



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:52 AM UTC

PDB ID : 2C2G / pdb_00002c2g
Title : Crystal structure of Threonine Synthase from Arabidopsis thaliana in complex with its cofactor pyridoxal phosphate
Authors : Mas-Droux, C.; Biou, V.; Dumas, R.
Deposited on : 2005-09-29
Resolution : 2.61 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

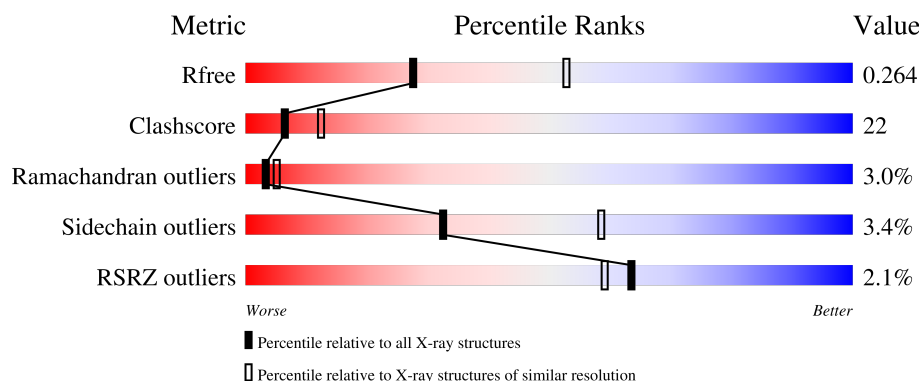
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	486	
1	B	486	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7015 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 THREONINE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3474	2211	595	646	22			
1	B	437	Total	C	N	O	S	0	0	0
			3390	2161	575	632	22			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



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

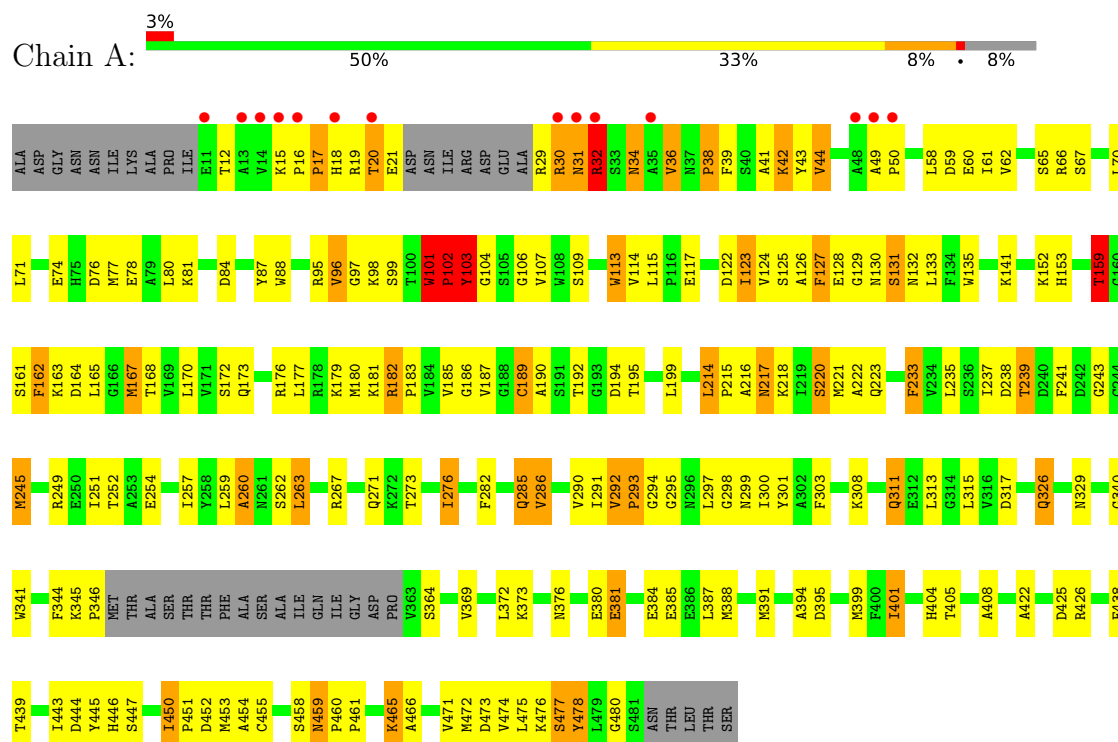
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total 72	O 72	0	0
3	B	49	Total 49	O 49	0	0

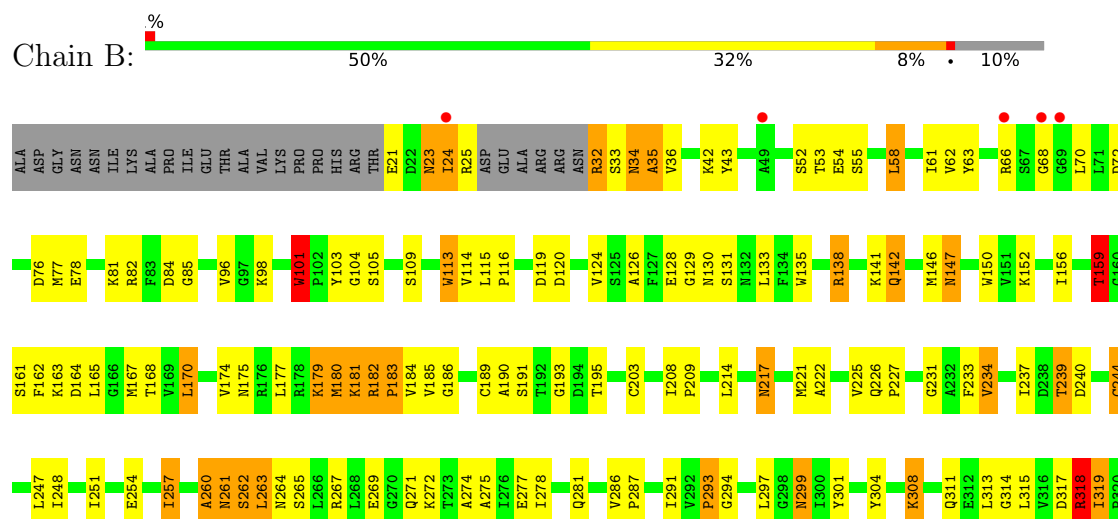
3 Residue-property plots

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: THREONINE SYNTHASE



• Molecule 1: THREONINE SYNTHASE



R321	M322		A325	Q326	A327	M331	P332	L335	H336	Y337		G340	W341	P346	MET	THR	ALA	SER	THR	THR	PHE	ALA	SER	ALA	ALA	ILE	GLN	ILE	GLY	ASP	PRO	V363	S364	I365	D366	R367		C375	N376		E381		E385	E386	L387	M388		M391		A394		M399	F400	I401		H404	T405
G406	V407	A408		A411	I412	F413		R416		P423		V428		T432	A433	H434	G435		T439		I443		S447		M453	A454	C455	R456		M459		K465	A466	D467	F468	G469	A470	V471	M472		K476	S477	Y478	L479	GLY	SER	ASN	THR	LEU	THR	SER						

