



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:29 AM UTC

PDB ID : 2CAN / pdb_00002can
Title : HUMAN ORNITHINE AMINOTRANSFERASE COMPLEXED WITH L-CANALINE
Authors : Shah, S.A.; Shen, B.W.; Brunger, A.T.
Deposited on : 1997-05-29
Resolution : 2.30 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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

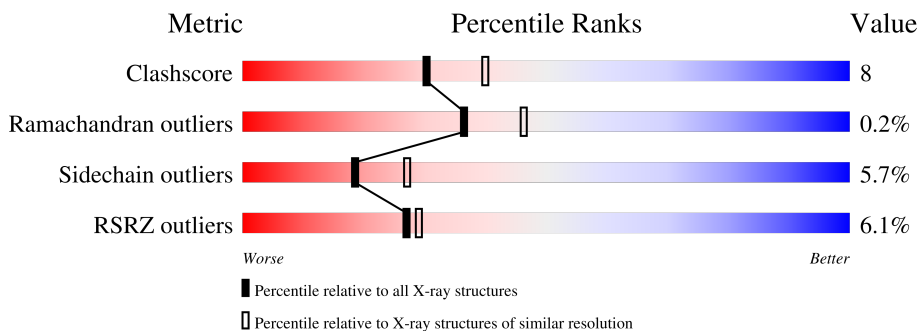
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

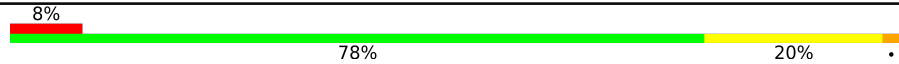


The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	402	 8% 78% 20% •
1	B	402	 6% 80% 18% •
1	C	402	 5% 81% 18% •

2 Entry composition [i](#)

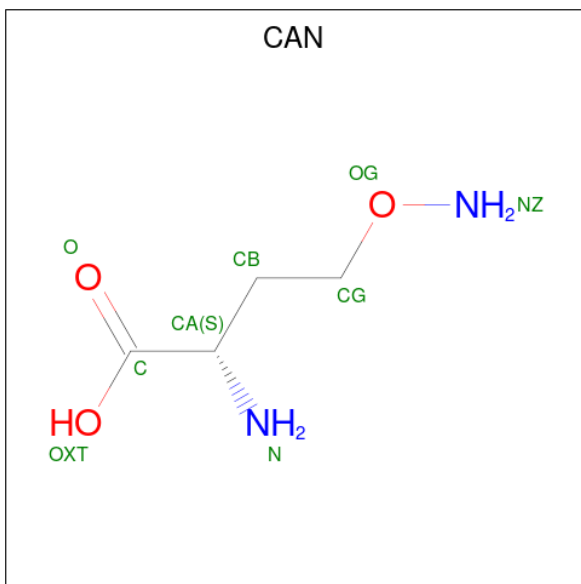
There are 4 unique types of molecules in this entry. The entry contains 11832 atoms, of which 2034 are hydrogens and 0 are deuteriums.

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 ORNITHINE AMINOTRANSFERASE.

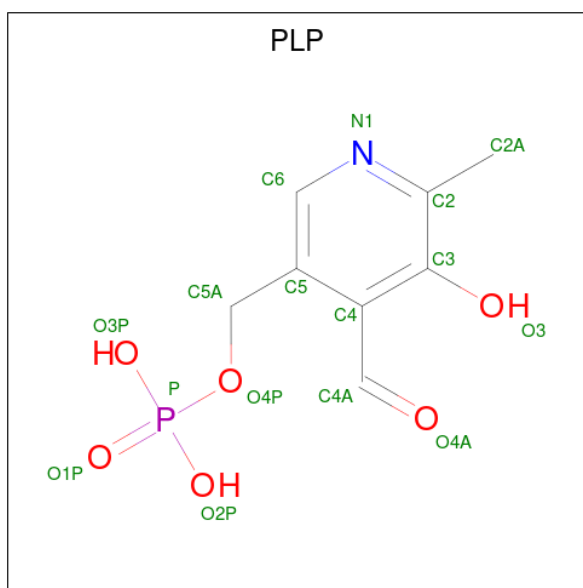
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	402	Total 3828	C 2023	H 678	N 531	O 584	S 12	0	0	0
1	B	402	Total 3828	C 2023	H 678	N 531	O 584	S 12	0	0	0
1	C	402	Total 3828	C 2023	H 678	N 531	O 584	S 12	0	0	0

