



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 11:30 PM UTC

PDB ID : 1K7E / pdb_00001k7e
Title : CRYSTAL STRUCTURE OF WILD-TYPE TRYPTOPHAN SYNTHASE
COMPLEXED WITH N-[1H-INDOL-3-YL-ACETYL]GLYCINE ACID
Authors : Weyand, M.; Schlichting, I.; Marabotti, A.; Mozzarelli, A.
Deposited on : 2001-10-19
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

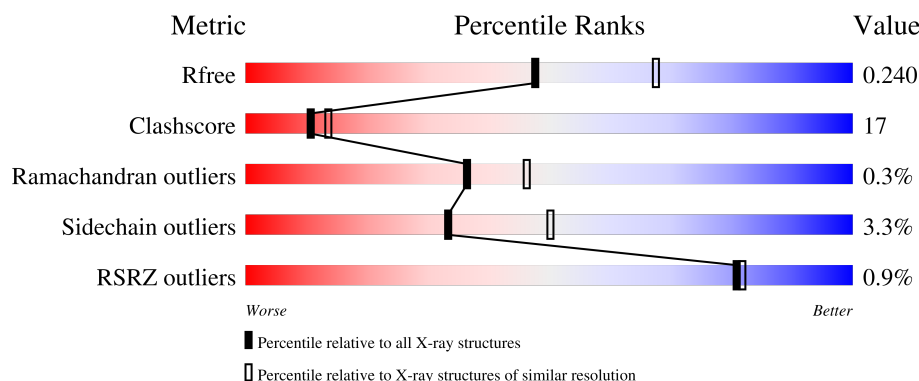
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	268	% 27% 50% 19% ..
2	B	396	% 32% 52% 15% ..

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5217 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 TRYPTOPHAN SYNTHASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	1	0
			1970	1251	341	370	8			

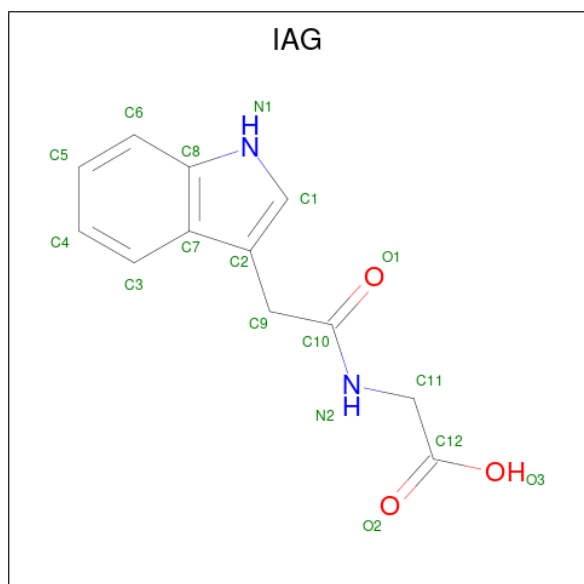
- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	393	Total	C	N	O	S	0	0	0
			2977	1871	523	564	19			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	34	SER	ARG	cloning artifact	UNP P0A2K1

- Molecule 3 is N-[1H-INDOL-3-YL-ACETYL]GLYCINE ACID (CCD ID: IAG) (formula: $C_{12}H_{12}N_2O_3$).

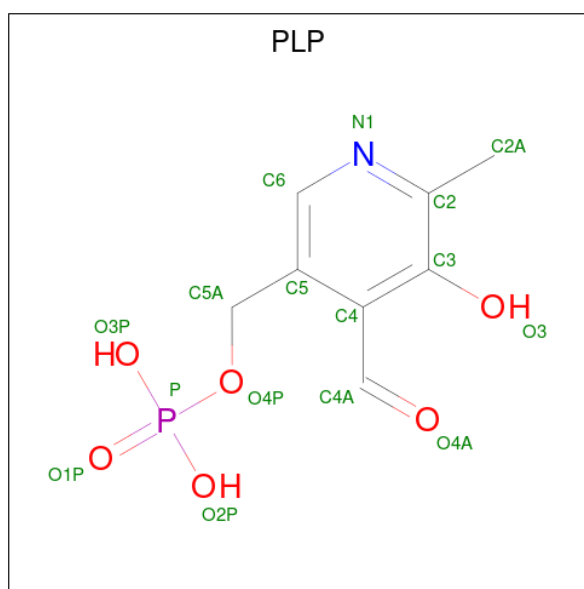


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	12	2	3		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		

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



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

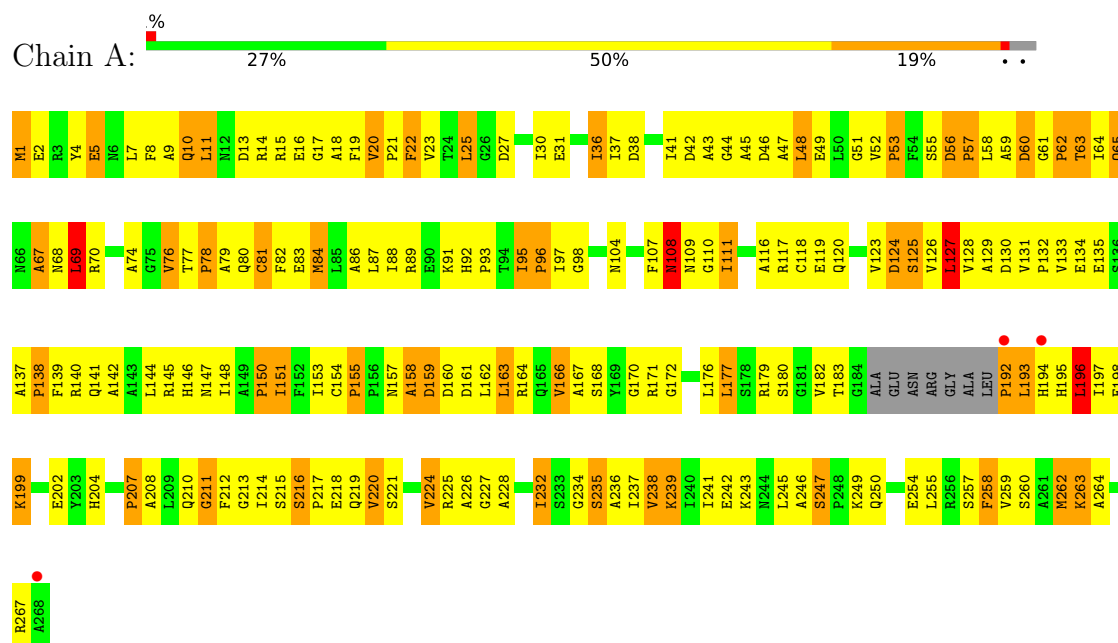
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	82	Total	O	0	0
			82	82		
6	B	155	Total	O	0	0
			155	155		

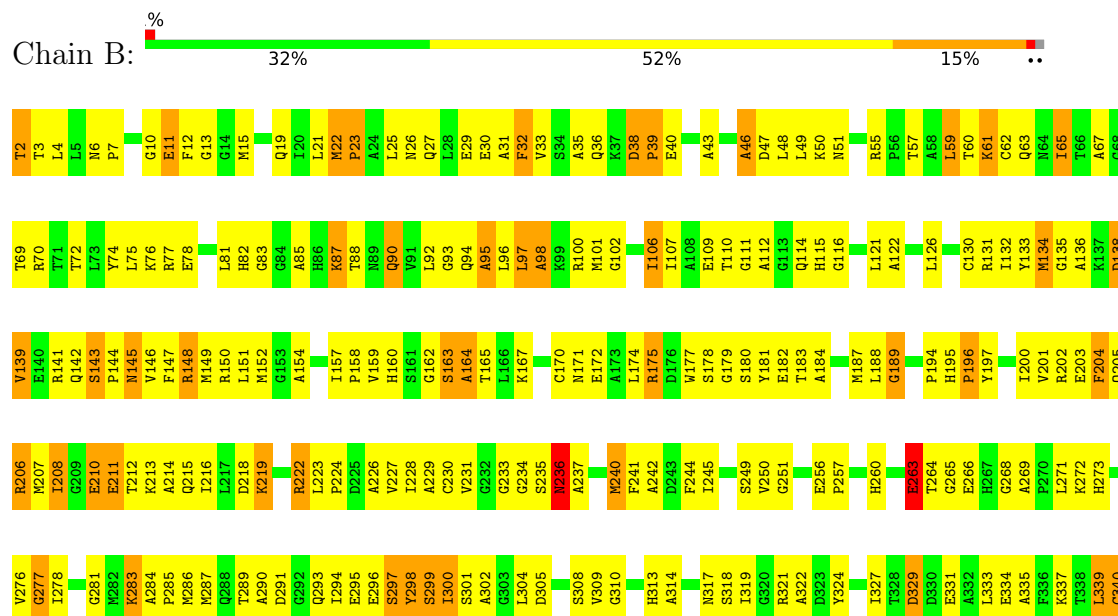
3 Residue-property plots

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

• Molecule 1: TRYPTOPHAN SYNTHASE ALPHA CHAIN



• Molecule 2: TRYPTOPHAN SYNTHASE BETA CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.65Å 59.08Å 67.30Å 90.00° 94.55° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.0 (20.00-2.30) 90.8 (20.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.29Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.167 , 0.244 0.167 , 0.240	Depositor DCC
R_{free} test set	1475 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.870	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5217	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IAG, NA, PLP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.89	161/2014 (8.0%)	2.29	93/2733 (3.4%)
2	B	2.87	238/3035 (7.8%)	2.26	146/4100 (3.6%)
All	All	2.88	399/5049 (7.9%)	2.27	239/6833 (3.5%)