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.63Å 61.01Å 76.68Å 108.96° 102.00° 107.36°	Depositor
Resolution (Å)	20.63 – 2.61 20.63 – 2.61	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.63-2.61) 95.4 (20.63-2.61)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.187 , 0.264 0.188 , 0.264	Depositor DCC
R_{free} test set	1311 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7015	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 5.71% 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

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	1.36	14/3554 (0.4%)	1.74	77/4817 (1.6%)
1	B	1.19	4/3467 (0.1%)	1.71	81/4699 (1.7%)
All	All	1.28	18/7021 (0.3%)	1.72	158/9516 (1.7%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	41	ALA	CA-CB	-7.08	1.41	1.53
1	A	216	ALA	CA-CB	-6.80	1.42	1.53
1	A	123	ILE	CA-CB	-6.62	1.47	1.54
1	A	291	ILE	CA-C	-6.53	1.44	1.52
1	A	102	PRO	CA-C	6.37	1.61	1.52
1	A	172	SER	CA-C	-6.23	1.45	1.52
1	A	408	ALA	CA-CB	-6.16	1.43	1.53
1	A	96	VAL	C-O	-5.97	1.17	1.24
1	A	167	MET	CA-C	-5.87	1.44	1.52
1	B	115	LEU	CA-C	-5.78	1.44	1.52
1	B	293	PRO	CA-C	-5.68	1.44	1.52
1	A	107	VAL	CA-CB	5.47	1.61	1.54
1	B	275	ALA	CA-CB	-5.41	1.44	1.53
1	A	127	PHE	CG-CD1	5.36	1.50	1.38
1	A	292	VAL	CA-C	-5.16	1.48	1.53
1	B	274	ALA	CA-CB	-5.16	1.44	1.53
1	A	114	VAL	CA-CB	5.11	1.61	1.54
1	A	189	CYS	CB-SG	-5.01	1.64	1.81

