Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 05:35 PM EDT

PDB ID	:	1GPB
Title	:	GLYCOGEN PHOSPHORYLASE B: DESCRIPTION OF THE PROTEIN STRUCTURE
Authors	:	Johnson, L.N.; Acharya, K.R.; Stuart, D.I.
Deposited on	:	1990-06-04
Resolution	:	1.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

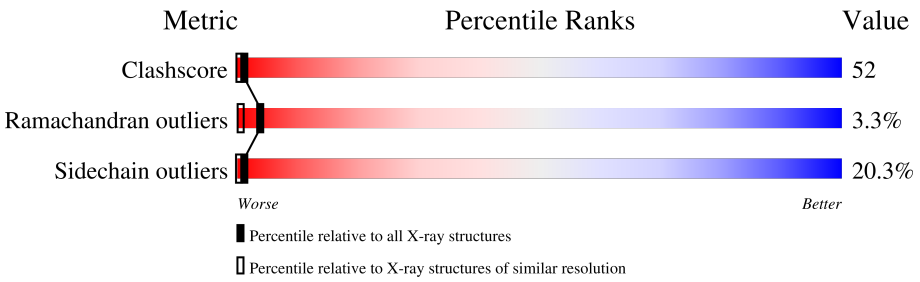
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	33% 39% 20% 6% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7397 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.

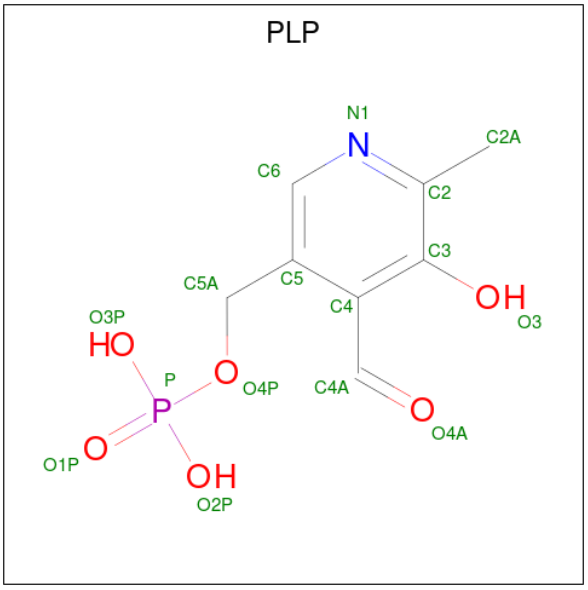
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	823	6691	4264	1178	1219	30	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	CONFLICT	UNP P00489

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	15	8	1	5	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	691	691	691	0	0

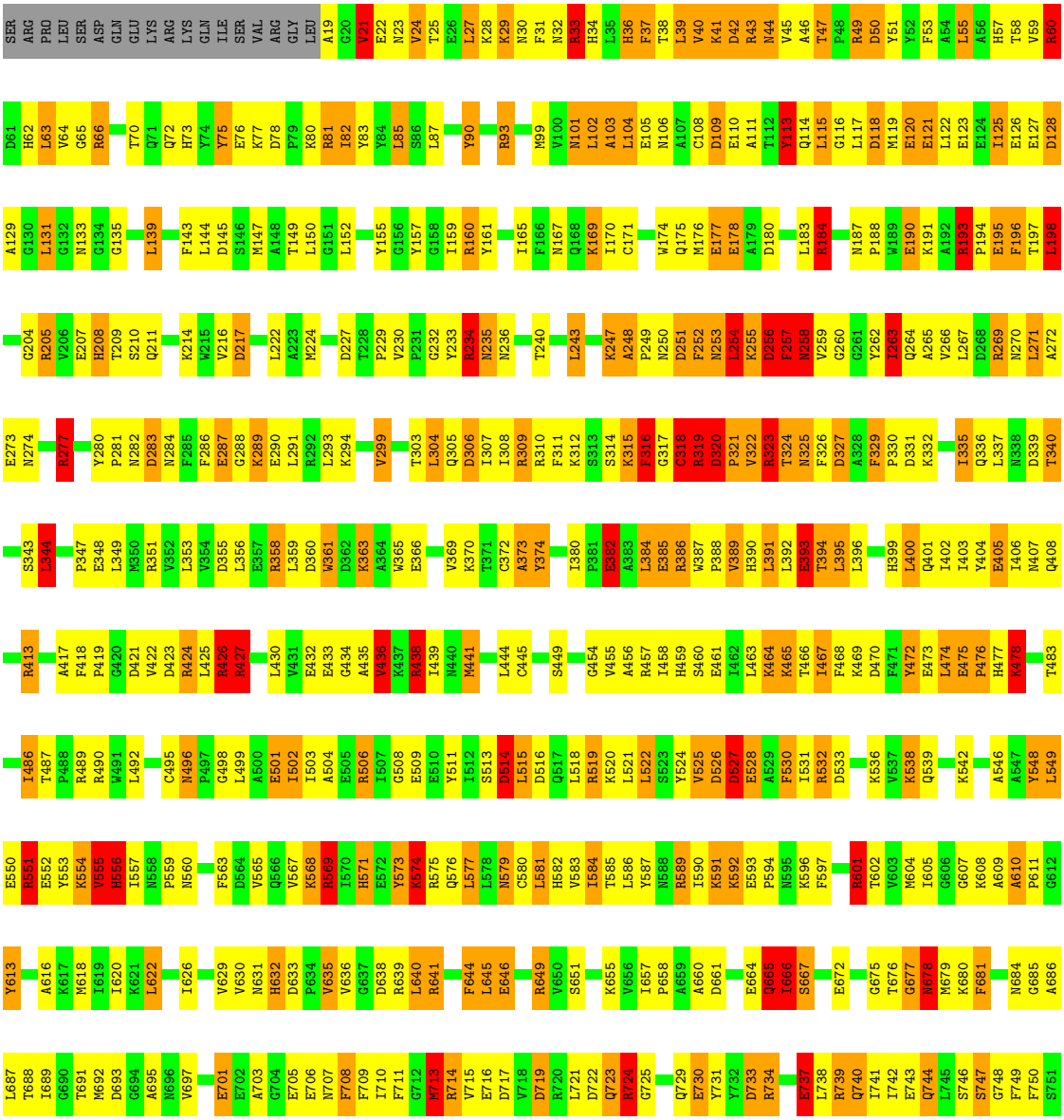
3 Residue-property plots (i)

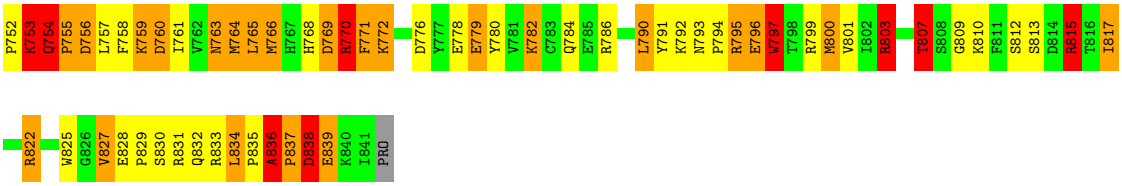
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: GLYCOGEN PHOSPHORYLASE B

Chain A: 33% 39% 20% 6% •




P752
K753
Q754
P755
D756
L757
F758
K759
D760
I761
V762
N763
M764
L765
M766
H767
H768
D769
R770
F771
K772
D776
Y777
E778
E779
Y780
V781
K782
C783
Q784
E785
R786
L790
Y791
K792
N793
P794
R795
E796
W797
T798
R799
M800
V801
I802
R803
T807
S808
G809
K810
F811
S812
S813
D814
R815
T816
I817
R822
W825
G826
V827
E828
P829
S830
R831
Q832
R833
L834
P835
A836
P837
D838
E839
K840
I841
PRO

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	128.50Å 128.50Å 116.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7397	wwPDB-VP
Average B, all atoms ($Å^2$)	38.0	wwPDB-VP

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: PLP

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	1.17	9/6844 (0.1%)	2.25	299/9265 (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	17

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	372	CYS	CB-SG	7.59	1.95	1.82
1	A	490	ARG	NE-CZ	6.67	1.41	1.33
1	A	678	ASN	CA-CB	6.49	1.70	1.53
1	A	675	GLY	N-CA	5.75	1.54	1.46
1	A	195	GLU	CG-CD	-5.71	1.43	1.51
1	A	230	VAL	N-CA	5.51	1.57	1.46
1	A	496	ASN	N-CA	5.26	1.56	1.46
1	A	836	ALA	N-CA	-5.24	1.35	1.46
1	A	178	GLU	CD-OE2	-5.02	1.20	1.25

