:X:738:ARG:O	1:X:745:PHE:CE2	2.66	0.48
1:X:45:ASP:OD1	1:X:677:ARG:NH2	2.36	0.48
1:X:582:GLN:O	4:X:2190:HOH:O	2.20	0.48
1:X:8:THR:CG2	1:X:9:SER:N	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:11:TYR:CD1	1:X:15:LEU:HD12	2.48	0.48
1:X:213:GLN:CG	4:X:2078:HOH:O	2.52	0.48
1:X:359:PHE:C	4:X:2127:HOH:O	2.55	0.48
1:X:529:LEU:HD23	1:X:529:LEU:O	2.14	0.48
1:X:577:VAL:HG11	1:X:579:TYR:OH	2.13	0.48
1:X:668:GLU:C	1:X:670:LYS:N	2.71	0.48
1:X:708:LEU:HD22	1:X:730:LEU:HD21	1.96	0.48
1:X:166:MET:HE1	1:X:247:PHE:HD2	1.78	0.48
1:X:529:LEU:HD23	1:X:529:LEU:C	2.39	0.48
1:X:736:GLN:O	1:X:747:ARG:CA	2.62	0.48
1:X:389:LEU:O	1:X:393:LEU:HB2	2.13	0.48
1:X:515:ASP:HA	1:X:518:ASP:OD1	2.14	0.48
1:X:385:ASN:HA	1:X:386:PRO:HD3	1.70	0.48
1:X:547:LEU:O	1:X:558:TYR:OH	2.32	0.48
1:X:8:THR:O	1:X:9:SER:C	2.56	0.47
1:X:274:THR:C	4:X:2099:HOH:O	2.54	0.47
1:X:472:ASN:O	1:X:473:TYR:C	2.56	0.47
1:X:706:TYR:HD2	4:X:2219:HOH:O	1.74	0.47
1:X:737:TYR:HB2	1:X:747:ARG:H	1.78	0.47
1:X:89:GLU:HG3	1:X:109:ARG:HH12	1.78	0.47
1:X:132:ILE:HD13	4:X:2050:HOH:O	2.03	0.47
1:X:187:GLU:HB3	4:X:2068:HOH:O	2.08	0.47
1:X:265:LYS:O	1:X:268:VAL:CG1	2.58	0.47
1:X:692:PHE:CD2	1:X:748:ALA:N	2.82	0.47
1:X:727:LEU:O	1:X:731:ASN:HA	2.14	0.47
1:X:734:PRO:CD	4:X:2241:HOH:O	2.59	0.47
1:X:22:SER:N	4:X:2012:HOH:O	2.41	0.47
1:X:23:ASP:OD1	1:X:23:ASP:N	2.46	0.47
1:X:66:ASP:HB2	1:X:68:GLN:OE1	2.14	0.47
1:X:569:GLY:HA2	1:X:577:VAL:O	2.13	0.47
1:X:378:ALA:O	1:X:379:SER:C	2.57	0.47
1:X:689:ARG:HG3	1:X:693:PRO:HG3	1.92	0.47
1:X:736:GLN:HA	1:X:747:ARG:HD2	1.95	0.47
1:X:85:PHE:N	1:X:85:PHE:CD1	2.81	0.47
1:X:377:ALA:HA	1:X:380:THR:OG1	2.15	0.47
1:X:84:LYS:HB3	1:X:755:GLU:OE2	2.14	0.47
1:X:395:GLU:HG3	1:X:408:HIS:CG	2.49	0.47
1:X:458:PHE:C	4:X:2148:HOH:O	2.57	0.47
1:X:572:HIS:C	1:X:574:ALA:N	2.71	0.47
1:X:739:PHE:CE1	1:X:744:ILE:HD11	2.50	0.47
1:X:14:TYR:CB	4:X:2004:HOH:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:254:SER:OG	1:X:255:GLY:N	2.41	0.47
1:X:276:ARG:HG2	1:X:277:ASN:N	2.30	0.47
1:X:544:ILE:HD13	1:X:581:ILE:CD1	2.41	0.47
1:X:564:SER:OG	1:X:567:GLU:HG3	2.15	0.47
1:X:600:PHE:C	1:X:602:ASP:H	2.23	0.47
1:X:622:LYS:C	1:X:628:ILE:HD11	2.40	0.47
1:X:698:TYR:OH	1:X:719:SER:C	2.57	0.47
2:X:1001:ADP:C2	4:X:2256:HOH:O	2.55	0.47
1:X:85:PHE:HA	4:X:2039:HOH:O	2.09	0.47
1:X:347:ILE:HD12	1:X:608:VAL:HG23	1.96	0.47
1:X:47:TYR:CD1	1:X:47:TYR:N	2.82	0.47
1:X:74:LYS:HD3	4:X:2029:HOH:O	2.15	0.47
1:X:390:GLU:O	1:X:393:LEU:N	2.48	0.47
1:X:550:HIS:O	1:X:554:LYS:HG3	2.15	0.47
1:X:559:GLU:OE2	1:X:560:GLU:O	2.33	0.47
1:X:756:GLU:O	1:X:756:GLU:HG3	2.15	0.47
1:X:81:ASN:ND2	1:X:101:ALA:HB1	2.29	0.47
