



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:03 AM UTC

PDB ID : 1K8Y / pdb_00001k8y
Title : CRYSTAL STRUCTURE OF THE TRYPTOPHAN SYNTHASE BETA-SER178PRO MUTANT COMPLEXED WITH D,L-ALPHA-GLYCEROL-3-PHOSPHATE
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Deposited on : 2001-10-26
Resolution : 1.50 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

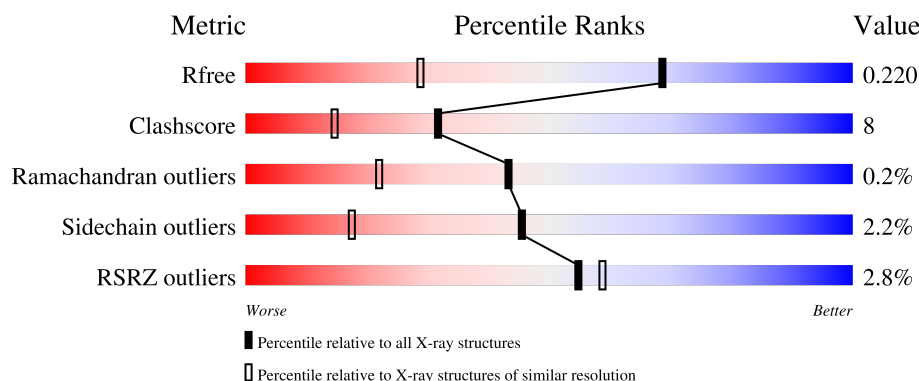
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	
2	B	396	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	13P	A	701	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5617 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	255	Total	C	N	O	S	0	6	0
			1947	1237	335	367	8			

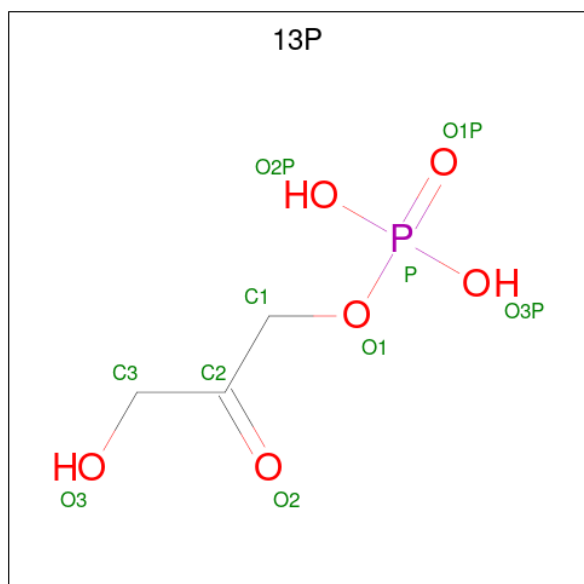
- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	390	Total	C	N	O	S	0	9	0
			2986	1873	527	566	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	34	SER	ARG	cloning artifact	UNP P0A2K1
B	178	PRO	SER	engineered mutation	UNP P0A2K1

- Molecule 3 is 1,3-DIHYDROXYACETONEPHOSPHATE (CCD ID: 13P) (formula: $C_3H_7O_6P$).

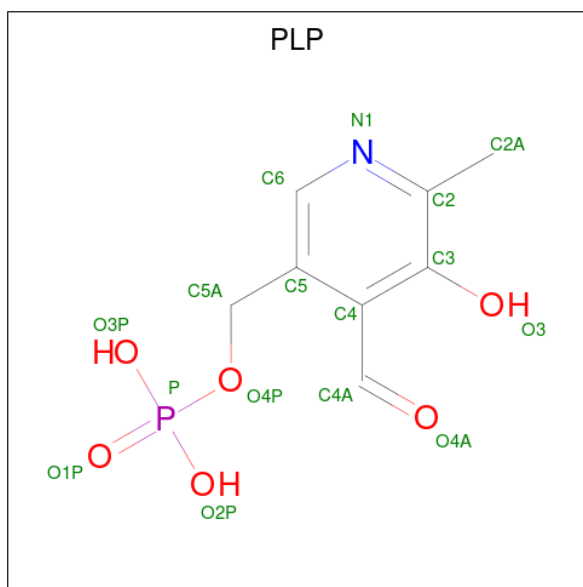


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			10	3	6	1		

- 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		

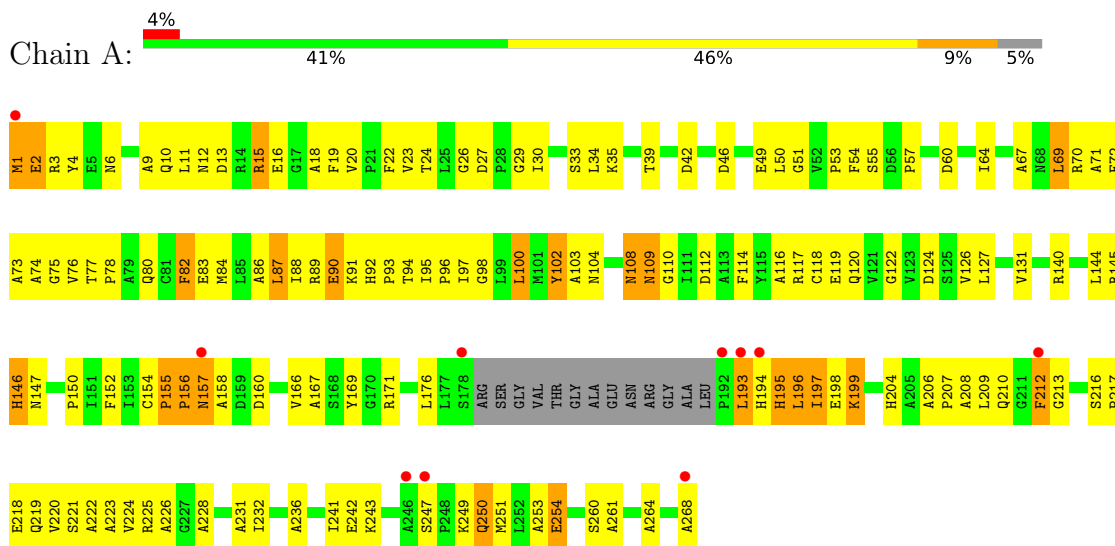
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	214	Total	O	0	0
			214	214		
6	B	444	Total	O	0	0
			444	444		