- Molecule 2 is CANALINE (CCD ID: CAN) (formula: C₄H₁₀N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 9	C 4	N 2	O 3	0	0
2	B	1	Total 9	C 4	N 2	O 3	0	0
2	C	1	Total 9	C 4	N 2	O 3	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



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

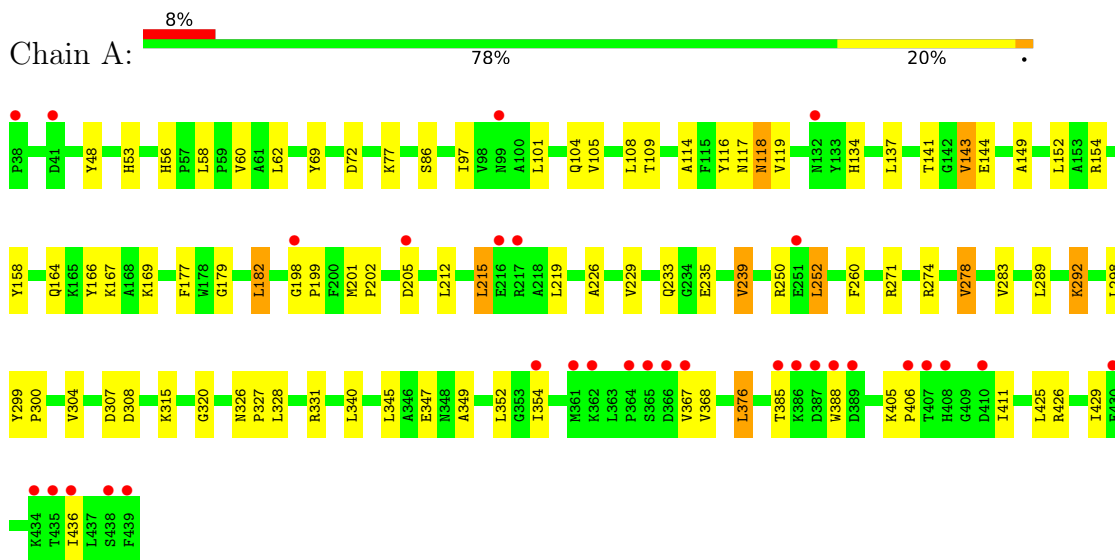
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	83	Total	83	0	0
4	B	99	Total	99	0	0
4	C	94	Total	94	0	0

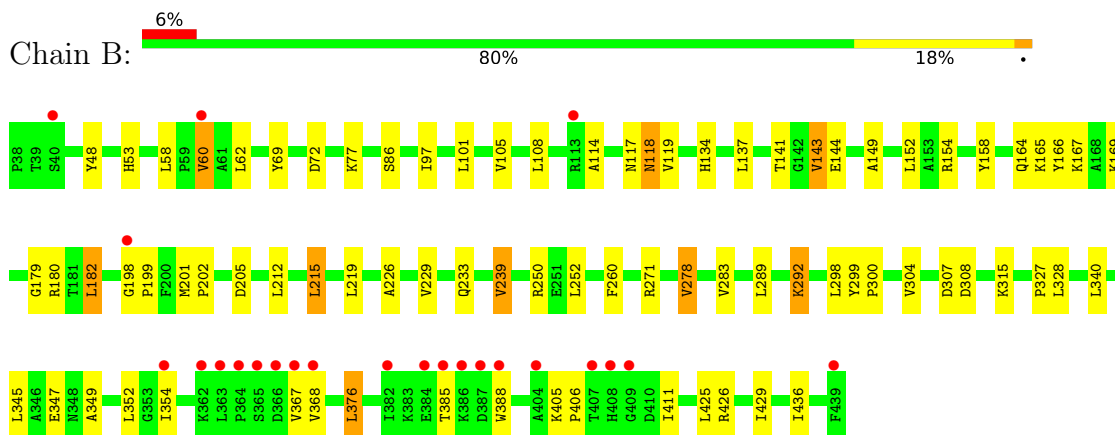
3 Residue-property plots [i](#)

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.

