



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:24 PM UTC

PDB ID : 2AAT / pdb_00002aat
Title : 2.8-ANGSTROMS-RESOLUTION CRYSTAL STRUCTURE OF AN
ACTIVE-SITE MUTANT OF ASPARTATE AMINOTRANSFERASE FROM
ESCHERICHIA COLI
Authors : Smith, D.; Almo, S.C.; Toney, M.; Ringe, D.
Deposited on : 1989-05-30
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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

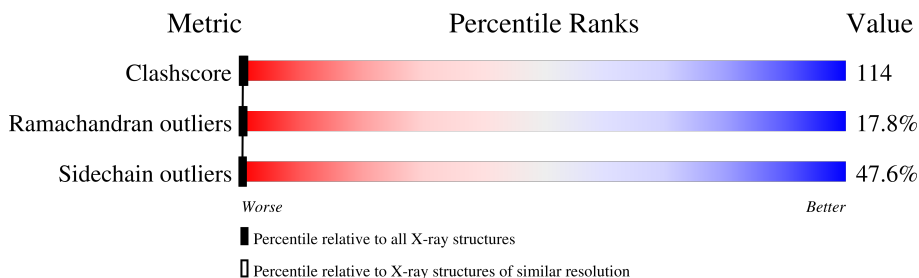
1 Overall quality at a glance

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)

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 $\leq 5\%$.

Note EDS was not executed.

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 3086 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.

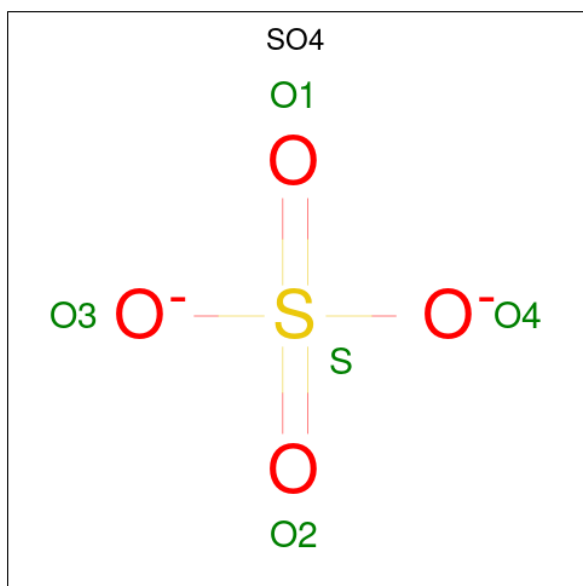
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	396	3065	1933	535	584	13	0	0	0

There is a discrepancy between the modelled and reference sequences:

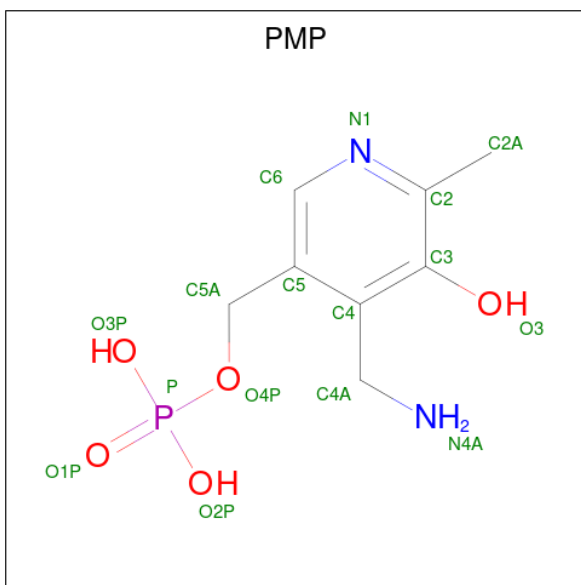
Chain	Residue	Modelled	Actual	Comment	Reference
A	258	ALA	LYS	engineered mutation	UNP P00509

- 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 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (CCD ID: PMP) (formula: C₈H₁₃N₂O₅P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	16	8	2	5	1	0	0

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	156.80Å 86.74Å 79.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3086	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PMP, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.96	0/3126	3.90	633/4236 (14.9%)

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	9

There are no bond length outliers.