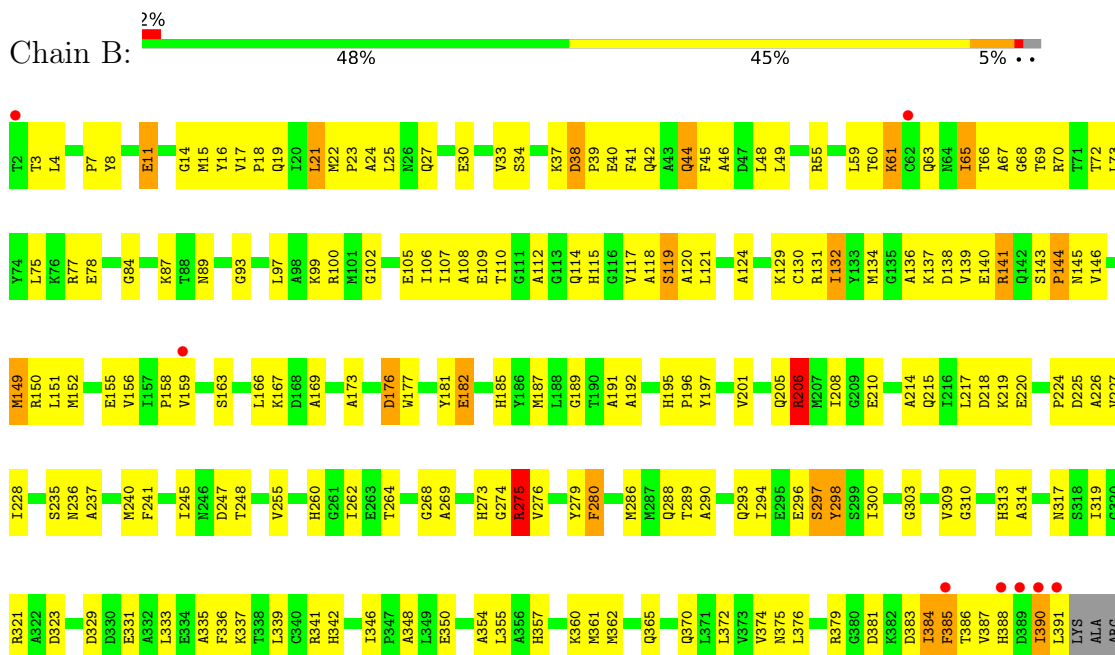
3 Residue-property plots

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



GLY
GLU
ILE

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.14Å 60.47Å 67.44Å 90.00° 94.63° 90.00°	Depositor
Resolution (Å)	20.00 – 1.50 20.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.1 (20.00-1.50) 95.1 (20.00-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 1.50Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.171 , 0.209 0.186 , 0.220	Depositor DCC
R_{free} test set	5721 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.697	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5617	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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: PLP, 13P, NA

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	2.67	134/2014 (6.7%)	2.30	107/2733 (3.9%)
2	B	2.71	186/3100 (6.0%)	2.25	117/4185 (2.8%)
All	All	2.69	320/5114 (6.3%)	2.27	224/6918 (3.2%)

