



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:22 AM UTC

PDB ID : 3VBE / pdb_00003vbe
Title : Crystal structure of beta-cyanoalanine synthase in soybean
Authors : Yi, H.; Jez, J.M.
Deposited on : 2012-01-02
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)	:	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

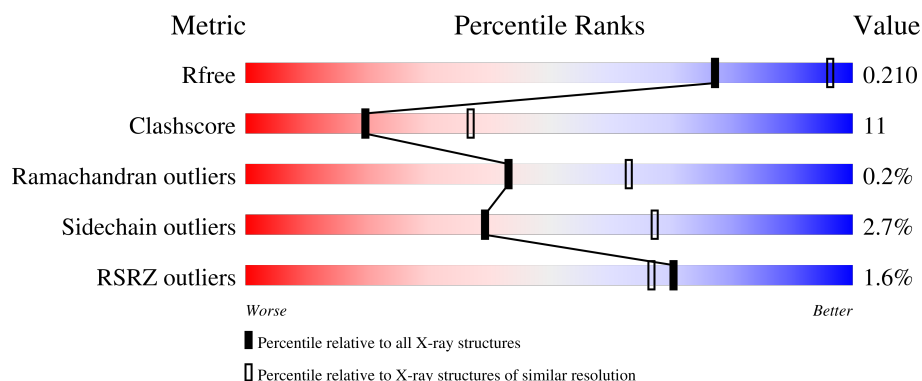
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	344	 79% 11% • 8%
1	B	344	 74% 18% • 7%
1	C	344	 74% 19% • •
1	D	344	 71% 19% •• 8%

2 Entry composition [i](#)

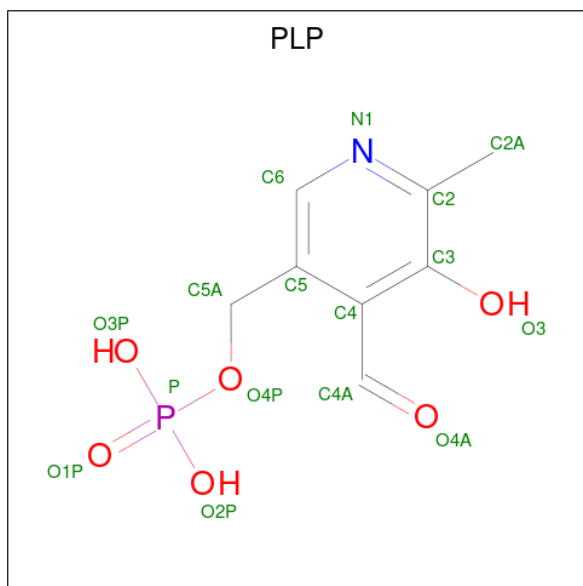
There are 3 unique types of molecules in this entry. The entry contains 9973 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 beta-cyanoalnine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2394	1507	407	462	18			
1	B	321	Total	C	N	O	S	0	0	0
			2423	1527	412	466	18			
1	C	329	Total	C	N	O	S	0	0	0
			2488	1570	423	477	18			
1	D	317	Total	C	N	O	S	0	0	0
			2394	1507	407	462	18			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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		

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

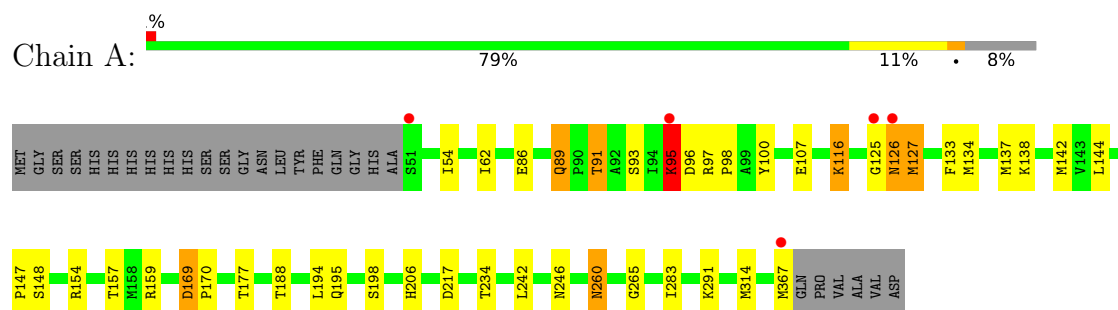
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total	O	0	0
			51	51		
3	B	54	Total	O	0	0
			54	54		
3	C	50	Total	O	0	0
			50	50		
3	D	59	Total	O	0	0
			59	59		