All (299) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	66	ARG	CD-NE-CZ	34.03	171.24	123.60
1	A	277	ARG	CD-NE-CZ	21.36	153.51	123.60
1	A	490	ARG	NE-CZ-NH2	-19.50	110.55	120.30
1	A	193	ARG	CD-NE-CZ	17.29	147.81	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	277	ARG	NE-CZ-NH1	16.17	128.39	120.30
1	A	207	GLU	CA-CB-CG	16.16	148.96	113.40
1	A	193	ARG	NE-CZ-NH1	15.86	128.23	120.30
1	A	269	ARG	NE-CZ-NH1	14.99	127.80	120.30
1	A	81	ARG	NE-CZ-NH1	13.99	127.30	120.30
1	A	384	LEU	CB-CA-C	13.96	136.72	110.20
1	A	506	ARG	NE-CZ-NH1	13.73	127.16	120.30
1	A	50	ASP	CB-CG-OD2	13.67	130.60	118.30
1	A	532	ARG	NE-CZ-NH1	13.46	127.03	120.30
1	A	386	ARG	NE-CZ-NH1	12.72	126.66	120.30
1	A	269	ARG	NE-CZ-NH2	-12.48	114.06	120.30
1	A	123	GLU	OE1-CD-OE2	-12.35	108.48	123.30
1	A	309	ARG	CA-CB-CG	12.17	140.17	113.40
1	A	93	ARG	NE-CZ-NH1	12.10	126.35	120.30
1	A	478	LYS	CA-CB-CG	11.73	139.22	113.40
1	A	519	ARG	NE-CZ-NH2	11.73	126.16	120.30
1	A	198	LEU	CA-CB-CG	11.40	141.52	115.30
1	A	50	ASP	CB-CG-OD1	-11.40	108.04	118.30
1	A	665	GLN	CB-CA-C	11.28	132.96	110.40
1	A	309	ARG	CD-NE-CZ	11.06	139.08	123.60
1	A	575	ARG	NE-CZ-NH1	11.05	125.83	120.30
1	A	438	ARG	CD-NE-CZ	10.98	138.97	123.60
1	A	321	PRO	N-CA-C	10.87	140.35	112.10
1	A	822	ARG	NE-CZ-NH1	-10.61	114.99	120.30
1	A	834	LEU	CB-CA-C	10.57	130.29	110.20
1	A	839	GLU	CB-CG-CD	10.44	142.38	114.20
1	A	490	ARG	NH1-CZ-NH2	10.24	130.67	119.40
1	A	556	HIS	N-CA-CB	10.19	128.93	110.60
1	A	475	GLU	OE1-CD-OE2	-10.07	111.21	123.30
1	A	33	ARG	NE-CZ-NH1	-10.03	115.29	120.30
1	A	586	LEU	CA-CB-CG	9.87	138.00	115.30
1	A	835	PRO	C-N-CA	9.81	146.22	121.70
1	A	532	ARG	CD-NE-CZ	9.78	137.29	123.60
1	A	33	ARG	CD-NE-CZ	-9.62	110.14	123.60
1	A	310	ARG	NE-CZ-NH1	-9.56	115.52	120.30
1	A	413	ARG	NE-CZ-NH2	-9.53	115.54	120.30
1	A	678	ASN	N-CA-CB	-9.48	93.53	110.60
1	A	569	ARG	NE-CZ-NH2	-9.41	115.59	120.30
1	A	731	TYR	CB-CG-CD1	-9.40	115.36	121.00
1	A	815	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	A	836	ALA	N-CA-C	9.19	135.81	111.00
1	A	632	HIS	CA-CB-CG	-9.18	97.99	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ASP	CB-CG-OD2	-9.05	110.15	118.30
1	A	178	GLU	CA-CB-CG	8.79	132.75	113.40
1	A	770	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	A	117	LEU	N-CA-C	8.79	134.73	111.00
1	A	519	ARG	CA-CB-CG	8.78	132.71	113.40
1	A	822	ARG	CD-NE-CZ	-8.74	111.37	123.60
1	A	340	THR	OG1-CB-CG2	8.74	130.09	110.00
1	A	506	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	A	66	ARG	NE-CZ-NH2	8.71	124.65	120.30
1	A	118	ASP	CB-CG-OD2	8.69	126.12	118.30
1	A	475	GLU	CG-CD-OE1	8.62	135.53	118.30
1	A	554	LYS	N-CA-CB	8.56	126.01	110.60
1	A	115	LEU	CA-CB-CG	8.44	134.70	115.30
1	A	807	THR	N-CA-CB	-8.43	94.28	110.30
1	A	526	ASP	N-CA-C	-8.32	88.52	111.00
1	A	791	TYR	CB-CG-CD1	8.30	125.98	121.00
1	A	81	ARG	NE-CZ-NH2	-8.27	116.16	120.30
1	A	340	THR	N-CA-CB	-8.24	94.64	110.30
1	A	113	TYR	CB-CG-CD1	-8.24	116.06	121.00
1	A	90	TYR	CB-CG-CD2	-8.23	116.06	121.00
1	A	160	ARG	NE-CZ-NH2	8.22	124.41	120.30
1	A	78	ASP	CB-CG-OD1	8.20	125.68	118.30
1	A	586	LEU	CB-CA-C	8.18	125.75	110.20
1	A	472	TYR	CB-CG-CD2	-8.07	116.16	121.00
1	A	24	VAL	CA-CB-CG2	8.03	122.95	110.90
1	A	646	GLU	CA-CB-CG	8.01	131.02	113.40
1	A	269	ARG	CD-NE-CZ	8.00	134.80	123.60
1	A	478	LYS	CG-CD-CE	7.98	135.84	111.90
1	A	90	TYR	CB-CG-CD1	7.96	125.77	121.00
1	A	803	ARG	CD-NE-CZ	-7.91	112.53	123.60
1	A	208	HIS	CA-CB-CG	-7.85	100.25	113.60
1	A	686	ALA	CB-CA-C	7.84	121.87	110.10
1	A	83	TYR	CB-CG-CD1	-7.76	116.34	121.00
1	A	43	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	A	737	GLU	CA-CB-CG	7.62	130.16	113.40
1	A	287	GLU	CA-CB-CG	7.60	130.12	113.40
1	A	610	ALA	CB-CA-C	7.60	121.49	110.10
1	A	800	MET	CG-SD-CE	7.58	112.33	100.20
1	A	589	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	A	254	LEU	CA-CB-CG	7.53	132.62	115.30
1	A	93	ARG	NH1-CZ-NH2	-7.46	111.20	119.40
1	A	42	ASP	CB-CG-OD1	7.43	124.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	310	ARG	CD-NE-CZ	-7.35	113.31	123.60
1	A	386	ARG	CD-NE-CZ	7.33	133.87	123.60
1	A	145	ASP	CB-CG-OD1	7.32	124.89	118.30
1	A	740	GLN	CB-CG-CD	7.30	130.57	111.60
1	A	360	ASP	N-CA-CB	-7.29	97.48	110.60
1	A	128	ASP	CB-CG-OD1	-7.28	111.75	118.30
1	A	253	ASN	N-CA-CB	-7.27	97.51	110.60
1	A	113	TYR	CB-CG-CD2	7.26	125.36	121.00
1	A	649	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	A	490	ARG	CD-NE-CZ	-7.19	113.53	123.60
1	A	511	TYR	CB-CG-CD1	7.15	125.29	121.00
1	A	807	THR	OG1-CB-CG2	7.12	126.37	110.00
1	A	323	ARG	C-N-CA	7.11	139.49	121.70
1	A	62	HIS	CA-CB-CG	-7.08	101.56	113.60
1	A	800	MET	CA-CB-CG	-7.08	101.26	113.30
1	A	438	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	A	37	PHE	CB-CG-CD1	-7.04	115.88	120.80
1	A	234	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	A	731	TYR	CB-CG-CD2	7.03	125.22	121.00
1	A	118	ASP	N-CA-CB	7.00	123.20	110.60
1	A	230	VAL	CA-CB-CG2	6.97	121.35	110.90
1	A	838	ASP	N-CA-C	6.96	129.80	111.00
1	A	321	PRO	CA-C-N	6.94	132.47	117.20
1	A	589	ARG	CD-NE-CZ	6.93	133.30	123.60
1	A	310	ARG	NE-CZ-NH2	6.92	123.76	120.30
1	A	324	THR	N-CA-CB	6.92	123.44	110.30
1	A	121	GLU	CA-CB-CG	6.91	128.60	113.40
1	A	160	ARG	CD-NE-CZ	-6.90	113.94	123.60
1	A	678	ASN	CA-CB-CG	-6.86	98.31	113.40
1	A	527	ASP	N-CA-CB	6.84	122.91	110.60
1	A	509	GLU	N-CA-C	6.80	129.37	111.00
1	A	601	ARG	CA-CB-CG	6.80	128.35	113.40
1	A	613	TYR	N-CA-C	-6.79	92.68	111.00
1	A	316	PHE	N-CA-CB	6.78	122.80	110.60
1	A	772	LYS	N-CA-CB	-6.76	98.44	110.60
1	A	344	LEU	CA-CB-CG	6.75	130.83	115.30
1	A	719	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	A	769	ASP	CB-CG-OD1	-6.67	112.30	118.30
1	A	551	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	A	714	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	A	457	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	803	ARG	NE-CZ-NH1	6.52	123.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	501	GLU	O-C-N	6.52	133.13	122.70
1	A	639	ARG	CB-CA-C	6.51	123.42	110.40
1	A	424	ARG	CD-NE-CZ	-6.51	114.49	123.60
1	A	190	GLU	OE1-CD-OE2	-6.50	115.50	123.30
1	A	190	GLU	CG-CD-OE2	6.50	131.30	118.30
1	A	609	ALA	CB-CA-C	-6.48	100.38	110.10
1	A	248	ALA	N-CA-CB	-6.43	101.10	110.10
1	A	178	GLU	CB-CA-C	6.40	123.21	110.40
1	A	526	ASP	CB-CA-C	6.40	123.20	110.40
1	A	532	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	234	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	666	ILE	N-CA-C	6.38	128.24	111.00
1	A	753	LYS	N-CA-CB	-6.38	99.11	110.60
1	A	571	HIS	CA-CB-CG	6.38	124.45	113.60
1	A	613	TYR	CB-CG-CD2	-6.38	117.17	121.00
1	A	217	ASP	CB-CA-C	6.37	123.14	110.40
1	A	834	LEU	CA-CB-CG	6.35	129.91	115.30
1	A	331	ASP	CB-CA-C	6.34	123.07	110.40
1	A	646	GLU	CB-CA-C	-6.33	97.73	110.40
1	A	555	VAL	CA-CB-CG1	6.31	120.36	110.90
1	A	613	TYR	CB-CG-CD1	6.28	124.77	121.00
1	A	348	GLU	CA-CB-CG	6.27	127.20	113.40
1	A	678	ASN	CA-C-O	6.26	133.26	120.10
1	A	316	PHE	N-CA-C	-6.25	94.13	111.00
1	A	433	GLU	CA-CB-CG	6.23	127.11	113.40
1	A	427	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	178	GLU	CG-CD-OE1	-6.18	105.94	118.30
1	A	472	TYR	CA-CB-CG	-6.17	101.67	113.40
1	A	224	MET	N-CA-CB	-6.17	99.50	110.60
1	A	299	VAL	CG1-CB-CG2	-6.14	101.08	110.90
1	A	373	ALA	N-CA-CB	6.13	118.69	110.10
1	A	574	LYS	CB-CG-CD	-6.13	95.66	111.60
1	A	739	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	A	374	TYR	CB-CG-CD2	6.12	124.67	121.00
1	A	257	PHE	CA-C-O	6.11	132.94	120.10
1	A	360	ASP	CB-CG-OD2	-6.11	112.81	118.30
1	A	63	LEU	N-CA-CB	-6.09	98.23	110.40
1	A	456	ALA	N-CA-CB	6.09	118.62	110.10
1	A	677	GLY	C-N-CA	6.05	136.83	121.70
1	A	514	ASP	CB-CA-C	6.03	122.46	110.40
1	A	436	VAL	N-CA-CB	6.02	124.75	111.50
1	A	713	MET	CG-SD-CE	-5.99	90.62	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	701	GLU	CB-CA-C	5.98	122.35	110.40
1	A	797	TRP	CA-CB-CG	5.95	125.00	113.70
1	A	160	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	A	666	ILE	CB-CG1-CD1	5.93	130.51	113.90
1	A	109	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	331	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	272	ALA	CB-CA-C	5.91	118.97	110.10
1	A	782	LYS	CB-CA-C	5.90	122.20	110.40
1	A	532	ARG	O-C-N	5.89	132.12	122.70
1	A	257	PHE	C-N-CA	5.88	136.40	121.70
1	A	265	ALA	CB-CA-C	-5.88	101.28	110.10
1	A	516	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	601	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	836	ALA	CB-CA-C	-5.86	101.31	110.10
1	A	75	TYR	CB-CG-CD1	-5.86	117.49	121.00
1	A	506	ARG	CD-NE-CZ	5.86	131.80	123.60
1	A	247	LYS	CB-CA-C	5.84	122.07	110.40
1	A	779	GLU	CA-CB-CG	5.83	126.23	113.40
1	A	120	GLU	CG-CD-OE2	5.83	129.96	118.30
1	A	325	ASN	CA-CB-CG	-5.81	100.61	113.40
1	A	754	GLN	CB-CA-C	-5.80	98.79	110.40
1	A	589	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	573	TYR	CG-CD1-CE1	5.73	125.89	121.30
1	A	252	PHE	CA-C-O	5.73	132.13	120.10
1	A	725	GLY	N-CA-C	-5.72	98.81	113.10
1	A	495	CYS	O-C-N	5.71	131.84	122.70
1	A	438	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	184	ARG	CD-NE-CZ	5.70	131.57	123.60
1	A	519	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	A	538	LYS	CG-CD-CE	5.70	128.98	111.90
1	A	321	PRO	CA-C-O	-5.69	106.54	120.20
1	A	722	ASP	O-C-N	5.69	131.81	122.70
1	A	433	GLU	N-CA-CB	5.69	120.84	110.60
1	A	129	ALA	N-CA-C	-5.68	95.66	111.00
1	A	198	LEU	N-CA-CB	-5.68	99.03	110.40
1	A	318	CYS	CB-CA-C	5.68	121.76	110.40
1	A	511	TYR	CB-CG-CD2	-5.68	117.59	121.00
1	A	454	GLY	N-CA-C	-5.67	98.92	113.10
1	A	257	PHE	N-CA-C	-5.66	95.71	111.00
1	A	83	TYR	CB-CG-CD2	5.66	124.39	121.00
1	A	277	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	791	TYR	CB-CG-CD2	-5.66	117.61	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	681	PHE	CB-CG-CD1	-5.65	116.85	120.80
1	A	66	ARG	NH1-CZ-NH2	-5.64	113.19	119.40
1	A	234	ARG	N-CA-CB	-5.63	100.47	110.60
1	A	325	ASN	CB-CA-C	5.62	121.64	110.40
1	A	457	ARG	CB-CA-C	5.62	121.64	110.40
1	A	771	PHE	CB-CA-C	5.62	121.63	110.40
1	A	526	ASP	N-CA-CB	5.59	120.67	110.60
1	A	489	ARG	CD-NE-CZ	5.58	131.41	123.60
1	A	577	LEU	O-C-N	5.57	131.62	122.70
1	A	27	LEU	CA-CB-CG	5.56	128.09	115.30
1	A	519	ARG	N-CA-CB	5.54	120.58	110.60
1	A	723	GLN	CB-CA-C	5.54	121.48	110.40
1	A	573	TYR	CB-CG-CD2	5.53	124.32	121.00
1	A	121	GLU	N-CA-CB	5.52	120.54	110.60
1	A	739	ARG	CD-NE-CZ	5.49	131.28	123.60
1	A	81	ARG	O-C-N	5.48	131.46	122.70
1	A	731	TYR	CA-CB-CG	-5.47	103.01	113.40
1	A	551	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	252	PHE	CA-C-N	-5.46	105.19	117.20
1	A	822	ARG	O-C-N	5.45	131.42	122.70
1	A	639	ARG	CG-CD-NE	5.45	123.24	111.80
1	A	256	ASP	CB-CG-OD1	-5.43	113.41	118.30
1	A	135	GLY	N-CA-C	5.41	126.63	113.10
1	A	382	GLU	CG-CD-OE2	-5.39	107.52	118.30
1	A	553	TYR	C-N-CA	5.38	135.15	121.70
1	A	324	THR	N-CA-C	-5.37	96.50	111.00
1	A	358	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	807	THR	CA-CB-CG2	5.36	119.91	112.40
1	A	114	GLN	CB-CG-CD	5.35	125.52	111.60
1	A	724	ARG	CA-CB-CG	5.35	125.17	113.40
1	A	316	PHE	CB-CA-C	-5.35	99.70	110.40
1	A	744	GLN	CA-CB-CG	5.34	125.14	113.40
1	A	39	LEU	O-C-N	5.32	131.21	122.70
1	A	701	GLU	CA-CB-CG	5.32	125.10	113.40
1	A	193	ARG	NH1-CZ-NH2	-5.32	113.55	119.40
1	A	40	VAL	N-CA-CB	-5.31	99.82	111.50
1	A	322	VAL	N-CA-CB	5.30	123.17	111.50
1	A	113	TYR	N-CA-CB	5.29	120.12	110.60
1	A	587	TYR	CB-CG-CD1	-5.29	117.83	121.00
1	A	766	MET	CB-CA-C	-5.28	99.84	110.40
1	A	263	ILE	O-C-N	5.28	131.15	122.70
1	A	430	LEU	CB-CA-C	-5.28	100.17	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	831	ARG	CD-NE-CZ	5.26	130.97	123.60
1	A	251	ASP	N-CA-C	5.25	125.16	111.00
1	A	393	GLU	CA-CB-CG	5.24	124.93	113.40
1	A	796	GLU	CB-CA-C	5.24	120.87	110.40
1	A	139	LEU	CA-CB-CG	-5.23	103.27	115.30
1	A	230	VAL	CG1-CB-CG2	-5.22	102.55	110.90
1	A	339	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	257	PHE	CA-C-N	-5.21	105.73	117.20
1	A	489	ARG	CB-CA-C	5.21	120.81	110.40
1	A	133	ASN	O-C-N	5.21	132.05	123.20
1	A	608	LYS	O-C-N	5.20	131.02	122.70
1	A	509	GLU	CB-CA-C	-5.20	100.00	110.40
1	A	436	VAL	CA-C-N	-5.19	105.78	117.20
1	A	312	LYS	CB-CA-C	-5.18	100.04	110.40
1	A	386	ARG	NH1-CZ-NH2	-5.17	113.71	119.40
1	A	103	ALA	N-CA-CB	-5.17	102.87	110.10
1	A	556	HIS	CA-C-N	-5.16	105.84	117.20
1	A	385	GLU	CG-CD-OE2	-5.16	107.97	118.30
1	A	649	ARG	N-CA-CB	-5.16	101.31	110.60
1	A	87	LEU	CB-CA-C	5.16	120.00	110.20
1	A	646	GLU	OE1-CD-OE2	-5.15	117.12	123.30
1	A	734	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	737	GLU	N-CA-CB	5.14	119.85	110.60
1	A	120	GLU	OE1-CD-OE2	-5.14	117.13	123.30
1	A	101	ASN	CB-CA-C	5.12	120.65	110.40
1	A	254	LEU	CB-CA-C	5.12	119.94	110.20
1	A	329	PHE	CB-CA-C	5.12	120.64	110.40
1	A	502	ILE	CA-CB-CG1	5.10	120.69	111.00
1	A	207	GLU	N-CA-CB	5.10	119.77	110.60
1	A	348	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	A	283	ASP	N-CA-CB	-5.09	101.44	110.60
1	A	644	PHE	CB-CG-CD2	-5.08	117.25	120.80
1	A	472	TYR	CB-CG-CD1	5.07	124.04	121.00
1	A	51	TYR	CB-CA-C	5.06	120.52	110.40
1	A	149	THR	CA-CB-CG2	5.06	119.49	112.40
1	A	602	THR	N-CA-C	-5.06	97.34	111.00
1	A	675	GLY	N-CA-C	-5.06	100.45	113.10
1	A	317	GLY	CA-C-N	-5.05	106.09	117.20
1	A	21	VAL	N-CA-C	5.04	124.61	111.00
1	A	82	ILE	O-C-N	5.04	130.76	122.70
1	A	677	GLY	N-CA-C	-5.04	100.50	113.10
1	A	176	MET	O-C-N	5.04	130.76	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	835	PRO	CA-C-O	5.00	132.21	120.20

