



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:39 AM UTC

PDB ID : 3AAT / pdb_00003aat
Title : ACTIVITY AND STRUCTURE OF THE ACTIVE-SITE MUTANTS R386Y AND R386F OF ESCHERICHIA COLI ASPARTATE AMINOTRANSFERASE
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Deposited on : 1990-12-06
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
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

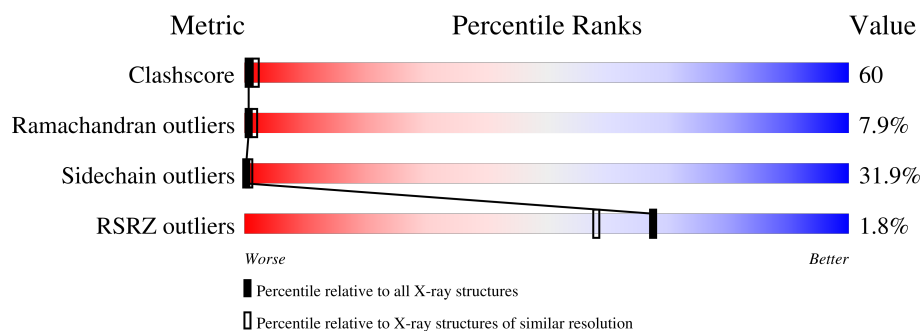
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	396	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3088 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 ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	396	3068	1939	533	583	13	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	PHE	ARG	engineered mutation	UNP P00509

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).

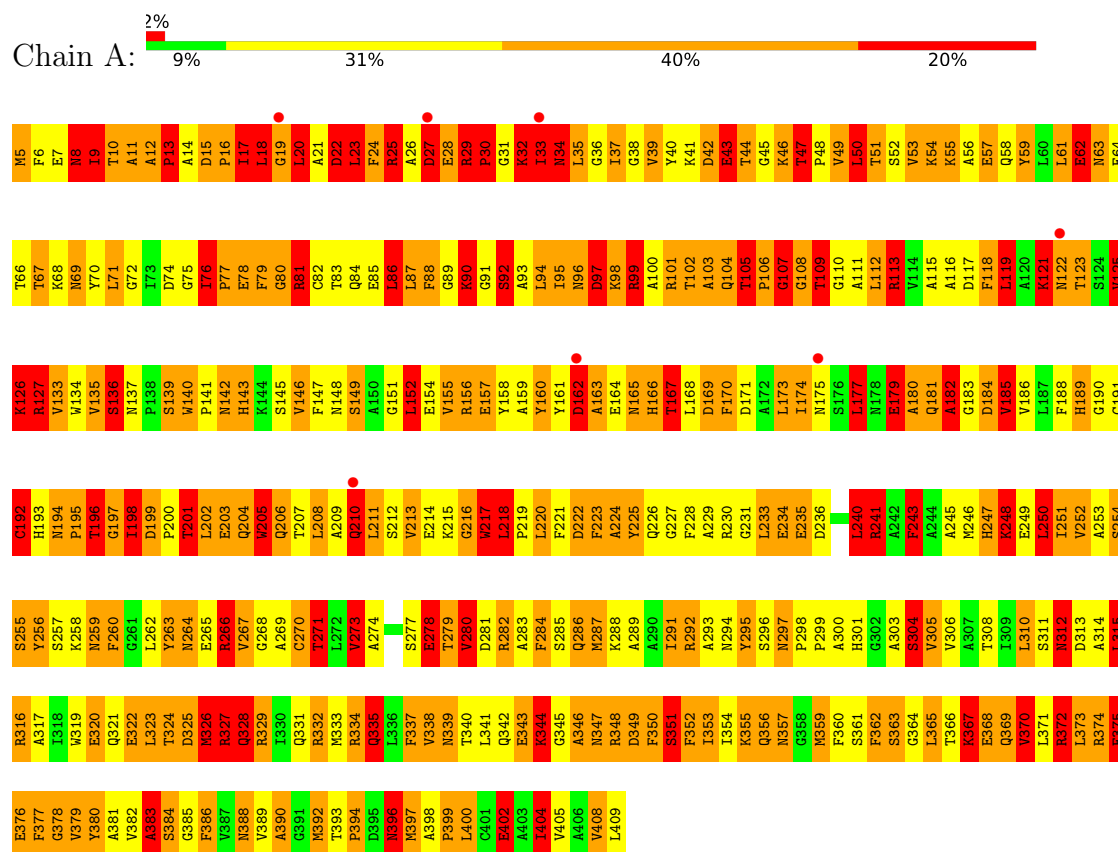


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	15	8	1	5	1	0	0

3 Residue-property plots

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

• Molecule 1: ASPARTATE AMINOTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	156.00Å 87.60Å 78.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80 10.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.80) 63.9 (10.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.78 (at 2.48Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.215 , (Not available) 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.648	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 104.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.029 for -1/2*h+3/2*k,1/2*h+1/2*k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3088	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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: SO4, 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	1.09	3/3130 (0.1%)	3.79	700/4242 (16.5%)

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	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	386	PHE	CA-C	-8.98	1.40	1.52
1	A	386	PHE	CA-CB	-7.73	1.41	1.53
1	A	386	PHE	CB-CG	-5.01	1.39	1.50

