



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 04:48 AM UTC

PDB ID : 3IZP / pdb_00003izp
Title : Conformation of EF-G during translocation
Authors : Li, W.; Trabuco, L.G.; Schulten, K.; Frank, J.
Deposited on : 2010-11-15
Resolution : Not provided
Based on initial model : 1FNM

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB entry.

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

A user guide is available at

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

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
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

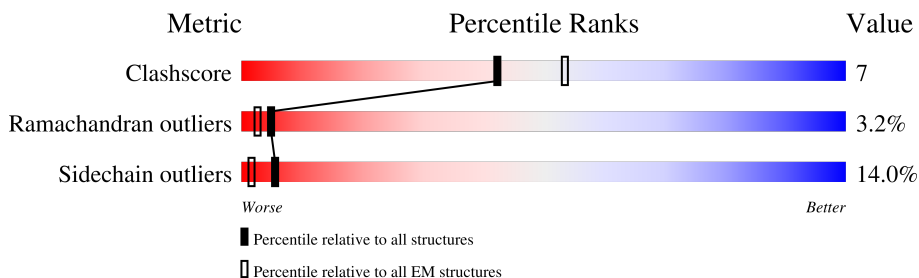
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	E	688	35% 44% 18% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5382 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E	688	5382	3416	920	1025	21	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	573	ALA	HIS	conflict	UNP P13551

4 Data and refinement statistics

Xtrriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – (Not available)	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-(Not available))	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5382	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	E	2.17	171/5482 (3.1%)	2.54	421/7421 (5.7%)

