



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:57 AM UTC

PDB ID : 2JGU / pdb_00002jgu
Title : crystal structure of DNA-directed DNA polymerase
Authors : Kim, D.U.; Cho, H.S.
Deposited on : 2007-02-15
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

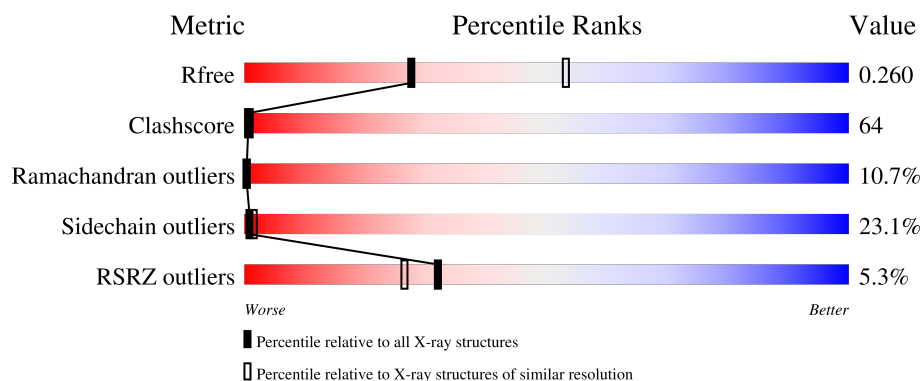
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	775	5% 22% 35% 27% 8% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5859 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 DNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	712	Total	C	N	O	S	0	0	1
			5826	3777	963	1072	14			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	LEU	ILE	conflict	UNP P61875
A	169	ARG	LYS	conflict	UNP P61875
A	183	SER	VAL	conflict	UNP P61875
A	186	THR	SER	conflict	UNP P61875
A	188	LYS	ARG	conflict	UNP P61875
A	265	ARG	THR	conflict	UNP P61875
A	266	THR	ARG	conflict	UNP P61875
A	406	TYR	PHE	conflict	UNP P61875
A	407	LYS	ARG	conflict	UNP P61875
A	408	SER	ALA	conflict	UNP P61875

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		

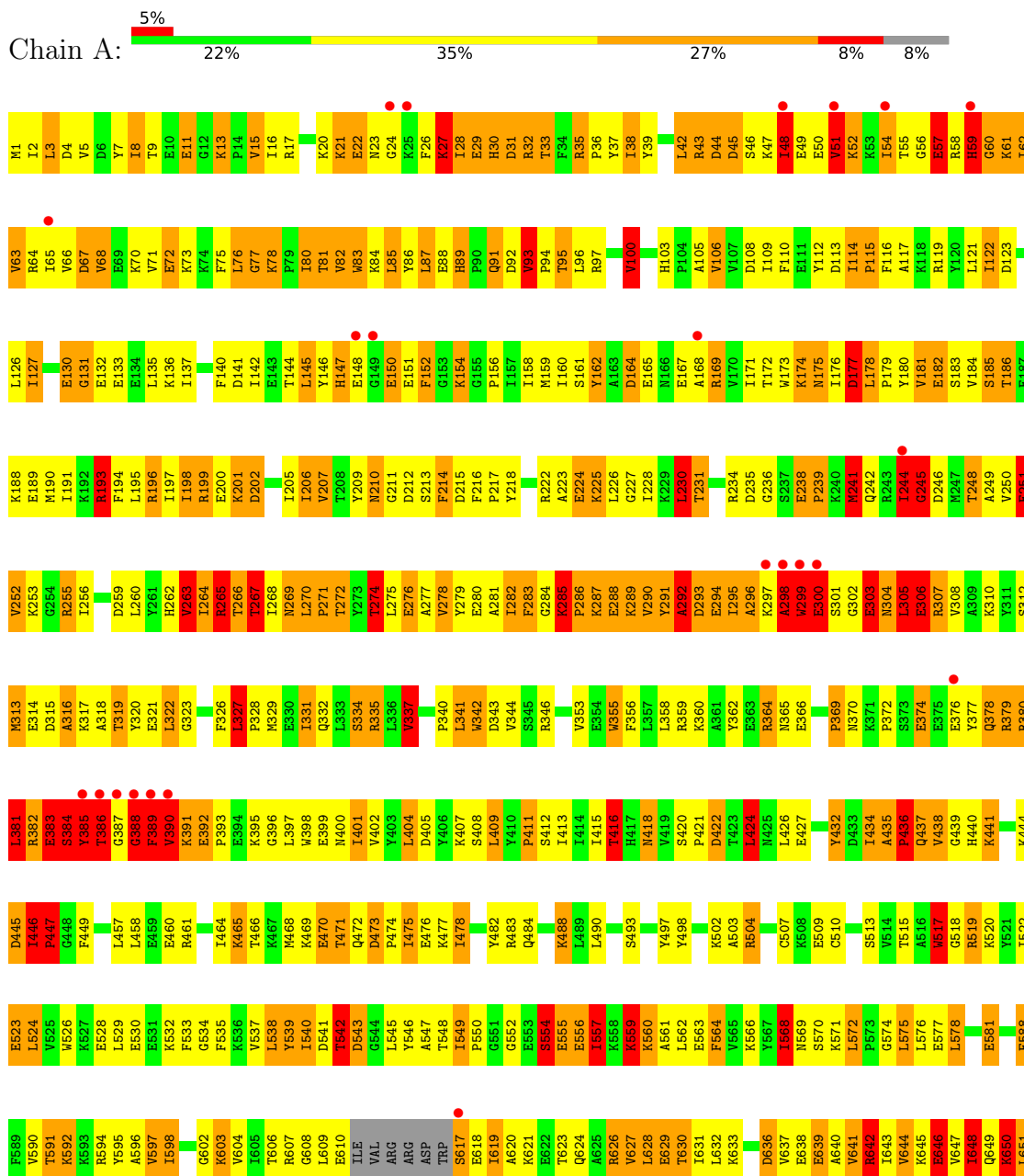
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	31	Total	O	0	0
			31	31		

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: DNA POLYMERASE



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.18Å 127.92Å 89.21Å 90.00° 109.11° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.2 (15.00-2.60) 93.6 (15.00-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.42Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.275 , 0.271 (Not available) , 0.260	Depositor DCC
R_{free} test set	1413 reflections (4.16%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5859	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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: MN

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	1.18	42/5953 (0.7%)	1.92	256/8024 (3.2%)

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	2

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	LYS	C-N	-11.54	1.06	1.33
1	A	299	TRP	CA-C	-8.99	1.40	1.52
1	A	386	THR	CA-C	8.43	1.64	1.52
1	A	385	TYR	C-N	8.30	1.45	1.33
1	A	384	SER	CA-C	-8.23	1.41	1.52
1	A	251	GLU	CB-CG	7.67	1.75	1.52
1	A	386	THR	N-CA	7.49	1.55	1.46
1	A	251	GLU	CA-CB	7.39	1.65	1.53
1	A	389	PHE	CA-C	-6.92	1.43	1.52
1	A	703	ILE	CA-CB	6.86	1.63	1.54
1	A	387	GLY	CA-C	6.70	1.61	1.51
1	A	389	PHE	N-CA	-6.63	1.38	1.45
1	A	757	ARG	C-N	-6.44	1.24	1.33
1	A	31	ASP	C-O	6.44	1.31	1.24
1	A	298	ALA	C-N	6.32	1.42	1.33
1	A	387	GLY	N-CA	6.29	1.54	1.45
1	A	384	SER	N-CA	-6.22	1.38	1.46
1	A	35	ARG	CA-C	6.06	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	741	ALA	C-O	-6.03	1.16	1.24
1	A	250	VAL	CA-CB	5.89	1.61	1.53
1	A	298	ALA	CA-C	5.78	1.60	1.52
1	A	383	GLU	N-CA	-5.69	1.38	1.46
1	A	251	GLU	CG-CD	5.66	1.66	1.52
1	A	390	VAL	CA-C	5.65	1.59	1.52
1	A	300	GLU	C-N	-5.63	1.27	1.33
1	A	133	GLU	CA-C	-5.53	1.46	1.52
1	A	31	ASP	CA-C	-5.44	1.46	1.52
1	A	694	ILE	CA-CB	5.43	1.61	1.54
1	A	390	VAL	C-N	5.42	1.41	1.33
1	A	42	LEU	C-O	-5.39	1.17	1.23
1	A	301	SER	N-CA	-5.36	1.40	1.46
1	A	384	SER	C-O	-5.27	1.17	1.24
1	A	699	VAL	CA-CB	5.27	1.59	1.54
1	A	695	LYS	C-O	-5.24	1.18	1.24
1	A	382	ARG	CA-C	-5.22	1.46	1.52
1	A	300	GLU	N-CA	-5.19	1.39	1.46
1	A	476	GLU	CA-CB	5.19	1.61	1.53
1	A	3	LEU	CA-C	-5.15	1.46	1.52
1	A	130	GLU	N-CA	-5.14	1.40	1.46
1	A	383	GLU	CA-C	-5.13	1.45	1.52
1	A	661	LEU	CA-C	5.12	1.59	1.52
1	A	241	MET	SD-CE	5.09	1.92	1.79