All (700) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	ARG	CD-NE-CZ	21.45	154.44	124.40
1	A	14	ALA	N-CA-C	19.35	134.18	110.19
1	A	13	PRO	CB-CA-C	18.94	142.81	111.56
1	A	122	ASN	CA-CB-CG	18.37	130.97	112.60
1	A	43	GLU	CB-CG-CD	18.14	143.43	112.60
1	A	199	ASP	CA-CB-CG	17.70	130.29	112.60
1	A	35	LEU	N-CA-C	-17.56	87.11	111.87
1	A	386	PHE	CA-CB-CG	17.40	131.20	113.80
1	A	162	ASP	CA-CB-CG	17.30	129.90	112.60
1	A	10	THR	CA-C-N	16.60	153.25	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	THR	C-N-CA	16.60	153.25	121.54
1	A	22	ASP	CA-CB-CG	-16.49	96.11	112.60
1	A	363	SER	CA-C-O	-16.36	103.07	120.58
1	A	321	GLN	OE1-CD-NE2	-16.18	106.42	122.60
1	A	122	ASN	CB-CG-ND2	16.02	140.43	116.40
1	A	12	ALA	N-CA-C	15.17	143.33	109.81
1	A	75	GLY	CA-C-N	15.04	133.42	122.59
1	A	75	GLY	C-N-CA	15.04	133.42	122.59
1	A	39	VAL	N-CA-CB	-15.01	93.23	112.60
1	A	357	ASN	CA-CB-CG	15.01	127.61	112.60
1	A	34	ASN	N-CA-C	-14.87	87.09	110.14
1	A	127	ARG	NE-CZ-NH2	14.40	132.16	119.20
1	A	350	PHE	CA-CB-CG	14.31	128.11	113.80
1	A	89	GLY	CA-C-O	13.94	136.06	122.26
1	A	322	GLU	CA-C-O	13.77	135.15	120.55
1	A	146	VAL	CB-CA-C	13.76	129.32	111.70
1	A	171	ASP	CA-C-O	-13.60	106.72	121.00
1	A	125	VAL	O-C-N	13.49	136.90	123.14
1	A	122	ASN	OD1-CG-ND2	-13.48	109.12	122.60
1	A	194	ASN	CA-CB-CG	13.32	125.92	112.60
1	A	105	THR	N-CA-CB	-12.96	89.14	111.17
1	A	192	CYS	CA-C-O	12.94	139.01	120.51
1	A	192	CYS	CA-C-N	12.84	141.59	121.56
1	A	192	CYS	C-N-CA	12.84	141.59	121.56
1	A	96	ASN	N-CA-C	-12.76	89.72	109.25
1	A	196	THR	OG1-CB-CG2	12.66	134.61	109.30
1	A	189	HIS	CA-C-O	-12.51	106.56	120.32
1	A	356	GLN	OE1-CD-NE2	12.43	135.03	122.60
1	A	122	ASN	N-CA-CB	12.37	131.39	110.49
1	A	125	VAL	N-CA-C	-12.30	90.69	108.53
1	A	22	ASP	CA-C-O	-12.13	106.61	120.20
1	A	279	THR	CA-C-O	-12.01	107.69	120.42
1	A	369	GLN	N-CA-C	-11.99	98.13	113.12
1	A	349	ASP	CA-CB-CG	-11.97	100.63	112.60
1	A	312	ASN	OD1-CG-ND2	11.97	134.57	122.60
1	A	327	ARG	NE-CZ-NH2	11.90	129.91	119.20
1	A	162	ASP	N-CA-C	-11.88	98.81	113.18
1	A	200	PRO	N-CA-C	-11.72	92.11	111.68
1	A	214	GLU	CB-CG-CD	11.58	132.29	112.60
1	A	14	ALA	CA-C-O	11.56	134.15	122.01
1	A	223	PHE	CA-CB-CG	11.50	125.30	113.80
1	A	10	THR	CB-CA-C	11.23	132.76	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	PRO	CA-C-N	11.00	142.96	121.41
1	A	106	PRO	C-N-CA	11.00	142.96	121.41
1	A	96	ASN	CB-CA-C	10.92	128.20	110.29
1	A	349	ASP	CB-CA-C	10.87	127.74	109.48
1	A	351	SER	N-CA-C	-10.87	99.97	113.01
1	A	241	ARG	N-CA-C	10.86	123.12	111.28
1	A	224	ALA	CA-C-O	-10.83	108.87	121.11
1	A	321	GLN	CB-CG-CD	10.78	130.92	112.60
1	A	312	ASN	CA-C-O	-10.73	108.68	121.02
1	A	278	GLU	CA-C-O	10.69	131.75	120.42
1	A	66	THR	N-CA-CB	-10.57	94.99	110.53
1	A	279	THR	O-C-N	10.55	134.18	122.15
1	A	377	PHE	N-CA-CB	10.52	128.75	110.44
1	A	127	ARG	CA-CB-CG	10.34	134.78	114.10
1	A	13	PRO	CA-C-N	10.32	139.25	121.29
1	A	13	PRO	C-N-CA	10.32	139.25	121.29
1	A	174	ILE	CA-C-O	10.11	131.56	121.05
1	A	402	GLU	CA-C-O	10.08	131.34	120.55
1	A	292	ARG	NE-CZ-NH1	10.08	131.58	121.50
1	A	297	ASN	CA-C-O	-10.06	111.48	120.13
1	A	388	ASN	CB-CG-ND2	-10.02	101.37	116.40
1	A	299	PRO	CB-CA-C	-9.90	103.55	111.87
1	A	189	HIS	O-C-N	9.88	134.93	123.27
1	A	210	GLN	N-CA-C	-9.78	100.31	110.97
1	A	192	CYS	CB-CA-C	9.78	129.88	110.42
1	A	304	SER	O-C-N	9.78	133.30	122.15
1	A	280	VAL	N-CA-CB	9.77	123.82	110.54
1	A	28	GLU	N-CA-C	9.76	125.02	108.23
1	A	235	GLU	CA-C-O	9.76	131.19	119.97
1	A	337	PHE	CA-C-O	9.74	130.74	120.70
1	A	325	ASP	N-CA-C	-9.73	100.23	111.03
1	A	247	HIS	CA-CB-CG	-9.67	104.13	113.80
1	A	377	PHE	CA-CB-CG	-9.64	104.16	113.80
1	A	8	ASN	CA-C-N	9.62	139.28	121.97
1	A	8	ASN	C-N-CA	9.62	139.28	121.97
1	A	96	ASN	CA-CB-CG	-9.61	102.99	112.60
1	A	278	GLU	CB-CG-CD	9.60	128.92	112.60
1	A	135	VAL	CA-C-O	-9.60	110.61	120.69
1	A	57	GLU	CA-CB-CG	9.54	133.18	114.10
1	A	39	VAL	CA-C-O	-9.54	111.56	121.67
1	A	126	LYS	CA-C-O	-9.53	108.72	119.67
1	A	112	LEU	N-CA-C	-9.51	100.79	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	HIS	CA-C-O	-9.50	108.75	119.67
1	A	103	ALA	CA-C-O	9.46	130.74	120.71
1	A	184	ASP	CA-CB-CG	-9.45	103.15	112.60
1	A	113	ARG	CD-NE-CZ	9.45	137.62	124.40
1	A	228	PHE	CA-CB-CG	9.44	123.24	113.80
1	A	117	ASP	CA-CB-CG	9.42	122.02	112.60
1	A	7	GLU	CB-CG-CD	9.29	128.39	112.60
1	A	313	ASP	N-CA-C	9.29	124.24	113.19
1	A	292	ARG	N-CA-CB	9.27	124.78	110.14
1	A	139	SER	CA-CB-OG	9.26	129.63	111.10
1	A	157	GLU	CB-CG-CD	9.26	128.34	112.60
1	A	24	PHE	O-C-N	9.20	134.19	122.23
1	A	210	GLN	CB-CG-CD	9.19	128.23	112.60
1	A	135	VAL	N-CA-C	9.17	120.38	111.67
1	A	334	ARG	NE-CZ-NH1	9.15	130.65	121.50
1	A	18	LEU	CA-C-O	9.14	130.93	119.05
1	A	51	THR	CA-CB-OG1	-9.13	95.91	109.60
1	A	175	ASN	CA-C-O	-9.13	111.30	120.70
1	A	334	ARG	N-CA-CB	9.06	123.43	109.94
1	A	165	ASN	CA-CB-CG	-9.05	103.55	112.60
1	A	87	LEU	CA-C-O	-9.02	111.41	120.70
1	A	110	GLY	CA-C-O	9.02	130.34	121.05
1	A	146	VAL	CA-CB-CG1	8.99	125.69	110.40
1	A	195	PRO	N-CD-CG	-8.96	93.05	103.80
1	A	121	LYS	N-CA-C	-8.93	95.66	108.96
1	A	127	ARG	NH1-CZ-NH2	-8.90	107.73	119.30
1	A	250	LEU	N-CA-CB	-8.82	98.16	111.56
1	A	106	PRO	CA-C-O	8.80	136.61	120.60
1	A	193	HIS	N-CA-CB	-8.75	95.95	109.34
1	A	174	ILE	CA-C-N	8.75	132.34	120.44
1	A	174	ILE	C-N-CA	8.75	132.34	120.44
1	A	79	PHE	CA-CB-CG	-8.74	105.06	113.80
1	A	113	ARG	NE-CZ-NH1	-8.74	112.76	121.50
1	A	191	CYS	CA-C-O	8.72	129.78	120.36
1	A	216	GLY	O-C-N	-8.63	111.47	122.70
1	A	113	ARG	NE-CZ-NH2	8.61	126.95	119.20
1	A	223	PHE	CA-C-O	8.57	134.61	120.81
1	A	348	ARG	CA-C-O	8.54	130.88	121.40
1	A	169	ASP	CA-C-O	-8.53	112.04	122.36
1	A	305	VAL	N-CA-C	-8.51	101.39	110.23
1	A	207	THR	CA-C-O	-8.36	110.96	120.24
1	A	297	ASN	N-CA-C	-8.34	100.62	108.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	ARG	CA-C-O	-8.27	109.28	119.28
1	A	51	THR	CA-C-O	-8.25	112.20	120.70
1	A	62	GLU	CA-CB-CG	8.22	130.55	114.10
1	A	356	GLN	N-CA-CB	-8.21	99.05	110.38
1	A	81	ARG	NE-CZ-NH1	-8.21	113.29	121.50
1	A	254	SER	N-CA-C	8.18	122.83	110.14
1	A	350	PHE	CA-C-O	8.18	127.67	119.08
1	A	377	PHE	O-C-N	8.18	132.15	122.09
1	A	165	ASN	OD1-CG-ND2	8.17	130.77	122.60
1	A	94	LEU	O-C-N	8.16	131.74	122.27
1	A	280	VAL	O-C-N	8.14	129.76	121.87
1	A	189	HIS	N-CA-C	-8.11	95.31	108.52
1	A	383	ALA	CA-C-O	-8.09	108.94	120.51
1	A	29	ARG	CA-C-N	8.09	129.95	119.84
1	A	29	ARG	C-N-CA	8.09	129.95	119.84
1	A	304	SER	N-CA-C	-8.08	102.56	111.36
1	A	317	ALA	O-C-N	8.08	130.68	122.12
1	A	37	ILE	CA-C-N	-8.07	110.04	122.30
1	A	37	ILE	C-N-CA	-8.07	110.04	122.30
1	A	44	THR	CA-CB-OG1	-8.07	97.49	109.60
1	A	234	GLU	O-C-N	-8.07	112.35	122.27
1	A	247	HIS	N-CA-C	8.06	123.70	113.55
1	A	356	GLN	CA-CB-CG	-8.05	98.01	114.10
1	A	179	GLU	CB-CG-CD	8.04	126.27	112.60
1	A	94	LEU	N-CA-C	-8.04	102.95	114.12
1	A	27	ASP	CA-CB-CG	8.03	120.63	112.60
1	A	328	GLN	CA-CB-CG	-8.03	98.04	114.10
1	A	365	LEU	CA-CB-CG	8.01	144.34	116.30
1	A	210	GLN	N-CA-CB	8.01	121.60	109.91
1	A	57	GLU	CA-C-O	8.00	129.17	119.97
1	A	198	ILE	N-CA-CB	7.97	122.09	111.25
1	A	342	GLN	CA-C-O	7.97	131.91	120.51
1	A	295	TYR	N-CA-C	-7.96	95.95	109.24
1	A	246	MET	N-CA-C	7.96	122.54	111.56
1	A	8	ASN	CA-C-O	7.95	131.88	120.51
1	A	314	ALA	N-CA-C	-7.95	101.71	111.40
1	A	109	THR	CB-CA-C	7.94	123.97	110.79