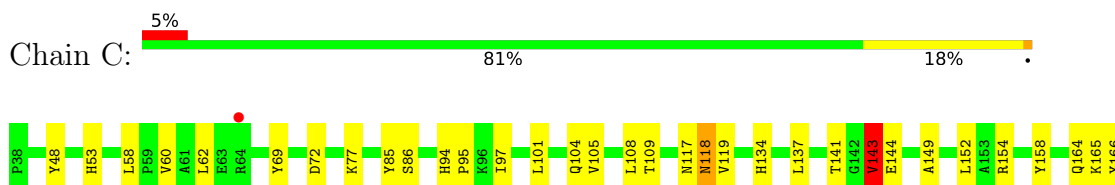
- Molecule 1: ORNITHINE AMINOTRANSFERASE

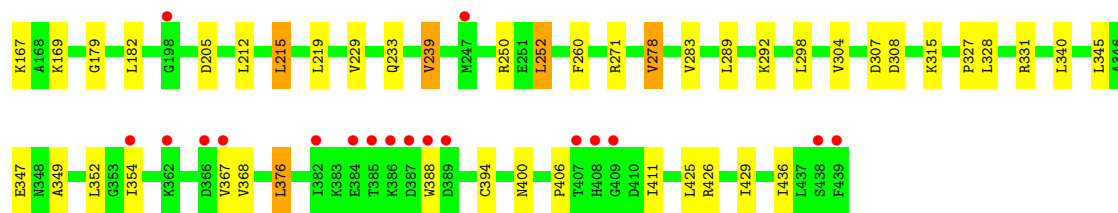


- Molecule 1: ORNITHINE AMINOTRANSFERASE



- Molecule 1: ORNITHINE AMINOTRANSFERASE





4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.92Å 115.92Å 185.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	84.1 (50.00-2.30) 86.4 (50.00-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.71 (at 2.29Å)	Xtrriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.212 , 0.238 0.222 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtrriage
Anisotropy	0.228	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.053 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11832	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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, CAN

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	0.41	0/3223	0.91	7/4375 (0.2%)
1	B	0.43	0/3223	0.91	4/4375 (0.1%)
1	C	0.43	0/3223	0.91	4/4375 (0.1%)
All	All	0.42	0/9669	0.91	15/13125 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	119	VAL	N-CA-C	7.62	118.21	110.82
1	B	119	VAL	N-CA-C	7.48	118.07	110.82
1	A	119	VAL	N-CA-C	7.43	118.03	110.82
1	A	58	LEU	N-CA-C	-5.52	101.38	109.50
1	B	58	LEU	N-CA-C	-5.46	101.48	109.50
1	C	58	LEU	N-CA-C	-5.45	101.49	109.50
1	A	326	ASN	CA-C-N	5.29	124.74	119.24
1	A	326	ASN	C-N-CA	5.29	124.74	119.24
1	C	165	LYS	N-CA-C	5.24	118.39	110.64
1	B	226	ALA	N-CA-C	5.19	116.18	108.60
1	A	56	HIS	CA-C-N	5.15	125.13	120.03
1	A	56	HIS	C-N-CA	5.15	125.13	120.03
1	B	165	LYS	N-CA-C	5.12	118.22	110.64
1	C	143	VAL	CB-CA-C	-5.05	105.33	112.14
1	A	226	ALA	N-CA-C	5.00	115.90	108.60