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	ARG	Sidechain
1	A	234	ARG	Sidechain
1	A	323	ARG	Sidechain
1	A	33	ARG	Sidechain
1	A	358	ARG	Sidechain
1	A	413	ARG	Sidechain
1	A	426	ARG	Sidechain
1	A	427	ARG	Sidechain
1	A	49	ARG	Sidechain
1	A	569	ARG	Sidechain
1	A	60	ARG	Sidechain
1	A	601	ARG	Sidechain
1	A	649	ARG	Sidechain
1	A	770	ARG	Sidechain
1	A	803	ARG	Sidechain
1	A	822	ARG	Sidechain
1	A	833	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6691	0	6614	696	1
2	A	15	0	7	1	0
3	A	691	0	0	56	0
All	All	7397	0	6621	696	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 52.

All (696) 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:99:MET:CE	1:A:119:MET:HE1	1.37	1.51
1:A:99:MET:HE1	1:A:119:MET:CE	1.41	1.46
1:A:666:ILE:HG21	1:A:711:PHE:CZ	1.53	1.44
1:A:320:ASP:HB3	1:A:321:PRO:CD	1.48	1.36
1:A:320:ASP:CB	1:A:321:PRO:HD3	1.55	1.36
1:A:584:ILE:HD11	1:A:741:ILE:CD1	1.61	1.31
1:A:322:VAL:HG11	1:A:325:ASN:CB	1.63	1.29
1:A:322:VAL:CG1	1:A:325:ASN:HB2	1.65	1.26
1:A:160:ARG:NH1	1:A:190:GLU:OE1	1.70	1.24
1:A:251:ASP:O	1:A:255:LYS:N	1.71	1.20
1:A:756:ASP:HB2	1:A:759:LYS:CE	1.71	1.20
1:A:666:ILE:CG2	1:A:711:PHE:HZ	1.56	1.19
1:A:549:LEU:C	1:A:555:VAL:HG21	1.64	1.16
1:A:666:ILE:CG2	1:A:711:PHE:CZ	2.29	1.16
1:A:474:LEU:HD13	1:A:474:LEU:O	1.48	1.14
1:A:256:ASP:HB2	1:A:258:ASN:HB2	1.30	1.13
1:A:474:LEU:HD12	1:A:475:GLU:HG3	1.24	1.13
1:A:687:LEU:HD21	1:A:801:VAL:HG23	1.31	1.11
1:A:832:GLN:HG3	3:A:1038:HOH:O	1.49	1.10
1:A:404:TYR:HB3	3:A:1267:HOH:O	1.50	1.10
1:A:160:ARG:HH12	1:A:190:GLU:CD	1.55	1.09
1:A:555:VAL:HG13	1:A:557:ILE:HG23	1.21	1.08
1:A:474:LEU:O	1:A:474:LEU:CD1	2.01	1.07
1:A:85:LEU:HG	1:A:335:ILE:HD13	1.38	1.06
1:A:687:LEU:HD21	1:A:801:VAL:CG2	1.85	1.06
1:A:723:GLN:HA	3:A:1375:HOH:O	1.54	1.05
1:A:536:LYS:HD2	1:A:539:GLN:HE21	1.18	1.04
1:A:584:ILE:CD1	1:A:741:ILE:HD13	1.88	1.04
1:A:198:LEU:HD21	1:A:305:GLN:CB	1.87	1.03
1:A:527:ASP:O	1:A:531:ILE:HD13	1.60	1.02
1:A:311:PHE:CE1	1:A:316:PHE:HE2	1.76	1.02
1:A:316:PHE:HD1	1:A:319:ARG:CB	1.72	1.02
1:A:316:PHE:CD1	1:A:319:ARG:HG3	1.94	1.02
1:A:518:LEU:O	1:A:521:LEU:HB2	1.60	1.02
1:A:555:VAL:CG1	1:A:557:ILE:HG23	1.91	1.01
1:A:198:LEU:HD21	1:A:305:GLN:HB2	1.44	1.00
1:A:778:GLU:HB3	3:A:1540:HOH:O	1.60	1.00
1:A:256:ASP:CB	1:A:258:ASN:HB2	1.92	0.99
1:A:99:MET:CE	1:A:119:MET:CE	2.14	0.98
1:A:325:ASN:HD22	1:A:326:PHE:H	1.12	0.98
1:A:106:ASN:OD1	3:A:1406:HOH:O	1.81	0.97
1:A:316:PHE:HD1	1:A:319:ARG:CG	1.76	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:MET:CE	1:A:108:CYS:CB	2.43	0.96
1:A:43:ARG:NH1	3:A:1002:HOH:O	1.94	0.96
1:A:316:PHE:HE1	1:A:319:ARG:NE	1.63	0.96
1:A:756:ASP:HB2	1:A:759:LYS:HE3	1.45	0.96
1:A:426:ARG:NH1	1:A:427:ARG:HG3	1.81	0.95
1:A:314:SER:HB3	3:A:1581:HOH:O	1.65	0.95
1:A:82:ILE:HD11	1:A:827:VAL:HG21	1.49	0.95
1:A:427:ARG:NH1	1:A:470:ASP:OD1	1.99	0.95
1:A:719:ASP:O	1:A:723:GLN:HG3	1.67	0.95
1:A:549:LEU:HB3	1:A:555:VAL:HG21	1.47	0.95
1:A:24:VAL:HG12	1:A:28:LYS:HE2	1.49	0.94
1:A:251:ASP:O	1:A:254:LEU:C	2.05	0.94
1:A:316:PHE:CE1	1:A:319:ARG:NE	2.36	0.94
1:A:426:ARG:HH12	1:A:427:ARG:CG	1.81	0.94
1:A:742:ILE:HG21	1:A:766:MET:HE3	1.48	0.94
1:A:834:LEU:HD23	1:A:836:ALA:HB2	1.48	0.93
1:A:108:CYS:HB3	1:A:119:MET:CE	1.98	0.93
1:A:252:PHE:C	1:A:254:LEU:H	1.66	0.92
1:A:150:LEU:HD12	1:A:817:ILE:HG22	1.52	0.92
1:A:536:LYS:HD2	1:A:539:GLN:NE2	1.83	0.92
1:A:593:GLU:OE2	1:A:596:LYS:HD2	1.69	0.92
1:A:678:ASN:HB3	1:A:679:MET:HG3	1.52	0.92
1:A:646:GLU:HG3	3:A:1127:HOH:O	1.68	0.92
1:A:666:ILE:HG23	1:A:691:THR:HG23	1.51	0.91
1:A:108:CYS:HB3	1:A:119:MET:HE3	1.52	0.91
1:A:549:LEU:C	1:A:555:VAL:CG2	2.39	0.91
1:A:584:ILE:HD11	1:A:741:ILE:HD13	0.93	0.90
1:A:421:ASP:O	1:A:425:LEU:HD13	1.70	0.90
1:A:361:TRP:CH2	1:A:406:ILE:HD13	2.05	0.90
1:A:316:PHE:CD1	1:A:319:ARG:CG	2.53	0.90
1:A:550:GLU:N	1:A:555:VAL:HG21	1.87	0.90
1:A:256:ASP:HB2	1:A:258:ASN:CB	2.01	0.90
1:A:779:GLU:HG2	3:A:1684:HOH:O	1.72	0.89
1:A:335:ILE:HD11	1:A:337:LEU:HD13	1.55	0.89
1:A:463:LEU:CD2	1:A:467:ILE:HD11	2.02	0.88
1:A:252:PHE:HA	1:A:255:LYS:HB2	1.54	0.87
1:A:271:LEU:O	1:A:274:ASN:HB2	1.74	0.87
1:A:435:ALA:O	1:A:436:VAL:HG23	1.75	0.87
1:A:304:LEU:O	1:A:308:ILE:HG12	1.73	0.86
1:A:311:PHE:CE1	1:A:316:PHE:CE2	2.63	0.86
1:A:211:GLN:O	3:A:1068:HOH:O	1.94	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:TYR:CD2	1:A:655:LYS:HE2	2.09	0.86
1:A:474:LEU:HD12	1:A:475:GLU:CG	2.05	0.86
1:A:551:ARG:HG3	1:A:552:GLU:H	1.41	0.85
1:A:790:LEU:O	1:A:790:LEU:CD1	2.24	0.85
1:A:316:PHE:HA	1:A:319:ARG:HB2	1.58	0.85
1:A:198:LEU:HD23	1:A:305:GLN:CD	1.96	0.85
1:A:252:PHE:HA	1:A:255:LYS:CB	2.07	0.85
1:A:666:ILE:CG2	1:A:691:THR:HG23	2.05	0.85
1:A:790:LEU:O	1:A:790:LEU:HD13	1.75	0.85
1:A:455:VAL:H	1:A:459:HIS:HD2	1.24	0.85
1:A:546:ALA:HB2	1:A:557:ILE:HD11	1.58	0.85
1:A:752:PRO:HB2	1:A:753:LYS:HZ3	1.42	0.85
1:A:474:LEU:CD1	1:A:474:LEU:C	2.41	0.84
1:A:252:PHE:CA	1:A:255:LYS:HB2	2.08	0.84
1:A:80:LYS:HE2	1:A:825:TRP:O	1.78	0.84
1:A:752:PRO:HB2	1:A:753:LYS:NZ	1.92	0.84
1:A:759:LYS:O	1:A:763:ASN:ND2	2.10	0.83
1:A:549:LEU:HB3	1:A:555:VAL:CG2	2.06	0.83
1:A:515:LEU:HB3	1:A:809:GLY:HA2	1.61	0.82
1:A:584:ILE:HD13	1:A:585:THR:N	1.94	0.82
1:A:549:LEU:CB	1:A:555:VAL:HG21	2.09	0.82
1:A:311:PHE:CZ	1:A:316:PHE:CE2	2.68	0.82
1:A:102:LEU:HB3	1:A:104:LEU:HD22	1.62	0.82
1:A:426:ARG:HH12	1:A:427:ARG:HG3	1.38	0.81
1:A:756:ASP:HB2	1:A:759:LYS:CD	2.11	0.81
1:A:63:LEU:HD21	1:A:229:PRO:HG3	1.62	0.81
1:A:85:LEU:HG	1:A:335:ILE:CD1	2.10	0.81
1:A:555:VAL:HG12	1:A:556:HIS:H	1.45	0.81
1:A:322:VAL:O	1:A:323:ARG:HG2	1.81	0.81
1:A:316:PHE:CD1	1:A:319:ARG:CB	2.64	0.80
1:A:423:ASP:HB3	3:A:1289:HOH:O	1.81	0.80
1:A:266:VAL:O	1:A:269:ARG:HG3	1.82	0.80
1:A:311:PHE:CZ	1:A:316:PHE:HE2	1.98	0.80
1:A:549:LEU:CA	1:A:555:VAL:HG21	2.11	0.80
1:A:743:GLU:O	1:A:747:SER:OG	1.99	0.80
1:A:584:ILE:CD1	1:A:741:ILE:CD1	2.55	0.80
1:A:111:ALA:O	1:A:115:LEU:HD13	1.82	0.80
1:A:361:TRP:CZ2	1:A:406:ILE:HD13	2.16	0.80
1:A:463:LEU:HD22	1:A:467:ILE:HD11	1.63	0.79
1:A:579:ASN:O	1:A:583:VAL:HG23	1.83	0.79
1:A:322:VAL:CG2	1:A:325:ASN:OD1	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ILE:CG1	1:A:299:VAL:HG23	2.13	0.79
1:A:99:MET:CE	1:A:108:CYS:HB2	2.11	0.78