1:X:328:ARG:HG2	1:X:341:GLN:OE1	2.15	0.47
1:X:523:PRO:HB3	1:X:527:ALA:HB1	1.97	0.47
1:X:544:ILE:HD13	1:X:581:ILE:HG12	1.79	0.47
1:X:735:GLU:HA	1:X:738:ARG:NH1	2.30	0.47
1:X:432:TRP:NE1	1:X:610:LYS:CE	2.78	0.46
1:X:689:ARG:CG	1:X:693:PRO:CG	2.90	0.46
1:X:223:GLU:HG3	1:X:227:ASN:HD22	1.80	0.46
1:X:398:ILE:HD13	1:X:407:GLN:CD	2.39	0.46
1:X:703:LYS:O	4:X:2219:HOH:O	2.15	0.46
1:X:706:TYR:CE1	1:X:714:ARG:N	2.83	0.46
1:X:33:ARG:HH22	1:X:753:ARG:HA	1.80	0.46
1:X:420:ALA:HB1	1:X:592:LEU:HD13	1.97	0.46
1:X:477:LYS:HG3	1:X:638:LEU:HD21	1.98	0.46
1:X:671:VAL:O	1:X:675:GLN:HG3	2.16	0.46
1:X:696:ILE:HD11	1:X:701:PHE:HB2	1.97	0.46
1:X:706:TYR:OH	1:X:714:ARG:HG3	2.16	0.46
1:X:733:ASP:OD1	1:X:734:PRO:N	2.48	0.46
1:X:736:GLN:OE1	1:X:747:ARG:HD3	2.15	0.46
1:X:42:LYS:HG3	1:X:43:GLU:N	2.31	0.46
1:X:60:PHE:HE1	1:X:74:LYS:HZ2	1.61	0.46
1:X:745:PHE:HE1	4:X:2157:HOH:O	1.95	0.46
1:X:116:TYR:HE2	1:X:134:ILE:HD12	1.80	0.46
1:X:460:ILE:C	1:X:461:PHE:CD1	2.94	0.46
1:X:731:ASN:ND2	1:X:731:ASN:C	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:83:ILE:C	1:X:85:PHE:N	2.69	0.46
1:X:341:GLN:O	1:X:345:PHE:HD2	1.97	0.46
1:X:398:ILE:HD12	1:X:398:ILE:N	2.31	0.46
1:X:425:LEU:O	1:X:429:LEU:CB	2.64	0.46
1:X:11:TYR:HD1	1:X:15:LEU:HD12	1.81	0.46
1:X:120:GLY:CA	4:X:2049:HOH:O	2.64	0.46
1:X:347:ILE:HD11	1:X:605:ASP:OD2	2.16	0.46
1:X:747:ARG:HG2	1:X:750:GLN:H	1.81	0.46
1:X:83:ILE:HD13	1:X:86:ASP:OD2	2.16	0.46
1:X:712:VAL:HG22	1:X:722:ALA:O	2.16	0.46
1:X:52:ILE:CG2	1:X:55:GLU:OE2	2.63	0.46
1:X:136:THR:HG23	4:X:2051:HOH:O	2.15	0.46
1:X:159:SER:O	1:X:163:TYR:N	2.49	0.46
1:X:188:ASN:C	1:X:190:LYS:N	2.73	0.46
1:X:389:LEU:O	1:X:389:LEU:HD23	2.16	0.46
1:X:559:GLU:C	1:X:559:GLU:CD	2.84	0.46
1:X:710:PRO:CG	4:X:2221:HOH:O	2.61	0.46
1:X:752:ALA:HB1	1:X:756:GLU:HG2	1.98	0.46
1:X:306:TYR:C	1:X:307:LEU:HD12	2.41	0.46
1:X:313:VAL:CG2	1:X:314:ASP:N	2.48	0.46
1:X:348:ILE:HG13	1:X:349:ALA:H	1.80	0.46
1:X:121:LEU:O	4:X:2048:HOH:O	2.11	0.45
1:X:148:ARG:HA	4:X:2058:HOH:O	2.16	0.45
1:X:249:SER:C	4:X:2063:HOH:O	2.56	0.45
1:X:540:ASP:O	1:X:541:ASN:C	2.58	0.45
1:X:724:ASP:CB	4:X:2235:HOH:O	2.31	0.45
1:X:188:ASN:O	1:X:191:LYS:N	2.47	0.45
1:X:345:PHE:CA	1:X:348:ILE:HG12	2.38	0.45
1:X:22:SER:HB2	4:X:2012:HOH:O	2.16	0.45
1:X:276:ARG:HG3	1:X:282:TYR:OH	2.14	0.45
1:X:396:PRO:O	1:X:398:ILE:CD1	2.65	0.45
1:X:428:ARG:O	1:X:611:LEU:HD21	2.16	0.45
1:X:668:GLU:CD	1:X:670:LYS:CE	2.89	0.45
1:X:739:PHE:CD1	1:X:744:ILE:HG13	2.51	0.45
1:X:15:LEU:HD21	1:X:134:ILE:HB	1.97	0.45
1:X:84:LYS:HZ1	1:X:704:ARG:CD	2.25	0.45
1:X:187:GLU:HB2	4:X:2068:HOH:O	2.11	0.45
1:X:215:ILE:HA	1:X:441:LEU:HD11	1.98	0.45