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	3150	678	3156	70	0
1	B	3150	678	3156	61	0
1	C	3150	678	3156	46	0
2	A	9	0	7	1	0
2	B	9	0	8	2	0
2	C	9	0	7	0	0
3	A	15	0	7	3	0
3	B	15	0	7	1	0
3	C	15	0	7	1	0
4	A	83	0	0	3	0
4	B	99	0	0	0	0
4	C	94	0	0	1	0
All	All	9798	2034	9511	159	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (159) 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:367:VAL:HG13	1:A:388:TRP:HH2	1.31	0.96
1:B:367:VAL:HG13	1:B:388:TRP:HH2	1.34	0.92
1:C:367:VAL:HG13	1:C:388:TRP:HH2	1.34	0.91
1:A:367:VAL:HG13	1:A:388:TRP:CH2	2.09	0.87
1:C:367:VAL:HG13	1:C:388:TRP:CH2	2.11	0.85
1:B:367:VAL:HG13	1:B:388:TRP:CH2	2.11	0.84
1:B:118:ASN:HD22	1:B:118:ASN:H	1.38	0.72
1:A:118:ASN:HD22	1:A:118:ASN:H	1.37	0.71
1:C:118:ASN:H	1:C:118:ASN:HD22	1.38	0.70
1:C:97:ILE:HG22	1:C:298:LEU:HD22	1.74	0.69
1:A:97:ILE:HG22	1:A:298:LEU:HD22	1.76	0.67
1:B:97:ILE:HG22	1:B:298:LEU:HD22	1.75	0.66
1:B:292:LYS:NZ	2:B:1:CAN:HNZ1	1.93	0.66
1:A:158:TYR:OH	1:B:198:GLY:HA2	1.97	0.65
1:A:101:LEU:HD12	1:A:328:LEU:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:VAL:HG13	1:B:179:GLY:HA3	1.82	0.62
1:B:101:LEU:HD12	1:B:328:LEU:HD11	1.82	0.62
1:C:340:LEU:HD23	1:C:345:LEU:HD12	1.81	0.61
1:B:340:LEU:HD23	1:B:345:LEU:HD12	1.83	0.60
1:A:114:ALA:HB1	1:B:405:LYS:HG3	1.83	0.60
1:A:250:ARG:O	1:A:250:ARG:HD3	2.01	0.60
1:A:86:SER:OG	1:A:271:ARG:HD3	2.01	0.60
1:B:250:ARG:O	1:B:250:ARG:HD3	2.01	0.60
1:A:340:LEU:HD23	1:A:345:LEU:HD12	1.84	0.59
1:C:158:TYR:OH	1:C:166:TYR:HA	2.02	0.59
1:B:385:THR:HG1	1:B:388:TRP:CD1	2.20	0.59
1:C:86:SER:OG	1:C:271:ARG:HD3	2.03	0.59
1:C:250:ARG:O	1:C:250:ARG:HD3	2.02	0.59
1:C:101:LEU:HD12	1:C:328:LEU:HD11	1.84	0.58
1:A:158:TYR:OH	1:A:166:TYR:HA	2.04	0.58
1:B:134:HIS:HB2	1:B:307:ASP:HA	1.86	0.58
1:B:164:GLN:HB3	1:B:167:LYS:HD2	1.85	0.58
1:B:158:TYR:OH	1:B:166:TYR:HA	2.04	0.58
1:C:406:PRO:HA	1:C:411:ILE:O	2.05	0.57
1:B:406:PRO:HA	1:B:411:ILE:O	2.05	0.57
1:A:406:PRO:HA	1:A:411:ILE:O	2.05	0.56
1:C:367:VAL:HG12	1:C:368:VAL:HG23	1.88	0.56
1:A:134:HIS:HB2	1:A:307:ASP:HA	1.86	0.56
1:B:86:SER:OG	1:B:271:ARG:HD3	2.04	0.56
1:A:143:VAL:HG13	1:A:179:GLY:HA3	1.87	0.56
1:A:385:THR:HG1	1:A:388:TRP:CD1	2.24	0.56
1:B:385:THR:HG1	1:B:388:TRP:HD1	1.52	0.56
1:C:134:HIS:HB2	1:C:307:ASP:HA	1.88	0.55
1:A:116:TYR:HB2	1:B:60:VAL:O	2.07	0.55
1:A:283:VAL:HG12	4:A:495:HOH:O	2.06	0.55
1:B:48:TYR:O	1:B:53:HIS:HE1	1.89	0.55
1:B:292:LYS:HZ1	2:B:1:CAN:HNZ1	1.52	0.55
1:B:367:VAL:HG12	1:B:368:VAL:HG23	1.89	0.55
1:C:349:ALA:HA	1:C:376:LEU:CD2	2.36	0.55
1:A:105:VAL:HG11	1:B:101:LEU:HD23	1.88	0.55
1:C:143:VAL:HG13	1:C:179:GLY:HA3	1.87	0.55
1:C:48:TYR:O	1:C:53:HIS:HE1	1.90	0.55
1:A:101:LEU:HD23	1:B:105:VAL:HG11	1.88	0.55
1:A:48:TYR:O	1:A:53:HIS:HE1	1.90	0.54
1:A:349:ALA:HA	1:A:376:LEU:CD2	2.37	0.54
1:A:198:GLY:HA2	1:B:158:TYR:OH	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:MET:HE3	1:B:182:LEU:HB3	1.89	0.54
1:B:349:ALA:HA	1:B:376:LEU:CD2	2.37	0.54
1:A:367:VAL:HG12	1:A:368:VAL:HG23	1.89	0.53
1:B:62:LEU:HA	1:B:72:ASP:HA	1.90	0.53
1:C:164:GLN:HB3	1:C:167:LYS:HD2	1.90	0.53
1:A:164:GLN:HB3	1:A:167:LYS:HD2	1.89	0.53
1:B:143:VAL:HG23	3:B:2:PLP:O1P	2.09	0.53
1:A:274:ARG:NH1	4:A:470:HOH:O	2.42	0.53
1:C:143:VAL:HG23	3:C:2:PLP:O1P	2.09	0.53
1:A:158:TYR:HE2	1:B:198:GLY:H	1.57	0.52
1:A:158:TYR:HH	1:A:166:TYR:HA	1.75	0.52
1:A:62:LEU:HA	1:A:72:ASP:HA	1.92	0.52
1:A:69:TYR:CD1	1:A:77:LYS:HE2	2.44	0.51
1:A:143:VAL:HG23	3:A:2:PLP:O1P	2.10	0.51
1:C:349:ALA:HA	1:C:376:LEU:HD23	1.92	0.51
1:B:149:ALA:HB2	1:B:289:LEU:HD21	1.93	0.51
1:C:69:TYR:CD1	1:C:77:LYS:HE2	2.46	0.51
1:A:405:LYS:HG3	1:B:114:ALA:HB1	1.93	0.51
1:B:367:VAL:HG11	1:B:436:ILE:HG23	1.93	0.50
1:A:199:PRO:HB2	1:B:202:PRO:HG2	1.94	0.50
1:C:62:LEU:HA	1:C:72:ASP:HA	1.92	0.50
1:B:69:TYR:CD1	1:B:77:LYS:HE2	2.46	0.50
1:A:201:MET:HE2	1:B:201:MET:HE2	1.92	0.50
1:A:149:ALA:HB2	1:A:289:LEU:HD21	1.94	0.49
1:A:349:ALA:HA	1:A:376:LEU:HD23	1.94	0.49