All (399) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	240	MET	SD-CE	-23.38	1.21	1.79
2	B	46	ALA	CA-CB	14.72	1.77	1.53
2	B	59	LEU	CA-C	14.03	1.70	1.52
1	A	1	MET	SD-CE	13.55	2.13	1.79
2	B	371	LEU	C-O	-13.31	1.08	1.24
1	A	60	ASP	C-O	13.13	1.40	1.23
2	B	143	SER	C-O	-13.10	1.11	1.24
2	B	214	ALA	CA-CB	12.18	1.73	1.53
1	A	87	LEU	CA-CB	12.14	1.73	1.53
2	B	180	SER	CA-C	-11.79	1.38	1.52
2	B	361	MET	C-O	-11.29	1.10	1.24
1	A	263	LYS	C-O	11.28	1.37	1.24
2	B	351	SER	C-O	-10.91	1.10	1.24
2	B	269	ALA	CA-CB	-10.87	1.41	1.53
2	B	346	ILE	C-O	-10.87	1.10	1.24
1	A	140	ARG	NE-CZ	-10.54	1.21	1.33
2	B	59	LEU	C-O	-10.52	1.11	1.24
2	B	295	GLU	CD-OE1	10.41	1.45	1.25
1	A	59	ALA	CA-C	10.29	1.66	1.52
1	A	237	ILE	CA-CB	-10.25	1.42	1.54
1	A	214	ILE	CA-CB	-9.98	1.41	1.53
2	B	4	LEU	CA-C	9.92	1.66	1.52
1	A	17	GLY	C-O	9.92	1.39	1.23
1	A	133	VAL	CA-CB	9.90	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	100	ARG	N-CA	-9.60	1.34	1.46
2	B	107	ILE	CA-CB	-9.50	1.42	1.54
1	A	52	VAL	CA-CB	-9.44	1.42	1.54
2	B	27	GLN	CD-OE1	9.39	1.41	1.23
1	A	148	ILE	CA-CB	-9.29	1.43	1.54
2	B	322	ALA	C-O	-9.28	1.11	1.23
1	A	95	ILE	CA-C	9.21	1.62	1.52
2	B	308	SER	C-O	-9.18	1.15	1.24
2	B	48	LEU	N-CA	9.18	1.58	1.46
1	A	224	VAL	C-O	-9.14	1.13	1.24
2	B	226	ALA	N-CA	-9.11	1.34	1.45
2	B	154	ALA	CA-CB	-9.10	1.39	1.53
1	A	216	SER	C-O	9.08	1.33	1.24
2	B	373	VAL	CA-CB	9.07	1.65	1.54
2	B	202	ARG	CZ-NH1	9.04	1.45	1.32
2	B	362	MET	N-CA	-9.03	1.35	1.46
2	B	216	ILE	N-CA	-8.98	1.35	1.46
2	B	3	THR	CA-CB	-8.93	1.39	1.53
2	B	263	GLU	CD-OE1	8.91	1.42	1.25
2	B	309	VAL	CA-CB	-8.87	1.46	1.55
1	A	47	ALA	CA-CB	8.87	1.68	1.53
2	B	147	PHE	CA-C	8.87	1.64	1.52
1	A	84	MET	SD-CE	-8.84	1.57	1.79
1	A	18	ALA	CA-CB	-8.82	1.39	1.53
1	A	93	PRO	C-O	-8.70	1.12	1.24
2	B	346	ILE	CA-CB	-8.62	1.43	1.54
2	B	346	ILE	CG1-CD1	8.61	1.85	1.51
1	A	22	PHE	C-O	-8.61	1.13	1.24
1	A	235	SER	C-O	-8.57	1.14	1.24
1	A	96	PRO	CA-CB	-8.57	1.42	1.53
1	A	95	ILE	C-O	-8.48	1.13	1.24
1	A	21	PRO	C-O	8.43	1.32	1.23
1	A	254	GLU	C-O	-8.42	1.13	1.24
2	B	365	GLN	N-CA	-8.42	1.37	1.46
2	B	62	CYS	CA-C	8.31	1.61	1.53
1	A	176	LEU	CA-C	-8.31	1.42	1.52
1	A	10	GLN	N-CA	-8.23	1.35	1.46
1	A	141	GLN	CA-CB	8.23	1.66	1.53
2	B	107	ILE	C-O	-8.19	1.15	1.24
2	B	31	ALA	CA-CB	-8.07	1.39	1.53
2	B	11	GLU	CD-OE2	8.04	1.40	1.25
1	A	116	ALA	CA-CB	8.02	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	138	ASP	C-N	-8.00	1.24	1.33
2	B	346	ILE	N-CA	-7.99	1.36	1.46
2	B	263	GLU	CA-C	-7.97	1.41	1.52
1	A	45	ALA	C-O	7.94	1.33	1.23
1	A	183	THR	CA-CB	7.90	1.66	1.53
2	B	61	LYS	C-O	-7.89	1.14	1.24
2	B	134	MET	C-O	7.88	1.32	1.23
1	A	53	PRO	CA-C	-7.87	1.43	1.52
2	B	263	GLU	C-O	-7.87	1.14	1.24
2	B	272	LYS	C-O	-7.86	1.14	1.24
2	B	139	VAL	CB-CG2	7.85	1.78	1.52
2	B	213	LYS	CA-C	-7.80	1.43	1.52
2	B	150	ARG	NE-CZ	7.79	1.41	1.33
2	B	30	GLU	CA-CB	7.75	1.65	1.53
2	B	208	ILE	CA-C	7.74	1.62	1.52
1	A	27	ASP	C-O	-7.73	1.15	1.24
2	B	194	PRO	CA-CB	-7.70	1.43	1.53
2	B	194	PRO	C-O	-7.69	1.15	1.23
1	A	25	LEU	CG-CD1	7.67	1.77	1.52
1	A	239	LYS	CE-NZ	7.66	1.72	1.49
2	B	145	ASN	N-CA	-7.64	1.36	1.46
2	B	204	PHE	CA-C	7.63	1.64	1.52
2	B	334	GLU	C-O	7.59	1.33	1.24
2	B	251	GLY	CA-C	7.56	1.62	1.51
2	B	87	LYS	C-O	-7.55	1.14	1.24
2	B	281	GLY	CA-C	-7.55	1.40	1.51
1	A	124	ASP	CA-C	-7.53	1.43	1.52
2	B	112	ALA	CA-CB	7.52	1.66	1.53
1	A	81	CYS	N-CA	-7.48	1.36	1.46
2	B	293	GLN	N-CA	-7.48	1.36	1.46
2	B	291	ASP	CA-C	7.44	1.62	1.52
2	B	344	GLY	C-O	7.41	1.34	1.24
2	B	21	LEU	C-O	-7.41	1.14	1.24
1	A	43	ALA	CA-CB	7.40	1.66	1.53
2	B	379	ARG	CZ-NH1	7.38	1.43	1.32
2	B	150	ARG	CZ-NH2	7.35	1.43	1.33
2	B	317	ASN	CG-OD1	7.34	1.37	1.23
2	B	360	LYS	CG-CD	7.33	1.74	1.52
1	A	5	GLU	C-O	-7.30	1.15	1.24
2	B	60	THR	CA-CB	7.29	1.63	1.53
1	A	232	ILE	CA-C	-7.26	1.43	1.52
2	B	31	ALA	N-CA	-7.22	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	335	ALA	CA-C	7.20	1.62	1.52
2	B	340	CYS	CA-C	7.18	1.61	1.52
1	A	45	ALA	CA-CB	7.15	1.65	1.53
1	A	126	VAL	C-O	7.15	1.31	1.23
2	B	207	MET	CG-SD	-7.11	1.62	1.80
1	A	19	PHE	C-O	-7.08	1.16	1.24
2	B	337	LYS	CA-C	-7.08	1.43	1.52
2	B	67	ALA	CA-CB	7.07	1.65	1.53
1	A	166	VAL	CA-CB	-7.04	1.45	1.54
2	B	374	VAL	C-O	-7.04	1.15	1.24
2	B	15	MET	SD-CE	7.02	1.97	1.79
1	A	23	VAL	CA-C	-7.00	1.45	1.52
2	B	308	SER	CA-C	7.00	1.60	1.53
2	B	360	LYS	C-O	6.97	1.32	1.24
1	A	250	GLN	CA-C	6.96	1.62	1.52
1	A	151	ILE	CA-CB	-6.94	1.45	1.54
1	A	232	ILE	CG1-CD1	6.94	1.78	1.51
2	B	341	ARG	CZ-NH1	6.93	1.42	1.32
1	A	126	VAL	N-CA	-6.93	1.38	1.46
2	B	369	GLU	N-CA	-6.91	1.37	1.46
2	B	165	THR	N-CA	-6.87	1.37	1.46
1	A	78	PRO	C-O	-6.87	1.16	1.24
2	B	331	GLU	N-CA	-6.87	1.38	1.46