1:X:300:GLY:O	1:X:302:GLU:N	2.49	0.45
1:X:361:LYS:HD2	1:X:361:LYS:H	1.82	0.45
1:X:720:GLN:NE2	1:X:741:ILE:HG13	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:85:PHE:HE1	1:X:755:GLU:CD	2.25	0.45
1:X:375:LEU:C	1:X:377:ALA:N	2.71	0.45
1:X:546:LYS:NZ	1:X:550:HIS:CE1	2.77	0.45
1:X:79:GLN:N	4:X:2036:HOH:O	2.28	0.45
1:X:144:LYS:NZ	1:X:144:LYS:CB	2.80	0.45
1:X:193:ILE:HG23	1:X:245:ILE:HD11	1.98	0.45
1:X:276:ARG:CD	1:X:282:TYR:CE2	3.00	0.45
1:X:752:ALA:HA	1:X:755:GLU:HB3	1.99	0.45
1:X:36:TRP:N	1:X:78:ASN:O	2.47	0.45
1:X:40:ASP:C	1:X:42:LYS:N	2.74	0.45
1:X:423:LYS:O	1:X:427:GLY:N	2.43	0.45
1:X:650:PRO:HB2	1:X:652:PHE:CZ	2.52	0.45
1:X:7:ARG:NH1	4:X:2003:HOH:O	2.25	0.45
1:X:211:LEU:HA	1:X:214:GLN:OE1	2.16	0.45
1:X:491:GLN:C	1:X:491:GLN:CD	2.85	0.45
1:X:90:ASP:OD1	1:X:118:TYR:HB3	2.17	0.45
1:X:166:MET:SD	1:X:448:TYR:HB2	2.54	0.45
1:X:747:ARG:HG2	1:X:750:GLN:O	2.16	0.45
1:X:60:PHE:HD1	1:X:60:PHE:HA	1.65	0.45
1:X:85:PHE:O	1:X:86:ASP:C	2.59	0.45
1:X:91:MET:SD	1:X:117:THR:HG21	2.57	0.45
1:X:264:GLU:HG3	1:X:267:ARG:CB	2.47	0.45
1:X:267:ARG:O	1:X:268:VAL:C	2.59	0.45
1:X:291:GLU:O	1:X:295:ALA:HB2	2.16	0.45
1:X:583:ASP:O	1:X:584:TRP:C	2.60	0.45
1:X:641:LEU:O	1:X:644:THR:CB	2.63	0.45
1:X:654:ARG:CB	1:X:681:VAL:CG1	2.95	0.45
1:X:671:VAL:HG12	1:X:675:GLN:NE2	2.32	0.45
1:X:64:THR:CG2	1:X:68:GLN:HB2	2.48	0.44
1:X:128:PRO:O	1:X:129:PHE:HB2	2.18	0.44
1:X:463:VAL:O	1:X:463:VAL:HG23	2.16	0.44
1:X:477:LYS:HD2	1:X:514:ILE:HD12	1.98	0.44
1:X:520:ARG:O	1:X:523:PRO:CG	2.59	0.44
1:X:14:TYR:CE2	4:X:2005:HOH:O	2.42	0.44
1:X:365:GLU:OE1	1:X:365:GLU:HA	2.17	0.44
1:X:455:ILE:HG13	1:X:456:SER:N	2.33	0.44
1:X:702:VAL:HG11	1:X:719:SER:OG	2.17	0.44
1:X:702:VAL:HG21	1:X:719:SER:OG	2.17	0.44
1:X:132:ILE:HG22	1:X:133:PRO:HD2	1.97	0.44
1:X:180:GLU:CD	1:X:675:GLN:HG2	2.42	0.44
1:X:379:SER:HB2	1:X:386:PRO:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:620:ARG:NH1	1:X:628:ILE:O	2.24	0.44
1:X:654:ARG:CB	1:X:681:VAL:HG11	2.47	0.44
1:X:4:ILE:HD11	1:X:146:ARG:HH12	1.82	0.44
1:X:14:TYR:OH	1:X:133:PRO:HG3	2.17	0.44
1:X:15:LEU:CD1	1:X:143:PHE:HZ	2.29	0.44
1:X:223:GLU:O	1:X:227:ASN:HB2	2.17	0.44
1:X:246:GLN:O	1:X:247:PHE:HD1	2.00	0.44
1:X:294:LYS:C	1:X:296:LEU:N	2.74	0.44
1:X:530:ASP:OD1	1:X:629:THR:OG1	2.33	0.44
1:X:746:PHE:O	1:X:747:ARG:O	2.35	0.44
1:X:96:TYR:HE2	4:X:2042:HOH:O	1.99	0.44
1:X:189:THR:HG23	1:X:452:VAL:HG11	1.99	0.44
1:X:717:GLU:HG3	1:X:718:ASP:N	2.32	0.44
1:X:53:VAL:HG21	1:X:62:PHE:O	2.17	0.44
1:X:184:GLY:HA2	2:X:1001:ADP:O1A	2.18	0.44
1:X:431:LEU:O	1:X:435:LYS:HG2	2.17	0.44
1:X:2:ASN:HB2	1:X:5:HIS:NE2	2.32	0.44
1:X:239:PHE:CD1	1:X:240:GLY:O	2.59	0.44