All (320) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	319	ILE	C-O	25.28	1.52	1.24
2	B	152	MET	SD-CE	-16.73	1.37	1.79
2	B	388	HIS	CA-C	-14.82	1.33	1.52
2	B	149	MET	CG-SD	13.99	2.15	1.80
1	A	84	MET	SD-CE	-13.75	1.45	1.79
2	B	22	MET	SD-CE	-13.43	1.46	1.79
1	A	82	PHE	CD1-CE1	13.21	1.78	1.38
2	B	362	MET	SD-CE	-12.33	1.48	1.79
2	B	385	PHE	CA-CB	-12.22	1.33	1.53
2	B	45	PHE	CG-CD1	11.75	1.63	1.38
2	B	55	ARG	CA-C	-10.66	1.40	1.53
2	B	39	PRO	C-O	10.53	1.37	1.24
2	B	158	PRO	C-O	10.39	1.35	1.23
1	A	225	ARG	NE-CZ	10.07	1.44	1.33
2	B	143	SER	CA-C	10.06	1.65	1.52
2	B	41	PHE	C-O	9.82	1.35	1.24
1	A	96	PRO	C-O	9.60	1.34	1.23
2	B	173	ALA	CA-CB	9.22	1.67	1.53
2	B	145	ASN	C-O	9.12	1.34	1.24
1	A	251	MET	C-O	9.04	1.34	1.24
2	B	141	ARG	C-O	8.79	1.36	1.24
2	B	21	LEU	C-O	8.74	1.35	1.24
2	B	275	ARG	N-CA	8.71	1.56	1.45
1	A	144	LEU	C-O	8.66	1.34	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	109	ASN	CA-C	-8.64	1.41	1.52
1	A	103	ALA	CA-C	-8.60	1.41	1.52
1	A	120	GLN	N-CA	8.37	1.56	1.46
1	A	108	ASN	CG-ND2	-8.34	1.15	1.33
2	B	138	ASP	C-O	8.23	1.34	1.24
2	B	385	PHE	CB-CG	-8.21	1.31	1.50
1	A	109	ASN	N-CA	-8.20	1.36	1.46
1	A	261	ALA	C-O	8.19	1.33	1.24
2	B	139	VAL	N-CA	8.16	1.56	1.46
1	A	15	ARG	CA-CB	8.10	1.66	1.53
2	B	237	ALA	CA-CB	8.06	1.66	1.53
2	B	140	GLU	C-O	8.05	1.34	1.24
1	A	169	TYR	CD1-CE1	8.05	1.62	1.38
1	A	109	ASN	CG-OD1	8.04	1.38	1.23
1	A	89	ARG	CZ-NH2	8.04	1.43	1.33
2	B	100	ARG	CZ-NH1	-8.01	1.21	1.32
1	A	199	LYS	C-O	8.01	1.33	1.24
1	A	24	THR	C-O	7.97	1.33	1.24
2	B	61	LYS	N-CA	7.95	1.56	1.46
2	B	296	GLU	N-CA	7.93	1.55	1.45
2	B	44	GLN	CA-C	7.89	1.62	1.52
2	B	276	VAL	CA-CB	-7.84	1.46	1.54
2	B	30	GLU	C-O	7.82	1.33	1.24
1	A	131	VAL	C-O	7.80	1.31	1.23
2	B	360	LYS	CB-CG	-7.77	1.29	1.52
2	B	18	PRO	CA-C	-7.76	1.43	1.52
2	B	372	LEU	N-CA	7.75	1.55	1.46
1	A	254[A]	GLU	CA-C	7.74	1.63	1.52
1	A	254[B]	GLU	CA-C	7.74	1.63	1.52
1	A	30	ILE	CA-CB	-7.72	1.45	1.54
2	B	341	ARG	CZ-NH1	7.67	1.43	1.32
2	B	339	LEU	N-CA	7.65	1.55	1.46
2	B	132	ILE	CA-CB	-7.63	1.44	1.54
2	B	290	ALA	N-CA	7.55	1.55	1.46
1	A	78	PRO	C-O	7.51	1.33	1.24
1	A	217	PRO	C-O	7.48	1.33	1.24
2	B	109	GLU	CA-CB	7.48	1.65	1.53
1	A	207	PRO	CA-CB	7.41	1.64	1.53
1	A	39	THR	C-N	7.40	1.43	1.33
1	A	104	ASN	CA-CB	7.38	1.65	1.53
1	A	120	GLN	CD-OE1	7.38	1.37	1.23
2	B	149	MET	CA-CB	7.37	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	HIS	C-O	7.36	1.33	1.24
2	B	375	ASN	CG-OD1	7.35	1.37	1.23
2	B	37	LYS	C-O	7.33	1.34	1.23
1	A	55	SER	C-O	7.33	1.32	1.24
2	B	11	GLU	CD-OE2	7.31	1.39	1.25
2	B	17	VAL	CA-CB	7.29	1.61	1.55
2	B	280	PHE	CA-C	-7.26	1.43	1.52
1	A	264	ALA	CA-CB	7.23	1.65	1.53
2	B	192	ALA	CA-CB	7.21	1.63	1.53
2	B	72	THR	CA-CB	-7.20	1.43	1.53
2	B	99	LYS	C-O	7.14	1.33	1.24
2	B	155	GLU	N-CA	7.13	1.54	1.46
2	B	102	GLY	CA-C	-7.12	1.41	1.51
1	A	228	ALA	C-O	7.11	1.33	1.23
1	A	4	TYR	N-CA	-7.08	1.37	1.46
1	A	220	VAL	N-CA	-7.05	1.38	1.46
2	B	124	ALA	C-O	7.04	1.32	1.24
1	A	73	ALA	N-CA	7.03	1.55	1.46
2	B	151	LEU	N-CA	7.02	1.54	1.46
2	B	146	VAL	N-CA	-6.98	1.38	1.46
2	B	354	ALA	CA-CB	6.98	1.64	1.53
1	A	11	LEU	CA-C	6.97	1.62	1.52
1	A	260	SER	C-O	6.95	1.32	1.24
2	B	262	ILE	CA-CB	-6.92	1.46	1.54
1	A	98	GLY	N-CA	6.91	1.53	1.45
1	A	93	PRO	C-O	-6.90	1.15	1.24
2	B	67	ALA	C-O	-6.88	1.15	1.23
2	B	375	ASN	CG-ND2	-6.87	1.18	1.33
1	A	88	ILE	CA-CB	6.87	1.63	1.54
2	B	323	ASP	C-O	6.87	1.32	1.24
2	B	136	ALA	CA-CB	6.86	1.64	1.53
1	A	249	LYS	C-O	6.85	1.32	1.24
2	B	121	LEU	C-O	6.85	1.32	1.24
2	B	390	ILE	CA-C	-6.82	1.44	1.52
2	B	158	PRO	CA-CB	6.82	1.62	1.53
1	A	87	LEU	CG-CD1	6.81	1.75	1.52
1	A	11	LEU	C-O	6.78	1.32	1.24
2	B	240	MET	CA-C	-6.76	1.44	1.52
1	A	152	PHE	CA-C	-6.76	1.44	1.52
1	A	69	LEU	N-CA	6.75	1.54	1.46
1	A	212	PHE	C-O	6.74	1.32	1.24
1	A	73	ALA	C-O	6.74	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	117	VAL	CA-C	-6.73	1.44	1.52
2	B	39	PRO	C-N	-6.71	1.24	1.33
1	A	11	LEU	N-CA	-6.71	1.37	1.46
2	B	73	LEU	N-CA	6.71	1.54	1.46
2	B	181	TYR	C-O	-6.69	1.15	1.24
1	A	251	MET	N-CA	6.69	1.54	1.46
2	B	388	HIS	N-CA	6.67	1.54	1.46
2	B	105	GLU	CA-C	6.66	1.60	1.52
1	A	82	PHE	CE2-CZ	6.64	1.58	1.38
1	A	117	ARG	CD-NE	6.64	1.55	1.46
1	A	222	ALA	CA-C	6.62	1.61	1.52
1	A	231	ALA	C-N	6.61	1.42	1.33
1	A	42	ASP	N-CA	6.60	1.54	1.46
1	A	226	ALA	CA-CB	-6.55	1.41	1.53
1	A	206	ALA	CA-CB	6.54	1.63	1.53
2	B	68	GLY	C-O	6.54	1.32	1.24
2	B	314	ALA	N-CA	6.54	1.54	1.46
2	B	331	GLU	CD-OE2	6.52	1.37	1.25
1	A	4	TYR	CA-C	6.51	1.61	1.52
1	A	90[A]	GLU	C-O	6.48	1.32	1.24
1	A	90[B]	GLU	C-O	6.48	1.32	1.24
2	B	30	GLU	CA-CB	6.46	1.63	1.53
2	B	224	PRO	CA-CB	6.46	1.63	1.53
1	A	160	ASP	N-CA	-6.44	1.38	1.46
1	A	250	GLN	C-O	6.43	1.31	1.24
1	A	220	VAL	CA-C	6.42	1.60	1.52
2	B	288	GLN	N-CA	6.41	1.54	1.45
2	B	296	GLU	CA-C	6.41	1.62	1.53
2	B	106	ILE	N-CA	6.40	1.53	1.46
2	B	60	THR	C-N	6.37	1.42	1.33
1	A	18	ALA	CA-CB	6.36	1.63	1.53
1	A	71	ALA	CA-CB	6.36	1.63	1.53
2	B	119	SER	N-CA	-6.34	1.38	1.46
2	B	134	MET	SD-CE	6.33	1.95	1.79
2	B	386	THR	C-O	6.30	1.31	1.24
2	B	329	ASP	CA-C	6.29	1.61	1.52
1	A	145	ARG	CZ-NH2	6.28	1.41	1.33
2	B	132	ILE	C-O	6.27	1.30	1.24
2	B	108	ALA	CA-C	-6.26	1.45	1.52
2	B	4	LEU	C-N	6.26	1.42	1.33
2	B	260	HIS	CG-ND1	6.23	1.45	1.38
1	A	83	GLU	CA-CB	6.21	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	MET	CA-CB	6.20	1.65	1.53
2	B	245	ILE	CA-CB	-6.19	1.46	1.54
1	A	77	THR	CA-CB	-6.18	1.46	1.54
2	B	132	ILE	CB-CG1	6.18	1.65	1.53
2	B	156	VAL	CA-CB	6.16	1.61	1.54
2	B	297	SER	C-O	6.15	1.31	1.23
1	A	100[A]	LEU	CA-C	-6.14	1.45	1.52
1	A	100[B]	LEU	CA-C	-6.14	1.45	1.52
2	B	205	GLN	CA-C	6.11	1.60	1.52