All (633) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	PHE	CA-CB-CG	40.65	154.44	113.80
1	A	88	ARG	CD-NE-CZ	39.63	179.89	124.40
1	A	349	ASP	CA-CB-CG	26.60	139.20	112.60
1	A	372	ARG	CD-NE-CZ	23.98	157.97	124.40
1	A	347	ASN	CA-CB-CG	23.22	135.82	112.60
1	A	379	VAL	CB-CA-C	21.15	143.25	111.31
1	A	193	CYS	CA-C-O	19.79	142.08	120.70
1	A	328	GLN	CB-CG-CD	19.32	145.45	112.60
1	A	21	PRO	N-CA-C	19.02	144.89	111.03
1	A	193	CYS	CA-C-N	18.90	157.63	121.54
1	A	193	CYS	C-N-CA	18.90	157.63	121.54
1	A	298	PRO	N-CA-C	17.58	132.15	110.70
1	A	187	VAL	N-CA-CB	16.92	131.36	112.07
1	A	403	ALA	CA-C-N	16.01	143.11	120.53
1	A	403	ALA	C-N-CA	16.01	143.11	120.53
1	A	76	ASN	CA-CB-CG	15.68	128.28	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	ILE	N-CA-CB	15.37	136.59	111.23
1	A	159	TYR	CA-C-O	-15.28	98.66	120.51
1	A	207	GLN	CB-CG-CD	15.20	138.43	112.60
1	A	213	SER	N-CA-CB	15.19	132.45	110.12
1	A	234	GLU	CA-C-O	-15.16	104.97	120.89
1	A	260	PHE	CA-CB-CG	14.74	128.54	113.80
1	A	309	ILE	N-CA-CB	14.58	130.37	110.54
1	A	71	ASN	CA-CB-CG	14.23	126.83	112.60
1	A	155	GLU	N-CA-CB	14.09	133.60	110.63
1	A	211	GLN	N-CA-CB	14.06	132.35	110.14
1	A	85	GLU	N-CA-C	-13.78	96.60	113.41
1	A	189	PHE	CA-CB-CG	13.77	127.57	113.80
1	A	357	ASN	CA-CB-CG	13.50	126.10	112.60
1	A	136	TRP	N-CA-CB	13.44	132.34	110.43
1	A	211	GLN	CA-CB-CG	13.35	140.80	114.10
1	A	125	PHE	N-CA-C	-13.24	96.84	111.14
1	A	366	THR	N-CA-CB	13.24	132.87	110.49
1	A	206	TRP	N-CA-C	-13.23	96.85	111.14
1	A	291	ILE	CB-CA-C	-13.18	95.33	111.81
1	A	296	SER	CA-C-O	-12.83	107.63	122.13
1	A	41	ILE	N-CA-CB	12.71	132.21	111.23
1	A	322	GLU	CB-CG-CD	12.60	134.02	112.60
1	A	144	ASN	CA-CB-CG	12.56	125.16	112.60
1	A	190	HIS	CA-CB-CG	12.26	126.06	113.80
1	A	18	THR	N-CA-C	-12.18	97.05	108.75
1	A	231	ARG	N-CA-CB	-12.05	90.13	110.49
1	A	104	ASP	N-CA-C	-11.91	98.88	113.41
1	A	376	GLU	CA-CB-CG	11.83	137.75	114.10
1	A	330	ILE	N-CA-C	-11.78	101.98	113.53
1	A	334	ARG	CD-NE-CZ	11.68	140.75	124.40
1	A	23	ASP	N-CA-CB	11.63	128.97	110.01
1	A	23	ASP	N-CA-C	-11.53	95.12	109.65
1	A	26	LEU	N-CA-C	-11.26	99.27	113.23
1	A	292	ARG	NE-CZ-NH2	11.24	129.31	119.20
1	A	278	GLU	CB-CG-CD	11.15	131.56	112.60
1	A	125	PHE	O-C-N	11.15	134.13	122.09
1	A	51	GLU	CB-CG-CD	11.14	131.54	112.60
1	A	340	THR	CB-CA-C	11.09	128.29	110.88
1	A	309	ILE	CB-CA-C	-11.05	97.22	112.14
1	A	185	ASP	CA-CB-CG	10.99	123.59	112.60
1	A	171	PHE	CA-C-N	10.88	134.59	120.44
1	A	171	PHE	C-N-CA	10.88	134.59	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	PHE	N-CA-CB	10.85	128.82	110.49
1	A	47	VAL	N-CA-CB	-10.80	93.14	110.96
1	A	14	PHE	N-CA-C	-10.79	98.19	114.16
1	A	281	ASP	CA-C-N	10.79	135.30	120.63
1	A	281	ASP	C-N-CA	10.79	135.30	120.63
1	A	238	GLU	N-CA-C	-10.76	96.80	111.96
1	A	125	PHE	N-CA-CB	10.71	125.61	110.07
1	A	101	LEU	N-CA-C	-10.65	99.46	111.71
1	A	340	THR	CA-CB-OG1	-10.62	93.67	109.60
1	A	36	GLU	CA-CB-CG	10.61	135.32	114.10
1	A	33	ARG	CD-NE-CZ	10.58	139.21	124.40
1	A	41	ILE	O-C-N	10.56	135.77	122.57
1	A	245	ALA	CA-C-O	10.53	131.88	119.56
1	A	177	SER	N-CA-C	-10.51	99.62	111.82
1	A	40	LYS	N-CA-CB	10.51	128.25	110.49
1	A	322	GLU	CA-CB-CG	10.48	135.06	114.10
1	A	338	VAL	N-CA-C	10.47	121.29	110.72
1	A	20	ALA	N-CA-C	10.33	132.64	109.81
1	A	62	LYS	N-CA-C	-10.31	99.01	111.69
1	A	210	ALA	CA-C-O	-10.30	109.53	120.55
1	A	235	GLU	CB-CG-CD	10.28	130.07	112.60
1	A	403	ALA	CA-C-O	10.26	131.27	120.70
1	A	393	THR	CA-CB-OG1	-10.23	94.25	109.60
1	A	281	ASP	CA-CB-CG	10.21	122.81	112.60
1	A	158	GLU	CB-CG-CD	10.18	129.91	112.60
1	A	172	ASP	CA-CB-CG	-10.13	102.47	112.60
1	A	69	LEU	N-CA-C	-9.99	101.22	113.50
1	A	122	ALA	CA-C-N	9.96	133.62	120.28
1	A	122	ALA	C-N-CA	9.96	133.62	120.28
1	A	374	ARG	N-CA-CB	-9.93	93.72	110.49
1	A	16	ASN	N-CA-C	9.85	124.39	110.50
1	A	15	GLU	CB-CG-CD	9.83	129.32	112.60
1	A	43	LEU	CB-CA-C	9.80	126.56	110.88
1	A	21	PRO	CA-C-N	9.79	140.24	121.54
1	A	21	PRO	C-N-CA	9.79	140.24	121.54
1	A	181	ALA	CA-C-N	9.73	135.13	120.82
1	A	181	ALA	C-N-CA	9.73	135.13	120.82
1	A	79	GLY	N-CA-C	-9.71	101.64	112.33
1	A	71	ASN	N-CA-CB	9.69	128.04	110.60
1	A	190	HIS	CA-C-N	9.67	140.37	121.41
1	A	190	HIS	C-N-CA	9.67	140.37	121.41
1	A	404	ILE	N-CA-C	9.61	121.58	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	ASP	O-C-N	9.60	131.96	122.07
1	A	182	GLN	N-CA-C	9.59	122.71	110.24
1	A	396	ASN	O-C-N	9.58	133.07	122.15
1	A	376	GLU	CA-C-O	9.56	138.17	121.53
1	A	293	ALA	CA-C-O	-9.52	108.41	120.31
1	A	309	ILE	O-C-N	9.51	131.10	121.87
1	A	371	LEU	N-CA-C	-9.51	100.79	111.82
1	A	395	ASP	CA-CB-CG	9.51	122.11	112.60
1	A	211	GLN	CB-CG-CD	9.49	128.74	112.60
1	A	262	LEU	N-CA-C	9.49	126.55	114.31
1	A	86	PHE	N-CA-C	-9.47	101.04	111.36
1	A	85	GLU	CA-C-O	9.47	130.11	119.41
1	A	331	GLN	N-CA-C	-9.46	98.42	112.04
1	A	144	ASN	N-CA-C	-9.42	101.92	113.50
1	A	69	LEU	CB-CA-C	9.41	126.41	109.29
1	A	407	VAL	CA-C-O	9.36	130.36	120.25
1	A	349	ASP	CA-C-O	-9.33	111.07	122.36
1	A	235	GLU	N-CA-CB	9.26	126.13	110.49
1	A	223	ASP	CA-CB-CG	9.23	121.83	112.60
1	A	291	ILE	O-C-N	9.17	131.39	121.94
1	A	43	LEU	N-CA-C	-9.14	94.01	108.63
1	A	233	LEU	CA-C-N	9.13	134.58	120.89
1	A	233	LEU	C-N-CA	9.13	134.58	120.89
1	A	245	ALA	CB-CA-C	9.13	125.99	110.56
1	A	221	LEU	N-CA-CB	9.12	125.89	110.49
1	A	231	ARG	N-CA-C	9.11	130.21	110.80
1	A	132	VAL	CB-CA-C	9.09	124.10	111.38
1	A	70	GLU	N-CA-CB	9.08	124.27	110.19
1	A	290	ALA	CA-C-N	9.08	132.05	120.70
1	A	290	ALA	C-N-CA	9.08	132.05	120.70
1	A	200	ASP	N-CA-C	9.06	129.84	109.81
1	A	90	THR	CA-C-N	9.06	138.85	121.54
1	A	90	THR	C-N-CA	9.06	138.85	121.54
1	A	193	CYS	O-C-N	-9.05	111.46	123.23
1	A	206	TRP	CB-CA-C	9.05	125.19	110.90
1	A	127	ALA	N-CA-CB	9.04	123.11	109.91
1	A	374	ARG	NH1-CZ-NH2	9.04	131.05	119.30
1	A	25	ILE	N-CA-CB	-9.03	96.33	111.23
1	A	42	ASN	N-CA-CB	9.02	124.22	110.60
1	A	303	ALA	O-C-N	9.01	131.67	122.12
1	A	90	THR	CA-C-O	8.98	130.95	121.07
1	A	358	GLY	O-C-N	8.95	130.31	122.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	LYS	CA-C-O	-8.94	107.73	120.51
1	A	171	PHE	CA-C-O	8.91	130.00	120.55
1	A	155	GLU	CB-CG-CD	8.87	127.68	112.60
1	A	342	GLN	CB-CG-CD	8.86	127.66	112.60
1	A	111	GLN	CB-CG-CD	-8.84	97.57	112.60
1	A	46	GLY	N-CA-C	-8.84	101.06	115.46
1	A	208	THR	N-CA-C	8.82	120.50	111.07
1	A	362	PHE	CB-CA-C	8.77	124.28	109.80
1	A	308	THR	CA-C-O	-8.76	111.80	121.00
1	A	76	ASN	OD1-CG-ND2	-8.75	113.85	122.60
1	A	173	ALA	N-CA-C	-8.75	101.67	111.82
1	A	204	GLU	CA-CB-CG	8.75	131.59	114.10
1	A	297	ASN	CA-CB-CG	8.75	121.35	112.60
1	A	43	LEU	CA-C-O	8.74	131.07	121.02
1	A	295	TYR	CA-C-O	-8.73	111.10	121.05
1	A	193	CYS	CB-CA-C	8.71	126.00	109.37
1	A	26	LEU	N-CA-CB	8.69	124.00	110.44
1	A	332	ARG	CD-NE-CZ	8.68	136.55	124.40
1	A	320	GLU	N-CA-CB	8.67	125.06	110.32
1	A	313	ASP	CA-CB-CG	-8.66	103.94	112.60
1	A	207	GLN	OE1-CD-NE2	-8.65	113.95	122.60
1	A	163	ASP	CB-CA-C	8.62	124.48	110.09
1	A	142	TRP	CB-CA-C	8.60	127.11	110.17
1	A	249	GLU	N-CA-CB	8.58	126.49	111.13
1	A	368	GLU	CA-C-N	8.50	132.35	120.29
1	A	368	GLU	C-N-CA	8.50	132.35	120.29
1	A	225	ALA	N-CA-C	-8.48	97.92	110.46
1	A	236	ASP	CA-CB-CG	-8.47	104.13	112.60
1	A	355	LYS	CA-C-O	8.46	131.24	120.57
1	A	51	GLU	CA-C-N	8.46	137.70	121.54
1	A	51	GLU	C-N-CA	8.46	137.70	121.54
1	A	100	ALA	N-CA-C	-8.44	102.99	113.20
1	A	348	ARG	CA-C-N	8.44	136.07	122.32
1	A	348	ARG	C-N-CA	8.44	136.07	122.32
1	A	127	ALA	N-CA-C	-8.42	101.79	110.97
1	A	280	VAL	CB-CA-C	8.41	123.40	110.95
1	A	355	LYS	CA-C-N	8.41	137.60	121.54
1	A	355	LYS	C-N-CA	8.41	137.60	121.54
1	A	181	ALA	N-CA-C	8.39	122.88	109.79
1	A	213	SER	N-CA-C	-8.39	102.14	111.28
1	A	396	ASN	OD1-CG-ND2	8.35	130.95	122.60
1	A	267	VAL	N-CA-C	8.35	120.14	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	GLN	CA-C-N	8.35	137.48	121.54
1	A	356	GLN	C-N-CA	8.35	137.48	121.54
1	A	322	GLU	N-CA-CB	8.34	122.11	110.01
1	A	343	GLU	CB-CA-C	-8.33	96.31	110.64
1	A	98	GLY	N-CA-C	8.32	124.15	113.24
1	A	219	LEU	CA-C-N	8.29	128.22	119.85
1	A	219	LEU	C-N-CA	8.29	128.22	119.85
1	A	327	ARG	N-CA-CB	8.29	122.00	109.98
1	A	396	ASN	N-CA-CB	8.29	122.42	110.16
1	A	72	GLU	CA-C-N	8.28	137.35	121.54
1	A	72	GLU	C-N-CA	8.28	137.35	121.54
1	A	276	ASP	CA-C-O	-8.26	111.43	120.43
1	A	210	ALA	O-C-N	8.26	132.16	122.17
1	A	396	ASN	CA-C-O	-8.26	111.67	120.42
1	A	47	VAL	N-CA-C	8.22	119.42	107.75
1	A	314	ALA	CA-C-N	8.20	131.94	120.29
1	A	314	ALA	C-N-CA	8.20	131.94	120.29
1	A	95	PHE	CA-CB-CG	-8.20	105.60	113.80
1	A	178	LEU	O-C-N	8.19	131.77	122.11
1	A	342	GLN	N-CA-CB	8.18	124.71	110.39
1	A	376	GLU	CB-CA-C	8.18	122.06	111.50
1	A	247	HIS	N-CA-C	8.16	128.19	110.80
1	A	393	THR	CA-CB-CG2	8.16	124.38	110.50
1	A	265	GLU	CA-CB-CG	8.15	130.40	114.10
1	A	205	GLN	OE1-CD-NE2	8.14	130.75	122.60
1	A	376	GLU	CB-CG-CD	8.12	126.41	112.60
1	A	309	ILE	CA-CB-CG1	8.10	124.17	110.40
1	A	393	THR	CA-C-O	8.10	129.12	120.94
1	A	281	ASP	CA-C-O	8.09	129.28	119.97
1	A	277	SER	N-CA-C	-8.06	103.34	113.01
1	A	21	PRO	O-C-N	-8.06	114.29	123.23
1	A	231	ARG	CB-CA-C	-8.04	94.42	110.42
1	A	407	VAL	CB-CA-C	8.04	125.26	112.16
1	A	211	GLN	N-CA-C	-8.02	101.48	111.75
1	A	328	GLN	OE1-CD-NE2	-8.02	114.58	122.60
1	A	44	GLY	N-CA-C	-7.99	94.24	113.18
1	A	355	LYS	N-CA-CB	7.99	123.87	110.69
1	A	22	ALA	N-CA-C	7.98	127.79	110.80
1	A	18	THR	CA-CB-OG1	-7.97	97.65	109.60
1	A	150	ASN	N-CA-C	-7.94	103.08	114.12
1	A	371	LEU	CA-C-O	7.90	129.06	119.97
1	A	176	ASN	O-C-N	7.89	131.72	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	LYS	O-C-N	7.87	133.06	122.59
1	A	188	LEU	CA-C-N	-7.86	111.63	122.95
1	A	188	LEU	C-N-CA	-7.86	111.63	122.95
1	A	376	GLU	CA-C-N	7.85	136.53	121.54
1	A	376	GLU	C-N-CA	7.85	136.53	121.54
1	A	182	GLN	CA-C-O	7.85	129.92	121.44
1	A	357	ASN	N-CA-C	7.80	127.42	110.80
1	A	370	VAL	CA-C-O	-7.77	110.72	119.42
1	A	318	ILE	CA-C-N	7.77	130.54	120.44
1	A	318	ILE	C-N-CA	7.77	130.54	120.44
1	A	32	PHE	CA-CB-CG	-7.76	106.03	113.80
1	A	172	ASP	N-CA-C	7.76	119.38	111.07
1	A	308	THR	O-C-N	7.73	130.07	122.03
1	A	47	VAL	CA-C-O	7.73	127.43	121.09
1	A	76	ASN	CB-CG-ND2	7.71	127.96	116.40
1	A	161	TYR	CA-CB-CG	7.70	127.75	113.90
1	A	373	LEU	CA-C-O	7.70	129.13	120.90
1	A	86	PHE	CA-C-N	7.68	128.31	119.94
1	A	86	PHE	C-N-CA	7.68	128.31	119.94
1	A	222	PHE	O-C-N	7.66	132.78	122.59
1	A	265	GLU	CA-C-N	7.66	136.17	121.54
1	A	265	GLU	C-N-CA	7.66	136.17	121.54
1	A	207	GLN	CA-CB-CG	7.62	129.35	114.10
1	A	14	PHE	CA-CB-CG	7.62	121.42	113.80
1	A	231	ARG	NE-CZ-NH1	-7.60	113.90	121.50
1	A	264	ASN	CA-C-N	7.58	134.37	123.14
1	A	264	ASN	C-N-CA	7.58	134.37	123.14
1	A	252	VAL	CB-CA-C	7.58	122.13	110.83
1	A	304	SER	O-C-N	7.57	130.15	122.12
1	A	189	PHE	CA-C-N	7.56	131.48	120.82
1	A	189	PHE	C-N-CA	7.56	131.48	120.82
1	A	208	THR	CA-C-N	7.56	136.32	121.58
1	A	208	THR	C-N-CA	7.56	136.32	121.58
1	A	218	TRP	N-CA-C	7.55	126.88	110.80
1	A	298	PRO	CA-C-O	7.50	131.44	120.56
1	A	158	GLU	CB-CA-C	7.49	121.93	110.62
1	A	350	PHE	CA-CB-CG	7.48	121.28	113.80
1	A	207	GLN	CG-CD-NE2	7.45	127.57	116.40
1	A	68	LEU	CA-C-O	7.44	128.18	119.32
1	A	80	ILE	CB-CA-C	-7.44	99.09	111.29
1	A	386	ARG	N-CA-C	7.43	120.62	109.25
1	A	372	ARG	CB-CA-C	-7.39	99.16	110.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	ASP	CA-CB-CG	7.35	119.95	112.60
1	A	310	LEU	N-CA-C	7.32	121.47	112.54
1	A	200	ASP	CA-CB-CG	7.32	119.92	112.60
1	A	135	VAL	N-CA-CB	7.31	121.76	111.82
1	A	13	MET	CA-C-N	7.31	132.61	120.70
1	A	13	MET	C-N-CA	7.31	132.61	120.70
1	A	23	ASP	O-C-N	7.30	129.16	121.42
1	A	209	LEU	N-CA-CB	-7.28	98.17	110.41
1	A	169	LEU	N-CA-CB	-7.28	98.19	110.49
1	A	103	ASN	CA-C-O	7.26	129.91	121.34
1	A	387	VAL	CA-C-O	7.26	128.80	120.67
1	A	96	GLY	CA-C-O	7.25	127.54	121.88
1	A	190	HIS	N-CA-CB	7.24	120.76	109.69
1	A	160	ALA	N-CA-CB	7.24	122.72	110.49
1	A	21	PRO	CA-C-O	7.22	130.84	121.96
1	A	297	ASN	CA-C-N	7.19	127.79	120.38
1	A	297	ASN	C-N-CA	7.19	127.79	120.38
1	A	180	GLU	CA-C-O	-7.17	110.25	120.51
1	A	369	GLN	CA-C-O	7.17	128.02	120.42
1	A	353	ILE	N-CA-CB	7.16	123.05	111.23
1	A	268	GLY	N-CA-C	-7.15	101.16	110.45
1	A	294	ASN	N-CA-CB	7.13	122.54	110.49
1	A	225	ALA	CA-C-O	-7.13	112.84	121.89
1	A	189	PHE	CB-CA-C	7.13	122.15	111.17
1	A	19	ALA	CA-C-O	-7.12	110.32	120.51
1	A	377	PHE	CA-C-O	-7.12	110.33	120.51
1	A	295	TYR	N-CA-C	-7.11	98.97	110.20
1	A	155	GLU	CG-CD-OE1	7.11	134.74	118.40
1	A	209	LEU	N-CA-C	7.10	121.77	113.18
1	A	238	GLU	CB-CA-C	-7.09	98.32	110.88
1	A	229	PHE	CA-CB-CG	7.09	120.89	113.80
1	A	104	ASP	CA-C-O	7.07	127.40	119.41
1	A	142	TRP	N-CA-C	-7.06	94.21	109.81
1	A	334	ARG	NE-CZ-NH1	7.06	128.56	121.50
1	A	198	GLY	CA-C-N	7.04	134.65	121.97
1	A	198	GLY	C-N-CA	7.04	134.65	121.97
1	A	389	VAL	CB-CA-C	7.04	125.24	111.79
1	A	36	GLU	CB-CG-CD	7.03	124.55	112.60
1	A	19	ALA	CB-CA-C	7.01	124.37	110.42
1	A	393	THR	CB-CA-C	7.00	120.12	109.56
1	A	146	LYS	CA-CB-CG	6.98	128.07	114.10
1	A	346	ALA	CA-C-O	6.95	130.46	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	PRO	CB-CA-C	-6.94	101.47	113.20
1	A	340	THR	N-CA-CB	-6.92	99.98	110.01
1	A	110	ALA	CA-C-O	-6.91	113.11	121.89
1	A	289	ALA	CB-CA-C	6.90	120.66	109.07
1	A	300	ALA	N-CA-C	6.89	125.48	110.80
1	A	214	VAL	N-CA-C	6.89	123.67	109.34
