



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5CE8 / pdb_00005ce8
Title : Crystal structure of branched-chain aminotransferase from thermophilic archaea *Thermoproteus uzoniensis*
Authors : Boyko, K.M.; Nikolaeva, A.Y.; Stekhanova, T.N.; Mardanov, A.V.; Rakitin, A.L.; Ravin, N.V.; Popov, V.O.
Deposited on : 2015-07-06
Resolution : 2.00 Å(reported)

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

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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

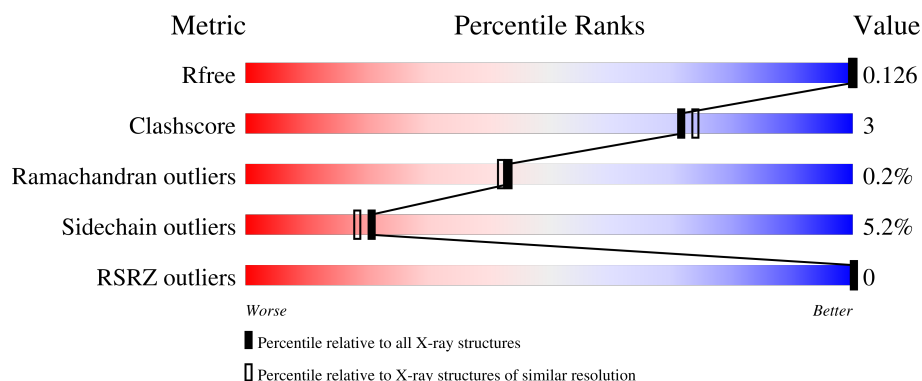
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	307	
1	B	307	
1	C	307	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7219 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	296	Total	C	N	O	S	0	0	0
			2281	1468	382	423	8			
1	B	296	Total	C	N	O	S	0	0	0
			2278	1465	382	424	7			
1	C	295	Total	C	N	O	S	0	1	0
			2275	1467	385	415	8			

There are 36 discrepancies between the modelled and reference sequences:

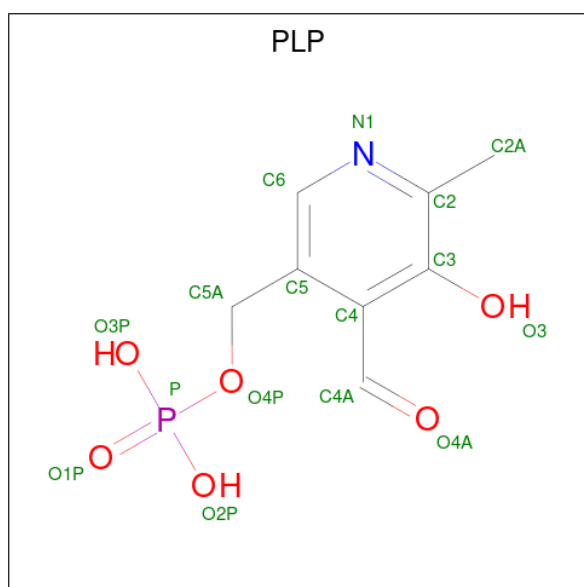
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP F2L0W0
A	-10	ARG	-	expression tag	UNP F2L0W0
A	-9	GLY	-	expression tag	UNP F2L0W0
A	-8	SER	-	expression tag	UNP F2L0W0
A	-7	HIS	-	expression tag	UNP F2L0W0
A	-6	HIS	-	expression tag	UNP F2L0W0
A	-5	HIS	-	expression tag	UNP F2L0W0
A	-4	HIS	-	expression tag	UNP F2L0W0
A	-3	HIS	-	expression tag	UNP F2L0W0
A	-2	HIS	-	expression tag	UNP F2L0W0
A	-1	GLY	-	expression tag	UNP F2L0W0
A	0	SER	-	expression tag	UNP F2L0W0
B	-11	MET	-	initiating methionine	UNP F2L0W0
B	-10	ARG	-	expression tag	UNP F2L0W0
B	-9	GLY	-	expression tag	UNP F2L0W0
B	-8	SER	-	expression tag	UNP F2L0W0
B	-7	HIS	-	expression tag	UNP F2L0W0
B	-6	HIS	-	expression tag	UNP F2L0W0
B	-5	HIS	-	expression tag	UNP F2L0W0
B	-4	HIS	-	expression tag	UNP F2L0W0
B	-3	HIS	-	expression tag	UNP F2L0W0
B	-2	HIS	-	expression tag	UNP F2L0W0
B	-1	GLY	-	expression tag	UNP F2L0W0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP F2L0W0
C	-11	MET	-	initiating methionine	UNP F2L0W0
C	-10	ARG	-	expression tag	UNP F2L0W0
C	-9	GLY	-	expression tag	UNP F2L0W0
C	-8	SER	-	expression tag	UNP F2L0W0
C	-7	HIS	-	expression tag	UNP F2L0W0
C	-6	HIS	-	expression tag	UNP F2L0W0
C	-5	HIS	-	expression tag	UNP F2L0W0
C	-4	HIS	-	expression tag	UNP F2L0W0
C	-3	HIS	-	expression tag	UNP F2L0W0
C	-2	HIS	-	expression tag	UNP F2L0W0
C	-1	GLY	-	expression tag	UNP F2L0W0
C	0	SER	-	expression tag	UNP F2L0W0