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	TRP	CA-C-N	-16.03	99.80	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	TRP	C-N-CA	-16.03	99.80	119.84
1	B	36	VAL	N-CA-C	-15.47	77.16	109.34
1	A	101	TRP	CA-C-N	-14.04	102.29	119.84
1	A	101	TRP	C-N-CA	-14.04	102.29	119.84
1	A	295	GLY	N-CA-C	-11.55	97.99	112.77
1	B	68	GLY	N-CA-C	-10.78	100.06	115.27
1	A	285	GLN	CA-C-N	-10.68	114.90	122.59
1	A	285	GLN	C-N-CA	-10.68	114.90	122.59
1	A	182	ARG	CA-C-N	-10.13	107.18	119.84
1	A	182	ARG	C-N-CA	-10.13	107.18	119.84
1	A	32	ARG	N-CA-C	9.63	123.53	108.79
1	B	262	SER	N-CA-C	-9.52	96.28	111.04
1	A	381	GLU	N-CA-C	9.05	124.17	110.14
1	B	401	ILE	N-CA-C	8.60	122.53	109.20
1	A	286	VAL	N-CA-C	8.43	116.27	107.76
1	A	237	ILE	N-CA-C	8.40	120.67	108.58
1	A	251	ILE	CB-CA-C	-8.18	101.31	111.87
1	A	459	ASN	CA-C-N	-8.02	112.12	120.38
1	A	459	ASN	C-N-CA	-8.02	112.12	120.38
1	A	18	HIS	N-CA-C	7.88	122.09	109.24
1	B	405	THR	N-CA-C	-7.88	102.67	111.82
1	B	214	LEU	N-CA-C	7.81	122.02	108.82
1	A	214	LEU	N-CA-C	7.71	121.85	108.82
1	A	301	TYR	N-CA-C	-7.46	103.09	111.07
1	B	321	ARG	N-CA-C	-7.45	99.46	110.48
1	B	381	GLU	N-CA-C	7.40	122.08	110.17
1	A	364	SER	N-CA-C	7.38	121.60	108.24
1	B	35	ALA	N-CA-C	7.38	121.10	110.10
1	A	215	PRO	N-CA-C	-7.32	99.74	111.38
1	A	115	LEU	CA-C-N	7.30	127.31	119.28
1	A	115	LEU	C-N-CA	7.30	127.31	119.28
1	A	249	ARG	N-CA-C	-7.25	103.06	110.97
1	A	297	LEU	N-CA-C	7.18	121.14	112.38
1	A	276	ILE	N-CA-C	-7.17	103.53	110.42
1	B	126	ALA	N-CA-C	-7.17	102.55	112.30
1	B	469	GLY	N-CA-C	-7.14	104.22	112.50
1	B	115	LEU	N-CA-C	-7.12	97.08	108.82
1	B	161	SER	CA-C-N	7.08	130.08	120.38
1	B	161	SER	C-N-CA	7.08	130.08	120.38
1	A	267	ARG	CB-CA-C	-6.88	99.38	110.79
1	A	106	GLY	N-CA-C	-6.86	107.12	114.67
1	B	319	ILE	N-CA-C	-6.86	94.05	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	SER	N-CA-C	6.86	119.28	108.79
1	B	432	THR	N-CA-C	6.79	121.65	113.23
1	A	326	GLN	N-CA-C	6.73	120.42	109.59
1	B	115	LEU	N-CA-CB	6.67	119.70	111.23
1	A	401	ILE	N-CA-C	6.65	123.18	109.34
1	B	105	SER	N-CA-C	6.65	120.00	110.10
1	A	450	ILE	N-CA-C	6.62	114.44	107.76
1	B	109	SER	N-CA-C	-6.59	104.34	112.38
1	A	460	PRO	CA-C-N	6.56	126.58	119.89
1	A	460	PRO	C-N-CA	6.56	126.58	119.89
1	B	455	CYS	N-CA-C	-6.55	102.43	111.28
1	A	115	LEU	N-CA-CB	6.52	119.51	111.23
1	B	103	TYR	N-CA-C	6.51	124.66	110.80
1	B	265	SER	N-CA-C	6.46	121.24	113.23
1	B	326	GLN	N-CA-C	6.41	120.08	110.14
1	B	291	ILE	CA-C-N	-6.40	116.36	123.02
1	B	291	ILE	C-N-CA	-6.40	116.36	123.02
1	B	124	VAL	N-CA-C	-6.39	98.42	107.75
1	A	34	ASN	N-CA-C	6.35	118.99	110.35
1	B	174	VAL	N-CA-C	-6.35	104.32	110.42
1	A	311	GLN	CA-CB-CG	-6.35	101.40	114.10
1	B	400	PHE	N-CA-C	-6.34	97.30	110.80
1	A	425	ASP	N-CA-C	6.29	118.20	109.15
1	A	260	ALA	N-CA-C	-6.28	98.30	108.41
1	B	104	GLY	N-CA-C	-6.25	105.23	112.73
1	A	439	THR	N-CA-C	6.20	118.55	111.11
1	B	308	LYS	CA-CB-CG	6.19	126.47	114.10
1	A	103	TYR	N-CA-C	6.18	123.96	110.80
1	B	404	HIS	N-CA-CB	6.11	119.20	110.16
1	B	234	VAL	CB-CA-C	-6.11	103.57	110.96
1	A	161	SER	CA-C-N	6.09	129.27	120.38
1	A	161	SER	C-N-CA	6.09	129.27	120.38
1	B	459	ASN	CA-C-N	-6.06	114.14	120.38
1	B	459	ASN	C-N-CA	-6.06	114.14	120.38
1	B	101	TRP	N-CA-C	6.01	123.09	109.81
1	A	126	ALA	N-CA-C	-5.96	104.14	113.02
1	A	239	THR	CB-CA-C	-5.96	98.56	110.42
1	B	133	LEU	N-CA-C	-5.96	95.25	107.70
1	B	239	THR	N-CA-CB	5.95	118.95	110.51
1	B	257	ILE	N-CA-C	-5.91	99.23	107.80
1	A	475	LEU	N-CA-C	5.91	117.52	111.14
1	A	422	ALA	CA-C-N	5.90	125.60	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	422	ALA	C-N-CA	5.90	125.60	119.05
1	B	113	TRP	N-CA-CB	-5.89	101.96	110.56
1	A	161	SER	N-CA-C	5.86	117.16	108.60
1	A	61	ILE	N-CA-C	-5.85	98.20	107.15
1	A	162	PHE	N-CA-CB	-5.85	100.90	110.14
1	A	452	ASP	CB-CA-C	-5.83	101.52	111.26
1	A	405	THR	N-CA-C	-5.83	105.06	111.82
1	A	239	THR	N-CA-CB	5.81	120.30	110.49
1	B	331	ASN	CA-C-N	-5.80	113.83	119.87
1	B	331	ASN	C-N-CA	-5.80	113.83	119.87
1	A	159	THR	N-CA-C	5.78	120.99	113.88
1	B	84	ASP	CA-C-N	5.75	126.32	119.94
1	B	84	ASP	C-N-CA	5.75	126.32	119.94
1	B	159	THR	N-CA-C	5.74	120.00	112.89
1	A	117	GLU	N-CA-C	5.71	120.37	113.17
1	B	58	LEU	N-CA-CB	-5.71	100.61	110.32
1	A	364	SER	CA-C-N	5.71	128.28	120.46
1	A	364	SER	C-N-CA	5.71	128.28	120.46
1	B	456	ARG	CB-CA-C	-5.69	100.11	110.63
1	B	365	ILE	CB-CA-C	-5.68	104.47	112.14
1	A	113	TRP	N-CA-CB	-5.66	102.30	110.56
1	A	84	ASP	N-CA-C	5.63	117.34	110.41
1	B	237	ILE	N-CA-C	5.62	116.68	108.58
1	B	131	SER	CA-C-N	5.61	128.82	120.90
1	B	131	SER	C-N-CA	5.61	128.82	120.90
1	B	439	THR	N-CA-C	5.57	117.03	111.07
1	B	456	ARG	CA-C-N	-5.55	114.36	122.86
1	B	456	ARG	C-N-CA	-5.55	114.36	122.86
1	B	61	ILE	N-CA-C	-5.55	98.97	106.85
1	A	245	MET	N-CA-C	-5.54	105.33	111.36
1	A	317	ASP	N-CA-C	5.53	120.30	113.50
1	A	291	ILE	CA-C-N	-5.48	114.70	123.46
1	A	291	ILE	C-N-CA	-5.48	114.70	123.46
1	B	406	GLY	N-CA-C	-5.45	106.19	112.73
1	B	114	VAL	N-CA-C	5.44	115.92	111.62
1	A	376	ASN	N-CA-CB	-5.42	103.69	111.70
1	A	220	SER	N-CA-C	-5.41	99.29	110.80
1	B	244	CYS	N-CA-C	-5.34	105.12	111.69
1	B	58	LEU	CB-CG-CD2	-5.33	94.72	110.70
1	B	116	PRO	CA-C-N	-5.32	113.77	122.54
1	B	116	PRO	C-N-CA	-5.32	113.77	122.54
1	A	384	GLU	N-CA-C	-5.28	105.44	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	ALA	N-CA-C	-5.27	105.44	111.14
1	B	162	PHE	N-CA-CB	-5.27	102.15	110.06
1	B	174	VAL	N-CA-CB	5.27	116.72	110.55
1	B	180	MET	N-CA-C	-5.26	102.54	110.70
1	A	131	SER	N-CA-CB	-5.26	102.12	110.06
1	B	52	SER	N-CA-C	5.26	116.98	108.26
1	B	70	LEU	N-CA-C	5.25	116.86	110.41
1	B	147	ASN	CA-C-N	-5.24	114.08	122.62
1	B	147	ASN	C-N-CA	-5.24	114.08	122.62
1	A	290	VAL	N-CA-C	-5.23	100.59	108.12
1	A	233	PHE	N-CA-C	-5.20	99.32	108.20
1	A	30	ARG	N-CA-C	5.18	121.38	113.61
1	B	183	PRO	CA-C-N	5.17	131.28	121.97
1	B	183	PRO	C-N-CA	5.17	131.28	121.97
1	A	480	GLY	N-CA-C	5.16	117.32	111.85
1	A	438	PHE	N-CA-C	5.16	119.14	111.87
1	B	318	ARG	CA-CB-CG	5.15	124.39	114.10
1	A	38	PRO	CA-C-N	-5.14	113.90	122.64
1	A	38	PRO	C-N-CA	-5.14	113.90	122.64
1	B	335	LEU	N-CA-CB	5.13	117.75	110.06
1	A	135	TRP	CB-CA-C	5.10	119.10	110.79
1	B	182	ARG	CB-CA-C	5.10	115.49	109.47
1	B	318	ARG	N-CA-C	-5.08	101.96	109.18
1	A	42	LYS	CA-CB-CG	5.08	124.26	114.10
1	A	450	ILE	CA-C-N	5.08	124.99	119.76
1	A	450	ILE	C-N-CA	5.08	124.99	119.76
1	B	327	ALA	N-CA-C	-5.04	101.75	109.76
1	B	193	GLY	CA-C-N	5.02	127.27	120.44
1	B	193	GLY	C-N-CA	5.02	127.27	120.44
1	B	318	ARG	CB-CA-C	-5.02	100.57	111.11
1	A	195	THR	CB-CA-C	-5.01	102.47	110.79