1	A	89	CYS	N-CA-C	-6.88	104.70	113.23
1	A	77	TYR	O-C-N	6.88	131.74	122.59
1	A	165	GLU	CA-C-O	-6.87	108.14	118.65
1	A	148	VAL	O-C-N	6.85	128.25	122.09
1	A	17	ILE	CA-C-N	-6.84	115.81	123.13
1	A	17	ILE	C-N-CA	-6.84	115.81	123.13
1	A	374	ARG	NE-CZ-NH1	-6.83	114.67	121.50
1	A	102	ILE	O-C-N	6.81	128.84	121.83
1	A	239	GLY	CA-C-N	6.81	129.70	120.44
1	A	239	GLY	C-N-CA	6.81	129.70	120.44
1	A	118	ALA	O-C-N	6.80	131.61	122.49
1	A	91	GLN	CA-CB-CG	6.79	127.67	114.10
1	A	402	GLU	CA-CB-CG	6.77	127.65	114.10
1	A	60	SER	CA-C-N	6.77	131.32	120.82
1	A	60	SER	C-N-CA	6.77	131.32	120.82
1	A	173	ALA	CB-CA-C	6.76	123.66	110.67
1	A	59	THR	N-CA-CB	6.75	121.89	110.49
1	A	329	ARG	N-CA-C	6.74	122.67	113.37
1	A	134	ARG	NE-CZ-NH1	-6.73	114.77	121.50
1	A	66	GLN	CB-CG-CD	6.72	124.02	112.60
1	A	44	GLY	CA-C-O	6.70	132.23	120.57
1	A	229	PHE	CA-C-N	6.70	132.69	122.37
1	A	229	PHE	C-N-CA	6.70	132.69	122.37
1	A	164	ALA	CA-C-O	6.67	130.05	120.51
1	A	303	ALA	CB-CA-C	-6.67	99.34	110.68
1	A	297	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	A	388	ASN	CA-CB-CG	6.66	119.26	112.60
1	A	111	GLN	N-CA-C	-6.65	101.58	110.55
1	A	85	GLU	N-CA-CB	6.64	120.16	110.47
1	A	105	LYS	N-CA-C	-6.63	96.67	110.80
1	A	166	ASN	N-CA-C	-6.63	96.67	110.80
1	A	58	LEU	N-CA-C	6.62	124.90	110.80
1	A	347	ASN	N-CA-CB	-6.60	100.71	111.01
1	A	187	VAL	N-CA-C	-6.59	100.36	109.46
1	A	396	ASN	CB-CA-C	-6.59	99.65	110.85
1	A	349	ASP	OD1-CG-OD2	-6.57	107.13	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	GLU	CB-CG-CD	6.56	123.75	112.60
1	A	371	LEU	CA-C-N	6.56	129.91	120.79
1	A	371	LEU	C-N-CA	6.56	129.91	120.79
1	A	405	VAL	CB-CA-C	6.54	120.08	111.70
1	A	238	GLU	O-C-N	6.54	129.90	122.19
1	A	45	ILE	CB-CA-C	6.53	120.47	110.55
1	A	397	MET	CA-C-O	6.53	129.84	120.51
1	A	126	LEU	CB-CA-C	6.50	122.66	110.63
1	A	407	VAL	CA-C-N	6.50	133.40	121.70
1	A	407	VAL	C-N-CA	6.50	133.40	121.70
1	A	101	LEU	CA-C-O	6.49	127.44	120.10
1	A	154	LEU	CA-C-O	-6.48	111.24	120.51
1	A	396	ASN	CA-CB-CG	6.46	119.06	112.60
1	A	376	GLU	N-CA-C	-6.45	102.52	111.81
1	A	210	ALA	N-CA-C	-6.45	103.53	111.40
1	A	336	LEU	N-CA-CB	-6.44	98.77	109.72
1	A	42	ASN	O-C-N	6.43	130.99	122.56
1	A	34	ALA	CA-C-N	6.43	132.95	120.99
1	A	34	ALA	C-N-CA	6.43	132.95	120.99
1	A	216	LYS	CB-CA-C	6.42	120.96	110.88
1	A	344	LYS	N-CA-CB	6.41	121.32	110.49
1	A	398	ALA	CB-CA-C	6.41	122.80	110.17
1	A	227	GLN	OE1-CD-NE2	6.40	129.00	122.60
1	A	28	LEU	N-CA-CB	6.39	121.29	110.49
1	A	19	ALA	N-CA-C	-6.38	97.21	110.80
1	A	112	THR	CB-CA-C	6.36	118.57	109.92
1	A	309	ILE	CA-C-O	-6.35	114.34	120.95
1	A	393	THR	CA-C-N	6.35	125.85	119.24
1	A	393	THR	C-N-CA	6.35	125.85	119.24
1	A	215	GLU	N-CA-CB	6.33	120.10	110.28
1	A	318	ILE	N-CA-C	-6.33	104.68	110.82
1	A	166	ASN	CB-CA-C	6.32	123.00	110.42
1	A	69	LEU	N-CA-CB	-6.31	101.25	110.53
1	A	320	GLU	CA-C-O	-6.30	111.86	119.49
1	A	338	VAL	CA-C-O	-6.30	114.17	120.85
1	A	89	CYS	N-CA-CB	6.29	120.26	110.44
1	A	159	TYR	CB-CA-C	6.29	122.95	110.42
1	A	134	ARG	N-CA-C	6.29	118.11	108.42
1	A	162	TYR	N-CA-CB	6.29	121.12	110.49
1	A	389	VAL	CA-CB-CG1	6.28	121.08	110.40
1	A	374	ARG	CA-CB-CG	6.27	126.64	114.10
1	A	219	LEU	CA-CB-CG	6.25	138.19	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	PHE	N-CA-CB	-6.25	102.73	110.98
1	A	335	GLN	CA-C-O	6.25	127.38	120.82
1	A	255	SER	N-CA-CB	6.24	121.03	110.49
1	A	137	VAL	N-CA-C	6.22	122.28	109.34
1	A	213	SER	CA-CB-OG	6.22	123.53	111.10
1	A	324	THR	O-C-N	6.21	128.70	122.12
1	A	177	SER	O-C-N	6.21	129.91	122.27
1	A	379	VAL	N-CA-C	-6.21	99.35	108.97
1	A	165	GLU	N-CA-C	-6.21	98.31	108.67
1	A	148	VAL	N-CA-C	-6.20	106.47	112.29
1	A	402	GLU	N-CA-CB	6.20	119.92	110.44
1	A	399	PRO	CA-C-N	6.16	129.15	120.28
1	A	399	PRO	C-N-CA	6.16	129.15	120.28
1	A	18	THR	CB-CA-C	6.16	125.58	116.53
1	A	187	VAL	O-C-N	6.15	127.84	122.12
1	A	402	GLU	CB-CG-CD	6.14	123.05	112.60
1	A	244	ALA	N-CA-C	6.14	121.43	113.88
1	A	240	LEU	N-CA-C	6.14	117.77	111.14
1	A	110	ALA	O-C-N	6.13	129.95	122.84
1	A	166	ASN	N-CA-CB	6.12	120.83	110.49
1	A	80	ILE	N-CA-CB	6.11	121.31	111.23
1	A	155	GLU	CA-C-O	6.10	128.48	121.28
1	A	129	ASN	N-CA-CB	6.09	120.79	110.49
1	A	103	ASN	CB-CA-C	6.09	121.88	111.46
1	A	116	THR	CA-CB-CG2	6.09	120.86	110.50
1	A	279	THR	N-CA-C	6.09	118.72	111.71
1	A	24	PRO	CA-C-N	6.08	132.91	121.97
1	A	24	PRO	C-N-CA	6.08	132.91	121.97
1	A	283	ALA	CA-C-N	6.07	128.90	120.29
1	A	283	ALA	C-N-CA	6.07	128.90	120.29
1	A	40	LYS	O-C-N	6.06	130.65	122.59
1	A	328	GLN	N-CA-CB	6.06	120.74	110.49
1	A	276	ASP	CA-CB-CG	6.05	118.66	112.60
1	A	74	THR	CA-CB-OG1	-6.04	100.54	109.60
1	A	247	HIS	CA-CB-CG	-6.04	107.76	113.80
1	A	393	THR	N-CA-CB	-6.04	99.16	110.09
1	A	162	TYR	CA-C-N	-6.02	112.61	122.54
1	A	162	TYR	C-N-CA	-6.02	112.61	122.54
1	A	326	MET	CB-CA-C	6.02	122.40	110.42
1	A	292	ARG	NE-CZ-NH1	-6.01	115.48	121.50
1	A	81	ASP	CA-C-O	6.01	125.39	119.08
1	A	366	THR	CA-CB-OG1	6.01	118.62	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	HIS	O-C-N	6.00	130.69	122.41
1	A	402	GLU	CA-C-O	-6.00	112.02	119.28
1	A	312	ASN	CB-CG-ND2	-6.00	107.41	116.40
1	A	200	ASP	CB-CA-C	-5.99	98.38	110.17
1	A	188	LEU	CA-C-O	-5.98	113.87	120.33
1	A	358	GLY	N-CA-C	-5.97	102.02	112.53
1	A	387	VAL	CB-CA-C	5.97	119.69	110.50
1	A	274	ALA	O-C-N	5.96	130.42	122.73
1	A	95	PHE	O-C-N	5.95	130.51	122.59
1	A	291	ILE	CA-C-O	-5.94	114.94	121.29
1	A	131	SER	CB-CA-C	-5.93	102.90	111.14
1	A	229	PHE	CA-C-O	5.91	128.96	120.51
1	A	278	GLU	N-CA-CB	5.90	118.74	110.07
1	A	18	THR	O-C-N	5.90	126.54	121.65
1	A	123	ALA	N-CA-C	5.90	117.71	111.28
1	A	142	TRP	N-CA-CB	5.90	120.86	110.37
1	A	20	ALA	CA-C-N	5.89	127.21	120.85
1	A	20	ALA	C-N-CA	5.89	127.21	120.85
1	A	237	ALA	CA-C-O	5.89	128.93	120.51
1	A	26	LEU	CA-C-N	5.88	132.94	121.41
1	A	26	LEU	C-N-CA	5.88	132.94	121.41
1	A	162	TYR	N-CA-C	-5.88	98.28	110.80
1	A	69	LEU	CA-C-O	5.87	125.60	119.14
1	A	119	LEU	O-C-N	5.86	130.19	122.33
1	A	178	LEU	CB-CA-C	-5.86	102.07	111.39
1	A	136	TRP	CA-C-O	5.85	126.81	120.43
1	A	127	ALA	CA-C-O	-5.84	114.86	121.00
1	A	237	ALA	CA-C-N	5.84	131.47	122.42
1	A	237	ALA	C-N-CA	5.84	131.47	122.42
1	A	312	ASN	N-CA-CB	5.83	119.63	110.71
1	A	70	GLU	CA-C-O	-5.83	113.03	120.31
1	A	384	SER	N-CA-CB	5.83	120.33	110.49
1	A	352	PHE	CA-CB-CG	5.81	119.61	113.80
1	A	376	GLU	N-CA-CB	5.81	118.97	110.25
1	A	59	THR	CA-C-O	-5.81	112.21	120.51
1	A	102	ILE	N-CA-C	-5.81	104.85	110.72
1	A	252	VAL	N-CA-CB	-5.81	103.35	111.25
1	A	190	HIS	CA-C-O	5.80	127.54	120.92
1	A	331	GLN	N-CA-CB	5.77	119.14	110.19
1	A	259	ASN	CA-CB-CG	5.77	118.37	112.60
1	A	129	ASN	CA-CB-CG	5.76	118.36	112.60
1	A	90	THR	N-CA-C	-5.76	104.00	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	ASN	CA-C-O	5.74	125.46	119.14
1	A	353	ILE	O-C-N	5.73	129.74	122.57
1	A	16	ASN	N-CA-CB	5.73	118.43	110.17
1	A	301	HIS	O-C-N	5.72	128.18	122.12
1	A	284	PHE	O-C-N	-5.71	115.64	122.15
1	A	320	GLU	CA-CB-CG	5.69	125.49	114.10
1	A	376	GLU	CG-CD-OE1	5.69	131.49	118.40
1	A	161	TYR	CA-C-O	-5.68	114.99	121.58
1	A	182	GLN	OE1-CD-NE2	-5.68	116.92	122.60
1	A	282	ARG	N-CA-C	5.67	117.33	111.03
1	A	28	LEU	O-C-N	5.67	130.13	122.59
1	A	175	ILE	CB-CG1-CD1	5.67	125.70	113.80
1	A	240	LEU	N-CA-CB	-5.66	101.86	110.07
1	A	46	GLY	CA-C-N	-5.65	115.78	122.11
1	A	46	GLY	C-N-CA	-5.65	115.78	122.11
1	A	348	ARG	CD-NE-CZ	-5.64	116.50	124.40
1	A	100	ALA	N-CA-CB	5.64	119.56	110.42
1	A	122	ALA	CA-C-O	5.64	126.39	120.42
1	A	388	ASN	N-CA-C	-5.64	98.54	108.23
1	A	288	LYS	N-CA-CB	5.63	122.39	110.67
1	A	130	THR	O-C-N	-5.62	116.01	122.93
1	A	309	ILE	CB-CG1-CD1	5.62	125.60	113.80
1	A	96	GLY	CA-C-N	5.61	132.25	121.54
1	A	96	GLY	C-N-CA	5.61	132.25	121.54
1	A	213	SER	O-C-N	5.61	128.06	122.12
1	A	244	ALA	CB-CA-C	5.61	118.11	109.03
1	A	147	SER	CA-C-O	-5.60	113.05	119.60
1	A	307	ALA	N-CA-C	-5.59	104.81	111.69
1	A	135	VAL	CA-CB-CG1	5.59	119.91	110.40
1	A	358	GLY	CA-C-O	-5.59	112.99	122.43
1	A	106	ARG	CD-NE-CZ	-5.59	116.58	124.40
1	A	363	SER	N-CA-C	5.58	117.45	109.14
1	A	167	HIS	ND1-CG-CD2	5.56	111.66	106.10
1	A	248	LYS	N-CA-CB	5.56	119.89	110.49
1	A	141	SER	CA-C-O	5.56	128.46	120.51
1	A	221	LEU	N-CA-C	-5.56	98.96	110.80
1	A	264	ASN	N-CA-CB	-5.56	101.09	110.49
1	A	194	HIS	N-CA-CB	-5.55	101.10	110.49
1	A	50	ASP	N-CA-C	5.54	118.54	110.17
1	A	135	VAL	CB-CA-C	5.53	117.89	110.42
1	A	378	GLY	CA-C-O	5.53	130.19	120.57
1	A	86	PHE	O-C-N	5.53	128.45	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	PHE	CA-C-O	-5.52	112.61	120.51
1	A	321	GLN	OE1-CD-NE2	-5.52	117.08	122.60
1	A	157	ARG	CD-NE-CZ	5.52	132.12	124.40
1	A	400	LEU	N-CA-C	-5.51	105.37	111.71
1	A	374	ARG	NE-CZ-NH2	-5.51	114.24	119.20
1	A	307	ALA	CB-CA-C	5.51	120.78	110.70
1	A	245	ALA	CA-C-N	5.50	132.95	122.60
1	A	245	ALA	C-N-CA	5.50	132.95	122.60
1	A	398	ALA	CA-C-N	5.49	124.95	119.24
1	A	398	ALA	C-N-CA	5.49	124.95	119.24
1	A	71	ASN	CA-C-N	-5.48	113.47	123.34
1	A	71	ASN	C-N-CA	-5.48	113.47	123.34
1	A	405	VAL	N-CA-CB	-5.48	104.87	110.62
1	A	343	GLU	O-C-N	5.47	128.81	122.19
1	A	238	GLU	N-CA-CB	5.47	120.06	110.27
1	A	129	ASN	CA-C-O	-5.46	112.70	120.51
1	A	66	GLN	N-CA-CB	5.45	118.38	110.26
1	A	124	ASP	N-CA-C	-5.45	106.48	113.23
1	A	227	GLN	CB-CG-CD	5.44	121.84	112.60
1	A	127	ALA	O-C-N	5.42	127.67	122.03
1	A	300	ALA	CB-CA-C	-5.42	99.63	110.42
1	A	313	ASP	O-C-N	5.42	128.94	122.27
1	A	88	ARG	N-CA-CB	5.41	118.67	110.28
1	A	216	LYS	N-CA-C	-5.40	105.29	111.07
1	A	144	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	A	375	GLU	N-CA-C	5.38	122.26	110.80
1	A	91	GLN	OE1-CD-NE2	5.38	127.98	122.60
1	A	36	GLU	N-CA-C	5.37	122.25	110.80
1	A	51	GLU	CA-CB-CG	5.37	124.83	114.10
1	A	114	GLY	N-CA-C	5.36	125.88	113.18
1	A	193	CYS	CA-CB-SG	-5.36	102.08	114.40
1	A	108	ARG	CD-NE-CZ	-5.34	116.92	124.40
1	A	32	PHE	N-CA-CB	5.34	117.72	109.98
1	A	340	THR	CA-C-O	-5.33	115.22	120.82
1	A	104	ASP	CA-CB-CG	-5.32	107.28	112.60
1	A	278	GLU	N-CA-C	-5.32	104.38	111.24
1	A	228	GLY	O-C-N	5.31	129.60	122.70
1	A	406	ALA	O-C-N	5.30	129.28	122.39
1	A	20	ALA	N-CA-CB	-5.29	100.95	110.37
1	A	246	MET	CA-C-O	-5.29	112.72	120.13
1	A	395	ASP	CB-CA-C	5.29	119.26	110.90
1	A	137	VAL	N-CA-CB	-5.28	102.51	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ASN	CA-C-O	5.28	128.06	120.51
1	A	212	LEU	CA-C-N	-5.28	113.21	120.28
1	A	212	LEU	C-N-CA	-5.28	113.21	120.28
1	A	60	SER	CB-CA-C	5.27	120.91	110.42
1	A	393	THR	N-CA-C	5.27	118.44	109.06
1	A	227	GLN	CG-CD-NE2	-5.26	108.51	116.40
1	A	348	ARG	CB-CA-C	5.25	119.25	110.43
1	A	294	ASN	CB-CG-ND2	-5.25	108.53	116.40
1	A	339	ASN	N-CA-CB	5.25	118.41	110.28
1	A	74	THR	N-CA-CB	-5.23	101.65	110.49
1	A	119	LEU	CA-C-O	-5.22	113.63	119.79
1	A	292	ARG	CD-NE-CZ	-5.22	117.09	124.40
1	A	368	GLU	N-CA-CB	-5.21	101.68	110.49
1	A	121	VAL	CA-C-O	5.21	126.31	119.85
1	A	35	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	157	ARG	CA-C-O	-5.20	114.71	121.73
1	A	279	THR	CA-CB-OG1	-5.20	101.80	109.60
1	A	145	HIS	ND1-CG-CD2	5.20	111.30	106.10
1	A	55	THR	CA-CB-OG1	-5.19	101.81	109.60
1	A	337	PHE	CB-CA-C	5.19	119.36	110.74
1	A	121	VAL	CB-CA-C	5.19	123.55	111.77
1	A	173	ALA	O-C-N	5.19	128.65	122.27
1	A	216	LYS	CA-C-N	5.19	131.58	121.41
1	A	216	LYS	C-N-CA	5.19	131.58	121.41
1	A	57	VAL	CB-CA-C	5.18	118.62	110.95
1	A	212	LEU	CA-C-O	-5.18	113.54	119.60
1	A	194	HIS	ND1-CG-CD2	5.18	111.28	106.10
1	A	112	THR	N-CA-CB	-5.17	103.58	110.77
1	A	59	THR	N-CA-C	-5.17	99.78	110.80
1	A	167	HIS	ND1-CE1-NE2	5.17	113.57	108.40
1	A	84	PRO	CB-CA-C	5.17	120.09	111.56
1	A	51	GLU	CA-C-O	5.17	127.90	120.51
1	A	70	GLU	O-C-N	5.16	129.27	122.30
1	A	342	GLN	O-C-N	5.16	129.59	122.46
1	A	386	ARG	CD-NE-CZ	5.16	131.63	124.40
1	A	106	ARG	O-C-N	5.15	129.44	122.59
1	A	109	THR	CA-CB-OG1	-5.15	101.87	109.60
1	A	334	ARG	NH1-CZ-NH2	-5.15	112.60	119.30
1	A	403	ALA	O-C-N	-5.14	116.53	122.09
1	A	31	LEU	CB-CA-C	5.14	120.65	110.42
1	A	129	ASN	O-C-N	5.13	129.41	122.59
1	A	312	ASN	O-C-N	5.13	130.01	123.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	PRO	N-CA-C	-5.12	102.20	110.55
1	A	344	LYS	CA-CB-CG	5.12	124.33	114.10
1	A	287	MET	CB-CA-C	-5.11	101.99	110.68
1	A	365	LEU	CA-C-N	-5.11	111.78	121.54
1	A	365	LEU	C-N-CA	-5.11	111.78	121.54
1	A	75	LYS	CA-CB-CG	5.11	124.31	114.10
1	A	273	VAL	N-CA-CB	-5.11	101.92	111.62
1	A	343	GLU	CA-C-O	-5.10	113.47	119.48
1	A	224	PHE	N-CA-C	5.08	116.51	109.54
1	A	65	GLU	N-CA-C	-5.08	106.92	113.01
1	A	321	GLN	CB-CA-C	5.08	119.87	109.67
1	A	369	GLN	CA-C-N	5.07	128.68	121.02
1	A	369	GLN	C-N-CA	5.07	128.68	121.02
1	A	40	LYS	CA-C-O	-5.07	113.26	120.51
1	A	150	ASN	O-C-N	5.07	128.15	122.27
1	A	196	PRO	CB-CA-C	-5.06	99.35	112.00
1	A	88	ARG	NE-CZ-NH1	5.05	126.56	121.50
1	A	32	PHE	CB-CA-C	5.05	118.78	110.95
1	A	59	THR	CA-CB-CG2	5.04	119.08	110.50
1	A	230	ALA	N-CA-CB	-5.04	102.66	110.98
1	A	264	ASN	CA-CB-CG	5.03	117.63	112.60
1	A	108	ARG	CA-CB-CG	5.03	124.15	114.10
1	A	376	GLU	O-C-N	-5.02	114.75	122.08
1	A	186	VAL	CB-CA-C	5.02	118.06	110.63
1	A	248	LYS	CG-CD-CE	5.02	122.84	111.30
1	A	94	LEU	CA-C-O	5.01	127.67	120.51
1	A	89	CYS	CB-CA-C	5.01	119.72	109.55
1	A	86	PHE	N-CA-CB	5.01	117.57	110.16
1	A	278	GLU	CA-CB-CG	5.00	124.10	114.10

