



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:25 PM GMT

PDB ID : 1K7E
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

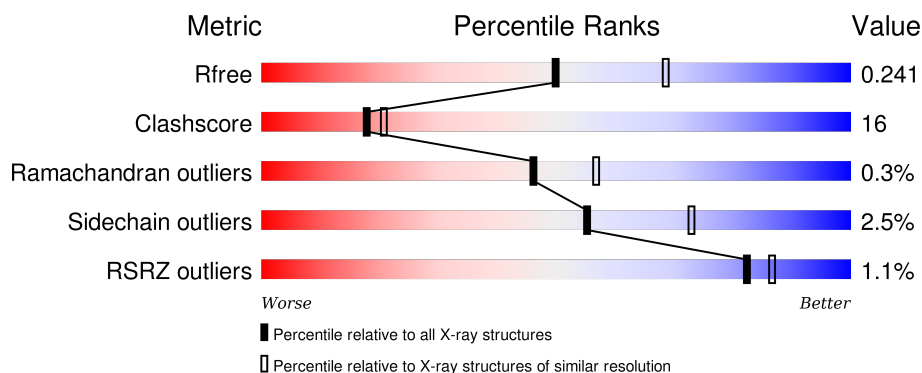
1 Overall quality at a glance

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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div></div> <div> <div></div> <div>43%</div> <div>41%</div> <div>13%</div> <div></div> </div> <div></div> </div>
2	B	396	<div> <div></div> <div> <div></div> <div>51%</div> <div>39%</div> <div>9%</div> <div></div> </div> <div></div> </div>

2 Entry composition

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			

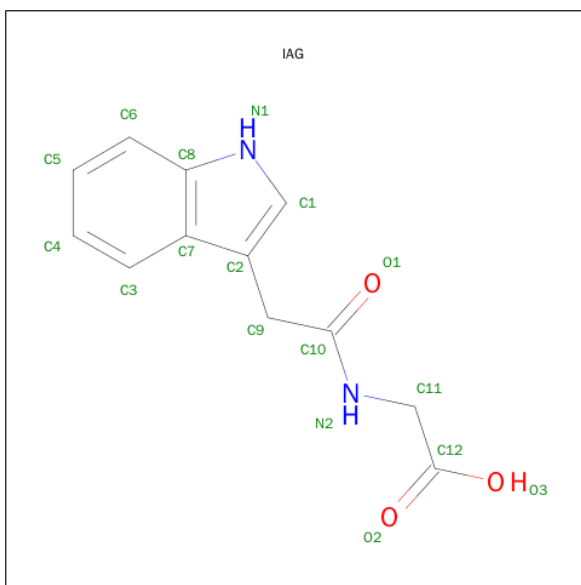
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	34	SER	ARG	CLONING ARTIFACT	UNP P0A2K1

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

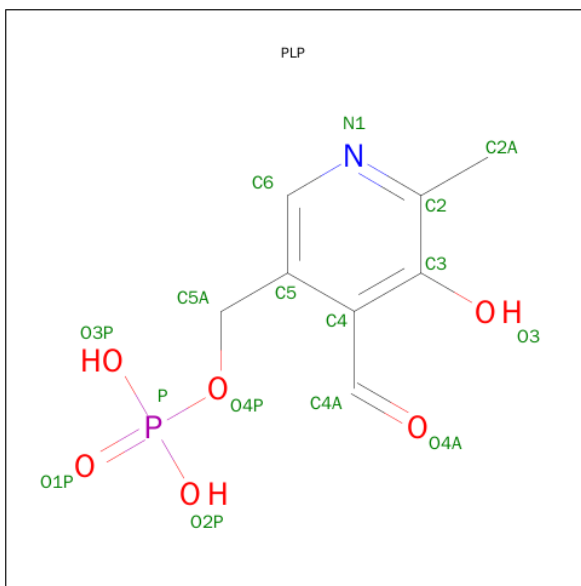
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is N-[1H-INDOL-3-YL-ACETYL]GLYCINE ACID (three-letter code: IAG) (formula: C₁₂H₁₂N₂O₃).



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

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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

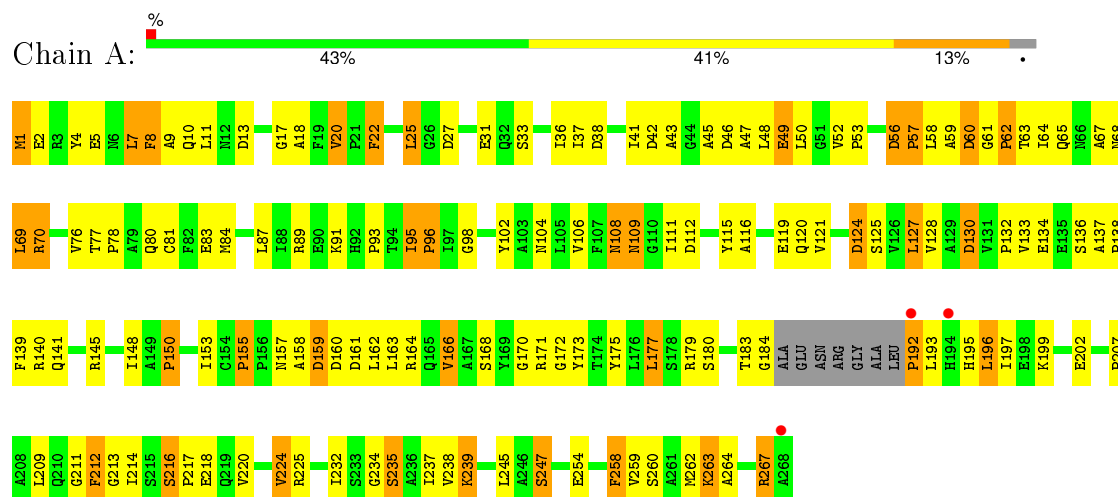
- Molecule 6 is water.