2	B	245	ILE	CA-CB	6.87	1.62	1.54
1	A	177	LEU	C-O	-6.82	1.15	1.23
2	B	236	ASN	C-O	6.82	1.32	1.24
1	A	44	GLY	C-O	-6.80	1.17	1.24
2	B	69	THR	CA-C	-6.80	1.43	1.52
1	A	163	LEU	CA-C	-6.80	1.43	1.52
1	A	56	ASP	CA-C	-6.78	1.44	1.52
2	B	219	LYS	CD-CE	6.72	1.72	1.52
2	B	77	ARG	CZ-NH1	6.71	1.42	1.32
1	A	198	GLU	CA-C	6.70	1.61	1.52
1	A	120	GLN	CG-CD	6.69	1.68	1.52
2	B	19	GLN	C-O	-6.67	1.15	1.24
2	B	131	ARG	CA-CB	-6.66	1.43	1.53
2	B	152	MET	SD-CE	-6.66	1.62	1.79
1	A	62	PRO	CB-CG	6.66	1.82	1.49
2	B	197	TYR	CA-C	6.64	1.60	1.52
1	A	204	HIS	CA-C	6.64	1.61	1.53
1	A	141	GLN	CA-C	6.61	1.61	1.52
1	A	241	ILE	C-O	6.61	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49[A]	GLU	N-CA	-6.61	1.38	1.46
1	A	49[B]	GLU	N-CA	-6.61	1.38	1.46
1	A	138	PRO	C-O	6.60	1.32	1.24
1	A	88	ILE	CA-CB	-6.60	1.46	1.54
2	B	386	THR	C-O	-6.59	1.15	1.24
2	B	215	GLN	CD-OE1	6.57	1.36	1.23
1	A	129	ALA	CA-CB	-6.54	1.42	1.53
2	B	160	HIS	C-O	-6.54	1.15	1.24
2	B	381	ASP	CA-C	-6.54	1.44	1.52
2	B	13	GLY	C-O	-6.54	1.15	1.23
2	B	375	ASN	CG-OD1	6.53	1.35	1.23
1	A	245	LEU	CG-CD2	6.53	1.74	1.52
2	B	184	ALA	CA-CB	-6.51	1.42	1.53
1	A	48	LEU	C-O	6.50	1.32	1.23
2	B	27	GLN	C-O	6.47	1.31	1.24
2	B	122	ALA	CA-CB	6.47	1.64	1.53
1	A	139	PHE	CA-C	6.45	1.61	1.52
1	A	207	PRO	CA-C	6.45	1.60	1.52
2	B	51	ASN	C-O	-6.44	1.15	1.24
2	B	363	ARG	N-CA	-6.44	1.38	1.46
1	A	119	GLU	C-O	6.44	1.31	1.24
2	B	139	VAL	C-O	6.42	1.31	1.24
1	A	155	PRO	CA-C	-6.41	1.46	1.52
2	B	378	GLY	C-O	6.41	1.30	1.23
1	A	131	VAL	CA-CB	-6.40	1.46	1.54
1	A	183	THR	CB-CG2	6.40	1.73	1.52
1	A	215	SER	C-N	-6.40	1.25	1.33
2	B	309	VAL	CA-C	-6.38	1.45	1.52
2	B	367	GLU	C-O	6.37	1.32	1.24
2	B	197	TYR	C-O	-6.33	1.18	1.24
2	B	286	MET	CA-C	6.33	1.60	1.52
2	B	298	TYR	CZ-OH	6.33	1.51	1.38
2	B	264	THR	CA-C	-6.31	1.44	1.52
2	B	201	VAL	C-O	-6.30	1.16	1.24
2	B	317	ASN	N-CA	-6.30	1.38	1.46
1	A	20	VAL	N-CA	-6.29	1.41	1.45
2	B	364	GLU	CD-OE2	-6.29	1.13	1.25
2	B	65	ILE	CA-C	-6.29	1.44	1.52
2	B	358	ALA	CA-C	-6.26	1.44	1.52
2	B	136	ALA	CA-C	-6.26	1.44	1.52
2	B	76	LYS	C-O	6.25	1.31	1.24
1	A	46	ASP	CA-C	-6.25	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	48	LEU	CA-C	6.24	1.61	1.52
1	A	14	ARG	CA-C	-6.23	1.43	1.52
2	B	133	TYR	C-N	-6.20	1.25	1.33
2	B	40	GLU	CA-CB	6.20	1.63	1.53
1	A	126	VAL	CA-CB	6.19	1.63	1.54
1	A	11	LEU	CA-C	6.18	1.61	1.52
2	B	206	ARG	CG-CD	6.17	1.71	1.52
1	A	218	GLU	C-O	6.17	1.31	1.24
1	A	36	ILE	CG1-CD1	6.17	1.75	1.51
2	B	327	ILE	CA-CB	-6.16	1.46	1.54
1	A	16	GLU	N-CA	-6.15	1.38	1.46
2	B	133	TYR	C-O	-6.15	1.16	1.24
1	A	57	PRO	CB-CG	6.13	1.80	1.49
2	B	182	GLU	CD-OE1	6.13	1.36	1.25
2	B	15	MET	CA-C	-6.13	1.46	1.53
1	A	228	ALA	CA-CB	-6.12	1.43	1.53
2	B	290	ALA	CA-C	6.12	1.61	1.52
2	B	143	SER	CA-C	-6.11	1.44	1.52
1	A	219	GLN	C-O	6.09	1.31	1.24
2	B	283	LYS	CA-C	-6.09	1.45	1.52
1	A	142	ALA	N-CA	-6.07	1.39	1.46
2	B	202	ARG	CD-NE	-6.07	1.37	1.46
1	A	164	ARG	NE-CZ	-6.06	1.26	1.33
1	A	226	ALA	CA-CB	-6.06	1.42	1.53
2	B	319	ILE	N-CA	-6.05	1.38	1.46
1	A	111	ILE	CA-CB	6.05	1.61	1.54
2	B	250	VAL	CA-CB	-6.04	1.46	1.53
1	A	214	ILE	C-O	6.02	1.29	1.23
2	B	39	PRO	CA-C	-6.02	1.42	1.52
2	B	90	GLN	CA-CB	6.00	1.62	1.53
2	B	256	GLU	CA-C	6.00	1.60	1.52
1	A	10	GLN	CB-CG	5.99	1.70	1.52
2	B	2	THR	N-CA	5.97	1.57	1.46
2	B	216	ILE	CA-CB	-5.97	1.46	1.54
2	B	291	ASP	CB-CG	-5.97	1.37	1.52
2	B	369	GLU	CA-CB	-5.97	1.45	1.53
2	B	76	LYS	N-CA	5.96	1.53	1.46
2	B	385	PHE	CG-CD1	5.96	1.51	1.38
1	A	243	LYS	C-O	-5.96	1.16	1.24
2	B	72	THR	N-CA	-5.96	1.38	1.46
2	B	187	MET	N-CA	5.95	1.54	1.46
2	B	339	LEU	CA-C	5.95	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6	ASN	C-N	-5.92	1.27	1.34
1	A	59	ALA	CA-CB	-5.92	1.44	1.53
1	A	67	ALA	CA-CB	5.92	1.62	1.53
2	B	296	GLU	CA-CB	-5.91	1.44	1.53
2	B	212	THR	C-O	5.89	1.31	1.24
2	B	50	LYS	N-CA	5.88	1.53	1.46
2	B	167	LYS	CD-CE	5.88	1.70	1.52
2	B	273	HIS	N-CA	-5.88	1.39	1.46
1	A	22	PHE	CA-C	5.87	1.59	1.52
2	B	110	THR	C-O	5.86	1.31	1.23
1	A	120	GLN	CD-OE1	5.85	1.34	1.23
2	B	219	LYS	C-O	-5.85	1.16	1.24
2	B	228	ILE	N-CA	5.85	1.52	1.46
2	B	346	ILE	CB-CG2	5.84	1.71	1.52
2	B	284	ALA	CA-CB	5.83	1.62	1.54
1	A	262	MET	C-O	5.83	1.30	1.24
2	B	75	LEU	C-N	-5.82	1.25	1.33
2	B	35	ALA	C-O	-5.81	1.17	1.24
2	B	188	LEU	C-O	5.81	1.30	1.23
1	A	131	VAL	C-O	-5.81	1.17	1.24
2	B	32	PHE	CA-C	5.80	1.60	1.52
1	A	65	GLN	C-O	-5.80	1.17	1.24
2	B	234	GLY	C-O	5.79	1.31	1.24
2	B	47	ASP	C-O	5.79	1.30	1.24
1	A	20	VAL	C-N	-5.78	1.26	1.33
2	B	203	GLU	C-O	-5.78	1.16	1.24
1	A	196	LEU	C-O	-5.76	1.17	1.24
1	A	227	GLY	CA-C	5.75	1.59	1.51
1	A	247	SER	C-N	-5.74	1.26	1.33
1	A	218	GLU	CA-C	5.73	1.60	1.52
1	A	125	SER	C-O	-5.73	1.16	1.23