1:X:395:GLU:HG2	1:X:407:GLN:O	2.17	0.44
1:X:448:TYR:N	1:X:448:TYR:CD1	2.86	0.44
1:X:466:PHE:O	1:X:467:GLU:C	2.60	0.44
1:X:747:ARG:N	4:X:2250:HOH:O	2.51	0.44
1:X:122:PHE:CE2	1:X:681:VAL:HA	2.53	0.44
1:X:294:LYS:O	1:X:296:LEU:N	2.50	0.44
1:X:344:ILE:O	1:X:348:ILE:HG23	2.18	0.44
1:X:689:ARG:CG	1:X:693:PRO:HG3	2.48	0.44
1:X:703:LYS:CB	4:X:2224:HOH:O	2.65	0.44
1:X:747:ARG:HB2	4:X:2250:HOH:O	2.00	0.44
1:X:283:GLN:OE1	1:X:323:GLU:OE1	2.36	0.44
1:X:497:GLU:O	1:X:498:LYS:CB	2.64	0.44
1:X:516:LEU:O	1:X:525:ILE:HG12	2.18	0.44
1:X:737:TYR:CD1	1:X:739:PHE:CD1	3.05	0.44
1:X:35:ILE:CG1	1:X:78:ASN:O	2.66	0.43
1:X:129:PHE:CE2	1:X:662:GLN:HA	2.53	0.43
1:X:285:LEU:HD21	1:X:298:LEU:HD22	1.99	0.43
1:X:410:ASN:OD1	1:X:412:GLU:N	2.44	0.43
1:X:410:ASN:C	1:X:412:GLU:H	2.26	0.43
1:X:410:ASN:C	1:X:412:GLU:N	2.75	0.43
1:X:449:PHE:CZ	1:X:648:THR:HG22	2.48	0.43
1:X:708:LEU:N	1:X:759:GLU:OXT	2.50	0.43
1:X:750:GLN:O	1:X:750:GLN:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:16:LYS:C	1:X:18:LYS:N	2.75	0.43
1:X:37:TYR:CE1	1:X:39:PRO:HG3	2.54	0.43
1:X:109:ARG:HE	1:X:109:ARG:HB3	1.66	0.43
1:X:336:PHE:HD1	1:X:336:PHE:HA	1.58	0.43
1:X:469:LEU:HD22	1:X:584:TRP:HH2	1.83	0.43
1:X:704:ARG:O	1:X:704:ARG:HG3	2.18	0.43
1:X:37:TYR:CD1	1:X:37:TYR:C	2.97	0.43
1:X:53:VAL:N	1:X:61:THR:OG1	2.46	0.43
1:X:273:GLU:HA	1:X:310:SER:O	2.18	0.43
1:X:102:VAL:O	1:X:106:LEU:HD22	2.19	0.43
1:X:274:THR:CG2	4:X:2098:HOH:O	2.54	0.43
1:X:363:ALA:O	1:X:364:GLY:C	2.60	0.43
1:X:614:ASP:HA	1:X:615:PRO:HD2	1.87	0.43
1:X:672:VAL:O	1:X:676:LEU:HD22	2.12	0.43
1:X:424:ALA:O	1:X:428:ARG:CG	2.67	0.43
1:X:449:PHE:CE1	1:X:648:THR:HG21	2.44	0.43
1:X:491:GLN:HA	1:X:494:TYR:HB2	2.01	0.43
1:X:697:ILE:O	1:X:698:TYR:HB3	2.19	0.43
1:X:11:TYR:CE1	1:X:152:ALA:HB2	2.54	0.43
1:X:217:GLN:HB3	1:X:330:ALA:CB	2.47	0.43
1:X:250:ALA:N	4:X:2094:HOH:O	2.51	0.43
1:X:590:ASP:O	1:X:590:ASP:CG	2.49	0.43
1:X:315:ILE:HG21	1:X:318:VAL:HG21	2.01	0.43
1:X:474:THR:C	1:X:476:GLU:H	2.27	0.43
1:X:522:PRO:HA	1:X:523:PRO:HD3	1.72	0.43
1:X:577:VAL:HG13	1:X:577:VAL:O	2.17	0.43
1:X:587:LYS:O	1:X:590:ASP:HB2	2.18	0.43
1:X:361:LYS:O	1:X:361:LYS:HD3	2.11	0.43
1:X:501:TRP:CZ2	1:X:738:ARG:HG3	2.54	0.43
1:X:597:GLU:O	1:X:601:LYS:HG3	2.19	0.43
1:X:664:PRO:O	1:X:665:ALA:CB	2.66	0.43
1:X:689:ARG:HD2	1:X:693:PRO:HG3	1.99	0.43
1:X:62:PHE:CZ	1:X:72:VAL:HG12	2.54	0.43
1:X:72:VAL:HG22	1:X:73:LYS:H	1.84	0.43
1:X:210:VAL:HG12	1:X:214:GLN:OE1	2.19	0.43
1:X:629:THR:O	1:X:632:ALA:HB3	2.19	0.43
1:X:17:VAL:O	1:X:18:LYS:CB	2.66	0.43
1:X:37:TYR:OH	1:X:64:THR:HB	2.19	0.43
1:X:73:LYS:HE2	1:X:75:ASP:HB2	2.01	0.43