1:A:474:LEU:O	1:A:474:LEU:HD12	1.83	0.78
1:A:474:LEU:HD12	1:A:474:LEU:C	2.04	0.78
1:A:19:ALA:N	1:A:106:ASN:HB3	1.98	0.78
1:A:159:ILE:HG13	1:A:299:VAL:CG2	2.14	0.77
1:A:536:LYS:HE3	3:A:1321:HOH:O	1.82	0.77
1:A:661:ASP:O	1:A:797:TRP:HH2	1.66	0.77
1:A:316:PHE:CA	1:A:319:ARG:HB2	2.15	0.77
1:A:160:ARG:NH1	1:A:190:GLU:CD	2.28	0.77
1:A:236:ASN:ND2	1:A:834:LEU:O	2.12	0.77
1:A:99:MET:HE2	1:A:108:CYS:CB	2.15	0.77
1:A:322:VAL:HG21	1:A:325:ASN:OD1	1.84	0.77
1:A:402:ILE:O	1:A:406:ILE:HG12	1.85	0.77
1:A:75:TYR:HE1	3:A:1557:HOH:O	1.67	0.76
1:A:716:GLU:HA	3:A:1527:HOH:O	1.85	0.76
1:A:177:GLU:OE1	1:A:611:PRO:HG3	1.85	0.76
1:A:248:ALA:HB1	1:A:253:ASN:OD1	1.86	0.76
1:A:630:VAL:HG11	1:A:640:LEU:HD13	1.68	0.75
1:A:251:ASP:HB2	1:A:255:LYS:HG3	1.68	0.75
1:A:555:VAL:HG13	1:A:557:ILE:CG2	2.12	0.75
1:A:666:ILE:HG21	1:A:711:PHE:HZ	0.66	0.75
1:A:208:HIS:O	1:A:209:THR:OG1	2.05	0.74
1:A:340:THR:HG23	1:A:374:TYR:HE1	1.50	0.74
1:A:528:GLU:O	1:A:532:ARG:HG3	1.87	0.74
1:A:304:LEU:HD12	1:A:307:ILE:HD12	1.69	0.74
1:A:426:ARG:NH1	1:A:427:ARG:CG	2.46	0.74
1:A:327:ASP:HA	1:A:363:LYS:HZ1	1.53	0.74
1:A:380:ILE:O	1:A:384:LEU:HD12	1.87	0.74
1:A:756:ASP:HB2	1:A:759:LYS:HE2	1.67	0.74
1:A:314:SER:C	1:A:316:PHE:H	1.89	0.74
1:A:322:VAL:O	1:A:323:ARG:CG	2.35	0.73
1:A:549:LEU:HD23	1:A:557:ILE:HG21	1.70	0.73
1:A:322:VAL:HG11	1:A:325:ASN:HB2	0.78	0.73
1:A:43:ARG:HD3	3:A:1412:HOH:O	1.89	0.73
1:A:340:THR:HG23	1:A:374:TYR:CE1	2.23	0.73
1:A:729:GLN:O	1:A:733:ASP:HB2	1.88	0.73
1:A:756:ASP:HA	1:A:759:LYS:HG3	1.70	0.73
1:A:160:ARG:NH1	1:A:190:GLU:OE2	2.16	0.73
1:A:522:LEU:O	1:A:525:VAL:HG22	1.87	0.73
1:A:737:GLU:O	1:A:740:GLN:HG2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ILE:HD11	1:A:680:LYS:HE3	1.71	0.72
1:A:546:ALA:CB	1:A:557:ILE:HD11	2.18	0.72
1:A:589:ARG:NH2	1:A:737:GLU:OE1	2.22	0.72
1:A:834:LEU:HD23	1:A:836:ALA:CB	2.18	0.72
1:A:486:ILE:CD1	1:A:676:THR:HB	2.18	0.72
1:A:763:ASN:N	1:A:763:ASN:HD22	1.87	0.72
1:A:499:LEU:HD12	1:A:502:ILE:HD11	1.71	0.72
1:A:633:ASP:OD1	1:A:635:VAL:HG23	1.89	0.72
1:A:198:LEU:HD21	1:A:305:GLN:HB3	1.70	0.71
1:A:498:GLY:O	1:A:501:GLU:HB3	1.90	0.71
1:A:19:ALA:HB1	3:A:1206:HOH:O	1.89	0.71
1:A:76:GLU:HA	1:A:315:LYS:NZ	2.05	0.71
1:A:21:VAL:HG23	3:A:1592:HOH:O	1.91	0.71
1:A:108:CYS:CB	1:A:119:MET:HE1	2.19	0.71
1:A:665:GLN:NE2	3:A:1400:HOH:O	2.22	0.71
1:A:31:PHE:CD2	1:A:115:LEU:HD21	2.26	0.71
1:A:30:ASN:HB3	1:A:58:THR:HG23	1.73	0.70
1:A:82:ILE:HD13	1:A:825:TRP:CE3	2.25	0.70
1:A:325:ASN:HD22	1:A:326:PHE:N	1.86	0.70
1:A:630:VAL:HG11	1:A:640:LEU:CD1	2.22	0.70
1:A:549:LEU:HB3	1:A:555:VAL:CG1	2.22	0.70
1:A:742:ILE:CG2	1:A:766:MET:HE3	2.22	0.70
1:A:198:LEU:HD23	1:A:305:GLN:NE2	2.06	0.70
1:A:335:ILE:HD11	1:A:337:LEU:CD1	2.22	0.70
1:A:687:LEU:CD2	1:A:801:VAL:CG2	2.69	0.70
1:A:75:TYR:O	1:A:315:LYS:HE3	1.92	0.69
1:A:193:ARG:HD3	1:A:196:PHE:HE2	1.57	0.69
1:A:604:MET:HB3	1:A:645:LEU:HD22	1.73	0.69
1:A:288:GLY:C	1:A:289:LYS:HD2	2.13	0.69
1:A:661:ASP:O	1:A:797:TRP:CH2	2.45	0.69
1:A:752:PRO:CB	1:A:753:LYS:HZ3	2.04	0.69
1:A:460:SER:O	1:A:464:LYS:HG3	1.91	0.69
1:A:252:PHE:C	1:A:254:LEU:N	2.45	0.69
1:A:551:ARG:CG	1:A:552:GLU:H	2.05	0.69
1:A:99:MET:HE2	1:A:108:CYS:HB2	1.73	0.69
1:A:250:ASN:HA	1:A:269:ARG:NH2	2.08	0.69
1:A:198:LEU:CD2	1:A:305:GLN:HB2	2.19	0.69
1:A:43:ARG:HB2	3:A:1412:HOH:O	1.91	0.69
1:A:198:LEU:CD2	1:A:305:GLN:CD	2.61	0.69
1:A:380:ILE:CG2	1:A:382:GLU:CD	2.61	0.69
1:A:63:LEU:HD21	1:A:229:PRO:CG	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:MET:HE2	1:A:108:CYS:SG	2.34	0.68
1:A:108:CYS:HB3	1:A:119:MET:HE1	1.73	0.68
1:A:426:ARG:HH12	1:A:427:ARG:HG2	1.57	0.68
1:A:730:GLU:O	1:A:734:ARG:HG3	1.92	0.68
1:A:687:LEU:HD21	1:A:801:VAL:HG22	1.73	0.68
1:A:744:GLN:HB3	1:A:749:PHE:HB3	1.73	0.68
1:A:252:PHE:N	1:A:255:LYS:HB2	2.09	0.68
1:A:466:THR:HA	1:A:469:LYS:HD3	1.75	0.68
1:A:118:ASP:HB3	1:A:121:GLU:HG3	1.75	0.67
1:A:584:ILE:HD13	1:A:585:THR:H	1.56	0.67
1:A:251:ASP:O	1:A:255:LYS:CA	2.42	0.67
1:A:538:LYS:NZ	1:A:684:ASN:O	2.28	0.67
1:A:289:LYS:HD2	1:A:289:LYS:N	2.08	0.67
1:A:85:LEU:CG	1:A:335:ILE:HD13	2.22	0.67
1:A:208:HIS:C	1:A:209:THR:OG1	2.34	0.67
1:A:380:ILE:HG23	1:A:382:GLU:CD	2.16	0.67
1:A:513:SER:O	1:A:514:ASP:HB2	1.94	0.67
1:A:790:LEU:HD12	1:A:797:TRP:CD1	2.30	0.67
1:A:665:GLN:NE2	1:A:678:ASN:HA	2.09	0.66
1:A:763:ASN:HB3	3:A:1083:HOH:O	1.95	0.66
1:A:633:ASP:HB3	1:A:636:VAL:HG23	1.77	0.66
1:A:152:LEU:HD11	1:A:829:PRO:HA	1.77	0.66
1:A:270:ASN:O	1:A:271:LEU:C	2.33	0.66
1:A:504:ALA:O	1:A:508:GLY:N	2.27	0.66
1:A:99:MET:HE3	1:A:119:MET:CE	2.18	0.65
1:A:426:ARG:HG3	1:A:427:ARG:N	2.11	0.65
1:A:31:PHE:CD2	1:A:115:LEU:CD2	2.79	0.65
1:A:475:GLU:HB3	1:A:477:HIS:CE1	2.31	0.65
1:A:828:GLU:CD	3:A:1405:HOH:O	2.35	0.65
1:A:250:ASN:HA	1:A:269:ARG:HH22	1.60	0.65
1:A:361:TRP:HH2	1:A:406:ILE:HD13	1.59	0.65
1:A:466:THR:O	1:A:469:LYS:HD3	1.96	0.65
1:A:591:LYS:NZ	3:A:1100:HOH:O	2.29	0.65
1:A:581:LEU:O	1:A:584:ILE:CD1	2.43	0.65
1:A:404:TYR:CB	3:A:1267:HOH:O	2.23	0.65
1:A:761:ILE:HG22	1:A:765:LEU:CD2	2.26	0.65
1:A:351:ARG:O	1:A:355:ASP:HB2	1.97	0.65
1:A:549:LEU:HB3	1:A:555:VAL:HG11	1.77	0.65
1:A:790:LEU:HD11	1:A:797:TRP:N	2.12	0.65
1:A:834:LEU:CD2	1:A:836:ALA:HB2	2.26	0.65
1:A:438:ARG:HG2	1:A:438:ARG:HH11	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ARG:O	1:A:43:ARG:HG3	1.94	0.64
1:A:55:LEU:HD11	1:A:119:MET:CE	2.27	0.64
1:A:113:TYR:O	1:A:116:GLY:HA2	1.96	0.64
1:A:753:LYS:HB2	1:A:754:GLN:HE21	1.63	0.64
1:A:538:LYS:O	1:A:538:LYS:HG3	1.98	0.64
1:A:582:HIS:HB2	1:A:780:TYR:HE2	1.61	0.64
1:A:167:ASN:ND2	1:A:180:ASP:HA	2.12	0.64
1:A:316:PHE:HD1	1:A:319:ARG:HB2	1.62	0.64
1:A:657:ILE:HG23	1:A:681:PHE:CD1	2.32	0.64
1:A:569:ARG:O	1:A:574:LYS:HE2	1.98	0.64
1:A:525:VAL:O	1:A:531:ILE:HD11	1.97	0.64
1:A:552:GLU:O	3:A:1326:HOH:O	2.15	0.64
1:A:687:LEU:HD23	1:A:797:TRP:CZ3	2.33	0.63
1:A:159:ILE:HG13	1:A:299:VAL:HG23	1.75	0.63
1:A:519:ARG:C	1:A:521:LEU:H	2.01	0.63
1:A:102:LEU:HB3	1:A:104:LEU:CD2	2.27	0.63
1:A:101:ASN:ND2	1:A:233:TYR:HA	2.14	0.63
1:A:810:LYS:O	1:A:810:LYS:HG3	1.97	0.63
1:A:99:MET:CE	1:A:108:CYS:HB3	2.27	0.62
1:A:113:TYR:O	1:A:116:GLY:N	2.30	0.62
1:A:335:ILE:HD12	1:A:336:GLN:N	2.14	0.62
