



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:31 AM UTC

PDB ID : 1A3G / pdb_00001a3g
Title : BRANCHED-CHAIN AMINO ACID AMINOTRANSFERASE FROM ES-
CHERICHIA COLI
Authors : Okada, K.; Hirotsu, K.; Sato, M.; Hayashi, H.; Kagamiyama, H.
Deposited on : 1998-01-21
Resolution : 2.50 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

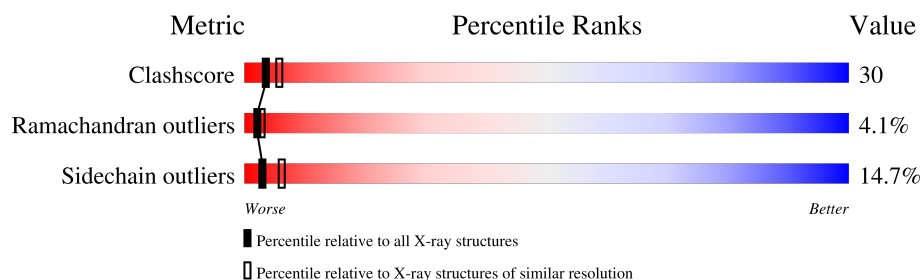
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	308	
1	B	308	
1	C	308	

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
2	PLP	A	413	-	X	-	-
2	PLP	B	413	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	C	413	-	X	-	-

2 Entry composition [i](#)

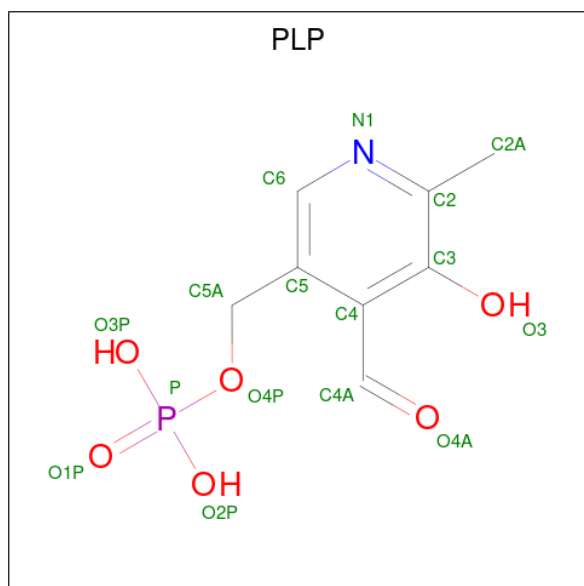
There are 3 unique types of molecules in this entry. The entry contains 7474 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BRANCHED-CHAIN AMINO ACID AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2303	1460	402	431	10			
1	B	295	Total	C	N	O	S	0	0	0
			2303	1460	402	431	10			
1	C	295	Total	C	N	O	S	0	0	0
			2303	1460	402	431	10			

- 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		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is water.

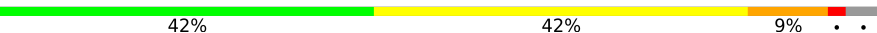
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	155	Total 155	O 155	0	0
3	B	191	Total 191	O 191	0	0
3	C	174	Total 174	O 174	0	0

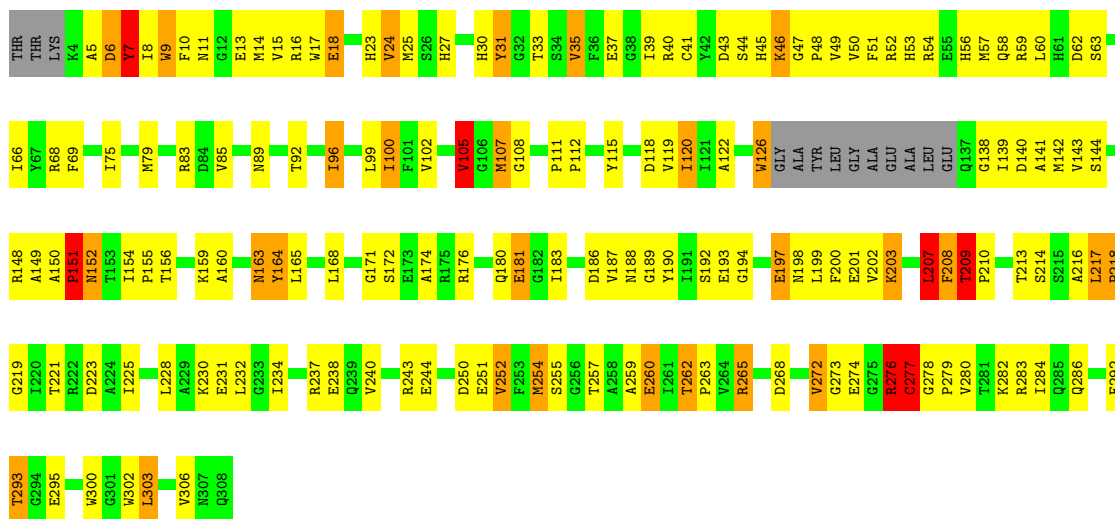
3 Residue-property plots

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. 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. 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.

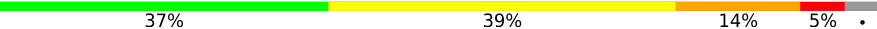
Note EDS was not executed.

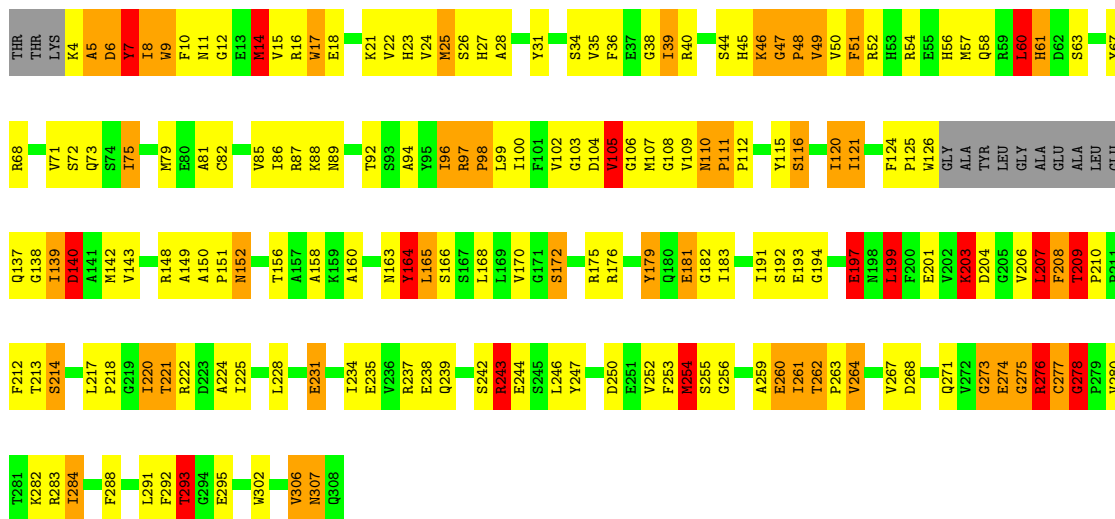
• Molecule 1: BRANCHED-CHAIN AMINO ACID AMINOTRANSFERASE

Chain A: 



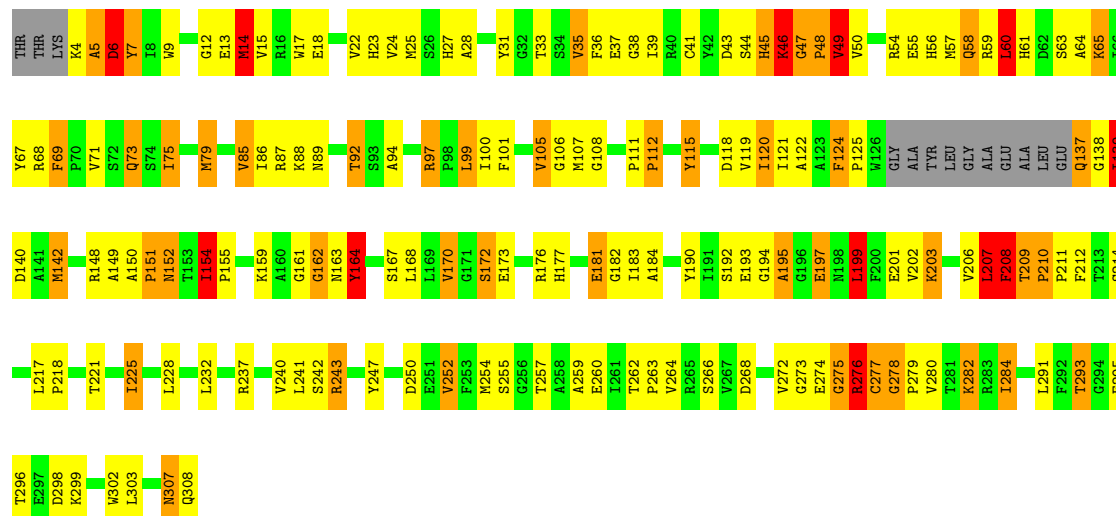
• Molecule 1: BRANCHED-CHAIN AMINO ACID AMINOTRANSFERASE