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

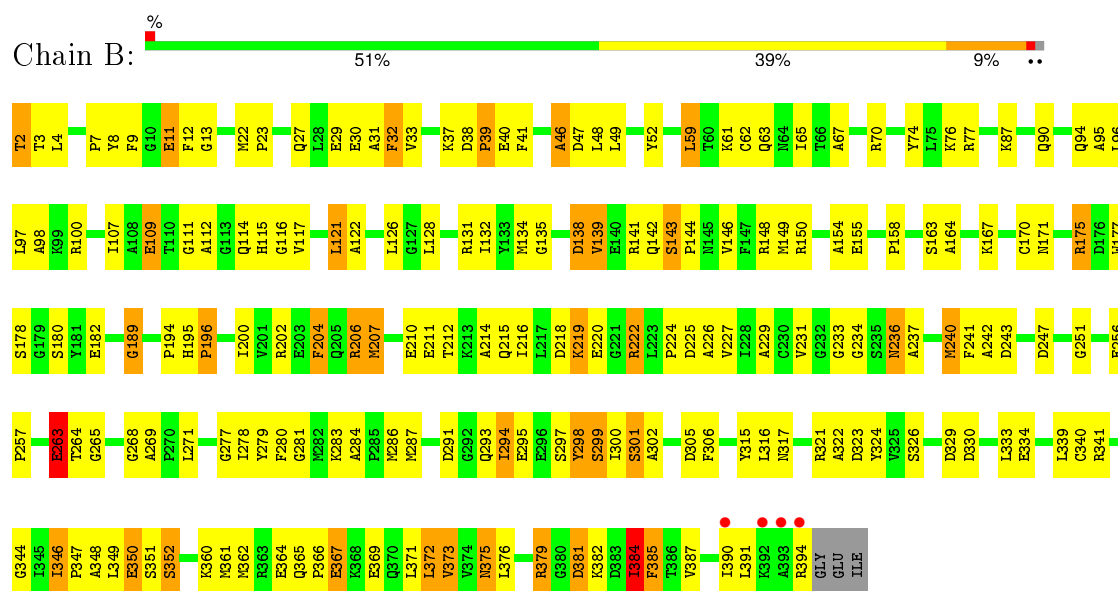
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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 34.94 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.0 (20.00-2.30) 91.0 (34.94-2.30)	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	REFMAC	Depositor
R, R_{free}	0.167 , 0.244 0.170 , 0.241	Depositor DCC
R_{free} test set	1475 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.870	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 29178 reflections (0.003%)	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, IAG, 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	2.29	79/2014 (3.9%)	1.86	49/2733 (1.8%)
2	B	2.34	123/3035 (4.1%)	1.82	62/4100 (1.5%)
All	All	2.32	202/5049 (4.0%)	1.83	111/6833 (1.6%)