1	A	92	HIS	C-O	-5.73	1.16	1.24
2	B	302	ALA	N-CA	5.73	1.53	1.46
2	B	26	ASN	C-O	-5.72	1.17	1.24
2	B	194	PRO	N-CA	-5.71	1.40	1.47
1	A	141	GLN	C-O	5.71	1.30	1.24
1	A	30	ILE	C-O	5.69	1.30	1.24
2	B	98	ALA	CA-C	5.69	1.60	1.52
1	A	86	ALA	CA-CB	5.68	1.62	1.53
2	B	223	LEU	CA-CB	-5.68	1.44	1.53
1	A	67	ALA	C-O	5.66	1.30	1.24
1	A	194	HIS	N-CA	-5.66	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	239	LYS	CG-CD	5.66	1.69	1.52
2	B	374	VAL	CA-CB	-5.66	1.47	1.54
1	A	238	VAL	N-CA	5.64	1.53	1.46
1	A	118	CYS	C-O	-5.64	1.17	1.24
1	A	170	GLY	N-CA	-5.63	1.38	1.45
2	B	299	SER	CA-CB	5.61	1.63	1.53
2	B	189	GLY	C-O	5.61	1.30	1.24
2	B	107	ILE	N-CA	-5.60	1.39	1.46
2	B	310	GLY	C-O	-5.59	1.16	1.24
2	B	40	GLU	N-CA	5.58	1.53	1.46
2	B	290	ALA	C-N	-5.58	1.25	1.33
1	A	208	ALA	C-O	-5.58	1.17	1.23
2	B	230	CYS	CA-C	-5.58	1.45	1.53
2	B	26	ASN	C-N	-5.57	1.26	1.33
2	B	285	PRO	N-CA	5.57	1.53	1.47
2	B	50	LYS	CA-C	5.55	1.59	1.52
1	A	192	PRO	CB-CG	5.54	1.77	1.49
1	A	236	ALA	C-O	-5.53	1.17	1.24
1	A	235	SER	N-CA	-5.53	1.39	1.46
1	A	239	LYS	CD-CE	5.51	1.69	1.52
2	B	339	LEU	CA-CB	5.51	1.62	1.53
2	B	11	GLU	CG-CD	5.51	1.65	1.52
2	B	172	GLU	N-CA	5.50	1.53	1.46
2	B	223	LEU	C-O	-5.50	1.16	1.23
1	A	51	GLY	C-N	5.49	1.38	1.32
1	A	132	PRO	CG-CD	5.48	1.69	1.50
2	B	264	THR	N-CA	-5.48	1.38	1.46
1	A	214	ILE	CG1-CD1	5.47	1.73	1.51
2	B	76	LYS	CA-CB	5.47	1.60	1.53
1	A	11	LEU	N-CA	-5.47	1.39	1.46
2	B	174	LEU	CA-C	-5.47	1.45	1.52
2	B	269	ALA	C-O	-5.47	1.17	1.24
1	A	202	GLU	CD-OE1	5.46	1.35	1.25
2	B	63	GLN	CG-CD	5.44	1.65	1.52
2	B	134	MET	CA-C	5.44	1.58	1.52
1	A	117	ARG	C-O	5.42	1.30	1.24
1	A	232	ILE	CA-CB	-5.42	1.47	1.54
2	B	210	GLU	C-O	-5.42	1.17	1.24
1	A	74	ALA	C-N	-5.42	1.25	1.33
2	B	302	ALA	C-O	-5.42	1.17	1.24
2	B	379	ARG	N-CA	-5.41	1.39	1.45
1	A	97	ILE	CG1-CD1	5.41	1.72	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	345	ILE	CG1-CD1	5.41	1.72	1.51
2	B	321	ARG	C-N	5.40	1.41	1.33
1	A	108	ASN	CA-CB	5.40	1.62	1.53
1	A	226	ALA	N-CA	-5.39	1.39	1.46
2	B	93	GLY	N-CA	5.38	1.52	1.45
2	B	297	SER	CA-C	5.38	1.59	1.52
1	A	150	PRO	CB-CG	5.36	1.76	1.49
1	A	158	ALA	N-CA	-5.36	1.39	1.46
2	B	130	CYS	C-O	-5.35	1.17	1.24
2	B	70	ARG	CG-CD	5.34	1.68	1.52
1	A	145	ARG	CA-C	-5.34	1.45	1.52
2	B	77	ARG	CA-CB	5.34	1.59	1.52
1	A	135	GLU	CA-C	5.33	1.59	1.52
1	A	150	PRO	C-O	5.33	1.30	1.24
2	B	30	GLU	N-CA	-5.32	1.40	1.46
2	B	289	THR	CA-CB	5.32	1.60	1.53
2	B	297	SER	C-O	5.30	1.30	1.23
2	B	340	CYS	C-O	5.30	1.30	1.24
2	B	201	VAL	N-CA	5.30	1.52	1.46
1	A	145	ARG	C-O	-5.29	1.17	1.24
2	B	324	TYR	CA-C	-5.29	1.46	1.52
1	A	148	ILE	C-O	5.29	1.30	1.24
1	A	220	VAL	C-O	5.28	1.30	1.24
1	A	107	PHE	CA-C	-5.27	1.45	1.52
2	B	106	ILE	CA-CB	-5.27	1.47	1.54
2	B	223	LEU	CA-C	-5.27	1.45	1.52
1	A	2	GLU	CD-OE2	5.26	1.35	1.25
1	A	97	ILE	N-CA	-5.26	1.39	1.46
2	B	381	ASP	CG-OD2	-5.26	1.15	1.25
1	A	55	SER	N-CA	5.25	1.53	1.46
2	B	314	ALA	N-CA	-5.25	1.40	1.46
1	A	9	ALA	C-O	-5.25	1.17	1.24
1	A	183	THR	C-O	5.25	1.29	1.23
2	B	178	SER	N-CA	-5.25	1.39	1.46
1	A	199	LYS	C-O	5.24	1.30	1.24
2	B	49	LEU	CG-CD2	5.22	1.69	1.52
2	B	22	MET	C-O	5.22	1.30	1.24
2	B	78	GLU	CA-C	5.22	1.60	1.52
1	A	120	GLN	CA-C	5.21	1.59	1.52
2	B	136	ALA	CA-CB	5.21	1.61	1.53
2	B	287	MET	CB-CG	5.20	1.68	1.52
2	B	313	HIS	C-O	-5.17	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	300	ILE	C-O	-5.17	1.17	1.24
1	A	226	ALA	CA-C	5.16	1.60	1.52
2	B	95	ALA	CA-CB	-5.16	1.44	1.53
1	A	76	VAL	CA-CB	5.15	1.60	1.54
1	A	15	ARG	CA-CB	5.15	1.61	1.53
1	A	255	LEU	C-N	-5.14	1.27	1.33
2	B	377	SER	CA-C	5.13	1.59	1.52
1	A	142	ALA	C-O	-5.13	1.18	1.24
1	A	225	ARG	CZ-NH1	5.13	1.40	1.32
2	B	372	LEU	N-CA	-5.13	1.39	1.46
1	A	221	SER	C-N	-5.12	1.27	1.33
2	B	329	ASP	CA-C	5.12	1.60	1.52
2	B	300	ILE	CA-CB	5.12	1.61	1.54
1	A	246	ALA	C-O	-5.12	1.17	1.24
1	A	144	LEU	CA-CB	5.11	1.61	1.53
1	A	83	GLU	CD-OE1	5.10	1.35	1.25
2	B	293	GLN	CD-OE1	5.10	1.33	1.23
2	B	384	ILE	CB-CG2	-5.10	1.35	1.52
2	B	350	GLU	CD-OE2	-5.09	1.15	1.25
2	B	134	MET	SD-CE	5.09	1.92	1.79
1	A	259	VAL	N-CA	-5.08	1.40	1.46
2	B	141	ARG	CZ-NH2	-5.08	1.26	1.33
2	B	2	THR	CB-OG1	5.07	1.51	1.43
2	B	383	ASP	C-O	5.07	1.30	1.24
1	A	167	ALA	N-CA	-5.07	1.40	1.46
2	B	244	PHE	CA-C	5.07	1.59	1.52
2	B	82	HIS	N-CA	5.06	1.52	1.46
2	B	85	ALA	N-CA	5.05	1.52	1.45
2	B	361	MET	SD-CE	-5.04	1.67	1.79
2	B	188	LEU	C-N	-5.04	1.25	1.33
1	A	161	ASP	CB-CG	5.04	1.64	1.52
2	B	277	GLY	C-O	5.03	1.29	1.23
2	B	375	ASN	C-O	5.03	1.30	1.24
2	B	196	PRO	C-O	5.03	1.33	1.23
2	B	131	ARG	CG-CD	5.03	1.67	1.52
2	B	178	SER	CA-CB	-5.03	1.44	1.53
2	B	355	LEU	C-O	-5.02	1.18	1.24
1	A	199	LYS	N-CA	-5.00	1.40	1.46
2	B	367	GLU	CD-OE1	5.00	1.34	1.25