1:B:349:ALA:HA	1:B:376:LEU:HD23	1.95	0.49
1:A:367:VAL:HG11	1:A:436:ILE:HG23	1.95	0.49
1:B:169:LYS:HD3	1:B:205:ASP:OD2	2.12	0.49
1:A:278:VAL:HG22	1:A:283:VAL:CG2	2.43	0.49
1:A:202:PRO:HG2	1:B:199:PRO:HB2	1.95	0.48
1:A:292:LYS:HZ1	3:A:2:PLP:C4A	2.26	0.48
1:C:367:VAL:HG11	1:C:436:ILE:HG23	1.96	0.48
1:C:425:LEU:O	1:C:429:ILE:HG13	2.12	0.48
1:A:385:THR:HG1	1:A:388:TRP:HD1	1.61	0.48
1:C:278:VAL:HG22	1:C:283:VAL:CG2	2.44	0.48
1:C:149:ALA:HB2	1:C:289:LEU:HD21	1.94	0.47
1:C:134:HIS:HD2	1:C:308:ASP:H	1.63	0.47
1:B:233:GLN:HB2	1:B:239:VAL:HG22	1.97	0.47
1:B:278:VAL:HG22	1:B:283:VAL:CG2	2.45	0.46
1:A:292:LYS:NZ	3:A:2:PLP:C4A	2.78	0.46
1:A:182:LEU:HB3	1:B:201:MET:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:TYR:CD1	1:B:166:TYR:N	2.78	0.46
1:C:166:TYR:CD1	1:C:166:TYR:N	2.81	0.45
1:B:250:ARG:HD3	1:B:250:ARG:C	2.42	0.45
1:A:250:ARG:HD3	1:A:250:ARG:C	2.42	0.45
1:A:141:THR:OG1	1:A:144:GLU:HG3	2.16	0.45
1:A:166:TYR:N	1:A:166:TYR:CD1	2.82	0.45
1:C:141:THR:OG1	1:C:144:GLU:HG3	2.17	0.45
1:A:315:LYS:N	1:A:315:LYS:HD2	2.32	0.44
1:C:104:GLN:HB2	1:C:331:ARG:HG3	1.99	0.44
1:C:315:LYS:N	1:C:315:LYS:HD2	2.33	0.44
1:A:104:GLN:HB2	1:A:331:ARG:HG3	1.98	0.44
1:A:118:ASN:HD22	1:A:118:ASN:N	2.11	0.44
1:B:425:LEU:O	1:B:429:ILE:HG13	2.17	0.44
1:A:109:THR:O	1:A:327:PRO:HD2	2.17	0.44
1:A:169:LYS:HD3	1:A:205:ASP:OD2	2.15	0.44
1:B:134:HIS:HD2	1:B:308:ASP:H	1.64	0.44
1:C:250:ARG:HD3	1:C:250:ARG:C	2.42	0.44
1:A:300:PRO:HD3	1:B:299:TYR:CZ	2.51	0.44
1:C:169:LYS:HD3	1:C:205:ASP:OD2	2.17	0.44
1:A:215:LEU:HD22	1:A:219:LEU:HG	1.99	0.44
1:B:134:HIS:CD2	1:B:308:ASP:H	2.36	0.44
1:C:134:HIS:CD2	1:C:308:ASP:H	2.35	0.44
1:C:367:VAL:HG11	1:C:436:ILE:CG2	2.48	0.44
1:A:134:HIS:HD2	1:A:308:ASP:H	1.66	0.43
1:A:425:LEU:O	1:A:429:ILE:HG13	2.18	0.43
1:A:252:LEU:HD12	1:A:252:LEU:HA	1.90	0.43
1:C:233:GLN:HB2	1:C:239:VAL:HG22	1.99	0.43
1:A:367:VAL:HG11	1:A:436:ILE:CG2	2.49	0.43
1:C:252:LEU:HD12	1:C:252:LEU:HA	1.89	0.43
1:C:352:LEU:HB3	1:C:425:LEU:HD22	2.00	0.43
1:B:158:TYR:HH	1:B:166:TYR:HA	1.84	0.43
1:A:233:GLN:HB2	1:A:239:VAL:HG22	2.00	0.43
1:B:141:THR:OG1	1:B:144:GLU:HG3	2.18	0.43
1:C:215:LEU:HD22	1:C:219:LEU:HG	2.00	0.43
1:A:109:THR:HG21	1:B:298:LEU:HG	2.00	0.43
1:A:177:PHE:CE1	2:A:1:CAN:NZ	2.86	0.43
1:A:260:PHE:CD1	1:A:260:PHE:C	2.97	0.43
1:A:134:HIS:CD2	1:A:308:ASP:H	2.37	0.42
1:A:352:LEU:HB3	1:A:425:LEU:HD22	2.00	0.42
1:B:367:VAL:HG11	1:B:436:ILE:CG2	2.48	0.42
1:B:315:LYS:N	1:B:315:LYS:HD2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:LEU:HD22	1:B:219:LEU:HG	2.01	0.42
1:A:235:GLU:HG2	4:A:476:HOH:O	2.18	0.42
1:B:101:LEU:O	1:B:105:VAL:HG13	2.19	0.42
1:A:320:GLY:H	1:B:180:ARG:HG3	1.85	0.42
1:C:109:THR:O	1:C:327:PRO:HD2	2.19	0.41
1:B:260:PHE:C	1:B:260:PHE:CD1	2.98	0.41
1:A:198:GLY:H	1:B:158:TYR:HE2	1.68	0.41
1:A:299:TYR:CZ	1:B:300:PRO:HD3	2.56	0.41
1:C:394:CYS:SG	1:C:406:PRO:HD3	2.60	0.41
1:C:101:LEU:O	1:C:105:VAL:HG13	2.20	0.41
1:C:118:ASN:HD22	1:C:118:ASN:N	2.12	0.41
1:C:400:ASN:ND2	4:C:510:HOH:O	2.54	0.41
1:C:260:PHE:C	1:C:260:PHE:CD1	2.98	0.41
1:A:117:ASN:CG	1:A:327:PRO:HG3	2.46	0.40
1:B:352:LEU:HB3	1:B:425:LEU:HD22	2.02	0.40
1:C:94:HIS:HA	1:C:95:PRO:HD2	1.85	0.40
1:C:117:ASN:CG	1:C:327:PRO:HG3	2.46	0.40
1:B:117:ASN:CG	1:B:327:PRO:HG3	2.46	0.40
1:A:376:LEU:HD13	1:A:376:LEU:HA	1.88	0.40
1:C:85:TYR:O	1:C:86:SER:HB3	2.22	0.40
1:A:101:LEU:O	1:A:105:VAL:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	400/402 (100%)	372 (93%)	27 (7%)	1 (0%)	36	46
1	B	400/402 (100%)	371 (93%)	28 (7%)	1 (0%)	36	46
1	C	400/402 (100%)	372 (93%)	27 (7%)	1 (0%)	36	46
All	All	1200/1206 (100%)	1115 (93%)	82 (7%)	3 (0%)	36	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	LYS
1	B	292	LYS
1	C	292	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	336/336 (100%)	317 (94%)	19 (6%)	18	27
1	B	336/336 (100%)	317 (94%)	19 (6%)	18	27
1	C	336/336 (100%)	317 (94%)	19 (6%)	18	27
All	All	1008/1008 (100%)	951 (94%)	57 (6%)	18	27