All (256) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	684	ALA	N-CA-C	-18.63	82.65	109.11
1	A	554	SER	N-CA-C	15.76	131.94	113.19
1	A	154	LYS	N-CA-C	-14.57	95.52	114.31
1	A	641	VAL	N-CA-C	-14.39	96.18	110.72
1	A	392	GLU	CA-C-N	14.12	133.88	119.76
1	A	392	GLU	C-N-CA	14.12	133.88	119.76
1	A	150	GLU	N-CA-C	13.48	131.99	107.73
1	A	650	LYS	N-CA-C	-13.39	94.35	114.16
1	A	291	TYR	N-CA-C	12.50	128.94	109.81
1	A	702	TYR	N-CA-C	11.81	126.89	110.24
1	A	742	VAL	N-CA-C	-11.19	102.17	113.47
1	A	27	LYS	N-CA-C	11.18	123.64	107.88
1	A	60	GLY	N-CA-C	-11.15	97.72	116.01
1	A	652	ALA	N-CA-C	-10.92	99.41	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	730	ALA	N-CA-C	-10.92	98.74	112.72
1	A	648	ILE	N-CA-C	-10.88	98.94	112.76
1	A	619	ILE	N-CA-C	-10.69	100.25	111.58
1	A	682	ALA	CA-C-N	-9.97	104.02	121.97
1	A	682	ALA	C-N-CA	-9.97	104.02	121.97
1	A	557	ILE	N-CA-C	-9.95	100.67	110.72
1	A	28	ILE	N-CA-C	9.95	122.04	108.11
1	A	555	GLU	N-CA-C	-9.79	96.13	109.54
1	A	626	ARG	N-CA-C	-9.79	100.69	111.36
1	A	475	ILE	N-CA-C	-9.77	101.85	110.74
1	A	653	ASN	N-CA-C	-9.71	101.56	113.41
1	A	293	ASP	N-CA-C	-9.54	101.84	112.72
1	A	636	ASP	N-CA-C	9.37	126.08	107.62
1	A	568	ILE	N-CA-C	9.29	119.33	110.42
1	A	224	GLU	N-CA-C	-9.19	100.68	113.37
1	A	581	GLU	N-CA-C	9.16	122.96	111.69
1	A	285	LYS	CA-C-N	9.16	131.29	119.84
1	A	285	LYS	C-N-CA	9.16	131.29	119.84
1	A	251	GLU	N-CA-C	-8.86	98.59	110.55
1	A	278	VAL	N-CA-C	8.80	118.86	110.42
1	A	471	THR	N-CA-C	8.65	123.81	109.46
1	A	274	THR	N-CA-C	-8.62	98.92	110.55
1	A	342	TRP	N-CA-C	-8.50	102.02	111.28
1	A	322	LEU	N-CA-C	-8.48	101.98	111.14
1	A	210	ASN	N-CA-C	-8.46	100.96	113.40
1	A	42	LEU	N-CA-C	8.46	123.36	109.24
1	A	607	ARG	N-CA-C	-8.43	96.59	109.41
1	A	278	VAL	CB-CA-C	-8.42	101.19	111.97
1	A	216	PHE	CA-C-N	-8.40	110.96	120.04
1	A	216	PHE	C-N-CA	-8.40	110.96	120.04
1	A	434	ILE	N-CA-C	8.39	120.00	107.75
1	A	22	GLU	N-CA-C	8.39	121.23	107.23
1	A	82	VAL	N-CA-C	8.34	120.16	108.23
1	A	100	VAL	N-CA-C	8.33	118.90	110.82
1	A	592	LYS	CA-C-N	-8.19	109.44	122.79
1	A	592	LYS	C-N-CA	-8.19	109.44	122.79
1	A	572	LEU	CA-C-N	8.19	128.12	119.85
1	A	572	LEU	C-N-CA	8.19	128.12	119.85
1	A	387	GLY	N-CA-C	8.07	132.31	113.18
1	A	211	GLY	N-CA-C	-8.06	102.57	113.37
1	A	747	GLU	N-CA-C	-7.95	98.26	111.37
1	A	382	ARG	CA-C-N	7.83	136.49	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	ARG	C-N-CA	7.83	136.49	121.54
1	A	305	LEU	N-CA-C	-7.82	103.00	112.54
1	A	362	TYR	N-CA-C	-7.75	102.43	111.03
1	A	133	GLU	N-CA-C	-7.74	98.14	110.14
1	A	477	LYS	N-CA-C	7.73	120.39	111.11
1	A	382	ARG	CA-C-O	7.70	128.55	120.54
1	A	306	GLU	N-CA-C	-7.69	102.90	111.28
1	A	127	ILE	CB-CA-C	-7.67	102.00	110.52
1	A	742	VAL	N-CA-CB	-7.67	103.21	112.33
1	A	62	ILE	N-CA-C	7.65	119.94	108.23
1	A	248	THR	N-CA-C	7.64	120.88	108.34
1	A	424	LEU	N-CA-C	7.60	120.45	108.67
1	A	331	ILE	N-CA-C	-7.58	103.15	110.42
1	A	316	ALA	N-CA-C	7.47	119.32	111.03
1	A	746	LEU	N-CA-C	7.46	122.14	112.89
1	A	642	ARG	N-CA-C	-7.45	103.94	112.87
1	A	389	PHE	CA-C-N	-7.43	108.59	121.97
1	A	389	PHE	C-N-CA	-7.43	108.59	121.97
1	A	661	LEU	N-CA-C	7.43	122.47	113.41
1	A	386	THR	N-CA-C	7.41	126.59	110.80
1	A	608	GLY	N-CA-C	7.41	125.18	115.47
1	A	437	GLN	N-CA-C	7.39	122.05	112.89
1	A	389	PHE	CB-CA-C	-7.37	97.64	109.80
1	A	543	ASP	CB-CA-C	-7.36	97.64	109.13
1	A	178	LEU	CA-C-N	7.34	127.02	119.82
1	A	178	LEU	C-N-CA	7.34	127.02	119.82
1	A	249	ALA	N-CA-C	7.34	121.32	110.46
1	A	388	GLY	CA-C-N	-7.28	109.50	122.74
1	A	388	GLY	C-N-CA	-7.28	109.50	122.74
1	A	427	GLU	N-CA-C	7.25	121.01	110.28
1	A	329	MET	N-CA-C	-7.24	103.08	110.97
1	A	472	GLN	CA-C-N	-7.07	111.31	121.20
1	A	472	GLN	C-N-CA	-7.07	111.31	121.20
1	A	321	GLU	N-CA-C	7.03	119.84	111.33
1	A	384	SER	CA-C-O	-7.02	110.47	120.51
1	A	299	TRP	N-CA-CB	6.96	122.25	110.49
1	A	382	ARG	N-CA-CB	6.89	121.75	110.37
1	A	556	GLU	N-CA-CB	-6.89	98.84	110.49
1	A	21	LYS	N-CA-C	-6.89	97.67	108.90
1	A	245	GLY	N-CA-C	-6.85	96.94	113.18
1	A	382	ARG	O-C-N	6.85	131.20	123.05
1	A	253	LYS	N-CA-C	6.83	120.55	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	TRP	N-CA-C	-6.77	96.38	110.80
1	A	447	PRO	CA-C-N	-6.74	117.53	122.18
1	A	447	PRO	C-N-CA	-6.74	117.53	122.18
1	A	178	LEU	N-CA-C	6.72	120.12	109.64
1	A	473	ASP	CA-C-N	-6.71	112.89	119.87
1	A	473	ASP	C-N-CA	-6.71	112.89	119.87
1	A	683	VAL	N-CA-C	6.69	123.25	109.34
1	A	687	LEU	N-CA-C	-6.68	104.39	112.54
1	A	465	LYS	N-CA-C	-6.67	103.10	111.11
1	A	130	GLU	N-CA-C	6.63	119.48	111.40
1	A	560	LYS	N-CA-C	-6.60	104.17	111.36
1	A	289	LYS	CA-C-N	6.57	133.80	121.97
1	A	289	LYS	C-N-CA	6.57	133.80	121.97
1	A	269	ASN	N-CA-C	-6.56	100.57	110.28
1	A	533	PHE	N-CA-C	6.55	121.33	112.88
1	A	396	GLY	N-CA-C	6.55	120.30	111.72
1	A	238	GLU	CA-C-N	6.54	126.50	119.76
1	A	238	GLU	C-N-CA	6.54	126.50	119.76
1	A	411	PRO	N-CA-C	-6.52	104.85	113.65
1	A	690	LYS	N-CA-C	6.50	124.65	110.80
1	A	694	ILE	CB-CA-C	6.48	120.55	111.34
1	A	218	TYR	N-CA-C	-6.47	104.15	111.14
1	A	692	VAL	N-CA-C	6.47	122.80	109.34
1	A	416	THR	N-CA-C	6.46	118.32	111.28
1	A	387	GLY	CA-C-N	6.42	133.99	121.41
1	A	387	GLY	C-N-CA	6.42	133.99	121.41
1	A	24	GLY	N-CA-C	-6.41	106.39	115.43
1	A	35	ARG	N-CA-C	6.41	120.03	109.58
1	A	248	THR	N-CA-CB	-6.38	100.75	110.77
1	A	83	TRP	N-CA-C	6.36	119.08	108.20
1	A	292	ALA	N-CA-C	-6.34	97.29	110.80
1	A	42	LEU	CA-C-N	6.28	129.01	120.54
1	A	42	LEU	C-N-CA	6.28	129.01	120.54
1	A	87	LEU	N-CA-C	6.27	116.73	108.07
1	A	541	ASP	N-CA-C	6.25	119.50	107.44
1	A	655	GLU	CA-C-N	-6.20	117.45	122.85
1	A	655	GLU	C-N-CA	-6.20	117.45	122.85
1	A	89	HIS	CA-C-N	-6.20	112.10	119.84
1	A	89	HIS	C-N-CA	-6.20	112.10	119.84
1	A	272	THR	CB-CA-C	-6.17	98.65	110.24
1	A	239	PRO	N-CA-C	-6.14	101.56	111.14
1	A	355	TRP	N-CA-C	-6.14	104.70	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	735	GLU	N-CA-C	6.12	122.44	110.56
1	A	235	ASP	N-CA-C	-6.11	106.08	112.93
1	A	466	THR	N-CA-C	6.09	117.59	111.07
1	A	52	LYS	N-CA-C	-6.08	106.50	114.04
1	A	97	ARG	N-CA-C	6.06	123.70	110.80
1	A	145	LEU	N-CA-C	-6.02	98.46	108.34
1	A	202	ASP	CA-C-N	-6.01	113.77	120.14
1	A	202	ASP	C-N-CA	-6.01	113.77	120.14
1	A	538	LEU	N-CA-C	6.01	120.68	113.23
1	A	201	LYS	N-CA-C	6.00	117.90	111.36
1	A	510	CYS	N-CA-C	-6.00	104.81	111.36
1	A	11	GLU	N-CA-C	5.95	123.48	110.80
1	A	691	GLY	N-CA-C	-5.95	105.74	114.61
1	A	285	LYS	C-N-CD	-5.95	100.62	125.00
1	A	37	TYR	N-CA-C	5.91	117.13	108.14
1	A	225	LYS	N-CA-CB	-5.88	103.19	111.00
1	A	366	GLU	N-CA-CB	-5.86	101.21	110.77
1	A	207	VAL	N-CA-C	5.86	116.73	108.36
1	A	181	VAL	N-CA-C	-5.85	100.16	109.17
1	A	376	GLU	N-CA-C	-5.84	104.91	111.28
1	A	22	GLU	CA-C-N	5.84	130.70	122.46
1	A	22	GLU	C-N-CA	5.84	130.70	122.46
1	A	185	SER	N-CA-C	5.84	123.23	110.80
1	A	23	ASN	N-CA-CB	5.80	119.92	111.62
1	A	382	ARG	CA-CB-CG	-5.79	102.51	114.10
1	A	745	ILE	CB-CA-C	-5.78	101.81	111.29
1	A	739	LEU	CA-C-N	-5.75	112.80	119.47
1	A	739	LEU	C-N-CA	-5.75	112.80	119.47
1	A	657	PRO	N-CA-C	5.75	117.71	110.70
1	A	48	ILE	CA-C-N	-5.75	111.37	122.06
1	A	48	ILE	C-N-CA	-5.75	111.37	122.06
1	A	122	ILE	CB-CA-C	-5.69	104.56	112.02
1	A	517	TRP	N-CA-C	-5.67	105.18	111.71
1	A	207	VAL	CB-CA-C	-5.64	103.17	110.84
1	A	490	LEU	N-CA-C	5.63	117.10	111.07
1	A	251	GLU	CA-CB-CG	5.62	125.33	114.10
1	A	8	ILE	CA-C-N	-5.62	115.19	123.05
1	A	8	ILE	C-N-CA	-5.62	115.19	123.05
1	A	383	GLU	N-CA-C	5.59	122.72	110.80
1	A	661	LEU	N-CA-CB	-5.59	102.31	110.47
1	A	30	HIS	N-CA-C	-5.57	99.81	108.90
1	A	591	THR	CB-CA-C	-5.56	102.37	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	441	LYS	N-CA-C	5.55	117.74	108.02
1	A	540	ILE	N-CA-C	5.54	116.56	108.58
1	A	32	ARG	CA-C-N	-5.54	113.82	122.73
1	A	32	ARG	C-N-CA	-5.54	113.82	122.73
1	A	91	GLN	N-CA-C	-5.53	106.57	113.38
1	A	212	ASP	CB-CA-C	-5.51	102.22	110.88
1	A	327	LEU	CA-C-N	5.51	125.34	119.28
1	A	327	LEU	C-N-CA	5.51	125.34	119.28
1	A	369	PRO	N-CA-C	-5.50	102.81	111.34
1	A	657	PRO	CA-C-N	5.50	126.72	119.84
1	A	657	PRO	C-N-CA	5.50	126.72	119.84
1	A	435	ALA	CA-C-N	5.50	126.71	119.84
1	A	435	ALA	C-N-CA	5.50	126.71	119.84
1	A	54	ILE	N-CA-C	5.47	120.73	109.34
1	A	436	PRO	CA-C-N	-5.47	111.56	121.14
1	A	436	PRO	C-N-CA	-5.47	111.56	121.14
1	A	77	GLY	CA-C-N	5.47	128.09	120.65
1	A	77	GLY	C-N-CA	5.47	128.09	120.65
1	A	738	VAL	N-CA-C	5.47	120.72	109.34
1	A	390	VAL	CA-C-N	5.47	131.99	121.54
1	A	390	VAL	C-N-CA	5.47	131.99	121.54
1	A	174	LYS	N-CA-C	-5.46	101.16	108.86
1	A	289	LYS	N-CA-C	5.45	122.41	110.80
1	A	267	THR	N-CA-C	-5.44	99.20	110.80
1	A	383	GLU	O-C-N	5.41	129.78	122.59
1	A	285	LYS	O-C-N	-5.39	115.12	121.32
1	A	559	LYS	CB-CG-CD	-5.38	98.91	111.30
1	A	409	LEU	N-CA-C	5.38	117.56	111.11
1	A	299	TRP	CA-CB-CG	-5.36	103.42	113.60
1	A	194	PHE	N-CA-C	-5.35	104.50	111.02
1	A	300	GLU	N-CA-C	-5.35	99.41	110.80
1	A	504	ARG	N-CA-C	-5.34	105.62	111.82
1	A	230	LEU	N-CA-C	-5.34	99.27	108.56
1	A	106	VAL	CA-C-N	5.33	127.39	120.88
1	A	106	VAL	C-N-CA	5.33	127.39	120.88
1	A	48	ILE	CB-CA-C	-5.32	102.57	111.29
1	A	193	ARG	N-CA-C	-5.31	105.39	111.07
1	A	205	ILE	CA-C-N	-5.31	116.22	123.12
1	A	205	ILE	C-N-CA	-5.31	116.22	123.12
1	A	59	HIS	N-CA-C	5.28	122.05	110.80
1	A	438	VAL	N-CA-C	5.28	117.26	111.77
1	A	576	LEU	N-CA-C	-5.26	101.89	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	446	ILE	N-CA-CB	-5.25	103.86	111.21
1	A	681	VAL	N-CA-CB	-5.22	102.62	111.23
1	A	110	PHE	N-CA-C	5.21	117.11	109.24
1	A	488	LYS	CG-CD-CE	-5.21	99.31	111.30
1	A	564	PHE	N-CA-C	5.20	117.69	111.71
1	A	389	PHE	N-CA-C	5.20	118.48	110.42
1	A	588	PHE	N-CA-C	-5.20	100.55	108.76
1	A	386	THR	CA-C-O	-5.18	113.10	120.51
1	A	422	ASP	N-CA-C	5.18	119.31	113.15
1	A	214	PHE	N-CA-C	5.17	119.04	111.34
1	A	334	SER	CB-CA-C	-5.15	102.24	110.79
1	A	114	ILE	CB-CA-C	-5.15	101.99	111.36
1	A	263	VAL	N-CA-C	5.11	117.00	111.58
1	A	246	ASP	N-CA-CB	-5.11	101.86	110.49
1	A	346	ARG	N-CA-C	5.10	119.66	111.81
1	A	44	ASP	N-CA-C	-5.09	99.95	110.80
1	A	93	VAL	N-CA-C	5.09	119.86	108.88
1	A	216	PHE	N-CA-C	5.08	121.04	109.81
1	A	520	LYS	N-CA-C	5.08	117.55	111.71
1	A	44	ASP	CB-CA-C	5.07	120.52	110.42
1	A	337	VAL	N-CA-C	5.05	117.41	111.09
1	A	196	ARG	CA-CB-CG	-5.05	104.00	114.10
1	A	542	THR	N-CA-C	5.04	121.54	110.80
1	A	51	VAL	N-CA-C	5.04	119.82	109.34
1	A	15	VAL	N-CA-C	5.03	115.36	108.12
1	A	632	LEU	CA-C-N	5.03	127.43	120.29
1	A	632	LEU	C-N-CA	5.03	127.43	120.29
1	A	404	LEU	N-CA-C	5.02	116.70	108.52
1	A	305	LEU	CA-CB-CG	5.01	133.84	116.30
1	A	559	LYS	N-CA-C	5.01	117.63	111.82
1	A	687	LEU	CA-CB-CG	5.01	133.82	116.30
1	A	341	LEU	N-CA-C	5.00	117.46	111.71