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	ARG	Sidechain
1	A	120	ARG	Sidechain
1	A	231	ARG	Sidechain
1	A	241	ARG	Sidechain
1	A	266	ARG	Sidechain
1	A	292	ARG	Sidechain
1	A	316	ARG	Sidechain
1	A	327	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	348	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3065	0	3009	694	12
2	A	5	0	0	0	0
3	A	16	0	10	5	0
All	All	3086	0	3019	695	12

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 114.

All (695) 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:199:ILE:O	1:A:200:ASP:HB3	1.38	1.20
1:A:202:THR:N	1:A:205:GLN:HE21	1.39	1.19
1:A:202:THR:H	1:A:205:GLN:NE2	1.42	1.16
1:A:198:GLY:HA3	1:A:357:ASN:O	1.49	1.09
1:A:26:LEU:HD22	1:A:29:ALA:HB3	1.34	1.08
1:A:146:LYS:HB2	1:A:156:VAL:HG21	1.35	1.07
1:A:47:VAL:HG13	1:A:55:THR:HG21	1.30	1.07
1:A:116:THR:HB	1:A:142:TRP:HH2	1.19	1.06
1:A:128:LYS:HZ3	1:A:286:GLN:HB3	1.20	1.04
1:A:74:THR:O	1:A:75:LYS:HB3	1.49	1.04
1:A:37:ARG:HB2	1:A:38:PRO:HD2	1.40	1.01
1:A:59:THR:O	1:A:61:VAL:N	1.94	1.01
1:A:61:VAL:HG12	1:A:309:ILE:HD11	1.42	1.01
1:A:338:VAL:HG11	1:A:354:ILE:HD11	1.43	1.00
1:A:20:ALA:HB3	1:A:21:PRO:HD3	1.42	1.00
1:A:104:ASP:HB3	1:A:106:ARG:HG2	1.38	0.99
1:A:26:LEU:CD2	1:A:29:ALA:HB3	1.92	0.99
1:A:335:GLN:HA	1:A:354:ILE:CG2	1.94	0.98
1:A:263:TYR:O	1:A:265:GLU:N	1.96	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:THR:HG23	1:A:75:LYS:H	1.27	0.97
1:A:312:ASN:O	1:A:316:ARG:HB2	1.67	0.95
1:A:40:LYS:HZ2	1:A:40:LYS:C	1.73	0.95
1:A:51:GLU:N	1:A:329:ARG:HH12	1.65	0.93
1:A:41:ILE:HG22	1:A:43:LEU:HD12	1.47	0.92
1:A:27:GLY:C	1:A:28:LEU:HD22	1.94	0.92
1:A:172:ASP:O	1:A:176:ASN:ND2	2.02	0.91
1:A:125:PHE:O	1:A:128:LYS:HG3	1.69	0.91
1:A:42:ASN:HA	1:A:380:TYR:HB2	1.53	0.91
1:A:57:VAL:O	1:A:58:LEU:HB2	1.71	0.90
1:A:128:LYS:O	1:A:130:THR:N	2.05	0.90
1:A:197:THR:O	1:A:199:ILE:N	2.05	0.89
1:A:54:LYS:O	1:A:56:PRO:HD3	1.72	0.89
1:A:192:CYS:HB3	1:A:231:ARG:NH1	1.88	0.89
1:A:47:VAL:CG1	1:A:55:THR:HG21	2.04	0.88
1:A:112:THR:HG21	1:A:118:ALA:HB2	1.55	0.88
1:A:128:LYS:HE3	1:A:129:ASN:N	1.89	0.88
1:A:45:ILE:CG2	1:A:47:VAL:H	1.87	0.86
1:A:327:ARG:HG2	1:A:327:ARG:HH11	1.40	0.86
1:A:64:ALA:O	1:A:68:LEU:HD13	1.76	0.86
1:A:82:GLY:HA3	1:A:111:GLN:HB2	1.58	0.85
1:A:220:PRO:HD3	1:A:247:HIS:CE1	2.11	0.85
1:A:144:ASN:O	1:A:148:VAL:HG13	1.77	0.85
1:A:43:LEU:HD21	1:A:392:MET:HG3	1.58	0.84
1:A:48:TYR:CZ	1:A:326:MET:HG3	2.13	0.84
1:A:221:LEU:O	1:A:222:PHE:HB2	1.77	0.84
1:A:329:ARG:O	1:A:333:MET:HB2	1.77	0.83
1:A:116:THR:HB	1:A:142:TRP:CH2	2.11	0.83
1:A:80:ILE:HD12	1:A:288:LYS:HB3	1.60	0.83
1:A:50:ASP:C	1:A:52:THR:H	1.84	0.83
1:A:40:LYS:HE3	1:A:400:LEU:HD22	1.58	0.82
1:A:175:ILE:O	1:A:179:ASN:HB3	1.80	0.82
1:A:335:GLN:HA	1:A:354:ILE:HG23	1.58	0.82
1:A:48:TYR:O	1:A:49:LYS:HG3	1.80	0.82
1:A:335:GLN:HA	1:A:354:ILE:HG21	1.61	0.81
1:A:39:GLY:O	1:A:41:ILE:N	2.14	0.81
1:A:228:GLY:HA3	1:A:233:LEU:HD12	1.61	0.81
1:A:365:LEU:HB3	1:A:369:GLN:HB3	1.63	0.81
1:A:36:GLU:O	1:A:37:ARG:HB3	1.79	0.81
1:A:109:THR:HB	1:A:271:THR:HB	1.61	0.81
1:A:230:ALA:HB1	1:A:357:ASN:OD1	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LEU:O	1:A:72:GLU:HB2	1.81	0.80
1:A:100:ALA:O	1:A:104:ASP:N	2.15	0.80
1:A:58:LEU:O	1:A:59:THR:HG22	1.82	0.79
1:A:338:VAL:CG1	1:A:354:ILE:HD11	2.12	0.79
1:A:135:VAL:O	1:A:156:VAL:HA	1.81	0.79
1:A:40:LYS:NZ	1:A:40:LYS:O	2.15	0.79
1:A:339:ASN:C	1:A:339:ASN:HD22	1.89	0.79
1:A:111:GLN:NE2	1:A:303:ALA:HB2	1.99	0.78
1:A:388:ASN:ND2	1:A:390:ALA:HB3	1.98	0.78
1:A:128:LYS:HD2	1:A:286:GLN:HG2	1.64	0.78
1:A:42:ASN:HA	1:A:380:TYR:CB	2.13	0.78
1:A:50:ASP:OD1	1:A:52:THR:HB	1.83	0.78
1:A:142:TRP:O	1:A:145:HIS:HB2	1.84	0.78
1:A:116:THR:HG22	3:A:1:PMP:H5A1	1.65	0.77
1:A:152:ALA:O	1:A:154:LEU:N	2.16	0.77
1:A:296:SER:O	1:A:297:ASN:ND2	2.16	0.77
1:A:121:VAL:CG2	1:A:291:ILE:HD13	2.15	0.77
1:A:124:ASP:OD1	1:A:124:ASP:N	2.14	0.77
1:A:276:ASP:HB2	1:A:279:THR:H	1.49	0.77
1:A:115:GLY:HA3	3:A:1:PMP:H5A2	1.66	0.76
1:A:210:ALA:HB2	1:A:243:PHE:CE1	2.19	0.76
1:A:404:ILE:O	1:A:407:VAL:HG22	1.84	0.76
1:A:30:ASP:O	1:A:32:PHE:N	2.19	0.76
1:A:352:PHE:HD2	1:A:356:GLN:HE22	1.30	0.76
1:A:106:ARG:NE	1:A:274:ALA:O	2.18	0.76
1:A:165:GLU:O	1:A:166:ASN:C	2.28	0.76
1:A:45:ILE:HG22	1:A:47:VAL:H	1.50	0.76
1:A:310:LEU:O	1:A:316:ARG:NH1	2.19	0.76
1:A:348:ARG:NH2	1:A:348:ARG:HG3	2.01	0.76
1:A:235:GLU:HG3	1:A:235:GLU:O	1.83	0.76
1:A:130:THR:CG2	1:A:132:VAL:HB	2.16	0.75
1:A:144:ASN:HD22	1:A:148:VAL:CG1	1.99	0.75
1:A:23:ASP:OD2	1:A:25:ILE:HB	1.86	0.75
1:A:59:THR:O	1:A:62:LYS:N	2.16	0.75
1:A:67:TYR:HD1	1:A:68:LEU:HD12	1.51	0.75
1:A:30:ASP:C	1:A:32:PHE:N	2.43	0.75
1:A:366:THR:O	1:A:368:GLU:N	2.18	0.75
1:A:182:GLN:O	1:A:185:ASP:HB2	1.87	0.74
1:A:392:MET:HG2	1:A:400:LEU:HD21	1.68	0.74
1:A:28:LEU:HD21	1:A:381:ALA:O	1.88	0.74
1:A:35:ASP:O	1:A:37:ARG:NH2	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:PRO:HA	1:A:87:GLY:HA3	1.69	0.74
1:A:341:LEU:HD23	1:A:401:CYS:SG	2.26	0.74
1:A:112:THR:HG22	1:A:269:ALA:HA	1.70	0.74
1:A:202:THR:OG1	1:A:205:GLN:HG3	1.86	0.74
1:A:86:PHE:HE2	1:A:269:ALA:HB2	1.50	0.74
1:A:394:PRO:HG2	1:A:395:ASP:H	1.53	0.73
1:A:135:VAL:HA	1:A:186:VAL:O	1.89	0.73
1:A:375:GLU:C	1:A:377:PHE:H	1.96	0.73
1:A:49:LYS:HB3	1:A:53:GLY:HA2	1.72	0.72
1:A:30:ASP:C	1:A:32:PHE:H	1.97	0.72
1:A:221:LEU:O	1:A:251:ILE:O	2.06	0.72
1:A:396:ASN:HD22	1:A:396:ASN:N	1.86	0.72
1:A:150:ASN:OD1	1:A:155:GLU:HG2	1.90	0.72
1:A:110:ALA:O	1:A:269:ALA:HB1	1.90	0.72
1:A:365:LEU:HD22	1:A:365:LEU:N	2.05	0.71
1:A:47:VAL:HG13	1:A:55:THR:CG2	2.15	0.71
1:A:365:LEU:N	1:A:365:LEU:CD2	2.54	0.71
1:A:14:PHE:CD1	1:A:14:PHE:C	2.69	0.71
1:A:229:PHE:HE2	1:A:359:MET:HE1	1.55	0.71
1:A:237:ALA:O	1:A:241:ARG:HB3	1.91	0.71
1:A:45:ILE:CG2	1:A:47:VAL:O	2.39	0.71
1:A:167:HIS:O	1:A:168:THR:HG23	1.90	0.71
1:A:241:ARG:O	1:A:244:ALA:N	2.20	0.71
1:A:41:ILE:HG23	1:A:42:ASN:N	2.05	0.70
1:A:192:CYS:C	1:A:193:CYS:SG	2.72	0.70
1:A:312:ASN:O	1:A:316:ARG:N	2.25	0.70
1:A:74:THR:CG2	1:A:75:LYS:H	2.03	0.70
1:A:45:ILE:HG23	1:A:47:VAL:H	1.56	0.70
1:A:128:LYS:NZ	1:A:286:GLN:HB3	2.02	0.70
1:A:372:ARG:O	1:A:375:GLU:HB3	1.92	0.69
1:A:26:LEU:O	1:A:28:LEU:N	2.25	0.69
1:A:58:LEU:HD22	1:A:260:PHE:O	1.93	0.69
1:A:404:ILE:HA	1:A:407:VAL:HG22	1.73	0.69
1:A:314:ALA:O	1:A:318:ILE:HG13	1.92	0.69
1:A:59:THR:HG23	1:A:60:SER:H	1.57	0.69
1:A:74:THR:HG23	1:A:75:LYS:N	2.06	0.69
1:A:122:ALA:O	1:A:126:LEU:HB2	1.93	0.69
1:A:134:ARG:HB2	1:A:155:GLU:O	1.92	0.69
1:A:165:GLU:O	1:A:167:HIS:N	2.25	0.69
1:A:229:PHE:HE1	1:A:326:MET:HG2	1.55	0.69
1:A:47:VAL:HG22	1:A:263:TYR:OH	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LYS:HZ1	1:A:396:ASN:CG	2.01	0.68
1:A:192:CYS:HG	1:A:236:ASP:CG	2.00	0.68
1:A:365:LEU:O	1:A:367:LYS:N	2.26	0.68
1:A:199:ILE:HG22	1:A:200:ASP:H	1.58	0.68
1:A:43:LEU:HD11	1:A:391:GLY:C	2.19	0.68
1:A:327:ARG:HG2	1:A:327:ARG:NH1	2.09	0.68
1:A:256:TYR:HD2	1:A:260:PHE:CE2	2.11	0.68
1:A:315:LEU:HD12	1:A:318:ILE:HD12	1.76	0.68
1:A:67:TYR:CD1	1:A:68:LEU:HD12	2.29	0.68
1:A:373:LEU:O	1:A:377:PHE:HB2	1.94	0.68
1:A:190:HIS:HA	1:A:223:ASP:O	1.94	0.68
1:A:306:VAL:O	1:A:310:LEU:HB2	1.94	0.68
1:A:45:ILE:HG21	1:A:47:VAL:O	1.94	0.67
1:A:396:ASN:O	1:A:397:MET:C	2.37	0.67
1:A:50:ASP:O	1:A:53:GLY:N	2.27	0.67
1:A:103:ASN:ND2	1:A:105:LYS:HG2	2.08	0.67
1:A:136:TRP:CE3	1:A:157:ARG:HB3	2.29	0.67
1:A:260:PHE:HB3	1:A:262:LEU:HD22	1.77	0.67
1:A:13:MET:SD	1:A:13:MET:N	2.68	0.67
1:A:51:GLU:N	1:A:329:ARG:NH1	2.40	0.67
1:A:140:PRO:HG2	1:A:194:HIS:HE1	1.60	0.67
1:A:370:VAL:HG13	1:A:381:ALA:HB3	1.77	0.67
1:A:262:LEU:O	1:A:263:TYR:O	2.13	0.67
1:A:14:PHE:C	1:A:14:PHE:HD1	2.02	0.66
1:A:231:ARG:NE	1:A:235:GLU:HG2	2.10	0.66
1:A:315:LEU:HA	1:A:318:ILE:HD12	1.78	0.66
1:A:372:ARG:O	1:A:375:GLU:HG2	1.94	0.66
1:A:87:GLY:O	1:A:91:GLN:HB2	1.95	0.66
1:A:20:ALA:CB	1:A:21:PRO:HD3	2.14	0.66
1:A:210:ALA:HB2	1:A:243:PHE:CD1	2.30	0.66
1:A:178:LEU:HD23	1:A:218:TRP:CH2	2.31	0.66
1:A:309:ILE:HG22	1:A:309:ILE:O	1.95	0.65
1:A:112:THR:CG2	1:A:118:ALA:HB2	2.26	0.65
1:A:276:ASP:O	1:A:280:VAL:HG12	1.97	0.65
1:A:373:LEU:HG	1:A:379:VAL:HG22	1.76	0.65
1:A:348:ARG:HG3	1:A:348:ARG:HH21	1.61	0.65
1:A:145:HIS:O	1:A:149:PHE:HB2	1.95	0.65
1:A:367:LYS:HD3	1:A:368:GLU:OE1	1.96	0.65
1:A:276:ASP:HB2	1:A:279:THR:OG1	1.97	0.65
1:A:232:GLY:H	1:A:327:ARG:NH1	1.95	0.65
1:A:126:LEU:HD12	1:A:130:THR:OG1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:THR:HG23	1:A:394:PRO:HD2	1.78	0.65
1:A:28:LEU:HD22	1:A:28:LEU:N	2.12	0.64
1:A:116:THR:CB	1:A:142:TRP:HH2	2.04	0.64
1:A:128:LYS:CD	1:A:286:GLN:HG2	2.27	0.64
1:A:334:ARG:NH2	1:A:360:PHE:O	2.31	0.64
1:A:231:ARG:CZ	1:A:235:GLU:HG2	2.27	0.64
1:A:339:ASN:C	1:A:339:ASN:ND2	2.56	0.64
1:A:256:TYR:O	1:A:260:PHE:HB2	1.98	0.63
1:A:344:LYS:O	1:A:345:GLY:C	2.40	0.63
1:A:315:LEU:CD1	1:A:318:ILE:HD12	2.29	0.63
1:A:150:ASN:OD1	1:A:155:GLU:CG	2.45	0.63
1:A:194:HIS:HB3	1:A:197:THR:O	1.99	0.63
1:A:203:LEU:O	1:A:207:GLN:HB2	1.98	0.63
1:A:330:ILE:O	1:A:334:ARG:HB2	1.99	0.63
1:A:382:VAL:CG1	1:A:386:ARG:HB3	2.29	0.63
1:A:327:ARG:HH11	1:A:327:ARG:CG	2.10	0.62
1:A:396:ASN:HD22	1:A:396:ASN:H	1.47	0.62
1:A:197:THR:O	1:A:197:THR:OG1	2.16	0.62
1:A:125:PHE:CD1	1:A:128:LYS:HE2	2.34	0.62
1:A:321:GLN:C	1:A:321:GLN:HE21	2.07	0.62
1:A:336:LEU:O	1:A:337:PHE:C	2.42	0.62
1:A:339:ASN:ND2	1:A:339:ASN:O	2.33	0.62
1:A:327:ARG:NH1	1:A:327:ARG:CG	2.61	0.62
1:A:337:PHE:CD1	1:A:392:MET:CE	2.82	0.62
1:A:148:VAL:HG23	1:A:148:VAL:O	1.97	0.62
1:A:328:GLN:O	1:A:332:ARG:HB3	2.00	0.62
1:A:334:ARG:NH1	1:A:389:VAL:HG21	2.15	0.62
1:A:382:VAL:O	1:A:382:VAL:HG13	1.98	0.62
1:A:402:GLU:O	1:A:402:GLU:HG2	1.99	0.62
1:A:40:LYS:HZ3	1:A:396:ASN:HB3	1.64	0.62
1:A:179:ASN:HB2	1:A:216:LYS:CE	2.30	0.62
1:A:179:ASN:HB2	1:A:216:LYS:NZ	2.15	0.62
1:A:232:GLY:N	1:A:327:ARG:NH1	2.48	0.62
1:A:356:GLN:O	1:A:356:GLN:HG2	2.00	0.62
1:A:136:TRP:HZ2	1:A:181:ALA:HB3	1.64	0.61
1:A:103:ASN:HD22	1:A:105:LYS:HG2	1.64	0.61
1:A:321:GLN:HE22	1:A:325:ASP:CG	2.08	0.61
1:A:226:TYR:CZ	1:A:360:PHE:HE2	2.17	0.61
1:A:309:ILE:HG21	1:A:319:TRP:HB2	1.83	0.61
1:A:367:LYS:O	1:A:370:VAL:N	2.33	0.61