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	VAL
1	A	108	LEU
1	A	118	ASN
1	A	137	LEU
1	A	143	VAL
1	A	152	LEU
1	A	154	ARG
1	A	182	LEU
1	A	212	LEU
1	A	215	LEU
1	A	229	VAL
1	A	239	VAL
1	A	252	LEU
1	A	278	VAL
1	A	304	VAL
1	A	347	GLU
1	A	354	ILE
1	A	376	LEU

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Mol	Chain	Res	Type
1	A	426	ARG
1	B	60	VAL
1	B	108	LEU
1	B	118	ASN
1	B	137	LEU
1	B	143	VAL
1	B	152	LEU
1	B	154	ARG
1	B	182	LEU
1	B	212	LEU
1	B	215	LEU
1	B	229	VAL
1	B	239	VAL
1	B	252	LEU
1	B	278	VAL
1	B	304	VAL
1	B	347	GLU
1	B	354	ILE
1	B	376	LEU
1	B	426	ARG
1	C	60	VAL
1	C	108	LEU
1	C	118	ASN
1	C	137	LEU
1	C	143	VAL
1	C	152	LEU
1	C	154	ARG
1	C	182	LEU
1	C	212	LEU
1	C	215	LEU
1	C	229	VAL
1	C	239	VAL
1	C	252	LEU
1	C	278	VAL
1	C	304	VAL
1	C	347	GLU
1	C	354	ILE
1	C	376	LEU
1	C	426	ARG