All (239) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	HIS	CA-C-N	16.96	136.88	119.24
1	A	92	HIS	C-N-CA	16.96	136.88	119.24
1	A	20	VAL	CA-C-O	13.38	126.90	119.94
1	A	20	VAL	CB-CA-C	-12.91	97.12	110.16
2	B	208	ILE	N-CA-C	-12.10	99.09	110.82
2	B	260	HIS	N-CA-C	-11.35	99.44	113.18
2	B	364	GLU	CA-C-N	-10.63	111.47	122.74
2	B	364	GLU	C-N-CA	-10.63	111.47	122.74
2	B	304	LEU	N-CA-C	-10.14	98.45	112.25
2	B	265	GLY	CA-C-N	-9.60	108.15	123.23
2	B	265	GLY	C-N-CA	-9.60	108.15	123.23
1	A	214	ILE	CB-CA-C	-9.41	101.09	111.35
1	A	164	ARG	NE-CZ-NH2	-8.96	111.13	119.20
1	A	211	GLY	N-CA-C	8.90	124.22	110.96
2	B	340	CYS	N-CA-C	-8.86	101.59	111.07
1	A	142	ALA	N-CA-C	-8.80	101.69	111.28
2	B	264	THR	CA-C-N	-8.60	109.47	122.28
2	B	264	THR	C-N-CA	-8.60	109.47	122.28
2	B	379	ARG	NE-CZ-NH2	-8.49	111.56	119.20
1	A	98	GLY	O-C-N	-8.43	114.22	123.49
2	B	384	ILE	N-CA-C	8.10	119.86	110.62
2	B	284	ALA	N-CA-CB	-8.02	103.03	111.29
2	B	263	GLU	CG-CD-OE2	-7.94	100.15	118.40
2	B	318	SER	CA-C-N	-7.93	110.11	121.52
2	B	318	SER	C-N-CA	-7.93	110.11	121.52
2	B	249	SER	CA-C-N	-7.82	112.69	122.93
2	B	249	SER	C-N-CA	-7.82	112.69	122.93
2	B	138	ASP	CA-C-N	-7.79	110.55	120.60
2	B	138	ASP	C-N-CA	-7.79	110.55	120.60
2	B	386	THR	N-CA-C	-7.70	102.89	111.82
2	B	212	THR	OG1-CB-CG2	-7.61	94.09	109.30
2	B	98	ALA	N-CA-C	-7.60	102.97	111.71
2	B	49	LEU	N-CA-C	-7.59	103.08	111.36
2	B	100	ARG	N-CA-C	-7.57	103.04	111.82
1	A	237	ILE	N-CA-C	-7.54	103.45	110.53
2	B	240	MET	N-CA-C	-7.53	102.42	111.69
2	B	367	GLU	CA-C-N	-7.50	110.70	121.42
2	B	367	GLU	C-N-CA	-7.50	110.70	121.42
1	A	249	LYS	N-CA-C	7.46	120.06	111.11
2	B	92	LEU	N-CA-C	-7.42	102.57	111.69
2	B	143	SER	N-CA-C	7.38	123.72	113.45
2	B	352	SER	CA-CB-OG	-7.23	96.65	111.10
1	A	183	THR	CA-C-O	-7.22	113.20	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	PRO	O-C-N	7.21	129.96	122.18
2	B	364	GLU	N-CA-C	-7.19	103.17	112.23
1	A	146	HIS	CA-C-N	-7.17	112.01	122.40
1	A	146	HIS	C-N-CA	-7.17	112.01	122.40
2	B	354	ALA	N-CA-C	-7.04	103.54	111.14
1	A	247	SER	CA-C-O	7.02	128.08	120.08
1	A	213	GLY	CA-C-O	-7.01	111.24	119.02
1	A	147	ASN	N-CA-C	6.97	121.17	112.24
2	B	96	LEU	N-CA-C	-6.93	103.50	112.23
1	A	242	GLU	N-CA-C	-6.92	103.81	111.36
1	A	89	ARG	NE-CZ-NH1	-6.83	114.67	121.50
2	B	65	ILE	CB-CA-C	-6.83	103.08	112.24
1	A	79	ALA	N-CA-C	-6.83	103.90	111.82
1	A	9	ALA	CA-C-N	-6.82	108.92	120.58
1	A	9	ALA	C-N-CA	-6.82	108.92	120.58
1	A	263	LYS	CA-C-N	-6.76	110.54	120.28
1	A	263	LYS	C-N-CA	-6.76	110.54	120.28
2	B	157	ILE	CA-C-O	6.76	127.26	119.89
1	A	220	VAL	N-CA-C	-6.75	104.19	110.53
1	A	155	PRO	CB-CA-C	-6.73	102.70	110.92
2	B	276	VAL	N-CA-C	6.73	118.12	109.30
2	B	189	GLY	N-CA-C	6.69	126.51	115.34
1	A	78	PRO	N-CA-C	-6.68	104.44	113.40
2	B	151	LEU	N-CA-C	-6.64	104.08	111.71
2	B	177	TRP	CA-C-N	-6.64	110.37	122.38
2	B	177	TRP	C-N-CA	-6.64	110.37	122.38
1	A	260	SER	N-CA-CB	-6.63	100.37	110.12
2	B	25	LEU	N-CA-C	-6.58	103.94	112.23
1	A	14	ARG	CA-C-N	-6.56	112.69	122.07
1	A	14	ARG	C-N-CA	-6.56	112.69	122.07
2	B	264	THR	N-CA-C	-6.56	105.31	113.38
1	A	154	CYS	CA-C-N	6.54	127.11	120.38
1	A	154	CYS	C-N-CA	6.54	127.11	120.38
1	A	69	LEU	N-CA-C	-6.48	104.30	111.36
2	B	181	TYR	N-CA-C	6.46	120.01	111.75
2	B	12	PHE	N-CA-CB	-6.43	100.14	110.63
1	A	87	LEU	CA-C-N	-6.40	112.49	120.56
1	A	87	LEU	C-N-CA	-6.40	112.49	120.56
1	A	134	GLU	CA-C-N	-6.38	112.47	122.49
1	A	134	GLU	C-N-CA	-6.38	112.47	122.49
1	A	214	ILE	N-CA-CB	-6.38	104.63	111.46
2	B	281	GLY	CA-C-N	-6.37	111.42	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	281	GLY	C-N-CA	-6.37	111.42	121.87
2	B	30	GLU	CA-C-N	-6.37	110.63	120.31
2	B	30	GLU	C-N-CA	-6.37	110.63	120.31
1	A	239	LYS	CD-CE-NZ	6.36	132.25	111.90
1	A	193	LEU	CA-C-O	6.36	125.89	118.90
1	A	168	SER	N-CA-CB	-6.34	100.87	110.07
1	A	110	GLY	CA-C-N	6.31	128.74	120.60
1	A	110	GLY	C-N-CA	6.31	128.74	120.60
2	B	7	PRO	N-CD-CG	-6.31	93.73	103.20
2	B	224	PRO	N-CD-CG	-6.29	93.76	103.20
2	B	23	PRO	N-CA-C	-6.28	105.17	113.65
2	B	206	ARG	CD-NE-CZ	6.27	133.18	124.40
2	B	381	ASP	O-C-N	6.26	128.76	122.12
2	B	38	ASP	N-CA-C	6.24	118.53	109.04
1	A	43	ALA	CA-C-N	-6.24	112.38	122.30
1	A	43	ALA	C-N-CA	-6.24	112.38	122.30
2	B	32	PHE	N-CA-C	-6.21	104.59	111.36
2	B	394	ARG	NE-CZ-NH1	-6.19	115.31	121.50
2	B	11	GLU	N-CA-C	-6.17	105.78	113.38
2	B	43	ALA	N-CA-C	-6.16	104.11	111.69
1	A	182	VAL	CB-CA-C	-6.10	102.83	111.19
2	B	384	ILE	CA-C-N	-6.09	110.33	120.68
2	B	384	ILE	C-N-CA	-6.09	110.33	120.68
2	B	122	ALA	N-CA-C	-6.05	104.81	111.82
2	B	228	ILE	N-CA-C	6.04	117.18	108.48
1	A	42	ASP	N-CA-C	-6.04	105.17	112.54
1	A	215	SER	CA-C-O	6.04	125.61	118.79
2	B	183	THR	N-CA-C	-6.01	106.55	114.31
1	A	59	ALA	CA-C-N	-5.97	113.26	122.87
1	A	59	ALA	C-N-CA	-5.97	113.26	122.87
2	B	10	GLY	CA-C-O	-5.96	113.23	121.46
1	A	263	LYS	N-CA-C	-5.95	104.88	111.36
1	A	124	ASP	CA-C-N	-5.93	112.15	121.87
1	A	124	ASP	C-N-CA	-5.93	112.15	121.87