All (202) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	295	GLU	CD-OE1	17.72	1.45	1.25
2	B	263	GLU	CD-OE1	15.11	1.42	1.25
2	B	11	GLU	CD-OE2	13.61	1.40	1.25
2	B	139	VAL	CB-CG2	12.20	1.78	1.52
2	B	46	ALA	CA-CB	11.91	1.77	1.52
2	B	364	GLU	CD-OE2	-11.14	1.13	1.25
2	B	182	GLU	CD-OE1	10.31	1.36	1.25
2	B	240	MET	SD-CE	-10.13	1.21	1.77
2	B	214	ALA	CA-CB	9.92	1.73	1.52
1	A	17	GLY	C-O	9.58	1.39	1.23
2	B	202	ARG	CZ-NH1	9.51	1.45	1.33
1	A	239	LYS	CE-NZ	9.32	1.72	1.49
2	B	11	GLU	CG-CD	9.24	1.65	1.51
1	A	202	GLU	CD-OE1	9.15	1.35	1.25
2	B	350	GLU	CD-OE2	-9.07	1.15	1.25
1	A	140	ARG	NE-CZ	-8.92	1.21	1.33
2	B	279	TYR	CD2-CE2	-8.90	1.25	1.39
1	A	2	GLU	CD-OE2	8.82	1.35	1.25
1	A	60	ASP	C-O	8.71	1.40	1.23
1	A	87	LEU	CA-CB	8.56	1.73	1.53
1	A	83	GLU	CD-OE1	8.54	1.35	1.25
2	B	219	LYS	CD-CE	8.54	1.72	1.51
2	B	41	PHE	CE1-CZ	8.52	1.53	1.37
2	B	385	PHE	CG-CD1	8.41	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	367	GLU	CD-OE1	8.37	1.34	1.25
2	B	9	PHE	CE1-CZ	8.27	1.53	1.37
1	A	31	GLU	CG-CD	7.98	1.64	1.51
2	B	117	VAL	CB-CG2	-7.96	1.36	1.52
2	B	298	TYR	CZ-OH	7.94	1.51	1.37
2	B	27	GLN	CD-OE1	7.93	1.41	1.24
2	B	40	GLU	CD-OE2	7.87	1.34	1.25
2	B	155	GLU	CD-OE1	7.83	1.34	1.25
2	B	379	ARG	CZ-NH1	7.72	1.43	1.33
1	A	120	GLN	CG-CD	7.71	1.68	1.51
2	B	150	ARG	CZ-NH2	7.66	1.43	1.33
2	B	298	TYR	CE1-CZ	7.62	1.48	1.38
2	B	371	LEU	C-O	-7.62	1.08	1.23
2	B	206	ARG	CG-CD	7.61	1.71	1.51
1	A	102	TYR	CD2-CE2	7.60	1.50	1.39
1	A	47	ALA	CA-CB	7.58	1.68	1.52
2	B	167	LYS	CD-CE	7.53	1.70	1.51
2	B	298	TYR	CD1-CE1	7.47	1.50	1.39
1	A	263	LYS	C-O	7.46	1.37	1.23
2	B	341	ARG	CZ-NH1	7.24	1.42	1.33
2	B	299	SER	CB-OG	7.18	1.51	1.42
1	A	239	LYS	CD-CE	7.10	1.69	1.51
1	A	25	LEU	CG-CD1	7.03	1.77	1.51
2	B	77	ARG	CZ-NH1	7.00	1.42	1.33
2	B	231	VAL	CB-CG2	7.00	1.67	1.52
2	B	344	GLY	C-O	7.00	1.34	1.23
2	B	207	MET	CG-SD	-6.99	1.62	1.81
2	B	291	ASP	CB-CG	-6.97	1.37	1.51
2	B	280	PHE	CD2-CE2	6.96	1.53	1.39
2	B	369	GLU	CG-CD	6.91	1.62	1.51
2	B	281	GLY	CA-C	-6.89	1.40	1.51
2	B	32	PHE	CG-CD1	-6.84	1.28	1.38
1	A	43	ALA	CA-CB	6.84	1.66	1.52
2	B	263	GLU	CD-OE2	6.81	1.33	1.25
2	B	299	SER	CA-CB	6.79	1.63	1.52
2	B	351	SER	C-O	-6.79	1.10	1.23
2	B	112	ALA	CA-CB	6.77	1.66	1.52
1	A	17	GLY	CA-C	6.73	1.62	1.51
2	B	251	GLY	CA-C	6.68	1.62	1.51
2	B	346	ILE	C-O	-6.64	1.10	1.23
1	A	175	TYR	CD2-CE2	6.62	1.49	1.39