Chain B: 



- Molecule 1: BRANCHED-CHAIN AMINO ACID AMINOTRANSFERASE

Chain C: 42% 36% 14% . .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.10Å 144.00Å 102.90Å 90.00° 136.10° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	83.6 (10.00-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.188 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7474	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	1.51	15/2357 (0.6%)	1.61	50/3193 (1.6%)
1	B	1.70	30/2357 (1.3%)	1.75	60/3193 (1.9%)
1	C	1.64	22/2357 (0.9%)	1.71	59/3193 (1.8%)
All	All	1.62	67/7071 (0.9%)	1.69	169/9579 (1.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	2
All	All	0	8

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	225	ILE	CA-CB	-10.49	1.42	1.54
1	B	100	ILE	CA-CB	-10.09	1.41	1.54
1	C	203	LYS	CA-C	-9.26	1.47	1.52
1	C	152	ASN	CA-C	-9.04	1.40	1.52
1	B	8	ILE	CA-CB	-8.13	1.44	1.54
1	C	210	PRO	CA-C	7.77	1.56	1.51
1	B	206	VAL	CA-CB	-7.76	1.44	1.54
1	B	34	SER	CA-C	-7.44	1.43	1.52
1	C	46	LYS	CA-C	-7.28	1.43	1.52
1	B	204	ASP	CA-C	-7.12	1.43	1.53
1	B	150	ALA	CA-CB	-6.98	1.43	1.53
1	A	149	ALA	CA-CB	-6.88	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	98	PRO	CA-C	6.80	1.60	1.52
1	B	179	TYR	C-O	-6.78	1.16	1.23
1	C	28	ALA	CA-CB	-6.71	1.42	1.53
1	B	152	ASN	CA-C	-6.70	1.43	1.52
1	C	97	ARG	N-CA	-6.70	1.39	1.46
1	A	192	SER	CA-C	-6.67	1.48	1.52
1	A	208	PHE	N-CA	6.66	1.54	1.46
1	C	181	GLU	CD-OE2	6.61	1.38	1.25
1	B	60	LEU	C-O	-6.44	1.16	1.24
1	C	122	ALA	CA-C	-6.38	1.44	1.52
1	A	280	VAL	CA-CB	-6.27	1.46	1.54
1	B	28	ALA	CA-CB	-6.25	1.42	1.53
1	C	201	GLU	C-O	-6.17	1.16	1.23
1	A	13	GLU	CA-C	-6.11	1.45	1.52
1	B	25	MET	SD-CE	-6.10	1.64	1.79
1	C	262	THR	CA-CB	-6.02	1.44	1.53
1	C	14	MET	SD-CE	-5.96	1.64	1.79
1	B	293	THR	CA-CB	-5.94	1.43	1.53
1	C	121	ILE	CA-CB	-5.94	1.47	1.54
1	B	267	VAL	CA-CB	-5.91	1.47	1.54
1	A	174	ALA	CA-CB	-5.88	1.44	1.53
1	C	206	VAL	CA-CB	-5.88	1.46	1.54
1	C	75	ILE	CA-CB	-5.84	1.46	1.54
1	A	144	SER	CA-C	-5.82	1.44	1.53
1	B	306	VAL	CA-CB	-5.78	1.48	1.54
1	B	261	ILE	C-O	-5.77	1.17	1.24
1	B	164	TYR	CA-C	-5.75	1.45	1.52
1	C	184	ALA	CA-CB	-5.75	1.44	1.53
1	A	151	PRO	C-N	-5.71	1.26	1.33
1	C	79	MET	SD-CE	-5.71	1.65	1.79
1	C	208	PHE	N-CA	5.67	1.53	1.46
1	A	216	ALA	CA-CB	-5.64	1.44	1.53
1	C	43	ASP	C-O	-5.51	1.17	1.24
1	B	170	VAL	CA-CB	-5.44	1.48	1.54
1	C	149	ALA	CA-CB	-5.43	1.44	1.53
1	A	57	MET	SD-CE	-5.41	1.66	1.79
1	A	181	GLU	CD-OE1	5.40	1.35	1.25
1	B	208	PHE	N-CA	5.38	1.53	1.46
1	B	160	ALA	CA-CB	-5.31	1.44	1.53
1	B	239	GLN	N-CA	-5.26	1.39	1.45
1	A	187	VAL	CA-C	-5.23	1.45	1.52
1	B	49	VAL	CA-C	5.23	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	182	GLY	CA-C	-5.23	1.48	1.52
1	C	31	TYR	CA-C	-5.19	1.45	1.52
1	B	17	TRP	CA-C	-5.15	1.45	1.52
1	A	122	ALA	CA-CB	-5.13	1.44	1.53
1	B	63	SER	N-CA	-5.08	1.40	1.46
1	B	140	ASP	N-CA	5.08	1.52	1.46
1	C	50	VAL	CA-CB	-5.07	1.47	1.54
1	C	139	ILE	CA-CB	-5.06	1.47	1.54
1	B	264	VAL	CA-CB	5.05	1.60	1.54
1	B	181	GLU	CD-OE2	5.05	1.34	1.25
1	B	261	ILE	CA-C	-5.05	1.48	1.53
1	A	54	ARG	CA-C	-5.04	1.46	1.52
1	A	150	ALA	CA-CB	-5.03	1.46	1.53