2	B	222	ARG	NE-CZ-NH2	-5.92	113.87	119.20
2	B	205	GLN	N-CA-C	-5.91	105.81	114.39
1	A	89	ARG	NE-CZ-NH2	5.89	124.50	119.20
1	A	145	ARG	CA-C-N	-5.89	113.24	122.49
1	A	145	ARG	C-N-CA	-5.89	113.24	122.49
1	A	141	GLN	N-CA-C	5.89	118.18	111.11
2	B	33	VAL	CA-CB-CG1	5.87	120.38	110.40
1	A	159	ASP	O-C-N	-5.85	116.39	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	PHE	CA-C-N	-5.82	112.15	120.42
1	A	258	PHE	C-N-CA	-5.82	112.15	120.42
2	B	175	ARG	N-CA-C	-5.81	104.85	111.07
2	B	90	GLN	N-CA-C	-5.80	105.30	112.90
1	A	155	PRO	N-CD-CG	-5.79	94.52	103.20
1	A	13	ASP	CA-C-N	-5.78	113.41	122.65
1	A	13	ASP	C-N-CA	-5.78	113.41	122.65
2	B	266	GLU	CA-CB-CG	-5.71	102.67	114.10
2	B	65	ILE	N-CA-C	-5.69	104.80	111.00
1	A	166	VAL	CA-CB-CG2	-5.67	100.76	110.40
2	B	180	SER	O-C-N	5.66	129.33	122.20
2	B	355	LEU	CB-CA-C	-5.61	101.83	110.81
1	A	69	LEU	CA-C-N	-5.61	112.77	120.28
1	A	69	LEU	C-N-CA	-5.61	112.77	120.28
2	B	366	PRO	CA-C-N	-5.60	113.68	122.65
2	B	366	PRO	C-N-CA	-5.60	113.68	122.65
1	A	10	GLN	CA-C-N	-5.60	112.22	120.28
1	A	10	GLN	C-N-CA	-5.60	112.22	120.28
1	A	250	GLN	N-CA-C	5.58	118.08	111.33
2	B	298	TYR	CA-CB-CG	-5.56	103.89	113.90
2	B	263	GLU	CA-C-N	-5.56	112.65	122.26
2	B	263	GLU	C-N-CA	-5.56	112.65	122.26
1	A	108	ASN	N-CA-C	5.55	122.63	110.80
2	B	240	MET	CG-SD-CE	-5.55	88.69	100.90
2	B	27	GLN	CG-CD-NE2	-5.54	108.09	116.40
2	B	384	ILE	CA-CB-CG1	-5.54	100.98	110.40
2	B	182	GLU	CA-C-N	-5.53	113.55	122.24
2	B	182	GLU	C-N-CA	-5.53	113.55	122.24
2	B	83	GLY	CA-C-O	5.53	125.19	119.27
2	B	386	THR	O-C-N	-5.53	115.47	122.27
2	B	287	MET	N-CA-C	-5.53	100.17	108.96
1	A	224	VAL	CB-CA-C	-5.52	104.69	112.14
2	B	29	GLU	CB-CA-C	-5.50	101.66	110.79
2	B	167	LYS	N-CA-C	-5.50	105.44	111.82
1	A	70	ARG	NE-CZ-NH1	-5.50	116.00	121.50
2	B	321	ARG	CB-CG-CD	5.49	123.93	111.30
2	B	206	ARG	N-CA-C	5.48	119.59	113.01
1	A	16	GLU	CA-C-N	-5.46	113.43	121.30
1	A	16	GLU	C-N-CA	-5.46	113.43	121.30
2	B	327	ILE	N-CA-CB	-5.45	103.56	111.52
2	B	285	PRO	CA-C-O	-5.45	115.38	121.32
2	B	36	GLN	CA-C-N	-5.42	113.97	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	36	GLN	C-N-CA	-5.42	113.97	122.65
2	B	337	LYS	O-C-N	5.42	127.66	122.07
2	B	61	LYS	CA-C-O	-5.38	114.56	120.69
2	B	163	SER	CA-C-N	-5.36	114.62	122.40
2	B	163	SER	C-N-CA	-5.36	114.62	122.40
2	B	159	VAL	N-CA-C	5.36	115.31	107.37
2	B	107	ILE	CB-CA-C	-5.36	102.70	110.63
1	A	82	PHE	N-CA-C	-5.35	105.49	112.23
2	B	162	GLY	CA-C-N	-5.34	113.38	122.56
2	B	162	GLY	C-N-CA	-5.34	113.38	122.56
2	B	164	ALA	CA-C-O	-5.33	114.20	120.81
1	A	260	SER	CA-CB-OG	-5.32	100.45	111.10
2	B	286	MET	CA-CB-CG	5.31	124.72	114.10
2	B	201	VAL	CA-C-N	5.31	127.39	120.28
2	B	201	VAL	C-N-CA	5.31	127.39	120.28
2	B	70	ARG	CB-CA-C	-5.30	102.48	111.02
2	B	183	THR	OG1-CB-CG2	-5.30	98.69	109.30
2	B	237	ALA	CB-CA-C	-5.30	102.53	110.90
2	B	300	ILE	CA-C-N	-5.29	115.64	123.05
2	B	300	ILE	C-N-CA	-5.29	115.64	123.05
1	A	51	GLY	CA-C-N	-5.28	118.18	123.04
1	A	51	GLY	C-N-CA	-5.28	118.18	123.04
2	B	148	ARG	N-CA-C	-5.28	105.42	111.07
2	B	293	GLN	CB-CA-C	-5.28	100.82	109.53
2	B	235	SER	CA-C-N	-5.26	113.23	120.28
2	B	235	SER	C-N-CA	-5.26	113.23	120.28
1	A	257	SER	CA-C-O	-5.25	115.31	120.82
2	B	218	ASP	N-CA-C	5.24	116.99	111.28
2	B	231	VAL	CA-C-O	-5.24	115.01	120.51
2	B	74	TYR	N-CA-C	-5.23	100.50	109.24
1	A	207	PRO	CA-C-N	-5.23	114.36	122.09
1	A	207	PRO	C-N-CA	-5.23	114.36	122.09
2	B	4	LEU	CA-C-O	5.21	125.94	119.79
2	B	290	ALA	N-CA-C	5.20	118.88	112.54
2	B	363	ARG	N-CA-C	5.20	117.69	111.71
2	B	101	MET	N-CA-C	-5.19	106.92	113.20
2	B	163	SER	N-CA-C	-5.19	106.79	113.02
1	A	52	VAL	CG1-CB-CG2	-5.18	99.40	110.80
2	B	211	GLU	N-CA-C	-5.17	105.72	111.36
2	B	321	ARG	NE-CZ-NH1	-5.14	116.36	121.50
2	B	102	GLY	N-CA-C	-5.14	108.53	115.36
1	A	63	THR	N-CA-C	5.13	117.28	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ILE	N-CA-C	5.13	116.67	108.87
2	B	139	VAL	N-CA-C	5.12	115.73	110.36
1	A	210	GLN	CA-CB-CG	-5.11	103.89	114.10
2	B	216	ILE	CG1-CB-CG2	-5.11	95.38	110.70
1	A	166	VAL	N-CA-C	5.10	115.82	110.62
2	B	49	LEU	CA-C-O	5.10	125.83	120.42
2	B	384	ILE	CA-C-O	5.09	126.34	121.05
2	B	222	ARG	NE-CZ-NH1	5.08	126.58	121.50
2	B	379	ARG	N-CA-C	-5.07	102.56	110.42
1	A	127	LEU	CA-C-N	-5.07	116.22	123.11
1	A	127	LEU	C-N-CA	-5.07	116.22	123.11
2	B	341	ARG	CA-C-N	-5.06	114.21	122.26
2	B	341	ARG	C-N-CA	-5.06	114.21	122.26
2	B	373	VAL	CA-CB-CG1	-5.06	101.80	110.40
1	A	119	GLU	N-CA-C	-5.04	105.86	111.36
2	B	284	ALA	N-CA-C	5.04	112.56	108.07
1	A	146	HIS	N-CA-C	-5.03	105.87	112.41
2	B	386	THR	CA-C-N	-5.02	112.06	120.30
2	B	386	THR	C-N-CA	-5.02	112.06	120.30
1	A	133	VAL	O-C-N	5.02	126.74	121.87
2	B	61	LYS	CA-C-N	5.02	129.51	122.79
2	B	61	LYS	C-N-CA	5.02	129.51	122.79
2	B	97	LEU	CA-C-N	-5.01	113.07	120.28
2	B	97	LEU	C-N-CA	-5.01	113.07	120.28
2	B	57	THR	N-CA-C	-5.01	102.11	110.17
2	B	179	GLY	O-C-N	-5.01	116.19	122.70
2	B	81	LEU	N-CA-C	-5.00	103.08	110.48
1	A	57	PRO	CA-N-CD	5.00	119.00	112.00