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	TYR	Sidechain
1	A	389	PHE	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	5826	0	5919	757	0
2	A	2	0	0	0	0
3	A	31	0	0	5	0
All	All	5859	0	5919	757	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 64.

All (757) 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:389:PHE:CE1	1:A:519:ARG:HG2	1.30	1.65
1:A:389:PHE:HE1	1:A:519:ARG:CG	1.08	1.63
1:A:251:GLU:CG	1:A:251:GLU:CB	1.75	1.54
1:A:617:SER:OG	1:A:737:GLN:NE2	1.65	1.26
1:A:389:PHE:O	1:A:390:VAL:HG23	1.40	1.22
1:A:389:PHE:CE1	1:A:519:ARG:CG	2.00	1.22
1:A:384:SER:O	1:A:385:TYR:O	1.65	1.15
1:A:176:ILE:HD11	1:A:305:LEU:CD2	1.76	1.14
1:A:178:LEU:CD2	1:A:179:PRO:HD2	1.76	1.14
1:A:289:LYS:O	1:A:290:VAL:HG23	1.47	1.13
1:A:651:LEU:HD23	1:A:734:ILE:HG13	1.19	1.13
1:A:178:LEU:HD23	1:A:179:PRO:HD2	1.28	1.13
1:A:386:THR:HG22	1:A:386:THR:O	1.39	1.10
1:A:45:ASP:O	1:A:48:ILE:HG23	1.51	1.10
1:A:52:LYS:O	1:A:65:ILE:HG21	1.49	1.10
1:A:377:TYR:HE1	1:A:502:LYS:HG2	1.06	1.10
1:A:176:ILE:HD11	1:A:305:LEU:HD23	1.14	1.08
1:A:528:GLU:OE1	1:A:532:LYS:HD2	1.55	1.06
1:A:244:ILE:CG2	1:A:245:GLY:H	1.67	1.06
1:A:737:GLN:O	1:A:740:PRO:HD2	1.56	1.04
1:A:389:PHE:O	1:A:390:VAL:CG2	2.05	1.03
1:A:303:GLU:C	1:A:305:LEU:H	1.63	1.02
1:A:377:TYR:CE1	1:A:502:LYS:HG2	1.93	1.02
1:A:383:GLU:HG3	1:A:384:SER:N	1.75	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:GLU:O	1:A:643:ILE:HG12	1.59	1.01
1:A:144:THR:HG22	1:A:145:LEU:H	1.25	1.00
1:A:298:ALA:O	1:A:299:TRP:C	2.00	1.00
1:A:182:GLU:HG2	1:A:193:ARG:HH22	1.26	0.99
1:A:731:GLU:O	1:A:735:GLU:HB2	1.62	0.98
1:A:299:TRP:O	1:A:300:GLU:HB2	1.61	0.98
1:A:182:GLU:HG2	1:A:193:ARG:NH2	1.79	0.97
1:A:144:THR:HG22	1:A:145:LEU:N	1.79	0.97
1:A:729:ASP:HB3	1:A:732:TYR:HB2	1.44	0.97
1:A:460:GLU:OE2	1:A:483:ARG:NH2	1.98	0.97
1:A:739:LEU:O	1:A:743:LEU:HB2	1.64	0.96
1:A:45:ASP:O	1:A:48:ILE:CG2	2.13	0.96
1:A:176:ILE:CD1	1:A:305:LEU:HD23	1.94	0.96
1:A:70:LYS:HB2	1:A:83:TRP:CZ3	2.00	0.96
1:A:390:VAL:O	1:A:391:LYS:O	1.84	0.96
1:A:223:ALA:C	1:A:225:LYS:H	1.71	0.96
1:A:231:THR:HG22	1:A:231:THR:O	1.66	0.95
1:A:270:LEU:HD22	1:A:271:PRO:HD2	1.48	0.95
1:A:244:ILE:CG2	1:A:245:GLY:N	2.27	0.94
1:A:296:ALA:HB1	1:A:305:LEU:HB2	1.48	0.94
1:A:303:GLU:O	1:A:305:LEU:N	2.00	0.94
1:A:648:ILE:HG21	1:A:757:ARG:O	1.68	0.93
1:A:383:GLU:HG3	1:A:384:SER:H	1.33	0.93
1:A:384:SER:O	1:A:385:TYR:C	2.11	0.93
1:A:389:PHE:CD2	1:A:540:ILE:HG21	2.02	0.93
1:A:389:PHE:CE1	1:A:519:ARG:HG3	2.04	0.92
1:A:685:LYS:HE3	1:A:685:LYS:HA	1.50	0.92
1:A:78:LYS:HD3	1:A:80:ILE:HD12	1.51	0.91
1:A:71:VAL:HG12	1:A:72:GLU:N	1.83	0.91
1:A:78:LYS:HD3	1:A:80:ILE:CD1	2.00	0.91
1:A:244:ILE:HG23	1:A:245:GLY:H	1.31	0.90
1:A:285:LYS:HG2	1:A:286:PRO:HD2	1.53	0.90
1:A:680:HIS:O	1:A:681:VAL:HB	1.71	0.90
1:A:3:LEU:HD22	1:A:256:ILE:HD11	1.54	0.89
1:A:437:GLN:HE22	1:A:519:ARG:HH21	1.16	0.89
1:A:89:HIS:HD2	1:A:91:GLN:HG2	1.38	0.88
1:A:144:THR:CG2	1:A:145:LEU:H	1.86	0.88
1:A:298:ALA:O	1:A:299:TRP:O	1.91	0.88
1:A:302:GLY:O	1:A:303:GLU:O	1.92	0.87
1:A:360:LYS:O	1:A:364:ARG:HG2	1.74	0.87
1:A:48:ILE:HG13	1:A:49:GLU:N	1.88	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:TYR:HD1	1:A:432:TYR:O	1.58	0.87
1:A:383:GLU:CG	1:A:384:SER:N	2.28	0.86
1:A:386:THR:O	1:A:386:THR:CG2	2.16	0.86
1:A:89:HIS:CD2	1:A:91:GLN:HG2	2.11	0.86
1:A:474:PRO:O	1:A:478:ILE:HG22	1.74	0.86
1:A:52:LYS:O	1:A:65:ILE:CG2	2.23	0.86
1:A:755:ASP:CG	1:A:756:LEU:H	1.84	0.86
1:A:89:HIS:HD2	1:A:91:GLN:CG	1.89	0.86
1:A:651:LEU:HD23	1:A:734:ILE:CG1	2.06	0.86
1:A:227:GLY:O	1:A:228:ILE:HD12	1.75	0.85
1:A:244:ILE:HG22	1:A:245:GLY:N	1.89	0.85
1:A:147:HIS:CG	1:A:148:GLU:H	1.94	0.85
1:A:178:LEU:HD23	1:A:179:PRO:CD	2.06	0.85
1:A:303:GLU:C	1:A:305:LEU:N	2.29	0.85
1:A:379:ARG:O	1:A:382:ARG:N	2.07	0.85
1:A:122:ILE:HA	1:A:359:ARG:HH12	1.41	0.85
1:A:195:LEU:HA	1:A:198:ILE:CD1	2.06	0.85
1:A:378:GLN:OE1	1:A:378:GLN:HA	1.74	0.85
1:A:58:ARG:O	1:A:60:GLY:N	2.08	0.85
1:A:641:VAL:HA	1:A:644:VAL:HG23	1.59	0.84
1:A:437:GLN:HE22	1:A:519:ARG:NH2	1.75	0.84
1:A:42:LEU:CD1	1:A:106:VAL:HG12	2.07	0.84
1:A:47:LYS:O	1:A:49:GLU:N	2.11	0.83
1:A:158:ILE:HG22	1:A:159:MET:HG3	1.58	0.83
1:A:377:TYR:HE1	1:A:502:LYS:CG	1.91	0.83
1:A:745:ILE:HG22	1:A:746:LEU:HD23	1.59	0.83
1:A:51:VAL:O	1:A:51:VAL:HG23	1.78	0.83
1:A:57:GLU:N	1:A:63:VAL:HG23	1.94	0.83
1:A:323:GLY:O	1:A:327:LEU:HB2	1.78	0.82
1:A:289:LYS:HG2	1:A:290:VAL:N	1.93	0.82
1:A:298:ALA:C	1:A:299:TRP:O	2.20	0.82
1:A:270:LEU:HD22	1:A:271:PRO:CD	2.10	0.82
1:A:680:HIS:O	1:A:682:ALA:N	2.12	0.82
1:A:648:ILE:HD12	1:A:757:ARG:HA	1.60	0.81
1:A:732:TYR:O	1:A:735:GLU:N	2.13	0.81
1:A:653:ASN:O	1:A:654:TYR:HB2	1.79	0.81
1:A:160:ILE:CG2	1:A:171:ILE:HB	2.11	0.81
1:A:461:ARG:HH21	1:A:484:GLN:HE21	1.28	0.81
1:A:266:THR:OG1	1:A:267:THR:N	2.11	0.80
1:A:58:ARG:NH1	1:A:91:GLN:HB2	1.97	0.80
1:A:303:GLU:OE2	1:A:306:GLU:HB3	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ARG:C	1:A:382:ARG:H	1.88	0.80
1:A:432:TYR:HA	1:A:444:LYS:HG3	1.63	0.79
1:A:244:ILE:C	1:A:245:GLY:O	2.21	0.79
1:A:545:LEU:N	1:A:545:LEU:HD23	1.98	0.79
1:A:464:ILE:HD11	1:A:483:ARG:CZ	2.12	0.78
1:A:178:LEU:HD22	1:A:179:PRO:HD2	1.62	0.78
1:A:518:GLY:O	1:A:522:ILE:HG12	1.83	0.78
1:A:171:ILE:O	1:A:190:MET:HE2	1.83	0.77
1:A:284:GLY:O	1:A:285:LYS:O	2.02	0.77
1:A:266:THR:O	1:A:267:THR:O	2.03	0.77
1:A:223:ALA:C	1:A:225:LYS:N	2.40	0.77
1:A:168:ALA:HB3	1:A:313:MET:HE1	1.65	0.77
1:A:692:VAL:HG12	1:A:692:VAL:O	1.82	0.77
1:A:315:ASP:O	1:A:319:THR:OG1	2.02	0.77
1:A:383:GLU:O	1:A:385:TYR:N	2.19	0.76
1:A:568:ILE:HD13	1:A:568:ILE:O	1.86	0.76
1:A:42:LEU:HD13	1:A:106:VAL:HG12	1.65	0.76
1:A:169:ARG:HH12	1:A:182:GLU:CD	1.93	0.76
1:A:380:ARG:C	1:A:382:ARG:N	2.38	0.76
1:A:389:PHE:HD2	1:A:540:ILE:CG2	1.98	0.76
1:A:405:ASP:HB2	1:A:581:GLU:CG	2.15	0.76
1:A:100:VAL:O	1:A:106:VAL:HG21	1.87	0.75
1:A:209:TYR:O	1:A:210:ASN:HB3	1.85	0.75
1:A:227:GLY:C	1:A:228:ILE:HD12	2.11	0.75
1:A:432:TYR:O	1:A:432:TYR:CD1	2.40	0.75
1:A:374:GLU:OE1	1:A:374:GLU:HA	1.85	0.75
1:A:640:ALA:C	1:A:643:ILE:H	1.95	0.75
1:A:71:VAL:CG1	1:A:72:GLU:N	2.50	0.75
1:A:89:HIS:CD2	1:A:91:GLN:CG	2.70	0.74
1:A:389:PHE:CZ	1:A:391:LYS:NZ	2.55	0.74
1:A:252:VAL:HG12	1:A:255:ARG:HG3	1.69	0.74
1:A:20:LYS:NZ	1:A:29:GLU:HG2	2.03	0.74
1:A:389:PHE:CZ	1:A:519:ARG:HG2	2.16	0.74
1:A:473:ASP:OD2	1:A:475:ILE:N	2.17	0.74
1:A:736:ASN:C	1:A:736:ASN:HD22	1.95	0.74
1:A:66:VAL:O	1:A:67:ASP:O	2.05	0.74
1:A:641:VAL:HA	1:A:644:VAL:CG2	2.16	0.73
1:A:692:VAL:O	1:A:694:ILE:N	2.20	0.73
1:A:122:ILE:HA	1:A:359:ARG:NH1	2.01	0.73
1:A:36:PRO:HD3	1:A:116:PHE:CE1	2.23	0.73
1:A:372:PRO:HG3	1:A:380:ARG:NH1	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:VAL:O	1:A:266:THR:HG23	1.87	0.73
1:A:3:LEU:CD2	1:A:256:ILE:HD11	2.18	0.73
1:A:340:PRO:O	1:A:343:ASP:HB2	1.89	0.73
1:A:682:ALA:O	1:A:685:LYS:HB2	1.89	0.73
1:A:464:ILE:HD11	1:A:483:ARG:NE	2.03	0.72
1:A:630:THR:HG21	1:A:639:GLU:HG3	1.72	0.72
1:A:61:LYS:HG3	1:A:62:ILE:H	1.52	0.72
1:A:20:LYS:HE2	3:A:2003:HOH:O	1.89	0.72
1:A:35:ARG:NH1	1:A:67:ASP:OD2	2.23	0.72
1:A:680:HIS:C	1:A:681:VAL:HG23	2.15	0.71
1:A:736:ASN:C	1:A:736:ASN:ND2	2.47	0.71
1:A:70:LYS:HB2	1:A:83:TRP:CH2	2.25	0.71
1:A:388:GLY:H	1:A:515:THR:HG23	1.54	0.71
1:A:405:ASP:HB2	1:A:581:GLU:HG3	1.70	0.71
1:A:271:PRO:HG2	1:A:272:THR:H	1.54	0.71
1:A:58:ARG:HH11	1:A:91:GLN:HB2	1.53	0.71
1:A:195:LEU:HA	1:A:198:ILE:HD13	1.72	0.71
1:A:437:GLN:NE2	1:A:519:ARG:HH21	1.88	0.71
1:A:568:ILE:CD1	1:A:572:LEU:HG	2.20	0.71
1:A:298:ALA:O	1:A:300:GLU:O	2.08	0.70
1:A:641:VAL:CA	1:A:644:VAL:HG23	2.21	0.70
1:A:27:LYS:C	1:A:28:ILE:HG13	2.15	0.70
1:A:289:LYS:HA	1:A:291:TYR:CE2	2.26	0.70
1:A:172:THR:HA	1:A:190:MET:CE	2.22	0.70
1:A:389:PHE:CD2	1:A:540:ILE:CG2	2.72	0.70
1:A:64:ARG:CG	1:A:65:ILE:N	2.54	0.70
1:A:278:VAL:O	1:A:282:ILE:HG23	1.91	0.70
1:A:438:VAL:HG22	1:A:438:VAL:O	1.90	0.70
1:A:378:GLN:O	1:A:381:LEU:HD12	1.92	0.69
1:A:754:GLU:O	1:A:755:ASP:C	2.35	0.69
1:A:47:LYS:O	1:A:50:GLU:N	2.18	0.69
1:A:230:LEU:O	1:A:238:GLU:HG2	1.92	0.69
1:A:465:LYS:HA	1:A:468:MET:HE3	1.73	0.69
1:A:692:VAL:O	1:A:692:VAL:CG1	2.41	0.69
1:A:383:GLU:HG3	1:A:384:SER:CB	2.23	0.69
1:A:383:GLU:HG3	1:A:384:SER:CA	2.22	0.69