- 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 DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	113	Total	O	0	0
			113	113		
4	B	104	Total	O	0	0
			104	104		
4	C	116	Total	O	0	0
			116	116		

- Molecule 1: Branched-chain amino acid aminotransferase

[illegible][illegible]

M148	M155	L156	M157	D171	E172	A173	L174	M175	G180	K181	V182	V183	E188	H189	V190	V193	R194	L198	P201	P202	L203	E209	R213	D222	I225	R234	L237	V246	G247	E251	L258	I268	K271	L273	Y276	Y295	
NET	ARG	GLY	SER	HIS	HIS	HIS	HIS	GLY	SER	M1	W4	L9	V10	S23	G29	G33	I34	R35	M52	A59	P66	P67	S74	G85	E88	I92	I98	S99	Q102	I103	S104	L110	A115	L119	K123	V130	V147

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	93.54Å 93.54Å 212.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	75.69 – 2.00 75.69 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (75.69-2.00) 99.9 (75.69-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.120 , 0.168 0.126 , 0.126	Depositor DCC
R_{free} test set	3602 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 18.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.460 for -h,-k,l	Xtriage
Reported twinning fraction	0.491 for H, K, L 0.509 for K, H, -L	Depositor
Outliers	0 of 72105 reflections	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	7219	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	1.67	28/2324 (1.2%)	1.47	11/3158 (0.3%)
1	B	1.72	36/2320 (1.6%)	1.45	19/3151 (0.6%)
1	C	1.67	25/2323 (1.1%)	1.48	7/3156 (0.2%)
All	All	1.69	89/6967 (1.3%)	1.47	37/9465 (0.4%)