1:X:108:VAL:O	1:X:111:ASN:CB	2.64	0.43
1:X:197:ALA:O	1:X:201:GLY:HA3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:247:PHE:O	1:X:447:ALA:O	2.37	0.43
1:X:615:PRO:C	1:X:617:ILE:N	2.70	0.43
1:X:687:ILE:O	1:X:690:LYS:CB	2.64	0.43
1:X:739:PHE:CD2	1:X:744:ILE:CD1	3.01	0.43
1:X:146:ARG:HD3	1:X:151:VAL:CG1	2.49	0.42
1:X:273:GLU:C	1:X:274:THR:HG22	2.31	0.42
1:X:360:GLU:O	1:X:367:ALA:HB1	2.18	0.42
1:X:35:ILE:CD1	1:X:77:ALA:HB3	2.36	0.42
1:X:83:ILE:O	1:X:84:LYS:C	2.62	0.42
1:X:421:LEU:O	1:X:425:LEU:HD22	2.13	0.42
1:X:521:GLN:HA	1:X:522:PRO:HA	1.76	0.42
1:X:595:ASP:HA	1:X:598:LEU:HB3	2.00	0.42
1:X:122:PHE:CD1	1:X:654:ARG:HG3	2.50	0.42
1:X:276:ARG:HD2	1:X:282:TYR:CE1	2.54	0.42
1:X:516:LEU:HD23	1:X:555:ASN:HD22	1.84	0.42
1:X:692:PHE:CE2	1:X:747:ARG:NH2	2.80	0.42
1:X:2:ASN:O	1:X:5:HIS:CD2	2.73	0.42
1:X:60:PHE:CE1	1:X:74:LYS:NZ	2.85	0.42
1:X:351:ILE:HD11	1:X:425:LEU:HB2	2.00	0.42
1:X:529:LEU:HD22	1:X:588:ASN:ND2	2.29	0.42
1:X:614:ASP:C	1:X:616:ASN:H	2.27	0.42
1:X:664:PRO:HA	4:X:2044:HOH:O	2.19	0.42
1:X:667:LEU:CD1	1:X:672:VAL:HG21	2.47	0.42
1:X:683:GLU:O	1:X:683:GLU:HG3	2.19	0.42
1:X:702:VAL:HG21	1:X:719:SER:CB	2.49	0.42
1:X:25:PHE:O	1:X:25:PHE:CG	2.71	0.42
1:X:372:LYS:N	4:X:2129:HOH:O	2.37	0.42
1:X:544:ILE:CG1	1:X:581:ILE:HG13	2.47	0.42
1:X:692:PHE:CE2	1:X:737:TYR:HA	2.54	0.42
1:X:88:VAL:HG22	1:X:105:ASN:HD21	1.84	0.42
1:X:166:MET:HG3	1:X:448:TYR:HD2	1.84	0.42
1:X:389:LEU:C	1:X:389:LEU:HD23	2.43	0.42
1:X:645:LEU:C	1:X:647:THR:H	2.28	0.42
1:X:697:ILE:O	1:X:697:ILE:HG12	2.20	0.42
1:X:35:ILE:O	1:X:50:GLY:N	2.43	0.42
1:X:479:GLN:HG3	4:X:2171:HOH:O	2.19	0.42
1:X:531:GLU:O	1:X:535:PHE:CE1	2.73	0.42
1:X:687:ILE:HD12	1:X:687:ILE:HA	1.91	0.42
1:X:35:ILE:HD11	1:X:77:ALA:C	2.45	0.42
1:X:172:ASN:N	4:X:2067:HOH:O	2.47	0.42
1:X:384:VAL:CG1	1:X:385:ASN:H	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:480:GLN:NE2	1:X:511:GLN:OE1	2.53	0.42
1:X:517:ILE:HA	1:X:525:ILE:HG12	2.01	0.42
1:X:548:HIS:CG	1:X:560:GLU:HG3	2.55	0.42
1:X:751:LEU:CA	4:X:2252:HOH:O	2.17	0.42
1:X:47:TYR:CE1	1:X:673:LEU:HD21	2.55	0.42
1:X:264:GLU:CG	1:X:267:ARG:HB2	2.50	0.42
1:X:454:ASP:OD1	1:X:454:ASP:O	2.38	0.42
1:X:695:ARG:CG	1:X:745:PHE:CD1	3.02	0.42
1:X:712:VAL:HG23	1:X:725:ALA:HB3	2.02	0.42
1:X:76:ASP:CG	4:X:2032:HOH:O	2.61	0.42
1:X:375:LEU:O	1:X:377:ALA:N	2.52	0.42
1:X:516:LEU:C	1:X:516:LEU:HD13	2.45	0.42
1:X:529:LEU:C	1:X:529:LEU:CD2	2.93	0.41
1:X:732:ILE:N	1:X:732:ILE:CD1	2.78	0.41
1:X:219:ASN:O	1:X:221:ILE:N	2.52	0.41
1:X:296:LEU:HD11	1:X:298:LEU:HD12	1.90	0.41
1:X:361:LYS:HB3	1:X:411:VAL:HG13	2.01	0.41
1:X:476:GLU:HG3	1:X:514:ILE:HD11	2.02	0.41
1:X:745:PHE:CD1	1:X:745:PHE:N	2.88	0.41