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	E	0	51

All (171) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	553	GLY	C-N	-10.33	1.25	1.33
1	E	600	VAL	N-CA	-9.65	1.34	1.46
1	E	343	ASN	CA-CB	9.25	1.65	1.53
1	E	463	VAL	CA-C	-8.69	1.42	1.52
1	E	612	THR	CA-CB	8.68	1.64	1.53
1	E	243	VAL	CA-CB	-8.35	1.44	1.54
1	E	469	GLU	N-CA	-8.30	1.36	1.46
1	E	485	GLU	N-CA	8.23	1.55	1.45
1	E	465	ARG	CD-NE	8.18	1.57	1.46
1	E	87	HIS	ND1-CE1	7.93	1.40	1.32
1	E	455	GLY	CA-C	-7.91	1.44	1.51
1	E	125	ALA	CA-C	-7.78	1.42	1.52
1	E	123	ARG	CD-NE	7.70	1.57	1.46
1	E	237	PRO	N-CD	-7.59	1.37	1.47
1	E	150	ILE	CA-CB	-7.47	1.45	1.54
1	E	4	LYS	N-CA	-7.45	1.37	1.46
1	E	237	PRO	CA-C	-7.43	1.44	1.52
1	E	19	ALA	CA-C	7.35	1.61	1.52
1	E	677	GLN	CA-C	-7.32	1.43	1.52
1	E	484	ARG	CA-C	-7.29	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	152	THR	CA-C	-7.28	1.43	1.52
1	E	179	ASP	N-CA	-7.24	1.37	1.46
1	E	517	LEU	CA-C	7.20	1.60	1.52
1	E	470	PHE	CA-C	-7.17	1.43	1.52
1	E	105	ILE	C-N	7.06	1.42	1.33
1	E	167	PRO	N-CA	-7.06	1.40	1.46
1	E	186	TYR	N-CA	-7.05	1.37	1.46
1	E	459	LEU	CA-CB	7.03	1.64	1.53
1	E	539	ILE	N-CA	6.89	1.55	1.46
1	E	484	ARG	CD-NE	6.88	1.55	1.46
1	E	359	HIS	ND1-CE1	6.84	1.39	1.32
1	E	430	ARG	CA-CB	6.83	1.64	1.53
1	E	451	ILE	N-CA	-6.83	1.38	1.46
1	E	674	ASP	CA-C	-6.77	1.45	1.52
1	E	598	ASP	C-O	-6.75	1.20	1.23
1	E	440	VAL	C-N	6.72	1.41	1.33
1	E	349	LYS	CA-CB	-6.69	1.43	1.53
1	E	494	GLU	CA-C	-6.57	1.44	1.52
1	E	111	SER	C-N	6.55	1.42	1.33
1	E	302	HIS	ND1-CE1	6.51	1.39	1.32
1	E	504	ARG	NE-CZ	6.46	1.40	1.33
1	E	626	ALA	N-CA	-6.43	1.38	1.46
1	E	467	LYS	CA-C	-6.41	1.44	1.52
1	E	565	VAL	CA-C	-6.38	1.44	1.52
1	E	242	LEU	CA-CB	6.37	1.63	1.53
1	E	123	ARG	CA-C	6.35	1.61	1.52
1	E	628	ARG	CA-CB	6.34	1.62	1.53
1	E	31	ARG	N-CA	-6.31	1.37	1.46
1	E	668	SER	C-N	6.30	1.41	1.33
1	E	329	ARG	CA-C	6.29	1.60	1.52
1	E	682	GLN	C-N	6.29	1.41	1.33
1	E	242	LEU	C-N	6.25	1.41	1.33
1	E	90	PHE	N-CA	-6.25	1.38	1.46
1	E	190	ASN	N-CA	-6.25	1.38	1.46
1	E	104	ALA	C-O	-6.24	1.16	1.24
1	E	28	THR	CA-C	6.24	1.61	1.52
1	E	181	LEU	CA-C	-6.20	1.44	1.52
1	E	513	LYS	N-CA	-6.19	1.38	1.46
1	E	132	ARG	CD-NE	6.16	1.54	1.46
1	E	227	ILE	CA-C	-6.15	1.44	1.52
1	E	660	ARG	N-CA	6.13	1.54	1.46
1	E	348	ARG	N-CA	6.12	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	129	LYS	CA-C	6.12	1.60	1.52
1	E	471	LYS	CA-CB	6.12	1.62	1.53
1	E	126	GLU	CA-C	-6.11	1.45	1.52
1	E	107	VAL	CA-CB	6.09	1.61	1.54
1	E	330	VAL	N-CA	-6.08	1.38	1.46
1	E	535	PRO	CA-CB	6.07	1.62	1.53
1	E	145	ASP	CA-C	-6.06	1.45	1.52
1	E	326	THR	N-CA	-6.06	1.38	1.46
1	E	672	PHE	CA-C	-6.02	1.45	1.52
1	E	554	PRO	C-O	-6.01	1.17	1.23
1	E	672	PHE	C-N	6.00	1.41	1.33
1	E	506	GLN	N-CA	5.99	1.53	1.46
1	E	42	ILE	CA-C	-5.99	1.46	1.52
1	E	420	ASP	C-N	5.99	1.42	1.33
1	E	164	MET	CA-CB	5.95	1.64	1.53
1	E	213	HIS	CA-C	-5.93	1.45	1.52
1	E	36	THR	N-CA	5.92	1.53	1.46
1	E	441	SER	N-CA	-5.86	1.38	1.46
1	E	9	LEU	CA-C	-5.86	1.44	1.52
1	E	173	THR	CA-C	-5.85	1.45	1.52
1	E	267	LYS	N-CA	-5.85	1.39	1.46
1	E	56	GLU	N-CA	-5.85	1.39	1.46
1	E	70	THR	CA-C	-5.85	1.45	1.52
1	E	468	ARG	NE-CZ	5.84	1.39	1.33
1	E	676	TYR	CB-CG	-5.83	1.38	1.51
1	E	575	VAL	N-CA	5.81	1.53	1.46
1	E	594	VAL	N-CA	5.80	1.53	1.46
1	E	475	ASN	N-CA	-5.77	1.39	1.46
1	E	456	GLU	N-CA	-5.76	1.39	1.46
1	E	286	ILE	CA-C	5.75	1.58	1.52
1	E	341	VAL	N-CA	-5.70	1.39	1.46
1	E	373	ASP	N-CA	-5.70	1.38	1.45
1	E	509	HIS	CB-CG	-5.67	1.42	1.50
1	E	227	ILE	N-CA	-5.66	1.39	1.46
1	E	666	ARG	CD-NE	5.66	1.54	1.46
1	E	551	GLN	C-N	-5.65	1.25	1.33
1	E	436	PRO	N-CA	-5.64	1.41	1.47
1	E	659	LEU	C-N	5.61	1.41	1.33
1	E	555	LEU	CA-C	-5.61	1.49	1.52
1	E	286	ILE	N-CA	-5.58	1.39	1.46
1	E	335	LEU	N-CA	-5.58	1.39	1.46
1	E	472	VAL	CA-C	5.58	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	449	THR	CA-C	-5.57	1.45	1.52
1	E	605	ILE	CA-C	-5.57	1.45	1.52
1	E	389	LEU	N-CA	-5.56	1.39	1.46
1	E	222	ASP	C-N	5.54	1.42	1.33
1	E	199	ILE	N-CA	-5.54	1.39	1.46
1	E	515	GLU	CA-CB	5.53	1.62	1.54
1	E	303	PRO	CA-CB	-5.51	1.46	1.53
1	E	420	ASP	C-O	-5.48	1.17	1.24
1	E	327	PHE	N-CA	5.47	1.52	1.46
1	E	151	ARG	CD-NE	5.46	1.53	1.46
1	E	439	ARG	N-CA	-5.45	1.39	1.46
1	E	322	VAL	C-N	5.43	1.40	1.32
1	E	171	GLU	C-N	-5.42	1.26	1.33
1	E	111	SER	N-CA	5.41	1.53	1.46
1	E	618	GLY	C-N	-5.40	1.26	1.33
1	E	12	LEU	CA-CB	5.40	1.62	1.53
1	E	17	ILE	C-O	5.39	1.30	1.24
1	E	577	SER	C-N	5.38	1.40	1.33
1	E	439	ARG	NE-CZ	5.38	1.39	1.33
1	E	14	ASN	N-CA	-5.37	1.39	1.46
1	E	270	GLN	CA-CB	5.37	1.61	1.53
1	E	160	ARG	CD-NE	5.34	1.53	1.46
1	E	405	PRO	N-CA	5.33	1.54	1.47
1	E	462	ILE	CA-C	-5.33	1.46	1.52
1	E	256	THR	C-O	-5.32	1.19	1.24
1	E	511	LYS	CA-C	-5.32	1.46	1.53
1	E	69	VAL	CA-C	-5.31	1.46	1.52
1	E	126	GLU	C-N	5.30	1.40	1.33
1	E	423	LYS	N-CA	5.30	1.53	1.46
1	E	278	ASP	N-CA	-5.30	1.39	1.46
1	E	513	LYS	C-N	5.29	1.40	1.33
1	E	36	THR	CA-C	-5.27	1.45	1.52
1	E	255	ILE	CA-C	-5.27	1.46	1.52
1	E	98	MET	CA-CB	5.27	1.62	1.53
1	E	677	GLN	N-CA	-5.25	1.39	1.45
1	E	373	ASP	CA-C	5.25	1.59	1.52
1	E	555	LEU	CA-CB	5.25	1.60	1.53
1	E	178	ILE	CA-CB	-5.24	1.47	1.54
1	E	363	ARG	CA-C	5.24	1.59	1.52
1	E	428	LEU	C-O	-5.23	1.18	1.24
1	E	163	VAL	N-CA	5.22	1.52	1.46
1	E	209	ALA	C-O	-5.21	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	617	MET	CA-C	-5.21	1.46	1.52
1	E	397	VAL	C-O	-5.20	1.17	1.24
1	E	149	VAL	CA-C	5.20	1.59	1.52
1	E	607	ARG	CD-NE	5.20	1.53	1.46
1	E	41	LYS	C-O	5.20	1.29	1.24
1	E	92	ILE	N-CA	5.20	1.52	1.46
1	E	559	PRO	N-CD	-5.20	1.40	1.47
1	E	58	GLU	N-CA	5.19	1.52	1.46
1	E	7	TYR	C-N	5.18	1.41	1.34
1	E	166	LEU	CA-C	5.17	1.59	1.52
1	E	210	ARG	NE-CZ	5.15	1.38	1.33
1	E	342	TYR	CA-CB	5.14	1.60	1.53
1	E	93	GLU	C-N	5.13	1.40	1.33
1	E	465	ARG	CA-CB	-5.13	1.45	1.53
1	E	474	ALA	N-CA	-5.13	1.39	1.46
1	E	448	GLN	CA-CB	5.12	1.61	1.53
1	E	534	ILE	C-N	-5.10	1.27	1.33
1	E	443	HIS	C-N	-5.08	1.29	1.34
1	E	355	LEU	C-O	-5.05	1.18	1.24
1	E	527	ASN	C-N	5.03	1.40	1.33
1	E	334	THR	N-CA	5.02	1.52	1.46
1	E	669	PHE	CA-CB	5.02	1.62	1.53
1	E	175	SER	CA-C	5.01	1.58	1.52
1	E	308	PRO	CA-C	-5.01	1.45	1.52
1	E	362	HIS	ND1-CE1	5.01	1.37	1.32