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105	VAL	N-CA-C	-13.44	92.43	108.82
1	C	210	PRO	CA-C-N	11.21	131.62	120.52
1	C	210	PRO	C-N-CA	11.21	131.62	120.52
1	B	60	LEU	N-CA-C	-11.01	99.25	111.14
1	B	203	LYS	CA-C-N	-10.88	108.18	123.20
1	B	203	LYS	C-N-CA	-10.88	108.18	123.20
1	C	65	LYS	N-CA-C	-9.46	100.95	111.07
1	A	118	ASP	N-CA-C	-8.91	95.78	109.95
1	C	58	GLN	N-CA-C	-8.83	101.63	111.07
1	A	165	LEU	N-CA-C	-8.75	101.82	111.36
1	A	105	VAL	N-CA-C	-8.64	91.37	109.34
1	B	151	PRO	CA-C-N	-8.56	105.19	121.54
1	B	151	PRO	C-N-CA	-8.56	105.19	121.54
1	A	152	ASN	N-CA-CB	-8.39	99.88	110.45
1	B	105	VAL	N-CA-CB	-8.29	103.17	112.45
1	B	151	PRO	N-CA-C	8.22	129.41	112.47
1	A	69	PHE	N-CA-C	-8.16	97.90	109.24
1	C	69	PHE	N-CA-C	-8.13	99.56	109.72
1	C	151	PRO	N-CA-C	8.11	129.17	112.47
1	C	207	LEU	N-CA-C	8.06	123.89	111.56
1	A	163	ASN	N-CA-C	-7.96	102.69	111.36
1	A	151	PRO	N-CA-C	7.94	128.82	112.47
1	C	6	ASP	N-CA-C	-7.68	97.37	109.50
1	B	73	GLN	N-CA-C	7.67	121.95	109.76
1	C	274	GLU	N-CA-C	7.61	119.81	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	TYR	N-CA-C	7.44	121.79	112.87
1	B	139	ILE	N-CA-C	7.37	120.33	112.96
1	A	203	LYS	CA-C-N	-7.25	111.32	122.05
1	A	203	LYS	C-N-CA	-7.25	111.32	122.05
1	B	207	LEU	N-CA-C	7.20	126.13	110.80
1	A	43	ASP	N-CA-C	-7.17	97.56	108.96
1	C	49	VAL	CB-CA-C	7.15	119.84	110.12
1	A	154	ILE	CA-C-N	7.03	128.63	119.84
1	A	154	ILE	C-N-CA	7.03	128.63	119.84
1	A	18	GLU	N-CA-C	7.01	121.58	112.89
1	B	208	PHE	N-CA-C	6.99	125.68	110.80
1	C	201	GLU	CA-C-N	-6.98	114.00	123.14
1	C	201	GLU	C-N-CA	-6.98	114.00	123.14
1	B	243	ARG	NE-CZ-NH1	-6.93	114.56	121.50
1	C	115	TYR	N-CA-C	-6.91	101.62	110.53
1	C	308	GLN	N-CA-C	-6.86	91.79	111.00
1	C	203	LYS	CA-C-N	-6.85	111.81	122.08
1	C	203	LYS	C-N-CA	-6.85	111.81	122.08
1	B	209	THR	CA-C-N	6.78	127.36	120.38
1	B	209	THR	C-N-CA	6.78	127.36	120.38
1	B	116	SER	N-CA-C	6.76	120.56	109.06
1	A	221	THR	N-CA-C	-6.73	103.19	111.40
1	A	152	ASN	CB-CA-C	6.68	121.29	111.88
1	B	14	MET	N-CA-C	-6.62	99.52	110.17
1	C	207	LEU	O-C-N	-6.57	114.76	122.32
1	B	210	PRO	CA-C-N	-6.53	113.99	120.98
1	B	210	PRO	C-N-CA	-6.53	113.99	120.98
1	B	165	LEU	N-CA-C	-6.52	104.02	112.23
1	B	209	THR	CB-CA-C	-6.50	99.35	109.55
1	A	9	TRP	N-CA-C	-6.49	100.68	110.28
1	B	278	GLY	N-CA-C	6.48	125.56	112.34
1	C	272	VAL	N-CA-C	-6.37	99.12	108.54
1	B	204	ASP	N-CA-C	-6.35	99.59	108.54
1	B	307	ASN	N-CA-C	6.34	119.59	108.56
1	C	275	GLY	N-CA-C	6.33	128.17	113.18
1	A	250	ASP	N-CA-C	-6.31	106.12	113.88
1	C	49	VAL	N-CA-CB	-6.31	102.66	111.99
1	B	284	ILE	CB-CA-C	-6.30	103.77	112.02
1	C	307	ASN	CA-C-N	6.29	133.03	121.70
1	C	307	ASN	C-N-CA	6.29	133.03	121.70
1	B	5	ALA	N-CA-C	-6.28	97.42	110.80
1	B	197	GLU	N-CA-C	6.28	118.85	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	151	PRO	CA-C-N	-6.26	109.58	121.54
1	C	151	PRO	C-N-CA	-6.26	109.58	121.54
1	A	208	PHE	N-CA-C	6.24	124.08	110.80
1	A	105	VAL	N-CA-CB	-6.22	100.97	111.23
1	C	118	ASP	N-CA-C	-6.21	98.27	108.76
1	A	151	PRO	CA-C-N	-6.14	112.86	122.08
1	A	151	PRO	C-N-CA	-6.14	112.86	122.08
1	C	92	THR	CA-C-N	-6.13	114.47	123.05
1	C	92	THR	C-N-CA	-6.13	114.47	123.05
1	A	284	ILE	CB-CA-C	-6.12	104.13	111.97
1	C	28	ALA	N-CA-C	6.07	119.52	111.75
1	B	100	ILE	N-CA-C	-6.07	98.73	107.78
1	B	47	GLY	N-CA-C	-6.05	99.99	112.34
1	C	31	TYR	N-CA-C	6.05	119.62	112.72
1	B	51	PHE	N-CA-C	6.04	118.49	109.25
1	A	46	LYS	N-CA-C	-6.01	107.18	114.75
1	C	232	LEU	N-CA-C	-5.97	105.97	113.20
1	B	111	PRO	CA-C-N	5.97	127.30	119.84
1	B	111	PRO	C-N-CA	5.97	127.30	119.84
1	C	43	ASP	N-CA-C	-5.95	99.53	109.24
1	C	5	ALA	N-CA-C	-5.95	100.39	108.24
1	C	199	LEU	CA-CB-CG	5.93	137.07	116.30
1	B	221	THR	N-CA-C	-5.91	104.47	111.03
1	A	111	PRO	CA-C-N	5.88	125.79	119.85
1	A	111	PRO	C-N-CA	5.88	125.79	119.85
1	B	208	PHE	CB-CA-C	-5.87	98.73	110.42
1	B	28	ALA	N-CA-C	5.84	119.22	111.75
1	A	31	TYR	N-CA-C	5.83	121.11	113.30
1	B	97	ARG	CG-CD-NE	-5.81	99.21	112.00
1	B	140	ASP	CB-CA-C	-5.81	98.86	110.42
1	C	272	VAL	CB-CA-C	-5.73	104.37	111.08
1	A	100	ILE	N-CA-C	-5.70	99.33	107.77
1	B	143	VAL	N-CA-CB	5.70	116.93	110.72
1	A	217	LEU	CA-C-N	5.69	126.95	119.84
1	A	217	LEU	C-N-CA	5.69	126.95	119.84
1	A	8	ILE	N-CA-C	-5.65	99.92	108.17
1	A	149	ALA	N-CA-C	5.64	118.54	110.24
1	A	62	ASP	N-CA-C	5.63	118.35	111.82
1	A	58	GLN	N-CA-C	-5.59	105.19	112.23
1	A	189	GLY	N-CA-C	-5.55	107.54	115.64
1	A	244	GLU	CB-CA-C	-5.54	101.26	110.68
1	C	207	LEU	CA-C-N	-5.54	110.96	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	207	LEU	C-N-CA	-5.54	110.96	121.54
1	C	119	VAL	N-CA-C	-5.53	100.63	109.20
1	B	92	THR	N-CA-C	-5.49	105.70	112.72
1	C	60	LEU	N-CA-C	-5.48	105.31	111.28
1	B	104	ASP	N-CA-CB	5.46	118.57	110.49
1	B	291	LEU	N-CA-C	-5.44	105.38	112.23
1	B	224	ALA	N-CA-C	-5.43	104.40	111.02
1	C	214	SER	N-CA-C	-5.42	107.23	112.97
1	B	261	ILE	N-CA-CB	-5.41	107.24	112.65
1	B	9	TRP	N-CA-C	-5.38	103.80	110.41
1	B	254	MET	CB-CA-C	-5.38	100.93	109.80
1	C	262	THR	CB-CA-C	-5.38	102.70	109.31
1	A	11	ASN	CA-C-N	-5.35	117.62	123.30
1	A	11	ASN	C-N-CA	-5.35	117.62	123.30
1	B	110	ASN	CB-CA-C	-5.35	103.93	110.08
1	C	87	ARG	CB-CA-C	-5.34	102.73	110.96
1	C	150	ALA	CA-C-N	5.34	126.51	119.84
1	C	150	ALA	C-N-CA	5.34	126.51	119.84
1	B	264	VAL	N-CA-C	-5.33	100.80	108.53
1	C	154	ILE	CA-C-N	5.33	126.50	119.84
1	C	154	ILE	C-N-CA	5.33	126.50	119.84
1	C	73	GLN	N-CA-C	5.32	118.60	110.20
1	B	8	ILE	N-CA-C	-5.31	100.67	108.11
1	A	208	PHE	CB-CA-C	-5.31	99.85	110.42
1	A	207	LEU	N-CA-C	5.30	122.08	110.80
1	A	92	THR	N-CA-C	-5.28	105.96	112.72
1	A	164	TYR	N-CA-C	5.28	122.04	110.80
1	A	141	ALA	N-CA-C	-5.28	101.62	109.96
1	B	235	GLU	CA-C-N	-5.27	115.79	123.06
1	B	235	GLU	C-N-CA	-5.27	115.79	123.06
1	C	154	ILE	N-CA-C	-5.26	97.53	108.88
1	B	36	PHE	N-CA-C	5.25	116.96	109.14
1	B	302	TRP	N-CA-C	5.25	119.55	113.20
1	A	234	ILE	N-CA-C	5.23	116.24	108.23
1	C	47	GLY	N-CA-C	-5.21	101.72	112.34
1	B	58	GLN	N-CA-C	-5.21	105.50	111.07
1	C	195	ALA	N-CA-C	5.15	116.89	111.28
1	B	267	VAL	N-CA-C	-5.13	100.72	108.12
1	C	208	PHE	N-CA-C	5.13	121.72	110.80
1	C	307	ASN	O-C-N	5.12	128.98	122.84
1	A	300	TRP	N-CA-C	5.11	118.67	112.23
1	A	238	GLU	CB-CA-C	-5.10	101.93	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	ALA	N-CA-C	-5.09	102.99	110.52
1	C	124	PHE	N-CA-C	-5.08	102.35	108.25
1	C	111	PRO	CA-C-N	5.08	126.19	119.84
1	C	111	PRO	C-N-CA	5.08	126.19	119.84
1	A	210	PRO	CA-C-N	-5.07	115.56	120.98
1	A	210	PRO	C-N-CA	-5.07	115.56	120.98
1	B	34	SER	N-CA-C	-5.07	102.06	109.81
1	C	170	VAL	CB-CA-C	-5.06	104.31	112.16
1	C	97	ARG	CG-CD-NE	-5.06	100.86	112.00
1	A	209	THR	N-CA-C	-5.05	100.66	108.55
1	A	171	GLY	N-CA-C	5.04	118.34	112.50
1	C	202	VAL	CA-C-N	-5.04	115.18	121.98
1	C	202	VAL	C-N-CA	-5.04	115.18	121.98
1	B	262	THR	CA-C-N	5.03	127.04	120.25
1	B	262	THR	C-N-CA	5.03	127.04	120.25
1	A	262	THR	CA-C-O	5.02	124.21	119.59
1	B	199	LEU	CA-CB-CG	5.02	133.88	116.30
1	B	182	GLY	N-CA-C	-5.01	103.05	110.71

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	TYR	Sidechain
1	A	31	TYR	Sidechain
1	A	7	TYR	Sidechain
1	B	247	TYR	Sidechain
1	B	260	GLU	Mainchain
1	B	7	TYR	Sidechain
1	C	164	TYR	Sidechain
1	C	307	ASN	Mainchain

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	2303	0	2243	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2303	0	2242	151	0
1	C	2303	0	2243	134	0
2	A	15	0	7	2	0
2	B	15	0	6	2	0
2	C	15	0	6	3	0
3	A	155	0	0	8	0
3	B	191	0	0	16	0
3	C	174	0	0	15	0
All	All	7474	0	6747	405	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 30.