1:A:64:ARG:HG3	1:A:65:ILE:H	1.55	0.69
1:A:71:VAL:CG1	1:A:72:GLU:H	2.06	0.69
1:A:534:GLY:O	1:A:549:ILE:HG23	1.91	0.69
1:A:231:THR:O	1:A:231:THR:CG2	2.38	0.68
1:A:434:ILE:HG12	1:A:441:LYS:HG2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:GLU:O	1:A:526:TRP:N	2.25	0.68
1:A:645:LYS:C	1:A:647:VAL:H	1.99	0.68
1:A:165:GLU:HG2	1:A:320:TYR:OH	1.93	0.68
1:A:680:HIS:O	1:A:681:VAL:CB	2.39	0.68
1:A:528:GLU:CD	1:A:532:LYS:HD2	2.18	0.68
1:A:460:GLU:CD	1:A:483:ARG:NH2	2.52	0.68
1:A:647:VAL:C	1:A:649:GLN:N	2.49	0.68
1:A:62:ILE:HD12	1:A:62:ILE:N	2.09	0.67
1:A:71:VAL:HG12	1:A:72:GLU:H	1.56	0.67
1:A:263:VAL:O	1:A:266:THR:CG2	2.41	0.67
1:A:184:VAL:HG11	1:A:189:GLU:HB3	1.76	0.67
1:A:5:VAL:HG21	1:A:121:LEU:HD21	1.77	0.67
1:A:119:ARG:NH1	1:A:123:ASP:OD1	2.26	0.67
1:A:755:ASP:CG	1:A:756:LEU:N	2.50	0.67
1:A:546:TYR:N	1:A:546:TYR:CD2	2.63	0.67
1:A:36:PRO:HD3	1:A:116:PHE:HE1	1.59	0.67
1:A:172:THR:O	1:A:183:SER:HA	1.95	0.67
1:A:680:HIS:CG	1:A:681:VAL:HG23	2.29	0.67
1:A:184:VAL:HG12	1:A:189:GLU:HB2	1.75	0.66
1:A:389:PHE:CE1	1:A:519:ARG:CD	2.77	0.66
1:A:687:LEU:CD2	1:A:692:VAL:HG11	2.25	0.66
1:A:389:PHE:HD2	1:A:540:ILE:HG21	1.48	0.66
1:A:398:TRP:HB2	1:A:401:ILE:HD11	1.76	0.66
1:A:661:LEU:CD2	1:A:733:TYR:CE2	2.79	0.66
1:A:295:ILE:O	1:A:300:GLU:O	2.12	0.66
1:A:647:VAL:C	1:A:649:GLN:H	2.03	0.66
1:A:147:HIS:CG	1:A:148:GLU:N	2.63	0.66
1:A:598:ILE:HD11	1:A:602:GLY:HA2	1.78	0.66
1:A:144:THR:O	1:A:158:ILE:HD12	1.95	0.66
1:A:294:GLU:CG	1:A:294:GLU:O	2.44	0.66
1:A:51:VAL:O	1:A:51:VAL:CG2	2.44	0.65
1:A:64:ARG:CG	1:A:65:ILE:H	2.09	0.65
1:A:464:ILE:CG2	1:A:468:MET:HE2	2.27	0.65
1:A:70:LYS:HD2	1:A:83:TRP:CZ2	2.32	0.65
1:A:248:THR:O	1:A:248:THR:HG23	1.96	0.65
1:A:661:LEU:HD23	1:A:733:TYR:HE2	1.61	0.65
1:A:44:ASP:C	1:A:46:SER:N	2.51	0.65
1:A:52:LYS:HA	1:A:65:ILE:HD13	1.78	0.65
1:A:298:ALA:O	1:A:300:GLU:C	2.39	0.65
1:A:172:THR:HA	1:A:190:MET:HE3	1.78	0.65
1:A:389:PHE:HE1	1:A:519:ARG:HG2	0.48	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:MET:O	1:A:471:THR:HG22	1.96	0.65
1:A:21:LYS:O	1:A:22:GLU:HG2	1.97	0.65
1:A:624:GLN:O	1:A:624:GLN:HG2	1.97	0.65
1:A:446:ILE:HG12	1:A:446:ILE:O	1.97	0.64
1:A:335:ARG:NH1	1:A:335:ARG:HG2	2.11	0.64
1:A:169:ARG:CG	1:A:169:ARG:HH11	2.10	0.64
1:A:609:LEU:O	1:A:610:GLU:C	2.39	0.64
1:A:289:LYS:HG2	1:A:290:VAL:H	1.62	0.64
1:A:38:ILE:HG13	1:A:39:TYR:N	2.07	0.64
1:A:31:ASP:C	1:A:31:ASP:OD1	2.40	0.64
1:A:66:VAL:HG12	1:A:67:ASP:N	2.13	0.64
1:A:360:LYS:O	1:A:364:ARG:CG	2.46	0.64
1:A:181:VAL:HG12	1:A:182:GLU:N	2.12	0.64
1:A:244:ILE:HG22	1:A:245:GLY:H	1.51	0.64
1:A:657:PRO:C	1:A:659:GLU:H	2.05	0.64
1:A:386:THR:O	1:A:515:THR:HG21	1.98	0.64
1:A:737:GLN:O	1:A:740:PRO:CD	2.41	0.64
1:A:568:ILE:HD12	1:A:572:LEU:HG	1.80	0.63
1:A:595:TYR:CD1	1:A:595:TYR:C	2.76	0.63
1:A:660:LYS:C	1:A:661:LEU:HG	2.07	0.63
1:A:147:HIS:ND1	1:A:148:GLU:N	2.46	0.63
1:A:754:GLU:HA	1:A:754:GLU:OE1	1.99	0.63
1:A:66:VAL:HG12	1:A:67:ASP:H	1.62	0.63
1:A:262:HIS:HA	3:A:2014:HOH:O	1.98	0.63
1:A:657:PRO:HB3	1:A:659:GLU:HG3	1.80	0.63
1:A:383:GLU:CG	1:A:384:SER:H	1.80	0.63
1:A:390:VAL:O	1:A:390:VAL:HG12	1.97	0.63
1:A:184:VAL:CG1	1:A:189:GLU:CB	2.77	0.63
1:A:202:ASP:OD1	1:A:255:ARG:NH2	2.32	0.63
1:A:746:LEU:O	1:A:747:GLU:C	2.41	0.63
1:A:16:ILE:HD11	1:A:116:PHE:CE2	2.34	0.63
1:A:285:LYS:CG	1:A:286:PRO:HD2	2.28	0.63
1:A:45:ASP:HB2	1:A:83:TRP:HZ2	1.64	0.62
1:A:648:ILE:CD1	1:A:757:ARG:HA	2.29	0.62
1:A:653:ASN:HB2	1:A:655:GLU:OE2	1.99	0.62
1:A:112:TYR:CE1	1:A:370:ASN:OD1	2.53	0.62
1:A:372:PRO:HB2	1:A:377:TYR:HB2	1.81	0.62
1:A:687:LEU:HG	1:A:692:VAL:HG11	1.82	0.62
1:A:151:GLU:O	1:A:152:PHE:HB3	2.00	0.62
1:A:265:ARG:HD3	3:A:2014:HOH:O	1.99	0.62
1:A:464:ILE:HG22	1:A:468:MET:HE2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:VAL:HG12	1:A:592:LYS:HD2	1.82	0.62
1:A:680:HIS:C	1:A:682:ALA:H	2.05	0.61
1:A:405:ASP:HB2	1:A:581:GLU:HG2	1.82	0.61
1:A:530:GLU:HG2	1:A:535:PHE:O	2.00	0.61
1:A:160:ILE:HG22	1:A:171:ILE:HB	1.82	0.61
1:A:244:ILE:O	1:A:245:GLY:C	2.42	0.61
1:A:42:LEU:CD1	1:A:106:VAL:CG1	2.78	0.61
1:A:7:TYR:HA	1:A:15:VAL:O	2.00	0.61
1:A:209:TYR:O	1:A:210:ASN:CB	2.48	0.61
1:A:264:ILE:HA	1:A:326:PHE:CE2	2.35	0.61
1:A:159:MET:HE1	1:A:308:VAL:HG12	1.82	0.60
1:A:364:ARG:CD	1:A:449:PHE:HE1	2.14	0.60
1:A:58:ARG:NH1	1:A:91:GLN:CB	2.64	0.60
1:A:655:GLU:OE2	1:A:655:GLU:N	2.34	0.60
1:A:680:HIS:CB	1:A:681:VAL:HG23	2.31	0.60
1:A:43:ARG:HB2	1:A:105:ALA:O	2.02	0.60
1:A:650:LYS:HE2	1:A:655:GLU:O	2.02	0.60
1:A:735:GLU:CD	1:A:757:ARG:HH21	2.10	0.60
1:A:269:ASN:O	1:A:270:LEU:HD23	2.02	0.60
1:A:294:GLU:O	1:A:294:GLU:OE1	2.19	0.60
1:A:598:ILE:HA	1:A:603:LYS:O	2.02	0.60
1:A:78:LYS:CD	1:A:80:ILE:CD1	2.76	0.60
1:A:313:MET:HE2	1:A:317:LYS:HD2	1.84	0.60
1:A:61:LYS:HG3	1:A:62:ILE:N	2.16	0.60
1:A:287:LYS:O	1:A:288:GLU:HG2	2.02	0.60
1:A:380:ARG:O	1:A:382:ARG:N	2.35	0.60
1:A:538:LEU:O	1:A:539:TYR:HB2	2.02	0.60
1:A:289:LYS:HA	1:A:291:TYR:HE2	1.64	0.59
1:A:114:ILE:HG22	1:A:115:PRO:O	2.03	0.59
1:A:335:ARG:HH11	1:A:335:ARG:CG	2.14	0.59
1:A:438:VAL:HG13	1:A:440:HIS:CD2	2.38	0.59
1:A:296:ALA:HA	1:A:302:GLY:O	2.02	0.59
1:A:661:LEU:HD23	1:A:733:TYR:CE2	2.37	0.59
1:A:9:THR:HG23	1:A:13:LYS:O	2.02	0.59
1:A:20:LYS:HZ3	1:A:29:GLU:HG2	1.67	0.59
1:A:184:VAL:CG1	1:A:189:GLU:HB3	2.32	0.59
1:A:390:VAL:O	1:A:390:VAL:CG1	2.51	0.58
1:A:545:LEU:N	1:A:545:LEU:CD2	2.66	0.58
1:A:58:ARG:N	1:A:61:LYS:O	2.36	0.58
1:A:244:ILE:O	1:A:245:GLY:O	2.21	0.58
1:A:17:ARG:HG2	1:A:30:HIS:CD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ARG:HG3	1:A:255:ARG:NH1	2.18	0.58
1:A:390:VAL:HG12	1:A:592:LYS:CD	2.33	0.58
1:A:620:ALA:O	1:A:621:LYS:C	2.46	0.58
1:A:214:PHE:O	1:A:217:PRO:HD2	2.03	0.58
1:A:293:ASP:C	1:A:295:ILE:H	2.10	0.58
1:A:661:LEU:HD22	1:A:733:TYR:CE2	2.38	0.58
1:A:169:ARG:NH2	1:A:182:GLU:OE1	2.37	0.58
1:A:754:GLU:OE1	1:A:754:GLU:CA	2.50	0.58
1:A:100:VAL:O	1:A:106:VAL:CG2	2.52	0.58
1:A:729:ASP:CB	1:A:732:TYR:HB2	2.28	0.58
1:A:1:MET:HG2	1:A:2:ILE:N	2.19	0.58
1:A:196:ARG:HA	1:A:199:ARG:CZ	2.34	0.58
1:A:264:ILE:C	1:A:266:THR:H	2.12	0.58
1:A:687:LEU:CG	1:A:692:VAL:HG11	2.33	0.58
1:A:733:TYR:O	1:A:737:GLN:HB3	2.03	0.58
1:A:432:TYR:CD1	1:A:432:TYR:C	2.79	0.57
1:A:66:VAL:HG12	1:A:67:ASP:CG	2.28	0.57
1:A:206:ILE:HD12	1:A:207:VAL:N	2.19	0.57
1:A:569:ASN:HD21	1:A:578:LEU:H	1.50	0.57
1:A:644:VAL:HG13	1:A:742:VAL:HG11	1.86	0.57
1:A:7:TYR:HB2	1:A:15:VAL:O	2.04	0.57
1:A:184:VAL:CG1	1:A:189:GLU:HB2	2.33	0.57
1:A:294:GLU:O	1:A:294:GLU:HG2	2.04	0.57
1:A:440:HIS:CE1	1:A:509:GLU:HG2	2.38	0.57
1:A:264:ILE:HG12	1:A:326:PHE:CZ	2.39	0.57
1:A:424:LEU:C	1:A:424:LEU:HD22	2.29	0.57
1:A:159:MET:CE	1:A:308:VAL:HG12	2.35	0.57
1:A:169:ARG:HH22	1:A:182:GLU:CD	2.12	0.57
1:A:176:ILE:CD1	1:A:305:LEU:CD2	2.63	0.57
1:A:473:ASP:OD2	1:A:473:ASP:C	2.47	0.57
1:A:641:VAL:C	1:A:643:ILE:N	2.59	0.57
1:A:752:ARG:HD2	1:A:753:LYS:HG2	1.86	0.57
1:A:377:TYR:O	1:A:377:TYR:CD2	2.58	0.57
1:A:460:GLU:CD	1:A:483:ARG:HH21	2.13	0.57
1:A:618:GLU:HB3	1:A:660:LYS:HB3	1.87	0.57
1:A:145:LEU:HG	1:A:156:PRO:HD2	1.86	0.56
1:A:260:LEU:HD11	1:A:322:LEU:HB2	1.86	0.56
1:A:119:ARG:HD2	1:A:123:ASP:OD2	2.05	0.56
1:A:529:LEU:HD13	1:A:564:PHE:CE2	2.40	0.56
1:A:175:ASN:OD1	1:A:175:ASN:N	2.37	0.56
1:A:289:LYS:O	1:A:290:VAL:CG2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:LYS:HE3	1:A:685:LYS:CA	2.30	0.56
1:A:294:GLU:CB	3:A:2016:HOH:O	2.53	0.56
1:A:122:ILE:HG12	1:A:359:ARG:NH1	2.20	0.56
1:A:252:VAL:CG1	1:A:255:ARG:HG3	2.35	0.56
1:A:299:TRP:O	1:A:300:GLU:CB	2.38	0.56
1:A:196:ARG:HA	1:A:199:ARG:NH2	2.21	0.56
1:A:87:LEU:HD21	1:A:96:LEU:HG	1.87	0.56
1:A:432:TYR:CE2	1:A:441:LYS:HD2	2.40	0.56
1:A:446:ILE:O	1:A:447:PRO:O	2.24	0.56
1:A:620:ALA:O	1:A:623:THR:N	2.39	0.56
1:A:58:ARG:HH12	1:A:91:GLN:HG3	1.70	0.55
1:A:137:ILE:N	1:A:137:ILE:HD12	2.21	0.55
1:A:169:ARG:HH11	1:A:169:ARG:HG3	1.71	0.55
1:A:389:PHE:CD1	1:A:519:ARG:HG3	2.40	0.55
1:A:274:THR:HB	1:A:276:GLU:HG2	1.88	0.55
1:A:335:ARG:HG2	1:A:335:ARG:HH11	1.68	0.55
1:A:755:ASP:O	1:A:757:ARG:N	2.39	0.55
1:A:122:ILE:HG12	1:A:359:ARG:HH11	1.70	0.55
1:A:446:ILE:C	1:A:447:PRO:O	2.47	0.55
1:A:735:GLU:O	1:A:740:PRO:HD3	2.07	0.55
1:A:68:VAL:HG12	1:A:68:VAL:O	2.05	0.55
1:A:407:LYS:HG3	1:A:577:GLU:HG2	1.87	0.55