All (421) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	373	ASP	CA-CB-CG	12.07	124.67	112.60
1	E	248	LYS	CA-C-N	11.81	133.05	119.94
1	E	248	LYS	C-N-CA	11.81	133.05	119.94
1	E	14	ASN	CA-CB-CG	-11.41	101.19	112.60
1	E	40	HIS	CA-CB-CG	11.38	125.19	113.80
1	E	438	PHE	CA-CB-CG	10.83	124.63	113.80
1	E	7	TYR	CB-CG-CD1	10.71	136.86	120.80
1	E	46	HIS	CA-CB-CG	-10.21	103.59	113.80
1	E	598	ASP	CA-CB-CG	-10.05	102.55	112.60
1	E	117	GLN	CA-C-N	9.99	133.43	120.44
1	E	117	GLN	C-N-CA	9.99	133.43	120.44
1	E	609	GLU	CA-C-N	9.87	135.19	122.95
1	E	609	GLU	C-N-CA	9.87	135.19	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	88	VAL	N-CA-C	-9.33	104.39	113.53
1	E	152	THR	N-CA-CB	9.28	124.67	110.28
1	E	61	ARG	NE-CZ-NH2	9.19	127.47	119.20
1	E	126	GLU	N-CA-CB	9.07	123.23	110.07
1	E	4	LYS	N-CA-C	9.03	122.09	111.71
1	E	422	GLU	CA-C-O	9.00	130.27	120.82
1	E	293	THR	O-C-N	-8.85	112.22	121.60
1	E	365	GLU	N-CA-C	8.74	123.66	109.76
1	E	276	VAL	N-CA-C	8.58	119.37	110.36
1	E	686	LYS	N-CA-C	-8.58	100.94	111.40
1	E	26	THR	CA-C-O	8.52	129.77	119.97
1	E	231	TYR	CA-C-N	8.44	131.58	120.28
1	E	231	TYR	C-N-CA	8.44	131.58	120.28
1	E	272	LEU	CA-C-N	8.30	132.24	120.28
1	E	272	LEU	C-N-CA	8.30	132.24	120.28
1	E	427	ALA	N-CA-C	8.24	121.30	111.33
1	E	582	PHE	CA-CB-CG	-8.16	105.64	113.80
1	E	132	ARG	NE-CZ-NH1	8.10	129.60	121.50
1	E	655	TYR	N-CA-C	8.05	120.14	111.36
1	E	89	ASP	CA-CB-CG	-7.96	104.64	112.60
1	E	464	ASP	CA-C-N	7.93	131.25	120.38
1	E	464	ASP	C-N-CA	7.93	131.25	120.38
1	E	443	HIS	ND1-CE1-NE2	7.87	116.27	108.40
1	E	586	GLY	CA-C-O	7.82	128.95	120.66
1	E	344	THR	N-CA-C	7.77	119.38	111.07
1	E	206	LEU	N-CA-C	7.76	120.43	111.11
1	E	121	VAL	N-CA-CB	7.76	121.10	110.54
1	E	4	LYS	CA-C-N	7.75	130.60	120.60
1	E	4	LYS	C-N-CA	7.75	130.60	120.60
1	E	615	GLU	CB-CA-C	7.74	123.38	109.29
1	E	236	GLU	CA-C-N	7.71	127.75	119.89
1	E	236	GLU	C-N-CA	7.71	127.75	119.89
1	E	149	VAL	CA-C-O	7.70	129.01	120.85
1	E	408	VAL	O-C-N	-7.63	113.03	122.57
1	E	527	ASN	CA-CB-CG	7.63	120.23	112.60
1	E	610	VAL	N-CA-C	7.61	118.45	106.88
1	E	678	GLU	CA-C-N	7.58	134.95	119.72
1	E	678	GLU	C-N-CA	7.58	134.95	119.72
1	E	316	ILE	N-CA-C	7.57	119.05	107.99
1	E	157	LEU	N-CA-C	-7.54	104.10	113.38
1	E	390	VAL	CA-C-O	-7.49	114.30	121.64
1	E	587	SER	CA-C-N	7.36	130.01	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	587	SER	C-N-CA	7.36	130.01	120.44
1	E	685	GLU	CA-C-N	7.34	132.97	120.71
1	E	685	GLU	C-N-CA	7.34	132.97	120.71
1	E	343	ASN	CA-C-O	-7.30	112.94	120.54
1	E	581	ALA	CA-C-N	7.29	130.65	120.29
1	E	581	ALA	C-N-CA	7.29	130.65	120.29
1	E	562	ASP	CA-CB-CG	-7.29	105.31	112.60
1	E	456	GLU	CA-C-N	7.28	130.53	120.63
1	E	456	GLU	C-N-CA	7.28	130.53	120.63
1	E	443	HIS	CE1-NE2-CD2	-7.24	101.76	109.00
1	E	149	VAL	O-C-N	-7.24	114.37	121.83
1	E	87	HIS	CE1-NE2-CD2	-7.19	101.81	109.00
1	E	30	GLU	O-C-N	-7.19	113.47	122.17
1	E	427	ALA	CB-CA-C	-7.17	98.48	110.68
1	E	654	GLY	O-C-N	-7.16	112.58	122.68
1	E	61	ARG	CA-C-O	7.10	128.01	119.78
1	E	207	ASP	O-C-N	-7.08	114.07	122.15
1	E	627	ARG	CG-CD-NE	-7.06	96.47	112.00
1	E	132	ARG	NE-CZ-NH2	-7.05	112.86	119.20
1	E	390	VAL	N-CA-C	-7.04	98.45	108.65
1	E	124	GLN	CA-C-N	7.02	129.69	120.28
1	E	124	GLN	C-N-CA	7.02	129.69	120.28
1	E	513	LYS	N-CA-CB	7.00	121.58	110.65
1	E	26	THR	N-CA-C	7.00	119.94	111.82
1	E	122	TRP	CA-CB-CG	7.00	126.89	113.60
1	E	391	GLY	CA-C-N	6.99	129.96	120.38
1	E	391	GLY	C-N-CA	6.99	129.96	120.38
1	E	610	VAL	CA-C-O	-6.93	112.72	120.97
1	E	70	THR	O-C-N	-6.89	114.96	123.44
1	E	446	THR	N-CA-C	-6.86	105.04	113.41
1	E	370	LYS	N-CA-CB	-6.86	98.90	110.49
1	E	678	GLU	N-CA-C	6.86	120.25	109.96
1	E	53	ASP	N-CA-C	6.85	120.12	111.69
1	E	368	GLU	CA-C-O	6.84	128.65	121.06
1	E	568	TYR	N-CA-C	6.83	123.12	114.31
1	E	634	MET	CG-SD-CE	-6.79	85.97	100.90
1	E	7	TYR	CB-CG-CD2	-6.78	110.62	120.80
1	E	216	LEU	CA-C-O	-6.78	113.23	120.42
1	E	473	ASP	CA-C-O	6.78	127.55	120.30
1	E	444	PRO	CA-C-N	6.78	129.25	120.44
1	E	444	PRO	C-N-CA	6.78	129.25	120.44
1	E	655	TYR	CA-C-N	6.76	130.96	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	655	TYR	C-N-CA	6.76	130.96	120.82
1	E	612	THR	O-C-N	-6.76	117.39	121.71
1	E	682	GLN	CA-C-N	6.75	129.07	120.56
1	E	682	GLN	C-N-CA	6.75	129.07	120.56
1	E	211	GLU	N-CA-C	-6.74	103.94	111.28
1	E	62	GLY	CA-C-N	6.71	134.04	121.97
1	E	62	GLY	C-N-CA	6.71	134.04	121.97
1	E	440	VAL	O-C-N	-6.70	115.99	123.03
1	E	54	PHE	CA-C-N	6.70	129.80	120.29
1	E	54	PHE	C-N-CA	6.70	129.80	120.29
1	E	521	SER	CB-CA-C	-6.67	99.52	110.85
1	E	300	GLU	CA-C-N	6.66	130.17	120.91
1	E	300	GLU	C-N-CA	6.66	130.17	120.91
1	E	146	LEU	CA-C-O	6.66	127.62	120.10
1	E	164	MET	N-CA-CB	-6.64	100.66	110.49
1	E	650	ALA	N-CA-C	6.64	120.83	112.87
1	E	215	LYS	N-CA-CB	6.63	119.87	110.12
1	E	542	VAL	CA-C-N	6.62	131.90	120.58
1	E	542	VAL	C-N-CA	6.62	131.90	120.58
1	E	172	ASP	CA-CB-CG	6.61	119.21	112.60
1	E	135	PHE	CA-CB-CG	6.59	120.39	113.80
1	E	636	PRO	N-CA-C	6.59	121.68	111.21
1	E	603	GLU	O-C-N	-6.58	115.18	121.57
1	E	682	GLN	CB-CA-C	6.56	121.19	110.88
1	E	483	TYR	CA-C-N	6.54	133.43	121.85
1	E	483	TYR	C-N-CA	6.54	133.43	121.85
1	E	160	ARG	CD-NE-CZ	-6.53	115.26	124.40
1	E	356	LEU	CA-C-N	-6.53	113.99	123.00
1	E	356	LEU	C-N-CA	-6.53	113.99	123.00
1	E	686	LYS	N-CA-CB	6.53	119.79	110.13
1	E	20	HIS	N-CA-C	-6.51	100.11	109.29
1	E	473	ASP	O-C-N	-6.50	115.73	123.27
1	E	95	GLU	CB-CA-C	-6.50	99.80	110.85
1	E	368	GLU	O-C-N	-6.48	117.58	123.41
1	E	534	ILE	N-CA-CB	6.47	120.27	111.21
1	E	20	HIS	CE1-NE2-CD2	-6.46	102.54	109.00
1	E	191	ASP	O-C-N	6.45	131.07	122.43
1	E	262	SER	N-CA-CB	6.44	121.37	110.49
1	E	282	SER	CA-C-O	-6.42	113.97	120.96
1	E	241	GLU	CA-C-N	6.40	128.76	120.44
1	E	241	GLU	C-N-CA	6.40	128.76	120.44
1	E	371	ALA	CB-CA-C	-6.39	100.65	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	348	ARG	NE-CZ-NH1	6.38	127.88	121.50