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	3474	0	3428	178	0
1	B	3390	0	3341	148	0
2	A	15	0	6	0	0
2	B	15	0	6	1	0
3	A	72	0	0	6	0
3	B	49	0	0	2	0
All	All	7015	0	6781	299	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 22.

All (299) 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:252:THR:HG21	1:A:259:LEU:CD1	1.74	1.17
1:B:138:ARG:HH11	1:B:138:ARG:CG	1.60	1.14
1:B:261:ASN:HB2	1:B:264:ASN:HB2	1.09	1.05
1:A:252:THR:HG21	1:A:259:LEU:HD11	1.02	1.00
1:B:32:ARG:HD3	1:B:33:SER:H	1.26	0.99
1:B:182:ARG:HG3	1:B:183:PRO:HD2	1.46	0.97
1:B:317:ASP:HB2	1:B:318:ARG:NH1	1.80	0.95
1:B:138:ARG:HH11	1:B:138:ARG:HG2	1.32	0.92
1:B:394:ALA:HB1	1:B:399:MET:HE3	1.49	0.91
1:B:263:LEU:HD12	1:B:364:SER:OG	1.72	0.88
1:B:138:ARG:HH11	1:B:138:ARG:HG3	1.39	0.87
1:A:252:THR:CG2	1:A:259:LEU:HD11	1.97	0.87
1:A:32:ARG:HB2	1:A:38:PRO:HD2	1.58	0.86
1:A:31:ASN:O	1:A:31:ASN:ND2	2.07	0.86
1:A:238:ASP:OD2	1:B:465:LYS:NZ	2.09	0.85
1:B:78:GLU:OE2	1:B:78:GLU:HA	1.78	0.84
1:B:261:ASN:HB2	1:B:264:ASN:CB	2.03	0.82
1:A:32:ARG:CB	1:A:38:PRO:HD2	2.10	0.81
1:A:113:TRP:CZ2	1:A:313:LEU:HD12	2.16	0.80
1:B:152:LYS:NZ	1:B:277:GLU:OE1	2.14	0.78
1:B:142:GLN:HE21	1:B:142:GLN:HA	1.47	0.78
1:A:141:LYS:NZ	1:A:141:LYS:HB3	1.99	0.77
1:B:138:ARG:CG	1:B:138:ARG:NH1	2.36	0.77
1:A:241:PHE:CZ	1:A:245:MET:HE3	2.20	0.77
1:A:446:HIS:HD2	1:A:459:ASN:H	1.33	0.77
1:A:472:MET:O	1:A:476:LYS:HG2	1.85	0.76
1:A:159:THR:HB	1:A:164:ASP:OD1	1.86	0.75
1:B:180:MET:O	1:B:182:ARG:N	2.18	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ALA:HB1	1:A:50:PRO:HD2	1.69	0.75
1:A:385:GLU:HA	1:A:453:MET:HE2	1.70	0.74
1:A:31:ASN:C	1:A:31:ASN:HD22	1.93	0.74
1:A:326:GLN:HA	1:A:326:GLN:NE2	2.03	0.74
1:B:32:ARG:CD	1:B:33:SER:H	2.00	0.74
1:B:180:MET:O	1:B:181:LYS:C	2.31	0.73
1:A:15:LYS:HB2	1:A:19:ARG:HE	1.52	0.73
1:B:175:ASN:O	1:B:179:LYS:HG2	1.89	0.73
1:A:326:GLN:HE21	1:A:326:GLN:CA	2.00	0.73
1:A:466:ALA:CB	1:B:239:THR:HG23	2.19	0.73
1:A:477:SER:O	1:A:478:TYR:C	2.31	0.72
1:B:217:ASN:H	1:B:217:ASN:HD22	1.37	0.72
1:B:262:SER:HB2	1:B:263:LEU:HD22	1.71	0.72
1:B:416:ARG:NH2	1:B:423:PRO:HD3	2.06	0.71
1:B:311:GLN:NE2	1:B:319:ILE:HG23	2.05	0.70
1:B:299:ASN:HD22	1:B:299:ASN:N	1.89	0.70
1:A:128:GLU:CD	1:A:128:GLU:H	1.98	0.70
1:A:32:ARG:HB2	1:A:38:PRO:CD	2.21	0.70
1:A:473:ASP:O	1:A:474:VAL:C	2.36	0.69
1:A:466:ALA:HB2	1:B:239:THR:HG23	1.73	0.69
1:A:127:PHE:CE1	3:A:2028:HOH:O	2.44	0.69
1:B:472:MET:O	1:B:476:LYS:HG2	1.93	0.69
1:A:388:MET:HE1	1:A:391:MET:HE1	1.75	0.68
1:A:141:LYS:HB3	1:A:141:LYS:HZ3	1.56	0.68
1:A:173:GLN:OE1	1:A:173:GLN:HA	1.93	0.68
1:A:391:MET:HA	1:A:401:ILE:HD11	1.76	0.67
1:B:32:ARG:HD3	1:B:33:SER:N	2.06	0.67
1:A:326:GLN:HA	1:A:326:GLN:HE21	1.58	0.67
1:A:88:TRP:HB2	1:A:315:LEU:HD21	1.75	0.66
1:A:394:ALA:HB1	1:A:399:MET:HE3	1.76	0.66
1:B:299:ASN:HD22	1:B:299:ASN:H	1.42	0.66
1:B:465:LYS:HE2	1:B:465:LYS:HA	1.77	0.65
1:B:189:CYS:SG	1:B:191:SER:HB3	2.36	0.65
1:A:99:SER:HB3	1:B:281:GLN:O	1.95	0.65
1:A:443:ILE:HD11	1:B:222:ALA:HA	1.78	0.65
1:B:77:MET:O	1:B:81:LYS:HG3	1.96	0.65
1:B:138:ARG:HG3	1:B:138:ARG:NH1	2.07	0.64
1:A:16:PRO:O	1:A:17:PRO:C	2.37	0.64
1:B:167:MET:HA	1:B:167:MET:HE2	1.80	0.64
1:A:167:MET:HE2	1:A:167:MET:HA	1.79	0.64
1:A:31:ASN:OD1	1:A:87:TYR:HE2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PHE:CD1	1:A:80:LEU:HD23	2.34	0.63