1	A	150	PRO	CA-C	6.10	1.58	1.52
2	B	117	VAL	CA-CB	-6.07	1.46	1.54
2	B	25	LEU	N-CA	6.06	1.53	1.46
1	A	223	ALA	N-CA	6.05	1.53	1.46
1	A	210	GLN	CA-C	-6.02	1.45	1.52
2	B	42	GLN	N-CA	-5.99	1.39	1.46
2	B	150	ARG	CA-C	5.98	1.60	1.52
2	B	177	TRP	CA-CB	5.98	1.62	1.53
2	B	381	ASP	N-CA	5.97	1.53	1.46
1	A	253	ALA	C-O	5.95	1.31	1.24
2	B	24	ALA	CA-CB	-5.94	1.44	1.53
2	B	63	GLN	C-O	5.93	1.31	1.24
1	A	108	ASN	CA-CB	5.90	1.63	1.53
1	A	232	ILE	CA-CB	5.89	1.62	1.54
1	A	91	LYS	C-N	5.89	1.40	1.33
2	B	141	ARG	CZ-NH1	5.88	1.41	1.32
2	B	191	ALA	N-CA	5.88	1.54	1.46
2	B	218	ASP	C-O	5.88	1.30	1.24
1	A	67	ALA	CA-C	-5.86	1.45	1.52
1	A	15	ARG	N-CA	5.85	1.55	1.46
2	B	143	SER	CA-CB	5.85	1.62	1.53
2	B	225	ASP	C-O	5.85	1.31	1.24
2	B	34	SER	C-O	5.82	1.30	1.24
1	A	110	GLY	CA-C	5.81	1.56	1.52
1	A	87	LEU	N-CA	5.81	1.53	1.46
1	A	204	HIS	C-N	-5.80	1.25	1.33
2	B	214	ALA	CA-C	-5.80	1.45	1.52
1	A	217	PRO	CA-C	-5.80	1.43	1.52
2	B	264	THR	C-O	5.80	1.31	1.24
1	A	104	ASN	C-O	-5.78	1.16	1.24
2	B	69	THR	CA-CB	5.77	1.63	1.54
1	A	212	PHE	N-CA	5.76	1.53	1.46
2	B	89	ASN	C-O	5.76	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	191	ALA	CA-CB	5.76	1.60	1.52
2	B	37	LYS	CG-CD	5.75	1.69	1.52
2	B	118	ALA	N-CA	-5.72	1.39	1.46
2	B	341	ARG	CZ-NH2	5.71	1.40	1.33
1	A	9	ALA	N-CA	5.71	1.53	1.46
2	B	208	ILE	N-CA	5.71	1.53	1.46
2	B	152	MET	CA-CB	5.70	1.62	1.53
1	A	261	ALA	N-CA	5.69	1.53	1.46
1	A	104	ASN	CG-ND2	5.69	1.45	1.33
1	A	140[A]	ARG	CA-C	-5.69	1.45	1.52
1	A	140[B]	ARG	CA-C	-5.69	1.45	1.52
2	B	65	ILE	CA-CB	5.69	1.62	1.54
2	B	383	ASP	CA-CB	5.67	1.63	1.53
1	A	236	ALA	CA-CB	-5.67	1.44	1.53
2	B	280	PHE	C-O	5.67	1.31	1.24
2	B	41	PHE	CB-CG	5.66	1.63	1.50
1	A	11	LEU	CA-CB	5.66	1.62	1.53
1	A	217	PRO	N-CA	-5.66	1.40	1.47
2	B	17	VAL	N-CA	5.66	1.51	1.46
1	A	26	GLY	CA-C	-5.65	1.43	1.51
2	B	130	CYS	CA-C	-5.65	1.45	1.52
1	A	76	VAL	N-CA	5.64	1.53	1.46
2	B	341	ARG	C-O	5.63	1.31	1.24
2	B	146	VAL	C-O	5.60	1.30	1.24
2	B	93	GLY	CA-C	5.60	1.58	1.52
2	B	167	LYS	CA-CB	5.60	1.62	1.53
2	B	374	VAL	CA-CB	-5.60	1.47	1.54
1	A	243	LYS	N-CA	5.57	1.53	1.46
2	B	379[A]	ARG	N-CA	5.57	1.52	1.45
2	B	379[B]	ARG	N-CA	5.57	1.52	1.45
2	B	195	HIS	CE1-NE2	5.57	1.38	1.32
2	B	195	HIS	CA-C	-5.56	1.47	1.53
2	B	136	ALA	N-CA	5.56	1.53	1.46
1	A	167	ALA	CA-CB	5.56	1.61	1.53
1	A	55	SER	N-CA	5.55	1.53	1.46
2	B	197	TYR	C-O	5.55	1.30	1.24
2	B	169	ALA	CA-CB	5.53	1.62	1.53
1	A	213	GLY	CA-C	5.53	1.59	1.51
2	B	360	LYS	CG-CD	5.53	1.69	1.52
1	A	16	GLU	CA-C	5.51	1.59	1.52
1	A	120	GLN	CG-CD	5.51	1.65	1.52
2	B	370	GLN	CG-CD	5.51	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	ASN	CG-OD1	5.50	1.33	1.23
1	A	152	PHE	N-CA	5.49	1.52	1.45
1	A	197	ILE	CA-CB	-5.49	1.47	1.54
2	B	341	ARG	CD-NE	5.48	1.53	1.46
1	A	212	PHE	CA-CB	5.48	1.62	1.53
2	B	289	THR	CB-OG1	5.48	1.52	1.43
2	B	255	VAL	C-O	5.47	1.30	1.24
2	B	376	LEU	CA-CB	5.47	1.59	1.52
2	B	129	LYS	C-O	5.46	1.30	1.24
1	A	204	HIS	N-CA	-5.45	1.38	1.46
2	B	27	GLN	CB-CG	5.44	1.68	1.52
2	B	41	PHE	CD1-CE1	5.44	1.54	1.38
2	B	350	GLU	CA-CB	5.44	1.61	1.53
1	A	195	HIS	CA-C	5.44	1.59	1.52
1	A	127	LEU	C-N	5.43	1.40	1.33
2	B	303	GLY	C-O	-5.43	1.17	1.23
1	A	19	PHE	C-N	5.42	1.39	1.33
2	B	167	LYS	CE-NZ	5.42	1.65	1.49
2	B	3	THR	N-CA	5.41	1.52	1.45
2	B	118	ALA	CA-CB	5.39	1.61	1.53
1	A	94	THR	C-O	5.39	1.31	1.24
1	A	145	ARG	C-O	5.37	1.30	1.24
2	B	34	SER	N-CA	5.37	1.52	1.46
1	A	171	ARG	C-O	-5.37	1.17	1.23
1	A	116	ALA	N-CA	5.36	1.52	1.46
2	B	336	PHE	CA-CB	5.36	1.61	1.53
2	B	159	VAL	CA-CB	-5.35	1.47	1.54
1	A	208	ALA	CA-C	-5.35	1.45	1.52
2	B	293	GLN	CD-NE2	5.34	1.44	1.33
2	B	286	MET	CB-CG	5.34	1.68	1.52
1	A	176	LEU	CA-C	-5.33	1.46	1.52
2	B	44	GLN	C-O	-5.33	1.17	1.24
2	B	206[A]	ARG	N-CA	5.33	1.53	1.46
2	B	206[B]	ARG	N-CA	5.33	1.53	1.46
2	B	274	GLY	C-O	-5.33	1.19	1.24
1	A	92	HIS	N-CA	-5.32	1.41	1.46
2	B	387	VAL	C-O	-5.31	1.17	1.24
2	B	310	GLY	N-CA	5.31	1.51	1.44
1	A	206	ALA	N-CA	-5.30	1.38	1.45
1	A	209	LEU	CA-C	-5.30	1.46	1.52
2	B	107	ILE	C-O	-5.29	1.18	1.24
1	A	4	TYR	CA-CB	5.28	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	269	ALA	CA-CB	5.28	1.58	1.53
1	A	50	LEU	C-O	-5.28	1.18	1.24
2	B	268	GLY	C-O	5.27	1.31	1.23
2	B	63	GLN	N-CA	5.27	1.53	1.46
2	B	70	ARG	NE-CZ	5.27	1.38	1.33
2	B	226	ALA	N-CA	5.27	1.52	1.46
1	A	93	PRO	CG-CD	5.26	1.68	1.50
2	B	59	LEU	C-O	5.25	1.30	1.24
2	B	100	ARG	C-O	5.23	1.30	1.24
1	A	27	ASP	CA-C	5.23	1.59	1.52
1	A	80	GLN	C-O	5.22	1.30	1.24
1	A	169	TYR	CG-CD1	-5.21	1.28	1.39
1	A	60	ASP	CG-OD1	5.21	1.35	1.25
2	B	97	LEU	CG-CD2	5.21	1.69	1.52
2	B	360	LYS	CE-NZ	5.20	1.65	1.49
2	B	8	TYR	CA-C	-5.19	1.46	1.52
2	B	146	VAL	CA-C	5.18	1.59	1.52
2	B	275	ARG	CA-CB	5.18	1.64	1.54
2	B	67	ALA	CA-CB	5.18	1.61	1.53
2	B	201	VAL	CA-C	-5.17	1.46	1.52
1	A	23	VAL	N-CA	5.17	1.51	1.46
2	B	78	GLU	C-O	5.16	1.30	1.24
2	B	201	VAL	C-O	5.16	1.30	1.24
2	B	317	ASN	N-CA	5.15	1.52	1.46
1	A	126	VAL	CA-C	5.15	1.58	1.52
2	B	357	HIS	CD2-NE2	5.14	1.43	1.37
1	A	219	GLN	CA-CB	5.13	1.62	1.53
2	B	228	ILE	C-O	5.13	1.29	1.24
2	B	66	THR	N-CA	5.12	1.52	1.46
1	A	93	PRO	N-CD	5.12	1.54	1.47
1	A	108	ASN	CA-C	-5.11	1.46	1.52
1	A	210	GLN	CG-CD	-5.10	1.39	1.52
2	B	217	LEU	C-O	5.10	1.30	1.24
2	B	39	PRO	N-CA	5.08	1.54	1.47
1	A	242	GLU	C-O	5.07	1.29	1.24
1	A	20	VAL	C-N	-5.07	1.27	1.33
2	B	75	LEU	CG-CD1	5.05	1.69	1.52
2	B	182	GLU	C-O	5.05	1.30	1.24
2	B	365	GLN	N-CA	5.03	1.52	1.46
2	B	227	VAL	N-CA	5.03	1.51	1.46
2	B	248	THR	CA-CB	5.02	1.62	1.53
2	B	290	ALA	CA-CB	5.01	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	333	LEU	N-CA	5.01	1.52	1.46
1	A	46	ASP	C-N	5.00	1.39	1.33