All (405) 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:49:VAL:HG11	1:A:303:LEU:HB3	1.27	1.14
1:B:120:ILE:HG21	3:B:1621:HOH:O	1.51	1.10
1:B:181:GLU:HG2	1:B:254:MET:HE3	1.41	1.01
1:C:105:VAL:HG13	1:C:112:PRO:HD2	1.49	0.95
1:A:7:TYR:HA	1:A:15:VAL:O	1.68	0.94
1:A:282:LYS:O	1:A:286:GLN:HG3	1.67	0.93
1:C:41:CYS:SG	3:C:1961:HOH:O	2.25	0.93
1:A:265:ARG:HH11	1:A:265:ARG:HG2	1.31	0.92
1:A:47:GLY:CA	1:A:49:VAL:HG23	2.01	0.90
1:B:264:VAL:HG23	3:B:1780:HOH:O	1.72	0.89
1:C:7:TYR:HA	1:C:15:VAL:O	1.73	0.89
1:C:293:THR:HG21	1:C:295:GLU:OE1	1.73	0.89
1:C:137:GLN:HG3	1:C:276:ARG:HB3	1.52	0.88
1:B:276:ARG:HD3	1:B:277:CYS:N	1.88	0.88
1:A:208:PHE:HA	1:A:237:ARG:O	1.74	0.86
1:A:47:GLY:HA2	1:A:49:VAL:HG23	1.56	0.86
1:A:27:HIS:HE1	1:A:108:GLY:O	1.58	0.84
1:A:183:ILE:HD12	3:A:1901:HOH:O	1.78	0.83
1:C:92:THR:HG22	3:C:1927:HOH:O	1.79	0.82
1:A:75:ILE:HG22	1:A:79:MET:CE	2.09	0.81
1:A:183:ILE:HB	3:A:1901:HOH:O	1.80	0.80
1:A:197:GLU:HB2	1:A:255:SER:O	1.81	0.80
1:B:27:HIS:CE1	1:B:31:TYR:HD2	2.01	0.78
1:A:100:ILE:HG12	1:A:119:VAL:HG22	1.65	0.78
1:C:293:THR:HG22	1:C:295:GLU:H	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:LEU:O	1:B:209:THR:HG22	1.84	0.77
1:A:265:ARG:HG2	1:A:265:ARG:NH1	2.00	0.76
1:B:181:GLU:CG	1:B:254:MET:HE3	2.16	0.76
1:C:105:VAL:CG1	1:C:112:PRO:HD2	2.15	0.75
1:A:265:ARG:HB3	1:A:276:ARG:HB2	1.68	0.75
1:C:210:PRO:HD3	1:C:241:LEU:HD12	1.67	0.75
1:B:86:ILE:HG21	1:B:306:VAL:HG21	1.68	0.74
1:B:75:ILE:HG22	1:B:79:MET:HE2	1.71	0.73
1:A:202:VAL:HB	1:A:251:GLU:HB2	1.69	0.73
1:B:96:ILE:N	1:B:96:ILE:HD12	2.03	0.73
1:A:199:LEU:O	1:A:209:THR:HG22	1.88	0.73
1:C:302:TRP:HZ3	3:C:1985:HOH:O	1.72	0.72
1:B:44:SER:OG	1:B:47:GLY:N	2.21	0.72
1:B:94:ALA:HB1	1:B:124:PHE:O	1.88	0.72
1:A:75:ILE:HG22	1:A:79:MET:HE3	1.70	0.72
1:C:107:MET:HA	1:C:107:MET:HE3	1.72	0.72
1:A:139:ILE:HD13	1:A:262:THR:CG2	2.20	0.72
1:C:199:LEU:O	1:C:209:THR:HG22	1.88	0.71
1:B:27:HIS:CE1	1:B:31:TYR:CD2	2.77	0.71
1:A:207:LEU:O	1:A:208:PHE:HB2	1.90	0.71
1:B:44:SER:C	1:B:46:LYS:H	1.97	0.71
1:A:126:TRP:HA	1:A:126:TRP:CE3	2.24	0.71
1:A:139:ILE:HD13	1:A:262:THR:HG21	1.72	0.70
1:B:47:GLY:HA2	1:B:49:VAL:HB	1.74	0.69
1:B:21:LYS:HD2	3:B:1651:HOH:O	1.93	0.69
1:C:208:PHE:HA	1:C:237:ARG:O	1.93	0.69
1:B:208:PHE:HA	1:B:237:ARG:O	1.94	0.68
1:A:303:LEU:N	1:A:303:LEU:HD23	2.09	0.68
1:A:200:PHE:CD1	1:A:209:THR:HG23	2.28	0.67
1:C:137:GLN:HG3	1:C:276:ARG:CB	2.22	0.67
1:B:256:GLY:HA3	3:B:1769:HOH:O	1.94	0.67
1:B:7:TYR:HB3	1:B:14:MET:HE2	1.76	0.67
1:A:47:GLY:HA3	1:A:49:VAL:HG23	1.77	0.67
1:B:201:GLU:O	1:B:207:LEU:O	2.13	0.67
1:B:8:ILE:HD11	1:B:17:TRP:CE3	2.30	0.66
1:C:45:HIS:CD2	1:C:45:HIS:H	2.12	0.66
1:B:276:ARG:HE	1:B:278:GLY:N	1.94	0.66
1:A:37:GLU:OE1	1:A:56:HIS:HD2	1.79	0.65
1:A:274:GLU:HB2	1:A:277:CYS:SG	2.36	0.65
1:C:252:VAL:HG22	1:C:264:VAL:HB	1.77	0.65
1:C:255:SER:HA	1:C:260:GLU:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:LEU:HD11	3:C:1985:HOH:O	1.94	0.65
1:B:268:ASP:O	1:C:68:ARG:NH2	2.30	0.64
1:A:274:GLU:CB	1:A:277:CYS:SG	2.86	0.64
1:B:8:ILE:HG22	1:B:9:TRP:O	1.96	0.64
1:B:271:GLN:CD	1:B:275:GLY:H	2.05	0.64
1:C:139:ILE:O	1:C:140:ASP:HB2	1.98	0.64
1:C:181:GLU:HG2	1:C:254:MET:HE2	1.80	0.64
1:B:253:PHE:HA	3:B:1780:HOH:O	1.98	0.63
1:B:139:ILE:O	1:B:140:ASP:CB	2.44	0.63
1:C:45:HIS:O	1:C:46:LYS:HB3	1.98	0.63
1:A:268:ASP:O	1:B:68:ARG:NH2	2.32	0.62
1:B:120:ILE:HG23	1:B:121:ILE:N	2.13	0.62
1:B:207:LEU:O	1:B:208:PHE:HB2	1.99	0.62
1:C:60:LEU:HD13	1:C:100:ILE:HD11	1.82	0.62
1:C:37:GLU:HG3	1:C:38:GLY:N	2.14	0.62
1:A:49:VAL:HG11	1:A:303:LEU:CB	2.17	0.62
1:C:54:ARG:NH1	1:C:79:MET:HE1	2.15	0.62
1:A:190:TYR:CE1	1:B:213:THR:HB	2.35	0.61
1:C:217:LEU:C	1:C:217:LEU:HD23	2.26	0.61
1:B:139:ILE:O	1:B:140:ASP:HB2	2.00	0.61
1:B:96:ILE:HD12	1:B:96:ILE:H	1.65	0.60
1:A:159:LYS:NZ	2:A:413:PLP:O3	2.32	0.60
1:C:37:GLU:HG3	1:C:38:GLY:H	1.66	0.60
1:C:209:THR:HB	3:C:1506:HOH:O	2.00	0.60
1:B:6:ASP:O	1:B:7:TYR:HB2	2.01	0.60
1:A:75:ILE:HD12	1:A:75:ILE:N	2.17	0.60
1:C:45:HIS:CD2	1:C:45:HIS:N	2.69	0.60
1:C:39:ILE:HD11	1:C:57:MET:HE2	1.84	0.60
1:C:154:ILE:HG22	1:C:154:ILE:O	2.02	0.60
1:A:201:GLU:O	1:A:207:LEU:O	2.20	0.59
1:B:276:ARG:HE	1:B:278:GLY:HA3	1.67	0.59
1:B:26:SER:HA	1:B:103:GLY:O	2.02	0.59
1:B:27:HIS:ND1	1:B:31:TYR:HD2	1.98	0.59
1:C:49:VAL:CG1	1:C:303:LEU:HD22	2.33	0.59
1:A:207:LEU:O	1:A:208:PHE:CB	2.50	0.58
1:B:164:TYR:OH	2:B:413:PLP:O3	2.14	0.58
1:A:47:GLY:HA2	1:A:49:VAL:CG2	2.32	0.58
1:B:259:ALA:O	1:B:260:GLU:C	2.43	0.58
1:A:44:SER:OG	1:A:47:GLY:N	2.36	0.58
1:C:291:LEU:HD23	1:C:296:THR:HB	1.84	0.58
1:A:40:ARG:HG2	1:A:257:THR:CG2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:LEU:HD11	3:C:1985:HOH:O	2.03	0.58
1:C:159:LYS:NZ	2:C:413:PLP:O3	2.33	0.58
1:A:252:VAL:HG12	1:A:272:VAL:HG11	1.85	0.57
1:C:148:ARG:HD3	1:C:192:SER:OG	2.04	0.57
1:B:6:ASP:O	1:B:7:TYR:CB	2.52	0.57
1:C:75:ILE:HG22	1:C:79:MET:CE	2.35	0.57
1:C:139:ILE:O	1:C:140:ASP:CB	2.47	0.57
1:A:23:HIS:CD2	1:A:25:MET:H	2.22	0.57
1:A:302:TRP:C	1:A:303:LEU:HD23	2.29	0.57
1:C:164:TYR:OH	2:C:413:PLP:O3	2.23	0.57
1:C:207:LEU:O	1:C:208:PHE:HB2	2.05	0.57
1:C:302:TRP:CZ3	3:C:1985:HOH:O	2.53	0.57
1:A:209:THR:HB	3:A:1501:HOH:O	2.03	0.56
1:B:112:PRO:HG2	3:B:1878:HOH:O	2.04	0.56
1:B:191:ILE:HD11	1:B:246:LEU:HG	1.86	0.56
1:A:75:ILE:HD12	1:A:75:ILE:H	1.69	0.56
1:C:6:ASP:O	1:C:89:ASN:OD1	2.24	0.56
1:B:46:LYS:C	1:B:47:GLY:O	2.45	0.56
1:C:39:ILE:CD1	1:C:57:MET:HE2	2.36	0.56
1:C:293:THR:CG2	1:C:295:GLU:HG3	2.35	0.56
1:B:45:HIS:O	1:B:46:LYS:HB3	2.05	0.56
1:B:276:ARG:HE	1:B:278:GLY:CA	2.18	0.56
1:B:6:ASP:HA	1:B:17:TRP:HB2	1.88	0.55
1:A:274:GLU:HB3	1:A:277:CYS:SG	2.46	0.55
1:B:105:VAL:HA	3:B:1878:HOH:O	2.07	0.55
1:B:261:ILE:HG22	1:B:261:ILE:O	2.06	0.55
1:C:7:TYR:H	1:C:17:TRP:H	1.53	0.55
1:A:217:LEU:O	1:A:219:GLY:N	2.39	0.55