1	A	347	ASN	OD1-CG-ND2	7.94	130.54	122.60
1	A	119	LEU	CA-C-O	7.94	129.10	119.97
1	A	306	VAL	N-CA-C	7.93	118.69	110.36
1	A	394	PRO	CA-C-O	-7.93	107.50	119.55
1	A	230	ARG	CA-C-N	-7.93	110.61	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	ARG	C-N-CA	-7.93	110.61	120.92
1	A	84	GLN	OE1-CD-NE2	7.92	130.52	122.60
1	A	256	TYR	O-C-N	7.91	132.08	122.35
1	A	154	GLU	N-CA-CB	7.91	123.04	110.23
1	A	408	VAL	CA-C-N	7.90	135.91	121.70
1	A	408	VAL	C-N-CA	7.90	135.91	121.70
1	A	377	PHE	CA-C-O	-7.89	110.58	119.81
1	A	63	ASN	CB-CA-C	7.88	125.55	109.55
1	A	301	HIS	CA-CB-CG	-7.87	105.93	113.80
1	A	107	GLY	N-CA-C	7.86	131.81	113.18
1	A	69	ASN	CA-CB-CG	-7.86	104.75	112.60
1	A	308	THR	CA-CB-OG1	-7.85	97.82	109.60
1	A	59	TYR	CB-CG-CD2	-7.85	109.03	120.80
1	A	394	PRO	O-C-N	7.82	132.31	122.22
1	A	233	LEU	CB-CA-C	7.82	123.35	110.92
1	A	357	ASN	CA-C-O	7.81	130.25	121.11
1	A	63	ASN	N-CA-CB	-7.78	98.30	110.44
1	A	23	LEU	CA-C-O	7.77	128.94	119.38
1	A	146	VAL	CA-CB-CG2	-7.77	97.20	110.40
1	A	386	PHE	CB-CA-C	7.76	121.34	110.16
1	A	196	THR	CB-CA-C	-7.76	98.91	110.62
1	A	340	THR	CB-CA-C	7.76	125.51	110.46
1	A	316	ARG	N-CA-CB	7.75	121.31	110.07
1	A	230	ARG	NH1-CZ-NH2	-7.74	109.24	119.30
1	A	252	VAL	CA-C-O	-7.74	112.00	120.67
1	A	328	GLN	N-CA-C	7.73	119.79	111.36
1	A	347	ASN	CA-C-N	-7.73	110.08	122.53
1	A	347	ASN	C-N-CA	-7.73	110.08	122.53
1	A	312	ASN	CB-CG-ND2	-7.73	104.81	116.40
1	A	169	ASP	O-C-N	7.72	133.10	122.29
1	A	14	ALA	O-C-N	-7.72	112.02	122.36
1	A	321	GLN	CG-CD-OE1	7.71	136.21	120.80
1	A	6	PHE	CA-CB-CG	-7.69	106.11	113.80
1	A	368	GLU	CB-CG-CD	7.69	125.68	112.60
1	A	322	GLU	O-C-N	-7.68	113.98	122.12
1	A	52	SER	CA-C-N	7.67	130.37	120.56
1	A	52	SER	C-N-CA	7.67	130.37	120.56
1	A	28	GLU	CA-C-N	7.66	140.49	121.80
1	A	28	GLU	C-N-CA	7.66	140.49	121.80
1	A	222	ASP	CA-CB-CG	-7.66	104.94	112.60
1	A	193	HIS	CA-C-O	7.66	128.61	120.95
1	A	227	GLY	O-C-N	7.65	131.53	122.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	GLU	CB-CG-CD	7.65	125.60	112.60
1	A	66	THR	CA-CB-CG2	7.64	123.49	110.50
1	A	379	VAL	CB-CA-C	7.63	121.74	110.98
1	A	205	TRP	CA-C-N	7.63	131.13	120.29
1	A	205	TRP	C-N-CA	7.63	131.13	120.29
1	A	316	ARG	O-C-N	7.63	130.33	122.09
1	A	385	GLY	O-C-N	7.61	132.10	122.28
1	A	288	LYS	N-CA-C	-7.60	103.47	112.89
1	A	368	GLU	CG-CD-OE1	7.59	135.87	118.40
1	A	236	ASP	CB-CA-C	7.59	124.67	110.63
1	A	29	ARG	CD-NE-CZ	7.58	135.02	124.40
1	A	230	ARG	CA-C-O	-7.57	110.95	119.81
1	A	50	LEU	N-CA-C	7.57	126.92	110.80
1	A	291	ILE	CA-C-O	-7.56	111.17	121.15
1	A	148	ASN	N-CA-CB	7.55	121.85	110.22
1	A	101	ARG	NE-CZ-NH2	7.52	125.97	119.20
1	A	223	PHE	CA-C-N	7.51	134.61	122.81
1	A	223	PHE	C-N-CA	7.51	134.61	122.81
1	A	9	ILE	CB-CG1-CD1	7.49	129.53	113.80
1	A	322	GLU	CA-C-N	7.48	130.91	120.29
1	A	322	GLU	C-N-CA	7.48	130.91	120.29
1	A	346	ALA	N-CA-C	7.47	121.24	110.10
1	A	273	VAL	CB-CA-C	7.46	122.63	110.69
1	A	204	GLN	CA-C-O	7.42	128.84	120.90
1	A	316	ARG	CA-CB-CG	7.42	128.93	114.10
1	A	267	VAL	N-CA-C	7.41	119.25	108.58
1	A	283	ALA	N-CA-C	7.41	119.44	111.36
1	A	140	TRP	CB-CA-C	7.37	120.78	109.50
1	A	257	SER	CA-CB-OG	7.37	125.84	111.10
1	A	96	ASN	N-CA-CB	7.37	121.88	109.87
1	A	250	LEU	CB-CA-C	7.35	122.77	110.43
1	A	76	ILE	CB-CA-C	-7.34	102.86	110.71
1	A	196	THR	CA-C-O	-7.33	112.41	120.33
1	A	316	ARG	NE-CZ-NH1	-7.30	114.20	121.50
1	A	199	ASP	CB-CA-C	-7.29	98.55	108.68
1	A	148	ASN	CB-CG-ND2	7.29	127.33	116.40
1	A	265	GLU	CG-CD-OE1	7.28	135.15	118.40
1	A	188	PHE	CA-C-O	7.26	129.94	121.44
1	A	338	VAL	CA-C-O	-7.25	113.16	120.85
1	A	140	TRP	N-CA-C	-7.23	100.67	109.57
1	A	66	THR	CA-CB-OG1	-7.23	98.75	109.60
1	A	375	GLU	O-C-N	-7.22	112.98	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	SER	N-CA-C	-7.22	96.79	108.41
1	A	404	ILE	CA-C-O	-7.21	113.52	121.17
1	A	17	ILE	O-C-N	7.21	131.58	122.57
1	A	296	SER	CA-CB-OG	7.20	125.50	111.10
1	A	64	GLU	CA-C-N	7.20	134.37	121.92
1	A	64	GLU	C-N-CA	7.20	134.37	121.92
1	A	287	MET	N-CA-C	-7.19	103.49	112.90
1	A	222	ASP	O-C-N	7.18	132.18	123.13
1	A	326	MET	CA-CB-CG	-7.17	99.76	114.10
1	A	29	ARG	NH1-CZ-NH2	-7.16	110.00	119.30
1	A	221	PHE	N-CA-CB	7.15	121.81	110.23
1	A	257	SER	N-CA-CB	7.14	120.85	110.20
1	A	199	ASP	N-CA-C	7.14	120.17	110.31
1	A	143	HIS	CA-C-N	7.12	130.15	120.54
1	A	143	HIS	C-N-CA	7.12	130.15	120.54
1	A	207	THR	CA-CB-OG1	-7.12	98.93	109.60
1	A	335	GLN	CA-CB-CG	7.12	128.33	114.10
1	A	245	ALA	CB-CA-C	-7.11	97.48	110.63
1	A	363	SER	O-C-N	7.10	131.45	122.93
1	A	201	THR	N-CA-C	-7.10	101.38	110.53
1	A	241	ARG	NE-CZ-NH1	-7.09	114.41	121.50
1	A	122	ASN	N-CA-C	-7.09	95.70	110.80
1	A	105	THR	CA-C-N	7.07	128.68	119.84
1	A	105	THR	C-N-CA	7.07	128.68	119.84
1	A	404	ILE	N-CA-CB	7.07	118.82	110.55
1	A	12	ALA	N-CA-CB	-7.07	97.80	110.37
1	A	243	PHE	O-C-N	7.06	129.34	122.07
1	A	113	ARG	CA-CB-CG	-7.03	100.04	114.10
1	A	182	ALA	CA-C-O	-7.02	110.47	120.51
1	A	344	LYS	CG-CD-CE	7.01	127.43	111.30
1	A	98	LYS	CA-CB-CG	7.00	128.09	114.10
1	A	141	PRO	O-C-N	7.00	130.63	122.23
1	A	311	SER	CA-CB-OG	-7.00	97.11	111.10
1	A	56	ALA	N-CA-CB	6.99	121.12	110.28
1	A	140	TRP	CA-C-N	6.98	126.80	119.05
1	A	140	TRP	C-N-CA	6.98	126.80	119.05
1	A	360	PHE	N-CA-C	6.98	121.42	110.32
1	A	372	ARG	N-CA-C	-6.98	104.73	113.18
1	A	112	LEU	CA-C-N	-6.98	111.14	120.63
1	A	112	LEU	C-N-CA	-6.98	111.14	120.63
1	A	11	ALA	N-CA-CB	6.96	122.26	110.49
1	A	47	THR	CA-C-N	6.96	127.91	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	THR	C-N-CA	6.96	127.91	120.11
1	A	167	THR	O-C-N	6.96	131.06	122.92
1	A	255	SER	CB-CA-C	6.95	121.62	109.80
1	A	70	TYR	N-CA-CB	6.95	120.74	109.69
1	A	251	ILE	CB-CG1-CD1	-6.95	99.21	113.80
1	A	230	ARG	O-C-N	6.95	130.63	122.09
1	A	102	THR	CA-C-O	-6.94	112.67	120.66
1	A	217	TRP	CA-C-N	-6.94	111.48	121.20
1	A	217	TRP	C-N-CA	-6.94	111.48	121.20
1	A	105	THR	CA-CB-CG2	6.94	122.30	110.50
1	A	175	ASN	O-C-N	6.94	129.59	122.09
1	A	123	THR	O-C-N	6.94	132.61	122.97
1	A	15	ASP	N-CA-C	6.93	118.44	109.64
1	A	113	ARG	N-CA-CB	6.93	120.03	109.98
1	A	17	ILE	CA-C-O	-6.92	112.13	120.78
1	A	235	GLU	N-CA-C	6.92	119.85	111.82
1	A	374	ARG	CG-CD-NE	6.92	127.22	112.00
1	A	378	GLY	CA-C-O	-6.91	111.34	119.01
1	A	298	PRO	N-CA-CB	-6.90	96.39	103.08
1	A	297	ASN	O-C-N	6.90	129.41	122.17
1	A	313	ASP	OD1-CG-OD2	6.89	139.44	122.90
1	A	282	ARG	CB-CG-CD	6.88	127.11	111.30
1	A	49	VAL	CA-C-O	-6.87	112.70	120.26
1	A	181	GLN	CG-CD-NE2	-6.86	106.11	116.40
1	A	282	ARG	NE-CZ-NH1	6.85	128.35	121.50
1	A	190	GLY	O-C-N	-6.85	113.80	122.70
1	A	267	VAL	N-CA-CB	-6.84	103.26	110.72
1	A	312	ASN	CA-CB-CG	-6.83	105.77	112.60
1	A	75	GLY	N-CA-C	6.83	119.84	111.45
1	A	34	ASN	O-C-N	6.82	131.90	123.10
1	A	268	GLY	CA-C-O	-6.82	115.15	121.63
1	A	388	ASN	CB-CG-OD1	6.82	134.43	120.80
1	A	76	ILE	CA-C-O	6.81	123.17	119.15
1	A	59	TYR	CB-CG-CD1	6.81	131.01	120.80
1	A	191	CYS	CA-C-N	6.80	134.53	121.54
1	A	191	CYS	C-N-CA	6.80	134.53	121.54
1	A	202	LEU	CA-C-O	-6.80	113.63	120.90
1	A	127	ARG	CG-CD-NE	6.77	126.90	112.00
1	A	227	GLY	N-CA-C	-6.77	105.72	115.27
1	A	170	PHE	CB-CA-C	-6.75	100.02	110.81
1	A	195	PRO	CA-C-O	-6.74	104.03	120.20
1	A	177	LEU	N-CA-C	6.72	119.61	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	LEU	O-C-N	6.71	129.80	122.15
1	A	231	GLY	CA-C-O	-6.71	115.05	121.49