1:A:186:VAL:HG23	1:A:187:VAL:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:GLN:CA	1:A:354:ILE:HG23	2.31	0.61
1:A:119:LEU:HD13	1:A:145:HIS:NE2	2.15	0.61
1:A:13:MET:CG	1:A:13:MET:O	2.49	0.61
1:A:32:PHE:CE1	1:A:39:GLY:HA3	2.36	0.61
1:A:169:LEU:HD22	1:A:200:ASP:O	1.99	0.61
1:A:101:LEU:HA	1:A:104:ASP:HB2	1.83	0.61
1:A:121:VAL:HG21	1:A:291:ILE:HD13	1.82	0.61
1:A:363:SER:HB2	1:A:365:LEU:CD2	2.30	0.61
1:A:218:TRP:O	1:A:219:LEU:HB2	2.00	0.60
1:A:13:MET:SD	1:A:13:MET:O	2.59	0.60
1:A:209:LEU:O	1:A:213:SER:N	2.34	0.60
1:A:397:MET:HE3	1:A:397:MET:O	2.00	0.60
1:A:40:LYS:HE2	1:A:400:LEU:HB2	1.83	0.60
1:A:120:ARG:O	1:A:123:ALA:HB3	2.02	0.60
1:A:40:LYS:HD3	1:A:41:ILE:N	2.16	0.60
1:A:111:GLN:CD	1:A:303:ALA:HB2	2.26	0.60
1:A:135:VAL:HB	1:A:186:VAL:HG22	1.84	0.60
1:A:363:SER:HB2	1:A:365:LEU:HD23	1.83	0.60
1:A:37:ARG:O	1:A:39:GLY:N	2.34	0.60
1:A:152:ALA:C	1:A:154:LEU:H	2.07	0.60
1:A:19:ALA:O	1:A:20:ALA:HB2	2.00	0.60
1:A:40:LYS:CG	1:A:41:ILE:N	2.64	0.60
1:A:136:TRP:CZ2	1:A:181:ALA:HB3	2.37	0.60
1:A:113:PRO:HA	1:A:266:ARG:HB2	1.84	0.60
1:A:210:ALA:C	1:A:212:LEU:N	2.58	0.60
1:A:229:PHE:HE2	1:A:359:MET:CE	2.14	0.59
1:A:255:SER:OG	3:A:1:PMP:O2P	2.15	0.59
1:A:23:ASP:CG	1:A:24:PRO:HD2	2.27	0.59
1:A:40:LYS:CE	1:A:400:LEU:HD22	2.31	0.59
1:A:43:LEU:CD2	1:A:392:MET:HG3	2.31	0.59
1:A:83:ILE:O	1:A:86:PHE:HB3	2.01	0.59
1:A:128:LYS:O	1:A:129:ASN:C	2.45	0.59
1:A:393:THR:HG23	1:A:394:PRO:CD	2.31	0.59
1:A:119:LEU:O	1:A:122:ALA:HB3	2.02	0.59
1:A:238:GLU:O	1:A:239:GLY:C	2.46	0.59
1:A:367:LYS:HB2	1:A:368:GLU:OE1	2.03	0.59
1:A:287:MET:C	1:A:289:ALA:H	2.08	0.59
1:A:16:ASN:CG	1:A:17:ILE:H	2.11	0.59
1:A:46:GLY:O	1:A:47:VAL:HG23	2.02	0.59
1:A:369:GLN:O	1:A:372:ARG:HB3	2.03	0.59
1:A:13:MET:SD	1:A:13:MET:C	2.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LYS:HG3	1:A:41:ILE:H	1.68	0.59
1:A:101:LEU:HD23	1:A:106:ARG:HG3	1.83	0.59
1:A:146:LYS:O	1:A:150:ASN:ND2	2.36	0.59
1:A:49:LYS:CG	1:A:55:THR:HG23	2.33	0.58
1:A:257:SER:HB3	1:A:263:TYR:HD2	1.68	0.58
1:A:40:LYS:NZ	1:A:396:ASN:OD1	2.27	0.58
1:A:26:LEU:HD23	1:A:29:ALA:HB3	1.82	0.58
1:A:178:LEU:CD2	1:A:218:TRP:CH2	2.86	0.58
1:A:401:CYS:O	1:A:404:ILE:HG22	2.03	0.58
1:A:373:LEU:O	1:A:374:ARG:C	2.46	0.58
1:A:40:LYS:HG3	1:A:41:ILE:N	2.18	0.58
1:A:37:ARG:CB	1:A:38:PRO:HD2	2.17	0.58
1:A:128:LYS:HZ3	1:A:286:GLN:CB	2.06	0.58
1:A:312:ASN:HB3	1:A:315:LEU:HB2	1.84	0.58
1:A:32:PHE:HD1	1:A:380:TYR:CE1	2.22	0.58
1:A:174:LEU:O	1:A:178:LEU:N	2.30	0.58
1:A:40:LYS:NZ	1:A:396:ASN:HB3	2.18	0.58
1:A:199:ILE:HG22	1:A:200:ASP:N	2.19	0.58
1:A:175:ILE:CD1	1:A:209:LEU:HD12	2.34	0.57
1:A:272:LEU:C	1:A:273:VAL:HG12	2.29	0.57
1:A:50:ASP:C	1:A:329:ARG:HH12	2.12	0.57
1:A:27:GLY:O	1:A:28:LEU:HD13	2.04	0.57
1:A:128:LYS:NZ	1:A:129:ASN:HB2	2.19	0.57
1:A:375:GLU:CG	1:A:376:GLU:N	2.67	0.57
1:A:389:VAL:O	1:A:392:MET:HB2	2.05	0.57
1:A:202:THR:OG1	1:A:205:GLN:CG	2.52	0.57
1:A:306:VAL:O	1:A:310:LEU:HD22	2.05	0.57
1:A:26:LEU:C	1:A:28:LEU:H	2.13	0.57
1:A:101:LEU:CA	1:A:104:ASP:HB2	2.35	0.57
1:A:112:THR:HG21	1:A:118:ALA:CB	2.32	0.57
1:A:119:LEU:HD23	1:A:253:ALA:CB	2.35	0.57
1:A:200:ASP:OD2	1:A:201:PRO:O	2.23	0.57
1:A:144:ASN:HD22	1:A:148:VAL:HG12	1.70	0.57
1:A:388:ASN:HD21	1:A:390:ALA:HB3	1.70	0.57
1:A:78:LEU:HD22	1:A:300:ALA:HB2	1.87	0.56
1:A:193:CYS:SG	1:A:357:ASN:ND2	2.77	0.56
1:A:257:SER:O	1:A:258:ALA:HB2	2.05	0.56
1:A:32:PHE:HE1	1:A:39:GLY:HA3	1.70	0.56
1:A:171:PHE:O	1:A:174:LEU:HB3	2.03	0.56
1:A:32:PHE:CD1	1:A:32:PHE:C	2.81	0.56
1:A:140:PRO:CG	1:A:196:PRO:HD2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:CYS:SG	1:A:200:ASP:HB2	2.45	0.56
1:A:73:THR:HG23	1:A:74:THR:HB	1.88	0.56
1:A:40:LYS:C	1:A:40:LYS:CD	2.78	0.56
1:A:40:LYS:C	1:A:40:LYS:HD3	2.31	0.56
1:A:119:LEU:HD23	1:A:253:ALA:HB3	1.87	0.56
1:A:399:PRO:O	1:A:403:ALA:N	2.39	0.56
1:A:104:ASP:O	1:A:105:LYS:HB2	2.05	0.56
1:A:108:ARG:HB2	1:A:284:PHE:CD1	2.40	0.56
1:A:112:THR:CG2	1:A:269:ALA:HA	2.35	0.56
1:A:128:LYS:HE3	1:A:129:ASN:H	1.68	0.56
1:A:185:ASP:O	1:A:218:TRP:O	2.23	0.56
1:A:334:ARG:NH2	1:A:361:SER:OG	2.38	0.56
1:A:26:LEU:HD22	1:A:26:LEU:O	2.06	0.56
1:A:84:PRO:O	1:A:88:ARG:HG2	2.05	0.56
1:A:394:PRO:CG	1:A:395:ASP:H	2.17	0.56
1:A:321:GLN:NE2	1:A:325:ASP:OD1	2.38	0.56
1:A:404:ILE:HA	1:A:407:VAL:CG2	2.36	0.56
3:A:1:PMP:H4A2	3:A:1:PMP:O4P	2.04	0.55
1:A:260:PHE:HE1	1:A:309:ILE:HG13	1.71	0.55
1:A:353:ILE:CG1	1:A:354:ILE:N	2.69	0.55
1:A:41:ILE:CG2	1:A:42:ASN:N	2.68	0.55
1:A:179:ASN:HB2	1:A:216:LYS:HZ3	1.71	0.55
1:A:232:GLY:HA2	1:A:327:ARG:CZ	2.36	0.55
1:A:298:PRO:O	1:A:300:ALA:N	2.36	0.55
1:A:382:VAL:HG11	1:A:386:ARG:HB3	1.87	0.55
1:A:130:THR:HG23	1:A:132:VAL:HB	1.89	0.55
1:A:260:PHE:CE1	1:A:309:ILE:HG13	2.41	0.55
1:A:276:ASP:O	1:A:280:VAL:CG1	2.54	0.55
1:A:173:ALA:O	1:A:177:SER:HB2	2.06	0.55
1:A:353:ILE:HG13	1:A:354:ILE:N	2.18	0.55
1:A:327:ARG:O	1:A:328:GLN:C	2.49	0.55
1:A:404:ILE:C	1:A:407:VAL:HG22	2.31	0.55
1:A:220:PRO:HD3	1:A:247:HIS:HE1	1.66	0.54
1:A:234:GLU:C	1:A:236:ASP:N	2.64	0.54
1:A:23:ASP:OD1	1:A:24:PRO:HD2	2.07	0.54
1:A:393:THR:O	1:A:397:MET:N	2.35	0.54
1:A:196:PRO:HG2	1:A:362:PHE:CE1	2.42	0.54
1:A:107:ALA:HB2	1:A:273:VAL:HB	1.89	0.54
1:A:141:SER:OG	1:A:142:TRP:N	2.35	0.54
1:A:226:TYR:O	1:A:229:PHE:HB3	2.07	0.54
1:A:231:ARG:NH1	1:A:235:GLU:HG2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:VAL:HG22	1:A:263:TYR:CZ	2.43	0.54
1:A:89:CYS:O	1:A:93:LEU:HB2	2.08	0.54
1:A:263:TYR:C	1:A:265:GLU:N	2.66	0.54
1:A:120:ARG:O	1:A:124:ASP:OD1	2.26	0.54
1:A:349:ASP:C	1:A:351:SER:H	2.15	0.54
1:A:88:ARG:O	1:A:91:GLN:HB3	2.07	0.54
1:A:192:CYS:SG	1:A:236:ASP:OD2	2.66	0.54
1:A:48:TYR:O	1:A:49:LYS:CG	2.53	0.53
1:A:202:THR:H	1:A:205:GLN:HE21	0.64	0.53
1:A:126:LEU:HD12	1:A:130:THR:CB	2.38	0.53
1:A:241:ARG:HA	1:A:244:ALA:HB3	1.91	0.53
1:A:234:GLU:O	1:A:236:ASP:N	2.42	0.53
1:A:74:THR:CG2	1:A:75:LYS:N	2.67	0.53
1:A:51:GLU:H	1:A:329:ARG:NH1	2.06	0.53
1:A:92:GLU:HG3	1:A:97:LYS:HA	1.91	0.53
1:A:149:PHE:O	1:A:154:LEU:O	2.26	0.53
1:A:369:GLN:O	1:A:372:ARG:CB	2.57	0.53
1:A:136:TRP:HZ2	1:A:181:ALA:CB	2.21	0.53
1:A:356:GLN:OE1	1:A:361:SER:HB3	2.07	0.53
1:A:49:LYS:HG3	1:A:55:THR:HG23	1.91	0.53
1:A:128:LYS:HZ1	1:A:129:ASN:HB2	1.74	0.53
1:A:287:MET:C	1:A:289:ALA:N	2.67	0.53
1:A:50:ASP:C	1:A:52:THR:N	2.61	0.53
1:A:136:TRP:NE1	1:A:185:ASP:OD1	2.42	0.53
1:A:57:VAL:O	1:A:58:LEU:CB	2.50	0.52
1:A:174:LEU:C	1:A:176:ASN:N	2.65	0.52
1:A:256:TYR:HD1	1:A:268:GLY:HA2	1.72	0.52
1:A:256:TYR:CD2	1:A:260:PHE:CE2	2.96	0.52
1:A:352:PHE:HD2	1:A:356:GLN:NE2	2.05	0.52
1:A:234:GLU:O	1:A:235:GLU:C	2.52	0.52
1:A:179:ASN:OD1	1:A:180:GLU:N	2.43	0.52
1:A:335:GLN:CA	1:A:354:ILE:CG2	2.80	0.52
1:A:20:ALA:CB	1:A:21:PRO:CD	2.88	0.52
1:A:195:ASN:HD22	1:A:196:PRO:HA	1.73	0.52
1:A:43:LEU:HD23	1:A:387:VAL:HG23	1.91	0.52
1:A:178:LEU:CD2	1:A:218:TRP:CZ3	2.93	0.52
1:A:194:HIS:HB3	1:A:197:THR:C	2.34	0.52
1:A:261:GLY:O	1:A:262:LEU:HD13	2.09	0.52
1:A:333:MET:O	1:A:336:LEU:HB2	2.09	0.52
1:A:13:MET:O	1:A:13:MET:HG2	2.10	0.52
1:A:99:SER:O	1:A:102:ILE:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:SER:HG	1:A:142:TRP:H	1.58	0.52
1:A:272:LEU:CD2	1:A:280:VAL:HG23	2.39	0.52
1:A:27:GLY:O	1:A:28:LEU:HD22	2.10	0.52
1:A:209:LEU:O	1:A:212:LEU:HB2	2.10	0.52
1:A:206:TRP:O	1:A:243:PHE:HE1	1.93	0.52
1:A:179:ASN:OD1	1:A:179:ASN:C	2.52	0.51
1:A:276:ASP:C	1:A:278:GLU:N	2.65	0.51
1:A:282:ARG:O	1:A:285:SER:OG	2.20	0.51
1:A:61:VAL:HG12	1:A:309:ILE:CD1	2.29	0.51
1:A:203:LEU:C	1:A:207:GLN:HE21	2.19	0.51
1:A:321:GLN:NE2	1:A:325:ASP:CG	2.69	0.51
1:A:188:LEU:HD12	1:A:221:LEU:HG	1.92	0.51
1:A:351:SER:O	1:A:352:PHE:C	2.53	0.51
1:A:26:LEU:HD22	1:A:29:ALA:CB	2.24	0.51
1:A:99:SER:C	1:A:101:LEU:H	2.18	0.51
1:A:228:GLY:HA3	1:A:233:LEU:HA	1.92	0.51
1:A:393:THR:HG23	1:A:394:PRO:CG	2.41	0.51
1:A:204:GLU:HA	1:A:207:GLN:HB2	1.92	0.51
1:A:364:GLY:C	1:A:365:LEU:HD22	2.35	0.51
1:A:257:SER:HB3	1:A:263:TYR:CD2	2.45	0.51
1:A:309:ILE:HG21	1:A:319:TRP:CB	2.39	0.51
1:A:375:GLU:HG3	1:A:376:GLU:N	2.26	0.51
1:A:174:LEU:O	1:A:175:ILE:C	2.54	0.51
1:A:342:GLN:O	1:A:342:GLN:HG2	2.10	0.51
1:A:349:ASP:OD2	1:A:351:SER:OG	2.20	0.51
1:A:40:LYS:NZ	1:A:396:ASN:CG	2.67	0.51
1:A:128:LYS:HZ1	1:A:129:ASN:CB	2.24	0.51
1:A:83:ILE:HD11	1:A:303:ALA:HB3	1.93	0.50
1:A:136:TRP:HB3	1:A:157:ARG:HB3	1.93	0.50
1:A:37:ARG:HB2	1:A:38:PRO:CD	2.29	0.50
1:A:84:PRO:HA	1:A:87:GLY:CA	2.39	0.50
1:A:165:GLU:O	1:A:167:HIS:ND1	2.44	0.50
1:A:189:PHE:CE1	1:A:209:LEU:HD23	2.46	0.50
1:A:76:ASN:O	1:A:77:TYR:C	2.54	0.50
1:A:174:LEU:HD22	1:A:178:LEU:HB2	1.93	0.50
1:A:334:ARG:HH22	1:A:360:PHE:C	2.19	0.50
1:A:404:ILE:CA	1:A:407:VAL:HG22	2.41	0.50
1:A:58:LEU:O	1:A:322:GLU:OE2	2.29	0.50
1:A:165:GLU:O	1:A:167:HIS:CG	2.64	0.50
1:A:332:ARG:HH21	1:A:336:LEU:HD21	1.76	0.50
1:A:375:GLU:HG3	1:A:377:PHE:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLU:OE2	1:A:70:GLU:HA	2.11	0.50
1:A:274:ALA:HB3	1:A:280:VAL:HG12	1.94	0.50
1:A:352:PHE:HB2	1:A:356:GLN:NE2	2.27	0.50
1:A:20:ALA:HB3	1:A:21:PRO:CD	2.30	0.50
1:A:100:ALA:C	1:A:103:ASN:H	2.20	0.50
1:A:276:ASP:CB	1:A:279:THR:H	2.20	0.50
1:A:43:LEU:O	1:A:380:TYR:O	2.29	0.49
1:A:145:HIS:CE1	1:A:188:LEU:HD21	2.47	0.49
1:A:135:VAL:O	1:A:157:ARG:N	2.44	0.49
1:A:140:PRO:HG2	1:A:196:PRO:HD2	1.94	0.49
1:A:372:ARG:O	1:A:375:GLU:CB	2.58	0.49
1:A:107:ALA:HA	1:A:272:LEU:O	2.12	0.49
1:A:175:ILE:HD13	1:A:209:LEU:HD12	1.93	0.49
1:A:179:ASN:HA	1:A:218:TRP:HZ2	1.76	0.49
1:A:85:GLU:O	1:A:89:CYS:SG	2.68	0.49
1:A:309:ILE:O	1:A:316:ARG:HG2	2.13	0.49
1:A:382:VAL:HG12	1:A:386:ARG:HB3	1.95	0.49
1:A:100:ALA:O	1:A:103:ASN:C	2.56	0.49
1:A:337:PHE:CD1	1:A:392:MET:HE2	2.48	0.49
1:A:57:VAL:HG11	1:A:62:LYS:HE2	1.95	0.49
1:A:59:THR:CG2	1:A:322:GLU:OE1	2.61	0.49
1:A:137:VAL:O	1:A:138:SER:CB	2.60	0.49
1:A:193:CYS:SG	1:A:200:ASP:CB	3.01	0.49
1:A:263:TYR:C	1:A:265:GLU:H	2.13	0.49
1:A:347:ASN:O	1:A:348:ARG:HB3	2.11	0.49
1:A:183:ALA:O	1:A:185:ASP:N	2.46	0.48
1:A:212:LEU:O	1:A:213:SER:C	2.55	0.48
1:A:210:ALA:O	1:A:213:SER:N	2.46	0.48
1:A:366:THR:O	1:A:368:GLU:HG2	2.12	0.48
1:A:246:MET:HE2	1:A:246:MET:HA	1.96	0.48