1:A:192:THR:HG22	1:A:214:LEU:HD11	1.81	0.63
1:B:311:GLN:NE2	1:B:319:ILE:CG2	2.62	0.63
1:B:182:ARG:HG3	1:B:183:PRO:CD	2.25	0.63
1:A:177:LEU:O	1:A:182:ARG:HB3	1.99	0.63
1:B:317:ASP:HB2	1:B:318:ARG:HH11	1.63	0.62
1:B:138:ARG:HG2	1:B:138:ARG:NH1	2.08	0.62
1:A:263:LEU:N	1:A:263:LEU:HD22	2.14	0.62
1:A:445:TYR:CE1	1:A:455:CYS:HA	2.35	0.61
1:A:472:MET:HE2	1:B:254:GLU:HG2	1.81	0.61
1:A:88:TRP:HB2	1:A:315:LEU:CD2	2.29	0.61
1:A:170:LEU:C	1:A:170:LEU:HD23	2.25	0.61
1:A:97:GLY:C	3:A:2022:HOH:O	2.43	0.61
1:A:62:VAL:HG12	1:A:71:LEU:CD1	2.31	0.60
1:A:217:ASN:ND2	1:A:218:LYS:HG2	2.16	0.60
1:A:30:ARG:CB	1:A:32:ARG:HD2	2.31	0.60
1:A:385:GLU:HG3	1:A:453:MET:HG3	1.82	0.60
1:A:380:GLU:HG3	1:A:381:GLU:N	2.17	0.59
1:A:465:LYS:HE3	1:A:465:LYS:HA	1.85	0.59
1:A:239:THR:HG23	1:B:466:ALA:CB	2.32	0.59
1:A:65:SER:O	1:A:67:SER:N	2.35	0.59
1:A:162:PHE:CZ	1:A:271:GLN:HB3	2.38	0.58
1:B:376:ASN:C	1:B:376:ASN:HD22	2.11	0.58
1:A:387:LEU:HD12	1:A:387:LEU:C	2.29	0.58
1:B:203:CYS:HB3	1:B:208:ILE:O	2.04	0.58
1:A:388:MET:HE1	1:A:391:MET:CE	2.34	0.58
1:A:122:ASP:OD1	1:A:179:LYS:HD2	2.02	0.57
1:B:167:MET:HE1	1:B:170:LEU:HD13	1.85	0.57
1:B:135:TRP:HB2	1:B:150:TRP:CZ3	2.38	0.57
1:B:364:SER:HB3	1:B:367:ARG:HD2	1.87	0.57
1:B:185:VAL:O	1:B:209:PRO:HG2	2.05	0.56
1:A:133:LEU:HD21	1:A:282:PHE:CE2	2.40	0.56
1:B:240:ASP:O	1:B:244:CYS:HB2	2.05	0.56
1:A:388:MET:CE	1:A:391:MET:CE	2.83	0.56
1:B:128:GLU:CD	1:B:128:GLU:H	2.13	0.56
1:A:222:ALA:HA	1:B:443:ILE:HD11	1.88	0.56
1:A:233:PHE:CE2	1:A:235:LEU:HD21	2.41	0.56
1:B:177:LEU:O	1:B:182:ARG:HB3	2.06	0.56
1:B:293:PRO:HA	1:B:325:ALA:HB3	1.88	0.55
1:A:326:GLN:NE2	1:A:326:GLN:CA	2.58	0.55
1:B:53:THR:O	1:B:53:THR:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ALA:O	1:B:261:ASN:C	2.50	0.55
1:B:85:GLY:HA3	1:B:314:GLY:O	2.06	0.55
1:B:263:LEU:HD22	1:B:263:LEU:H	1.70	0.55
1:B:34:ASN:OD1	1:B:35:ALA:N	2.39	0.55
1:B:385:GLU:HG3	1:B:453:MET:HG3	1.88	0.55
1:A:345:LYS:HD2	1:A:346:PRO:HD2	1.89	0.55
1:B:119:ASP:OD1	1:B:120:ASP:N	2.39	0.55
1:B:195:THR:OG1	1:B:267:ARG:NH2	2.37	0.55
1:B:388:MET:HE1	1:B:391:MET:HE1	1.90	0.54
1:B:62:VAL:HG12	1:B:63:TYR:H	1.71	0.54
1:A:220:SER:OG	1:A:223:GLN:HG3	2.09	0.53
1:B:297:LEU:HD11	1:B:331:ASN:ND2	2.23	0.53
1:A:233:PHE:HE2	1:A:235:LEU:HD21	1.73	0.53
1:A:30:ARG:HB2	1:A:32:ARG:HD2	1.90	0.53
1:A:446:HIS:HA	1:A:458:SER:HB2	1.89	0.53
1:A:454:ALA:O	1:A:455:CYS:HB2	2.08	0.53
1:A:78:GLU:OE2	1:A:78:GLU:HA	2.08	0.53
1:A:243:GLY:HA2	3:A:2046:HOH:O	2.09	0.53
1:A:31:ASN:ND2	1:A:31:ASN:C	2.64	0.53
1:A:131:SER:HB3	1:A:152:LYS:NZ	2.23	0.53
1:A:241:PHE:CZ	1:A:245:MET:CE	2.92	0.53
1:A:292:VAL:O	1:A:293:PRO:O	2.26	0.53
1:A:163:LYS:HE3	1:A:194:ASP:HB2	1.90	0.53
1:B:159:THR:HB	1:B:164:ASP:OD1	2.09	0.53
1:A:132:ASN:HB3	1:A:153:HIS:HB2	1.91	0.52
1:A:299:ASN:O	1:A:303:PHE:HD1	1.92	0.52
1:A:466:ALA:HB1	1:B:239:THR:HG23	1.91	0.52
1:A:43:TYR:CE1	1:A:58:LEU:HA	2.44	0.52
1:A:101:TRP:HZ3	3:A:2028:HOH:O	1.93	0.52
1:B:388:MET:CE	1:B:391:MET:HE1	2.40	0.52
1:A:446:HIS:HD2	1:A:459:ASN:N	2.06	0.52
1:A:59:ASP:HA	1:A:177:LEU:HD21	1.91	0.52
1:A:70:LEU:CD2	1:A:263:LEU:HD12	2.40	0.52
1:A:185:VAL:HG12	1:B:479:LEU:HD22	1.92	0.51
1:A:459:ASN:HD22	1:B:231:GLY:HA2	1.74	0.51
1:B:170:LEU:C	1:B:170:LEU:HD23	2.35	0.51
1:B:180:MET:C	1:B:182:ARG:N	2.69	0.51