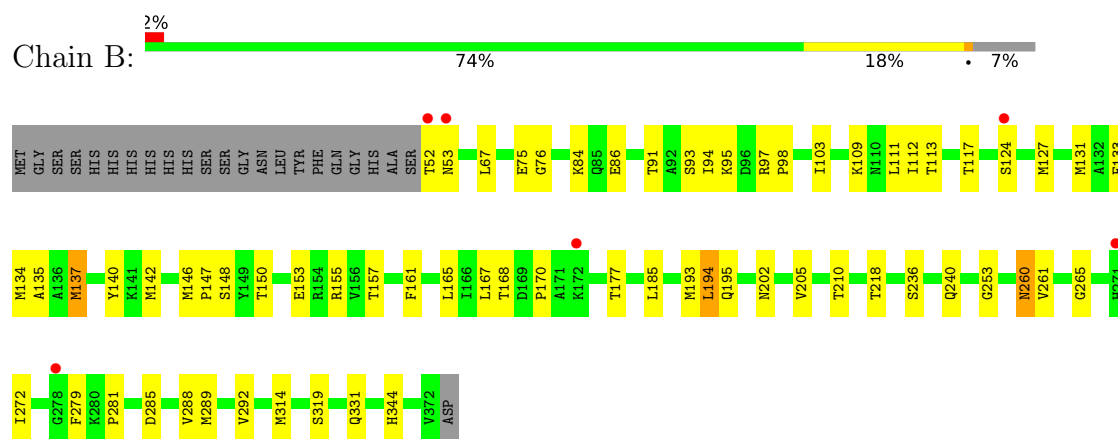
3 Residue-property plots [i](#)

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.

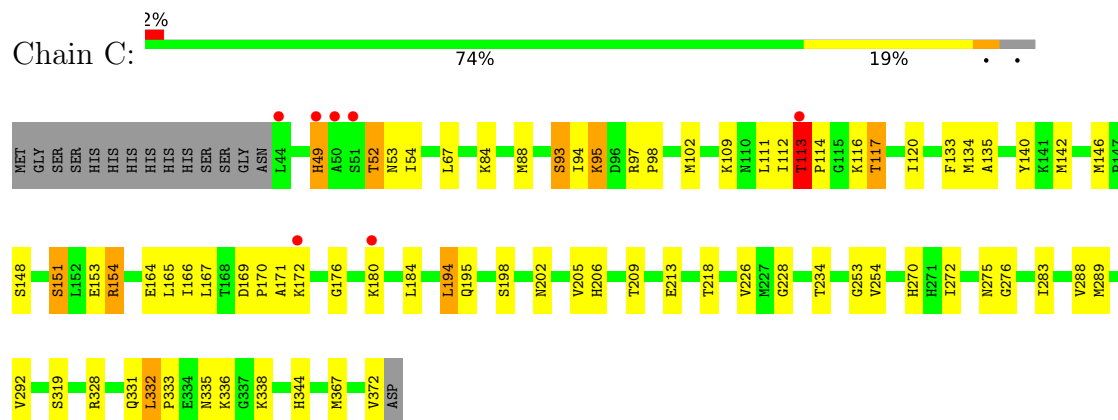
- Molecule 1: beta-cyanoalnine synthase



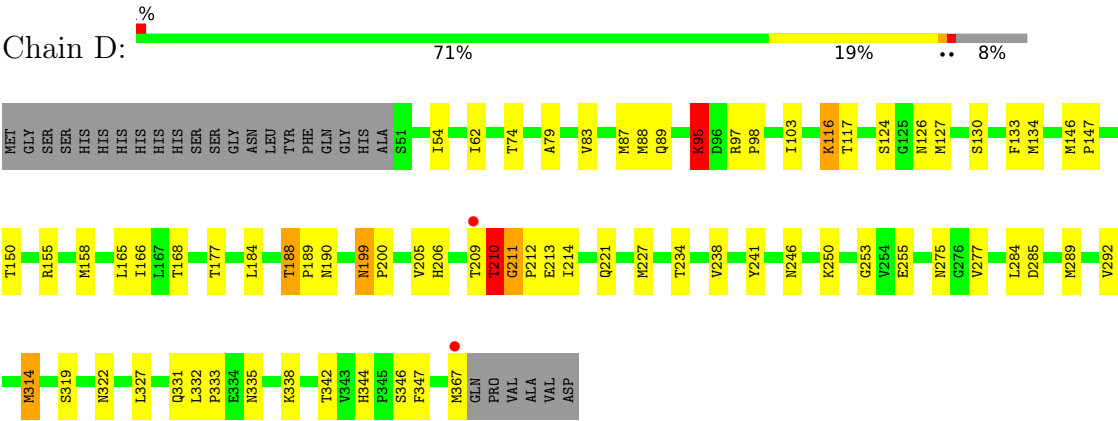
- Molecule 1: beta-cyanoalnine synthase



- Molecule 1: beta-cyanoalnine synthase



● Molecule 1: beta-cyanoalnine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	190.32Å 154.58Å 70.80Å 90.00° 101.89° 90.00°	Depositor
Resolution (Å)	49.16 – 2.50 49.16 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.16-2.50) 99.2 (49.16-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.95 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.167 , 0.210 0.172 , 0.210	Depositor DCC
R_{free} test set	3463 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9973	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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