1:A:272:LEU:HD23	1:A:280:VAL:HG23	1.94	0.48
1:A:276:ASP:C	1:A:278:GLU:H	2.20	0.48
1:A:334:ARG:HH12	1:A:361:SER:HB2	1.77	0.48
1:A:405:VAL:O	1:A:408:LEU:HA	2.13	0.48
1:A:97:LYS:HD2	1:A:98:GLY:H	1.78	0.48
1:A:179:ASN:HB2	1:A:216:LYS:HE2	1.94	0.48
1:A:45:ILE:HG22	1:A:47:VAL:N	2.24	0.48
1:A:94:LEU:O	1:A:237:ALA:HB1	2.14	0.48
1:A:136:TRP:HZ2	1:A:181:ALA:H	1.59	0.48
1:A:231:ARG:NH1	1:A:235:GLU:CG	2.76	0.48
1:A:213:SER:HA	1:A:218:TRP:HE3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:PRO:CD	1:A:247:HIS:CE1	2.91	0.48
1:A:370:VAL:CG1	1:A:381:ALA:HB3	2.44	0.48
1:A:49:LYS:HG2	1:A:55:THR:HG23	1.96	0.48
1:A:126:LEU:HG	1:A:130:THR:HG21	1.96	0.48
1:A:382:VAL:HG13	1:A:384:SER:OG	2.13	0.48
1:A:174:LEU:O	1:A:176:ASN:N	2.46	0.48
1:A:14:PHE:CD1	1:A:14:PHE:O	2.67	0.48
1:A:119:LEU:HD13	1:A:145:HIS:CD2	2.49	0.48
1:A:178:LEU:HD23	1:A:218:TRP:CZ3	2.49	0.48
1:A:223:ASP:OD1	3:A:1:PMP:N1	2.47	0.48
1:A:112:THR:HG22	1:A:269:ALA:CA	2.42	0.48
1:A:146:LYS:HA	1:A:156:VAL:HG11	1.96	0.48
1:A:202:THR:H	1:A:205:GLN:CG	2.27	0.47
1:A:213:SER:HA	1:A:218:TRP:CE3	2.49	0.47
1:A:228:GLY:O	1:A:323:LEU:HD21	2.14	0.47
1:A:310:LEU:HA	1:A:316:ARG:HH11	1.79	0.47
1:A:99:SER:C	1:A:101:LEU:N	2.73	0.47
1:A:232:GLY:HA2	1:A:327:ARG:NH1	2.30	0.47
1:A:305:VAL:HG13	1:A:305:VAL:O	2.14	0.47
1:A:393:THR:CB	1:A:394:PRO:HD2	2.42	0.47
1:A:37:ARG:CB	1:A:38:PRO:CD	2.91	0.47
1:A:50:ASP:O	1:A:52:THR:N	2.37	0.47
1:A:59:THR:O	1:A:60:SER:C	2.55	0.47
1:A:392:MET:HG2	1:A:400:LEU:CD2	2.41	0.47
1:A:32:PHE:HA	1:A:380:TYR:CE2	2.50	0.47
1:A:393:THR:CG2	1:A:394:PRO:HD2	2.44	0.47
1:A:357:ASN:OD1	1:A:358:GLY:N	2.47	0.47
1:A:365:LEU:HA	1:A:369:GLN:CD	2.40	0.47
1:A:118:ALA:HA	1:A:121:VAL:CG1	2.45	0.47
1:A:144:ASN:ND2	1:A:148:VAL:HG12	2.30	0.47
1:A:167:HIS:CD2	1:A:167:HIS:H	2.32	0.47
1:A:229:PHE:CE2	1:A:359:MET:CE	2.96	0.47
1:A:360:PHE:O	1:A:361:SER:OG	2.31	0.47
1:A:367:LYS:HD3	1:A:368:GLU:CD	2.40	0.47
1:A:75:LYS:HG3	1:A:75:LYS:O	2.14	0.47
1:A:86:PHE:O	1:A:90:THR:HB	2.15	0.47
1:A:100:ALA:O	1:A:104:ASP:HB2	2.15	0.47
1:A:171:PHE:CZ	1:A:208:THR:HG21	2.50	0.47
1:A:192:CYS:SG	1:A:236:ASP:OD1	2.73	0.47
1:A:26:LEU:HA	1:A:29:ALA:HB2	1.97	0.46
1:A:128:LYS:NZ	1:A:129:ASN:CB	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ASN:C	1:A:77:TYR:O	2.57	0.46
1:A:105:LYS:O	1:A:106:ARG:HB3	2.15	0.46
1:A:174:LEU:CD1	1:A:209:LEU:HD11	2.45	0.46
1:A:256:TYR:HA	1:A:259:ASN:OD1	2.15	0.46
1:A:372:ARG:O	1:A:375:GLU:CG	2.62	0.46
1:A:45:ILE:CG2	1:A:47:VAL:N	2.68	0.46
1:A:197:THR:C	1:A:199:ILE:H	2.15	0.46
1:A:231:ARG:CD	1:A:235:GLU:HG2	2.45	0.46
1:A:262:LEU:HD23	1:A:306:VAL:CG2	2.45	0.46
1:A:293:ALA:O	1:A:294:ASN:O	2.33	0.46
1:A:393:THR:HG23	1:A:394:PRO:HG2	1.96	0.46
1:A:333:MET:HE2	1:A:392:MET:HB3	1.98	0.46
1:A:348:ARG:NE	1:A:350:PHE:HE1	2.14	0.46
1:A:182:GLN:O	1:A:183:ALA:C	2.58	0.46
1:A:188:LEU:HD12	1:A:221:LEU:HB3	1.98	0.46
1:A:202:THR:N	1:A:205:GLN:HG3	2.30	0.46
1:A:256:TYR:HD2	1:A:260:PHE:CD2	2.34	0.46
1:A:342:GLN:O	1:A:342:GLN:CG	2.63	0.46
1:A:40:LYS:CD	1:A:41:ILE:N	2.79	0.46
1:A:83:ILE:HA	1:A:84:PRO:HD3	1.81	0.46
1:A:201:PRO:CB	1:A:205:GLN:HB2	2.46	0.46
1:A:377:PHE:HB3	1:A:379:VAL:HG13	1.98	0.46
1:A:397:MET:C	1:A:397:MET:HE3	2.41	0.46
1:A:142:TRP:CZ2	1:A:144:ASN:HB3	2.50	0.46
1:A:221:LEU:O	1:A:222:PHE:CB	2.55	0.46
1:A:352:PHE:O	1:A:353:ILE:C	2.59	0.46
1:A:32:PHE:CD1	1:A:32:PHE:O	2.70	0.45
1:A:120:ARG:HH11	1:A:120:ARG:HG2	1.81	0.45
1:A:202:THR:H	1:A:205:GLN:CD	2.16	0.45
1:A:204:GLU:O	1:A:208:THR:N	2.49	0.45
1:A:352:PHE:O	1:A:356:GLN:HB3	2.16	0.45
1:A:312:ASN:O	1:A:316:ARG:CB	2.53	0.45
1:A:334:ARG:NH1	1:A:361:SER:OG	2.50	0.45
1:A:136:TRP:HA	1:A:157:ARG:H	1.81	0.45
1:A:136:TRP:HH2	1:A:180:GLU:CD	2.24	0.45
1:A:208:THR:O	1:A:212:LEU:HD23	2.16	0.45
1:A:388:ASN:C	1:A:390:ALA:N	2.71	0.45
1:A:197:THR:C	1:A:199:ILE:N	2.72	0.45
1:A:377:PHE:CZ	1:A:403:ALA:O	2.69	0.45
1:A:396:ASN:N	1:A:396:ASN:ND2	2.60	0.45
1:A:158:GLU:C	1:A:159:TYR:O	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:HD12	1:A:78:LEU:HA	1.57	0.45
1:A:86:PHE:CE2	1:A:269:ALA:HB2	2.40	0.45
1:A:226:TYR:O	1:A:227:GLN:C	2.59	0.45
1:A:375:GLU:CG	1:A:376:GLU:H	2.30	0.45
1:A:70:GLU:OE2	1:A:70:GLU:CA	2.64	0.45
1:A:202:THR:N	1:A:205:GLN:NE2	2.22	0.45
1:A:116:THR:CG2	1:A:142:TRP:CH2	3.00	0.45
1:A:374:ARG:HH11	1:A:374:ARG:HD3	1.44	0.45
1:A:111:GLN:NE2	1:A:303:ALA:CB	2.73	0.45
1:A:140:PRO:HG2	1:A:140:PRO:O	2.16	0.45
1:A:199:ILE:O	1:A:200:ASP:CB	2.28	0.45
1:A:228:GLY:CA	1:A:233:LEU:HA	2.47	0.45
1:A:348:ARG:NH2	1:A:348:ARG:CG	2.69	0.45
1:A:398:ALA:HB3	1:A:399:PRO:HD2	1.99	0.45
1:A:32:PHE:CD1	1:A:380:TYR:CE1	3.05	0.45
1:A:291:ILE:HG23	1:A:295:TYR:CE2	2.52	0.45
1:A:48:TYR:O	1:A:49:LYS:CB	2.65	0.44
1:A:291:ILE:CG2	1:A:295:TYR:CE2	2.99	0.44
1:A:334:ARG:C	1:A:354:ILE:HG23	2.43	0.44
1:A:204:GLU:CA	1:A:207:GLN:HB2	2.47	0.44
1:A:235:GLU:HA	1:A:238:GLU:CD	2.42	0.44
1:A:334:ARG:HG2	1:A:353:ILE:HG13	1.98	0.44
1:A:363:SER:HB2	1:A:365:LEU:HD21	2.00	0.44
1:A:48:TYR:CE2	1:A:326:MET:HG3	2.51	0.44
1:A:50:ASP:HA	1:A:329:ARG:NH1	2.32	0.44
1:A:108:ARG:HH21	1:A:281:ASP:HA	1.82	0.44
1:A:206:TRP:CE3	1:A:206:TRP:HA	2.51	0.44
1:A:43:LEU:HD23	1:A:387:VAL:CG2	2.47	0.44
1:A:274:ALA:HB3	1:A:280:VAL:CG1	2.48	0.44
1:A:323:LEU:HA	1:A:323:LEU:HD12	1.69	0.44
1:A:136:TRP:CD2	1:A:157:ARG:HB3	2.53	0.44
1:A:247:HIS:HB3	1:A:248:LYS:H	1.26	0.44
1:A:255:SER:HA	1:A:268:GLY:HA3	1.98	0.44
1:A:393:THR:HB	1:A:396:ASN:ND2	2.32	0.44
1:A:192:CYS:SG	1:A:236:ASP:CG	3.01	0.44
1:A:312:ASN:HB3	1:A:315:LEU:CB	2.48	0.44
1:A:108:ARG:NH2	1:A:281:ASP:OD2	2.45	0.44
1:A:178:LEU:HD21	1:A:218:TRP:CZ3	2.53	0.44
1:A:210:ALA:O	1:A:211:GLN:C	2.61	0.44
1:A:394:PRO:CG	1:A:395:ASP:N	2.81	0.44
1:A:404:ILE:CG2	1:A:405:VAL:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLN:HG3	1:A:102:ILE:HD11	1.99	0.44
1:A:112:THR:HA	1:A:113:PRO:HD3	1.80	0.44
1:A:398:ALA:O	1:A:401:CYS:HB3	2.18	0.44
1:A:28:LEU:HD12	1:A:380:TYR:HD2	1.83	0.43
1:A:36:GLU:O	1:A:37:ARG:CB	2.54	0.43
1:A:396:ASN:H	1:A:396:ASN:ND2	2.13	0.43
1:A:26:LEU:O	1:A:29:ALA:N	2.50	0.43
1:A:86:PHE:CD2	1:A:111:GLN:HG3	2.53	0.43
1:A:179:ASN:CA	1:A:216:LYS:HE2	2.48	0.43
1:A:232:GLY:CA	1:A:327:ARG:NH1	2.81	0.43
1:A:287:MET:HE3	1:A:287:MET:HB2	1.83	0.43
1:A:335:GLN:N	1:A:354:ILE:HG23	2.32	0.43
1:A:367:LYS:O	1:A:370:VAL:HB	2.17	0.43
1:A:398:ALA:HB3	1:A:399:PRO:CD	2.48	0.43
1:A:174:LEU:HD11	1:A:209:LEU:HD11	2.00	0.43
1:A:224:PHE:CE2	1:A:227:GLN:HG2	2.53	0.43
1:A:366:THR:O	1:A:367:LYS:C	2.61	0.43
1:A:45:ILE:HG23	1:A:47:VAL:N	2.29	0.43
1:A:195:ASN:ND2	1:A:386:ARG:HD2	2.33	0.43
1:A:200:ASP:O	1:A:200:ASP:OD1	2.36	0.43
1:A:214:VAL:HG12	1:A:215:GLU:N	2.33	0.43
1:A:47:VAL:C	1:A:48:TYR:O	2.59	0.43
1:A:181:ALA:HB1	1:A:182:GLN:H	1.47	0.43
1:A:291:ILE:H	1:A:291:ILE:HG12	1.56	0.43
1:A:18:THR:HG22	1:A:19:ALA:H	1.84	0.43
1:A:225:ALA:O	1:A:226:TYR:HB2	2.18	0.43
1:A:231:ARG:HG3	1:A:236:ASP:CG	2.44	0.43
1:A:94:LEU:C	1:A:96:GLY:N	2.77	0.43
1:A:210:ALA:HB2	1:A:243:PHE:CZ	2.54	0.43
1:A:59:THR:C	1:A:61:VAL:N	2.70	0.43
1:A:202:THR:OG1	1:A:205:GLN:NE2	2.52	0.43
1:A:122:ALA:CB	1:A:251:ILE:HD11	2.48	0.43
1:A:149:PHE:CE2	1:A:188:LEU:HD13	2.54	0.42
1:A:234:GLU:C	1:A:236:ASP:H	2.27	0.42
1:A:174:LEU:C	1:A:176:ASN:H	2.26	0.42
1:A:136:TRP:CH2	1:A:180:GLU:HB3	2.54	0.42
1:A:173:ALA:O	1:A:177:SER:N	2.51	0.42
1:A:337:PHE:HE2	1:A:350:PHE:HD2	1.66	0.42
1:A:122:ALA:HB1	1:A:251:ILE:HD11	2.01	0.42
1:A:149:PHE:HB3	1:A:156:VAL:HG12	2.00	0.42
1:A:329:ARG:HE	1:A:329:ARG:HB3	1.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ARG:HG3	1:A:333:MET:N	2.33	0.42
1:A:26:LEU:C	1:A:28:LEU:N	2.74	0.42
1:A:32:PHE:CD1	1:A:380:TYR:CD1	3.07	0.42
1:A:40:LYS:NZ	1:A:396:ASN:CB	2.82	0.42
1:A:47:VAL:O	1:A:48:TYR:O	2.38	0.42
1:A:91:GLN:HB3	1:A:92:GLU:H	1.53	0.42
1:A:172:ASP:O	1:A:176:ASN:CG	2.61	0.42
1:A:252:VAL:HG13	1:A:271:THR:HG23	2.02	0.42
1:A:371:LEU:O	1:A:374:ARG:HB3	2.20	0.42
1:A:200:ASP:HA	1:A:201:PRO:HD3	1.76	0.42
1:A:260:PHE:CE1	1:A:306:VAL:HG22	2.54	0.42
1:A:377:PHE:HB3	1:A:379:VAL:CG1	2.50	0.42
1:A:30:ASP:O	1:A:31:LEU:C	2.62	0.42
1:A:99:SER:O	1:A:102:ILE:HB	2.19	0.42
1:A:266:ARG:H	1:A:266:ARG:HG2	1.43	0.42
1:A:379:VAL:HG11	1:A:403:ALA:CB	2.49	0.42
1:A:179:ASN:CB	1:A:216:LYS:HE2	2.50	0.42
1:A:334:ARG:HH12	1:A:361:SER:CB	2.32	0.42
1:A:59:THR:HG22	1:A:322:GLU:OE1	2.20	0.41
1:A:83:ILE:HD11	1:A:303:ALA:CB	2.50	0.41
1:A:111:GLN:HB3	1:A:298:PRO:HG3	2.02	0.41
1:A:321:GLN:NE2	1:A:321:GLN:O	2.47	0.41
1:A:398:ALA:CB	1:A:399:PRO:CD	2.98	0.41
1:A:92:GLU:O	1:A:96:GLY:CA	2.67	0.41
1:A:116:THR:CG2	1:A:142:TRP:HH2	2.32	0.41
1:A:162:TYR:CD2	1:A:162:TYR:C	2.98	0.41
1:A:225:ALA:C	1:A:227:GLN:H	2.28	0.41
1:A:227:GLN:HE21	1:A:228:GLY:N	2.18	0.41
1:A:61:VAL:O	1:A:65:GLU:CG	2.68	0.41
1:A:28:LEU:HD12	1:A:380:TYR:CD2	2.55	0.41
1:A:40:LYS:HE2	1:A:400:LEU:CB	2.51	0.41
1:A:85:GLU:HA	1:A:88:ARG:HG3	2.02	0.41
1:A:188:LEU:HD12	1:A:221:LEU:CB	2.50	0.41
1:A:41:ILE:HD12	1:A:41:ILE:HA	1.72	0.41
1:A:198:GLY:O	1:A:356:GLN:C	2.63	0.41
1:A:388:ASN:C	1:A:390:ALA:H	2.29	0.41
1:A:276:ASP:OD1	1:A:279:THR:OG1	2.39	0.41
1:A:40:LYS:C	1:A:40:LYS:NZ	2.60	0.41
1:A:59:THR:C	1:A:61:VAL:H	2.26	0.41
1:A:142:TRP:HA	1:A:143:PRO:HD3	1.84	0.41
1:A:78:LEU:HD22	1:A:300:ALA:CB	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ARG:NH2	1:A:281:ASP:HA	2.36	0.41
1:A:327:ARG:O	1:A:329:ARG:N	2.54	0.41
1:A:356:GLN:OE1	1:A:361:SER:CB	2.69	0.41
1:A:32:PHE:HB2	1:A:380:TYR:CD2	2.55	0.40
1:A:39:GLY:C	1:A:41:ILE:N	2.77	0.40
1:A:351:SER:O	1:A:354:ILE:N	2.54	0.40
1:A:51:GLU:HG3	1:A:329:ARG:NH1	2.36	0.40
1:A:350:PHE:HA	1:A:352:PHE:CE1	2.56	0.40
1:A:350:PHE:HA	1:A:352:PHE:HE1	1.85	0.40
1:A:404:ILE:HG23	1:A:405:VAL:N	2.36	0.40
1:A:231:ARG:NH2	1:A:357:ASN:ND2	2.70	0.40
1:A:276:ASP:HB2	1:A:279:THR:CB	2.51	0.40
1:A:41:ILE:HG23	1:A:42:ASN:C	2.47	0.40
1:A:118:ALA:HA	1:A:121:VAL:HG12	2.04	0.40
1:A:178:LEU:HD12	1:A:178:LEU:HA	1.84	0.40
1:A:250:LEU:HD12	1:A:273:VAL:HG11	2.03	0.40
1:A:40:LYS:HD2	1:A:43:LEU:HD13	2.02	0.40
1:A:43:LEU:O	1:A:381:ALA:HA	2.22	0.40
1:A:152:ALA:C	1:A:154:LEU:N	2.71	0.40
1:A:212:LEU:N	1:A:212:LEU:CD2	2.84	0.40