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	53	HIS
1	A	118	ASN
1	A	134	HIS
1	A	256	HIS
1	A	319	HIS
1	A	348	ASN
1	A	400	ASN
1	A	408	HIS
1	B	53	HIS
1	B	118	ASN
1	B	134	HIS
1	B	266	GLN
1	B	319	HIS
1	B	348	ASN
1	B	400	ASN
1	B	408	HIS
1	C	53	HIS
1	C	118	ASN
1	C	134	HIS
1	C	140	ASN
1	C	233	GLN
1	C	256	HIS
1	C	319	HIS
1	C	348	ASN
1	C	400	ASN
1	C	408	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

6 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
3	PLP	C	2	2	15,15,16	2.05	5 (33%)	21,22,23	1.70	4 (19%)
2	CAN	A	1	3	5,8,8	0.86	0	4,9,9	1.10	1 (25%)
3	PLP	A	2	2	15,15,16	1.89	4 (26%)	21,22,23	1.95	8 (38%)
2	CAN	B	1	3	5,8,8	0.87	0	4,9,9	0.82	0
3	PLP	B	2	2	15,15,16	1.85	2 (13%)	21,22,23	1.49	5 (23%)
2	CAN	C	1	3	5,8,8	0.85	0	4,9,9	1.16	1 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	C	2	2	-	0/6/6/8	0/1/1/1
2	CAN	A	1	3	-	2/7/8/8	-
3	PLP	A	2	2	-	0/6/6/8	0/1/1/1
2	CAN	B	1	3	-	2/7/8/8	-
3	PLP	B	2	2	-	0/6/6/8	0/1/1/1
2	CAN	C	1	3	-	2/7/8/8	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2	PLP	C4A-C4	-5.32	1.41	1.51
3	C	2	PLP	C4A-C4	-5.05	1.41	1.51
3	A	2	PLP	C4A-C4	-4.38	1.42	1.51
3	A	2	PLP	C3-C2	-3.79	1.37	1.41
3	B	2	PLP	C3-C2	-3.16	1.37	1.41
3	C	2	PLP	P-O2P	2.96	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2	PLP	P-O2P	2.57	1.64	1.54
3	A	2	PLP	C2-N1	2.39	1.38	1.33
3	C	2	PLP	P-O4P	2.30	1.67	1.60
3	C	2	PLP	C3-C2	-2.30	1.38	1.41
3	C	2	PLP	C6-N1	2.00	1.38	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	PLP	O3P-P-O4P	3.87	116.76	106.67
3	C	2	PLP	O2P-P-O4P	-3.79	96.78	106.67
3	A	2	PLP	C6-C5-C4	3.49	120.96	118.10
3	B	2	PLP	O4P-C5A-C5	3.47	115.86	109.36
3	A	2	PLP	O2P-P-O4P	-3.38	97.86	106.67
3	A	2	PLP	O4P-C5A-C5	2.75	114.51	109.36
3	A	2	PLP	C4A-C4-C5	-2.68	118.18	120.94
3	A	2	PLP	O3P-P-O1P	2.59	120.94	110.83
3	A	2	PLP	C5-C6-N1	-2.59	119.62	123.83
3	B	2	PLP	O2P-P-O1P	-2.57	100.81	110.83
3	A	2	PLP	O2P-P-O1P	-2.49	101.11	110.83
3	C	2	PLP	O4P-C5A-C5	2.45	113.95	109.36
3	C	2	PLP	C6-C5-C4	2.43	120.09	118.10
3	A	2	PLP	O4P-P-O1P	2.36	112.83	106.44
3	B	2	PLP	O3P-P-O4P	2.10	112.14	106.67
2	A	1	CAN	OG-CG-CB	2.08	114.27	107.63
2	C	1	CAN	OG-CG-CB	2.03	114.11	107.63
3	B	2	PLP	O3P-P-O1P	2.01	118.69	110.83
3	B	2	PLP	C4A-C4-C5	-2.01	118.87	120.94