1	A	10	GLN	CB-CG	6.62	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	70	ARG	CG-CD	6.61	1.68	1.51
1	A	62	PRO	CB-CG	6.60	1.82	1.50
1	A	5	GLU	CD-OE1	6.59	1.32	1.25
2	B	150	ARG	NE-CZ	6.59	1.41	1.33
1	A	254	GLU	CD-OE1	6.56	1.32	1.25
2	B	59	LEU	CA-C	6.55	1.70	1.52
2	B	361	MET	C-O	-6.54	1.10	1.23
2	B	8	TYR	CG-CD2	6.53	1.47	1.39
1	A	134	GLU	CD-OE1	6.50	1.32	1.25
1	A	116	ALA	CA-CB	6.47	1.66	1.52
2	B	360	LYS	CG-CD	6.47	1.74	1.52
1	A	183	THR	CB-CG2	6.46	1.73	1.52
2	B	204	PHE	CG-CD1	-6.44	1.29	1.38
1	A	218	GLU	CD-OE2	6.44	1.32	1.25
1	A	1	MET	SD-CE	6.36	2.13	1.77
2	B	63	GLN	CG-CD	6.35	1.65	1.51
2	B	143	SER	CB-OG	6.30	1.50	1.42
2	B	37	LYS	CD-CE	6.27	1.67	1.51
2	B	154	ALA	CA-CB	-6.25	1.39	1.52
1	A	258	PHE	CB-CG	-6.24	1.40	1.51
2	B	131	ARG	CG-CD	6.23	1.67	1.51
2	B	59	LEU	C-O	-6.23	1.11	1.23
1	A	121	VAL	CB-CG2	6.20	1.65	1.52
1	A	235	SER	CB-OG	-6.18	1.34	1.42
2	B	100	ARG	N-CA	-6.17	1.34	1.46
2	B	317	ASN	CG-OD1	6.16	1.37	1.24
1	A	18	ALA	CA-CB	-6.14	1.39	1.52
1	A	161	ASP	CB-CG	6.14	1.64	1.51
2	B	346	ILE	CB-CG2	6.12	1.71	1.52
2	B	143	SER	C-O	-6.10	1.11	1.23
1	A	57	PRO	CB-CG	6.07	1.80	1.50
1	A	159	ASP	CB-CG	6.02	1.64	1.51
1	A	245	LEU	CG-CD2	6.01	1.74	1.51
1	A	45	ALA	CA-CB	6.01	1.65	1.52
2	B	33	VAL	CB-CG2	-5.99	1.40	1.52
2	B	322	ALA	C-O	-5.98	1.11	1.23
1	A	247	SER	CB-OG	5.98	1.50	1.42
2	B	31	ALA	CA-CB	-5.98	1.39	1.52
2	B	29	GLU	CD-OE2	5.97	1.32	1.25
2	B	256	GLU	CD-OE2	5.96	1.32	1.25
1	A	119	GLU	CD-OE1	5.96	1.32	1.25
1	A	173	TYR	CE1-CZ	5.95	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	67	ALA	CA-CB	5.95	1.65	1.52
2	B	369	GLU	CB-CG	5.93	1.63	1.52
2	B	226	ALA	N-CA	-5.91	1.34	1.46
1	A	22	PHE	CD2-CE2	-5.90	1.27	1.39
2	B	175	ARG	CG-CD	5.86	1.66	1.51
2	B	48	LEU	N-CA	5.86	1.58	1.46
1	A	20	VAL	CB-CG2	5.84	1.65	1.52
1	A	212	PHE	CD1-CE1	5.84	1.50	1.39
2	B	52	TYR	CZ-OH	5.84	1.47	1.37
2	B	52	TYR	CD1-CE1	-5.82	1.30	1.39
2	B	306	PHE	CG-CD1	5.82	1.47	1.38
1	A	106	VAL	CB-CG1	5.82	1.65	1.52
1	A	8	PHE	CG-CD2	-5.79	1.30	1.38
1	A	168	SER	CB-OG	-5.78	1.34	1.42
1	A	133	VAL	CA-CB	5.76	1.66	1.54
1	A	109	ASN	CB-CG	5.74	1.64	1.51
2	B	180	SER	CA-C	-5.71	1.38	1.52
1	A	214	ILE	CA-CB	-5.69	1.41	1.54
1	A	96	PRO	CA-CB	-5.68	1.42	1.53
2	B	341	ARG	CG-CD	5.68	1.66	1.51
2	B	211	GLU	CD-OE2	5.68	1.31	1.25
1	A	132	PRO	CG-CD	5.68	1.69	1.50
1	A	52	VAL	CA-CB	-5.67	1.42	1.54
2	B	301	SER	CB-OG	-5.64	1.34	1.42
2	B	2	THR	N-CA	5.63	1.57	1.46
2	B	256	GLU	CD-OE1	5.60	1.31	1.25