1:A:730:ALA:C	1:A:732:TYR:H	2.14	0.55
1:A:732:TYR:O	1:A:733:TYR:C	2.49	0.55
1:A:72:GLU:OE2	1:A:72:GLU:O	2.24	0.55
1:A:264:ILE:HA	1:A:326:PHE:HE2	1.72	0.55
1:A:31:ASP:OD1	1:A:32:ARG:N	2.39	0.55
1:A:142:ILE:HD12	1:A:142:ILE:C	2.32	0.55
1:A:645:LYS:O	1:A:647:VAL:N	2.35	0.55
1:A:182:GLU:CG	1:A:193:ARG:HH22	2.11	0.54
1:A:188:LYS:HE3	1:A:226:LEU:HG	1.89	0.54
1:A:270:LEU:CD2	1:A:271:PRO:HD2	2.31	0.54
1:A:314:GLU:O	1:A:315:ASP:C	2.49	0.54
1:A:695:LYS:O	1:A:697:GLY:N	2.36	0.54
1:A:377:TYR:CD2	1:A:377:TYR:C	2.86	0.54
1:A:687:LEU:HD23	1:A:692:VAL:CG1	2.38	0.54
1:A:645:LYS:C	1:A:647:VAL:N	2.65	0.54
1:A:44:ASP:C	1:A:46:SER:H	2.15	0.54
1:A:617:SER:CB	1:A:737:GLN:HE21	2.17	0.54
1:A:66:VAL:HG12	1:A:67:ASP:OD2	2.07	0.54
1:A:596:ALA:O	1:A:597:VAL:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:THR:CG2	1:A:574:GLY:HA3	2.39	0.53
1:A:8:ILE:HG13	1:A:15:VAL:HB	1.90	0.53
1:A:464:ILE:HD11	1:A:483:ARG:NH2	2.22	0.53
1:A:312:SER:C	1:A:314:GLU:N	2.64	0.53
1:A:497:TYR:CZ	1:A:503:ALA:HB1	2.43	0.53
1:A:48:ILE:O	1:A:52:LYS:HG3	2.08	0.53
1:A:64:ARG:HG2	1:A:65:ILE:N	2.23	0.53
1:A:195:LEU:HA	1:A:198:ILE:HD11	1.88	0.53
1:A:559:LYS:O	1:A:563:GLU:HG3	2.08	0.53
1:A:639:GLU:O	1:A:642:ARG:HB3	2.08	0.53
1:A:294:GLU:CD	1:A:294:GLU:C	2.76	0.53
1:A:45:ASP:OD1	1:A:45:ASP:N	2.41	0.53
1:A:169:ARG:NH1	1:A:182:GLU:OE1	2.42	0.53
1:A:264:ILE:HG22	1:A:265:ARG:N	2.23	0.53
1:A:753:LYS:O	1:A:754:GLU:O	2.26	0.53
1:A:130:GLU:O	1:A:131:GLY:O	2.27	0.53
1:A:538:LEU:O	1:A:539:TYR:CB	2.55	0.53
1:A:549:ILE:CG1	1:A:557:ILE:HG12	2.38	0.53
1:A:335:ARG:NH1	1:A:335:ARG:CG	2.72	0.53
1:A:656:ILE:O	1:A:657:PRO:C	2.51	0.52
1:A:78:LYS:CD	1:A:80:ILE:HD12	2.31	0.52
1:A:388:GLY:H	1:A:515:THR:CG2	2.22	0.52
1:A:4:ASP:C	1:A:5:VAL:HG23	2.34	0.52
1:A:63:VAL:HG21	1:A:95:THR:HG21	1.91	0.52
1:A:195:LEU:CA	1:A:198:ILE:HD13	2.40	0.52
1:A:364:ARG:HD2	1:A:449:PHE:HE1	1.73	0.52
1:A:745:ILE:HG22	1:A:746:LEU:CD2	2.35	0.52
1:A:146:TYR:O	1:A:147:HIS:O	2.26	0.52
1:A:264:ILE:O	1:A:266:THR:N	2.33	0.52
1:A:241:MET:SD	1:A:241:MET:N	2.82	0.52
1:A:289:LYS:C	1:A:290:VAL:HG23	2.30	0.52
1:A:81:THR:O	1:A:82:VAL:CG1	2.58	0.52
1:A:81:THR:O	1:A:82:VAL:HG13	2.10	0.52
1:A:136:LYS:C	1:A:137:ILE:HD12	2.35	0.52
1:A:169:ARG:HH11	1:A:169:ARG:CB	2.23	0.52
1:A:222:ARG:O	1:A:222:ARG:HG3	2.10	0.52
1:A:45:ASP:HB2	1:A:83:TRP:CZ2	2.44	0.52
1:A:122:ILE:CA	1:A:359:ARG:HH12	2.18	0.52
1:A:148:GLU:OE1	1:A:148:GLU:HA	2.10	0.52
1:A:328:PRO:O	1:A:332:GLN:HG2	2.10	0.52
1:A:434:ILE:HG23	1:A:441:LYS:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:VAL:O	1:A:438:VAL:CG2	2.58	0.51
1:A:84:LYS:HD3	1:A:86:TYR:CZ	2.45	0.51
1:A:141:ASP:OD1	1:A:315:ASP:HB3	2.10	0.51
1:A:700:ILE:O	1:A:700:ILE:HD12	2.10	0.51
1:A:47:LYS:O	1:A:48:ILE:C	2.53	0.51
1:A:523:GLU:O	1:A:524:LEU:C	2.53	0.51
1:A:468:MET:C	1:A:470:GLU:H	2.19	0.51
1:A:687:LEU:HD23	1:A:692:VAL:HG11	1.92	0.51
1:A:169:ARG:HH11	1:A:169:ARG:HB3	1.76	0.51
1:A:436:PRO:HG2	1:A:517:TRP:HA	1.93	0.51
1:A:650:LYS:O	1:A:656:ILE:CD1	2.58	0.51
1:A:168:ALA:HB3	1:A:313:MET:CE	2.36	0.51
1:A:378:GLN:HA	1:A:381:LEU:HD12	1.92	0.51
1:A:184:VAL:HG11	1:A:189:GLU:CB	2.40	0.50
1:A:264:ILE:HD13	1:A:278:VAL:HG21	1.93	0.50
1:A:655:GLU:N	1:A:655:GLU:CD	2.69	0.50
1:A:7:TYR:CA	1:A:15:VAL:O	2.58	0.50
1:A:401:ILE:HD13	1:A:538:LEU:CD1	2.41	0.50
1:A:703:ILE:HG13	1:A:704:VAL:H	1.76	0.50
1:A:289:LYS:HG3	1:A:291:TYR:CE2	2.46	0.50
1:A:295:ILE:O	1:A:296:ALA:C	2.53	0.50
1:A:523:GLU:O	1:A:526:TRP:HB3	2.11	0.50
1:A:641:VAL:C	1:A:643:ILE:H	2.17	0.50
1:A:750:GLY:O	1:A:751:TYR:O	2.30	0.50
1:A:20:LYS:HZ2	1:A:29:GLU:HG2	1.72	0.50
1:A:48:ILE:CG1	1:A:49:GLU:N	2.67	0.50
1:A:56:GLY:C	1:A:63:VAL:HG23	2.36	0.50
1:A:264:ILE:HG12	1:A:326:PHE:CE2	2.46	0.50
1:A:730:ALA:C	1:A:732:TYR:N	2.68	0.50
1:A:151:GLU:O	1:A:152:PHE:CB	2.59	0.50
1:A:303:GLU:OE2	1:A:306:GLU:CB	2.54	0.50
1:A:644:VAL:CG1	1:A:742:VAL:HG11	2.41	0.50
1:A:754:GLU:O	1:A:757:ARG:HB2	2.12	0.50
1:A:89:HIS:CD2	1:A:91:GLN:HG3	2.46	0.50
1:A:225:LYS:HD3	1:A:226:LEU:HD13	1.94	0.50
1:A:280:GLU:HG3	1:A:284:GLY:O	2.11	0.50
1:A:76:LEU:O	1:A:422:ASP:HB2	2.12	0.49
1:A:294:GLU:O	1:A:294:GLU:CD	2.55	0.49
1:A:640:ALA:O	1:A:643:ILE:N	2.44	0.49
1:A:692:VAL:O	1:A:694:ILE:HB	2.12	0.49
1:A:214:PHE:C	1:A:217:PRO:HD2	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:ASN:HD22	1:A:572:LEU:HD12	1.77	0.49
1:A:735:GLU:OE1	1:A:757:ARG:NE	2.42	0.49
1:A:57:GLU:H	1:A:63:VAL:HG23	1.77	0.49
1:A:313:MET:CE	1:A:317:LYS:HD2	2.42	0.49
1:A:568:ILE:HD13	1:A:568:ILE:C	2.36	0.49
1:A:619:ILE:HD11	1:A:651:LEU:HD11	1.93	0.49
1:A:16:ILE:O	1:A:30:HIS:HA	2.12	0.49
1:A:404:LEU:HB3	1:A:578:LEU:HD13	1.94	0.49
1:A:377:TYR:O	1:A:381:LEU:CD1	2.61	0.49
1:A:617:SER:HG	1:A:737:GLN:NE2	2.02	0.49
1:A:409:LEU:HD11	1:A:413:ILE:HD11	1.94	0.49
1:A:528:GLU:OE1	1:A:532:LYS:CD	2.44	0.49
1:A:561:ALA:O	1:A:562:LEU:C	2.56	0.49
1:A:596:ALA:C	1:A:597:VAL:CG1	2.86	0.49
1:A:2:ILE:CG2	1:A:3:LEU:N	2.74	0.49
1:A:20:LYS:CE	3:A:2003:HOH:O	2.57	0.49
1:A:191:ILE:O	1:A:195:LEU:HG	2.13	0.49
1:A:288:GLU:O	1:A:289:LYS:HB2	2.13	0.49
1:A:415:ILE:CD1	1:A:458:LEU:HD12	2.42	0.49
1:A:468:MET:C	1:A:470:GLU:N	2.71	0.49
1:A:91:GLN:O	1:A:94:PRO:HD2	2.12	0.49
1:A:661:LEU:HB3	1:A:733:TYR:OH	2.13	0.49
1:A:63:VAL:HG11	1:A:92:ASP:HA	1.93	0.48
1:A:657:PRO:HB3	1:A:659:GLU:OE2	2.13	0.48
1:A:745:ILE:HG22	1:A:746:LEU:N	2.26	0.48
1:A:295:ILE:O	1:A:297:LYS:N	2.46	0.48
1:A:276:GLU:O	1:A:277:ALA:C	2.54	0.48
1:A:43:ARG:HD2	1:A:105:ALA:HA	1.95	0.48
1:A:392:GLU:OE2	1:A:591:THR:HG22	2.13	0.48
1:A:680:HIS:HB2	1:A:681:VAL:HG23	1.95	0.48
1:A:744:ARG:O	1:A:745:ILE:C	2.56	0.48
1:A:140:PHE:HB2	1:A:161:SER:O	2.12	0.48
1:A:264:ILE:CG1	1:A:326:PHE:CE2	2.97	0.48
1:A:93:VAL:HB	1:A:94:PRO:HD3	1.94	0.48
1:A:353:VAL:O	1:A:356:PHE:HB3	2.14	0.48
1:A:702:TYR:H	1:A:702:TYR:HD2	1.59	0.48
1:A:127:ILE:HD13	1:A:359:ARG:HH21	1.78	0.48
1:A:160:ILE:HG23	1:A:171:ILE:HB	1.92	0.48
1:A:76:LEU:HG	1:A:422:ASP:HB3	1.96	0.48
1:A:265:ARG:C	1:A:266:THR:HG22	2.39	0.48
1:A:468:MET:O	1:A:470:GLU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:MET:HA	1:A:471:THR:HG22	1.95	0.48
1:A:755:ASP:O	1:A:756:LEU:C	2.56	0.48
1:A:627:VAL:HG12	1:A:628:LEU:N	2.29	0.48
1:A:47:LYS:C	1:A:49:GLU:N	2.72	0.47
1:A:464:ILE:O	1:A:465:LYS:C	2.56	0.47
1:A:694:ILE:HA	1:A:698:MET:HG3	1.94	0.47
1:A:694:ILE:HG12	1:A:698:MET:HG3	1.95	0.47
1:A:230:LEU:O	1:A:238:GLU:HA	2.14	0.47
1:A:457:LEU:O	1:A:458:LEU:C	2.58	0.47
1:A:478:ILE:HG13	1:A:482:TYR:CE1	2.49	0.47
1:A:596:ALA:O	1:A:597:VAL:CG1	2.62	0.47
1:A:435:ALA:HA	1:A:436:PRO:HD2	1.73	0.47
1:A:732:TYR:CD1	1:A:736:ASN:HB3	2.50	0.47
1:A:405:ASP:CB	1:A:581:GLU:HG3	2.42	0.47
1:A:95:THR:O	1:A:95:THR:CG2	2.62	0.47
1:A:264:ILE:C	1:A:266:THR:N	2.72	0.47
1:A:271:PRO:CG	1:A:272:THR:H	2.26	0.47
1:A:369:PRO:O	1:A:504:ARG:HD3	2.13	0.47
1:A:181:VAL:CG1	1:A:182:GLU:N	2.78	0.47
1:A:182:GLU:HG2	1:A:193:ARG:CZ	2.40	0.47
1:A:445:ASP:C	1:A:446:ILE:HG23	2.40	0.47
1:A:549:ILE:HG12	1:A:557:ILE:HG12	1.97	0.47
1:A:703:ILE:HG13	1:A:704:VAL:N	2.30	0.47
1:A:287:LYS:O	1:A:288:GLU:CB	2.63	0.47
1:A:383:GLU:C	1:A:385:TYR:N	2.72	0.47
1:A:113:ASP:OD2	1:A:113:ASP:N	2.46	0.47
1:A:266:THR:C	1:A:267:THR:O	2.58	0.47
1:A:293:ASP:C	1:A:295:ILE:N	2.73	0.47
1:A:731:GLU:O	1:A:735:GLU:CB	2.50	0.47
1:A:432:TYR:OH	1:A:441:LYS:NZ	2.40	0.47
1:A:750:GLY:C	1:A:751:TYR:O	2.56	0.47
1:A:59:HIS:CD2	1:A:59:HIS:O	2.68	0.46
1:A:81:THR:C	1:A:82:VAL:HG13	2.40	0.46
1:A:264:ILE:HD13	1:A:278:VAL:HG11	1.97	0.46
1:A:341:LEU:HA	1:A:344:VAL:HB	1.97	0.46
1:A:62:ILE:H	1:A:62:ILE:HD12	1.77	0.46
1:A:177:ASP:O	1:A:177:ASP:CG	2.58	0.46
1:A:283:PHE:N	1:A:283:PHE:CD1	2.83	0.46
1:A:408:SER:HB2	1:A:411:PRO:HG2	1.97	0.46
1:A:445:ASP:OD1	1:A:445:ASP:N	2.48	0.46
1:A:202:ASP:HA	1:A:255:ARG:NH2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:GLU:OE1	1:A:148:GLU:CA	2.63	0.46
1:A:649:GLN:O	1:A:653:ASN:OD1	2.33	0.46
1:A:160:ILE:HG23	1:A:160:ILE:O	2.15	0.46
1:A:178:LEU:HD13	1:A:180:TYR:CZ	2.50	0.46
1:A:400:ASN:OD1	1:A:554:SER:HB2	2.16	0.46
1:A:522:ILE:O	1:A:523:GLU:C	2.58	0.46
1:A:731:GLU:HG3	1:A:735:GLU:HG3	1.97	0.46
1:A:58:ARG:C	1:A:60:GLY:H	2.14	0.46
1:A:513:SER:O	1:A:517:TRP:HB2	2.15	0.46