1:B:413:PHE:HD1	3:B:2036:HOH:O	1.94	0.51
1:A:344:PHE:CE2	1:A:369:VAL:HG21	2.46	0.51
1:B:21:GLU:HG2	1:B:101:TRP:CD1	2.45	0.51
1:B:226:GLN:O	1:B:227:PRO:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ASN:CG	1:A:87:TYR:OH	2.54	0.51
1:A:199:LEU:HD22	1:A:260:ALA:HB3	1.91	0.51
1:A:292:VAL:C	1:A:293:PRO:O	2.52	0.51
1:A:385:GLU:CA	1:A:453:MET:HE2	2.40	0.51
1:A:62:VAL:HG12	1:A:71:LEU:HD11	1.93	0.50
1:B:299:ASN:N	1:B:299:ASN:ND2	2.59	0.50
1:B:363:VAL:O	1:B:365:ILE:HG13	2.11	0.50
1:A:153:HIS:HE1	3:A:2035:HOH:O	1.95	0.50
1:A:60:GLU:HB2	1:A:62:VAL:HG23	1.93	0.50
1:A:19:ARG:O	1:A:20:THR:OG1	2.21	0.50
1:A:199:LEU:HD22	1:A:260:ALA:CB	2.42	0.50
1:A:446:HIS:CD2	1:A:459:ASN:H	2.20	0.49
1:B:387:LEU:C	1:B:387:LEU:HD12	2.37	0.49
1:A:31:ASN:OD1	1:A:87:TYR:CE2	2.63	0.49
1:A:32:ARG:HB3	1:A:38:PRO:HD2	1.91	0.49
1:B:260:ALA:C	1:B:261:ASN:O	2.55	0.49
1:A:141:LYS:NZ	1:A:141:LYS:CB	2.73	0.49
1:A:19:ARG:H	1:B:147:ASN:ND2	2.10	0.49
1:A:32:ARG:CB	1:A:38:PRO:CD	2.84	0.49
1:A:466:ALA:CB	1:B:239:THR:CG2	2.91	0.49
1:B:43:TYR:CE1	1:B:58:LEU:HA	2.48	0.49
1:A:395:ASP:HA	1:A:399:MET:O	2.13	0.48
1:A:478:TYR:CD1	1:B:233:PHE:CD1	3.02	0.48
1:B:261:ASN:CB	1:B:264:ASN:HB2	2.05	0.48
1:A:466:ALA:HB1	1:B:239:THR:CG2	2.42	0.48
1:B:299:ASN:H	1:B:299:ASN:ND2	2.06	0.48
1:B:317:ASP:CB	1:B:318:ARG:NH1	2.64	0.48
1:B:304:TYR:HB2	1:B:322:MET:HE1	1.95	0.48
1:B:293:PRO:CB	1:B:404:HIS:HB3	2.44	0.48
1:A:254:GLU:HG2	1:B:468:PHE:HZ	1.78	0.48
1:A:30:ARG:HB3	1:A:32:ARG:HD2	1.94	0.48
1:B:364:SER:HB3	1:B:367:ARG:CD	2.44	0.48
1:A:98:LYS:N	1:A:98:LYS:HD2	2.29	0.48
1:B:62:VAL:HG12	1:B:63:TYR:N	2.30	0.47
1:A:217:ASN:HD22	1:A:218:LYS:HG2	1.79	0.47
1:A:187:VAL:HG11	1:A:199:LEU:HD11	1.96	0.47
1:B:311:GLN:HE21	1:B:319:ILE:CG2	2.27	0.47
1:B:434:HIS:ND1	1:B:435:GLY:N	2.63	0.47
1:A:293:PRO:HB3	1:A:404:HIS:HB3	1.97	0.47
1:A:113:TRP:CZ2	1:A:313:LEU:CD1	2.92	0.47
1:A:162:PHE:HZ	1:A:271:GLN:HB3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ASP:OD1	1:B:78:GLU:HB3	2.15	0.46
1:B:24:ILE:O	1:B:25:ARG:HB2	2.15	0.46
1:B:190:ALA:HB2	1:B:248:ILE:HD11	1.97	0.46
1:B:454:ALA:O	1:B:455:CYS:HB2	2.14	0.46
1:A:263:LEU:N	1:A:263:LEU:CD2	2.79	0.46
1:B:387:LEU:HD12	1:B:388:MET:N	2.30	0.46
1:A:102:PRO:O	1:A:104:GLY:N	2.48	0.46
1:B:167:MET:CE	1:B:170:LEU:HD13	2.46	0.46
1:B:394:ALA:CB	1:B:399:MET:HE3	2.34	0.46
1:A:31:ASN:OD1	1:A:88:TRP:CZ3	2.68	0.46
1:A:29:ARG:O	1:A:103:TYR:OH	2.28	0.46
1:A:131:SER:HB3	1:A:152:LYS:HZ2	1.81	0.45
1:A:341:TRP:CE3	1:A:373:LYS:HE2	2.51	0.45
1:B:53:THR:O	1:B:53:THR:CG2	2.65	0.45
1:B:225:VAL:HG13	1:B:226:GLN:N	2.31	0.45
1:A:263:LEU:HD22	1:A:263:LEU:H	1.79	0.45
1:A:380:GLU:HG3	1:A:381:GLU:H	1.80	0.45
1:A:447:SER:HB3	1:B:221:MET:HE2	1.99	0.45
1:B:142:GLN:HA	1:B:142:GLN:NE2	2.25	0.45
1:A:345:LYS:HA	1:A:346:PRO:HD3	1.81	0.45
1:B:163:LYS:NZ	2:B:1163:PLP:O3	2.48	0.45
1:A:44:VAL:HG21	1:A:74:GLU:OE1	2.17	0.45
1:A:472:MET:CE	1:B:254:GLU:HG2	2.47	0.45
1:B:269:GLU:O	1:B:272:LYS:HG2	2.17	0.45
1:A:129:GLY:O	1:A:130:ASN:HB2	2.17	0.44
1:A:96:VAL:HG12	1:B:96:VAL:HG12	1.99	0.44
1:A:77:MET:O	1:A:81:LYS:HG3	2.18	0.44
1:B:138:ARG:NH1	3:B:2010:HOH:O	2.49	0.44
1:A:20:THR:OG1	1:B:141:LYS:NZ	2.45	0.44
1:A:70:LEU:HD22	1:A:263:LEU:HD12	2.00	0.44
1:B:277:GLU:O	1:B:278:ILE:C	2.60	0.44
1:A:273:THR:HG22	1:A:276:ILE:HD12	2.00	0.43