2	B	167	LYS	CE-NZ	5.59	1.63	1.49
1	A	141	GLN	CA-CB	5.59	1.66	1.53
1	A	237	ILE	CA-CB	-5.55	1.42	1.54
1	A	139	PHE	CD2-CE2	5.55	1.50	1.39
1	A	133	VAL	CB-CG1	-5.54	1.41	1.52
2	B	384	ILE	CB-CG2	-5.53	1.35	1.52
2	B	293	GLN	CB-CG	5.51	1.67	1.52
2	B	122	ALA	CA-CB	5.51	1.64	1.52
2	B	178	SER	CA-CB	-5.50	1.44	1.52
2	B	215	GLN	CD-OE1	5.49	1.36	1.24
2	B	29	GLU	CD-OE1	-5.49	1.19	1.25
1	A	192	PRO	CB-CG	5.48	1.77	1.50
1	A	212	PHE	CD2-CE2	5.48	1.50	1.39
1	A	83	GLU	CG-CD	5.47	1.60	1.51
2	B	375	ASN	CG-OD1	5.46	1.35	1.24
2	B	315	TYR	CZ-OH	5.44	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	SER	C-O	5.44	1.33	1.23
2	B	324	TYR	CZ-OH	5.44	1.47	1.37
2	B	109	GLU	CB-CG	5.43	1.62	1.52
2	B	362	MET	N-CA	-5.41	1.35	1.46
2	B	216	ILE	N-CA	-5.41	1.35	1.46
2	B	269	ALA	CA-CB	-5.40	1.41	1.52
1	A	93	PRO	C-O	-5.39	1.12	1.23
2	B	382	LYS	CD-CE	5.38	1.64	1.51
2	B	13	GLY	C-O	-5.35	1.15	1.23
1	A	112	ASP	CB-CG	-5.34	1.40	1.51
1	A	136	SER	CB-OG	-5.33	1.35	1.42
2	B	76	LYS	CD-CE	5.32	1.64	1.51
1	A	150	PRO	CB-CG	5.30	1.76	1.50
2	B	30	GLU	CA-CB	5.29	1.65	1.53
1	A	225	ARG	CZ-NH1	5.29	1.40	1.33
2	B	3	THR	CA-CB	-5.29	1.39	1.53
1	A	184	GLY	C-O	5.27	1.32	1.23
2	B	177	TRP	CE3-CZ3	5.27	1.47	1.38
1	A	56	ASP	CB-CG	5.25	1.62	1.51
1	A	22	PHE	C-O	-5.25	1.13	1.23
2	B	107	ILE	CA-CB	-5.24	1.42	1.54
2	B	39	PRO	CA-C	-5.23	1.42	1.52
1	A	59	ALA	CA-C	5.23	1.66	1.52
2	B	287	MET	CB-CG	5.22	1.68	1.51
2	B	177	TRP	CG-CD1	5.21	1.44	1.36
1	A	10	GLN	N-CA	-5.21	1.35	1.46
1	A	224	VAL	C-O	-5.20	1.13	1.23
1	A	254	GLU	C-O	-5.20	1.13	1.23
1	A	148	ILE	CA-CB	-5.19	1.43	1.54
2	B	373	VAL	CA-CB	5.19	1.65	1.54
2	B	234	GLY	C-O	5.18	1.31	1.23
2	B	279	TYR	CE2-CZ	5.17	1.45	1.38
1	A	33	SER	CB-OG	5.16	1.49	1.42
2	B	293	GLN	N-CA	-5.15	1.36	1.46
2	B	206	ARG	CZ-NH2	5.15	1.39	1.33
2	B	4	LEU	CA-C	5.14	1.66	1.52
1	A	45	ALA	C-O	5.14	1.33	1.23
2	B	346	ILE	CA-CB	-5.13	1.43	1.54
1	A	164	ARG	NE-CZ	-5.13	1.26	1.33
2	B	202	ARG	CD-NE	-5.11	1.37	1.46
2	B	220	GLU	CD-OE2	5.11	1.31	1.25
2	B	334	GLU	C-O	5.11	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	194	PRO	CA-CB	-5.08	1.43	1.53
1	A	10	GLN	CG-CD	5.08	1.62	1.51
1	A	95	ILE	C-O	-5.06	1.13	1.23
2	B	264	THR	CB-CG2	5.05	1.69	1.52
2	B	346	ILE	CG1-CD1	5.05	1.85	1.50
2	B	196	PRO	C-O	5.03	1.33	1.23
1	A	259	VAL	CB-CG1	5.01	1.63	1.52
2	B	294	ILE	CB-CG2	-5.01	1.37	1.52
2	B	326	SER	CA-CB	5.01	1.60	1.52
1	A	170	GLY	N-CA	-5.00	1.38	1.46