1:B:15:VAL:HG12	1:B:16:ARG:O	2.06	0.55
1:C:36:PHE:HB3	1:C:99:LEU:HD23	1.89	0.55
1:C:86:ILE:HD13	3:C:1961:HOH:O	2.05	0.55
1:B:44:SER:C	1:B:46:LYS:N	2.62	0.55
1:C:27:HIS:HE1	1:C:108:GLY:O	1.89	0.55
1:B:106:GLY:N	3:B:1878:HOH:O	2.40	0.55
1:B:47:GLY:CA	1:B:49:VAL:HB	2.36	0.55
1:B:273:GLY:O	1:B:274:GLU:HB2	2.07	0.54
1:C:259:ALA:O	1:C:260:GLU:C	2.48	0.54
1:A:112:PRO:O	1:A:115:TYR:HB3	2.07	0.54
1:B:197:GLU:HG3	1:B:254:MET:HB3	1.89	0.54
1:C:75:ILE:HG22	1:C:79:MET:HE3	1.89	0.54
1:A:156:THR:O	1:A:217:LEU:HD12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:LYS:C	1:C:47:GLY:O	2.47	0.54
1:A:276:ARG:HH12	1:A:282:LYS:HE2	1.72	0.54
1:A:293:THR:HG22	1:A:295:GLU:H	1.73	0.54
1:C:164:TYR:HE1	3:C:1592:HOH:O	1.89	0.54
1:A:199:LEU:HD23	1:A:254:MET:SD	2.47	0.54
1:A:53:HIS:CD2	1:A:79:MET:HG2	2.43	0.54
1:C:44:SER:OG	1:C:47:GLY:N	2.41	0.54
1:B:175:ARG:HG3	3:B:1648:HOH:O	2.08	0.53
1:B:280:VAL:O	1:B:284:ILE:HG12	2.09	0.53
1:B:255:SER:HA	1:B:260:GLU:O	2.09	0.53
1:C:23:HIS:HD2	1:C:25:MET:H	1.56	0.53
1:A:24:VAL:O	1:A:30:HIS:HE1	1.91	0.53
1:C:49:VAL:HG11	1:C:303:LEU:HD22	1.89	0.53
1:C:94:ALA:HB1	1:C:124:PHE:O	2.09	0.53
1:A:23:HIS:HD2	1:A:25:MET:H	1.56	0.53
1:A:138:GLY:HA2	1:A:263:PRO:O	2.08	0.53
1:A:6:ASP:OD1	1:A:6:ASP:N	2.42	0.52
1:A:68:ARG:NH2	1:C:268:ASP:O	2.43	0.52
1:B:67:TYR:O	1:B:68:ARG:HB2	2.08	0.52
1:B:203:LYS:O	1:B:250:ASP:OD2	2.27	0.52
1:B:212:PHE:CE1	1:B:218:PRO:HA	2.44	0.52
1:A:37:GLU:OE2	1:A:59:ARG:HB3	2.09	0.52
1:A:181:GLU:HG2	1:A:254:MET:CE	2.39	0.52
1:C:45:HIS:O	1:C:46:LYS:CB	2.57	0.52
1:C:99:LEU:HD13	1:C:101:PHE:CD1	2.44	0.52
1:A:255:SER:HA	1:A:260:GLU:O	2.10	0.52
1:C:6:ASP:O	1:C:7:TYR:HB2	2.10	0.52
1:A:259:ALA:O	1:A:260:GLU:HB2	2.08	0.51
1:A:213:THR:HB	1:C:190:TYR:CE1	2.44	0.51
1:A:252:VAL:CG1	1:A:272:VAL:HG11	2.40	0.51
1:A:9:TRP:HZ3	1:A:119:VAL:HG12	1.75	0.51
1:C:209:THR:CG2	3:C:1506:HOH:O	2.57	0.51
1:A:75:ILE:HD13	3:A:1777:HOH:O	2.10	0.51
1:B:60:LEU:HA	3:B:1649:HOH:O	2.09	0.51
1:B:81:ALA:O	1:B:85:VAL:HG23	2.09	0.51
1:B:179:TYR:CD1	1:B:179:TYR:N	2.79	0.51
1:C:27:HIS:HD2	1:C:33:THR:OG1	1.94	0.50
1:A:41:CYS:HA	1:A:50:VAL:HA	1.93	0.50
1:C:71:VAL:HG22	1:C:100:ILE:HD13	1.94	0.50
1:A:176:ARG:NH2	3:A:1697:HOH:O	2.44	0.50
1:B:197:GLU:HB2	1:B:255:SER:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:SER:HB2	1:B:244:GLU:OE1	2.11	0.50
1:C:279:PRO:O	1:C:282:LYS:HB2	2.12	0.50
1:B:39:ILE:HD11	1:B:57:MET:HE2	1.93	0.50
1:C:35:VAL:CG2	1:C:63:SER:HB3	2.41	0.50
1:C:170:VAL:HG12	1:C:170:VAL:O	2.10	0.50
1:C:280:VAL:O	1:C:284:ILE:HG13	2.12	0.50
1:C:44:SER:C	1:C:46:LYS:H	2.20	0.50
1:A:105:VAL:HG13	1:A:112:PRO:CD	2.42	0.50
1:B:276:ARG:CD	1:B:277:CYS:N	2.70	0.50
1:C:105:VAL:CG2	1:C:115:TYR:HB2	2.42	0.50
1:B:217:LEU:HD23	1:B:218:PRO:N	2.27	0.50
1:B:94:ALA:HA	1:B:126:TRP:H	1.77	0.49
1:A:27:HIS:HD2	1:A:33:THR:OG1	1.95	0.49
1:A:96:ILE:HD12	1:A:96:ILE:N	2.28	0.49
1:B:45:HIS:CE1	1:B:46:LYS:HD3	2.47	0.49
1:C:35:VAL:HG21	1:C:63:SER:HB3	1.93	0.49
1:A:139:ILE:O	1:A:140:ASP:CB	2.55	0.49
1:B:27:HIS:HB3	1:B:102:VAL:HB	1.93	0.49
1:B:61:HIS:CE1	1:B:71:VAL:HG11	2.48	0.49
1:B:172:SER:O	1:B:176:ARG:HB2	2.11	0.49
1:A:44:SER:H	1:A:47:GLY:HA3	1.77	0.49
1:A:75:ILE:H	1:A:75:ILE:CD1	2.25	0.49
1:A:126:TRP:HA	1:A:126:TRP:HE3	1.74	0.49
1:B:254:MET:HG2	3:B:1780:HOH:O	2.13	0.49
1:C:37:GLU:OE2	1:C:56:HIS:HD2	1.95	0.49
1:B:271:GLN:CG	1:B:275:GLY:H	2.26	0.48
1:A:75:ILE:HG22	1:A:79:MET:HE2	1.92	0.48
1:C:54:ARG:CZ	1:C:79:MET:HE1	2.43	0.48
1:A:6:ASP:O	1:A:89:ASN:OD1	2.31	0.48
1:A:52:ARG:HH12	1:A:223:ASP:HB3	1.77	0.48
1:A:181:GLU:HG2	1:A:254:MET:HE3	1.94	0.48
1:A:251:GLU:CD	1:A:278:GLY:HA2	2.39	0.48
1:B:39:ILE:CD1	1:B:57:MET:HE2	2.44	0.48
1:C:293:THR:HG22	1:C:295:GLU:N	2.25	0.48
1:B:14:MET:HE3	1:B:14:MET:HA	1.95	0.48
1:B:168:LEU:HD13	1:B:168:LEU:C	2.39	0.48
1:A:138:GLY:HA3	1:A:265:ARG:N	2.29	0.48
1:B:6:ASP:HB3	3:B:1681:HOH:O	2.12	0.48
1:C:293:THR:HG21	1:C:295:GLU:CD	2.39	0.48
1:A:10:PHE:CG	1:A:120:ILE:HD11	2.49	0.48
1:B:260:GLU:HG2	1:B:288:PHE:HE2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:LYS:NZ	3:C:1568:HOH:O	2.46	0.48
1:A:293:THR:CG2	1:A:295:GLU:HG3	2.44	0.47
1:B:23:HIS:CD2	1:B:25:MET:H	2.32	0.47
1:A:39:ILE:HB	1:A:96:ILE:HB	1.95	0.47
1:B:163:ASN:O	1:B:165:LEU:N	2.47	0.47
1:A:5:ALA:O	1:A:17:TRP:HB2	2.15	0.47
1:B:56:HIS:HE1	3:B:1505:HOH:O	1.95	0.47
1:B:207:LEU:O	1:B:208:PHE:CB	2.60	0.47
1:B:276:ARG:NH2	1:B:282:LYS:HG2	2.30	0.47
1:A:15:VAL:HG12	1:A:16:ARG:O	2.15	0.47
1:C:217:LEU:HD23	1:C:218:PRO:N	2.30	0.47
1:B:75:ILE:CG2	1:B:79:MET:HE2	2.40	0.47
1:B:274:GLU:O	1:B:276:ARG:N	2.48	0.47
1:C:23:HIS:CD2	1:C:25:MET:H	2.33	0.47
1:C:176:ARG:NH1	3:C:1685:HOH:O	2.48	0.47
1:C:197:GLU:HB2	1:C:255:SER:O	2.15	0.47
1:A:27:HIS:CE1	1:A:108:GLY:O	2.51	0.47
1:C:45:HIS:O	1:C:45:HIS:CG	2.64	0.47
1:C:61:HIS:CE1	1:C:71:VAL:HG11	2.50	0.47
1:A:276:ARG:HD3	1:A:276:ARG:C	2.40	0.47
1:A:240:VAL:HG12	1:B:213:THR:HG21	1.97	0.46
1:B:228:LEU:O	1:B:231:GLU:N	2.48	0.46
1:C:228:LEU:HD21	3:C:1985:HOH:O	2.14	0.46
1:A:30:HIS:CD2	1:A:107:MET:HE2	2.50	0.46
1:A:105:VAL:HG13	1:A:112:PRO:HD3	1.95	0.46
1:B:6:ASP:HB3	3:B:1873:HOH:O	2.15	0.46
1:C:44:SER:H	1:C:47:GLY:HA3	1.80	0.46
1:A:152:ASN:N	3:A:1547:HOH:O	2.42	0.46
1:B:222:ARG:HH11	1:B:222:ARG:HG2	1.81	0.46
1:A:14:MET:HE1	1:A:85:VAL:HA	1.97	0.46
1:B:9:TRP:CZ2	1:B:12:GLY:HA2	2.51	0.46
1:C:203:LYS:O	1:C:250:ASP:OD2	2.34	0.46
1:B:54:ARG:CZ	1:B:79:MET:HE1	2.46	0.46
1:A:96:ILE:N	1:A:96:ILE:CD1	2.79	0.46
1:B:7:TYR:HB3	1:B:14:MET:CE	2.44	0.46
1:B:96:ILE:H	1:B:96:ILE:CD1	2.29	0.46
1:C:4:LYS:HG2	1:C:5:ALA:N	2.31	0.46
1:B:7:TYR:HA	1:B:15:VAL:O	2.16	0.46
1:B:23:HIS:HD2	1:B:25:MET:H	1.64	0.46
1:B:96:ILE:N	1:B:96:ILE:CD1	2.73	0.46
1:B:276:ARG:HD3	1:B:277:CYS:CA	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:TRP:HB2	1:C:85:VAL:HG23	1.98	0.46