1:A:443:ILE:O	1:A:444:ASP:C	2.59	0.43
1:B:54:GLU:OE1	1:B:66:ARG:N	2.49	0.43
1:A:153:HIS:CE1	3:A:2035:HOH:O	2.71	0.43
1:A:192:THR:HG22	1:A:214:LEU:CD1	2.48	0.43
1:B:23:ASN:O	1:B:25:ARG:N	2.50	0.43
1:B:167:MET:HE1	1:B:170:LEU:CD1	2.48	0.43
1:A:30:ARG:O	1:A:32:ARG:HG3	2.18	0.43
1:B:294:GLY:O	1:B:326:GLN:OE1	2.37	0.43
1:A:15:LYS:HB2	1:A:16:PRO:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PHE:CE1	1:A:80:LEU:HD23	2.52	0.43
1:A:186:GLY:O	1:A:257:ILE:HA	2.18	0.43
1:B:101:TRP:O	1:B:101:TRP:CE3	2.72	0.43
1:B:247:LEU:O	1:B:251:ILE:HG12	2.18	0.43
1:A:21:GLU:HB2	1:A:101:TRP:HB2	1.99	0.43
1:B:113:TRP:CZ2	1:B:313:LEU:HD12	2.53	0.43
1:B:156:ILE:HG21	1:B:156:ILE:HD13	1.78	0.43
1:B:286:VAL:HA	1:B:287:PRO:HD3	1.97	0.43
1:B:317:ASP:HB2	1:B:318:ARG:CZ	2.46	0.43
1:A:180:MET:O	1:A:181:LYS:HB3	2.17	0.43
1:A:450:ILE:HA	1:A:451:PRO:HD3	1.88	0.43
1:B:165:LEU:O	1:B:168:THR:HG22	2.19	0.43
1:B:477:SER:O	1:B:478:TYR:C	2.61	0.43
1:A:443:ILE:CD1	1:B:222:ALA:HA	2.47	0.42
1:B:293:PRO:HB2	1:B:404:HIS:HB3	2.01	0.42
1:A:15:LYS:HD2	1:A:19:ARG:HG3	2.02	0.42
1:A:221:MET:HE2	1:B:447:SER:HB3	2.00	0.42
1:A:477:SER:OG	1:A:478:TYR:N	2.52	0.42
1:A:263:LEU:CD2	1:A:263:LEU:H	2.32	0.42
1:A:461:PRO:HA	1:B:234:VAL:HB	2.02	0.42
1:B:408:ALA:O	1:B:411:ALA:HB3	2.20	0.42
1:A:125:SER:OG	1:A:128:GLU:OE2	2.37	0.42
1:A:252:THR:HG21	1:A:259:LEU:HD12	1.86	0.42
1:A:471:VAL:HG21	1:B:247:LEU:HD13	2.01	0.42
1:B:467:ASP:O	1:B:470:ALA:HB3	2.20	0.42
1:B:337:TYR:HD1	1:B:341:TRP:CZ2	2.38	0.42
1:B:469:GLY:O	1:B:470:ALA:C	2.60	0.42
1:A:43:TYR:CD1	1:A:58:LEU:HD23	2.54	0.42
1:A:187:VAL:HG12	1:A:199:LEU:HD21	2.02	0.42
1:A:123:ILE:HG22	1:A:124:VAL:N	2.34	0.41
1:B:337:TYR:HD1	1:B:341:TRP:CH2	2.38	0.41
1:A:311:GLN:O	1:A:311:GLN:HG2	2.04	0.41
1:A:252:THR:CG2	1:A:259:LEU:CD1	2.69	0.41
1:A:262:SER:HB2	1:A:263:LEU:HD22	2.02	0.41
1:B:186:GLY:O	1:B:257:ILE:HA	2.20	0.41
1:B:217:ASN:HD22	1:B:217:ASN:N	2.03	0.41
1:A:34:ASN:C	1:A:36:VAL:N	2.79	0.41
1:A:60:GLU:HB2	1:A:62:VAL:CG2	2.49	0.41
1:A:222:ALA:HA	1:B:443:ILE:CD1	2.50	0.41
1:B:129:GLY:O	1:B:130:ASN:C	2.61	0.41
1:A:167:MET:HE1	1:A:170:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:CYS:SG	1:A:190:ALA:N	2.93	0.41
1:B:43:TYR:O	1:B:55:SER:HA	2.20	0.41
1:B:278:ILE:HD13	1:B:428:VAL:HG11	2.02	0.41
1:B:332:PRO:HB2	1:B:336:HIS:HD2	1.85	0.41
1:A:20:THR:O	1:A:20:THR:HG22	2.21	0.41
1:A:21:GLU:CG	1:A:101:TRP:HB2	2.51	0.41
1:A:43:TYR:CE1	1:A:58:LEU:HD23	2.56	0.41
1:B:375:CYS:O	1:B:376:ASN:C	2.63	0.41
1:A:173:GLN:O	1:A:176:ARG:HB3	2.20	0.41
1:A:298:GLY:O	1:A:299:ASN:C	2.63	0.41
1:A:465:LYS:HA	1:A:465:LYS:CE	2.51	0.41
1:A:472:MET:HE3	1:A:472:MET:HB3	1.94	0.41
1:A:472:MET:SD	1:B:251:ILE:HD12	2.60	0.41
1:B:72:ASP:OD2	1:B:301:TYR:OH	2.25	0.41
1:A:76:ASP:OD1	1:A:78:GLU:HB3	2.21	0.41
1:A:162:PHE:CE2	1:A:271:GLN:CD	2.99	0.41
1:A:95:ARG:NH1	1:A:109:SER:O	2.48	0.40
1:A:300:ILE:CD1	1:A:372:LEU:HD21	2.51	0.40
1:B:146:MET:SD	1:B:416:ARG:HD2	2.61	0.40
1:B:271:GLN:O	1:B:272:LYS:C	2.64	0.40
1:B:76:ASP:OD1	1:B:76:ASP:C	2.61	0.40
1:A:285:GLN:HB2	1:A:426:ARG:HH12	1.86	0.40
1:A:165:LEU:O	1:A:168:THR:HG22	2.21	0.40
1:A:459:ASN:ND2	1:B:231:GLY:HA2	2.36	0.40
1:B:98:LYS:HA	1:B:98:LYS:HD3	1.70	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	442/486 (91%)	391 (88%)	36 (8%)	15 (3%)	 