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	ARG	NE-CZ-NH2	-18.33	111.13	120.30
2	B	379	ARG	NE-CZ-NH2	-17.48	111.56	120.30
2	B	222	ARG	NE-CZ-NH2	-12.86	113.87	120.30
2	B	222	ARG	NE-CZ-NH1	12.55	126.58	120.30
1	A	46	ASP	CB-CG-OD2	11.89	129.00	118.30
2	B	379	ARG	NE-CZ-NH1	11.58	126.09	120.30
1	A	164	ARG	NE-CZ-NH1	11.52	126.06	120.30
1	A	89	ARG	NE-CZ-NH1	-11.27	114.67	120.30
2	B	202	ARG	NE-CZ-NH2	-10.50	115.05	120.30
2	B	394	ARG	NE-CZ-NH1	-9.97	115.31	120.30
2	B	202	ARG	NE-CZ-NH1	9.92	125.26	120.30
2	B	243	ASP	CB-CG-OD2	9.61	126.95	118.30
1	A	13	ASP	CB-CG-OD2	9.25	126.62	118.30
2	B	263	GLU	CG-CD-OE2	-9.08	100.15	118.30
1	A	239	LYS	CD-CE-NZ	8.93	132.25	111.70
1	A	70	ARG	NE-CZ-NH1	-8.60	116.00	120.30
2	B	141	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	A	89	ARG	NE-CZ-NH2	8.41	124.50	120.30
1	A	46	ASP	CB-CG-OD1	-8.38	110.76	118.30
1	A	225	ARG	NE-CZ-NH2	-8.38	116.11	120.30
2	B	218	ASP	CB-CG-OD2	8.23	125.70	118.30
2	B	291	ASP	CB-CG-OD1	-8.04	111.07	118.30
2	B	141	ARG	NE-CZ-NH2	-7.89	116.35	120.30
2	B	321	ARG	NE-CZ-NH1	-7.88	116.36	120.30
2	B	138	ASP	CB-CG-OD2	7.85	125.37	118.30
2	B	47	ASP	CB-CG-OD1	7.83	125.35	118.30
2	B	263	GLU	OE1-CD-OE2	7.57	132.38	123.30
1	A	20	VAL	CB-CA-C	-7.52	97.12	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49[A]	GLU	OE1-CD-OE2	-7.43	114.38	123.30
1	A	49[B]	GLU	OE1-CD-OE2	-7.43	114.38	123.30
2	B	376	LEU	CB-CG-CD1	-7.41	98.41	111.00
2	B	316	LEU	CB-CG-CD2	7.37	123.54	111.00
2	B	216	ILE	CG1-CB-CG2	-7.28	95.38	111.40
2	B	240	MET	CG-SD-CE	-7.19	88.69	100.20
1	A	52	VAL	CG1-CB-CG2	-7.19	99.40	110.90
1	A	112	ASP	CB-CG-OD1	7.08	124.67	118.30
1	A	42	ASP	CB-CG-OD2	6.92	124.53	118.30
2	B	212	THR	OG1-CB-CG2	-6.92	94.09	110.00
1	A	60	ASP	CB-CG-OD1	-6.89	112.10	118.30
2	B	206	ARG	CD-NE-CZ	6.84	133.18	123.60
2	B	74	TYR	CZ-CE2-CD2	-6.77	113.71	119.80
1	A	166	VAL	CA-CB-CG2	-6.76	100.76	110.90
1	A	260	SER	N-CA-CB	-6.75	100.37	110.50
1	A	124	ASP	CB-CG-OD2	6.73	124.36	118.30
2	B	286	MET	CA-CB-CG	6.72	124.72	113.30
2	B	364	GLU	OE1-CD-OE2	-6.65	115.32	123.30
2	B	49	LEU	CB-CG-CD1	6.61	122.23	111.00
2	B	107	ILE	CG1-CB-CG2	-6.59	96.89	111.40
2	B	381	ASP	CB-CG-OD1	6.55	124.20	118.30
1	A	168	SER	N-CA-CB	-6.42	100.87	110.50
2	B	96	LEU	CB-CG-CD1	-6.41	100.11	111.00
1	A	267	ARG	NE-CZ-NH1	-6.37	117.11	120.30
2	B	298	TYR	CD1-CE1-CZ	-6.35	114.08	119.80
2	B	33	VAL	CA-CB-CG1	6.32	120.38	110.90
2	B	7	PRO	N-CD-CG	-6.31	93.73	103.20
1	A	7	LEU	CB-CG-CD2	-6.30	100.29	111.00
2	B	224	PRO	N-CD-CG	-6.29	93.76	103.20
1	A	254	GLU	OE1-CD-OE2	6.21	130.75	123.30
1	A	11	LEU	CB-CG-CD1	-6.14	100.56	111.00
2	B	128	LEU	CB-CG-CD1	6.13	121.41	111.00
2	B	264	THR	C-N-CA	-6.11	109.47	122.30
1	A	11	LEU	CA-CB-CG	-6.10	101.28	115.30
1	A	112	ASP	CB-CG-OD2	-6.08	112.82	118.30
2	B	373	VAL	CA-CB-CG1	-6.07	101.80	110.90
2	B	32	PHE	CB-CG-CD1	-6.00	116.60	120.80
1	A	130	ASP	CB-CG-OD2	5.99	123.69	118.30
2	B	47	ASP	OD1-CG-OD2	-5.93	112.03	123.30
1	A	50	LEU	CB-CG-CD2	-5.88	101.01	111.00
1	A	209	LEU	CB-CG-CD1	-5.81	101.12	111.00
2	B	12	PHE	N-CA-CB	-5.81	100.14	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	ASP	CB-CG-OD2	5.80	123.52	118.30
2	B	100	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	A	155	PRO	N-CD-CG	-5.79	94.52	103.20
2	B	225	ASP	CB-CG-OD2	5.77	123.50	118.30
1	A	5	GLU	CG-CD-OE1	5.75	129.79	118.30
2	B	121	LEU	CB-CG-CD1	-5.62	101.45	111.00
1	A	209	LEU	CA-CB-CG	-5.57	102.49	115.30
1	A	13	ASP	OD1-CG-OD2	-5.56	112.74	123.30
2	B	33	VAL	CG1-CB-CG2	-5.51	102.08	110.90
2	B	62	CYS	CA-CB-SG	-5.45	104.19	114.00
2	B	96	LEU	CB-CG-CD2	-5.45	101.74	111.00
2	B	265	GLY	C-N-CA	-5.42	108.15	121.70
1	A	177	LEU	CB-CG-CD2	-5.42	101.79	111.00
1	A	60	ASP	CB-CG-OD2	5.39	123.15	118.30
2	B	247	ASP	CB-CG-OD1	5.39	123.15	118.30
2	B	352	SER	CA-CB-OG	-5.39	96.65	111.20
2	B	189	GLY	N-CA-C	5.36	126.51	113.10
2	B	330	ASP	CB-CG-OD2	5.35	123.12	118.30
2	B	225	ASP	CB-CG-OD1	-5.33	113.50	118.30
1	A	159	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	127	LEU	CB-CG-CD2	-5.31	101.98	111.00
1	A	98	GLY	O-C-N	-5.30	114.22	122.70
2	B	323	ASP	CB-CG-OD1	5.28	123.05	118.30
2	B	384	ILE	CA-CB-CG1	-5.28	100.98	111.00
1	A	214	ILE	CB-CA-C	-5.25	101.09	111.60
1	A	57	PRO	CA-N-CD	5.21	119.00	111.70
1	A	213	GLY	CA-C-O	-5.20	111.24	120.60
2	B	243	ASP	CB-CG-OD1	-5.20	113.62	118.30
2	B	372	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	A	145	ARG	NE-CZ-NH1	-5.19	117.71	120.30
2	B	321	ARG	NE-CZ-NH2	5.19	122.89	120.30
1	A	25	LEU	CB-CG-CD2	-5.14	102.26	111.00
1	A	9	ALA	C-N-CA	-5.11	108.92	121.70
1	A	130	ASP	OD1-CG-OD2	-5.11	113.59	123.30
1	A	140	ARG	NE-CZ-NH1	-5.09	117.76	120.30
2	B	237	ALA	CB-CA-C	-5.05	102.53	110.10
2	B	284	ALA	N-CA-CB	-5.05	103.03	110.10
2	B	302	ALA	C-N-CA	-5.04	111.72	122.30
1	A	115	TYR	CZ-CE2-CD2	5.02	124.32	119.80
2	B	100	ARG	NE-CZ-NH1	5.01	122.81	120.30
2	B	298	TYR	CA-CB-CG	-5.01	103.89	113.40