All (12) 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:14:PHE:CZ	1:A:273:VAL:O[4_566]	1.53	0.67
1:A:55:THR:O	1:A:74:THR:OG1[4_566]	1.61	0.59
1:A:264:ASN:OD1	1:A:300:ALA:CB[4_566]	1.79	0.41
1:A:264:ASN:O	1:A:298:PRO:O[4_566]	1.82	0.38
1:A:120:ARG:NE	1:A:294:ASN:ND2[4_566]	1.91	0.29
1:A:165:GLU:OE2	1:A:282:ARG:NH1[7_645]	1.92	0.28
1:A:116:THR:CG2	1:A:296:SER:OG[4_566]	1.98	0.22
1:A:15:GLU:OE1	1:A:274:ALA:CB[4_566]	2.03	0.17
1:A:13:MET:CB	1:A:366:THR:OG1[6_655]	2.08	0.12
1:A:18:THR:OG1	1:A:129:ASN:ND2[4_566]	2.12	0.08
1:A:120:ARG:CD	1:A:294:ASN:ND2[4_566]	2.15	0.05
1:A:15:GLU:OE2	1:A:249:GLU:CG[4_566]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	394/396 (100%)	249 (63%)	75 (19%)	70 (18%)	0 0

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	ALA
1	A	22	ALA
1	A	27	GLY
1	A	34	ALA
1	A	40	LYS
1	A	41	ILE
1	A	48	TYR
1	A	58	LEU
1	A	59	THR
1	A	60	SER
1	A	73	THR
1	A	75	LYS
1	A	97	LYS
1	A	114	GLY
1	A	129	ASN
1	A	138	SER
1	A	160	ALA
1	A	199	ILE
1	A	200	ASP
1	A	214	VAL
1	A	218	TRP
1	A	222	PHE
1	A	247	HIS
1	A	248	LYS
1	A	258	ALA
1	A	263	TYR
1	A	294	ASN
1	A	300	ALA