1:A:551:ARG:HG3	1:A:552:GLU:N	2.15	0.62
1:A:709:PHE:CZ	1:A:800:MET:HE1	2.34	0.62
1:A:327:ASP:CA	1:A:363:LYS:HZ1	2.11	0.62
1:A:253:ASN:O	1:A:254:LEU:HB3	1.98	0.62
1:A:631:ASN:O	1:A:632:HIS:CD2	2.52	0.62
1:A:527:ASP:O	1:A:531:ILE:CD1	2.44	0.61
1:A:582:HIS:HB2	1:A:780:TYR:CE2	2.34	0.61
1:A:803:ARG:O	1:A:807:THR:HB	2.00	0.61
1:A:436:VAL:O	1:A:438:ARG:HD2	1.99	0.61
1:A:170:ILE:HD11	1:A:644:PHE:CE1	2.35	0.61
1:A:790:LEU:O	1:A:790:LEU:HD12	2.00	0.61
1:A:455:VAL:H	1:A:459:HIS:CD2	2.12	0.61
1:A:756:ASP:CB	1:A:759:LYS:CE	2.64	0.61
1:A:753:LYS:CG	1:A:754:GLN:H	2.14	0.61
1:A:256:ASP:HB2	1:A:258:ASN:CG	2.20	0.61
1:A:423:ASP:O	1:A:426:ARG:HG2	2.00	0.61
1:A:555:VAL:HG12	1:A:556:HIS:N	2.14	0.61
1:A:550:GLU:N	1:A:555:VAL:CG2	2.61	0.61
1:A:519:ARG:C	1:A:521:LEU:N	2.53	0.61
1:A:756:ASP:CB	1:A:759:LYS:HE3	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:MET:CE	1:A:108:CYS:SG	2.89	0.60
1:A:687:LEU:CD2	1:A:801:VAL:HG22	2.30	0.60
1:A:746:SER:HB3	3:A:1534:HOH:O	2.01	0.60
1:A:24:VAL:O	1:A:28:LYS:HG3	2.01	0.60
1:A:108:CYS:CB	1:A:119:MET:CE	2.72	0.60
1:A:81:ARG:NH2	3:A:1581:HOH:O	2.34	0.60
1:A:110:GLU:O	1:A:113:TYR:N	2.35	0.60
1:A:325:ASN:ND2	1:A:326:PHE:H	1.92	0.60
1:A:542:LYS:HE3	1:A:661:ASP:OD2	2.01	0.60
1:A:703:ALA:CB	1:A:807:THR:HG21	2.32	0.60
1:A:426:ARG:NH1	3:A:1289:HOH:O	2.34	0.60
1:A:797:TRP:HZ3	3:A:1662:HOH:O	1.83	0.60
1:A:72:GLN:NE2	1:A:76:GLU:OE1	2.35	0.60
1:A:322:VAL:CG1	1:A:325:ASN:CB	2.47	0.60
1:A:790:LEU:HD12	1:A:797:TRP:HD1	1.67	0.59
1:A:99:MET:CE	1:A:119:MET:HE2	2.26	0.59
1:A:356:LEU:N	1:A:356:LEU:HD12	2.17	0.59
1:A:102:LEU:O	1:A:103:ALA:HB3	2.03	0.59
1:A:803:ARG:NH1	1:A:803:ARG:HG3	2.15	0.59
1:A:99:MET:HE1	1:A:108:CYS:HB2	1.84	0.59
1:A:667:SER:HB3	1:A:693:ASP:OD2	2.02	0.59
1:A:251:ASP:C	1:A:255:LYS:HB2	2.22	0.59
1:A:548:TYR:CD1	1:A:548:TYR:C	2.75	0.59
1:A:55:LEU:HD11	1:A:119:MET:HE2	1.84	0.59
1:A:463:LEU:HD22	1:A:467:ILE:CD1	2.31	0.59
1:A:705:GLU:HG2	1:A:710:ILE:HD12	1.84	0.59
1:A:169:LYS:HG3	1:A:170:ILE:N	2.17	0.59
1:A:75:TYR:CE1	3:A:1557:HOH:O	2.48	0.58
1:A:327:ASP:HA	1:A:363:LYS:NZ	2.18	0.58
1:A:716:GLU:HB2	3:A:1114:HOH:O	2.03	0.58
1:A:72:GLN:O	1:A:75:TYR:HB3	2.03	0.58
1:A:629:VAL:HG23	3:A:1536:HOH:O	2.03	0.58
1:A:758:PHE:C	1:A:760:ASP:H	2.06	0.58
1:A:709:PHE:HZ	1:A:800:MET:HE1	1.67	0.58
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.85	0.58
1:A:105:GLU:HB3	3:A:1428:HOH:O	2.04	0.58
1:A:536:LYS:HE2	3:A:1320:HOH:O	2.02	0.58
1:A:548:TYR:CE2	1:A:655:LYS:HE2	2.39	0.58
1:A:47:THR:N	1:A:50:ASP:OD2	2.29	0.58
1:A:60:ARG:O	1:A:63:LEU:HB3	2.04	0.58
1:A:235:ASN:HD22	1:A:235:ASN:H	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:LYS:HG2	1:A:754:GLN:H	1.68	0.57
1:A:175:GLN:HG2	1:A:177:GLU:OE2	2.04	0.57
1:A:198:LEU:CD2	1:A:305:GLN:CB	2.74	0.57
1:A:555:VAL:CG1	1:A:556:HIS:H	2.06	0.57
1:A:664:GLU:OE1	1:A:666:ILE:CD1	2.51	0.57
1:A:752:PRO:CG	1:A:753:LYS:HZ3	2.17	0.57
1:A:322:VAL:HG22	1:A:323:ARG:HG3	1.86	0.57
1:A:41:LYS:HE3	3:A:1576:HOH:O	2.04	0.57
1:A:709:PHE:CE2	1:A:800:MET:HE3	2.39	0.57
1:A:316:PHE:C	1:A:318:CYS:N	2.57	0.57
1:A:466:THR:O	1:A:469:LYS:CD	2.52	0.57
1:A:752:PRO:O	1:A:755:PRO:HD3	2.04	0.57
1:A:536:LYS:CE	3:A:1321:HOH:O	2.46	0.57
1:A:42:ASP:H	1:A:45:VAL:HG13	1.70	0.57
1:A:80:LYS:CE	1:A:825:TRP:O	2.49	0.57
1:A:205:ARG:HH21	1:A:216:VAL:HG21	1.69	0.57
1:A:251:ASP:OD2	1:A:255:LYS:NZ	2.36	0.57
1:A:763:ASN:CB	3:A:1083:HOH:O	2.52	0.57
1:A:150:LEU:CD1	1:A:817:ILE:HG22	2.32	0.57
1:A:380:ILE:HG23	1:A:382:GLU:OE2	2.05	0.57
1:A:476:PRO:HB3	3:A:1203:HOH:O	2.04	0.57
1:A:474:LEU:CD1	1:A:475:GLU:HG3	2.16	0.56
1:A:274:ASN:HA	1:A:277:ARG:HH11	1.70	0.56
1:A:761:ILE:HG22	1:A:765:LEU:HD22	1.85	0.56
1:A:101:ASN:HD22	1:A:232:GLY:C	2.09	0.56
1:A:280:TYR:OH	1:A:291:LEU:HB3	2.06	0.56
1:A:171:CYS:N	1:A:174:TRP:O	2.33	0.56
1:A:764:MET:HE1	3:A:1654:HOH:O	2.04	0.56
1:A:111:ALA:O	1:A:115:LEU:CD1	2.52	0.56
1:A:337:LEU:HD22	1:A:373:ALA:O	2.05	0.56
1:A:581:LEU:O	1:A:584:ILE:HD13	2.05	0.56
1:A:590:ILE:HD13	1:A:636:VAL:HG13	1.87	0.56
1:A:678:ASN:OD1	1:A:695:ALA:HB3	2.05	0.56
1:A:159:ILE:HG12	1:A:299:VAL:HG23	1.87	0.56
1:A:687:LEU:N	1:A:687:LEU:HD22	2.20	0.56
1:A:538:LYS:HE2	1:A:660:ALA:O	2.06	0.56
1:A:703:ALA:HB2	1:A:807:THR:HG21	1.88	0.56
1:A:705:GLU:HG2	1:A:710:ILE:CD1	2.36	0.56
1:A:108:CYS:HB2	1:A:119:MET:HE1	1.87	0.56
1:A:113:TYR:O	1:A:116:GLY:CA	2.53	0.56
1:A:538:LYS:CE	1:A:660:ALA:O	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:ILE:HG22	1:A:691:THR:HG23	1.88	0.56
1:A:837:PRO:HG2	1:A:838:ASP:H	1.70	0.56
1:A:666:ILE:CG2	1:A:711:PHE:CE1	2.87	0.55
1:A:756:ASP:CA	1:A:759:LYS:HG3	2.36	0.55
1:A:208:HIS:C	1:A:209:THR:HG1	2.04	0.55
1:A:252:PHE:C	1:A:255:LYS:H	2.09	0.55
1:A:349:LEU:HD12	1:A:353:LEU:HG	1.86	0.55
1:A:256:ASP:CA	1:A:258:ASN:HB2	2.37	0.55
1:A:251:ASP:OD1	1:A:252:PHE:N	2.40	0.55
1:A:65:GLY:HA3	1:A:838:ASP:OD1	2.05	0.55
1:A:343:SER:OG	1:A:441:MET:HG3	2.07	0.55
1:A:713:MET:HB2	1:A:717:ASP:HB2	1.88	0.55
1:A:252:PHE:CE2	1:A:255:LYS:HE2	2.41	0.55
1:A:340:THR:CG2	1:A:374:TYR:CE1	2.89	0.55
1:A:343:SER:HB3	1:A:445:CYS:SG	2.47	0.55
1:A:395:LEU:C	1:A:396:LEU:HG	2.26	0.55
1:A:532:ARG:O	1:A:536:LYS:HB2	2.08	0.54
1:A:183:LEU:HD23	1:A:187:ASN:HB2	1.89	0.54
1:A:252:PHE:CA	1:A:255:LYS:H	2.20	0.54
1:A:754:GLN:HB3	1:A:757:LEU:HB2	1.90	0.54
1:A:150:LEU:O	1:A:152:LEU:CD1	2.55	0.54
1:A:571:HIS:HB2	1:A:574:LYS:HD2	1.89	0.54
1:A:41:LYS:CE	3:A:1576:HOH:O	2.55	0.54
1:A:557:ILE:HG13	1:A:557:ILE:O	2.07	0.54
1:A:147:MET:HE2	1:A:825:TRP:CH2	2.43	0.54
1:A:22:GLU:O	1:A:25:THR:N	2.41	0.54
1:A:565:VAL:HG21	1:A:660:ALA:HB2	1.90	0.54
1:A:571:HIS:HB2	1:A:574:LYS:CD	2.37	0.54
1:A:36:HIS:HB2	3:A:1000:HOH:O	2.08	0.53
1:A:42:ASP:H	1:A:45:VAL:CG1	2.21	0.53
1:A:487:THR:HG23	1:A:487:THR:O	2.08	0.53
1:A:758:PHE:C	1:A:760:ASP:N	2.61	0.53
1:A:703:ALA:HA	1:A:807:THR:HG21	1.91	0.53
1:A:205:ARG:HE	1:A:216:VAL:HG23	1.72	0.53
1:A:314:SER:O	1:A:316:PHE:N	2.41	0.53
1:A:519:ARG:O	1:A:521:LEU:N	2.41	0.53
1:A:76:GLU:HA	1:A:315:LYS:CE	2.37	0.53
1:A:147:MET:CE	1:A:825:TRP:HH2	2.21	0.53
1:A:666:ILE:HG23	1:A:711:PHE:CZ	2.37	0.53
1:A:676:THR:CA	1:A:678:ASN:HB2	2.39	0.53
1:A:314:SER:C	1:A:316:PHE:N	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:GLU:OE1	1:A:532:ARG:NH2	2.37	0.53