All (224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	ARG	NE-CZ-NH2	-14.12	106.50	119.20
2	B	385	PHE	CB-CA-C	-11.45	86.30	109.55
1	A	196	LEU	N-CA-C	-10.39	99.14	112.23
1	A	221	SER	O-C-N	10.21	132.94	122.12
1	A	109	ASN	N-CA-CB	-9.20	98.20	111.54
2	B	286	MET	CA-CB-CG	9.10	132.31	114.10
1	A	216	SER	O-C-N	-8.96	115.58	121.85
2	B	390	ILE	CB-CA-C	-8.59	100.77	112.02
1	A	33	SER	O-C-N	8.57	131.20	122.12
1	A	155	PRO	N-CD-CG	-8.56	90.36	103.20
1	A	70	ARG	NE-CZ-NH1	8.46	129.96	121.50
1	A	74	ALA	N-CA-C	8.44	123.63	113.16
1	A	213	GLY	CA-C-O	-8.44	110.09	119.04
1	A	93	PRO	N-CD-CG	-8.32	90.72	103.20
1	A	55	SER	CA-C-O	-8.20	111.86	120.55
2	B	321	ARG	NE-CZ-NH2	-8.20	111.82	119.20
1	A	3	ARG	NE-CZ-NH1	8.12	129.62	121.50
2	B	131	ARG	NE-CZ-NH1	8.07	129.57	121.50
1	A	95	ILE	CA-C-N	-7.96	111.80	119.76
1	A	95	ILE	C-N-CA	-7.96	111.80	119.76
1	A	92	HIS	O-C-N	-7.85	114.99	121.27
2	B	84	GLY	CA-C-O	-7.80	110.09	119.06
2	B	298	TYR	CA-CB-CG	-7.77	99.92	113.90
2	B	388	HIS	N-CA-C	7.70	119.31	111.07
2	B	309	VAL	O-C-N	7.68	129.65	122.97
2	B	117	VAL	O-C-N	-7.58	114.52	121.87
2	B	384	ILE	CA-C-N	-7.52	108.42	121.66
2	B	384	ILE	C-N-CA	-7.52	108.42	121.66
2	B	201	VAL	O-C-N	-7.48	114.12	121.83
1	A	207	PRO	CB-CA-C	-7.38	101.78	111.23
1	A	13	ASP	N-CA-C	-7.38	103.23	111.71
2	B	132	ILE	O-C-N	7.34	131.10	123.18
2	B	19	GLN	O-C-N	7.29	129.84	122.12
2	B	145	ASN	CA-C-O	-7.26	112.72	120.42
2	B	55	ARG	O-C-N	-7.22	113.59	121.53
2	B	235	SER	N-CA-C	7.21	118.93	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	158	PRO	N-CD-CG	-7.11	92.53	103.20
2	B	144	PRO	N-CD-CG	-7.10	92.56	103.20
2	B	38	ASP	CA-C-O	-7.06	113.43	119.36
2	B	387	VAL	N-CA-C	-6.99	103.66	110.72
2	B	44	GLN	O-C-N	6.90	130.02	122.15
1	A	119	GLU	N-CA-C	-6.87	103.87	111.36
2	B	346	ILE	O-C-N	-6.80	117.08	121.37
1	A	213	GLY	CA-C-N	-6.80	112.28	121.80
1	A	213	GLY	C-N-CA	-6.80	112.28	121.80
2	B	197	TYR	O-C-N	-6.78	114.34	120.71
2	B	158	PRO	CB-CA-C	-6.75	102.24	111.21
1	A	93	PRO	O-C-N	-6.72	113.03	122.38
2	B	176	ASP	N-CA-CB	-6.70	100.22	110.20
2	B	40	GLU	N-CA-CB	6.65	120.01	110.16
2	B	4	LEU	CA-C-O	6.61	127.58	119.79
2	B	119	SER	N-CA-C	-6.57	104.20	111.36
1	A	117	ARG	CA-C-O	6.55	127.36	120.42
2	B	49	LEU	N-CA-C	-6.52	104.26	111.36
1	A	90[A]	GLU	N-CA-C	-6.51	104.60	112.54
1	A	90[B]	GLU	N-CA-C	-6.51	104.60	112.54
2	B	339	LEU	O-C-N	6.47	129.52	122.15
1	A	152	PHE	CA-CB-CG	-6.45	107.35	113.80
1	A	103	ALA	N-CA-C	6.41	119.09	111.33
1	A	9	ALA	CA-C-N	6.41	128.77	120.44
1	A	9	ALA	C-N-CA	6.41	128.77	120.44
2	B	66	THR	O-C-N	-6.38	114.36	122.34
1	A	96	PRO	CA-C-O	-6.37	113.66	121.31
1	A	167	ALA	N-CA-C	6.37	118.22	111.28
2	B	150	ARG	O-C-N	6.36	129.40	122.15
2	B	141	ARG	N-CA-CB	6.33	120.55	110.73
1	A	224	VAL	N-CA-C	6.33	117.11	110.72
2	B	14	GLY	O-C-N	6.31	129.17	122.86
2	B	97	LEU	CA-C-O	-6.28	113.89	120.55
1	A	104	ASN	CA-CB-CG	-6.28	106.32	112.60
2	B	286	MET	CG-SD-CE	-6.26	87.12	100.90
2	B	275	ARG	O-C-N	6.24	130.51	123.27
1	A	223	ALA	N-CA-C	-6.22	104.58	111.36
1	A	220	VAL	CA-C-O	6.14	127.68	121.17
2	B	87	LYS	CB-CG-CD	-6.14	97.17	111.30
1	A	232	ILE	O-C-N	-6.12	116.90	123.14
2	B	41	PHE	N-CA-C	-6.09	104.72	111.36
2	B	41	PHE	CA-C-O	-6.08	113.97	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	GLY	N-CA-C	-6.07	106.34	115.32
2	B	227	VAL	CA-CB-CG2	6.06	120.71	110.40
1	A	29	GLY	CA-C-O	-6.06	115.07	121.56
2	B	360	LYS	O-C-N	-6.03	115.27	122.15
1	A	64	ILE	CA-CB-CG1	-6.01	100.18	110.40
1	A	154	CYS	CA-C-N	5.99	126.55	120.38
1	A	154	CYS	C-N-CA	5.99	126.55	120.38
1	A	127	LEU	CA-C-N	-5.99	115.23	122.90
1	A	127	LEU	C-N-CA	-5.99	115.23	122.90
1	A	250	GLN	CB-CG-CD	5.98	122.76	112.60
1	A	218	GLU	CA-C-N	-5.95	110.73	121.14
1	A	218	GLU	C-N-CA	-5.95	110.73	121.14
2	B	166	LEU	CA-C-N	-5.95	111.27	120.31
2	B	166	LEU	C-N-CA	-5.95	111.27	120.31
2	B	152	MET	CG-SD-CE	-5.93	87.85	100.90
1	A	124	ASP	CA-CB-CG	-5.92	106.68	112.60
1	A	77	THR	CA-CB-OG1	5.92	118.47	109.60
2	B	357	HIS	CA-CB-CG	-5.91	107.89	113.80
1	A	247	SER	N-CA-CB	5.90	118.41	111.09
1	A	114	PHE	CA-C-O	-5.90	114.62	120.70
2	B	77	ARG	N-CA-C	5.89	118.86	110.68
2	B	67	ALA	O-C-N	5.88	130.07	122.89
1	A	212	PHE	CA-C-N	-5.86	112.19	122.09
1	A	212	PHE	C-N-CA	-5.86	112.19	122.09
1	A	2	GLU	N-CA-C	-5.84	100.78	109.83
1	A	96	PRO	O-C-N	5.84	130.11	123.10
2	B	44	GLN	CA-C-O	-5.83	114.24	120.42
1	A	242	GLU	N-CA-C	-5.83	104.84	111.07
1	A	210	GLN	CA-CB-CG	-5.82	102.47	114.10
1	A	12	ASN	N-CA-C	-5.81	105.08	111.82
2	B	34	SER	N-CA-CB	-5.81	101.59	110.01
2	B	355	LEU	O-C-N	5.80	128.26	122.12
2	B	309	VAL	CA-C-O	-5.76	116.12	120.96
2	B	131	ARG	NH1-CZ-NH2	-5.74	111.84	119.30