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	CAN	N-CA-CB-CG
2	B	1	CAN	CA-CB-CG-OG
2	A	1	CAN	C-CA-CB-CG
2	C	1	CAN	OXT-C-CA-N
2	B	1	CAN	O-C-CA-N
2	C	1	CAN	O-C-CA-N

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	PLP	1	0
2	A	1	CAN	1	0
3	A	2	PLP	3	0
2	B	1	CAN	2	0
3	B	2	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

6.1 Protein, DNA and RNA chains

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	402/402 (100%)	0.62	31 (7%) 19 21	11, 22, 41, 64	0
1	B	402/402 (100%)	0.54	23 (5%) 29 31	10, 21, 39, 65	0
1	C	402/402 (100%)	0.50	19 (4%) 36 38	9, 22, 40, 64	0
All	All	1206/1206 (100%)	0.55	73 (6%) 27 29	9, 22, 40, 65	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	388	TRP	6.2
1	C	198	GLY	6.1
1	B	198	GLY	6.0
1	A	407	THR	5.7
1	B	407	THR	5.6
1	C	409	GLY	5.5
1	B	409	GLY	4.9
1	B	408	HIS	4.7
1	A	387	ASP	4.6
1	B	388	TRP	4.6
1	A	367	VAL	4.3
1	B	387	ASP	4.3
1	C	388	TRP	4.0
1	C	408	HIS	4.0
1	A	386	LYS	4.0
1	C	407	THR	4.0
1	A	198	GLY	3.9
1	B	386	LYS	3.8
1	C	382	ILE	3.7
1	C	386	LYS	3.6
1	C	385	THR	3.6
1	B	382	ILE	3.5
1	B	364	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	436	ILE	3.3
1	C	387	ASP	3.3
1	B	385	THR	3.3
1	A	408	HIS	3.1
1	A	364	PRO	3.0
1	A	366	ASP	3.0
1	C	439	PHE	3.0
1	B	384	GLU	2.9
1	A	439	PHE	2.8
1	A	365	SER	2.8
1	A	406	PRO	2.7
1	A	385	THR	2.7
1	B	366	ASP	2.7
1	C	389	ASP	2.7
1	A	217	ARG	2.7
1	B	363	LEU	2.6
1	A	41	ASP	2.6
1	B	60	VAL	2.6
1	C	354	ILE	2.5
1	C	366	ASP	2.5
1	A	251	GLU	2.5
1	B	367	VAL	2.5
1	C	438	SER	2.5
1	A	438	SER	2.4
1	B	40	SER	2.4
1	A	354	ILE	2.4
1	B	404	ALA	2.4
1	B	354	ILE	2.4
1	B	439	PHE	2.4
1	C	367	VAL	2.3
1	A	216	GLU	2.3
1	A	430	GLU	2.3
1	C	247	MET	2.3
1	B	365	SER	2.3
1	B	362	LYS	2.3
1	A	38	PRO	2.2
1	B	368	VAL	2.2
1	A	362	LYS	2.2
1	C	362	LYS	2.2
1	A	99	ASN	2.1
1	A	361	MET	2.1
1	A	410	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	434	LYS	2.1
1	C	64	ARG	2.1
1	C	384	GLU	2.1
1	A	435	THR	2.1
1	A	132	ASN	2.1
1	A	205	ASP	2.1
1	A	389	ASP	2.1
1	B	113	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CAN	C	1	9/9	0.76	0.18	41,43,46,47	0
2	CAN	B	1	9/9	0.81	0.16	37,43,46,49	0
2	CAN	A	1	9/9	0.81	0.16	46,50,52,52	0
3	PLP	A	2	15/16	0.94	0.09	24,27,31,38	0
3	PLP	B	2	15/16	0.97	0.06	20,22,26,31	0
3	PLP	C	2	15/16	0.97	0.07	19,27,33,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.