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	B	0	2

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	28	PHE	C-O	9.06	1.35	1.23
1	C	157	ASN	C-O	7.78	1.33	1.24
1	A	202	PRO	N-CA	-7.75	1.39	1.46
1	B	35	ARG	CA-C	-7.70	1.43	1.52
1	C	148	MET	C-O	-7.34	1.14	1.24
1	B	140	VAL	C-O	7.31	1.33	1.24
1	A	193	VAL	C-O	-7.30	1.16	1.24
1	A	232	ILE	C-O	-7.22	1.16	1.24
1	B	99	SER	C-O	-7.07	1.14	1.24
1	B	34	ILE	N-CA	7.06	1.54	1.46
1	B	134	VAL	N-CA	7.00	1.54	1.46
1	B	140	VAL	CA-CB	6.98	1.61	1.54
1	A	134	VAL	CA-CB	6.97	1.62	1.54
1	C	234	ARG	CD-NE	-6.96	1.36	1.46
1	A	18	THR	C-O	6.79	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	15	ALA	CA-C	-6.68	1.45	1.53
1	C	188	GLU	CA-C	-6.68	1.44	1.52
1	B	5	LEU	CA-C	-6.67	1.45	1.52
1	A	74	SER	C-O	6.63	1.31	1.24
1	B	52	MET	N-CA	-6.59	1.38	1.46
1	B	224	GLY	N-CA	6.58	1.54	1.45
1	C	172	GLU	N-CA	6.56	1.54	1.46
1	B	135	VAL	CA-C	-6.54	1.45	1.52
1	B	149	ALA	CA-CB	-6.51	1.43	1.53
1	B	59	ALA	N-CA	-6.48	1.38	1.46
1	A	234	ARG	CD-NE	-6.47	1.37	1.46
1	A	206	GLY	C-O	-6.45	1.13	1.24
1	B	68	TYR	CA-C	-6.45	1.44	1.52
1	A	157	ASN	C-O	6.44	1.31	1.24
1	C	209	GLU	C-N	-6.44	1.26	1.33
1	C	276	TYR	C-O	-6.44	1.16	1.24
1	B	92	ILE	CA-CB	-6.37	1.46	1.54
1	B	55	LEU	C-O	6.23	1.31	1.24
1	A	36	ALA	CA-C	-6.20	1.44	1.52
1	C	88	GLU	C-O	-6.18	1.17	1.23
1	A	5	LEU	N-CA	-6.12	1.39	1.46
1	C	33	GLY	N-CA	6.09	1.54	1.45
1	B	220	ALA	N-CA	6.08	1.53	1.46
1	C	201	PRO	CA-C	6.08	1.57	1.52
1	C	155	TYR	C-O	6.05	1.31	1.24
1	B	215	THR	N-CA	-6.01	1.39	1.46
1	A	237	LEU	CA-C	5.99	1.60	1.52
1	C	85	GLY	C-O	-5.99	1.17	1.24
1	A	154	ILE	N-CA	5.92	1.53	1.46
1	B	250	ALA	CA-C	5.88	1.60	1.52
1	C	102	GLN	CA-C	5.80	1.58	1.52
1	C	59	ALA	C-O	-5.76	1.17	1.24
1	A	95	VAL	N-CA	-5.74	1.39	1.46
1	A	209	GLU	C-O	-5.74	1.17	1.23
1	C	23	SER	CA-C	-5.74	1.45	1.52
1	C	29	GLY	C-O	5.73	1.29	1.23
1	B	104	SER	N-CA	5.70	1.53	1.46
1	B	133	ALA	C-O	-5.68	1.17	1.24
1	B	239	ALA	C-O	-5.64	1.16	1.24
1	B	205	ASP	C-O	-5.60	1.15	1.24
1	C	213	ARG	N-CA	5.58	1.53	1.46
1	B	26	TYR	N-CA	5.58	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	174	ILE	N-CA	-5.55	1.39	1.46
1	C	66	VAL	CA-C	5.51	1.57	1.53
1	B	48	LEU	N-CA	-5.48	1.40	1.46
1	A	72	GLU	C-O	5.47	1.30	1.24
1	A	148	MET	C-O	-5.46	1.17	1.24
1	B	234	ARG	CD-NE	-5.45	1.38	1.46
1	B	288	LEU	C-O	-5.43	1.17	1.24
1	C	35	ARG	CA-C	-5.38	1.46	1.52
1	B	132	ALA	C-O	5.37	1.30	1.24