1	A	259	ASN	OD1-CG-ND2	6.71	129.31	122.60
1	A	167	THR	CA-C-O	-6.70	114.26	121.36
1	A	126	LYS	CG-CD-CE	6.69	126.68	111.30
1	A	123	THR	CA-C-O	-6.68	113.23	121.78
1	A	188	PHE	N-CA-CB	6.68	123.18	111.55
1	A	282	ARG	NH1-CZ-NH2	-6.68	110.61	119.30
1	A	82	CYS	CB-CA-C	6.67	121.35	110.88
1	A	257	SER	CA-C-O	-6.67	112.83	120.24
1	A	20	LEU	O-C-N	6.66	131.44	122.59
1	A	240	LEU	N-CA-C	-6.66	102.90	111.02
1	A	22	ASP	N-CA-C	6.65	120.26	111.75
1	A	193	HIS	N-CA-C	6.64	120.12	110.42
1	A	334	ARG	CA-C-O	-6.64	113.79	120.90
1	A	386	PHE	CA-C-O	-6.64	113.06	120.70
1	A	43	GLU	OE1-CD-OE2	-6.60	107.05	122.90
1	A	264	ASN	OD1-CG-ND2	6.58	129.18	122.60
1	A	399	PRO	CA-C-N	6.57	129.41	120.54
1	A	399	PRO	C-N-CA	6.57	129.41	120.54
1	A	100	ALA	CA-C-N	6.57	132.86	122.74
1	A	100	ALA	C-N-CA	6.57	132.86	122.74
1	A	396	ASN	N-CA-C	-6.57	105.23	113.18
1	A	29	ARG	N-CA-C	-6.57	95.29	109.81
1	A	194	ASN	CA-C-O	6.57	126.68	119.32
1	A	230	ARG	NE-CZ-NH2	6.57	125.11	119.20
1	A	27	ASP	O-C-N	6.56	131.32	122.59
1	A	95	ILE	CA-C-N	-6.55	112.23	121.72
1	A	95	ILE	C-N-CA	-6.55	112.23	121.72
1	A	34	ASN	N-CA-CB	6.54	120.92	110.85
1	A	121	LYS	CA-C-O	-6.53	114.47	121.45
1	A	92	SER	CA-C-O	-6.52	111.18	120.51
1	A	343	GLU	CG-CD-OE2	-6.52	103.41	118.40
1	A	402	GLU	CA-CB-CG	6.52	127.13	114.10
1	A	20	LEU	CA-C-O	-6.52	111.19	120.51
1	A	74	ASP	CB-CA-C	6.51	123.44	110.17
1	A	264	ASN	N-CA-C	6.50	121.05	113.18
1	A	43	GLU	N-CA-CB	6.49	121.84	110.42
1	A	151	GLY	CA-C-O	6.48	127.46	119.88
1	A	44	THR	CB-CA-C	-6.48	99.22	110.17
1	A	56	ALA	CA-C-O	-6.48	112.52	119.97
1	A	224	ALA	N-CA-C	-6.48	99.36	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	PHE	CA-C-N	-6.46	110.97	120.28
1	A	147	PHE	C-N-CA	-6.46	110.97	120.28
1	A	298	PRO	CB-CA-C	6.46	118.80	110.92
1	A	356	GLN	CG-CD-NE2	-6.44	106.74	116.40
1	A	118	PHE	CA-C-O	-6.44	113.09	120.24
1	A	122	ASN	O-C-N	6.42	131.13	122.59
1	A	402	GLU	CA-C-N	6.42	128.79	120.44
1	A	402	GLU	C-N-CA	6.42	128.79	120.44
1	A	266	ARG	NE-CZ-NH2	-6.42	113.42	119.20
1	A	282	ARG	CA-C-O	-6.42	113.70	120.63
1	A	345	GLY	N-CA-C	6.40	128.35	113.18
1	A	47	THR	N-CA-CB	-6.39	100.69	111.30
1	A	375	GLU	CB-CG-CD	6.38	123.45	112.60
1	A	380	TYR	CA-CB-CG	-6.36	102.44	113.90
1	A	18	LEU	CB-CA-C	6.35	123.13	110.17
1	A	222	ASP	N-CA-CB	6.35	121.01	110.47
1	A	190	GLY	CA-C-O	6.34	131.60	120.57
1	A	192	CYS	CA-CB-SG	-6.33	99.83	114.40
1	A	341	LEU	CA-C-O	-6.33	112.69	119.97
1	A	93	ALA	CA-C-O	-6.33	111.46	120.51
1	A	8	ASN	CA-CB-CG	6.33	118.92	112.60
1	A	348	ARG	N-CA-C	6.33	117.78	108.86
1	A	225	TYR	N-CA-C	6.32	124.27	110.80
1	A	376	GLU	N-CA-CB	6.32	121.43	109.93
1	A	139	SER	N-CA-CB	6.32	121.86	111.62
1	A	392	MET	CA-C-O	-6.29	113.38	120.43
1	A	99	ARG	CA-C-O	-6.29	112.37	119.79
1	A	322	GLU	N-CA-C	6.29	118.14	111.28
1	A	213	VAL	CB-CA-C	-6.29	103.81	112.24
1	A	106	PRO	O-C-N	-6.26	114.19	122.64
1	A	19	GLY	N-CA-C	-6.26	98.34	113.18
1	A	316	ARG	CB-CA-C	-6.25	101.02	110.90
1	A	356	GLN	CA-C-O	-6.25	114.82	121.88
1	A	12	ALA	CA-C-N	6.24	127.63	119.84
1	A	12	ALA	C-N-CA	6.24	127.63	119.84
1	A	28	GLU	CA-CB-CG	6.23	126.56	114.10
1	A	335	GLN	CB-CG-CD	6.23	123.19	112.60
1	A	294	ASN	CA-CB-CG	-6.22	106.38	112.60
1	A	38	GLY	N-CA-C	-6.21	105.00	115.80
1	A	143	HIS	CA-CB-CG	-6.21	107.59	113.80
1	A	161	TYR	CB-CA-C	-6.21	100.80	111.23
1	A	295	TYR	CA-C-O	-6.21	113.52	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	PHE	CA-C-N	6.20	129.47	120.11
1	A	260	PHE	C-N-CA	6.20	129.47	120.11
1	A	156	ARG	CA-CB-CG	6.18	126.47	114.10
1	A	214	GLU	CA-C-O	-6.18	111.02	119.12
1	A	292	ARG	NH1-CZ-NH2	-6.18	111.26	119.30
1	A	218	LEU	CA-C-N	6.18	127.11	120.13
1	A	218	LEU	C-N-CA	6.18	127.11	120.13
1	A	223	PHE	N-CA-C	6.16	120.11	107.37
1	A	332	ARG	CD-NE-CZ	6.14	133.00	124.40
1	A	198	ILE	O-C-N	6.14	129.62	123.18
1	A	177	LEU	O-C-N	6.13	129.81	122.27
1	A	227	GLY	CA-C-O	-6.11	112.23	119.01
1	A	304	SER	CA-C-O	-6.11	113.95	120.42
1	A	271	THR	CA-C-N	6.11	132.10	122.94
1	A	271	THR	C-N-CA	6.11	132.10	122.94
1	A	208	LEU	CA-C-N	6.10	128.37	120.44
1	A	208	LEU	C-N-CA	6.10	128.37	120.44
1	A	218	LEU	N-CA-C	-6.09	100.41	109.42
1	A	92	SER	CA-C-N	-6.08	109.93	121.54
1	A	92	SER	C-N-CA	-6.08	109.93	121.54
1	A	154	GLU	CA-C-O	-6.08	113.93	120.92
1	A	22	ASP	N-CA-CB	6.07	119.72	110.14
1	A	72	GLY	N-CA-C	-6.06	103.23	112.51
1	A	21	ALA	CA-C-O	-6.06	114.66	120.90
1	A	101	ARG	CA-C-O	-6.05	113.60	120.32
1	A	339	ASN	OD1-CG-ND2	6.05	128.65	122.60
1	A	252	VAL	O-C-N	6.04	129.56	123.10
1	A	304	SER	CA-C-N	-6.03	112.87	120.77
1	A	304	SER	C-N-CA	-6.03	112.87	120.77
1	A	152	LEU	CA-C-O	-6.03	114.19	120.70
1	A	286	GLN	CA-C-O	6.03	126.88	119.05
1	A	162	ASP	CB-CA-C	6.02	121.92	109.95
1	A	181	GLN	OE1-CD-NE2	6.01	128.61	122.60
1	A	385	GLY	CA-C-N	6.01	129.92	121.02
1	A	385	GLY	C-N-CA	6.01	129.92	121.02
1	A	93	ALA	N-CA-CB	6.01	120.65	110.49
1	A	30	PRO	CA-C-N	6.00	133.16	121.41
1	A	30	PRO	C-N-CA	6.00	133.16	121.41
1	A	102	THR	O-C-N	5.99	130.58	123.27
1	A	339	ASN	CB-CG-ND2	-5.99	107.42	116.40
1	A	137	ASN	N-CA-CB	5.99	120.22	110.05
1	A	109	THR	CA-C-N	5.98	126.75	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	THR	C-N-CA	5.98	126.75	119.99
1	A	125	VAL	N-CA-CB	5.98	122.28	111.21
1	A	92	SER	O-C-N	5.97	130.53	122.59
1	A	392	MET	O-C-N	5.96	129.99	123.13
1	A	223	PHE	O-C-N	-5.96	114.95	123.06
1	A	335	GLN	OE1-CD-NE2	-5.96	116.64	122.60
1	A	342	GLN	OE1-CD-NE2	-5.95	116.65	122.60
1	A	125	VAL	CA-C-O	-5.93	113.95	120.72
1	A	390	ALA	N-CA-C	5.93	119.62	112.38
1	A	112	LEU	O-C-N	5.93	129.56	122.27
1	A	208	LEU	CB-CA-C	5.93	120.19	110.88
1	A	235	GLU	CG-CD-OE1	5.93	132.04	118.40
1	A	375	GLU	N-CA-CB	5.93	120.51	110.49
1	A	281	ASP	CA-C-O	-5.92	114.60	120.70
1	A	112	LEU	CA-C-O	-5.92	113.17	119.97
1	A	126	LYS	O-C-N	5.92	131.00	122.13
1	A	12	ALA	CB-CA-C	-5.90	98.54	110.17
1	A	284	PHE	CB-CA-C	5.90	120.58	110.79
1	A	235	GLU	CG-CD-OE2	-5.89	104.85	118.40
1	A	170	PHE	O-C-N	5.89	128.21	122.09
1	A	270	CYS	CA-C-O	5.88	126.58	120.40
1	A	45	GLY	N-CA-C	-5.88	106.61	115.32
1	A	402	GLU	CB-CG-CD	5.88	122.59	112.60
1	A	99	ARG	N-CA-CB	5.88	119.35	110.30
1	A	186	VAL	CA-C-O	-5.88	113.78	120.66
1	A	86	LEU	CB-CA-C	5.87	120.18	110.90
1	A	136	SER	N-CA-CB	5.87	120.41	110.49
1	A	288	LYS	CA-CB-CG	5.86	125.82	114.10
1	A	361	SER	O-C-N	5.86	129.77	123.56
1	A	233	LEU	N-CA-CB	-5.86	100.92	109.82
1	A	133	VAL	N-CA-CB	5.85	121.03	111.44
1	A	89	GLY	N-CA-C	5.84	119.18	111.70
1	A	216	GLY	CA-C-N	5.84	132.70	121.54
1	A	216	GLY	C-N-CA	5.84	132.70	121.54
1	A	186	VAL	CA-C-N	5.83	130.18	121.72
1	A	186	VAL	C-N-CA	5.83	130.18	121.72
1	A	154	GLU	O-C-N	5.83	129.92	123.16
1	A	79	PHE	N-CA-CB	-5.82	101.33	110.06
1	A	79	PHE	CA-C-O	5.82	126.91	120.63
1	A	375	GLU	CG-CD-OE2	-5.81	105.04	118.40
1	A	27	ASP	CA-C-O	-5.80	112.22	120.51
1	A	107	GLY	O-C-N	5.79	130.23	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	PHE	N-CA-CB	5.78	119.02	110.53
1	A	21	ALA	N-CA-C	-5.77	104.63	111.03
1	A	135	VAL	N-CA-CB	-5.76	102.55	110.68
1	A	229	ALA	CA-C-O	-5.76	114.37	120.71
1	A	32	LYS	N-CA-C	-5.75	103.53	111.81
1	A	292	ARG	CD-NE-CZ	5.73	132.42	124.40
1	A	87	LEU	N-CA-C	5.73	117.33	111.14
1	A	214	GLU	O-C-N	5.73	130.87	122.39
1	A	115	ALA	N-CA-C	-5.71	105.13	111.36
1	A	62	GLU	N-CA-C	5.71	119.42	112.23
1	A	233	LEU	O-C-N	5.71	128.19	122.08