1	A	82	PHE	CE1-CZ-CE2	5.72	130.30	120.00
2	B	290	ALA	CA-C-N	-5.70	112.75	122.56
2	B	290	ALA	C-N-CA	-5.70	112.75	122.56
1	A	154	CYS	CA-C-O	5.70	124.15	119.36
1	A	221	SER	N-CA-C	5.70	117.49	111.28
1	A	196	LEU	CB-CG-CD1	5.69	127.78	110.70
1	A	3	ARG	O-C-N	-5.69	116.09	122.12
1	A	157	ASN	N-CA-CB	-5.68	102.34	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	MET	N-CA-CB	5.67	118.45	110.12
2	B	208	ILE	O-C-N	5.65	127.76	121.94
2	B	247	ASP	CA-CB-CG	-5.65	106.95	112.60
1	A	6	ASN	O-C-N	-5.64	116.26	122.07
1	A	77	THR	CB-CA-C	-5.61	100.50	109.08
1	A	146	HIS	N-CA-C	-5.60	105.75	112.59
2	B	37	LYS	CB-CG-CD	-5.60	98.41	111.30
1	A	1	MET	N-CA-C	-5.59	95.36	111.00
1	A	3	ARG	N-CA-C	5.58	117.36	111.28
1	A	55	SER	N-CA-C	-5.57	105.20	111.28
2	B	129	LYS	N-CA-CB	-5.56	100.82	110.17
2	B	297	SER	O-C-N	5.55	129.59	123.16
2	B	49	LEU	CA-C-O	-5.54	114.54	120.42
2	B	136	ALA	O-C-N	-5.54	115.45	122.27
1	A	122	GLY	CA-C-O	5.54	125.17	118.86
2	B	342	HIS	CA-CB-CG	-5.50	108.30	113.80
2	B	39	PRO	N-CD-CG	-5.50	94.95	103.20
2	B	8	TYR	CA-C-O	5.49	127.88	121.46
1	A	193	LEU	CB-CA-C	5.47	120.11	110.37
2	B	33	VAL	CA-C-O	-5.47	115.26	120.95
1	A	118	CYS	O-C-N	5.46	127.77	122.09
1	A	103	ALA	CA-C-N	-5.46	112.02	120.31
1	A	103	ALA	C-N-CA	-5.46	112.02	120.31
2	B	93	GLY	CA-C-N	-5.46	112.97	120.28
2	B	93	GLY	C-N-CA	-5.46	112.97	120.28
2	B	46	ALA	CA-C-O	-5.45	114.78	120.55
2	B	294	ILE	CA-C-O	5.42	127.56	121.11
2	B	309	VAL	CA-C-N	-5.42	113.37	121.87
2	B	309	VAL	C-N-CA	-5.42	113.37	121.87
2	B	339	LEU	CA-C-O	-5.40	114.69	120.42
1	A	54	PHE	CA-C-O	5.40	127.43	121.11
2	B	7	PRO	CB-CA-C	-5.40	103.27	110.88
1	A	34	LEU	O-C-N	-5.39	116.40	122.12
2	B	313	HIS	CA-C-N	-5.38	113.06	120.28
2	B	313	HIS	C-N-CA	-5.38	113.06	120.28
1	A	166	VAL	CA-CB-CG1	5.38	119.55	110.40
2	B	329	ASP	CB-CA-C	-5.37	101.55	110.68
2	B	220	GLU	N-CA-C	-5.37	106.61	114.39
2	B	185	HIS	CA-C-N	5.34	129.78	122.84
2	B	185	HIS	C-N-CA	5.34	129.78	122.84
1	A	147	ASN	CB-CG-ND2	5.34	124.40	116.40
1	A	88	ILE	CB-CA-C	-5.33	104.86	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	237	ALA	CA-C-N	-5.32	111.58	120.30
2	B	237	ALA	C-N-CA	-5.32	111.58	120.30
2	B	336	PHE	N-CA-CB	-5.32	102.31	110.12
2	B	16	TYR	O-C-N	5.31	128.78	122.46
2	B	110	THR	N-CA-CB	-5.31	103.33	111.56
1	A	176	LEU	CB-CG-CD2	-5.30	94.79	110.70
1	A	53	PRO	O-C-N	5.29	129.09	123.01
1	A	51	GLY	CA-C-N	-5.26	117.54	123.02
1	A	51	GLY	C-N-CA	-5.26	117.54	123.02
2	B	106	ILE	CA-C-O	5.25	125.92	120.36
1	A	156	PRO	CB-CA-C	-5.24	104.41	111.85
2	B	262	ILE	CA-C-O	-5.23	115.62	121.17
2	B	274	GLY	N-CA-C	-5.22	105.13	112.60
1	A	10	GLN	O-C-N	-5.22	116.70	122.07
2	B	335	ALA	CA-C-O	-5.21	113.98	119.97
2	B	300	ILE	O-C-N	5.21	127.13	121.87
1	A	80	GLN	N-CA-C	-5.21	105.69	111.36
2	B	132	ILE	CB-CG1-CD1	-5.20	102.88	113.80
2	B	273	HIS	CA-CB-CG	-5.20	108.60	113.80
1	A	102	TYR	CA-CB-CG	-5.19	104.56	113.90
2	B	141	ARG	NE-CZ-NH2	-5.18	114.53	119.20
1	A	78	PRO	N-CA-C	-5.18	106.33	113.53
1	A	35	LYS	CD-CE-NZ	5.17	128.46	111.90
1	A	72	PHE	CA-C-N	-5.16	112.85	120.28
1	A	72	PHE	C-N-CA	-5.16	112.85	120.28
2	B	15	MET	CA-CB-CG	-5.16	103.79	114.10
2	B	143	SER	CB-CA-C	5.16	120.33	110.17
2	B	139	VAL	N-CA-CB	-5.15	104.03	110.47
1	A	241	ILE	N-CA-C	-5.14	105.69	110.53
1	A	75	GLY	CA-C-N	-5.14	113.99	120.98
1	A	75	GLY	C-N-CA	-5.14	113.99	120.98
2	B	158	PRO	CA-CB-CG	-5.14	94.74	104.50
2	B	241	PHE	CA-C-O	-5.14	113.73	119.79
2	B	237	ALA	O-C-N	5.13	128.00	122.15
2	B	110	THR	CA-C-O	5.12	126.71	121.23
2	B	120	ALA	CA-C-O	-5.12	115.00	120.42
2	B	120	ALA	N-CA-C	-5.12	105.78	111.36
2	B	61	LYS	N-CA-CB	-5.11	102.34	110.06
1	A	253	ALA	N-CA-CB	-5.11	102.59	110.16
1	A	82	PHE	CB-CG-CD1	-5.11	112.02	120.70
1	A	247	SER	CA-CB-OG	-5.10	100.89	111.10
2	B	114	GLN	CB-CA-C	-5.09	102.19	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	341	ARG	CA-C-O	-5.09	113.78	119.79
1	A	90[A]	GLU	CA-C-O	-5.08	113.13	119.38
1	A	90[B]	GLU	CA-C-O	-5.08	113.13	119.38
2	B	182	GLU	CA-C-N	-5.08	114.36	122.29
2	B	182	GLU	C-N-CA	-5.08	114.36	122.29
2	B	348	ALA	CA-C-N	-5.08	112.23	120.72
2	B	348	ALA	C-N-CA	-5.08	112.23	120.72
1	A	225	ARG	CA-C-O	-5.08	115.17	120.55
2	B	48	LEU	CD1-CG-CD2	-5.07	99.65	110.80
2	B	390	ILE	CG1-CB-CG2	5.07	125.90	110.70
1	A	82	PHE	CD1-CE1-CZ	-5.06	110.89	120.00
1	A	97	ILE	CA-C-O	5.06	125.38	120.27
2	B	384	ILE	O-C-N	5.05	127.51	121.80
2	B	185	HIS	N-CA-C	-5.05	101.92	109.95
2	B	361	MET	N-CA-C	-5.05	105.78	111.28
1	A	109	ASN	N-CA-C	-5.05	104.59	111.56
1	A	176	LEU	N-CA-C	-5.04	100.51	108.73
1	A	88	ILE	CA-CB-CG1	-5.03	101.85	110.40
2	B	155	GLU	CB-CA-C	5.02	118.61	110.22
1	A	243	LYS	N-CA-C	5.02	118.51	112.38