1	A	192	ILE	C-O	-5.36	1.16	1.23
1	C	10	VAL	C-O	-5.36	1.18	1.23
1	B	23	SER	CA-C	-5.36	1.45	1.52
1	A	234	ARG	N-CA	-5.32	1.40	1.46
1	B	35	ARG	N-CA	-5.29	1.39	1.45
1	A	269	THR	N-CA	-5.24	1.40	1.46
1	B	234	ARG	CZ-NH2	-5.24	1.26	1.33
1	A	92	ILE	CA-C	5.21	1.59	1.52
1	A	124	TYR	N-CA	5.21	1.52	1.46
1	C	119	ILE	C-O	-5.21	1.17	1.24
1	C	52	MET	CA-C	-5.16	1.46	1.52
1	B	45	VAL	N-CA	-5.14	1.40	1.46
1	C	67	PRO	C-O	-5.13	1.17	1.24
1	A	115	ALA	C-O	5.12	1.30	1.24
1	B	276	TYR	CA-C	-5.11	1.46	1.52
1	B	284	GLU	CA-C	-5.11	1.46	1.52
1	A	274	GLU	N-CA	5.11	1.52	1.46
1	A	214	GLU	N-CA	-5.10	1.40	1.46
1	A	119	ILE	N-CA	-5.10	1.40	1.46
1	C	74	SER	N-CA	-5.06	1.40	1.46
1	A	137	TRP	C-O	-5.04	1.17	1.23
1	B	233	THR	C-O	-5.02	1.17	1.23
1	A	173	ALA	CA-C	-5.01	1.46	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ARG	NE-CZ-NH2	-11.38	108.96	119.20
1	C	234	ARG	NE-CZ-NH2	-9.57	110.58	119.20
1	B	183	VAL	N-CA-C	9.33	118.99	111.62
1	C	110	LEU	N-CA-C	8.96	122.22	111.82
1	B	234	ARG	NE-CZ-NH2	-7.94	112.05	119.20
1	A	201	PRO	O-C-N	7.50	124.76	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	ARG	N-CA-C	-7.08	103.61	111.82
1	A	183	VAL	N-CA-C	6.94	117.95	112.12
1	B	23	SER	N-CA-C	6.55	118.42	111.28
1	B	46	PHE	N-CA-C	6.29	118.53	108.41
1	B	161	ALA	N-CA-C	6.27	117.78	111.07
1	C	222	ASP	CB-CA-C	-6.09	100.50	110.85
1	C	180	GLY	N-CA-C	6.00	123.65	115.30
1	A	185	GLY	N-CA-C	-5.94	103.50	112.41
1	B	207	ILE	CB-CA-C	-5.93	104.81	111.45
1	B	153	GLY	N-CA-C	5.88	121.10	113.27
1	B	292	THR	CA-C-N	-5.78	113.75	119.99
1	B	292	THR	C-N-CA	-5.78	113.75	119.99
1	B	182	VAL	CA-C-N	-5.68	117.14	123.16
1	B	182	VAL	C-N-CA	-5.68	117.14	123.16
1	C	103	ILE	CB-CA-C	-5.48	104.90	112.24
1	B	200	THR	CB-CA-C	5.47	117.41	109.20
1	C	275	THR	N-CA-CB	5.47	118.25	110.16
1	B	275	THR	CB-CA-C	5.47	120.14	110.85
1	A	248	THR	N-CA-C	-5.41	105.28	111.07
1	A	261	ARG	CG-CD-NE	5.38	123.83	112.00
1	B	237	LEU	CB-CA-C	-5.33	102.50	110.88
1	B	234	ARG	NE-CZ-NH1	5.31	126.81	121.50
1	B	193	VAL	N-CA-C	-5.17	100.20	107.75
1	C	104	SER	N-CA-C	5.15	117.81	110.24
1	A	140	VAL	N-CA-C	-5.14	102.95	109.58
1	A	57	ARG	N-CA-C	-5.09	105.82	111.36
1	B	155	TYR	CA-CB-CG	-5.08	104.75	113.90
1	A	225	ILE	CA-C-O	5.05	122.13	119.15
1	B	177	ASN	N-CA-C	5.03	116.59	110.41
1	A	182	VAL	CA-C-N	-5.02	117.50	122.77
1	A	182	VAL	C-N-CA	-5.02	117.50	122.77