1	A	349	ASP	CA-C-O	5.71	127.13	120.80
1	A	19	GLY	O-C-N	5.70	130.11	122.70
1	A	202	LEU	O-C-N	5.70	128.01	122.09
1	A	48	PRO	O-C-N	5.69	129.54	122.71
1	A	56	ALA	O-C-N	5.68	129.26	122.27
1	A	222	ASP	N-CA-C	-5.68	97.93	107.99
1	A	21	ALA	CA-C-N	-5.68	112.09	120.38
1	A	21	ALA	C-N-CA	-5.68	112.09	120.38
1	A	343	GLU	N-CA-CB	-5.67	100.91	110.49
1	A	339	ASN	CA-CB-CG	-5.66	106.94	112.60
1	A	63	ASN	CA-CB-CG	-5.66	106.94	112.60
1	A	29	ARG	CA-CB-CG	5.66	125.41	114.10
1	A	340	THR	CA-CB-CG2	5.66	120.12	110.50
1	A	184	ASP	CA-C-O	-5.66	114.22	120.38
1	A	47	THR	CA-C-O	5.64	128.37	120.64
1	A	368	GLU	CG-CD-OE2	-5.64	105.42	118.40
1	A	24	PHE	N-CA-C	-5.63	104.77	111.69
1	A	286	GLN	O-C-N	-5.62	114.71	122.46
1	A	370	VAL	N-CA-C	-5.62	104.89	110.62
1	A	59	TYR	N-CA-C	-5.60	105.70	112.54
1	A	315	LEU	CA-C-O	5.60	126.26	119.49
1	A	48	PRO	CB-CG-CD	-5.59	88.20	106.10
1	A	294	ASN	CB-CA-C	5.58	119.68	111.65
1	A	349	ASP	CB-CG-OD2	-5.57	105.59	118.40
1	A	313	ASP	CB-CG-OD1	-5.55	105.64	118.40
1	A	30	PRO	O-C-N	-5.53	115.17	122.64
1	A	58	GLN	CA-C-O	5.53	126.31	119.79
1	A	298	PRO	CA-C-N	5.53	127.97	120.79
1	A	298	PRO	C-N-CA	5.53	127.97	120.79
1	A	205	TRP	N-CA-CB	-5.52	102.00	110.12
1	A	206	GLN	OE1-CD-NE2	-5.52	117.08	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ASN	CB-CG-OD1	-5.51	109.78	120.80
1	A	228	PHE	N-CA-CB	5.50	119.02	110.44
1	A	208	LEU	N-CA-C	-5.49	105.19	111.07
1	A	81	ARG	NH1-CZ-NH2	5.49	126.43	119.30
1	A	53	VAL	CA-CB-CG1	5.48	119.72	110.40
1	A	316	ARG	N-CA-C	-5.48	105.22	111.14
1	A	334	ARG	NE-CZ-NH2	-5.48	114.27	119.20
1	A	257	SER	N-CA-C	-5.47	104.97	111.69
1	A	324	THR	O-C-N	5.46	128.38	122.15
1	A	359	MET	O-C-N	5.46	128.37	122.15
1	A	166	HIS	N-CA-C	5.46	122.43	110.80
1	A	229	ALA	CB-CA-C	5.46	121.77	112.00
1	A	61	LEU	O-C-N	5.45	127.90	122.12
1	A	280	VAL	CG1-CB-CG2	-5.45	98.81	110.80
1	A	48	PRO	CB-CA-C	-5.44	103.02	111.40
1	A	367	LYS	N-CA-C	-5.44	104.78	111.75
1	A	41	LYS	CA-C-O	-5.44	114.07	120.60
1	A	300	ALA	N-CA-C	5.44	117.66	111.02
1	A	67	THR	CA-CB-OG1	5.43	117.75	109.60
1	A	195	PRO	CA-N-CD	-5.43	103.90	111.50
1	A	306	VAL	CA-C-N	5.43	127.55	120.28
1	A	306	VAL	C-N-CA	5.43	127.55	120.28
1	A	362	PHE	N-CA-CB	5.43	119.11	110.16
1	A	99	ARG	NH1-CZ-NH2	5.42	126.34	119.30
1	A	256	TYR	CA-CB-CG	-5.41	104.16	113.90
1	A	203	GLU	CA-C-N	5.41	127.84	120.54
1	A	203	GLU	C-N-CA	5.41	127.84	120.54
1	A	189	HIS	ND1-CE1-NE2	5.40	113.80	108.40
1	A	118	PHE	O-C-N	5.40	129.25	122.23
1	A	192	CYS	N-CA-C	5.40	122.30	110.80
1	A	203	GLU	O-C-N	-5.40	116.48	122.09
1	A	207	THR	CA-CB-CG2	5.40	119.68	110.50
1	A	13	PRO	CA-N-CD	-5.39	104.45	112.00
1	A	137	ASN	OD1-CG-ND2	-5.39	117.21	122.60
1	A	315	LEU	N-CA-CB	-5.39	101.16	110.32
1	A	278	GLU	CB-CA-C	-5.39	101.69	110.85
1	A	329	ARG	N-CA-C	-5.38	105.41	111.28
1	A	221	PHE	O-C-N	5.37	129.39	123.16
1	A	292	ARG	CA-CB-CG	5.37	124.83	114.10
1	A	70	TYR	CA-CB-CG	5.36	123.55	113.90
1	A	299	PRO	N-CA-CB	5.35	105.92	102.92
1	A	191	CYS	N-CA-C	-5.35	100.19	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	PRO	N-CA-C	-5.34	106.57	113.57
1	A	78	GLU	CA-C-O	5.34	126.21	120.55
1	A	279	THR	N-CA-C	-5.34	105.54	111.36
1	A	299	PRO	O-C-N	5.34	126.52	122.73
1	A	92	SER	CB-CA-C	-5.34	99.80	110.42
1	A	327	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	A	270	CYS	CB-CA-C	5.33	119.32	110.74
1	A	84	GLN	CG-CD-NE2	-5.32	108.42	116.40
1	A	90	LYS	CB-CA-C	5.32	121.00	110.42
1	A	372	ARG	NE-CZ-NH1	-5.31	116.19	121.50
1	A	57	GLU	CA-C-N	5.31	129.71	120.68
1	A	57	GLU	C-N-CA	5.31	129.71	120.68
1	A	152	LEU	N-CA-C	-5.30	100.75	109.40
1	A	54	LYS	CA-C-O	5.29	126.89	121.07
1	A	223	PHE	N-CA-CB	-5.29	101.16	111.11
1	A	203	GLU	CA-C-O	5.29	126.56	120.90
1	A	32	LYS	CB-CA-C	-5.29	104.68	111.50
1	A	99	ARG	NE-CZ-NH1	-5.28	116.22	121.50
1	A	47	THR	CB-CA-C	5.28	120.94	111.12
1	A	292	ARG	N-CA-C	-5.28	104.99	111.75
1	A	13	PRO	N-CA-C	-5.28	101.59	112.47
1	A	184	ASP	O-C-N	5.27	129.51	123.29
1	A	142	ASN	CA-C-O	-5.27	112.22	119.12
1	A	327	ARG	CB-CA-C	5.27	119.64	110.68
1	A	352	PHE	CA-CB-CG	-5.25	108.55	113.80
1	A	70	TYR	O-C-N	5.24	129.37	122.97
1	A	210	GLN	CG-CD-OE1	5.24	131.27	120.80
1	A	18	LEU	N-CA-C	-5.22	106.74	113.01
1	A	23	LEU	N-CA-C	-5.22	106.17	112.54
1	A	310	LEU	CB-CA-C	5.22	120.29	110.63
1	A	83	THR	OG1-CB-CG2	5.22	119.74	109.30
1	A	142	ASN	OD1-CG-ND2	5.21	127.81	122.60
1	A	384	SER	CA-CB-OG	-5.21	100.68	111.10
1	A	81	ARG	CD-NE-CZ	5.20	131.68	124.40
1	A	156	ARG	CD-NE-CZ	5.20	131.68	124.40
1	A	171	ASP	O-C-N	5.20	127.44	122.03
1	A	33	ILE	N-CA-CB	5.18	119.78	111.23
1	A	282	ARG	CB-CA-C	5.18	119.49	110.68
1	A	108	GLY	N-CA-C	-5.18	100.90	113.18
1	A	192	CYS	N-CA-CB	-5.18	101.73	110.49
1	A	243	PHE	CA-C-N	5.18	127.74	120.28
1	A	243	PHE	C-N-CA	5.18	127.74	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	ALA	N-CA-CB	-5.18	102.24	110.22
1	A	122	ASN	CB-CG-OD1	-5.18	110.44	120.80
1	A	251	ILE	N-CA-CB	-5.18	102.52	111.63
1	A	335	GLN	CA-C-N	5.17	127.73	120.28
1	A	335	GLN	C-N-CA	5.17	127.73	120.28
1	A	17	ILE	CA-CB-CG2	5.17	119.28	110.50
1	A	171	ASP	N-CA-C	-5.16	105.35	110.97
1	A	181	GLN	CB-CA-C	5.16	118.90	110.03
1	A	42	ASP	CA-C-O	-5.15	115.18	121.67
1	A	305	VAL	CB-CA-C	5.15	118.29	111.70
1	A	169	ASP	N-CA-C	-5.15	99.21	108.58
1	A	253	ALA	CA-C-N	5.14	131.97	122.92
1	A	253	ALA	C-N-CA	5.14	131.97	122.92
1	A	343	GLU	CA-CB-CG	5.14	124.38	114.10
1	A	11	ALA	CB-CA-C	-5.13	100.20	110.42
1	A	141	PRO	CA-C-N	-5.13	111.69	121.94
1	A	141	PRO	C-N-CA	-5.13	111.69	121.94
1	A	185	VAL	CB-CA-C	5.13	117.27	110.91
1	A	48	PRO	CA-N-CD	-5.12	104.83	112.00
1	A	68	LYS	N-CA-C	-5.12	103.98	111.30
1	A	104	GLN	N-CA-C	-5.12	100.96	109.46
1	A	196	THR	CA-CB-OG1	-5.12	101.92	109.60
1	A	288	LYS	CA-C-O	5.11	125.64	119.31
1	A	5	MET	CA-CB-CG	-5.09	103.91	114.10
1	A	248	LYS	O-C-N	5.09	129.37	122.59
1	A	349	ASP	OD1-CG-OD2	5.09	135.12	122.90
1	A	311	SER	CB-CA-C	-5.08	101.41	110.70
1	A	79	PHE	CA-C-N	5.08	131.36	121.41
1	A	79	PHE	C-N-CA	5.08	131.36	121.41
1	A	289	ALA	CA-C-N	5.07	129.19	120.72
1	A	289	ALA	C-N-CA	5.07	129.19	120.72
1	A	125	VAL	CA-C-N	-5.07	113.77	122.79
1	A	125	VAL	C-N-CA	-5.07	113.77	122.79
1	A	5	MET	CA-C-O	-5.07	112.19	120.80
1	A	188	PHE	CA-CB-CG	5.07	118.87	113.80
1	A	312	ASN	N-CA-CB	-5.06	101.88	109.88
1	A	37	ILE	N-CA-C	-5.06	101.36	109.20
1	A	292	ARG	CA-C-N	-5.05	113.23	122.38
1	A	292	ARG	C-N-CA	-5.05	113.23	122.38
1	A	236	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	194	ASN	CB-CA-C	5.05	115.61	109.85
1	A	241	ARG	CA-CB-CG	-5.05	104.00	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	HIS	CA-C-N	5.05	125.55	119.94
1	A	301	HIS	C-N-CA	5.05	125.55	119.94
1	A	271	THR	OG1-CB-CG2	-5.05	99.21	109.30
1	A	374	ARG	N-CA-C	-5.05	106.90	113.16
1	A	312	ASN	CB-CA-C	5.04	118.95	110.88
1	A	28	GLU	CB-CG-CD	5.04	121.17	112.60
1	A	210	GLN	CB-CA-C	5.03	118.71	110.96
1	A	320	GLU	CG-CD-OE1	5.03	129.98	118.40
1	A	55	LYS	N-CA-C	-5.03	105.25	111.33
1	A	16	PRO	CB-CA-C	5.02	119.85	111.56
1	A	63	ASN	OD1-CG-ND2	5.02	127.62	122.60
1	A	127	ARG	CB-CG-CD	5.02	122.84	111.30
1	A	137	ASN	CB-CG-OD1	5.02	130.84	120.80
1	A	367	LYS	CA-CB-CG	5.02	124.13	114.10
1	A	183	GLY	O-C-N	5.01	129.22	122.70
1	A	314	ALA	CA-C-O	5.01	125.91	120.55
1	A	156	ARG	N-CA-C	-5.01	101.76	109.52
1	A	146	VAL	N-CA-CB	-5.00	105.37	110.62