1:A:584:ILE:HG13	1:A:741:ILE:HG23	1.90	0.53
1:A:703:ALA:CA	1:A:807:THR:HG21	2.39	0.53
1:A:55:LEU:CD2	1:A:59:VAL:HG23	2.39	0.53
1:A:322:VAL:HG22	1:A:325:ASN:OD1	2.07	0.53
1:A:235:ASN:H	1:A:235:ASN:ND2	2.07	0.53
1:A:400:LEU:HD13	1:A:404:TYR:CE2	2.44	0.53
1:A:810:LYS:O	1:A:810:LYS:CG	2.56	0.53
1:A:263:ILE:O	1:A:267:LEU:HG	2.09	0.52
1:A:753:LYS:HG3	1:A:754:GLN:NE2	2.24	0.52
1:A:197:THR:CG2	1:A:222:LEU:HB3	2.40	0.52
1:A:763:ASN:HD22	1:A:763:ASN:H	1.58	0.52
1:A:347:PRO:HB3	1:A:402:ILE:HG22	1.91	0.52
1:A:486:ILE:HD12	1:A:676:THR:HB	1.90	0.52
1:A:147:MET:CE	1:A:825:TRP:CH2	2.93	0.52
1:A:306:ASP:HA	1:A:309:ARG:HD3	1.90	0.52
1:A:685:GLY:HA2	3:A:1667:HOH:O	2.09	0.52
1:A:387:TRP:HD1	1:A:441:MET:SD	2.33	0.52
1:A:549:LEU:HD23	1:A:557:ILE:HD13	1.92	0.52
1:A:689:ILE:CD1	1:A:784:GLN:HG2	2.40	0.52
1:A:259:VAL:HG22	1:A:260:GLY:H	1.75	0.52
1:A:316:PHE:CE1	1:A:319:ARG:CD	2.93	0.51
1:A:380:ILE:CG2	1:A:382:GLU:OE1	2.59	0.51
1:A:252:PHE:HA	1:A:255:LYS:H	1.75	0.51
1:A:577:LEU:O	1:A:580:CYS:HB2	2.09	0.51
1:A:692:MET:CE	1:A:710:ILE:HD13	2.41	0.51
1:A:483:THR:O	1:A:815:ARG:NH2	2.43	0.51
1:A:658:PRO:HA	1:A:684:ASN:HB3	1.91	0.51
1:A:664:GLU:HB3	1:A:666:ILE:HD12	1.92	0.51
1:A:455:VAL:N	1:A:459:HIS:HD2	2.02	0.51
1:A:551:ARG:CG	1:A:552:GLU:N	2.73	0.51
1:A:76:GLU:HA	1:A:315:LYS:HE3	1.93	0.51
1:A:198:LEU:CD2	1:A:305:GLN:NE2	2.72	0.51
1:A:311:PHE:CZ	1:A:325:ASN:O	2.63	0.51
1:A:31:PHE:CE2	1:A:115:LEU:HD23	2.45	0.50
1:A:472:TYR:O	1:A:476:PRO:HG3	2.11	0.50
1:A:590:ILE:HG22	1:A:591:LYS:N	2.25	0.50
1:A:557:ILE:HD12	1:A:563:PHE:CZ	2.45	0.50
1:A:753:LYS:HB2	1:A:754:GLN:NE2	2.27	0.50
1:A:55:LEU:HD11	1:A:119:MET:HE3	1.93	0.50
1:A:721:LEU:HA	1:A:724:ARG:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:LEU:O	1:A:742:ILE:HG12	2.12	0.50
1:A:147:MET:HE2	1:A:825:TRP:HH2	1.77	0.50
1:A:616:ALA:O	1:A:620:ILE:HG12	2.11	0.50
1:A:73:HIS:O	1:A:77:LYS:HB2	2.11	0.50
1:A:382:GLU:OE2	1:A:770:ARG:NH1	2.39	0.50
1:A:764:MET:HE1	1:A:769:ASP:HA	1.94	0.50
1:A:790:LEU:HD11	1:A:796:GLU:C	2.32	0.50
1:A:386:ARG:HA	1:A:439:ILE:O	2.12	0.50
1:A:810:LYS:O	1:A:815:ARG:HD2	2.12	0.50
1:A:384:LEU:HD23	3:A:1260:HOH:O	2.11	0.49
1:A:503:ILE:HG12	1:A:521:LEU:HD21	1.94	0.49
1:A:584:ILE:HG12	1:A:741:ILE:HG12	1.94	0.49
1:A:709:PHE:HE2	1:A:800:MET:HE3	1.77	0.49
1:A:191:LYS:HE3	1:A:193:ARG:NH2	2.28	0.49
1:A:402:ILE:O	1:A:405:GLU:HB2	2.13	0.49
1:A:70:THR:O	1:A:73:HIS:HB3	2.13	0.49
1:A:76:GLU:HA	1:A:315:LYS:HZ2	1.78	0.49
1:A:227:ASP:HB3	1:A:240:THR:HG23	1.94	0.49
1:A:666:ILE:HD13	1:A:780:TYR:CE1	2.47	0.49
1:A:198:LEU:HD23	1:A:305:GLN:OE1	2.13	0.49
1:A:322:VAL:C	1:A:323:ARG:CG	2.80	0.49
1:A:790:LEU:CD1	1:A:790:LEU:C	2.80	0.49
1:A:337:LEU:CD2	1:A:373:ALA:O	2.61	0.49
1:A:304:LEU:CD1	1:A:307:ILE:HD12	2.39	0.48
1:A:667:SER:OG	1:A:672:GLU:HB2	2.13	0.48
1:A:744:GLN:NE2	1:A:750:PHE:CZ	2.81	0.48
1:A:492:LEU:O	1:A:496:ASN:N	2.40	0.48
1:A:316:PHE:CD1	1:A:319:ARG:HB3	2.47	0.48
1:A:287:GLU:OE1	1:A:289:LYS:HG2	2.13	0.48
1:A:322:VAL:O	1:A:323:ARG:HG3	2.13	0.48
1:A:93:ARG:NE	1:A:126:GLU:O	2.46	0.48
1:A:99:MET:HE1	1:A:108:CYS:CB	2.28	0.48
1:A:408:GLN:OE1	3:A:1191:HOH:O	2.20	0.48
1:A:703:ALA:HB2	1:A:807:THR:CG2	2.43	0.48
1:A:793:ASN:HD21	1:A:796:GLU:HG3	1.78	0.48
1:A:320:ASP:CB	1:A:321:PRO:CD	2.37	0.48
1:A:790:LEU:HD12	1:A:797:TRP:CB	2.44	0.48
1:A:311:PHE:HZ	1:A:325:ASN:O	1.96	0.48
1:A:709:PHE:CE2	1:A:800:MET:CE	2.97	0.47
1:A:770:ARG:HD3	3:A:1469:HOH:O	2.13	0.47
1:A:131:LEU:HG	1:A:161:TYR:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:PHE:CE1	1:A:332:LYS:HD2	2.49	0.47
1:A:463:LEU:HD23	1:A:467:ILE:HD11	1.92	0.47
1:A:466:THR:O	1:A:469:LYS:CG	2.62	0.47
1:A:568:LYS:O	1:A:607:GLY:HA3	2.14	0.47
1:A:441:MET:HG2	3:A:1471:HOH:O	2.13	0.47
1:A:715:VAL:HG23	1:A:716:GLU:N	2.30	0.47
1:A:315:LYS:N	1:A:315:LYS:CD	2.76	0.47
1:A:387:TRP:HA	1:A:388:PRO:HD3	1.85	0.47
1:A:795:ARG:HE	1:A:795:ARG:HB3	1.21	0.47
1:A:46:ALA:HA	1:A:50:ASP:OD2	2.14	0.47
1:A:75:TYR:CE2	1:A:315:LYS:HE2	2.50	0.47
1:A:422:VAL:HG13	3:A:1643:HOH:O	2.13	0.47
1:A:678:ASN:HB3	1:A:679:MET:H	1.26	0.47
1:A:316:PHE:HA	1:A:319:ARG:CB	2.39	0.47
1:A:347:PRO:HB3	1:A:402:ILE:CG2	2.45	0.47
1:A:688:THR:HB	1:A:708:PHE:CE2	2.50	0.47
1:A:44:ASN:ND2	3:A:1001:HOH:O	2.47	0.47
1:A:315:LYS:H	1:A:315:LYS:HD3	1.79	0.47
1:A:427:ARG:NH1	1:A:470:ASP:CG	2.67	0.47
1:A:557:ILE:O	1:A:559:PRO:HD3	2.15	0.47
1:A:177:GLU:OE1	1:A:611:PRO:CG	2.60	0.47
1:A:113:TYR:O	1:A:113:TYR:HD1	1.98	0.46
1:A:113:TYR:C	1:A:113:TYR:CD1	2.86	0.46
1:A:193:ARG:HD3	1:A:196:PHE:CE2	2.43	0.46
1:A:424:ARG:NH2	1:A:473:GLU:OE1	2.48	0.46
1:A:315:LYS:N	1:A:315:LYS:HD3	2.31	0.46
1:A:390:HIS:O	1:A:394:THR:OG1	2.32	0.46
1:A:399:HIS:O	1:A:403:ILE:HG13	2.16	0.46
1:A:555:VAL:CG1	1:A:556:HIS:N	2.75	0.46
1:A:803:ARG:NH1	1:A:803:ARG:CG	2.74	0.46
1:A:101:ASN:ND2	1:A:233:TYR:CA	2.79	0.46
1:A:177:GLU:H	1:A:177:GLU:HG2	1.52	0.46
1:A:356:LEU:N	1:A:356:LEU:CD1	2.78	0.46
1:A:640:LEU:O	1:A:641:ARG:HD2	2.16	0.46
1:A:697:VAL:O	1:A:701:GLU:HB2	2.14	0.46
1:A:729:GLN:O	1:A:729:GLN:HG3	2.15	0.46
1:A:160:ARG:HH11	1:A:160:ARG:HD2	1.42	0.46
1:A:709:PHE:CZ	1:A:800:MET:CE	2.99	0.46
1:A:93:ARG:NH1	3:A:1014:HOH:O	2.41	0.46
1:A:159:ILE:HG13	1:A:299:VAL:HG21	1.96	0.46
1:A:257:PHE:HD1	1:A:257:PHE:HA	1.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:GLU:O	1:A:294:LYS:HG3	2.16	0.46
1:A:584:ILE:CG1	1:A:741:ILE:HG12	2.46	0.46
1:A:771:PHE:O	1:A:772:LYS:HB2	2.15	0.46
1:A:167:ASN:HD22	1:A:180:ASP:HA	1.79	0.46
1:A:252:PHE:CE2	1:A:255:LYS:CE	2.98	0.46
1:A:316:PHE:CD1	1:A:319:ARG:HB2	2.44	0.46
1:A:455:VAL:O	1:A:483:THR:HA	2.16	0.46
1:A:483:THR:HB	1:A:815:ARG:NH2	2.31	0.45
1:A:502:ILE:HG21	1:A:533:ASP:HB3	1.98	0.45
1:A:756:ASP:CB	1:A:759:LYS:HE2	2.41	0.45
1:A:28:LYS:O	1:A:32:ASN:ND2	2.49	0.45
1:A:309:ARG:HG2	3:A:1253:HOH:O	2.15	0.45
1:A:118:ASP:CB	1:A:121:GLU:HG3	2.43	0.45
1:A:103:ALA:HB2	1:A:234:ARG:NE	2.32	0.45
1:A:157:TYR:CG	1:A:303:THR:HG23	2.52	0.45
1:A:321:PRO:O	1:A:322:VAL:C	2.54	0.45
1:A:593:GLU:N	1:A:594:PRO:HD3	2.32	0.45
1:A:39:LEU:N	1:A:39:LEU:HD12	2.31	0.45
1:A:109:ASP:OD2	3:A:1205:HOH:O	2.21	0.45
1:A:467:ILE:HD12	1:A:468:PHE:CE2	2.52	0.45