1:C:58:GLN:O	1:C:59:ARG:C	2.57	0.46
1:C:124:PHE:HB2	1:C:125:PRO:HD2	1.97	0.45
1:B:276:ARG:HD3	1:B:276:ARG:C	2.41	0.45
1:B:38:GLY:O	1:B:56:HIS:CD2	2.69	0.45
1:B:124:PHE:CD1	1:B:124:PHE:N	2.84	0.45
1:C:140:ASP:HA	1:C:266:SER:O	2.15	0.45
1:B:94:ALA:HA	1:B:126:TRP:N	2.31	0.45
1:C:199:LEU:O	1:C:209:THR:CG2	2.63	0.45
1:C:193:GLU:OE1	2:C:413:PLP:N1	2.50	0.45
1:C:181:GLU:HG2	1:C:254:MET:CE	2.45	0.45
1:C:45:HIS:CD2	1:C:46:LYS:HG2	2.51	0.45
1:C:242:SER:O	1:C:243:ARG:C	2.59	0.45
1:A:230:LYS:O	1:A:231:GLU:C	2.59	0.45
1:C:9:TRP:CZ2	1:C:12:GLY:HA2	2.52	0.45
1:C:17:TRP:CD1	1:C:17:TRP:C	2.94	0.45
1:B:27:HIS:ND1	1:B:31:TYR:CD2	2.82	0.45
1:B:87:ARG:O	1:B:88:LYS:C	2.57	0.45
1:A:193:GLU:OE1	2:A:413:PLP:N1	2.49	0.45
1:C:59:ARG:O	1:C:60:LEU:C	2.58	0.44
1:A:44:SER:C	1:A:46:LYS:N	2.75	0.44
1:A:142:MET:HG2	1:A:143:VAL:N	2.30	0.44
1:B:10:PHE:O	1:B:11:ASN:C	2.57	0.44
1:B:199:LEU:O	1:B:209:THR:CG2	2.59	0.44
1:C:45:HIS:H	1:C:45:HIS:HD2	1.61	0.44
1:B:6:ASP:O	1:B:89:ASN:OD1	2.35	0.44
1:C:64:ALA:HB1	1:C:69:PHE:HB2	1.99	0.44
1:A:160:ALA:O	1:A:163:ASN:HB2	2.17	0.44
1:A:276:ARG:HD3	1:A:277:CYS:N	2.33	0.44
1:B:45:HIS:H	1:B:45:HIS:CD2	2.35	0.44
1:C:44:SER:C	1:C:46:LYS:N	2.76	0.44
1:A:75:ILE:N	1:A:75:ILE:CD1	2.81	0.44
1:B:115:TYR:H	1:B:115:TYR:HD1	1.65	0.44
1:B:193:GLU:OE1	2:B:413:PLP:N1	2.51	0.44
1:C:45:HIS:N	1:C:45:HIS:HD2	2.16	0.44
1:C:60:LEU:HD13	1:C:100:ILE:CD1	2.47	0.44
1:A:303:LEU:N	1:A:303:LEU:CD2	2.81	0.43
1:B:105:VAL:CA	3:B:1878:HOH:O	2.65	0.43
1:C:37:GLU:OE2	1:C:56:HIS:CD2	2.70	0.43
1:A:139:ILE:HD13	1:A:262:THR:HG22	1.99	0.43
1:B:57:MET:HE1	1:B:98:PRO:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ILE:HD13	1:B:262:THR:HG21	2.00	0.43
1:B:142:MET:HB3	1:B:179:TYR:CG	2.53	0.43
1:C:277:CYS:O	1:C:278:GLY:C	2.61	0.43
1:A:45:HIS:HD2	1:A:292:PHE:O	2.00	0.43
1:B:110:ASN:O	1:B:111:PRO:C	2.58	0.43
1:C:152:ASN:O	1:C:152:ASN:CG	2.59	0.43
1:C:209:THR:HG22	3:C:1506:HOH:O	2.17	0.43
1:C:14:MET:HE2	1:C:14:MET:HB3	1.56	0.43
1:C:278:GLY:O	1:C:279:PRO:C	2.60	0.43
1:B:39:ILE:HB	1:B:96:ILE:HB	2.01	0.43
1:B:47:GLY:CA	1:B:48:PRO:C	2.91	0.43
1:A:213:THR:HG21	1:C:240:VAL:HG12	2.00	0.43
1:B:97:ARG:O	1:B:97:ARG:HG3	2.19	0.43
1:B:120:ILE:HD12	1:B:120:ILE:HA	1.61	0.43
1:B:183:ILE:HA	1:B:194:GLY:HA2	2.00	0.43
1:C:58:GLN:O	1:C:61:HIS:N	2.51	0.43
1:A:23:HIS:HD2	1:A:25:MET:N	2.15	0.43
1:C:138:GLY:N	1:C:276:ARG:HG3	2.34	0.43
1:B:51:PHE:O	1:B:52:ARG:C	2.62	0.43
1:B:156:THR:C	1:B:158:ALA:H	2.27	0.43
1:C:67:TYR:OH	1:C:155:PRO:HG2	2.19	0.43
1:C:210:PRO:HA	1:C:211:PRO:HD3	1.75	0.43
1:A:9:TRP:O	1:A:120:ILE:HD13	2.19	0.42
1:A:279:PRO:O	1:A:283:ARG:HG3	2.19	0.42
1:A:68:ARG:NH1	3:A:1752:HOH:O	2.48	0.42
1:B:15:VAL:O	1:B:16:ARG:C	2.62	0.42
1:B:293:THR:HG22	1:B:295:GLU:H	1.84	0.42
1:A:75:ILE:CG2	1:A:79:MET:CE	2.91	0.42
1:A:272:VAL:O	1:A:272:VAL:HG12	2.18	0.42
1:B:86:ILE:HG21	1:B:306:VAL:CG2	2.44	0.42
1:C:162:GLY:O	1:C:163:ASN:C	2.57	0.42
1:A:51:PHE:CZ	1:A:52:ARG:HD2	2.54	0.42
1:A:183:ILE:HA	1:A:194:GLY:HA2	2.00	0.42
1:B:181:GLU:OE1	1:B:181:GLU:HA	2.18	0.42
1:C:172:SER:O	1:C:173:GLU:C	2.62	0.42
1:C:221:THR:O	1:C:225:ILE:HD12	2.19	0.42
1:A:148:ARG:NH1	3:A:1604:HOH:O	2.48	0.42
1:B:124:PHE:HB2	1:B:125:PRO:HD2	2.01	0.42
1:B:138:GLY:HA2	1:B:263:PRO:O	2.20	0.42
1:A:120:ILE:HD13	1:A:120:ILE:HA	1.81	0.42
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ARG:O	1:B:149:ALA:C	2.62	0.42
1:C:9:TRP:O	1:C:120:ILE:HA	2.20	0.42
1:A:208:PHE:H	1:A:237:ARG:H	1.67	0.42
1:B:94:ALA:CB	1:B:124:PHE:O	2.63	0.42
1:C:167:SER:OG	1:C:195:ALA:O	2.35	0.42
1:C:217:LEU:HD23	1:C:218:PRO:C	2.45	0.42
1:A:35:VAL:HG22	1:A:63:SER:HB3	2.01	0.42
1:B:242:SER:O	1:B:243:ARG:C	2.61	0.42
1:B:293:THR:CG2	1:B:295:GLU:HG3	2.50	0.42
1:C:47:GLY:CA	1:C:48:PRO:C	2.93	0.42
1:A:138:GLY:HA3	1:A:265:ARG:H	1.85	0.42
1:B:212:PHE:C	1:B:214:SER:N	2.75	0.42
1:B:243:ARG:CG	1:B:243:ARG:HH11	2.33	0.42
1:A:75:ILE:CG2	1:A:79:MET:HE2	2.50	0.41
1:C:142:MET:O	1:C:182:GLY:HA2	2.20	0.41
1:C:212:PHE:CE1	1:C:218:PRO:HB3	2.55	0.41
1:A:40:ARG:HG2	1:A:257:THR:HG22	2.02	0.41
1:A:139:ILE:O	1:A:140:ASP:HB2	2.20	0.41
1:B:79:MET:O	1:B:82:CYS:HB3	2.20	0.41
1:C:207:LEU:O	1:C:208:PHE:O	2.38	0.41
1:C:73:GLN:H	1:C:73:GLN:CD	2.29	0.41
1:A:27:HIS:HB3	1:A:102:VAL:HB	2.02	0.41
1:A:186:ASP:OD1	1:A:188:ASN:HB2	2.20	0.41
1:B:192:SER:O	1:B:193:GLU:HB3	2.18	0.41
1:C:88:LYS:O	1:C:88:LYS:CG	2.69	0.41
1:B:253:PHE:HB2	1:B:262:THR:O	2.20	0.41
1:B:108:GLY:O	1:B:109:VAL:C	2.64	0.41
1:B:54:ARG:NH2	1:B:79:MET:HE1	2.36	0.41
1:B:139:ILE:HD13	1:B:262:THR:CG2	2.51	0.41
1:C:4:LYS:HG2	1:C:5:ALA:H	1.86	0.41
1:C:243:ARG:NH1	1:C:247:TYR:OH	2.54	0.41
1:B:52:ARG:HD3	1:B:220:ILE:HG22	2.02	0.41
1:B:293:THR:HG22	1:B:295:GLU:HG3	2.03	0.41
1:C:183:ILE:HA	1:C:194:GLY:HA2	2.02	0.41
1:A:16:ARG:O	1:A:17:TRP:C	2.62	0.41
1:A:83:ARG:HD3	1:A:306:VAL:HA	2.03	0.41
1:B:259:ALA:O	1:B:261:ILE:N	2.54	0.41
1:C:73:GLN:CD	1:C:73:GLN:N	2.79	0.41
1:A:198:ASN:HD21	1:A:219:GLY:HA3	1.86	0.40
1:B:40:ARG:HD2	1:B:40:ARG:HA	1.84	0.40
1:B:282:LYS:O	1:B:283:ARG:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:MET:HE1	1:C:177:HIS:ND1	2.35	0.40
1:C:263:PRO:HB3	3:C:1583:HOH:O	2.20	0.40
1:A:9:TRP:HB2	1:A:85:VAL:CG2	2.51	0.40
1:C:7:TYR:HB3	1:C:14:MET:HE2	2.04	0.40
1:A:51:PHE:CZ	1:A:52:ARG:HG3	2.56	0.40
1:B:307:ASN:ND2	3:B:1933:HOH:O	2.54	0.40
1:C:55:GLU:OE1	1:C:55:GLU:N	2.43	0.40
1:B:45:HIS:HD2	1:B:292:PHE:O	2.04	0.40
1:B:209:THR:O	1:B:238:GLU:HA	2.21	0.40
1:B:45:HIS:N	1:B:292:PHE:O	2.50	0.40
1:B:221:THR:O	1:B:222:ARG:C	2.65	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	291/308 (94%)	256 (88%)	25 (9%)	10 (3%)	3	4
1	B	291/308 (94%)	245 (84%)	32 (11%)	14 (5%)	2	2
1	C	291/308 (94%)	251 (86%)	28 (10%)	12 (4%)	2	3
All	All	873/924 (94%)	752 (86%)	85 (10%)	36 (4%)	2	3