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	ARG	Sidechain
1	A	327	ARG	Sidechain
1	A	81	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	3068	0	3011	369	0
2	A	5	0	0	0	0
3	A	15	0	6	3	0
All	All	3088	0	3017	369	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 60.

All (369) 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:248:LYS:NZ	1:A:248:LYS:HB3	1.52	1.18
1:A:247:HIS:O	1:A:248:LYS:HB2	1.56	1.04
1:A:96:ASN:O	1:A:97:ASP:HB2	1.57	1.01
1:A:32:LYS:HE2	1:A:400:LEU:HD13	1.42	0.99
1:A:34:ASN:HB2	1:A:36:GLY:H	1.26	0.99
1:A:20:LEU:HD13	1:A:382:VAL:HG23	1.47	0.96
1:A:92:SER:HB3	1:A:95:ILE:HD12	1.47	0.95
1:A:125:VAL:HG11	1:A:185:VAL:HG12	1.48	0.94
1:A:195:PRO:HB2	1:A:362:PHE:HE1	1.31	0.94
1:A:34:ASN:HA	1:A:380:TYR:HB2	1.50	0.93
1:A:123:THR:HG22	1:A:125:VAL:HG22	1.51	0.93
1:A:375:GLU:CD	1:A:376:GLU:H	1.75	0.92
1:A:50:LEU:HD12	1:A:50:LEU:N	1.84	0.92
1:A:27:ASP:HB3	1:A:380:TYR:OH	1.71	0.90
1:A:248:LYS:HB3	1:A:248:LYS:HZ2	1.09	0.89
1:A:182:ALA:HA	1:A:216:GLY:HA3	1.56	0.87
1:A:32:LYS:HB2	1:A:379:VAL:HG12	1.57	0.85
1:A:20:LEU:HD11	1:A:382:VAL:HA	1.57	0.85
1:A:29:ARG:HH11	1:A:378:GLY:HA2	1.41	0.85
1:A:19:GLY:O	1:A:20:LEU:HB2	1.76	0.84
1:A:24:PHE:CZ	1:A:33:ILE:HA	2.11	0.84
1:A:346:ALA:HB2	1:A:405:VAL:HG12	1.61	0.82
1:A:347:ASN:HD21	1:A:409:LEU:HD13	1.43	0.82
1:A:160:TYR:O	1:A:168:LEU:HD12	1.79	0.81
1:A:123:THR:CG2	1:A:125:VAL:HG22	2.10	0.81
1:A:256:TYR:HB2	1:A:267:VAL:HG23	1.59	0.81
1:A:250:LEU:HD12	1:A:251:ILE:H	1.43	0.81
1:A:375:GLU:OE1	1:A:376:GLU:N	2.15	0.80
1:A:256:TYR:HB2	1:A:267:VAL:CG2	2.11	0.79
1:A:375:GLU:CD	1:A:376:GLU:N	2.40	0.79
1:A:29:ARG:HB3	1:A:30:PRO:CD	2.13	0.79
1:A:220:LEU:HA	1:A:251:ILE:HG23	1.63	0.79
1:A:180:ALA:O	1:A:181:GLN:HB3	1.83	0.78
1:A:20:LEU:CD1	1:A:382:VAL:HA	2.15	0.77
1:A:18:LEU:CD1	1:A:22:ASP:HB2	2.15	0.77
1:A:195:PRO:HB2	1:A:362:PHE:CE1	2.18	0.77
1:A:34:ASN:HB2	1:A:36:GLY:N	2.00	0.76
1:A:328:GLN:HG3	1:A:331:GLN:NE2	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ALA:O	1:A:13:PRO:C	2.28	0.76
1:A:205:TRP:HA	1:A:205:TRP:CE3	2.20	0.75
1:A:260:PHE:CZ	1:A:310:LEU:HD21	2.21	0.75
1:A:18:LEU:HD13	1:A:22:ASP:HB2	1.69	0.75
1:A:388:ASN:OD1	1:A:390:ALA:HB3	1.87	0.75
1:A:355:LYS:HB2	1:A:355:LYS:NZ	2.01	0.75
1:A:355:LYS:HB2	1:A:355:LYS:HZ3	1.52	0.75
1:A:26:ALA:O	1:A:28:GLU:HG2	1.87	0.74
1:A:44:THR:HB	1:A:46:LYS:NZ	2.01	0.74
1:A:102:THR:OG1	1:A:271:THR:HG23	1.87	0.74
1:A:256:TYR:O	1:A:260:PHE:HB2	1.87	0.74
1:A:33:ILE:HG22	1:A:34:ASN:H	1.52	0.73
1:A:248:LYS:HB3	1:A:248:LYS:HZ3	1.54	0.73
1:A:76:ILE:HG12	1:A:104:GLN:HE22	1.52	0.73
1:A:23:LEU:O	1:A:27:ASP:HB2	1.87	0.72
1:A:43:GLU:OE2	1:A:333:MET:HE3	1.88	0.72
1:A:397:MET:HE3	1:A:400:LEU:CD2	2.20	0.72
1:A:248:LYS:NZ	1:A:249:GLU:HG3	2.04	0.72
1:A:32:LYS:HE2	1:A:400:LEU:CD1	2.19	0.72
1:A:250:LEU:HD12	1:A:251:ILE:N	2.03	0.72
1:A:366:THR:HG22	1:A:369:GLN:HG3	1.72	0.72
1:A:46:LYS:NZ	1:A:46:LYS:HB2	2.05	0.72
1:A:32:LYS:HE2	1:A:400:LEU:HB2	1.70	0.71
1:A:32:LYS:CE	1:A:400:LEU:HD13	2.18	0.71
1:A:44:THR:HB	1:A:46:LYS:HZ2	1.56	0.71
1:A:192:CYS:SG	1:A:199:ASP:HA	2.30	0.71
1:A:23:LEU:HD12	1:A:23:LEU:H	1.54	0.70
1:A:223:PHE:HE1	1:A:240:LEU:HB2	1.54	0.70
1:A:248:LYS:NZ	1:A:248:LYS:CB	2.41	0.70
1:A:397:MET:HE3	1:A:400:LEU:HD23	1.71	0.70
1:A:127:ARG:NH2	1:A:179:GLU:OE2	2.24	0.70
1:A:374:ARG:HG2	1:A:379:VAL:O	1.91	0.70
1:A:173:LEU:HD12	1:A:177:LEU:HD22	1.73	0.70
1:A:43:GLU:OE2	1:A:329:ARG:HD2	1.91	0.69
1:A:27:ASP:CB	1:A:380:TYR:OH	2.40	0.69
1:A:9:ILE:O	1:A:10:THR:OG1	2.10	0.69
1:A:352:PHE:HD2	1:A:356:GLN:HE22	1.39	0.69
1:A:17:ILE:HG23	1:A:18:LEU:H	1.55	0.69
1:A:105:THR:HG22	1:A:107:GLY:HA2	1.75	0.69
1:A:34:ASN:HA	1:A:380:TYR:CB	2.23	0.68
1:A:32:LYS:CB	1:A:379:VAL:HG12	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:HIS:O	1:A:248:LYS:CB	2.35	0.68
1:A:121:LYS:HD2	1:A:121:LYS:C	2.18	0.68
1:A:121:LYS:HD2	1:A:122:ASN:N	2.09	0.68
1:A:209:ALA:HB2	1:A:243:PHE:CD1	2.29	0.67
1:A:196:THR:HB	1:A:198:ILE:HD11	1.76	0.67
1:A:392:MET:SD	1:A:397:MET:HE1	2.34	0.67
1:A:109:THR:HG22	1:A:140:TRP:CH2	2.30	0.67
1:A:160:TYR:HE1	1:A:198:ILE:HD13	1.60	0.67
1:A:173:LEU:CD1	1:A:177:LEU:HD22	2.25	0.67
1:A:20:LEU:HD21	1:A:381:ALA:C	2.19	0.67
1:A:233:LEU:HD21	1:A:319:TRP:CH2	2.29	0.67
1:A:260:PHE:HZ	1:A:310:LEU:HD21	1.59	0.67
1:A:29:ARG:HB3	1:A:30:PRO:HD3	1.75	0.67
1:A:362:PHE:CD1	1:A:386:PHE:HB3	2.31	0.66
1:A:9:ILE:HD13	1:A:10:THR:N	2.09	0.66
1:A:105:THR:HG21	1:A:111:ALA:HB2	1.76	0.66
1:A:29:ARG:CB	1:A:30:PRO:CD	2.74	0.66
1:A:87:LEU:HB3	1:A:240:LEU:HD11	1.76	0.66
1:A:125:VAL:CG1	1:A:185:VAL:HG12	2.26	0.66
1:A:352:PHE:HD2	1:A:356:GLN:NE2	1.94	0.65
1:A:87:LEU:O	1:A:241:ARG:HD2	1.96	0.65
1:A:62:GLU:HG3	1:A:63:ASN:ND2	2.11	0.65
1:A:121:LYS:C	1:A:123:THR:H	2.04	0.65
1:A:113:ARG:NH1	1:A:149:SER:OG	2.30	0.64
1:A:366:THR:HG22	1:A:369:GLN:CG	2.28	0.64
1:A:224:ALA:O	1:A:225:TYR:HB2	1.96	0.64
1:A:375:GLU:C	1:A:377:PHE:H	2.05	0.64
1:A:126:LYS:HD3	1:A:126:LYS:N	2.13	0.63
1:A:43:GLU:CD	1:A:329:ARG:HD2	2.24	0.63
1:A:135:VAL:O	1:A:136:SER:HB3	1.97	0.63
1:A:87:LEU:HB3	1:A:240:LEU:CD1	2.28	0.63
1:A:251:ILE:HG23	1:A:251:ILE:O	1.97	0.63
1:A:197:GLY:HA3	1:A:357:ASN:O	1.98	0.63
1:A:81:ARG:O	1:A:85:GLU:HG3	1.98	0.63
1:A:160:TYR:HE1	1:A:198:ILE:CD1	2.11	0.62
1:A:20:LEU:CD1	1:A:382:VAL:HG23	2.26	0.62
1:A:362:PHE:HA	1:A:386:PHE:HA	1.80	0.62
1:A:50:LEU:HD12	1:A:50:LEU:H	1.64	0.62
1:A:159:ALA:O	1:A:160:TYR:HB2	1.99	0.62
1:A:312:ASN:C	1:A:312:ASN:HD22	2.07	0.61
1:A:400:LEU:O	1:A:404:ILE:HD13	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLU:O	1:A:206:GLN:HB2	2.00	0.61
1:A:17:ILE:C	1:A:19:GLY:N	2.60	0.60
1:A:46:LYS:HB2	1:A:46:LYS:HZ3	1.66	0.60
1:A:181:GLN:O	1:A:184:ASP:HB2	2.01	0.60
1:A:23:LEU:HD12	1:A:23:LEU:N	2.17	0.60
1:A:404:ILE:O	1:A:408:VAL:HG22	2.02	0.60
1:A:43:GLU:HG3	1:A:394:PRO:HD3	1.83	0.59
1:A:62:GLU:HG3	1:A:63:ASN:HD22	1.66	0.59
1:A:90:LYS:NZ	1:A:90:LYS:HA	2.18	0.59
1:A:349:ASP:OD1	1:A:351:SER:HB3	2.03	0.58
1:A:398:ALA:HB3	1:A:399:PRO:CD	2.33	0.58
1:A:76:ILE:CG1	1:A:104:GLN:HE22	2.16	0.58
1:A:92:SER:CB	1:A:95:ILE:HD12	2.27	0.58
1:A:43:GLU:HG3	1:A:394:PRO:CD	2.33	0.58
1:A:408:VAL:O	1:A:409:LEU:HG	2.03	0.58
1:A:160:TYR:CE1	1:A:198:ILE:HD13	2.38	0.58
1:A:248:LYS:HZ1	1:A:249:GLU:HG3	1.68	0.58
1:A:328:GLN:HA	1:A:331:GLN:HE21	1.68	0.57
1:A:77:PRO:HG2	1:A:78:GLU:OE1	2.05	0.57
1:A:350:PHE:HA	1:A:352:PHE:CD1	2.40	0.57
1:A:328:GLN:O	1:A:332:ARG:HG3	2.03	0.57
1:A:103:ALA:O	1:A:269:ALA:HB1	2.05	0.57
1:A:163:ALA:O	1:A:165:ASN:N	2.38	0.57
1:A:165:ASN:OD1	1:A:165:ASN:C	2.47	0.57
1:A:96:ASN:O	1:A:97:ASP:CB	2.41	0.56
1:A:29:ARG:NH1	1:A:378:GLY:HA2	2.18	0.56
1:A:350:PHE:C	1:A:352:PHE:N	2.62	0.56
1:A:34:ASN:CB	1:A:36:GLY:H	2.07	0.56
1:A:196:THR:O	1:A:198:ILE:N	2.36	0.56
1:A:225:TYR:CE2	1:A:258:LYS:HG3	2.39	0.56
1:A:118:PHE:O	1:A:121:LYS:O	2.23	0.56
1:A:76:ILE:HB	1:A:79:PHE:HB3	1.89	0.55
1:A:50:LEU:N	1:A:50:LEU:CD1	2.63	0.55
1:A:359:MET:O	1:A:389:VAL:N	2.37	0.55
1:A:121:LYS:C	1:A:123:THR:N	2.63	0.55
1:A:17:ILE:HG12	1:A:18:LEU:N	2.21	0.55
1:A:196:THR:HB	1:A:198:ILE:CD1	2.36	0.55
1:A:346:ALA:HB2	1:A:405:VAL:CG1	2.35	0.55
1:A:135:VAL:C	1:A:158:TYR:CE2	2.85	0.54
1:A:119:LEU:O	1:A:123:THR:HB	2.08	0.54
1:A:192:CYS:SG	1:A:199:ASP:CA	2.95	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:HD12	1:A:22:ASP:HB2	1.87	0.54
1:A:34:ASN:N	1:A:34:ASN:OD1	2.38	0.54
1:A:40:TYR:O	1:A:47:THR:HB	2.06	0.54
1:A:355:LYS:NZ	1:A:355:LYS:CB	2.70	0.54
1:A:101:ARG:HB3	1:A:284:PHE:CD1	2.43	0.54
1:A:160:TYR:O	1:A:168:LEU:CD1	2.55	0.54
1:A:201:THR:OG1	1:A:204:GLN:NE2	2.39	0.54
1:A:121:LYS:NZ	1:A:122:ASN:HB2	2.22	0.53
1:A:328:GLN:HG3	1:A:331:GLN:HE22	1.70	0.53
1:A:335:GLN:HE21	1:A:354:ILE:HG21	1.71	0.53
1:A:337:PHE:HD1	1:A:397:MET:CE	2.21	0.53
1:A:105:THR:O	1:A:107:GLY:N	2.35	0.53
1:A:113:ARG:O	1:A:116:ALA:HB3	2.07	0.53
1:A:267:VAL:HG23	1:A:267:VAL:O	2.08	0.53
1:A:17:ILE:C	1:A:19:GLY:H	2.09	0.53
1:A:184:ASP:O	1:A:217:TRP:HA	2.08	0.53
1:A:42:ASP:OD1	1:A:44:THR:N	2.37	0.53
1:A:189:HIS:HA	1:A:222:ASP:O	2.08	0.53
1:A:350:PHE:HA	1:A:352:PHE:CE1	2.44	0.53