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	79	0
2	B	2977	0	2954	79	0
3	B	1	0	0	0	0
4	A	17	0	11	1	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	157	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 16.

All (157) 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:CB	2:B:46:ALA:CA	1.77	1.61
2:B:139:VAL:CG2	2:B:139:VAL:CB	1.78	1.60
1:A:25:LEU:CG	1:A:25:LEU:CD1	1.77	1.60
1:A:232:ILE:CG1	1:A:232:ILE:CD1	1.78	1.60
1:A:57:PRO:CG	1:A:57:PRO:CB	1.80	1.56
1:A:36:ILE:CG1	1:A:36:ILE:CD1	1.75	1.54
2:B:346:ILE:CD1	2:B:346:ILE:CG1	1.85	1.51
1:A:192:PRO:CG	1:A:192:PRO:CB	1.77	1.50
1:A:239:LYS:NZ	1:A:239:LYS:CE	1.72	1.49
1:A:150:PRO:CG	1:A:150:PRO:CB	1.76	1.44
1:A:62:PRO:CB	1:A:62:PRO:CG	1.83	1.43
1:A:1:MET:SD	1:A:1:MET:CE	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
1:A:196:LEU:CD1	1:A:196:LEU:H	1.61	1.13
2:B:240:MET:SD	2:B:240:MET:HE3	1.78	1.10
1:A:196:LEU:N	1:A:196:LEU:HD12	1.63	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:MET:HE1	2:B:240:MET:SD	1.78	1.09
2:B:240:MET:HE2	2:B:240:MET:SD	1.78	1.08
1:A:196:LEU:CD1	1:A:196:LEU:N	2.14	1.07
1:A:196:LEU:HD13	1:A:196:LEU:H	1.25	1.02
2:B:240:MET:HE2	2:B:240:MET:CG	1.90	0.92
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
2:B:240:MET:HG3	2:B:240:MET:HE2	1.57	0.85
1:A:220:VAL:O	1:A:224:VAL:HG23	1.77	0.84
1:A:25:LEU:CD2	1:A:25:LEU:CD1	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
1:A:232:ILE:CB	1:A:232:ILE:CD1	2.63	0.77
1:A:127:LEU:HD23	1:A:127:LEU:C	2.07	0.75
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:CB	1:A:36:ILE:CD1	2.72	0.65
1:A:25:LEU:CB	1:A:25:LEU:CD1	2.72	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
1:A:56:ASP:N	1:A:57:PRO:CD	2.64	0.60
2:B:263:GLU:CD	2:B:263:GLU:H	2.04	0.60
1:A:137:ALA:HB3	1:A:138:PRO:CD	2.32	0.59
1:A:127:LEU:CD2	1:A:127:LEU:C	2.70	0.59
1:A:56:ASP:N	1:A:57:PRO:HD3	2.19	0.57
2:B:121:LEU:C	2:B:121:LEU:HD12	2.26	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
2:B:300:ILE:HB	2:B:329:ASP:CG	2.25	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:N	1:A:157:ASN:OD1	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:ALA:C	2:B:46:ALA:CB	2.69	0.52
1:A:234:GLY:O	1:A:235:SER:C	2.45	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
1:A:195:HIS:O	1:A:196:LEU:C	2.46	0.51
2:B:116:GLY:CA	2:B:132:ILE:HD13	2.40	0.51
2:B:87:LYS:HD2	2:B:114:GLN:HG3	1.92	0.51
1:A:53:PRO:HA	1:A:68:ASN:OD1	2.09	0.51
2:B:271:LEU:HD23	2:B:271:LEU:C	2.31	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: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: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:138:ASP:O	2:B:139:VAL:C	2.48	0.48
2:B:32:PHE:CG	2:B:200:ILE:HG12	2.49	0.47
1:A:130:ASP:N	1:A:130:ASP:OD1	2.47	0.47
2:B:109:GLU:HG3	2:B:170:CYS:SG	2.55	0.47
1:A:157:ASN:O	1:A:158:ALA:C	2.52	0.47
1:A:171:ARG:HG2	1:A:171:ARG:NH1	2.24	0.47
1:A:58:LEU:HD12	1:A:58:LEU:C	2.35	0.47
2:B:143:SER:HB2	2:B:144:PRO:HD3	1.96	0.47
2:B:163:SER:O	2:B:164:ALA:HB3	2.14	0.47
2:B:298:TYR:OH	2:B:329:ASP:OD2	2.26	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
2:B:111:GLY:O	2:B:138:ASP:HB3	2.15	0.45
1:A:159:ASP:O	1:A:160:ASP:C	2.54	0.45
1:A:162:LEU:O	1:A:166:VAL:HG23	2.16	0.45
1:A:69:LEU:HD22	1:A:69:LEU:HA	1.71	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:144:PRO:HB2	2:B:148:ARG:HH12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:GLN:O	2:B:146:VAL:HG23	2.16	0.45
2:B:346:ILE:CD1	2:B:346:ILE:CB	2.83	0.45
1:A:108:ASN:ND2	1:A:109:ASN:ND2	2.65	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
2:B:305:ASP:HB3	6:B:555:HOH:O	2.17	0.44
2:B:346:ILE:HG21	2:B:384:ILE:HD11	1.99	0.44
1:A:264:ALA:HA	1:A:267:ARG:NH1	2.32	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
2:B:277:GLY:O	2:B:283:LYS:HA	2.18	0.44
1:A:8:PHE:CD2	1:A:207:PRO:HG2	2.53	0.44
2:B:87:LYS:HD3	2:B:115:HIS:HA	2.00	0.44
2:B:135:GLY:O	2:B:138:ASP:N	2.51	0.44
1:A:177:LEU:HD11	1:A:212:PHE:CG	2.53	0.43
1:A:153:ILE:HD11	4:A:401:IAG:HC4	2.01	0.43
1:A:104:ASN:HB2	2:B:278:ILE:O	2.18	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:O	2:B:11:GLU:HG2	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
2:B:97:LEU:O	2:B:98:ALA:C	2.55	0.42
2:B:65:ILE:HA	2:B:65:ILE:HD13	1.79	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:22:PHE:CD1	1:A:22:PHE:C	2.92	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: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:241:PHE:O	2:B:242:ALA:C	2.56	0.41
2:B:348:ALA:HB1	2:B:350:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ILE:HD13	1:A:111:ILE:HG21	1.86	0.41
1:A:155:PRO:HD2	1:A:158:ALA:HB2	2.02	0.41
1:A:69:LEU:O	1:A:70:ARG:C	2.58	0.41
1:A:7:LEU:O	1:A:8:PHE:C	2.56	0.41
2:B:339:LEU:O	2:B:340:CYS:C	2.59	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
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:365:GLN:HA	2:B:366:PRO:HD2	1.87	0.40
2:B:294:ILE:HG23	2:B:294:ILE:HD12	1.82	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 [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	258/268 (96%)	249 (96%)	7 (3%)	2 (1%)	24	27
2	B	391/396 (99%)	380 (97%)	11 (3%)	0	100	100
All	All	649/664 (98%)	629 (97%)	18 (3%)	2 (0%)	46	57