1	E	13	ARG	NH1-CZ-NH2	-6.36	111.03	119.30
1	E	472	VAL	CA-C-N	6.36	131.96	123.00
1	E	472	VAL	C-N-CA	6.36	131.96	123.00
1	E	470	PHE	N-CA-C	6.34	118.27	111.36
1	E	57	GLN	CG-CD-NE2	-6.33	106.90	116.40
1	E	273	LEU	O-C-N	-6.33	114.81	122.22
1	E	97	SER	N-CA-C	6.32	118.17	111.28
1	E	557	GLY	N-CA-C	-6.31	105.66	116.01
1	E	383	THR	N-CA-C	6.31	119.37	110.23
1	E	122	TRP	N-CA-C	6.30	117.81	111.07
1	E	580	MET	CA-C-N	6.30	128.72	120.28
1	E	580	MET	C-N-CA	6.30	128.72	120.28
1	E	214	GLU	CA-C-N	6.29	128.70	120.28
1	E	214	GLU	C-N-CA	6.29	128.70	120.28
1	E	291	GLY	N-CA-C	-6.28	101.60	110.96
1	E	180	VAL	CA-CB-CG1	-6.26	99.75	110.40
1	E	160	ARG	O-C-N	-6.22	113.90	120.68
1	E	314	PHE	O-C-N	-6.22	115.06	122.27
1	E	534	ILE	CA-CB-CG1	6.20	120.94	110.40
1	E	252	ASP	CA-CB-CG	6.20	118.80	112.60
1	E	590	ILE	CB-CA-C	-6.20	103.67	112.22
1	E	54	PHE	CB-CA-C	6.17	121.03	111.28
1	E	419	ALA	CA-C-N	6.17	129.69	120.31
1	E	419	ALA	C-N-CA	6.17	129.69	120.31
1	E	422	GLU	O-C-N	-6.16	115.72	122.07
1	E	558	PHE	N-CA-CB	-6.16	101.72	110.04
1	E	402	ILE	N-CA-C	6.15	122.13	109.34
1	E	463	VAL	CB-CA-C	6.14	119.74	111.88
1	E	310	ALA	CB-CA-C	6.13	119.19	110.24
1	E	582	PHE	CA-C-O	6.09	126.87	120.42
1	E	625	ASN	OD1-CG-ND2	-6.08	116.52	122.60
1	E	607	ARG	CA-C-N	6.08	131.03	123.12
1	E	607	ARG	C-N-CA	6.08	131.03	123.12
1	E	435	ASP	CA-C-N	6.07	128.03	121.00
1	E	435	ASP	C-N-CA	6.07	128.03	121.00
1	E	277	VAL	N-CA-CB	6.05	119.65	110.58
1	E	660	ARG	CA-C-O	6.05	126.81	119.49
1	E	582	PHE	O-C-N	-6.04	115.27	122.15
1	E	55	MET	N-CA-C	6.03	117.93	111.36
1	E	267	LYS	N-CA-C	6.02	118.58	108.23
1	E	648	PRO	CA-C-O	-6.02	114.17	121.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	165	GLN	O-C-N	-6.01	117.51	123.46
1	E	426	GLN	CB-CA-C	6.01	120.27	110.95
1	E	675	HIS	ND1-CE1-NE2	6.00	114.40	108.40
1	E	63	ILE	CA-C-N	5.99	132.97	121.54
1	E	63	ILE	C-N-CA	5.99	132.97	121.54
1	E	212	TYR	CA-CB-CG	-5.98	103.13	113.90
1	E	21	ILE	CA-CB-CG2	-5.98	100.33	110.50
1	E	644	ARG	NE-CZ-NH2	-5.98	113.82	119.20
1	E	519	ARG	N-CA-C	5.97	118.92	110.50
1	E	224	ASP	O-C-N	-5.97	115.16	123.34
1	E	213	HIS	N-CA-C	-5.97	104.86	111.36
1	E	190	ASN	CA-C-N	5.97	130.69	120.72
1	E	190	ASN	C-N-CA	5.97	130.69	120.72
1	E	65	ILE	CA-C-N	5.96	132.93	121.54
1	E	65	ILE	C-N-CA	5.96	132.93	121.54
1	E	395	PRO	N-CA-CB	-5.96	97.79	103.33
1	E	378	VAL	CA-CB-CG1	5.95	120.51	110.40
1	E	587	SER	N-CA-CB	5.94	118.63	110.01
1	E	436	PRO	N-CA-C	-5.94	107.85	114.92
1	E	293	THR	CA-C-N	5.93	125.61	119.56
1	E	293	THR	C-N-CA	5.93	125.61	119.56
1	E	635	GLU	O-C-N	-5.93	113.23	121.12
1	E	99	ARG	O-C-N	-5.92	115.84	122.12
1	E	417	THR	CA-C-N	5.91	132.83	121.54
1	E	417	THR	C-N-CA	5.91	132.83	121.54
1	E	17	ILE	O-C-N	-5.91	115.17	122.97
1	E	27	THR	OG1-CB-CG2	-5.89	97.51	109.30
1	E	558	PHE	CB-CA-C	5.89	117.94	109.11
1	E	540	PRO	CB-CA-C	5.88	122.33	112.62
1	E	351	ARG	CB-CA-C	-5.87	101.38	110.78
1	E	646	PHE	CA-C-O	-5.87	113.86	120.32
1	E	6	GLU	CB-CA-C	5.87	119.50	109.24
1	E	305	PRO	CA-C-N	5.86	128.62	120.29
1	E	305	PRO	C-N-CA	5.86	128.62	120.29
1	E	417	THR	N-CA-CB	5.86	119.26	110.53
1	E	424	LEU	O-C-N	-5.86	115.08	122.17
1	E	577	SER	N-CA-CB	5.85	118.60	110.17
1	E	21	ILE	CA-CB-CG1	5.85	120.34	110.40
1	E	554	PRO	CB-CA-C	-5.84	103.45	110.00
1	E	59	ARG	N-CA-C	5.84	117.34	110.97
1	E	570	GLY	CA-C-O	-5.84	114.19	121.02
1	E	396	ARG	NE-CZ-NH2	-5.83	113.95	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	122	TRP	N-CA-CB	5.83	118.46	110.01
1	E	538	TYR	CB-CG-CD1	5.83	129.54	120.80
1	E	77	HIS	CB-CG-CD2	-5.81	123.64	131.20
1	E	98	MET	CA-C-O	5.81	126.65	119.97
1	E	615	GLU	CA-C-O	5.81	125.53	119.14
1	E	455	GLY	CA-C-N	5.80	128.33	120.38
1	E	455	GLY	C-N-CA	5.80	128.33	120.38
1	E	300	GLU	N-CA-C	5.80	117.75	108.41
1	E	475	ASN	CA-C-N	-5.80	115.48	122.90
1	E	475	ASN	C-N-CA	-5.80	115.48	122.90
1	E	683	VAL	N-CA-CB	5.80	117.33	110.55
1	E	454	MET	CG-SD-CE	5.79	113.65	100.90
1	E	608	VAL	N-CA-C	5.79	116.20	107.80
1	E	397	VAL	CA-C-N	5.79	129.61	122.37
1	E	397	VAL	C-N-CA	5.79	129.61	122.37
1	E	568	TYR	CB-CG-CD2	-5.79	112.12	120.80
1	E	501	THR	O-C-N	-5.76	116.67	123.41
1	E	182	ARG	CA-C-O	5.76	126.25	119.28
1	E	393	ASP	N-CA-C	5.75	120.30	113.28
1	E	107	VAL	N-CA-C	5.75	116.58	108.36
1	E	683	VAL	CA-C-N	5.74	128.77	120.79
1	E	683	VAL	C-N-CA	5.74	128.77	120.79
1	E	369	LEU	N-CA-CB	-5.74	100.87	110.80
1	E	299	VAL	CB-CA-C	5.73	121.90	111.30
1	E	657	THR	N-CA-CB	5.72	118.36	110.07
1	E	321	TYR	N-CA-CB	5.71	120.14	110.49
1	E	38	ARG	NE-CZ-NH1	-5.70	115.80	121.50
1	E	359	HIS	CA-C-N	5.70	127.92	120.28
1	E	359	HIS	C-N-CA	5.70	127.92	120.28
1	E	430	ARG	CB-CA-C	-5.70	102.19	110.96
1	E	143	GLY	N-CA-C	-5.69	107.46	115.32
1	E	51	THR	N-CA-CB	5.69	118.87	109.88
1	E	133	ILE	N-CA-CB	5.69	120.49	112.52
1	E	28	THR	N-CA-C	5.68	118.68	111.69
1	E	190	ASN	CA-C-O	5.68	128.64	120.51
1	E	376	ALA	O-C-N	-5.67	116.55	123.30
1	E	137	ASN	CA-CB-CG	-5.66	106.94	112.60
1	E	306	ASN	CA-CB-CG	-5.65	106.95	112.60
1	E	530	VAL	CA-CB-CG1	5.64	119.99	110.40
1	E	675	HIS	CB-CA-C	-5.63	100.13	111.17
1	E	669	PHE	CA-C-O	-5.63	114.91	121.10
1	E	610	VAL	CB-CA-C	-5.61	104.12	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	302	HIS	CA-C-O	-5.61	115.11	119.99
1	E	609	GLU	N-CA-C	5.60	117.90	107.99
1	E	152	THR	O-C-N	-5.59	115.39	122.27
1	E	153	MET	CG-SD-CE	-5.59	88.60	100.90
1	E	422	GLU	CA-C-N	-5.59	112.26	122.38
1	E	422	GLU	C-N-CA	-5.59	112.26	122.38
1	E	207	ASP	CA-CB-CG	-5.58	107.02	112.60
1	E	383	THR	CA-C-N	5.57	130.47	122.45
1	E	383	THR	C-N-CA	5.57	130.47	122.45
1	E	331	TYR	N-CA-CB	5.57	118.94	110.42
1	E	509	HIS	N-CA-CB	-5.55	101.72	110.77
1	E	38	ARG	N-CA-C	5.55	119.09	111.54
1	E	137	ASN	CB-CA-C	5.55	119.54	109.83
1	E	285	ASP	CA-C-N	5.54	132.39	122.13
1	E	285	ASP	C-N-CA	5.54	132.39	122.13
1	E	652	MET	CG-SD-CE	-5.53	88.73	100.90