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	0.78	3/2435 (0.1%)	0.98	10/3293 (0.3%)
1	B	0.67	0/2465	0.88	6/3336 (0.2%)
1	C	0.57	0/2533	0.89	6/3428 (0.2%)
1	D	0.63	1/2435 (0.0%)	0.93	10/3293 (0.3%)
All	All	0.67	4/9868 (0.0%)	0.92	32/13350 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	GLN	C-O	-6.83	1.18	1.24
1	D	89	GLN	C-O	-5.54	1.19	1.24
1	A	169	ASP	C-O	-5.18	1.18	1.24
1	A	126	ASN	CA-C	-5.01	1.46	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	MET	N-CA-C	-13.10	96.93	113.43
1	A	126	ASN	CB-CA-C	-11.60	89.14	111.06
1	D	116	LYS	CA-C-N	9.10	133.66	120.82
1	D	116	LYS	C-N-CA	9.10	133.66	120.82
1	D	95	LYS	CG-CD-CE	7.97	129.63	111.30
1	C	194	LEU	N-CA-C	7.96	120.04	111.36
1	D	188	THR	CA-C-N	7.77	127.33	119.24
1	D	188	THR	C-N-CA	7.77	127.33	119.24
1	C	195	GLN	N-CA-C	7.53	121.44	111.28
1	B	195	GLN	N-CA-C	7.46	121.97	111.52
1	B	261	VAL	N-CA-C	-7.45	105.40	111.81
1	A	95	LYS	CB-CG-CD	7.30	128.08	111.30
1	A	194	LEU	N-CA-C	6.91	118.89	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	LEU	N-CA-C	6.80	118.78	111.36
1	A	188	THR	CA-C-N	6.31	127.72	119.84
1	A	188	THR	C-N-CA	6.31	127.72	119.84
1	C	332	LEU	CA-C-N	6.19	125.92	119.05
1	C	332	LEU	C-N-CA	6.19	125.92	119.05
1	D	116	LYS	O-C-N	6.13	128.81	121.76
1	A	195	GLN	N-CA-C	5.86	119.18	111.28
1	B	260	ASN	N-CA-C	-5.45	96.41	107.41
1	D	199	ASN	CA-C-N	5.44	125.11	119.56
1	D	199	ASN	C-N-CA	5.44	125.11	119.56
1	B	272	ILE	N-CA-C	5.40	111.98	106.21
1	D	117	THR	N-CA-CB	5.29	117.78	109.69
1	B	124	SER	N-CA-C	-5.26	101.44	108.86
1	D	346	SER	N-CA-C	5.24	116.11	108.14
1	A	169	ASP	CA-C-N	5.20	124.99	119.28
1	A	169	ASP	C-N-CA	5.20	124.99	119.28
1	A	260	ASN	N-CA-C	5.17	117.86	110.68
1	C	113	THR	CA-C-N	5.11	124.87	119.76
1	C	113	THR	C-N-CA	5.11	124.87	119.76

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	2394	0	2423	44	0
1	B	2423	0	2457	55	0
1	C	2488	0	2513	65	0
1	D	2394	0	2423	71	0
2	A	15	0	7	0	0
2	B	15	0	7	0	0
2	C	15	0	7	1	0
2	D	15	0	6	3	0
3	A	51	0	0	1	0
3	B	54	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	50	0	0	2	0
3	D	59	0	0	1	0
All	All	9973	0	9843	225	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 11.