1:A:25:ARG:CZ	1:A:25:ARG:O	2.57	0.52
1:A:23:LEU:H	1:A:23:LEU:CD1	2.22	0.52
1:A:76:ILE:HB	1:A:79:PHE:CB	2.40	0.52
1:A:370:VAL:HG11	1:A:383:ALA:HA	1.90	0.52
1:A:404:ILE:HD13	1:A:404:ILE:N	2.25	0.52
1:A:223:PHE:O	1:A:254:SER:HA	2.09	0.52
1:A:121:LYS:HZ2	1:A:122:ASN:CB	2.23	0.52
1:A:145:SER:O	1:A:149:SER:HB3	2.10	0.52
1:A:202:LEU:O	1:A:206:GLN:HG3	2.09	0.52
1:A:34:ASN:C	1:A:36:GLY:H	2.02	0.52
1:A:59:TYR:O	1:A:63:ASN:HB2	2.09	0.52
1:A:160:TYR:O	1:A:168:LEU:HA	2.10	0.52
1:A:373:LEU:HB3	1:A:379:VAL:HG22	1.92	0.52
1:A:363:SER:OG	1:A:365:LEU:HG	2.09	0.51
1:A:54:LYS:HA	1:A:57:GLU:HG3	1.92	0.51
1:A:205:TRP:HA	1:A:205:TRP:HE3	1.70	0.51
1:A:9:ILE:O	1:A:9:ILE:HG23	2.11	0.51
1:A:121:LYS:NZ	1:A:122:ASN:CB	2.74	0.51
1:A:119:LEU:HG	1:A:125:VAL:HG21	1.92	0.51
1:A:67:THR:OG1	1:A:69:ASN:HB2	2.10	0.51
1:A:80:GLY:O	1:A:81:ARG:C	2.53	0.51
1:A:109:THR:HG22	1:A:140:TRP:HH2	1.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:PHE:C	1:A:352:PHE:H	2.18	0.51
1:A:397:MET:HA	1:A:400:LEU:HD23	1.91	0.51
1:A:94:LEU:HD23	1:A:94:LEU:O	2.11	0.51
1:A:162:ASP:O	1:A:163:ALA:HB3	2.10	0.51
1:A:210:GLN:O	1:A:211:LEU:C	2.53	0.50
1:A:42:ASP:OD2	1:A:46:LYS:NZ	2.44	0.50
1:A:223:PHE:CE2	1:A:226:GLN:HB2	2.47	0.50
1:A:256:TYR:HB2	1:A:267:VAL:HG21	1.92	0.50
1:A:17:ILE:CG1	1:A:18:LEU:N	2.69	0.50
1:A:209:ALA:HB2	1:A:243:PHE:CE1	2.46	0.50
1:A:101:ARG:HG2	1:A:280:VAL:CG1	2.42	0.50
1:A:121:LYS:C	1:A:121:LYS:CD	2.82	0.50
1:A:168:LEU:O	1:A:170:PHE:N	2.45	0.50
1:A:224:ALA:O	1:A:225:TYR:CB	2.60	0.50
1:A:29:ARG:HB3	1:A:30:PRO:HD2	1.92	0.49
1:A:9:ILE:C	1:A:10:THR:OG1	2.55	0.49
1:A:24:PHE:CZ	1:A:33:ILE:CA	2.91	0.49
1:A:127:ARG:HH11	1:A:181:GLN:CD	2.21	0.49
1:A:404:ILE:N	1:A:404:ILE:CD1	2.75	0.49
1:A:353:ILE:HD12	1:A:353:ILE:O	2.12	0.49
1:A:363:SER:O	1:A:365:LEU:N	2.45	0.49
1:A:353:ILE:HD12	1:A:353:ILE:C	2.38	0.49
1:A:90:LYS:HA	1:A:90:LYS:HZ3	1.78	0.49
1:A:29:ARG:CB	1:A:30:PRO:HD2	2.43	0.49
1:A:99:ARG:NH2	1:A:274:ALA:O	2.45	0.49
1:A:165:ASN:O	1:A:167:THR:N	2.46	0.49
1:A:113:ARG:O	1:A:116:ALA:N	2.47	0.48
1:A:180:ALA:O	1:A:181:GLN:CB	2.53	0.48
1:A:217:TRP:N	1:A:217:TRP:CD1	2.80	0.48
1:A:31:GLY:C	1:A:33:ILE:H	2.21	0.48
1:A:19:GLY:O	1:A:20:LEU:CB	2.56	0.48
1:A:278:GLU:OE1	1:A:282:ARG:NH2	2.47	0.48
1:A:312:ASN:C	1:A:312:ASN:ND2	2.71	0.48
1:A:220:LEU:CD1	1:A:251:ILE:HG12	2.44	0.48
1:A:44:THR:HG22	1:A:44:THR:O	2.14	0.47
1:A:135:VAL:O	1:A:136:SER:CB	2.60	0.47
1:A:375:GLU:C	1:A:377:PHE:N	2.72	0.47
1:A:256:TYR:HA	1:A:259:ASN:OD1	2.15	0.47
1:A:334:ARG:HB3	1:A:353:ILE:HD12	1.96	0.47
1:A:30:PRO:O	1:A:30:PRO:HG2	2.14	0.47
1:A:158:TYR:HD1	1:A:173:LEU:HD13	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LYS:HE2	1:A:286:GLN:HB3	1.96	0.47
1:A:262:LEU:O	1:A:263:TYR:C	2.56	0.47
1:A:49:VAL:HG22	1:A:49:VAL:O	2.14	0.47
1:A:140:TRP:HE3	1:A:143:HIS:CD2	2.33	0.47
1:A:197:GLY:HA3	1:A:357:ASN:H	1.80	0.47
1:A:32:LYS:HE3	1:A:32:LYS:HB3	1.74	0.47
1:A:62:GLU:CG	1:A:63:ASN:HD22	2.28	0.47
1:A:119:LEU:HD12	1:A:119:LEU:HA	1.70	0.47
1:A:156:ARG:HH22	1:A:179:GLU:CD	2.23	0.47
1:A:105:THR:CG2	1:A:107:GLY:HA2	2.45	0.47
1:A:140:TRP:CZ2	1:A:142:ASN:HB3	2.50	0.46
1:A:344:LYS:O	1:A:344:LYS:HD3	2.14	0.46
1:A:99:ARG:O	1:A:280:VAL:HG21	2.15	0.46
1:A:106:PRO:HA	1:A:266:ARG:O	2.15	0.46
1:A:211:LEU:HA	1:A:211:LEU:HD22	1.66	0.46
1:A:24:PHE:C	1:A:26:ALA:H	2.22	0.46
1:A:337:PHE:HD1	1:A:397:MET:HE2	1.81	0.46
1:A:105:THR:C	1:A:107:GLY:H	2.21	0.46
1:A:160:TYR:O	1:A:169:ASP:N	2.46	0.46
1:A:32:LYS:NZ	1:A:400:LEU:HD22	2.30	0.46
1:A:304:SER:O	1:A:305:VAL:C	2.55	0.46
1:A:248:LYS:O	1:A:273:VAL:HG23	2.16	0.46
1:A:54:LYS:O	1:A:57:GLU:N	2.48	0.45
1:A:366:THR:HG22	1:A:369:GLN:CD	2.41	0.45
1:A:32:LYS:CE	1:A:400:LEU:HB2	2.41	0.45
1:A:71:LEU:HD12	1:A:71:LEU:HA	1.77	0.45
1:A:325:ASP:O	1:A:326:MET:C	2.60	0.45
1:A:88:PHE:HA	1:A:241:ARG:HD2	1.98	0.45
1:A:352:PHE:O	1:A:356:GLN:NE2	2.50	0.45
1:A:160:TYR:OH	1:A:198:ILE:O	2.30	0.45
1:A:177:LEU:HD12	1:A:177:LEU:HA	1.51	0.45
1:A:291:ILE:C	1:A:293:ALA:N	2.72	0.45
1:A:398:ALA:HB3	1:A:399:PRO:HD2	1.98	0.45
1:A:266:ARG:HH21	1:A:266:ARG:HD2	1.38	0.45
1:A:225:TYR:HE1	3:A:410:PLP:O3	1.99	0.45
1:A:352:PHE:O	1:A:356:GLN:HG3	2.17	0.45
1:A:338:VAL:HG21	1:A:354:ILE:HG23	1.99	0.44
1:A:248:LYS:HZ2	1:A:248:LYS:CB	2.02	0.44
1:A:9:ILE:HD13	1:A:10:THR:CA	2.47	0.44
1:A:15:ASP:OD2	1:A:17:ILE:HG22	2.18	0.44
1:A:185:VAL:HA	1:A:218:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:THR:C	1:A:368:GLU:N	2.74	0.44
1:A:25:ARG:HA	1:A:25:ARG:HD2	1.69	0.44
1:A:118:PHE:O	1:A:121:LYS:NZ	2.49	0.44
1:A:152:LEU:HD12	1:A:152:LEU:HA	1.79	0.44
1:A:344:LYS:HD3	1:A:344:LYS:HA	1.57	0.44
1:A:106:PRO:HD2	1:A:295:TYR:CZ	2.53	0.44
1:A:322:GLU:O	1:A:325:ASP:HB2	2.18	0.44
1:A:20:LEU:HD13	1:A:382:VAL:HA	1.98	0.44
1:A:222:ASP:OD1	3:A:410:PLP:N1	2.51	0.44
1:A:375:GLU:CG	1:A:376:GLU:H	2.21	0.44
1:A:328:GLN:HA	1:A:331:GLN:NE2	2.32	0.44
1:A:53:VAL:HG13	1:A:305:VAL:HG11	2.00	0.43
1:A:15:ASP:O	1:A:17:ILE:CG2	2.66	0.43
1:A:328:GLN:HG3	1:A:331:GLN:HE21	1.79	0.43
1:A:396:ASN:C	1:A:396:ASN:OD1	2.60	0.43
1:A:40:TYR:CZ	1:A:326:MET:HG2	2.52	0.43
1:A:15:ASP:O	1:A:17:ILE:HG22	2.18	0.43
1:A:32:LYS:CD	1:A:400:LEU:HB2	2.49	0.43
1:A:121:LYS:HZ2	1:A:122:ASN:HB3	1.84	0.43
1:A:123:THR:HG21	1:A:125:VAL:HG22	1.98	0.43
1:A:91:GLY:O	1:A:92:SER:C	2.62	0.43
1:A:274:ALA:HB1	1:A:279:THR:HB	2.01	0.43
1:A:316:ARG:HH21	1:A:316:ARG:HD2	1.69	0.43
1:A:105:THR:C	1:A:107:GLY:N	2.75	0.43
1:A:140:TRP:CE3	1:A:143:HIS:CD2	3.07	0.43
1:A:260:PHE:HB3	1:A:262:LEU:HD12	1.99	0.43
1:A:291:ILE:O	1:A:292:ARG:C	2.60	0.42
1:A:133:VAL:O	1:A:155:VAL:HA	2.19	0.42
1:A:380:TYR:CD1	1:A:380:TYR:N	2.86	0.42
1:A:393:THR:H	1:A:396:ASN:ND2	2.17	0.42
1:A:219:PRO:O	1:A:251:ILE:HG22	2.19	0.42
1:A:223:PHE:HE2	1:A:226:GLN:HB2	1.82	0.42
1:A:319:TRP:CZ2	1:A:323:LEU:HD22	2.55	0.42
1:A:112:LEU:HA	1:A:112:LEU:HD23	1.58	0.42
1:A:205:TRP:CE3	1:A:205:TRP:CA	2.98	0.42
1:A:127:ARG:HD2	1:A:134:TRP:NE1	2.35	0.42
1:A:248:LYS:O	1:A:274:ALA:C	2.61	0.42
1:A:284:PHE:O	1:A:285:SER:C	2.60	0.42
1:A:121:LYS:HZ3	1:A:122:ASN:HB2	1.84	0.42
1:A:243:PHE:O	1:A:247:HIS:CD2	2.73	0.42
1:A:375:GLU:O	1:A:377:PHE:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LEU:O	1:A:27:ASP:N	2.39	0.42
1:A:212:SER:HA	1:A:217:TRP:CE3	2.55	0.42
1:A:337:PHE:HD1	1:A:397:MET:HE1	1.85	0.42
1:A:44:THR:CB	1:A:46:LYS:NZ	2.77	0.41
1:A:156:ARG:NH2	1:A:179:GLU:CD	2.78	0.41
1:A:9:ILE:HD13	1:A:9:ILE:C	2.45	0.41
1:A:87:LEU:HD22	1:A:240:LEU:HD11	2.01	0.41
1:A:315:LEU:HA	1:A:315:LEU:HD12	1.75	0.41
1:A:373:LEU:O	1:A:378:GLY:N	2.53	0.41
1:A:195:PRO:CB	1:A:362:PHE:HE1	2.17	0.41
1:A:310:LEU:HD12	1:A:316:ARG:CZ	2.50	0.41
1:A:136:SER:HB3	1:A:158:TYR:CZ	2.55	0.41
1:A:220:LEU:HA	1:A:251:ILE:O	2.21	0.41
1:A:337:PHE:CD1	1:A:392:MET:HE1	2.55	0.41
1:A:24:PHE:C	1:A:26:ALA:N	2.77	0.41
1:A:37:ILE:HD13	1:A:37:ILE:HG21	1.77	0.41
1:A:40:TYR:OH	1:A:326:MET:HA	2.21	0.41
1:A:194:ASN:HA	1:A:195:PRO:HA	1.90	0.41
1:A:220:LEU:HB2	1:A:251:ILE:CG2	2.51	0.41
1:A:103:ALA:O	1:A:269:ALA:CB	2.67	0.41
1:A:366:THR:O	1:A:367:LYS:C	2.63	0.41
1:A:108:GLY:HA3	3:A:410:PLP:O2P	2.20	0.41
1:A:220:LEU:HD13	1:A:251:ILE:HG12	2.03	0.41
1:A:372:ARG:NH1	1:A:375:GLU:OE2	2.53	0.41
1:A:399:PRO:O	1:A:402:GLU:HB3	2.20	0.41
1:A:51:THR:O	1:A:55:LYS:HG3	2.21	0.41
1:A:119:LEU:HB3	1:A:125:VAL:HG21	2.03	0.41
1:A:270:CYS:SG	1:A:287:MET:HE2	2.61	0.41
1:A:76:ILE:O	1:A:79:PHE:HB3	2.21	0.40
1:A:101:ARG:HG2	1:A:280:VAL:HG13	2.03	0.40
1:A:174:ILE:HD13	1:A:174:ILE:HA	1.89	0.40
1:A:15:ASP:HA	1:A:16:PRO:HD3	1.69	0.40
1:A:32:LYS:HE2	1:A:400:LEU:CB	2.47	0.40
1:A:43:GLU:OE2	1:A:333:MET:CE	2.63	0.40
1:A:211:LEU:O	1:A:212:SER:C	2.64	0.40
1:A:233:LEU:HD21	1:A:319:TRP:CZ3	2.55	0.40
1:A:270:CYS:SG	1:A:287:MET:CE	3.09	0.40
1:A:233:LEU:HD12	1:A:233:LEU:HA	1.69	0.40
1:A:324:THR:O	1:A:328:GLN:HB2	2.22	0.40
1:A:373:LEU:HA	1:A:373:LEU:HD12	1.86	0.40
1:A:86:LEU:HA	1:A:86:LEU:HD23	1.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LEU:HA	1:A:219:PRO:HD3	1.85	0.40
1:A:260:PHE:CZ	1:A:310:LEU:CD2	2.99	0.40
1:A:370:VAL:O	1:A:374:ARG:HG3	2.22	0.40