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Mol	Chain	Res	Type
1	A	357	ASN
1	A	367	LYS
1	A	375	GLU
1	A	398	ALA
1	A	17	ILE
1	A	29	ALA
1	A	31	LEU
1	A	49	LYS
1	A	115	GLY
1	A	128	LYS
1	A	153	GLY
1	A	180	GLU
1	A	183	ALA
1	A	184	GLY
1	A	191	GLY
1	A	194	HIS
1	A	198	GLY
1	A	233	LEU
1	A	264	ASN
1	A	328	GLN
1	A	344	LYS
1	A	345	GLY
1	A	356	GLN
1	A	368	GLU
1	A	397	MET
1	A	38	PRO
1	A	51	GLU
1	A	74	THR
1	A	159	TYR
1	A	164	ALA
1	A	227	GLN
1	A	297	ASN
1	A	346	ALA
1	A	352	PHE
1	A	77	TYR
1	A	154	LEU
1	A	219	LEU
1	A	80	ILE
1	A	235	GLU
1	A	266	ARG
1	A	366	THR
1	A	44	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	319/319 (100%)	167 (52%)	152 (48%)	0 0

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	MET
1	A	14	PHE
1	A	15	GLU
1	A	17	ILE
1	A	24	PRO
1	A	25	ILE
1	A	26	LEU
1	A	28	LEU
1	A	31	LEU
1	A	33	ARG
1	A	35	ASP
1	A	36	GLU
1	A	40	LYS
1	A	41	ILE
1	A	42	ASN
1	A	43	LEU
1	A	45	ILE
1	A	47	VAL
1	A	51	GLU
1	A	54	LYS
1	A	55	THR
1	A	58	LEU
1	A	61	VAL
1	A	66	GLN
1	A	69	LEU
1	A	71	ASN
1	A	74	THR
1	A	75	LYS
1	A	76	ASN
1	A	80	ILE

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Mol	Chain	Res	Type
1	A	83	ILE
1	A	88	ARG
1	A	89	CYS
1	A	90	THR
1	A	93	LEU
1	A	97	LYS
1	A	99	SER
1	A	101	LEU
1	A	102	ILE
1	A	103	ASN
1	A	109	THR
1	A	111	GLN
1	A	112	THR
1	A	116	THR
1	A	124	ASP
1	A	128	LYS
1	A	132	VAL
1	A	134	ARG
1	A	135	VAL
1	A	136	TRP
1	A	144	ASN
1	A	145	HIS
1	A	146	LYS
1	A	148	VAL
1	A	154	LEU
1	A	157	ARG
1	A	161	TYR
1	A	169	LEU
1	A	170	ASP
1	A	172	ASP
1	A	174	LEU
1	A	177	SER
1	A	179	ASN
1	A	182	GLN
1	A	186	VAL
1	A	189	PHE
1	A	190	HIS
1	A	192	CYS
1	A	193	CYS
1	A	200	ASP
1	A	202	THR
1	A	203	LEU

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Mol	Chain	Res	Type
1	A	204	GLU
1	A	206	TRP
1	A	207	GLN
1	A	209	LEU
1	A	211	GLN
1	A	212	LEU
1	A	213	SER
1	A	215	GLU
1	A	219	LEU
1	A	221	LEU
1	A	224	PHE
1	A	227	GLN
1	A	235	GLU
1	A	236	ASP
1	A	240	LEU
1	A	241	ARG
1	A	243	PHE
1	A	246	MET
1	A	247	HIS
1	A	248	LYS
1	A	250	LEU
1	A	251	ILE
1	A	252	VAL
1	A	254	SER
1	A	255	SER
1	A	259	ASN
1	A	262	LEU
1	A	263	TYR
1	A	265	GLU
1	A	266	ARG
1	A	271	THR
1	A	273	VAL
1	A	277	SER
1	A	280	VAL
1	A	282	ARG
1	A	286	GLN
1	A	291	ILE
1	A	296	SER
1	A	305	VAL
1	A	306	VAL
1	A	310	LEU
1	A	312	ASN

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Mol	Chain	Res	Type
1	A	313	ASP
1	A	315	LEU
1	A	316	ARG
1	A	321	GLN
1	A	322	GLU
1	A	327	ARG
1	A	328	GLN
1	A	329	ARG
1	A	330	ILE
1	A	332	ARG
1	A	334	ARG
1	A	336	LEU
1	A	339	ASN
1	A	347	ASN
1	A	348	ARG
1	A	353	ILE
1	A	354	ILE
1	A	356	GLN
1	A	357	ASN
1	A	362	PHE
1	A	365	LEU
1	A	367	LYS
1	A	369	GLN
1	A	373	LEU
1	A	374	ARG
1	A	375	GLU
1	A	376	GLU
1	A	379	VAL
1	A	382	VAL
1	A	387	VAL
1	A	393	THR
1	A	396	ASN
1	A	397	MET
1	A	400	LEU
1	A	402	GLU
1	A	404	ILE
1	A	407	VAL
1	A	408	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	129	ASN
1	A	144	ASN
1	A	166	ASN
1	A	167	HIS
1	A	190	HIS
1	A	195	ASN
1	A	205	GLN
1	A	207	GLN
1	A	227	GLN
1	A	294	ASN
1	A	297	ASN
1	A	312	ASN
1	A	321	GLN
1	A	331	GLN
1	A	339	ASN
1	A	388	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
2	SO4	A	2	-	4,4,4	0.79	0	6,6,6	1.42	1 (16%)
3	PMP	A	1	-	16,16,16	1.16	3 (18%)	22,23,23	2.38	9 (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
3	PMP	A	1	-	-	6/8/8/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	PMP	C5-C4	-2.41	1.37	1.40
3	A	1	PMP	O3-C3	-2.27	1.31	1.36
3	A	1	PMP	C4A-C4	-2.02	1.44	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	PMP	O2P-P-O1P	4.37	127.84	110.83
3	A	1	PMP	C6-N1-C2	4.11	126.65	119.20
3	A	1	PMP	C3-C2-N1	-3.99	115.92	120.96
3	A	1	PMP	O4P-C5A-C5	3.73	116.35	109.36
3	A	1	PMP	C5-C6-N1	-3.35	118.38	123.83
3	A	1	PMP	C3-C4-C5	3.24	121.67	118.73
3	A	1	PMP	C5A-C5-C6	-2.49	115.31	119.36
2	A	2	SO4	O3-S-O2	2.40	122.08	109.56
3	A	1	PMP	O3P-P-O4P	2.29	112.63	106.67
3	A	1	PMP	O2P-P-O4P	-2.25	100.81	106.67

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	PMP	C3-C4-C4A-N4A
3	A	1	PMP	C5-C4-C4A-N4A
3	A	1	PMP	C4-C5-C5A-O4P
3	A	1	PMP	C6-C5-C5A-O4P

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Mol	Chain	Res	Type	Atoms
3	A	1	PMP	C5A-O4P-P-O2P
3	A	1	PMP	C5A-O4P-P-O3P

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	PMP	5	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.