1:A:159:MET:HA	1:A:190:MET:HE1	1.98	0.46
1:A:197:ILE:C	1:A:199:ARG:N	2.73	0.46
1:A:703:ILE:CG1	1:A:704:VAL:N	2.79	0.46
1:A:169:ARG:CG	1:A:169:ARG:NH1	2.78	0.46
1:A:223:ALA:O	1:A:225:LYS:N	2.48	0.46
1:A:61:LYS:CG	1:A:62:ILE:N	2.79	0.45
1:A:292:ALA:C	1:A:294:GLU:H	2.24	0.45
1:A:426:LEU:HD12	1:A:426:LEU:HA	1.63	0.45
1:A:461:ARG:HE	1:A:484:GLN:HG2	1.80	0.45
1:A:631:ILE:CD1	1:A:637:VAL:HA	2.46	0.45
1:A:735:GLU:OE1	1:A:757:ARG:NH2	2.48	0.45
1:A:4:ASP:O	1:A:5:VAL:CG2	2.64	0.45
1:A:73:LYS:NZ	1:A:365:ASN:OD1	2.28	0.45
1:A:119:ARG:O	1:A:119:ARG:HD3	2.16	0.45
1:A:263:VAL:O	1:A:266:THR:HG21	2.16	0.45
1:A:656:ILE:O	1:A:656:ILE:HG12	2.16	0.45
1:A:661:LEU:HD22	1:A:733:TYR:CZ	2.51	0.45
1:A:58:ARG:NH1	1:A:91:GLN:HG3	2.32	0.45
1:A:75:PHE:O	1:A:77:GLY:N	2.49	0.45
1:A:355:TRP:CZ3	1:A:358:LEU:HD13	2.51	0.45
1:A:359:ARG:NH1	1:A:359:ARG:HG3	2.30	0.45
1:A:7:TYR:CB	1:A:15:VAL:O	2.64	0.45
1:A:322:LEU:HD23	1:A:322:LEU:HA	1.70	0.45
1:A:327:LEU:O	1:A:331:ILE:HG12	2.17	0.45
1:A:302:GLY:O	1:A:303:GLU:C	2.60	0.45
1:A:653:ASN:O	1:A:654:TYR:CB	2.53	0.45
1:A:135:LEU:HA	1:A:135:LEU:HD23	1.65	0.45
1:A:176:ILE:HD13	1:A:176:ILE:HA	1.61	0.45
1:A:287:LYS:O	1:A:288:GLU:CG	2.64	0.45
1:A:303:GLU:O	1:A:304:ASN:C	2.59	0.45
1:A:412:SER:HB2	1:A:575:LEU:HD13	1.99	0.45
1:A:432:TYR:CZ	1:A:441:LYS:HD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:THR:HB	1:A:592:LYS:H	1.37	0.45
1:A:646:GLU:O	1:A:646:GLU:HG2	2.17	0.45
1:A:657:PRO:C	1:A:659:GLU:N	2.73	0.45
1:A:162:TYR:CE1	1:A:169:ARG:HG2	2.52	0.45
1:A:392:GLU:HA	1:A:393:PRO:HD3	1.72	0.45
1:A:177:ASP:O	1:A:177:ASP:OD2	2.35	0.45
1:A:378:GLN:C	1:A:381:LEU:HD12	2.42	0.45
1:A:638:GLU:O	1:A:639:GLU:C	2.61	0.45
1:A:1:MET:HG2	1:A:2:ILE:H	1.79	0.44
1:A:5:VAL:HG12	1:A:117:ALA:HB1	1.99	0.44
1:A:327:LEU:CD2	1:A:331:ILE:HD11	2.47	0.44
1:A:377:TYR:O	1:A:381:LEU:HD11	2.16	0.44
1:A:464:ILE:HG21	1:A:484:GLN:HB2	1.99	0.44
1:A:399:GLU:HG3	1:A:400:ASN:ND2	2.33	0.44
1:A:144:THR:HG22	1:A:145:LEU:C	2.43	0.44
1:A:341:LEU:O	1:A:342:TRP:C	2.58	0.44
1:A:267:THR:HB	1:A:268:ILE:H	1.41	0.44
1:A:296:ALA:HB1	1:A:305:LEU:CB	2.34	0.44
1:A:378:GLN:OE1	1:A:378:GLN:CA	2.56	0.44
1:A:650:LYS:O	1:A:656:ILE:HD12	2.17	0.44
1:A:17:ARG:HG2	1:A:30:HIS:HD2	1.80	0.44
1:A:89:HIS:C	1:A:91:GLN:N	2.74	0.44
1:A:279:TYR:CE1	1:A:283:PHE:CE1	3.06	0.44
1:A:461:ARG:NH2	1:A:484:GLN:HE21	2.07	0.44
1:A:164:ASP:HA	1:A:320:TYR:CE1	2.52	0.44
1:A:327:LEU:N	1:A:328:PRO:HD3	2.33	0.44
1:A:327:LEU:N	1:A:328:PRO:CD	2.80	0.44
1:A:702:TYR:N	1:A:702:TYR:CD2	2.86	0.44
1:A:70:LYS:HD2	1:A:83:TRP:CH2	2.53	0.44
1:A:421:PRO:O	1:A:424:LEU:HB3	2.18	0.44
1:A:736:ASN:HD22	1:A:737:GLN:N	2.16	0.44
1:A:739:LEU:O	1:A:740:PRO:C	2.60	0.44
1:A:141:ASP:OD1	1:A:315:ASP:CB	2.66	0.44
1:A:4:ASP:O	1:A:5:VAL:HG23	2.18	0.44
1:A:550:PRO:C	1:A:552:GLY:H	2.26	0.44
1:A:186:THR:OG1	1:A:188:LYS:N	2.50	0.43
1:A:259:ASP:O	1:A:260:LEU:C	2.57	0.43
1:A:285:LYS:HG2	1:A:286:PRO:CD	2.36	0.43
1:A:588:PHE:HE1	1:A:590:VAL:HG23	1.82	0.43
1:A:636:ASP:OD1	1:A:639:GLU:N	2.48	0.43
1:A:7:TYR:HB3	1:A:16:ILE:HD13	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLU:N	1:A:63:VAL:CG2	2.75	0.43
1:A:754:GLU:O	1:A:757:ARG:N	2.32	0.43
1:A:2:ILE:HG22	1:A:3:LEU:N	2.32	0.43
1:A:20:LYS:HD2	1:A:29:GLU:HG2	2.01	0.43
1:A:26:PHE:C	1:A:27:LYS:HG3	2.42	0.43
1:A:285:LYS:CB	1:A:286:PRO:HD2	2.49	0.43
1:A:529:LEU:HD13	1:A:564:PHE:CD2	2.53	0.43
1:A:39:TYR:O	1:A:109:ILE:HA	2.19	0.43
1:A:144:THR:HG22	1:A:145:LEU:O	2.18	0.43
1:A:750:GLY:O	1:A:751:TYR:C	2.60	0.43
1:A:21:LYS:O	1:A:22:GLU:CG	2.65	0.43
1:A:248:THR:O	1:A:248:THR:CG2	2.65	0.43
1:A:299:TRP:CD1	1:A:299:TRP:H	2.36	0.43
1:A:312:SER:C	1:A:314:GLU:H	2.27	0.43
1:A:195:LEU:O	1:A:198:ILE:HD13	2.17	0.43
1:A:416:THR:HG23	1:A:574:GLY:HA3	1.99	0.43
1:A:122:ILE:CG1	1:A:359:ARG:NH1	2.82	0.43
1:A:289:LYS:CA	1:A:291:TYR:HE2	2.31	0.43
1:A:389:PHE:HD2	1:A:540:ILE:HG22	1.80	0.43
1:A:626:ARG:O	1:A:630:THR:OG1	2.35	0.43
1:A:752:ARG:O	1:A:755:ASP:OD1	2.37	0.43
1:A:89:HIS:C	1:A:91:GLN:H	2.27	0.43
1:A:173:TRP:CD1	1:A:173:TRP:H	2.37	0.43
1:A:295:ILE:C	1:A:297:LYS:N	2.75	0.43
1:A:45:ASP:O	1:A:48:ILE:HG22	2.10	0.42
1:A:175:ASN:O	1:A:176:ILE:HD13	2.19	0.42
1:A:251:GLU:HA	1:A:342:TRP:CD1	2.53	0.42
1:A:648:ILE:O	1:A:734:ILE:HD11	2.19	0.42
1:A:285:LYS:HA	1:A:286:PRO:HD3	1.38	0.42
1:A:651:LEU:HD12	1:A:656:ILE:CD1	2.49	0.42
1:A:690:LYS:C	1:A:692:VAL:N	2.75	0.42
1:A:63:VAL:HG12	1:A:92:ASP:HB3	2.01	0.42
1:A:103:HIS:HB3	1:A:106:VAL:HG22	2.01	0.42
1:A:160:ILE:CG2	1:A:160:ILE:O	2.68	0.42
1:A:176:ILE:O	1:A:178:LEU:N	2.44	0.42
1:A:314:GLU:C	1:A:316:ALA:N	2.77	0.42
1:A:588:PHE:CE1	1:A:590:VAL:HG23	2.54	0.42
1:A:619:ILE:CD1	1:A:651:LEU:HD11	2.50	0.42
1:A:44:ASP:O	1:A:46:SER:N	2.52	0.42
1:A:378:GLN:CA	1:A:381:LEU:HD12	2.50	0.42
1:A:595:TYR:C	1:A:595:TYR:HD1	2.25	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:LYS:O	1:A:692:VAL:HG23	2.19	0.42
1:A:145:LEU:CG	1:A:156:PRO:HD2	2.49	0.42
1:A:690:LYS:O	1:A:691:GLY:C	2.62	0.42
1:A:142:ILE:HG22	1:A:160:ILE:HG13	2.01	0.42
1:A:641:VAL:O	1:A:644:VAL:HG23	2.20	0.42
1:A:58:ARG:HG2	1:A:59:HIS:H	1.85	0.42
1:A:337:VAL:O	1:A:359:ARG:HD2	2.19	0.42
1:A:594:ARG:O	1:A:595:TYR:HB3	2.20	0.42
1:A:55:THR:OG1	1:A:56:GLY:N	2.53	0.42
1:A:66:VAL:CG1	1:A:67:ASP:N	2.82	0.42
1:A:420:SER:O	1:A:421:PRO:C	2.61	0.42
1:A:522:ILE:O	1:A:523:GLU:O	2.38	0.42
1:A:596:ALA:C	1:A:597:VAL:HG13	2.43	0.42
1:A:270:LEU:HD13	1:A:271:PRO:HD2	2.02	0.42
1:A:732:TYR:CE1	1:A:736:ASN:HB3	2.55	0.41
1:A:497:TYR:O	1:A:498:TYR:C	2.63	0.41
1:A:657:PRO:HA	1:A:658:PRO:HD3	1.67	0.41
1:A:58:ARG:CG	1:A:59:HIS:H	2.33	0.41
1:A:93:VAL:C	1:A:95:THR:H	2.26	0.41
1:A:737:GLN:O	1:A:738:VAL:C	2.62	0.41
1:A:65:ILE:HG23	1:A:65:ILE:O	2.20	0.41
1:A:568:ILE:O	1:A:571:LYS:N	2.41	0.41
1:A:732:TYR:O	1:A:734:ILE:N	2.54	0.41
1:A:318:ALA:O	1:A:319:THR:C	2.63	0.41
1:A:334:SER:HA	1:A:344:VAL:HG21	2.02	0.41
1:A:497:TYR:CE2	1:A:503:ALA:HB1	2.56	0.41
1:A:562:LEU:O	1:A:563:GLU:C	2.64	0.41
1:A:629:GLU:O	1:A:633:LYS:HB3	2.20	0.41
1:A:657:PRO:CB	1:A:659:GLU:HG3	2.49	0.41
1:A:9:THR:CG2	1:A:13:LYS:O	2.68	0.41
1:A:209:TYR:HB2	1:A:319:THR:HG23	2.03	0.41
1:A:372:PRO:HG3	1:A:380:ARG:HH12	1.84	0.41
1:A:377:TYR:CD2	1:A:381:LEU:HD11	2.56	0.41
1:A:421:PRO:HD2	1:A:422:ASP:H	1.86	0.41
1:A:446:ILE:O	1:A:447:PRO:C	2.63	0.41
1:A:658:PRO:HA	1:A:661:LEU:CD1	2.51	0.41
1:A:31:ASP:OD1	1:A:33:THR:N	2.48	0.41
1:A:44:ASP:O	1:A:45:ASP:C	2.63	0.41
1:A:214:PHE:O	1:A:215:ASP:C	2.62	0.41
1:A:228:ILE:O	1:A:228:ILE:HG22	2.20	0.41
1:A:438:VAL:CG1	1:A:440:HIS:CD2	3.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:ILE:HD13	1:A:483:ARG:HB2	2.02	0.41
1:A:126:LEU:O	1:A:359:ARG:NH2	2.54	0.41
1:A:389:PHE:HZ	1:A:523:GLU:HG3	1.86	0.41
1:A:252:VAL:HG12	1:A:252:VAL:O	2.21	0.41
1:A:630:THR:HG21	1:A:639:GLU:CG	2.46	0.41
1:A:749:PHE:CD1	1:A:749:PHE:N	2.88	0.41
1:A:307:ARG:O	1:A:310:LYS:HB3	2.21	0.40
1:A:437:GLN:NE2	1:A:519:ARG:NH2	2.53	0.40
1:A:598:ILE:HB	1:A:604:VAL:HG22	2.02	0.40
1:A:651:LEU:HD12	1:A:656:ILE:HD11	2.03	0.40
1:A:141:ASP:OD1	1:A:315:ASP:CG	2.57	0.40
1:A:169:ARG:HG3	1:A:169:ARG:NH1	2.32	0.40
1:A:234:ARG:C	1:A:236:GLY:H	2.28	0.40
1:A:303:GLU:HB3	1:A:304:ASN:H	1.54	0.40
1:A:473:ASP:OD2	1:A:475:ILE:HB	2.20	0.40
1:A:547:ALA:O	1:A:548:THR:HB	2.22	0.40
1:A:569:ASN:HD22	1:A:569:ASN:HA	1.62	0.40
1:A:95:THR:O	1:A:95:THR:HG22	2.20	0.40
1:A:119:ARG:HD3	1:A:119:ARG:C	2.47	0.40
1:A:291:TYR:N	1:A:291:TYR:CD2	2.88	0.40
1:A:294:GLU:OE1	1:A:294:GLU:C	2.65	0.40
1:A:390:VAL:HG12	1:A:592:LYS:HD3	2.03	0.40
1:A:418:ASN:HD21	1:A:447:PRO:C	2.29	0.40
1:A:473:ASP:OD2	1:A:474:PRO:N	2.54	0.40
1:A:755:ASP:C	1:A:757:ARG:N	2.77	0.40
1:A:196:ARG:O	1:A:196:ARG:HG2	2.20	0.40
1:A:312:SER:O	1:A:313:MET:C	2.64	0.40
1:A:391:LYS:HE2	1:A:526:TRP:HZ3	1.86	0.40
1:A:3:LEU:HD22	1:A:256:ILE:CD1	2.38	0.40
1:A:58:ARG:C	1:A:60:GLY:N	2.78	0.40
1:A:83:TRP:O	1:A:85:LEU:HD23	2.22	0.40
1:A:173:TRP:CD1	1:A:173:TRP:N	2.90	0.40
1:A:173:TRP:HB3	1:A:184:VAL:O	2.22	0.40
1:A:270:LEU:O	1:A:271:PRO:C	2.63	0.40
1:A:364:ARG:HD3	1:A:449:PHE:CE1	2.56	0.40
1:A:461:ARG:NE	1:A:488:LYS:HB2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	684/775 (88%)	503 (74%)	108 (16%)	73 (11%)	0 0