1:A:753:LYS:O	1:A:755:PRO:HD2	2.17	0.45
1:A:150:LEU:HD12	1:A:817:ILE:CG2	2.35	0.45
1:A:461:GLU:HA	1:A:464:LYS:HD2	1.99	0.45
1:A:597:PHE:HD1	3:A:1327:HOH:O	1.98	0.45
1:A:666:ILE:HD13	1:A:780:TYR:HE1	1.82	0.45
1:A:837:PRO:CG	1:A:838:ASP:H	2.29	0.45
1:A:322:VAL:HG11	1:A:325:ASN:CG	2.32	0.45
1:A:322:VAL:C	1:A:323:ARG:HG3	2.37	0.45
1:A:487:THR:O	1:A:487:THR:CG2	2.65	0.45
1:A:57:HIS:HE1	3:A:1007:HOH:O	2.00	0.45
1:A:187:ASN:HA	1:A:188:PRO:HD2	1.85	0.45
1:A:252:PHE:CE1	1:A:255:LYS:HD2	2.52	0.45
1:A:204:GLY:HA2	1:A:217:ASP:O	2.16	0.45
1:A:363:LYS:HD2	1:A:363:LYS:C	2.37	0.45
1:A:382:GLU:OE2	1:A:770:ARG:NH2	2.47	0.45
1:A:382:GLU:H	1:A:382:GLU:HG3	1.23	0.45
1:A:417:ALA:HB3	1:A:418:PHE:CD1	2.51	0.45
1:A:39:LEU:HD21	1:A:53:PHE:HB3	1.99	0.44
1:A:249:PRO:O	1:A:269:ARG:NH2	2.50	0.44
1:A:466:THR:O	1:A:469:LYS:HG2	2.17	0.44
1:A:515:LEU:HD22	1:A:518:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:GLU:OE1	1:A:799:ARG:HD3	2.16	0.44
1:A:43:ARG:O	1:A:43:ARG:CG	2.62	0.44
1:A:262:TYR:O	1:A:266:VAL:HG23	2.17	0.44
1:A:335:ILE:CD1	1:A:337:LEU:HD13	2.35	0.44
1:A:390:HIS:CE1	1:A:391:LEU:HD12	2.53	0.44
1:A:752:PRO:HB2	1:A:753:LYS:HZ2	1.76	0.44
1:A:365:TRP:O	1:A:369:VAL:HG23	2.17	0.44
1:A:748:GLY:O	1:A:749:PHE:C	2.56	0.44
1:A:208:HIS:HB2	3:A:1268:HOH:O	2.18	0.44
1:A:549:LEU:CB	1:A:555:VAL:CG2	2.81	0.44
1:A:567:VAL:O	1:A:568:LYS:HB3	2.18	0.44
1:A:417:ALA:C	1:A:419:PRO:HD3	2.38	0.43
1:A:834:LEU:CD2	1:A:836:ALA:CB	2.91	0.43
1:A:306:ASP:OD1	1:A:309:ARG:HD3	2.18	0.43
1:A:713:MET:HG2	1:A:776:ASP:OD1	2.18	0.43
1:A:24:VAL:HG12	1:A:24:VAL:O	2.17	0.43
1:A:29:LYS:HB3	1:A:29:LYS:HE2	1.78	0.43
1:A:31:PHE:CE2	1:A:115:LEU:CD2	3.02	0.43
1:A:184:ARG:HE	1:A:184:ARG:HB2	1.25	0.43
1:A:550:GLU:O	1:A:551:ARG:C	2.54	0.43
1:A:36:HIS:O	1:A:40:VAL:N	2.52	0.43
1:A:744:GLN:HB3	1:A:749:PHE:CB	2.44	0.43
1:A:344:LEU:O	1:A:347:PRO:HD2	2.17	0.43
1:A:764:MET:C	1:A:764:MET:SD	2.97	0.43
1:A:36:HIS:CB	3:A:1000:HOH:O	2.65	0.43
1:A:170:ILE:HA	1:A:174:TRP:O	2.19	0.43
1:A:329:PHE:N	1:A:330:PRO:HD2	2.34	0.43
1:A:366:GLU:O	1:A:370:LYS:HG3	2.19	0.43
1:A:661:ASP:C	1:A:797:TRP:HH2	2.20	0.43
1:A:252:PHE:CZ	1:A:255:LYS:HD2	2.53	0.43
1:A:256:ASP:C	1:A:258:ASN:N	2.63	0.43
1:A:361:TRP:CZ2	1:A:406:ILE:CD1	2.94	0.43
1:A:389:VAL:O	1:A:393:GLU:HB2	2.19	0.43
1:A:678:ASN:HA	1:A:678:ASN:HD22	0.99	0.43
1:A:680:LYS:NZ	2:A:999:PLP:O3	2.52	0.43
1:A:515:LEU:HD22	1:A:518:LEU:CD2	2.49	0.43
1:A:193:ARG:N	1:A:194:PRO:CD	2.82	0.42
1:A:758:PHE:O	1:A:760:ASP:N	2.52	0.42
1:A:159:ILE:CG1	1:A:299:VAL:CG2	2.80	0.42
1:A:753:LYS:CG	1:A:754:GLN:N	2.80	0.42
1:A:75:TYR:CZ	1:A:315:LYS:HE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:LYS:HD2	1:A:465:LYS:HA	1.67	0.42
1:A:530:PHE:HD1	1:A:530:PHE:HA	1.47	0.42
1:A:665:GLN:HE21	1:A:678:ASN:HA	1.83	0.42
1:A:752:PRO:HG2	1:A:753:LYS:HZ3	1.82	0.42
1:A:763:ASN:ND2	1:A:763:ASN:N	2.59	0.42
1:A:49:ARG:HH11	1:A:49:ARG:HD2	1.67	0.42
1:A:283:ASP:O	1:A:284:ASN:HB2	2.19	0.42
1:A:688:THR:HG21	1:A:708:PHE:CE2	2.55	0.42
1:A:316:PHE:HE1	1:A:319:ARG:CD	2.27	0.42
1:A:103:ALA:HB2	1:A:234:ARG:HE	1.84	0.42
1:A:548:TYR:HA	1:A:551:ARG:HG2	2.02	0.42
1:A:584:ILE:HD11	1:A:741:ILE:CG1	2.40	0.42
1:A:139:LEU:HD21	1:A:143:PHE:CZ	2.53	0.42
1:A:160:ARG:HB2	1:A:243:LEU:HB3	2.02	0.42
1:A:688:THR:HG21	1:A:708:PHE:HE2	1.84	0.42
1:A:152:LEU:CD1	1:A:829:PRO:HA	2.46	0.42
1:A:605:ILE:O	1:A:644:PHE:HA	2.20	0.42
1:A:449:SER:O	1:A:478:LYS:HD3	2.20	0.42
1:A:778:GLU:HG2	1:A:782:LYS:HE3	2.02	0.42
1:A:36:HIS:HD2	1:A:37:PHE:CE2	2.38	0.42
1:A:113:TYR:C	1:A:113:TYR:HD1	2.23	0.42
1:A:33:ARG:HG2	1:A:37:PHE:HD2	1.85	0.41
1:A:119:MET:O	1:A:120:GLU:C	2.59	0.41
1:A:286:PHE:CD1	1:A:385:GLU:HG2	2.55	0.41
1:A:293:LEU:HD12	1:A:293:LEU:HA	1.73	0.41
1:A:464:LYS:HG3	1:A:464:LYS:H	1.65	0.41
1:A:322:VAL:CG1	1:A:325:ASN:OD1	2.68	0.41
1:A:592:LYS:C	1:A:594:PRO:HD3	2.40	0.41
1:A:631:ASN:C	1:A:632:HIS:CD2	2.93	0.41
1:A:786:ARG:HH11	1:A:786:ARG:HD3	1.75	0.41
1:A:355:ASP:C	1:A:356:LEU:HD12	2.39	0.41
1:A:363:LYS:HD2	1:A:363:LYS:O	2.19	0.41
1:A:365:TRP:CE3	1:A:365:TRP:HA	2.54	0.41
1:A:251:ASP:CG	1:A:255:LYS:NZ	2.73	0.41
1:A:252:PHE:HA	1:A:255:LYS:N	2.35	0.41
1:A:618:MET:HB3	1:A:761:ILE:HD11	2.03	0.41
1:A:304:LEU:HD12	1:A:304:LEU:HA	1.68	0.41
1:A:677:GLY:O	1:A:681:PHE:HD2	2.04	0.41
1:A:39:LEU:O	1:A:40:VAL:HB	2.20	0.41
1:A:316:PHE:CE1	1:A:319:ARG:HG3	2.50	0.41
1:A:524:TYR:CD1	1:A:524:TYR:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:LEU:HD12	1:A:549:LEU:HA	1.82	0.41
1:A:666:ILE:HG23	1:A:711:PHE:CE1	2.55	0.41
1:A:282:ASN:ND2	1:A:610:ALA:HB1	2.35	0.41
1:A:349:LEU:O	1:A:353:LEU:HG	2.20	0.41
1:A:522:LEU:HG	3:A:1312:HOH:O	2.20	0.41
1:A:676:THR:N	1:A:678:ASN:HB2	2.36	0.41
1:A:707:ASN:ND2	1:A:803:ARG:HD2	2.36	0.41
1:A:316:PHE:CD1	1:A:319:ARG:NE	2.87	0.41
1:A:325:ASN:HD22	1:A:325:ASN:HA	1.44	0.41
1:A:335:ILE:HD12	1:A:335:ILE:C	2.41	0.41
1:A:128:ASP:OD1	1:A:651:SER:OG	2.36	0.41
1:A:622:LEU:HD22	1:A:626:ILE:HD12	2.03	0.41
1:A:793:ASN:ND2	1:A:796:GLU:HB2	2.35	0.41
1:A:76:GLU:H	1:A:76:GLU:HG2	1.62	0.41
1:A:85:LEU:N	1:A:85:LEU:HD23	2.36	0.41
1:A:99:MET:O	1:A:103:ALA:N	2.54	0.41
1:A:254:LEU:O	1:A:254:LEU:HD13	2.21	0.41
1:A:273:GLU:C	1:A:277:ARG:NH1	2.74	0.41
1:A:407:ASN:O	1:A:408:GLN:C	2.60	0.41
1:A:458:ILE:CG2	1:A:459:HIS:N	2.84	0.41
1:A:593:GLU:OE2	1:A:596:LYS:CD	2.54	0.41
1:A:676:THR:C	1:A:678:ASN:N	2.72	0.41
1:A:125:ILE:O	1:A:125:ILE:HG22	2.21	0.40
1:A:676:THR:C	1:A:678:ASN:HB2	2.42	0.40
1:A:758:PHE:HD2	1:A:761:ILE:HD12	1.87	0.40
1:A:293:LEU:HB2	1:A:387:TRP:CH2	2.57	0.40
1:A:380:ILE:HG21	1:A:382:GLU:OE1	2.22	0.40
1:A:41:LYS:NZ	3:A:1576:HOH:O	2.54	0.40
1:A:170:ILE:HD11	1:A:644:PHE:HE1	1.84	0.40
1:A:254:LEU:O	1:A:254:LEU:CD1	2.69	0.40
1:A:269:ARG:O	1:A:273:GLU:HG3	2.22	0.40
1:A:322:VAL:CG1	1:A:325:ASN:CG	2.89	0.40
1:A:790:LEU:HD11	1:A:797:TRP:CA	2.51	0.40
1:A:81:ARG:HB3	1:A:155:TYR:HE1	1.87	0.40
1:A:400:LEU:CD2	1:A:439:ILE:HD11	2.50	0.40
1:A:175:GLN:HE21	1:A:177:GLU:CD	2.24	0.40
1:A:610:ALA:HA	1:A:611:PRO:HD3	1.80	0.40
1:A:715:VAL:HG23	1:A:716:GLU:H	1.86	0.40
1:A:790:LEU:CD1	1:A:797:TRP:N	2.83	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:O	1:A:254:LEU:CD1[7_556]	1.88	0.32