1:X:33:ARG:NH1	1:X:753:ARG:NH1	2.67	0.41
1:X:84:LYS:CB	1:X:755:GLU:OE2	2.69	0.41
1:X:112:GLN:O	1:X:113:ASP:CB	2.67	0.41
1:X:265:LYS:HB3	1:X:423:LYS:HD3	2.01	0.41
1:X:391:LYS:HB2	1:X:391:LYS:NZ	2.35	0.41
1:X:466:PHE:HB2	1:X:584:TRP:NE1	2.35	0.41
1:X:721:LYS:O	1:X:721:LYS:HD3	2.20	0.41
1:X:89:GLU:HG2	1:X:153:PRO:HD3	2.02	0.41
1:X:91:MET:O	1:X:94:LEU:HG	2.19	0.41
1:X:92:SER:C	1:X:94:LEU:H	2.28	0.41
1:X:213:GLN:HE22	1:X:333:ILE:HD12	1.81	0.41
1:X:398:ILE:CB	1:X:407:GLN:NE2	2.82	0.41
1:X:52:ILE:HG22	1:X:55:GLU:OE2	2.21	0.41
1:X:58:ASP:OD1	1:X:58:ASP:O	2.38	0.41
1:X:308:ASN:C	1:X:310:SER:N	2.78	0.41
1:X:358:LYS:HE3	1:X:359:PHE:O	2.20	0.41
1:X:6:ASP:OD1	1:X:8:THR:HG22	2.21	0.41
1:X:172:ASN:HB3	1:X:449:PHE:CD1	2.55	0.41
1:X:387:SER:OG	1:X:388:VAL:N	2.54	0.41
1:X:430:PHE:CD1	1:X:430:PHE:C	2.99	0.41
1:X:466:PHE:O	1:X:468:GLN:N	2.54	0.41
1:X:179:GLY:O	1:X:185:LYS:HE3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:223:GLU:HG3	1:X:227:ASN:ND2	2.35	0.41
1:X:263:LEU:HD11	1:X:430:PHE:CB	2.50	0.41
1:X:304:PHE:O	1:X:308:ASN:OD1	2.38	0.41
1:X:361:LYS:HD2	1:X:361:LYS:C	2.16	0.41
1:X:560:GLU:HG2	1:X:561:PRO:HD2	2.02	0.41
1:X:92:SER:C	1:X:94:LEU:N	2.78	0.41
1:X:132:ILE:CG2	1:X:133:PRO:HD2	2.50	0.41
1:X:147:ARG:HB2	1:X:150:GLU:CG	2.13	0.41
1:X:179:GLY:HA2	4:X:2213:HOH:O	2.20	0.41
1:X:197:ALA:O	1:X:201:GLY:CA	2.69	0.41
1:X:397:ARG:HG2	1:X:406:ALA:HB2	2.03	0.41
1:X:592:LEU:CD1	1:X:596:LEU:HD13	2.51	0.41
1:X:614:ASP:C	1:X:616:ASN:N	2.78	0.41
1:X:687:ILE:HG23	1:X:688:THR:N	2.36	0.41
1:X:692:PHE:HD2	1:X:747:ARG:C	2.29	0.41
1:X:76:ASP:HB3	4:X:2032:HOH:O	2.15	0.41
1:X:84:LYS:HE3	1:X:704:ARG:HD2	1.97	0.41
1:X:172:ASN:CB	1:X:449:PHE:CZ	2.99	0.41
1:X:239:PHE:CE2	1:X:430:PHE:CE2	3.08	0.41
1:X:245:ILE:HG22	1:X:247:PHE:CE1	2.55	0.41
1:X:331:MET:CG	1:X:336:PHE:CD2	3.00	0.41
1:X:353:HIS:C	1:X:355:GLY:H	2.26	0.41
1:X:474:THR:HG22	1:X:478:LEU:CD1	2.50	0.41
1:X:532:GLN:OE1	1:X:543:LEU:HB2	2.21	0.41
1:X:196:LEU:HD13	1:X:245:ILE:CD1	2.50	0.41
1:X:345:PHE:CA	1:X:348:ILE:CG1	2.97	0.41
1:X:360:GLU:O	1:X:367:ALA:HA	2.20	0.41
1:X:595:ASP:HA	1:X:598:LEU:HB2	2.03	0.41
1:X:668:GLU:HB3	1:X:670:LYS:CG	2.39	0.41
1:X:6:ASP:OD2	1:X:9:SER:HB3	2.21	0.40
1:X:399:LEU:HA	1:X:403:ASP:O	2.21	0.40
1:X:611:LEU:HD23	1:X:611:LEU:HA	1.93	0.40
1:X:154:HIS:CE1	1:X:156:PHE:H	2.39	0.40
1:X:174:SER:HA	1:X:451:GLY:O	2.21	0.40
1:X:213:GLN:N	4:X:2078:HOH:O	2.54	0.40
1:X:217:GLN:C	1:X:220:PRO:HD2	2.46	0.40
1:X:331:MET:HB3	1:X:336:PHE:CB	2.51	0.40
1:X:333:ILE:C	1:X:335:GLY:H	2.29	0.40
1:X:390:GLU:C	1:X:393:LEU:H	2.29	0.40
1:X:410:ASN:ND2	1:X:412:GLU:HG2	2.36	0.40