There are no symmetry-related clashes.

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	394/396 (100%)	319 (81%)	44 (11%)	31 (8%)	1 1

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ALA
1	A	13	PRO
1	A	17	ILE
1	A	29	ARG
1	A	33	ILE
1	A	50	LEU
1	A	90	LYS
1	A	136	SER
1	A	160	TYR
1	A	166	HIS
1	A	192	CYS
1	A	217	TRP
1	A	9	ILE
1	A	20	LEU
1	A	30	PRO
1	A	97	ASP
1	A	107	GLY
1	A	163	ALA

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Mol	Chain	Res	Type
1	A	164	GLU
1	A	182	ALA
1	A	197	GLY
1	A	364	GLY
1	A	383	ALA
1	A	8	ASN
1	A	92	SER
1	A	263	TYR
1	A	266	ARG
1	A	180	ALA
1	A	27	ASP
1	A	375	GLU
1	A	80	GLY

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	320/320 (100%)	218 (68%)	102 (32%)	0 1

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	8	ASN
1	A	9	ILE
1	A	17	ILE
1	A	18	LEU
1	A	20	LEU
1	A	22	ASP
1	A	23	LEU
1	A	25	ARG
1	A	27	ASP
1	A	30	PRO
1	A	32	LYS
1	A	34	ASN

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Mol	Chain	Res	Type
1	A	35	LEU
1	A	39	VAL
1	A	43	GLU
1	A	46	LYS
1	A	47	THR
1	A	61	LEU
1	A	62	GLU
1	A	71	LEU
1	A	76	ILE
1	A	86	LEU
1	A	90	LYS
1	A	97	ASP
1	A	98	LYS
1	A	99	ARG
1	A	105	THR
1	A	109	THR
1	A	113	ARG
1	A	119	LEU
1	A	121	LYS
1	A	125	VAL
1	A	126	LYS
1	A	127	ARG
1	A	136	SER
1	A	139	SER
1	A	146	VAL
1	A	149	SER
1	A	152	LEU
1	A	155	VAL
1	A	157	GLU
1	A	162	ASP
1	A	167	THR
1	A	173	LEU
1	A	177	LEU
1	A	179	GLU
1	A	185	VAL
1	A	196	THR
1	A	198	ILE
1	A	201	THR
1	A	205	TRP
1	A	208	LEU
1	A	210	GLN
1	A	211	LEU

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Mol	Chain	Res	Type
1	A	213	VAL
1	A	215	LYS
1	A	218	LEU
1	A	220	LEU
1	A	234	GLU
1	A	235	GLU
1	A	240	LEU
1	A	241	ARG
1	A	243	PHE
1	A	248	LYS
1	A	250	LEU
1	A	252	VAL
1	A	255	SER
1	A	264	ASN
1	A	271	THR
1	A	273	VAL
1	A	277	SER
1	A	278	GLU
1	A	280	VAL
1	A	297	ASN
1	A	304	SER
1	A	312	ASN
1	A	315	LEU
1	A	320	GLU
1	A	326	MET
1	A	327	ARG
1	A	328	GLN
1	A	335	GLN
1	A	339	ASN
1	A	343	GLU
1	A	344	LYS
1	A	348	ARG
1	A	351	SER
1	A	353	ILE
1	A	355	LYS
1	A	367	LYS
1	A	370	VAL
1	A	371	LEU
1	A	372	ARG
1	A	373	LEU
1	A	375	GLU
1	A	384	SER

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Mol	Chain	Res	Type
1	A	396	ASN
1	A	397	MET
1	A	400	LEU
1	A	402	GLU
1	A	404	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	104	GLN
1	A	181	GLN
1	A	206	GLN
1	A	247	HIS
1	A	264	ASN
1	A	312	ASN
1	A	331	GLN
1	A	335	GLN
1	A	342	GLN
1	A	357	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PLP	A	410	1	15,15,16	1.79	3 (20%)	21,22,23	2.67	11 (52%)
2	SO4	A	411	-	4,4,4	1.33	0	6,6,6	1.25	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	A	410	1	-	1/6/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	410	PLP	C5-C4	-3.83	1.36	1.40
3	A	410	PLP	C4A-C4	-3.41	1.44	1.51
3	A	410	PLP	O3-C3	-2.49	1.31	1.36

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	410	PLP	O4P-C5A-C5	7.02	122.52	109.36
3	A	410	PLP	O2P-P-O1P	3.75	125.45	110.83
3	A	410	PLP	O4P-P-O1P	3.66	116.33	106.44
3	A	410	PLP	C5-C6-N1	-3.31	118.44	123.83
3	A	410	PLP	C6-N1-C2	3.17	124.95	119.20
3	A	410	PLP	O2P-P-O4P	-3.06	98.68	106.67
3	A	410	PLP	C4A-C4-C5	2.76	123.78	120.94
3	A	410	PLP	C3-C2-N1	-2.74	117.50	120.96
3	A	410	PLP	C2A-C2-N1	2.54	122.43	117.64
3	A	410	PLP	O3P-P-O1P	-2.50	101.09	110.83
2	A	411	SO4	O4-S-O3	2.40	121.79	108.54
3	A	410	PLP	C4A-C4-C3	-2.25	116.77	120.52

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	410	PLP	C5A-O4P-P-O1P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	410	PLP	3	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](#)

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	396/396 (100%)	-0.04	7 (1%) 67 58	12, 12, 12, 12	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	19	GLY	3.8
1	A	162	ASP	3.0
1	A	33	ILE	2.5
1	A	122	ASN	2.5
1	A	210	GLN	2.5
1	A	175	ASN	2.3
1	A	27	ASP	2.2

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(Å ²)	Q<0.9
2	SO4	A	411	5/5	0.90	0.19	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PLP	A	410	15/16	0.95	0.09	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.