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	121	PHE	Peptide
1	B	207	ILE	Peptide

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	2281	0	2299	16	0
1	B	2278	0	2296	16	0
1	C	2275	0	2300	13	0
2	A	15	0	7	1	0
2	B	15	0	7	1	0
2	C	15	0	7	0	0
3	C	7	0	10	0	0
4	A	113	0	0	0	0
4	B	104	0	0	1	0
4	C	116	0	0	3	0
All	All	7219	0	6926	45	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 3.

All (45) 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:4:TRP:O	1:A:115:ALA:HA	1.99	0.63
1:B:203:LEU:HD12	1:B:207:ILE:HD11	1.82	0.60
1:C:99:SER:HB2	4:C:445:HOH:O	2.05	0.57
1:B:234:ARG:HD2	4:C:479:HOH:O	2.09	0.51
1:C:34:ILE:HB	1:C:92:ILE:HB	1.91	0.51
1:B:140:VAL:HG13	1:B:147:VAL:CG1	2.40	0.50
1:B:198:LEU:HD22	1:B:225:ILE:HG21	1.94	0.49
1:B:150:LYS:NZ	2:B:301:PLP:O3	2.45	0.49
1:A:174:ILE:HD13	1:A:237:LEU:HD11	1.94	0.47
1:A:246:VAL:HA	1:A:251:GLU:O	2.15	0.47
1:B:124:TYR:O	1:B:125:LEU:HD13	2.15	0.47
1:B:193:VAL:HG22	1:B:198:LEU:HD13	1.97	0.46
1:B:214:GLU:HG2	4:B:439:HOH:O	2.16	0.46
1:C:247:GLY:O	1:C:251:GLU:N	2.49	0.46
1:C:98:ILE:HD13	1:C:110:LEU:HD13	1.98	0.45
1:C:130:VAL:HB	1:C:171:ASP:HB2	1.98	0.45
1:B:20:LEU:HB2	1:B:101:PRO:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:VAL:HG22	1:C:198:LEU:HD13	1.99	0.45
1:C:271:LYS:O	1:C:275:THR:HG23	2.17	0.44
1:C:246:VAL:HA	1:C:251:GLU:O	2.17	0.44
1:B:125:LEU:HG	1:B:130:VAL:HG11	1.99	0.44
1:A:247:GLY:O	1:A:251:GLU:N	2.51	0.44
1:A:130:VAL:HB	1:A:171:ASP:HB2	1.99	0.43
1:A:294:VAL:HG12	1:A:295:TYR:CD2	2.53	0.43
1:A:201:PRO:HD3	1:A:232:ILE:HD12	2.00	0.43
1:A:42:ASN:HB3	1:A:44:TYR:CE2	2.54	0.43
1:B:271:LYS:O	1:B:275:THR:HG23	2.19	0.43
1:A:97:TYR:CD2	1:A:97:TYR:C	2.97	0.42
1:B:202:PRO:HD3	1:B:230:LYS:C	2.44	0.42
1:B:288:LEU:N	1:B:289:PRO:CD	2.82	0.42
1:C:237:LEU:HD22	1:C:258:ILE:CG1	2.49	0.42
1:A:52:MET:HE1	1:A:94:PRO:HG3	2.02	0.42
1:A:237:LEU:HD13	1:A:258:ILE:HG21	2.01	0.42
1:C:225:ILE:HD13	1:C:268:ILE:HG23	2.02	0.42
1:C:194:ARG:HG3	4:C:473:HOH:O	2.20	0.42
1:B:128:GLU:H	1:B:128:GLU:CD	2.28	0.42
1:A:198:LEU:HD23	1:A:227:LEU:HD12	2.02	0.41
1:B:106:ASP:OD1	1:B:106:ASP:C	2.62	0.41
1:A:288:LEU:N	1:A:289:PRO:CD	2.83	0.41
1:A:184:GLU:OE1	2:A:301:PLP:N1	2.53	0.41
1:C:4:TRP:O	1:C:115:ALA:HA	2.20	0.41
1:A:0:SER:O	1:A:1:MET:HG2	2.21	0.41
1:A:80:THR:O	1:A:84:ASN:ND2	2.45	0.40
1:B:131:ARG:HG2	1:B:257:GLU:HB3	2.03	0.40
1:C:175:MET:O	1:C:183:VAL:HG12	2.22	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	294/307 (96%)	287 (98%)	7 (2%)	0	100	100
1	B	294/307 (96%)	281 (96%)	11 (4%)	2 (1%)	18	14
1	C	294/307 (96%)	282 (96%)	12 (4%)	0	100	100
All	All	882/921 (96%)	850 (96%)	30 (3%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	121	PHE
1	B	67	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	233/253 (92%)	227 (97%)	6 (3%)	40	44
1	B	233/253 (92%)	218 (94%)	15 (6%)	16	12
1	C	231/253 (91%)	216 (94%)	15 (6%)	15	12
All	All	697/759 (92%)	661 (95%)	36 (5%)	21	18

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	56	LEU
1	A	71	GLU
1	A	119	ILE
1	A	203	LEU
1	A	237	LEU
1	B	0	SER
1	B	9	LEU
1	B	35	ARG
1	B	41	GLU
1	B	53	GLU