1	E	171	GLU	CA-C-N	5.53	130.89	122.37
1	E	171	GLU	C-N-CA	5.53	130.89	122.37
1	E	462	ILE	CA-C-N	5.53	127.73	120.60
1	E	462	ILE	C-N-CA	5.53	127.73	120.60
1	E	620	VAL	CB-CA-C	5.53	121.17	112.16
1	E	592	GLU	CB-CA-C	5.53	119.56	110.88
1	E	247	ARG	O-C-N	5.53	127.76	122.07
1	E	687	LEU	CA-C-N	5.52	131.64	121.70
1	E	687	LEU	C-N-CA	5.52	131.64	121.70
1	E	483	TYR	N-CA-C	5.52	117.64	109.69
1	E	493	VAL	N-CA-C	5.51	116.84	108.80
1	E	568	TYR	CB-CA-C	5.51	118.28	109.02
1	E	239	GLU	CA-CB-CG	-5.51	103.09	114.10
1	E	46	HIS	ND1-CE1-NE2	5.50	113.90	108.40
1	E	397	VAL	N-CA-C	5.49	118.32	110.09
1	E	208	GLN	N-CA-CB	5.48	118.28	110.16
1	E	596	LYS	N-CA-C	-5.48	106.44	113.23
1	E	306	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	E	328	ILE	CB-CA-C	-5.47	101.94	110.69
1	E	128	TYR	CA-CB-CG	-5.47	104.05	113.90
1	E	498	ILE	CA-C-N	5.47	131.53	121.85
1	E	498	ILE	C-N-CA	5.47	131.53	121.85
1	E	276	VAL	CA-C-O	5.47	126.96	121.27
1	E	20	HIS	ND1-CE1-NE2	5.46	113.86	108.40
1	E	40	HIS	ND1-CE1-NE2	5.46	113.86	108.40
1	E	323	GLY	CA-C-O	5.46	127.46	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	232	LEU	CA-C-N	5.46	127.53	120.44
1	E	232	LEU	C-N-CA	5.46	127.53	120.44
1	E	314	PHE	CA-CB-CG	5.46	119.26	113.80
1	E	29	THR	N-CA-C	5.45	118.14	111.82
1	E	216	LEU	CB-CA-C	5.45	120.11	110.85
1	E	44	GLU	CB-CA-C	-5.44	100.24	109.38
1	E	440	VAL	N-CA-C	-5.44	100.47	108.85
1	E	309	LEU	N-CA-C	5.43	118.16	110.50
1	E	390	VAL	N-CA-CB	5.43	120.44	112.35
1	E	49	ALA	CB-CA-C	-5.42	102.37	110.50
1	E	339	SER	N-CA-C	5.42	115.40	108.24
1	E	432	ALA	N-CA-C	5.41	118.09	111.82
1	E	68	ALA	N-CA-CB	-5.41	103.26	111.15
1	E	2	ALA	N-CA-C	-5.40	105.39	112.41
1	E	422	GLU	CB-CG-CD	5.40	121.77	112.60
1	E	661	SER	O-C-N	-5.40	115.20	122.43
1	E	201	ILE	O-C-N	-5.39	114.95	121.10
1	E	174	PHE	N-CA-C	5.39	118.13	110.10
1	E	481	VAL	N-CA-C	5.39	117.56	109.20
1	E	496	LYS	N-CA-C	5.38	118.18	109.40
1	E	202	PRO	CA-C-O	-5.38	115.32	121.56
1	E	260	LEU	CA-C-O	5.38	127.48	121.40
1	E	363	ARG	NE-CZ-NH1	5.37	126.87	121.50
1	E	51	THR	N-CA-C	5.37	117.22	108.63
1	E	321	TYR	O-C-N	-5.36	115.46	122.59
1	E	538	TYR	CB-CG-CD2	-5.36	112.76	120.80
1	E	287	PRO	N-CA-C	5.36	117.24	110.70
1	E	605	ILE	CA-C-N	5.36	130.02	122.09
1	E	605	ILE	C-N-CA	5.36	130.02	122.09
1	E	61	ARG	NH1-CZ-NH2	-5.35	112.34	119.30
1	E	480	GLN	OE1-CD-NE2	5.35	127.95	122.60
1	E	80	ASN	N-CA-C	5.34	118.17	109.24
1	E	291	GLY	O-C-N	-5.34	118.61	123.57
1	E	210	ARG	NH1-CZ-NH2	5.33	126.24	119.30
1	E	239	GLU	N-CA-C	5.33	117.50	111.11
1	E	45	VAL	O-C-N	-5.33	117.29	122.99
1	E	266	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	E	81	ILE	N-CA-CB	5.32	118.75	111.41
1	E	422	GLU	CB-CA-C	5.31	119.22	110.88
1	E	293	THR	N-CA-CB	5.31	117.69	110.05
1	E	40	HIS	CE1-NE2-CD2	-5.30	103.69	109.00
1	E	486	THR	CB-CA-C	-5.30	101.52	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	507	TYR	CA-CB-CG	5.30	123.43	113.90
1	E	528	ALA	O-C-N	-5.29	116.52	122.12
1	E	317	MET	N-CA-CB	-5.28	102.41	110.85
1	E	385	THR	CA-CB-OG1	5.28	117.51	109.60
1	E	672	PHE	O-C-N	-5.28	117.15	123.27
1	E	365	GLU	CA-C-N	5.27	131.06	122.69
1	E	365	GLU	C-N-CA	5.27	131.06	122.69
1	E	612	THR	CA-CB-OG1	5.27	117.50	109.60
1	E	684	GLN	CA-C-N	5.26	128.06	120.38
1	E	684	GLN	C-N-CA	5.26	128.06	120.38
1	E	73	PHE	CA-C-O	5.25	125.81	120.24
1	E	81	ILE	N-CA-C	-5.25	100.77	108.11
1	E	586	GLY	N-CA-C	5.24	119.48	112.77
1	E	115	GLU	CA-C-N	5.23	124.68	119.24
1	E	115	GLU	C-N-CA	5.23	124.68	119.24
1	E	245	ALA	CA-C-N	5.23	127.62	120.46
1	E	245	ALA	C-N-CA	5.23	127.62	120.46
1	E	20	HIS	O-C-N	-5.22	117.54	123.13
1	E	527	ASN	N-CA-CB	-5.22	101.78	110.39
1	E	47	GLU	CA-C-N	-5.21	114.77	121.96
1	E	47	GLU	C-N-CA	-5.21	114.77	121.96
1	E	514	VAL	CA-CB-CG2	-5.21	101.55	110.40
1	E	507	TYR	CB-CA-C	5.20	118.21	110.62
1	E	126	GLU	CB-CA-C	-5.20	102.69	110.90
1	E	556	ILE	N-CA-C	-5.20	105.95	113.07
1	E	213	HIS	CE1-NE2-CD2	-5.19	103.81	109.00
1	E	437	THR	N-CA-C	-5.19	106.26	112.59
1	E	239	GLU	CA-C-N	5.19	127.23	120.28
1	E	239	GLU	C-N-CA	5.19	127.23	120.28
1	E	543	GLN	N-CA-C	-5.18	105.32	111.69
1	E	182	ARG	CD-NE-CZ	5.17	131.64	124.40
1	E	220	ALA	CB-CA-C	-5.17	102.06	110.85
1	E	475	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	E	396	ARG	CB-CA-C	-5.17	103.68	112.00
1	E	366	VAL	N-CA-C	5.17	117.28	108.86
1	E	182	ARG	CA-C-N	5.16	129.47	122.19
1	E	182	ARG	C-N-CA	5.16	129.47	122.19
1	E	632	LEU	N-CA-C	-5.16	105.87	113.61
1	E	46	HIS	CE1-NE2-CD2	-5.16	103.84	109.00
1	E	525	PHE	CA-CB-CG	-5.14	108.66	113.80
1	E	349	LYS	CA-C-N	5.14	132.09	122.74
1	E	349	LYS	C-N-CA	5.14	132.09	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	190	ASN	N-CA-C	5.14	121.74	110.80
1	E	243	VAL	CA-CB-CG1	5.13	119.13	110.40
1	E	591	LYS	CA-C-N	5.13	127.11	120.44
1	E	591	LYS	C-N-CA	5.13	127.11	120.44
1	E	303	PRO	CA-N-CD	-5.13	104.82	112.00
1	E	523	PHE	N-CA-C	-5.12	101.40	109.50
1	E	17	ILE	N-CA-CB	5.12	117.20	111.21
1	E	80	ASN	CA-CB-CG	-5.11	107.49	112.60
1	E	516	PRO	CB-CA-C	5.11	118.06	111.46
1	E	142	THR	N-CA-C	5.11	121.69	110.80
1	E	556	ILE	CA-CB-CG1	5.11	119.09	110.40
1	E	606	MET	O-C-N	-5.11	117.23	123.16
1	E	341	VAL	O-C-N	-5.10	117.68	123.03
1	E	342	TYR	CA-C-N	5.10	129.47	122.84
1	E	342	TYR	C-N-CA	5.10	129.47	122.84
1	E	202	PRO	CB-CA-C	5.09	117.74	111.23
1	E	454	MET	CA-CB-CG	-5.09	103.92	114.10
1	E	458	HIS	CG-CD2-NE2	5.08	112.28	107.20
1	E	332	SER	CA-C-O	-5.08	116.01	121.45
1	E	217	VAL	N-CA-CB	5.08	117.44	110.54
1	E	151	ARG	NE-CZ-NH1	-5.07	116.43	121.50
1	E	555	LEU	N-CA-C	-5.06	100.08	108.12
1	E	7	TYR	CG-CD2-CE2	5.06	128.78	121.20
1	E	576	ASP	CA-C-N	5.04	128.86	120.94
1	E	576	ASP	C-N-CA	5.04	128.86	120.94
1	E	198	GLU	CA-C-O	5.02	126.79	121.02
1	E	58	GLU	CA-C-N	5.01	127.27	120.65
1	E	58	GLU	C-N-CA	5.01	127.27	120.65
1	E	362	HIS	CB-CA-C	-5.00	101.43	110.03
1	E	655	TYR	N-CA-CB	-5.00	102.76	110.16