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	821/842 (98%)	735 (90%)	59 (7%)	27 (3%)	4 0

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	LEU
1	A	256	ASP
1	A	258	ASN
1	A	315	LYS
1	A	319	ARG
1	A	320	ASP
1	A	436	VAL
1	A	837	PRO
1	A	838	ASP
1	A	21	VAL
1	A	323	ARG
1	A	527	ASP
1	A	551	ARG
1	A	271	LEU
1	A	324	THR
1	A	434	GLY
1	A	514	ASP
1	A	556	HIS
1	A	836	ALA
1	A	210	SER
1	A	555	VAL
1	A	36	HIS
1	A	131	LEU

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Mol	Chain	Res	Type
1	A	520	LYS
1	A	678	ASN
1	A	759	LYS
1	A	755	PRO

5.3.2 Protein sidechains (i)

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	711/731 (97%)	567 (80%)	144 (20%)	1 0

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

Mol	Chain	Res	Type
1	A	21	VAL
1	A	23	ASN
1	A	27	LEU
1	A	29	LYS
1	A	41	LYS
1	A	44	ASN
1	A	47	THR
1	A	55	LEU
1	A	60	ARG
1	A	64	VAL
1	A	66	ARG
1	A	85	LEU
1	A	90	TYR
1	A	102	LEU
1	A	104	LEU
1	A	113	TYR
1	A	122	LEU
1	A	125	ILE
1	A	127	GLU
1	A	144	LEU
1	A	165	ILE
1	A	169	LYS

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Mol	Chain	Res	Type
1	A	177	GLU
1	A	178	GLU
1	A	184	ARG
1	A	193	ARG
1	A	195	GLU
1	A	196	PHE
1	A	198	LEU
1	A	214	LYS
1	A	234	ARG
1	A	235	ASN
1	A	243	LEU
1	A	247	LYS
1	A	254	LEU
1	A	255	LYS
1	A	257	PHE
1	A	258	ASN
1	A	263	ILE
1	A	264	GLN
1	A	277	ARG
1	A	281	PRO
1	A	289	LYS
1	A	304	LEU
1	A	306	ASP
1	A	316	PHE
1	A	318	CYS
1	A	319	ARG
1	A	320	ASP
1	A	323	ARG
1	A	327	ASP
1	A	335	ILE
1	A	344	LEU
1	A	359	LEU
1	A	361	TRP
1	A	363	LYS
1	A	382	GLU
1	A	389	VAL
1	A	391	LEU
1	A	392	LEU
1	A	393	GLU
1	A	394	THR
1	A	395	LEU
1	A	400	LEU

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Mol	Chain	Res	Type
1	A	401	GLN
1	A	405	GLU
1	A	426	ARG
1	A	432	GLU
1	A	438	ARG
1	A	441	MET
1	A	444	LEU
1	A	464	LYS
1	A	465	LYS
1	A	467	ILE
1	A	474	LEU
1	A	476	PRO
1	A	478	LYS
1	A	486	ILE
1	A	506	ARG
1	A	515	LEU
1	A	522	LEU
1	A	525	VAL
1	A	526	ASP
1	A	528	GLU
1	A	530	PHE
1	A	548	TYR
1	A	549	LEU
1	A	551	ARG
1	A	554	LYS
1	A	560	ASN
1	A	568	LYS
1	A	573	TYR
1	A	574	LYS
1	A	576	GLN
1	A	579	ASN
1	A	581	LEU
1	A	584	ILE
1	A	591	LYS
1	A	592	LYS
1	A	601	ARG
1	A	613	TYR
1	A	622	LEU
1	A	635	VAL
1	A	638	ASP
1	A	640	LEU
1	A	641	ARG

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Mol	Chain	Res	Type
1	A	645	LEU
1	A	665	GLN
1	A	666	ILE
1	A	667	SER
1	A	678	ASN
1	A	706	GLU
1	A	708	PHE
1	A	713	MET
1	A	714	ARG
1	A	724	ARG
1	A	730	GLU
1	A	733	ASP
1	A	737	GLU
1	A	739	ARG
1	A	747	SER
1	A	753	LYS
1	A	754	GLN
1	A	756	ASP
1	A	760	ASP
1	A	763	ASN
1	A	764	MET
1	A	765	LEU
1	A	768	HIS
1	A	790	LEU
1	A	792	LYS
1	A	794	PRO
1	A	795	ARG
1	A	797	TRP
1	A	803	ARG
1	A	807	THR
1	A	812	SER
1	A	813	SER
1	A	815	ARG
1	A	817	ILE
1	A	827	VAL
1	A	830	SER
1	A	838	ASP
1	A	839	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	36	HIS
1	A	72	GLN
1	A	101	ASN
1	A	106	ASN
1	A	187	ASN
1	A	235	ASN
1	A	282	ASN
1	A	412	ASN
1	A	459	HIS
1	A	477	HIS
1	A	481	ASN
1	A	484	ASN
1	A	539	GLN
1	A	560	ASN
1	A	566	GLN
1	A	576	GLN
1	A	579	ASN
1	A	632	HIS
1	A	678	ASN
1	A	754	GLN
1	A	763	ASN
1	A	768	HIS
1	A	793	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PLP	A	999	1	15,15,16	1.98	4 (26%)	20,22,23	2.92	8 (40%)

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	PLP	A	999	1	-	2/6/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	999	PLP	C4A-C4	-3.90	1.43	1.51
2	A	999	PLP	P-O4P	3.28	1.70	1.60
2	A	999	PLP	C5A-C5	3.28	1.59	1.50
2	A	999	PLP	P-O2P	-2.28	1.46	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	999	PLP	C6-N1-C2	5.53	129.42	119.17
2	A	999	PLP	O4P-C5A-C5	-5.40	99.06	109.35
2	A	999	PLP	C5-C6-N1	-5.15	115.23	123.82
2	A	999	PLP	C3-C2-N1	-4.34	115.16	120.77
2	A	999	PLP	C2A-C2-N1	4.18	125.83	117.67
2	A	999	PLP	C6-C5-C4	4.08	121.37	118.16
2	A	999	PLP	O2P-P-O4P	-3.66	97.00	106.73
2	A	999	PLP	O2P-P-O1P	2.86	121.87	110.68

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	999	PLP	C4-C5-C5A-O4P
2	A	999	PLP	C6-C5-C5A-O4P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	999	PLP	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.