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Mol	Chain	Res	Type
1	B	60	LYS
1	B	87	LYS
1	B	125	LEU
1	B	128	GLU
1	B	198	LEU
1	B	203	LEU
1	B	208	LEU
1	B	234	ARG
1	B	246	VAL
1	B	275	THR
1	C	1	MET
1	C	9	LEU
1	C	35	ARG
1	C	67	PRO
1	C	99	SER
1	C	123	LYS
1	C	147	VAL
1	C	174	ILE
1	C	181	LYS
1	C	190	ILE
1	C	194	ARG
1	C	198	LEU
1	C	203	LEU
1	C	237	LEU
1	C	275	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	301	1	15,15,16	3.01	6 (40%)	21,22,23	1.47	3 (14%)
2	PLP	B	301	1	15,15,16	2.68	4 (26%)	21,22,23	1.74	4 (19%)
3	PEG	C	301	-	6,6,6	0.34	0	5,5,5	0.98	0
2	PLP	C	302	1	15,15,16	3.05	4 (26%)	21,22,23	2.15	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	301	1	-	0/6/6/8	0/1/1/1
2	PLP	B	301	1	-	0/6/6/8	0/1/1/1
3	PEG	C	301	-	-	4/4/4/4	-
2	PLP	C	302	1	-	0/6/6/8	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	PLP	C5-C4	7.97	1.49	1.40
2	C	302	PLP	C5-C4	7.40	1.48	1.40
2	B	301	PLP	C3-C2	7.24	1.48	1.41
2	C	302	PLP	C3-C2	6.83	1.48	1.41
2	B	301	PLP	C5-C4	4.97	1.46	1.40
2	A	301	PLP	C3-C2	4.92	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	PLP	C3-C4	4.84	1.49	1.40
2	C	302	PLP	C3-C4	4.26	1.48	1.40
2	B	301	PLP	C3-C4	3.46	1.46	1.40
2	A	301	PLP	C6-C5	2.55	1.42	1.37
2	B	301	PLP	C2-N1	2.23	1.37	1.33
2	C	302	PLP	C4A-C4	2.22	1.56	1.51
2	A	301	PLP	P-O1P	2.15	1.57	1.50
2	A	301	PLP	P-O2P	-2.02	1.47	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	302	PLP	C6-N1-C2	4.21	126.83	119.20
2	B	301	PLP	O3P-P-O4P	-4.04	96.15	106.67
2	C	302	PLP	C2A-C2-N1	3.76	124.73	117.64
2	C	302	PLP	O4P-C5A-C5	3.51	115.93	109.36
2	B	301	PLP	O3-C3-C2	3.49	124.81	117.58
2	C	302	PLP	C2A-C2-C3	-3.20	117.06	120.80
2	B	301	PLP	O4P-C5A-C5	2.89	114.77	109.36
2	A	301	PLP	C6-N1-C2	2.78	124.23	119.20
2	C	302	PLP	O3P-P-O4P	-2.61	99.86	106.67
2	A	301	PLP	C3-C4-C5	-2.50	115.58	118.59
2	C	302	PLP	C5-C6-N1	-2.49	119.78	123.83
2	C	302	PLP	C3-C2-N1	-2.36	117.99	120.96
2	A	301	PLP	C2A-C2-C3	-2.30	118.11	120.80
2	C	302	PLP	O4P-P-O1P	-2.28	100.28	106.44
2	B	301	PLP	C4A-C4-C5	-2.07	118.81	120.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	301	PEG	O1-C1-C2-O2
3	C	301	PEG	C1-C2-O2-C3
3	C	301	PEG	O2-C3-C4-O4
3	C	301	PEG	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	PLP	1	0
2	B	301	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	296/307 (96%)	-1.72	0 100 100	16, 24, 39, 47	0
1	B	296/307 (96%)	-1.70	0 100 100	16, 25, 40, 62	0
1	C	295/307 (96%)	-1.69	0 100 100	12, 26, 40, 51	1 (0%)
All	All	887/921 (96%)	-1.70	0 100 100	12, 25, 40, 62	1 (0%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
3	PEG	C	301	7/7	0.99	0.11	20,21,26,32	7
2	PLP	B	301	15/16	1.00	0.01	20,23,27,27	0
2	PLP	C	302	15/16	1.00	0.02	20,22,25,26	0
2	PLP	A	301	15/16	1.00	0.01	18,23,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.