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	108	PHE	Peptide,Sidechain
1	E	11	ARG	Sidechain
1	E	128	TYR	Sidechain
1	E	130	VAL	Peptide
1	E	132	ARG	Sidechain
1	E	151	ARG	Sidechain
1	E	158	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	E	160	ARG	Peptide,Sidechain
1	E	174	PHE	Sidechain
1	E	182	ARG	Sidechain
1	E	212	TYR	Sidechain
1	E	279	TYR	Sidechain
1	E	28	THR	Peptide
1	E	287	PRO	Peptide
1	E	298	VAL	Peptide
1	E	31	ARG	Sidechain
1	E	319	ASP	Peptide
1	E	321	TYR	Sidechain
1	E	329	ARG	Sidechain
1	E	351	ARG	Sidechain
1	E	363	ARG	Peptide
1	E	38	ARG	Sidechain
1	E	39	ILE	Peptide
1	E	394	ALA	Peptide
1	E	430	ARG	Sidechain
1	E	442	THR	Peptide
1	E	45	VAL	Peptide
1	E	453	GLY	Peptide
1	E	468	ARG	Sidechain
1	E	478	LYS	Peptide
1	E	50	ALA	Peptide
1	E	528	ALA	Peptide
1	E	534	ILE	Peptide
1	E	568	TYR	Sidechain
1	E	572	TYR	Sidechain
1	E	60	GLU	Peptide
1	E	607	ARG	Sidechain
1	E	61	ARG	Sidechain
1	E	637	ARG	Sidechain
1	E	652	MET	Peptide
1	E	654	GLY	Peptide
1	E	655	TYR	Peptide,Sidechain
1	E	666	ARG	Sidechain
1	E	676	TYR	Sidechain
1	E	7	TYR	Sidechain
1	E	78	ARG	Sidechain
1	E	91	THR	Mainchain
1	E	99	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	E	5382	0	5445	73	0
All	All	5382	0	5445	73	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 7.