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	PRO
1	B	46	LYS
1	B	275	GLY
1	C	46	LYS
1	C	275	GLY
1	C	277	CYS

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Mol	Chain	Res	Type
1	A	7	TYR
1	A	155	PRO
1	A	260	GLU
1	A	273	GLY
1	B	7	TYR
1	B	278	GLY
1	C	273	GLY
1	C	278	GLY
1	A	277	CYS
1	B	5	ALA
1	B	121	ILE
1	B	274	GLU
1	C	161	GLY
1	C	208	PHE
1	A	48	PRO
1	A	207	LEU
1	A	218	PRO
1	B	140	ASP
1	B	164	TYR
1	B	276	ARG
1	B	277	CYS
1	C	276	ARG
1	C	298	ASP
1	A	276	ARG
1	B	207	LEU
1	C	7	TYR
1	C	106	GLY
1	C	162	GLY
1	B	273	GLY
1	B	48	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	242/250 (97%)	210 (87%)	32 (13%)	4 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	242/250 (97%)	205 (85%)	37 (15%)	3	5
1	C	242/250 (97%)	204 (84%)	38 (16%)	2	5
All	All	726/750 (97%)	619 (85%)	107 (15%)	3	6

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	18	GLU
1	A	24	VAL
1	A	35	VAL
1	A	60	LEU
1	A	66	ILE
1	A	96	ILE
1	A	99	LEU
1	A	105	VAL
1	A	107	MET
1	A	120	ILE
1	A	126	TRP
1	A	151	PRO
1	A	168	LEU
1	A	172	SER
1	A	180	GLN
1	A	197	GLU
1	A	203	LYS
1	A	209	THR
1	A	214	SER
1	A	218	PRO
1	A	225	ILE
1	A	232	LEU
1	A	243	ARG
1	A	252	VAL
1	A	254	MET
1	A	265	ARG
1	A	272	VAL
1	A	276	ARG
1	A	277	CYS
1	A	293	THR
1	A	303	LEU
1	B	4	LYS
1	B	6	ASP