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	431/486 (89%)	377 (88%)	43 (10%)	11 (3%)	4	6
All	All	873/972 (90%)	768 (88%)	79 (9%)	26 (3%)	3	5

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	66	ARG
1	A	103	TYR
1	A	478	TYR
1	B	23	ASN
1	B	34	ASN
1	B	181	LYS
1	A	36	VAL
1	A	102	PRO
1	A	293	PRO
1	A	340	GLY
1	B	179	LYS
1	B	184	VAL
1	B	260	ALA
1	B	340	GLY
1	A	329	ASN
1	B	364	SER
1	A	12	THR
1	A	17	PRO
1	B	101	TRP
1	A	477	SER
1	B	261	ASN
1	A	294	GLY
1	B	24	ILE
1	A	101	TRP
1	A	183	PRO

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	373/403 (93%)	363 (97%)	10 (3%)	39	65
1	B	364/403 (90%)	349 (96%)	15 (4%)	27	52
All	All	737/806 (91%)	712 (97%)	25 (3%)	32	58

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	32	ARG
1	A	42	LYS
1	A	44	VAL
1	A	159	THR
1	A	217	ASN
1	A	263	LEU
1	A	286	VAL
1	A	308	LYS
1	A	465	LYS
1	B	32	ARG
1	B	42	LYS
1	B	82	ARG
1	B	138	ARG
1	B	142	GLN
1	B	159	THR
1	B	170	LEU
1	B	217	ASN
1	B	263	LEU
1	B	299	ASN
1	B	308	LYS
1	B	315	LEU
1	B	318	ARG
1	B	416	ARG
1	B	465	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	153	HIS
1	A	217	ASN
1	A	223	GLN
1	A	230	ASN

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Mol	Chain	Res	Type
1	A	326	GLN
1	A	376	ASN
1	A	393	GLN
1	A	418	GLN
1	A	446	HIS
1	A	448	ASN
1	B	47	ASN
1	B	132	ASN
1	B	142	GLN
1	B	217	ASN
1	B	226	GLN
1	B	230	ASN
1	B	299	ASN
1	B	311	GLN
1	B	326	GLN
1	B	376	ASN
1	B	393	GLN
1	B	446	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PLP	A	1163	1	15,15,16	1.85	4 (26%)	21,22,23	1.94	9 (42%)
2	PLP	B	1163	1	15,15,16	2.23	4 (26%)	21,22,23	2.34	3 (14%)

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
2	PLP	A	1163	1	-	0/6/6/8	0/1/1/1
2	PLP	B	1163	1	-	2/6/6/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1163	PLP	O3-C3	-5.42	1.24	1.36
2	A	1163	PLP	O3-C3	-5.36	1.24	1.36
2	B	1163	PLP	C2-N1	3.56	1.40	1.33
2	B	1163	PLP	C5-C4	3.16	1.44	1.40
2	B	1163	PLP	C6-N1	3.14	1.40	1.34
2	A	1163	PLP	C2-N1	2.63	1.38	1.33
2	A	1163	PLP	C6-N1	2.45	1.39	1.34
2	A	1163	PLP	P-O3P	-2.04	1.47	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1163	PLP	O4P-C5A-C5	8.67	125.60	109.36
2	A	1163	PLP	O4P-C5A-C5	4.72	118.20	109.36
2	A	1163	PLP	O3P-P-O4P	-3.22	98.26	106.67
2	A	1163	PLP	C3-C4-C5	2.55	121.65	118.59
2	A	1163	PLP	C4A-C4-C5	-2.47	118.39	120.94
2	A	1163	PLP	O3P-P-O2P	2.43	116.90	107.80
2	B	1163	PLP	C2A-C2-N1	2.38	122.13	117.64
2	A	1163	PLP	C3-C2-N1	-2.33	118.02	120.96
2	A	1163	PLP	C2A-C2-C3	2.25	123.43	120.80
2	A	1163	PLP	O3-C3-C2	2.24	122.23	117.58
2	A	1163	PLP	C5-C6-N1	-2.11	120.40	123.83
2	B	1163	PLP	O3P-P-O4P	-2.01	101.42	106.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1163	PLP	C4-C5-C5A-O4P
2	B	1163	PLP	C6-C5-C5A-O4P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1163	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	448/486 (92%)	0.02	14 (3%) 51 46	6, 18, 37, 73	0
1	B	437/486 (89%)	-0.12	5 (1%) 78 74	7, 18, 34, 55	0
All	All	885/972 (91%)	-0.05	19 (2%) 63 59	6, 18, 36, 73	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	ALA	5.6
1	A	14	VAL	4.3
1	A	31	ASN	3.4
1	B	68	GLY	3.3
1	A	20	THR	3.2
1	B	69	GLY	3.2
1	A	30	ARG	3.1
1	A	15	LYS	3.1
1	A	49	ALA	3.1
1	B	66	ARG	2.7
1	B	24	ILE	2.7
1	A	16	PRO	2.7
1	A	18	HIS	2.6
1	A	48	ALA	2.5
1	A	50	PRO	2.4
1	A	32	ARG	2.3
1	A	35	ALA	2.3
1	B	49	ALA	2.2
1	A	11	GLU	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 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
2	PLP	B	1163	15/16	0.75	0.13	47,52,54,56	0
2	PLP	A	1163	15/16	0.76	0.12	47,52,53,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.