All (73) 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:E:23:ALA:H	1:E:109:ASP:HB2	1.62	0.65
1:E:487:ILE:HG22	1:E:563:ILE:HG22	1.79	0.64
1:E:210:ARG:HA	1:E:213:HIS:CD2	2.34	0.62
1:E:534:ILE:HG23	1:E:570:GLY:HA3	1.83	0.61
1:E:454:MET:H	1:E:458:HIS:CG	2.20	0.59
1:E:143:GLY:H	1:E:171:GLU:CD	2.10	0.59
1:E:227:ILE:HG23	1:E:237:PRO:HG2	1.85	0.58
1:E:493:VAL:CG2	1:E:593:ALA:HB2	2.33	0.58
1:E:4:LYS:HA	1:E:7:TYR:CD1	2.39	0.56
1:E:302:HIS:H	1:E:332:SER:CB	2.20	0.54
1:E:166:LEU:HD11	1:E:208:GLN:HB3	1.90	0.53
1:E:487:ILE:HD12	1:E:594:VAL:HA	1.91	0.52
1:E:377:VAL:HG21	1:E:380:LEU:HD13	1.92	0.51
1:E:339:SER:H	1:E:352:VAL:HG13	1.75	0.51
1:E:632:LEU:HB2	1:E:644:ARG:HB2	1.93	0.51
1:E:58:GLU:HG2	1:E:64:THR:HA	1.91	0.50
1:E:405:PRO:O	1:E:454:MET:HE3	2.12	0.49
1:E:631:ILE:HG22	1:E:633:GLY:H	1.76	0.49
1:E:74:TRP:HE1	1:E:274:ASP:CG	2.21	0.49
1:E:508:GLY:HA2	1:E:582:PHE:CD1	2.48	0.49
1:E:350:GLU:HB3	1:E:380:LEU:HD23	1.94	0.48
1:E:46:HIS:CE1	1:E:55:MET:HB2	2.48	0.48
1:E:97:SER:HB3	1:E:101:LEU:HD23	1.96	0.48
1:E:293:THR:CG2	1:E:299:VAL:HG21	2.44	0.48
1:E:220:ALA:HB1	1:E:227:ILE:HD13	1.97	0.47
1:E:487:ILE:CG2	1:E:563:ILE:HG22	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:GLU:HA	1:E:122:TRP:CD1	2.50	0.46
1:E:39:ILE:O	1:E:40:HIS:HB2	2.15	0.46
1:E:145:ASP:HB3	1:E:148:LEU:HD23	1.97	0.46
1:E:454:MET:H	1:E:458:HIS:CD2	2.33	0.46
1:E:377:VAL:HG21	1:E:380:LEU:CD1	2.46	0.46
1:E:541:ALA:HB1	1:E:583:LYS:HB2	1.98	0.46
1:E:556:ILE:HG23	1:E:601:ILE:HD11	1.97	0.45
1:E:536:LYS:HA	1:E:539:ILE:HG12	1.98	0.45
1:E:602:LEU:HA	1:E:678:GLU:HA	1.98	0.45
1:E:151:ARG:HA	1:E:154:GLN:HE21	1.82	0.45
1:E:153:MET:C	1:E:153:MET:SD	3.00	0.45
1:E:201:ILE:HG22	1:E:202:PRO:O	2.17	0.45
1:E:602:LEU:HB3	1:E:676:TYR:HB3	1.99	0.44
1:E:210:ARG:HA	1:E:213:HIS:HD2	1.81	0.44
1:E:1:MET:HB2	1:E:6:GLU:HB3	2.00	0.44
1:E:260:LEU:N	1:E:260:LEU:HD13	2.33	0.44
1:E:348:ARG:HG2	1:E:349:LYS:C	2.42	0.44
1:E:493:VAL:HG21	1:E:593:ALA:HB2	1.99	0.43
1:E:44:GLU:HG2	1:E:67:ALA:H	1.83	0.43
1:E:534:ILE:HG22	1:E:582:PHE:HE2	1.83	0.43
1:E:93:GLU:CD	1:E:96:ARG:HH12	2.27	0.43
1:E:53:ASP:HB3	1:E:54:PHE:CE1	2.54	0.42
1:E:227:ILE:HG23	1:E:237:PRO:CG	2.48	0.42
1:E:114:VAL:HG23	1:E:118:SER:HB3	2.00	0.42
1:E:310:ALA:HB1	1:E:399:LEU:HD11	2.02	0.42
1:E:290:LYS:CG	1:E:298:VAL:HG22	2.48	0.42
1:E:227:ILE:HG23	1:E:237:PRO:CB	2.48	0.42
1:E:219:VAL:O	1:E:222:ASP:HB3	2.19	0.42
1:E:671:MET:HG2	1:E:672:PHE:N	2.35	0.41
1:E:35:TYR:CD1	1:E:266:ASN:HA	2.55	0.41
1:E:302:HIS:O	1:E:332:SER:HB2	2.20	0.41
1:E:493:VAL:HG22	1:E:593:ALA:HB2	2.01	0.41
1:E:20:HIS:O	1:E:63:ILE:HD13	2.20	0.41
1:E:487:ILE:CD1	1:E:594:VAL:HA	2.49	0.41
1:E:189:GLY:C	1:E:193:GLY:HA3	2.46	0.41
1:E:617:MET:HE2	1:E:634:MET:HE1	2.01	0.41
1:E:305:PRO:HG3	1:E:371:ALA:H	1.86	0.41
1:E:188:TYR:HA	1:E:195:ASP:O	2.20	0.41
1:E:290:LYS:HD2	1:E:290:LYS:HA	1.94	0.41
1:E:299:VAL:CG2	1:E:395:PRO:HB2	2.51	0.41
1:E:500:GLN:HA	1:E:505:GLY:HA2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:569:ASP:CG	1:E:570:GLY:H	2.28	0.40
1:E:374:LEU:HD12	1:E:374:LEU:C	2.47	0.40
1:E:118:SER:HA	1:E:121:VAL:HG22	2.03	0.40
1:E:341:VAL:O	1:E:349:LYS:HA	2.21	0.40
1:E:116:PRO:O	1:E:119:GLU:HB3	2.22	0.40
1:E:119:GLU:HB2	1:E:156:ARG:HH21	1.87	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 PDB entries followed by that with respect to all EM entries.