1:X:615:PRO:C	1:X:617:ILE:H	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:701:PHE:O	1:X:704:ARG:N	2.54	0.40
1:X:734:PRO:O	1:X:738:ARG:CZ	2.69	0.40
1:X:735:GLU:HA	1:X:738:ARG:CZ	2.51	0.40
1:X:212:GLU:O	1:X:216:LEU:CD1	2.70	0.40
1:X:348:ILE:O	1:X:351:ILE:N	2.48	0.40
1:X:361:LYS:CG	1:X:411:VAL:CG1	2.96	0.40
1:X:428:ARG:C	1:X:611:LEU:HD11	2.46	0.40
1:X:449:PHE:CD1	1:X:449:PHE:C	2.99	0.40
1:X:223:GLU:CG	1:X:227:ASN:HD22	2.34	0.40
1:X:336:PHE:HA	1:X:340:GLU:OE1	2.20	0.40
1:X:350:GLY:HA3	1:X:382:PHE:CZ	2.56	0.40
1:X:192:VAL:O	1:X:193:ILE:C	2.65	0.40
1:X:285:LEU:CD2	1:X:298:LEU:HD22	2.51	0.40
1:X:315:ILE:HB	1:X:318:VAL:HB	2.04	0.40
1:X:354:LEU:HD21	1:X:378:ALA:CB	2.51	0.40
1:X:491:GLN:C	1:X:494:TYR:HB2	2.47	0.40
1:X:557:LYS:O	1:X:558:TYR:HB2	2.22	0.40
1:X:747:ARG:HG2	1:X:750:GLN:N	2.35	0.40

All (4) 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)
1:X:397:ARG:NH1	1:X:402:ARG:O[2_556]	1.10	1.10
1:X:204:GLN:O	1:X:273:GLU:OE2[1_455]	1.56	0.64
1:X:402:ARG:CG	4:X:2255:HOH:O[3_645]	1.93	0.27
4:X:2065:HOH:O	4:X:2149:HOH:O[1_455]	2.02	0.18

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	X	756/758 (100%)	617 (82%)	114 (15%)	25 (3%)	3	14

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	46	SER
1	X	297	HIS
1	X	448	TYR
1	X	540	ASP
1	X	623	LYS
1	X	625	ALA
1	X	690	LYS
1	X	295	ALA
1	X	747	ARG
1	X	757	ALA
1	X	93	GLU
1	X	189	THR
1	X	302	GLU
1	X	601	LYS
1	X	710	PRO
1	X	731	ASN
1	X	183	ALA
1	X	354	LEU
1	X	573	TYR
1	X	65	VAL
1	X	691	GLY
1	X	411	VAL
1	X	615	PRO
1	X	362	GLY
1	X	630	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	X	662/662 (100%)	631 (95%)	31 (5%)	23	51

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	4	ILE
1	X	26	LYS
1	X	29	VAL
1	X	60	PHE
1	X	73	LYS
1	X	88	VAL
1	X	144	LYS
1	X	215	ILE
1	X	238	ARG
1	X	243	ILE
1	X	336	PHE
1	X	344	ILE
1	X	357	ILE
1	X	361	LYS
1	X	391	LYS
1	X	397	ARG
1	X	409	LEU
1	X	411	VAL
1	X	454	ASP
1	X	468	GLN
1	X	487	PHE
1	X	496	LYS
1	X	506	PHE
1	X	525	ILE
1	X	553	LYS
1	X	554	LYS
1	X	586	GLU
1	X	608	VAL
1	X	646	GLU
1	X	702	VAL
1	X	745	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	111	ASN
1	X	171	GLN
1	X	173	GLN
1	X	213	GLN
1	X	227	ASN
1	X	234	ASN

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Mol	Chain	Res	Type
1	X	235	ASN
1	X	246	GLN
1	X	259	GLN
1	X	305	ASN
1	X	353	HIS
1	X	376	ASN
1	X	407	GLN
1	X	439	ASN
1	X	464	ASN
1	X	468	GLN
1	X	472	ASN
1	X	479	GLN
1	X	484	HIS
1	X	550	HIS
1	X	588	ASN
1	X	679	ASN
1	X	711	ASN
1	X	720	GLN
1	X	731	ASN
1	X	750	GLN

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](#)

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	$\# Z > 2$