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	1947	0	1955	42	0
2	B	2986	0	2959	41	0
3	A	10	0	5	0	0
4	B	1	0	0	0	0
5	B	15	0	7	0	0
6	A	214	0	0	5	0
6	B	444	0	0	5	0
All	All	5617	0	4926	80	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 8.

All (80) 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:82:PHE:CD1	1:A:82:PHE:CE1	1.78	1.65
1:A:87:LEU:CG	1:A:87:LEU:CD1	1.75	1.63
2:B:149:MET:SD	2:B:149:MET:CG	2.15	1.34
1:A:49[B]:GLU:OE2	1:A:100[B]:LEU:CD2	1.89	1.17
2:B:337:LYS:HE2	2:B:391:LEU:HD11	1.31	1.12
1:A:49[B]:GLU:OE2	1:A:100[B]:LEU:HD21	0.94	1.08
1:A:49[B]:GLU:CD	1:A:100[B]:LEU:HD11	1.79	1.06
2:B:337:LYS:CE	2:B:391:LEU:HD11	1.92	0.99
1:A:82:PHE:CD1	1:A:82:PHE:CZ	2.52	0.96
1:A:49[B]:GLU:CD	1:A:100[B]:LEU:HD21	1.92	0.94
2:B:337:LYS:CE	2:B:391:LEU:CD1	2.51	0.88
1:A:108:ASN:HD21	2:B:275:ARG:HH22	1.18	0.87
2:B:337:LYS:HZ1	2:B:391:LEU:HD13	1.38	0.87
1:A:254[B]:GLU:HG3	6:A:909:HOH:O	1.74	0.86
2:B:337:LYS:HE3	2:B:391:LEU:HD21	1.57	0.86
2:B:337:LYS:NZ	2:B:391:LEU:HD13	1.91	0.86
2:B:337:LYS:HE2	2:B:391:LEU:CD1	2.05	0.85
2:B:206[A]:ARG:HD3	2:B:210:GLU:OE2	1.81	0.80
1:A:49[B]:GLU:CD	1:A:100[B]:LEU:CD1	2.56	0.79
1:A:49[A]:GLU:OE2	6:A:913:HOH:O	2.01	0.77
1:A:49[B]:GLU:OE1	1:A:100[B]:LEU:HD11	1.82	0.77
1:A:194:HIS:O	1:A:198:GLU:HG2	1.85	0.77
2:B:141:ARG:HD2	6:B:1028:HOH:O	1.84	0.77
1:A:108:ASN:OD1	1:A:109:ASN:ND2	2.19	0.76
2:B:337:LYS:HZ1	2:B:391:LEU:HD22	1.48	0.75
1:A:87:LEU:CD1	1:A:87:LEU:CD2	2.65	0.73
1:A:87:LEU:CD1	1:A:87:LEU:HG	2.12	0.71
2:B:337:LYS:HZ1	2:B:391:LEU:CD1	2.04	0.70
2:B:337:LYS:NZ	2:B:391:LEU:HD22	2.08	0.69
2:B:337:LYS:NZ	2:B:391:LEU:CD1	2.56	0.68
1:A:108:ASN:HD21	2:B:275:ARG:NH2	1.94	0.64
1:A:49[B]:GLU:HG2	1:A:100[B]:LEU:HG	1.80	0.64
2:B:337:LYS:HZ1	2:B:391:LEU:CD2	2.12	0.63
1:A:195:HIS:CE1	1:A:199:LYS:HE2	2.34	0.63
2:B:149:MET:SD	2:B:149:MET:CB	2.86	0.63
2:B:337:LYS:HE3	2:B:391:LEU:CD2	2.28	0.62
1:A:108:ASN:ND2	2:B:275:ARG:HH22	1.95	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:390:ILE:HG22	2:B:391:LEU:N	2.14	0.60
2:B:215:GLN:O	2:B:219[C]:LYS:HD2	2.02	0.59
2:B:44:GLN:HG3	6:B:969:HOH:O	2.05	0.56
2:B:132:ILE:HD13	2:B:149:MET:SD	2.46	0.56
1:A:22:PHE:CD2	1:A:100[B]:LEU:HD12	2.42	0.55
2:B:206[A]:ARG:CD	2:B:210:GLU:OE2	2.52	0.55
1:A:157:ASN:O	1:A:158:ALA:C	2.49	0.54
2:B:337:LYS:NZ	2:B:391:LEU:CD2	2.69	0.54
2:B:38:ASP:OD1	2:B:38:ASP:C	2.53	0.51
2:B:337:LYS:CE	2:B:391:LEU:CD2	2.88	0.51
1:A:112:ASP:OD1	1:A:146:HIS:HE1	1.94	0.51
1:A:49[B]:GLU:CD	1:A:100[B]:LEU:CG	2.84	0.50
1:A:49[B]:GLU:OE2	1:A:100[B]:LEU:HD11	2.09	0.50
1:A:195:HIS:HE1	1:A:199:LYS:HE2	1.77	0.50
1:A:49[B]:GLU:CD	1:A:100[B]:LEU:CD2	2.70	0.49
2:B:137:LYS:HE3	2:B:163:SER:O	2.12	0.49
1:A:1:MET:N	6:A:880:HOH:O	2.46	0.48
2:B:279:TYR:CG	2:B:280:PHE:N	2.82	0.47
1:A:100[A]:LEU:HD21	6:A:846:HOH:O	2.15	0.46
1:A:250:GLN:NE2	1:A:254[A]:GLU:OE2	2.39	0.46
1:A:254[B]:GLU:CG	6:A:909:HOH:O	2.50	0.46
2:B:61:LYS:HE2	6:B:1006:HOH:O	2.16	0.46
1:A:193:LEU:O	1:A:197:ILE:HG13	2.16	0.45
1:A:195:HIS:CE1	1:A:199:LYS:CE	2.99	0.45
1:A:22:PHE:CE2	1:A:100[B]:LEU:HD12	2.52	0.45
1:A:250:GLN:O	1:A:254[A]:GLU:HG3	2.17	0.45
2:B:112:ALA:HB3	6:B:1077:HOH:O	2.17	0.45
1:A:86:ALA:O	1:A:90[B]:GLU:HG3	2.16	0.44
2:B:176:ASP:OD1	2:B:176:ASP:C	2.61	0.44
2:B:11:GLU:O	2:B:11:GLU:HG2	2.17	0.44
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.53	0.43
1:A:1:MET:HB3	1:A:1:MET:HE3	1.62	0.43
2:B:337:LYS:HE3	2:B:391:LEU:HD11	1.94	0.42
1:A:49[B]:GLU:CG	1:A:100[B]:LEU:HG	2.47	0.42
1:A:155:PRO:HA	1:A:156:PRO:HD3	1.86	0.42
1:A:15:ARG:O	1:A:268:ALA:HB2	2.19	0.41
2:B:298:TYR:CD2	2:B:298:TYR:C	2.99	0.41
1:A:57:PRO:HA	1:A:102:TYR:CZ	2.55	0.41
2:B:21:LEU:HD23	2:B:21:LEU:HA	1.90	0.41
2:B:119:SER:HA	2:B:187[B]:MET:HE3	2.03	0.41
1:A:49[B]:GLU:HG2	1:A:100[B]:LEU:CG	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:384:ILE:HG13	2:B:385:PHE:N	2.36	0.40
2:B:182:GLU:HB3	6:B:871:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	257/268 (96%)	251 (98%)	5 (2%)	1 (0%)	30	12
2	B	398/396 (100%)	389 (98%)	9 (2%)	0	100	100
All	All	655/664 (99%)	640 (98%)	14 (2%)	1 (0%)	43	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	PHE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	205/208 (99%)	202 (98%)	3 (2%)	57	31
2	B	316/310 (102%)	307 (97%)	9 (3%)	38	11
All	All	521/518 (101%)	509 (98%)	12 (2%)	45	16