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	E	686/688 (100%)	611 (89%)	53 (8%)	22 (3%)	3 3

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	63	ILE
1	E	190	ASN
1	E	304	ASP
1	E	321	TYR
1	E	40	HIS
1	E	66	THR
1	E	110	SER
1	E	142	THR
1	E	189	GLY
1	E	408	VAL
1	E	529	ILE
1	E	530	VAL
1	E	562	ASP
1	E	64	THR
1	E	83	ASP

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Mol	Chain	Res	Type
1	E	308	PRO
1	E	402	ILE
1	E	288	PRO
1	E	195	ASP
1	E	86	GLY
1	E	281	PRO
1	E	39	ILE

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 PDB entries followed by that with respect to all EM entries.

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	E	579/579 (100%)	498 (86%)	81 (14%)	3 3

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	5	VAL
1	E	7	TYR
1	E	12	LEU
1	E	17	ILE
1	E	21	ILE
1	E	25	LYS
1	E	27	THR
1	E	30	GLU
1	E	31	ARG
1	E	32	ILE
1	E	51	THR
1	E	64	THR
1	E	73	PHE
1	E	76	ASP
1	E	78	ARG
1	E	107	VAL
1	E	117	GLN
1	E	124	GLN
1	E	141	LYS

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Mol	Chain	Res	Type
1	E	146	LEU
1	E	153	MET
1	E	157	LEU
1	E	173	THR
1	E	181	LEU
1	E	186	TYR
1	E	196	ILE
1	E	197	ARG
1	E	208	GLN
1	E	210	ARG
1	E	215	LYS
1	E	231	TYR
1	E	237	PRO
1	E	246	ILE
1	E	255	ILE
1	E	257	PRO
1	E	260	LEU
1	E	282	SER
1	E	289	ILE
1	E	298	VAL
1	E	299	VAL
1	E	300	GLU
1	E	303	PRO
1	E	308	PRO
1	E	312	LEU
1	E	314	PHE
1	E	317	MET
1	E	356	LEU
1	E	365	GLU
1	E	368	GLU
1	E	382	GLU
1	E	420	ASP
1	E	422	GLU
1	E	438	PHE
1	E	444	PRO
1	E	452	SER
1	E	454	MET
1	E	456	GLU
1	E	459	LEU
1	E	466	LEU
1	E	468	ARG
1	E	496	LYS

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Mol	Chain	Res	Type
1	E	507	TYR
1	E	510	VAL
1	E	529	ILE
1	E	534	ILE
1	E	544	LYS
1	E	555	LEU
1	E	559	PRO
1	E	563	ILE
1	E	574	GLU
1	E	582	PHE
1	E	603	GLU
1	E	608	VAL
1	E	615	GLU
1	E	620	VAL
1	E	635	GLU
1	E	646	PHE
1	E	655	TYR
1	E	680	PRO
1	E	682	GLN
1	E	684	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	20	HIS
1	E	40	HIS
1	E	46	HIS
1	E	77	HIS
1	E	87	HIS
1	E	154	GLN
1	E	302	HIS
1	E	426	GLN
1	E	443	HIS
1	E	500	GLN
1	E	639	ASN
1	E	664	GLN

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

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.