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Mol	Chain	Res	Type
1	B	14	MET
1	B	18	GLU
1	B	22	VAL
1	B	24	VAL
1	B	35	VAL
1	B	39	ILE
1	B	50	VAL
1	B	60	LEU
1	B	61	HIS
1	B	72	SER
1	B	75	ILE
1	B	96	ILE
1	B	99	LEU
1	B	105	VAL
1	B	107	MET
1	B	116	SER
1	B	120	ILE
1	B	137	GLN
1	B	152	ASN
1	B	166	SER
1	B	172	SER
1	B	197	GLU
1	B	199	LEU
1	B	203	LYS
1	B	207	LEU
1	B	209	THR
1	B	214	SER
1	B	220	ILE
1	B	231	GLU
1	B	234	ILE
1	B	243	ARG
1	B	252	VAL
1	B	254	MET
1	B	276	ARG
1	B	293	THR
1	C	6	ASP
1	C	13	GLU
1	C	14	MET
1	C	18	GLU
1	C	22	VAL
1	C	24	VAL
1	C	35	VAL

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Mol	Chain	Res	Type
1	C	45	HIS
1	C	46	LYS
1	C	48	PRO
1	C	49	VAL
1	C	60	LEU
1	C	85	VAL
1	C	97	ARG
1	C	99	LEU
1	C	105	VAL
1	C	112	PRO
1	C	120	ILE
1	C	137	GLN
1	C	139	ILE
1	C	142	MET
1	C	151	PRO
1	C	154	ILE
1	C	168	LEU
1	C	172	SER
1	C	197	GLU
1	C	199	LEU
1	C	207	LEU
1	C	209	THR
1	C	225	ILE
1	C	243	ARG
1	C	252	VAL
1	C	257	THR
1	C	276	ARG
1	C	282	LYS
1	C	284	ILE
1	C	293	THR
1	C	299	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	27	HIS
1	A	30	HIS
1	A	45	HIS
1	A	56	HIS
1	A	89	ASN
1	A	163	ASN

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Mol	Chain	Res	Type
1	A	198	ASN
1	B	23	HIS
1	B	30	HIS
1	B	45	HIS
1	B	56	HIS
1	B	61	HIS
1	B	163	ASN
1	B	177	HIS
1	B	239	GLN
1	C	23	HIS
1	C	27	HIS
1	C	45	HIS
1	C	58	GLN
1	C	61	HIS
1	C	89	ASN
1	C	147	ASN
1	C	198	ASN
1	C	271	GLN
1	C	308	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 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	413	1	15,15,16	2.71	5 (33%)	21,22,23	2.87	11 (52%)
2	PLP	C	413	1	15,15,16	4.00	10 (66%)	21,22,23	2.83	11 (52%)
2	PLP	B	413	1	15,15,16	3.62	9 (60%)	21,22,23	2.39	8 (38%)

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	413	1	-	2/6/6/8	0/1/1/1
2	PLP	C	413	1	-	3/6/6/8	0/1/1/1
2	PLP	B	413	1	-	1/6/6/8	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	413	PLP	C5-C4	-8.09	1.31	1.40
2	C	413	PLP	C3-C2	-7.85	1.32	1.41
2	B	413	PLP	C2A-C2	7.40	1.62	1.50
2	B	413	PLP	C3-C2	-7.35	1.33	1.41
2	A	413	PLP	C3-C4	-6.71	1.27	1.40
2	C	413	PLP	C3-C4	-5.55	1.29	1.40
2	C	413	PLP	O3-C3	-4.43	1.26	1.36
2	B	413	PLP	C6-N1	4.36	1.43	1.34
2	A	413	PLP	C6-N1	4.32	1.43	1.34
2	A	413	PLP	C2A-C2	-4.23	1.43	1.50
2	C	413	PLP	C2-N1	-4.01	1.26	1.33
2	C	413	PLP	C6-N1	3.55	1.41	1.34
2	B	413	PLP	C2-N1	3.50	1.40	1.33
2	B	413	PLP	O4P-C5A	-3.27	1.32	1.44
2	B	413	PLP	P-O1P	-3.01	1.41	1.50
2	B	413	PLP	P-O3P	-2.90	1.44	1.54
2	C	413	PLP	C5A-C5	2.74	1.58	1.50
2	C	413	PLP	C2A-C2	2.67	1.54	1.50
2	A	413	PLP	P-O3P	-2.63	1.45	1.54
2	B	413	PLP	P-O4P	-2.61	1.52	1.60
2	C	413	PLP	P-O1P	-2.57	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	413	PLP	C5-C4	2.43	1.43	1.40
2	A	413	PLP	C6-C5	-2.40	1.33	1.37
2	C	413	PLP	P-O2P	-2.37	1.46	1.54

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	413	PLP	O2P-P-O4P	-9.12	82.88	106.67
2	C	413	PLP	O4P-C5A-C5	6.21	121.00	109.36
2	B	413	PLP	O4P-C5A-C5	5.13	118.97	109.36
2	C	413	PLP	O2P-P-O4P	-5.05	93.51	106.67
2	A	413	PLP	O4P-P-O1P	4.52	118.67	106.44
2	B	413	PLP	C2A-C2-N1	4.30	125.75	117.64
2	B	413	PLP	C2A-C2-C3	-3.89	116.24	120.80
2	C	413	PLP	C4-C3-C2	3.54	125.17	119.89
2	C	413	PLP	O3P-P-O2P	3.53	121.03	107.80
2	C	413	PLP	O4P-P-O1P	-3.50	96.99	106.44
2	C	413	PLP	O3P-P-O4P	3.47	115.70	106.67
2	C	413	PLP	O3P-P-O1P	3.20	123.31	110.83
2	B	413	PLP	O2P-P-O4P	3.16	114.92	106.67
2	C	413	PLP	C6-C5-C4	-3.16	115.50	118.10
2	B	413	PLP	O3P-P-O2P	-3.12	96.09	107.80
2	A	413	PLP	C4A-C4-C3	-3.07	115.40	120.52
2	A	413	PLP	O3P-P-O1P	3.07	122.81	110.83
2	B	413	PLP	C4A-C4-C3	-2.97	115.57	120.52
2	A	413	PLP	O4P-C5A-C5	2.89	114.78	109.36
2	C	413	PLP	C3-C2-N1	-2.86	117.35	120.96
2	C	413	PLP	O2P-P-O1P	-2.76	100.10	110.83
2	A	413	PLP	O2P-P-O1P	-2.71	100.26	110.83
2	A	413	PLP	O3-C3-C2	2.43	122.62	117.58
2	B	413	PLP	C3-C2-N1	-2.39	117.95	120.96
2	A	413	PLP	C5-C6-N1	-2.33	120.03	123.83
2	A	413	PLP	O3P-P-O2P	2.30	116.43	107.80
2	A	413	PLP	C4A-C4-C5	2.30	123.31	120.94
2	C	413	PLP	C3-C4-C5	2.26	121.30	118.59
2	B	413	PLP	C5-C6-N1	-2.21	120.23	123.83
2	A	413	PLP	C3-C4-C5	2.04	121.03	118.59

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	413	PLP	C5A-O4P-P-O2P
2	A	413	PLP	C5A-O4P-P-O3P
2	C	413	PLP	C6-C5-C5A-O4P
2	C	413	PLP	C5A-O4P-P-O1P
2	B	413	PLP	C5A-O4P-P-O3P
2	C	413	PLP	C4-C5-C5A-O4P

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	413	PLP	2	0
2	C	413	PLP	3	0
2	B	413	PLP	2	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.