There are no chirality outliers.

There are no planarity outliers.

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	1970	0	1972	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2977	0	2954	85	0
3	A	17	0	11	1	0
4	B	1	0	0	0	0
5	B	15	0	6	1	0
6	A	82	0	0	1	0
6	B	155	0	0	4	0
All	All	5217	0	4943	166	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 17.

All (166) 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)
2:B:46:ALA:CA	2:B:46:ALA:CB	1.77	1.61
1:A:25:LEU:CG	1:A:25:LEU:CD1	1.77	1.60
2:B:139:VAL:CB	2:B:139:VAL:CG2	1.78	1.60
1:A:232:ILE:CD1	1:A:232:ILE:CG1	1.78	1.60
1:A:57:PRO:CG	1:A:57:PRO:CB	1.80	1.56
1:A:36:ILE:CD1	1:A:36:ILE:CG1	1.75	1.54
2:B:346:ILE:CD1	2:B:346:ILE:CG1	1.85	1.51
1:A:192:PRO:CB	1:A:192:PRO:CG	1.77	1.50
1:A:239:LYS:CE	1:A:239:LYS:NZ	1.72	1.49
1:A:150:PRO:CB	1:A:150:PRO:CG	1.76	1.44
1:A:62:PRO:CB	1:A:62:PRO:CG	1.83	1.43
1:A:1:MET:CE	1:A:1:MET:SD	2.13	1.37
2:B:240:MET:CE	2:B:240:MET:SD	1.21	1.29
2:B:240:MET:CE	2:B:240:MET:CG	2.23	1.16
2:B:240:MET:SD	2:B:240:MET:HE3	1.78	1.14
1:A:196:LEU:H	1:A:196:LEU:CD1	1.61	1.13
2:B:240:MET:SD	2:B:240:MET:HE1	1.78	1.13
1:A:196:LEU:HD12	1:A:196:LEU:N	1.63	1.09
2:B:240:MET:SD	2:B:240:MET:HE2	1.78	1.09
1:A:196:LEU:CD1	1:A:196:LEU:N	2.14	1.07
1:A:196:LEU:H	1:A:196:LEU:HD13	1.25	1.02
2:B:61:LYS:HE3	6:B:409:HOH:O	1.71	0.89
1:A:211:GLY:O	1:A:212:PHE:HB2	1.74	0.86
1:A:220:VAL:O	1:A:224:VAL:HG23	1.77	0.84
1:A:25:LEU:CD1	1:A:25:LEU:CD2	2.60	0.80
1:A:127:LEU:HD23	1:A:128:VAL:N	1.99	0.78
1:A:171:ARG:HH11	1:A:171:ARG:HG2	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LEU:HD23	1:A:127:LEU:C	2.07	0.77
1:A:232:ILE:CD1	1:A:232:ILE:CB	2.63	0.77
2:B:139:VAL:CG2	2:B:139:VAL:CG1	2.67	0.72
1:A:38:ASP:OD2	1:A:91:LYS:NZ	2.21	0.72
2:B:139:VAL:CG2	2:B:139:VAL:CA	2.69	0.70
1:A:108:ASN:HA	6:A:460:HOH:O	1.95	0.67
1:A:36:ILE:CD1	1:A:36:ILE:CB	2.72	0.65
2:B:263:GLU:H	2:B:263:GLU:CD	2.04	0.64
1:A:127:LEU:C	1:A:127:LEU:CD2	2.70	0.64
1:A:25:LEU:CD1	1:A:25:LEU:CB	2.72	0.63
2:B:240:MET:CE	2:B:240:MET:HG3	2.25	0.63
1:A:20:VAL:HB	1:A:232:ILE:HG12	1.80	0.62
2:B:116:GLY:HA2	2:B:132:ILE:HD13	1.81	0.62
2:B:121:LEU:C	2:B:121:LEU:HD12	2.26	0.61
2:B:300:ILE:HB	2:B:329:ASP:CG	2.25	0.60
1:A:56:ASP:N	1:A:57:PRO:CD	2.64	0.60
1:A:137:ALA:HB3	1:A:138:PRO:CD	2.32	0.59
2:B:46:ALA:CB	2:B:46:ALA:C	2.69	0.57
1:A:56:ASP:N	1:A:57:PRO:HD3	2.19	0.57
2:B:227:VAL:HG12	2:B:373:VAL:HB	1.87	0.56
1:A:41:ILE:HD11	1:A:48:LEU:HD11	1.86	0.56
1:A:195:HIS:O	1:A:196:LEU:C	2.46	0.56
1:A:234:GLY:O	1:A:235:SER:C	2.45	0.56
2:B:271:LEU:HD23	2:B:271:LEU:C	2.31	0.56
2:B:222:ARG:NH2	6:B:512:HOH:O	2.40	0.55
2:B:229:ALA:HB1	2:B:236:ASN:HD21	1.72	0.55
1:A:157:ASN:OD1	1:A:157:ASN:N	2.32	0.55
2:B:379:ARG:HD2	2:B:381:ASP:OD2	2.05	0.55
1:A:20:VAL:O	1:A:232:ILE:HA	2.07	0.55
2:B:240:MET:CG	2:B:240:MET:HE3	2.22	0.55
2:B:240:MET:HE3	2:B:240:MET:O	2.07	0.54
2:B:271:LEU:HD23	2:B:271:LEU:O	2.07	0.54
2:B:384:ILE:HG22	2:B:385:PHE:N	2.22	0.53
1:A:60:ASP:OD1	1:A:64:ILE:HG21	2.09	0.53
2:B:134:MET:O	2:B:158:PRO:HA	2.08	0.53
2:B:206:ARG:HD3	2:B:210:GLU:OE2	2.09	0.52
1:A:58:LEU:C	1:A:58:LEU:HD12	2.35	0.52
1:A:157:ASN:O	1:A:158:ALA:C	2.52	0.52
2:B:333:LEU:HD11	2:B:390:ILE:HD13	1.92	0.52
2:B:229:ALA:HB1	2:B:236:ASN:ND2	2.24	0.52
2:B:116:GLY:CA	2:B:132:ILE:HD13	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PRO:HA	1:A:68:ASN:OD1	2.09	0.51
2:B:87:LYS:HD2	2:B:114:GLN:HG3	1.92	0.51
2:B:138:ASP:O	2:B:139:VAL:C	2.48	0.51
2:B:59:LEU:O	2:B:219:LYS:NZ	2.45	0.50
1:A:193:LEU:O	1:A:197:ILE:HG13	2.11	0.50
2:B:240:MET:CG	2:B:240:MET:HE2	2.22	0.49
2:B:298:TYR:CG	2:B:299:SER:N	2.78	0.49
2:B:22:MET:N	2:B:23:PRO:CD	2.75	0.49
1:A:177:LEU:HD11	1:A:212:PHE:CD2	2.47	0.49
1:A:67:ALA:HB2	1:A:238:VAL:HG11	1.94	0.49
2:B:46:ALA:CB	2:B:46:ALA:N	2.67	0.49
2:B:143:SER:N	2:B:144:PRO:HD2	2.26	0.49
1:A:179:ARG:HG3	1:A:180:SER:O	2.13	0.49
1:A:159:ASP:O	1:A:160:ASP:C	2.54	0.48
1:A:4:TYR:HE2	1:A:125:SER:HB3	1.77	0.48
1:A:137:ALA:HB3	1:A:138:PRO:HD3	1.95	0.48
2:B:32:PHE:CG	2:B:200:ILE:HG12	2.49	0.47
1:A:130:ASP:OD1	1:A:130:ASP:N	2.47	0.47
2:B:109:GLU:HG3	2:B:170:CYS:SG	2.55	0.47
1:A:171:ARG:HG2	1:A:171:ARG:NH1	2.24	0.47
2:B:97:LEU:O	2:B:98:ALA:C	2.55	0.47
2:B:143:SER:HB2	2:B:144:PRO:HD3	1.96	0.47
1:A:7:LEU:O	1:A:8:PHE:C	2.56	0.47
2:B:163:SER:O	2:B:164:ALA:HB3	2.14	0.47
1:A:22:PHE:C	1:A:22:PHE:CD1	2.92	0.46
2:B:38:ASP:HA	2:B:39:PRO:HD2	1.88	0.46
2:B:257:PRO:HG2	2:B:268:GLY:HA3	1.98	0.46
1:A:162:LEU:O	1:A:166:VAL:HG23	2.16	0.45
2:B:111:GLY:O	2:B:138:ASP:HB3	2.15	0.45
1:A:69:LEU:HD22	1:A:69:LEU:HA	1.71	0.45
2:B:339:LEU:O	2:B:340:CYS:C	2.59	0.45
1:A:4:TYR:CE2	1:A:125:SER:HB3	2.51	0.45
2:B:300:ILE:HG12	2:B:300:ILE:O	2.16	0.45
1:A:211:GLY:O	1:A:212:PHE:CB	2.47	0.45
2:B:233:GLY:N	5:B:402:PLP:O2P	2.44	0.45
2:B:142:GLN:O	2:B:146:VAL:HG23	2.16	0.45
2:B:144:PRO:HB2	2:B:148:ARG:HH12	1.81	0.45
1:A:108:ASN:ND2	1:A:109:ASN:ND2	2.65	0.45
2:B:346:ILE:CD1	2:B:346:ILE:CB	2.83	0.45
1:A:95:ILE:O	1:A:95:ILE:HG23	2.17	0.45
2:B:132:ILE:HD12	2:B:149:MET:SD	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LYS:O	1:A:264:ALA:C	2.57	0.44
2:B:38:ASP:OD1	2:B:38:ASP:C	2.59	0.44
2:B:305:ASP:HB3	6:B:555:HOH:O	2.17	0.44
1:A:264:ALA:HA	1:A:267:ARG:NH1	2.32	0.44
2:B:346:ILE:HG21	2:B:384:ILE:HD11	1.99	0.44
1:A:216:SER:HA	1:A:217:PRO:HD3	1.84	0.44
1:A:77:THR:HB	1:A:78:PRO:CD	2.48	0.44
1:A:8:PHE:CD2	1:A:207:PRO:HG2	2.53	0.44
2:B:277:GLY:O	2:B:283:LYS:HA	2.18	0.44
2:B:87:LYS:HD3	2:B:115:HIS:HA	2.00	0.44
2:B:241:PHE:O	2:B:242:ALA:C	2.56	0.44
2:B:135:GLY:O	2:B:138:ASP:N	2.51	0.44
1:A:104:ASN:HB2	2:B:278:ILE:O	2.18	0.43
1:A:153:ILE:HD11	3:A:401:IAG:HC4	2.01	0.43
1:A:177:LEU:HD11	1:A:212:PHE:CG	2.53	0.43
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.53	0.43
2:B:372:LEU:N	2:B:372:LEU:HD23	2.31	0.43
1:A:61:GLY:O	1:A:65:GLN:HG3	2.19	0.43
2:B:195:HIS:CG	2:B:196:PRO:HA	2.53	0.43
1:A:163:LEU:HD13	1:A:199:LYS:HD3	2.01	0.43
2:B:95:ALA:CB	2:B:126:LEU:HD12	2.48	0.43
2:B:11:GLU:HG2	2:B:11:GLU:O	2.19	0.43
1:A:96:PRO:HA	1:A:124:ASP:OD2	2.19	0.42
2:B:346:ILE:HG21	2:B:384:ILE:CD1	2.48	0.42
1:A:10:GLN:O	1:A:11:LEU:C	2.60	0.42
1:A:62:PRO:O	1:A:63:THR:C	2.62	0.42
2:B:65:ILE:HD13	2:B:65:ILE:HA	1.79	0.42
2:B:371:LEU:C	2:B:372:LEU:HD23	2.44	0.42
2:B:143:SER:N	2:B:144:PRO:CD	2.82	0.42
1:A:258:PHE:O	1:A:262:MET:HG2	2.20	0.42
1:A:263:LYS:HA	1:A:263:LYS:HD2	1.93	0.42
2:B:61:LYS:CE	6:B:409:HOH:O	2.47	0.42
1:A:81:CYS:O	1:A:84:MET:HB2	2.19	0.41
2:B:339:LEU:HD23	2:B:347:PRO:HB3	2.02	0.41
1:A:37:ILE:HG23	1:A:48:LEU:HD13	2.01	0.41
2:B:55:ARG:HH21	2:B:211:GLU:CD	2.29	0.41
2:B:94:GLN:O	2:B:97:LEU:HB2	2.20	0.41
2:B:171:ASN:O	2:B:175:ARG:HG3	2.21	0.41
1:A:77:THR:HB	1:A:78:PRO:HD2	2.03	0.41
2:B:348:ALA:HB1	2:B:350:GLU:OE1	2.20	0.41
1:A:111:ILE:HD13	1:A:111:ILE:HG21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:PRO:O	2:B:145:ASN:C	2.59	0.41
1:A:5:GLU:H	1:A:5:GLU:CD	2.29	0.41
1:A:155:PRO:HD2	1:A:158:ALA:HB2	2.02	0.41
2:B:387:VAL:O	2:B:391:LEU:HG	2.21	0.41
1:A:63:THR:OG1	1:A:239:LYS:NZ	2.47	0.41
1:A:160:ASP:HA	1:A:163:LEU:HD12	2.03	0.41
2:B:206:ARG:C	2:B:208:ILE:H	2.29	0.41
1:A:195:HIS:CE1	1:A:199:LYS:NZ	2.89	0.40
2:B:32:PHE:CD1	2:B:200:ILE:HG12	2.56	0.40
2:B:294:ILE:HD12	2:B:294:ILE:HG23	1.82	0.40
2:B:365:GLN:HA	2:B:366:PRO:HD2	1.87	0.40
1:A:76:VAL:HA	1:A:80:GLN:OE1	2.22	0.40
2:B:90:GLN:HA	2:B:204:PHE:HB3	2.04	0.40
1:A:195:HIS:CE1	1:A:199:LYS:CE	3.05	0.40
2:B:349:LEU:O	2:B:352:SER:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	258/268 (96%)	249 (96%)	7 (3%)	2 (1%)	16	20
2	B	391/396 (99%)	380 (97%)	11 (3%)	0	100	100
All	All	649/664 (98%)	629 (97%)	18 (3%)	2 (0%)	36	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	GLY
1	A	108	ASN