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ILE
1	A	59	HIS
1	A	67	ASP
1	A	76	LEU
1	A	131	GLY
1	A	147	HIS
1	A	177	ASP
1	A	185	SER
1	A	265	ARG
1	A	267	THR
1	A	285	LYS
1	A	286	PRO
1	A	288	GLU
1	A	290	VAL
1	A	292	ALA
1	A	298	ALA
1	A	303	GLU
1	A	304	ASN
1	A	383	GLU
1	A	384	SER
1	A	385	TYR
1	A	391	LYS
1	A	436	PRO
1	A	523	GLU
1	A	539	TYR
1	A	542	THR
1	A	690	LYS
1	A	693	LYS

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Mol	Chain	Res	Type
1	A	738	VAL
1	A	748	GLY
1	A	754	GLU
1	A	51	VAL
1	A	164	ASP
1	A	244	ILE
1	A	299	TRP
1	A	395	LYS
1	A	447	PRO
1	A	524	LEU
1	A	646	GLU
1	A	733	TYR
1	A	751	TYR
1	A	753	LYS
1	A	755	ASP
1	A	756	LEU
1	A	45	ASP
1	A	439	GLY
1	A	507	CYS
1	A	654	TYR
1	A	657	PRO
1	A	757	ARG
1	A	54	ILE
1	A	152	PHE
1	A	296	ALA
1	A	379	ARG
1	A	380	ARG
1	A	469	LYS
1	A	696	PRO
1	A	57	GLU
1	A	245	GLY
1	A	281	ALA
1	A	300	GLU
1	A	381	LEU
1	A	386	THR
1	A	390	VAL
1	A	639	GLU
1	A	732	TYR
1	A	556	GLU
1	A	692	VAL
1	A	745	ILE
1	A	68	VAL