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%)	199 (98%)	5 (2%)	55	73
2	B	308/310 (99%)	299 (97%)	9 (3%)	50	66
All	All	512/518 (99%)	498 (97%)	14 (3%)	55	70

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49[A]	GLU
1	A	49[B]	GLU
1	A	69	LEU
1	A	196	LEU
1	A	247	SER
2	B	2	THR
2	B	207	MET
2	B	236	ASN
2	B	263	GLU
2	B	297	SER
2	B	301	SER
2	B	367	GLU
2	B	375	ASN
2	B	384	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	146	HIS
1	A	195	HIS
2	B	26	ASN
2	B	63	GLN
2	B	236	ASN
2	B	246	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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$
4	IAG	A	401	-	14,18,18	1.88	4 (28%)	13,24,24	3.87	5 (38%)
5	PLP	B	402	2	15,15,16	2.60	6 (40%)	21,22,23	2.69	7 (33%)

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	402	PLP	C3-C2	-7.43	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	402	PLP	C3-C4	-3.01	1.32	1.40
4	A	401	IAG	C3-C7	-2.95	1.36	1.42
5	B	402	PLP	P-O1P	-2.90	1.41	1.51
4	A	401	IAG	C6-C8	-2.39	1.37	1.41
5	B	402	PLP	O4P-C5A	-2.02	1.36	1.44
5	B	402	PLP	C6-N1	2.00	1.38	1.34
4	A	401	IAG	C1-N1	2.03	1.40	1.36
5	B	402	PLP	C5A-C5	2.92	1.59	1.50
4	A	401	IAG	O1-C10	4.28	1.32	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	IAG	C9-C10-N2	-11.91	99.39	116.11
5	B	402	PLP	O2P-P-O4P	-4.24	94.35	106.56
4	A	401	IAG	C11-N2-C10	-4.11	115.14	122.32
4	A	401	IAG	C9-C2-C1	-2.98	121.68	127.49
5	B	402	PLP	C6-C5-C4	-2.96	115.64	118.15
5	B	402	PLP	C4A-C4-C3	-2.40	116.01	120.36
5	B	402	PLP	C2A-C2-C3	-2.11	118.50	121.04
4	A	401	IAG	O1-C10-C9	2.73	129.51	121.88
4	A	401	IAG	O1-C10-N2	4.09	131.05	122.94
5	B	402	PLP	C3-C4-C5	4.43	123.61	118.78
5	B	402	PLP	O3P-P-O4P	5.19	121.52	106.56
5	B	402	PLP	O4P-C5A-C5	7.25	120.97	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.31	3 (1%) 82 86	11, 21, 43, 67	1 (0%)
2	B	393/396 (99%)	-0.48	4 (1%) 84 88	7, 15, 31, 78	0
All	All	654/664 (98%)	-0.41	7 (1%) 82 86	7, 18, 37, 78	1 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	ALA	2.8
2	B	392	LYS	2.8
2	B	394	ARG	2.7
1	A	192	PRO	2.6
2	B	393	ALA	2.5
1	A	194	HIS	2.3
2	B	390	ILE	2.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	NA	B	403	1/1	0.97	0.14	1.90	3,3,3,3	0
4	IAG	A	401	17/17	0.94	0.16	0.88	21,27,46,46	0
5	PLP	B	402	15/16	0.99	0.12	-0.49	3,15,23,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.