2	ADP	X	1001	-	28,29,29	1.77	9 (32%)	43,45,45	2.02	12 (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
2	ADP	X	1001	-	-	0/16/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	1001	ADP	C2'-C3'	-4.12	1.42	1.53
2	X	1001	ADP	PA-O3A	-3.75	1.55	1.59
2	X	1001	ADP	C6-N6	3.14	1.42	1.34
2	X	1001	ADP	O4'-C4'	-2.72	1.38	1.45
2	X	1001	ADP	C3'-C4'	-2.66	1.46	1.53
2	X	1001	ADP	C2'-C1'	-2.51	1.45	1.53
2	X	1001	ADP	PA-O2A	-2.39	1.44	1.55
2	X	1001	ADP	O5'-C5'	-2.30	1.35	1.44
2	X	1001	ADP	C5-N7	-2.22	1.35	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	1001	ADP	C5-C4-N3	-5.47	119.19	126.72
2	X	1001	ADP	N3-C2-N1	-5.24	120.65	128.58
2	X	1001	ADP	N3-C4-N9	4.20	134.31	127.17
2	X	1001	ADP	C2-N3-C4	3.89	121.33	111.83
2	X	1001	ADP	N9-C8-N7	-3.36	109.18	113.94
2	X	1001	ADP	O2A-PA-O3A	3.26	116.08	107.27
2	X	1001	ADP	C4-N9-C8	2.75	108.62	105.74
2	X	1001	ADP	C5-N7-C8	2.73	107.74	103.45
2	X	1001	ADP	C4-C5-N7	-2.30	107.95	110.58
2	X	1001	ADP	C5'-C4'-C3'	-2.24	107.16	115.21
2	X	1001	ADP	C3'-C2'-C1'	2.22	105.66	101.46
2	X	1001	ADP	O3B-PB-O3A	2.09	111.65	104.64

There are no chirality outliers.

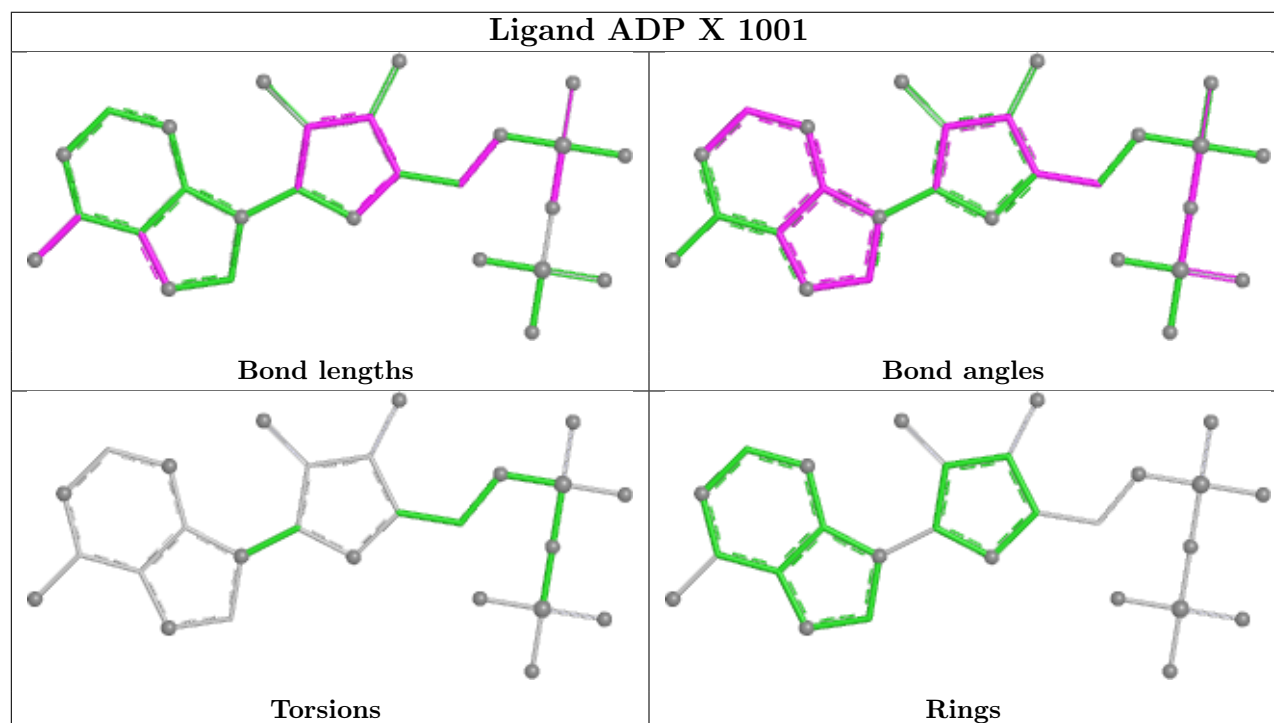
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	1001	ADP	5	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	755/758 (99%)	0.52	54 (7%) 21 11	2, 18, 71, 97	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	739	PHE	7.0
1	X	501	TRP	6.5
1	X	754	ILE	6.0
1	X	744	ILE	4.8
1	X	737	TYR	4.7
1	X	723	THR	4.4
1	X	693	PRO	4.4
1	X	493	GLU	4.2
1	X	755	GLU	4.1
1	X	497	GLU	3.7
1	X	261	TYR	3.7
1	X	726	VAL	3.5
1	X	756	GLU	3.4
1	X	623	LYS	3.4
1	X	713	PRO	3.3
1	X	752	ALA	3.3
1	X	625	ALA	3.3
1	X	745	PHE	3.2
1	X	113	ASP	3.1
1	X	730	LEU	3.0
1	X	732	ILE	3.0
1	X	3	PRO	3.0
1	X	729	HIS	2.9
1	X	701	PHE	2.9
1	X	180	GLU	2.9
1	X	759	GLU	2.9
1	X	505	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	X	494	TYR	2.8
1	X	312	CYS	2.8
1	X	725	ALA	2.7
1	X	602	ASP	2.7
1	X	499	ILE	2.7
1	X	702	VAL	2.7
1	X	727	LEU	2.7
1	X	65	VAL	2.6
1	X	696	ILE	2.6
1	X	724	ASP	2.6
1	X	247	PHE	2.5
1	X	705	TYR	2.5
1	X	173	GLN	2.5
1	X	743	LYS	2.4
1	X	443	GLN	2.3
1	X	248	ASN	2.3
1	X	59	SER	2.3
1	X	694	ASN	2.3
1	X	684	GLY	2.3
1	X	20	GLY	2.3
1	X	698	TYR	2.2
1	X	30	SER	2.2
1	X	539	THR	2.2
1	X	738	ARG	2.2
1	X	332	ASP	2.1
1	X	492	GLU	2.1
1	X	683	GLU	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.

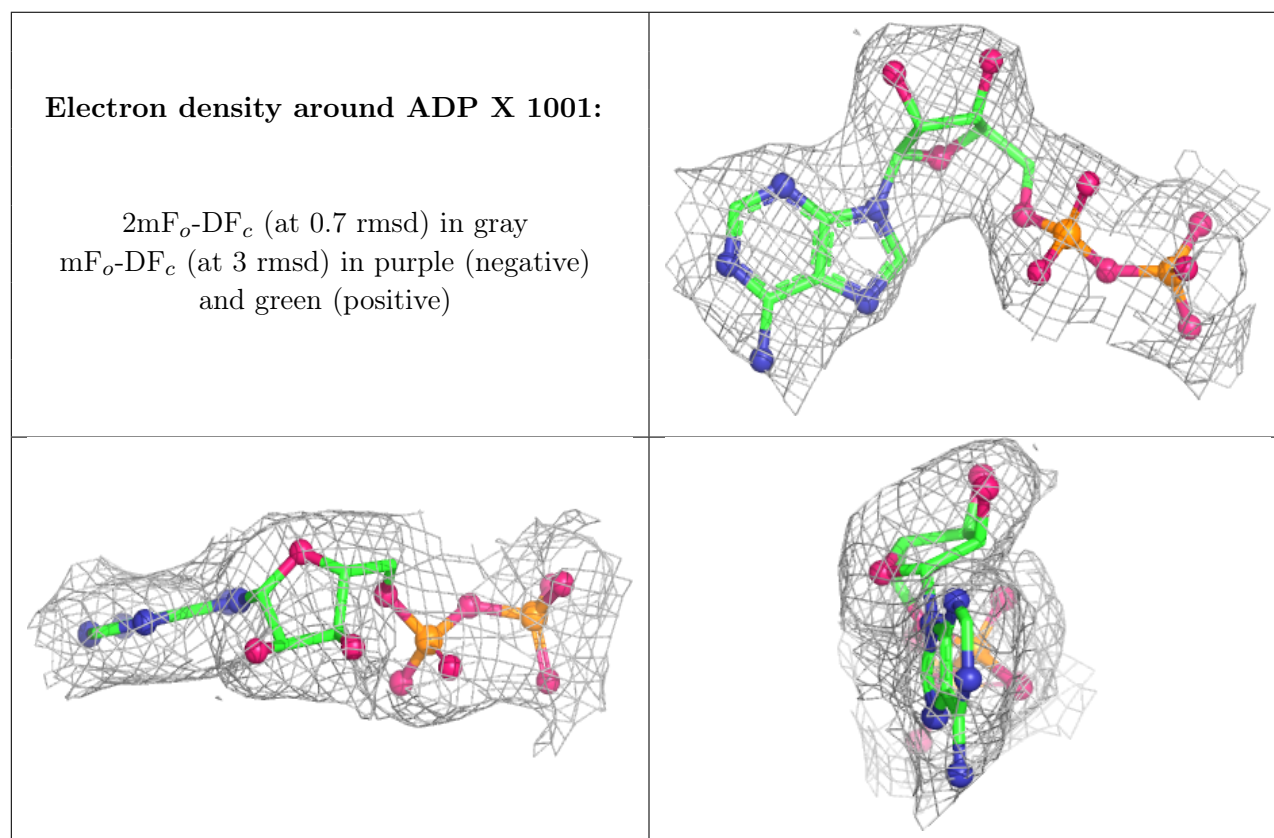
6.4 Ligands [i](#)

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	MG	X	1002	1/1	0.93	0.06	4,4,4,4	0
2	ADP	X	1001	27/27	0.95	0.10	4,8,12,13	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.