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	69	LEU
1	A	196	LEU
2	B	23	PRO
2	B	65	ILE
2	B	144	PRO
2	B	196	PRO
2	B	206[A]	ARG
2	B	206[B]	ARG
2	B	236	ASN
2	B	275	ARG
2	B	297	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	66	ASN
1	A	108	ASN
1	A	109	ASN
1	A	157	ASN
1	A	194	HIS
1	A	195	HIS
2	B	27	GLN
2	B	44	GLN
2	B	82	HIS
2	B	160	HIS
2	B	236	ASN
2	B	375	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	13P	A	701	-	9,9,9	4.70	6 (66%)	10,12,12	6.57	4 (40%)
5	PLP	B	702	2	15,15,16	2.99	6 (40%)	21,22,23	2.31	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	13P	A	701	-	-	2/8/8/8	-
5	PLP	B	702	2	-	0/6/6/8	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	13P	O2-C2	11.35	1.41	1.21
5	B	702	PLP	C3-C2	-9.04	1.31	1.41
3	A	701	13P	C1-C2	5.54	1.61	1.50
3	A	701	13P	C3-C2	3.98	1.60	1.50
5	B	702	PLP	C3-C4	-3.65	1.33	1.40
5	B	702	PLP	C6-N1	3.18	1.40	1.34
5	B	702	PLP	P-O4P	-3.05	1.50	1.60
3	A	701	13P	O3-C3	2.83	1.51	1.41
5	B	702	PLP	C5A-C5	2.39	1.57	1.50
5	B	702	PLP	C6-C5	-2.35	1.33	1.37
3	A	701	13P	P-O2P	2.28	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	13P	P-O1P	2.21	1.57	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	13P	O2-C2-C3	-16.81	94.07	120.91
3	A	701	13P	O2-C2-C1	-11.45	100.97	120.77
5	B	702	PLP	C2A-C2-C3	6.55	128.46	120.80
5	B	702	PLP	O4P-C5A-C5	4.26	117.35	109.36
5	B	702	PLP	C4A-C4-C5	-3.52	117.31	120.94
5	B	702	PLP	C2A-C2-N1	-3.30	111.43	117.64
3	A	701	13P	O3-C3-C2	-3.15	102.07	112.22
5	B	702	PLP	C6-C5-C4	-2.75	115.84	118.10
3	A	701	13P	O3P-P-O2P	2.31	116.46	107.80
5	B	702	PLP	C4-C3-C2	2.30	123.33	119.89

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	13P	O2-C2-C3-O3
3	A	701	13P	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	255/268 (95%)	0.40	10 (3%) 43 47	13, 22, 44, 79	7 (2%)
2	B	390/396 (98%)	-0.06	8 (2%) 63 67	10, 16, 28, 46	9 (2%)
All	All	645/664 (97%)	0.12	18 (2%) 55 59	10, 19, 37, 79	16 (2%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	ASN	5.6
2	B	391	LEU	5.4
1	A	192	PRO	4.6
1	A	193	LEU	4.1
2	B	385	PHE	3.7
1	A	268	ALA	3.6
2	B	62	CYS	3.2
1	A	246	ALA	3.1
1	A	194	HIS	3.0
2	B	389	ASP	3.0
1	A	178	SER	2.7
2	B	390	ILE	2.6
1	A	247	SER	2.4
1	A	1	MET	2.2
1	A	212	PHE	2.1
2	B	159	VAL	2.1
2	B	2	THR	2.0
2	B	388	HIS	2.0

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	13P	A	701	10/10	0.91	0.11	24,26,33,38	0
5	PLP	B	702	15/16	0.98	0.05	12,13,24,29	0
4	NA	B	703	1/1	0.99	0.04	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.