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Mol	Chain	Res	Type
1	A	388	GLY
1	A	697	GLY
1	A	271	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	624/682 (92%)	480 (77%)	144 (23%)	1 1

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	13	LYS
1	A	27	LYS
1	A	29	GLU
1	A	33	THR
1	A	38	ILE
1	A	43	ARG
1	A	48	ILE
1	A	51	VAL
1	A	57	GLU
1	A	61	LYS
1	A	63	VAL
1	A	72	GLU
1	A	78	LYS
1	A	80	ILE
1	A	81	THR
1	A	85	LEU
1	A	88	GLU
1	A	93	VAL
1	A	95	THR
1	A	100	VAL
1	A	108	ASP
1	A	115	PRO

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Mol	Chain	Res	Type
1	A	132	GLU
1	A	150	GLU
1	A	154	LYS
1	A	167	GLU
1	A	169	ARG
1	A	174	LYS
1	A	175	ASN
1	A	177	ASP
1	A	182	GLU
1	A	186	THR
1	A	193	ARG
1	A	198	ILE
1	A	199	ARG
1	A	200	GLU
1	A	201	LYS
1	A	206	ILE
1	A	213	SER
1	A	224	GLU
1	A	230	LEU
1	A	231	THR
1	A	239	PRO
1	A	241	MET
1	A	242	GLN
1	A	244	ILE
1	A	251	GLU
1	A	252	VAL
1	A	255	ARG
1	A	263	VAL
1	A	264	ILE
1	A	265	ARG
1	A	266	THR
1	A	267	THR
1	A	270	LEU
1	A	274	THR
1	A	275	LEU
1	A	276	GLU
1	A	282	ILE
1	A	283	PHE
1	A	287	LYS
1	A	294	GLU
1	A	295	ILE
1	A	300	GLU

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Mol	Chain	Res	Type
1	A	303	GLU
1	A	305	LEU
1	A	306	GLU
1	A	307	ARG
1	A	313	MET
1	A	319	THR
1	A	327	LEU
1	A	335	ARG
1	A	337	VAL
1	A	364	ARG
1	A	374	GLU
1	A	378	GLN
1	A	381	LEU
1	A	383	GLU
1	A	397	LEU
1	A	401	ILE
1	A	402	VAL
1	A	416	THR
1	A	418	ASN
1	A	424	LEU
1	A	432	TYR
1	A	436	PRO
1	A	445	ASP
1	A	446	ILE
1	A	470	GLU
1	A	478	ILE
1	A	493	SER
1	A	517	TRP
1	A	519	ARG
1	A	537	VAL
1	A	542	THR
1	A	543	ASP
1	A	549	ILE
1	A	554	SER
1	A	555	GLU
1	A	557	ILE
1	A	559	LYS
1	A	560	LYS
1	A	566	LYS
1	A	568	ILE
1	A	570	SER
1	A	575	LEU

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Mol	Chain	Res	Type
1	A	578	LEU
1	A	597	VAL
1	A	598	ILE
1	A	603	LYS
1	A	606	THR
1	A	617	SER
1	A	627	VAL
1	A	628	LEU
1	A	629	GLU
1	A	630	THR
1	A	642	ARG
1	A	644	VAL
1	A	646	GLU
1	A	648	ILE
1	A	650	LYS
1	A	651	LEU
1	A	656	ILE
1	A	657	PRO
1	A	661	LEU
1	A	680	HIS
1	A	683	VAL
1	A	685	LYS
1	A	687	LEU
1	A	694	ILE
1	A	695	LYS
1	A	699	VAL
1	A	700	ILE
1	A	703	ILE
1	A	729	ASP
1	A	731	GLU
1	A	736	ASN
1	A	739	LEU
1	A	742	VAL
1	A	743	LEU
1	A	744	ARG
1	A	745	ILE
1	A	752	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS

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Mol	Chain	Res	Type
1	A	59	HIS
1	A	89	HIS
1	A	257	HIS
1	A	351	ASN
1	A	417	HIS
1	A	418	ASN
1	A	437	GLN
1	A	462	GLN
1	A	484	GLN
1	A	569	ASN
1	A	736	ASN
1	A	737	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	285:LYS	C	286:PRO	N	1.06

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	712/775 (91%)	0.30	38 (5%) 32 26	21, 59, 91, 101	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	299	TRP	7.0
1	A	687	LEU	5.7
1	A	389	PHE	4.8
1	A	390	VAL	4.5
1	A	617	SER	4.0
1	A	385	TYR	3.7
1	A	25	LYS	3.6
1	A	689	ALA	3.5
1	A	386	THR	3.5
1	A	699	VAL	3.4
1	A	388	GLY	3.4
1	A	694	ILE	3.3
1	A	24	GLY	3.2
1	A	691	GLY	3.2
1	A	48	ILE	2.8
1	A	703	ILE	2.8
1	A	148	GLU	2.6
1	A	681	VAL	2.6
1	A	300	GLU	2.6
1	A	688	ALA	2.6
1	A	168	ALA	2.5
1	A	387	GLY	2.5
1	A	149	GLY	2.5
1	A	682	ALA	2.4
1	A	376	GLU	2.4
1	A	704	VAL	2.4
1	A	702	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	298	ALA	2.3
1	A	244	ILE	2.3
1	A	54	ILE	2.2
1	A	65	ILE	2.2
1	A	692	VAL	2.2
1	A	59	HIS	2.1
1	A	662	ALA	2.1
1	A	297	LYS	2.1
1	A	680	HIS	2.1
1	A	51	VAL	2.0
1	A	661	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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
2	MN	A	1758	1/1	0.57	0.27	61,61,61,61	0
2	MN	A	1759	1/1	0.91	0.07	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.