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	204/208 (98%)	197 (97%)	7 (3%)	32	49
2	B	308/310 (99%)	298 (97%)	10 (3%)	34	51
All	All	512/518 (99%)	495 (97%)	17 (3%)	33	50

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	69	LEU
1	A	123	VAL
1	A	127	LEU
1	A	151	ILE
1	A	196	LEU
1	A	247	SER
2	B	2	THR
2	B	88	THR
2	B	106	ILE
2	B	236	ASN
2	B	263	GLU
2	B	297	SER
2	B	301	SER
2	B	367	GLU
2	B	384	ILE
2	B	386	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	66	ASN
1	A	195	HIS
2	B	26	ASN
2	B	63	GLN

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Mol	Chain	Res	Type
2	B	160	HIS
2	B	236	ASN
2	B	246	ASN
2	B	365	GLN
2	B	375	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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	IAG	A	401	-	18,18,18	1.85	7 (38%)	24,24,24	3.39	9 (37%)
5	PLP	B	402	2	15,15,16	2.37	7 (46%)	21,22,23	2.61	6 (28%)

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	IAG	A	401	-	-	3/9/9/9	0/2/2/2
5	PLP	B	402	2	-	0/6/6/8	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	402	PLP	C3-C2	-5.14	1.35	1.41
3	A	401	IAG	O1-C10	4.54	1.32	1.23
5	B	402	PLP	C3-C4	-4.02	1.32	1.40
5	B	402	PLP	C5A-C5	3.23	1.59	1.50
3	A	401	IAG	C7-C2	-3.11	1.38	1.44
5	B	402	PLP	P-O1P	-2.85	1.41	1.50
3	A	401	IAG	C9-C10	-2.64	1.48	1.51
3	A	401	IAG	C3-C7	-2.44	1.36	1.39
5	B	402	PLP	O4P-C5A	-2.34	1.36	1.44
3	A	401	IAG	C1-N1	2.24	1.40	1.37
5	B	402	PLP	C6-N1	2.13	1.38	1.34
5	B	402	PLP	C4A-C4	2.05	1.55	1.51
3	A	401	IAG	C9-C2	2.02	1.52	1.50
3	A	401	IAG	O2-C12	2.01	1.28	1.22

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	IAG	C9-C10-N2	-12.85	99.39	116.25
5	B	402	PLP	O4P-C5A-C5	6.20	120.97	109.36
5	B	402	PLP	O3P-P-O4P	5.69	121.52	106.67
3	A	401	IAG	O1-C10-C9	5.15	129.51	121.40
5	B	402	PLP	O2P-P-O4P	-4.72	94.35	106.67
5	B	402	PLP	C3-C4-C5	4.19	123.61	118.59
3	A	401	IAG	O1-C10-N2	4.09	131.05	123.03
3	A	401	IAG	C9-C2-C1	-3.78	121.68	126.84
3	A	401	IAG	O3-C12-C11	3.62	126.56	112.81
3	A	401	IAG	C7-C2-C1	3.03	109.26	106.16
5	B	402	PLP	C6-C5-C4	-3.00	115.64	118.10
5	B	402	PLP	C4A-C4-C3	-2.71	116.01	120.52
3	A	401	IAG	C2-C1-N1	-2.63	107.42	110.31
3	A	401	IAG	O3-C12-O2	-2.37	117.23	123.33
3	A	401	IAG	C11-N2-C10	-2.19	115.14	121.49

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	IAG	C1-C2-C9-C10
3	A	401	IAG	O1-C10-C9-C2
3	A	401	IAG	N2-C10-C9-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	IAG	1	0
5	B	402	PLP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	261/268 (97%)	-0.44	3 (1%) 78 79	11, 21, 43, 67	2 (0%)
2	B	393/396 (99%)	-0.67	3 (0%) 82 83	7, 15, 31, 78	0
All	All	654/664 (98%)	-0.58	6 (0%) 81 82	7, 18, 37, 78	2 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	394	ARG	2.9
1	A	194	HIS	2.8
2	B	393	ALA	2.6
1	A	192	PRO	2.5
1	A	268	ALA	2.4
2	B	385	PHE	2.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	IAG	A	401	17/17	0.91	0.09	21,27,46,46	0
5	PLP	B	402	15/16	0.97	0.07	3,15,23,30	0
4	NA	B	403	1/1	0.98	0.22	3,3,3,3	0

6.5 Other polymers [i](#)

There are no such residues in this entry.