All (225) 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:D:146:MET:HE2	1:D:150:THR:HG21	1.26	1.12
1:B:289:MET:HE1	1:B:292:VAL:HG22	1.36	1.07
1:D:289:MET:HE1	1:D:292:VAL:HG22	1.39	1.04
1:C:289:MET:HE1	1:C:292:VAL:HG22	1.44	1.00
1:D:124:SER:HB3	1:D:146:MET:HE3	1.44	1.00
1:B:253:GLY:H	1:B:289:MET:HE3	1.29	0.97
1:D:146:MET:CE	1:D:150:THR:HG21	1.95	0.95
1:A:125:GLY:O	1:A:126:ASN:HB2	1.65	0.95
1:D:146:MET:HE1	1:D:158:MET:HE1	1.50	0.94
1:A:95:LYS:CG	1:A:126:ASN:O	2.17	0.92
1:A:95:LYS:HG3	1:A:126:ASN:O	1.70	0.92
1:C:134:MET:HE2	1:C:134:MET:HA	1.52	0.92
1:C:253:GLY:H	1:C:289:MET:HE3	1.40	0.86
1:B:134:MET:HE2	1:B:134:MET:HA	1.58	0.86
1:D:168:THR:OG1	1:D:177:THR:HG22	1.79	0.83
1:D:146:MET:HE2	1:D:150:THR:CG2	2.07	0.83
1:D:124:SER:CB	1:D:146:MET:HE3	2.10	0.82
1:D:95:LYS:HG3	1:D:127:MET:HA	1.62	0.80
1:C:52:THR:HG23	1:C:54:ILE:H	1.45	0.80
1:C:133:PHE:CE2	1:C:134:MET:HE3	2.16	0.79
1:C:253:GLY:N	1:C:289:MET:HE3	1.99	0.78
1:C:289:MET:CE	1:C:292:VAL:HG22	2.13	0.78
1:B:94:ILE:HG12	1:B:94:ILE:O	1.82	0.77
1:B:97:ARG:HB2	1:B:98:PRO:CD	2.16	0.76
1:D:289:MET:CE	1:D:292:VAL:HG22	2.15	0.75
1:C:112:ILE:HG22	1:C:117:THR:HG21	1.68	0.74
1:B:253:GLY:N	1:B:289:MET:HE3	2.03	0.72
1:B:133:PHE:CE2	1:B:134:MET:HE3	2.26	0.71
1:D:133:PHE:CE2	1:D:134:MET:HE2	2.25	0.70
1:A:91:THR:HB	1:A:96:ASP:OD1	1.91	0.70
1:B:289:MET:CE	1:B:292:VAL:HG22	2.18	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ARG:O	1:C:331:GLN:HG2	1.92	0.70
1:B:135:ALA:HB2	1:B:142:MET:HE3	1.75	0.69
1:B:135:ALA:HB2	1:B:142:MET:CE	2.23	0.69
1:B:147:PRO:HD3	1:B:177:THR:HG21	1.75	0.69
1:B:155:ARG:HG2	1:B:165:LEU:HD23	1.74	0.68
1:A:148:SER:OG	1:A:170:PRO:HG3	1.94	0.67
1:C:165:LEU:O	1:D:367:MET:HE1	1.93	0.67
1:B:148:SER:OG	1:B:170:PRO:HG3	1.94	0.67
1:B:91:THR:OG1	3:B:619:HOH:O	2.12	0.67
1:A:100:TYR:HB2	1:A:134:MET:HE3	1.75	0.67
1:B:52:THR:HG22	1:B:53:ASN:N	2.10	0.67
1:D:209:THR:O	1:D:212:PRO:HD2	1.95	0.67
1:C:272:ILE:HG22	1:C:275:ASN:HB3	1.77	0.67
1:A:95:LYS:HG2	1:A:126:ASN:O	1.96	0.66
1:D:209:THR:O	1:D:210:THR:C	2.40	0.65
1:C:113:THR:HG23	1:C:116:LYS:CE	2.26	0.65
1:C:94:ILE:HG12	1:C:94:ILE:O	1.97	0.64
1:A:367:MET:HE2	3:B:650:HOH:O	1.98	0.63
1:A:147:PRO:HD3	1:A:177:THR:HG21	1.79	0.63
1:A:95:LYS:HG3	1:A:127:MET:HA	1.79	0.63
1:A:95:LYS:HD2	1:A:127:MET:HE2	1.81	0.62
1:B:52:THR:HG22	1:B:53:ASN:H	1.64	0.62
1:D:95:LYS:HG3	1:D:127:MET:CA	2.29	0.62
1:D:87:MET:HE2	1:D:347:PHE:HD1	1.64	0.62
1:A:62:ILE:HD11	1:A:134:MET:CE	2.31	0.61
1:C:49:HIS:HB2	1:D:221:GLN:HG3	1.83	0.61
1:C:154:ARG:NH1	3:C:540:HOH:O	2.35	0.60
1:D:335:ASN:HA	1:D:338:LYS:HE3	1.83	0.60
1:B:97:ARG:HB2	1:B:98:PRO:HD3	1.83	0.60
1:B:185:LEU:HD22	1:B:193:MET:HE3	1.84	0.60
1:A:54:ILE:HD11	1:B:218:THR:HG22	1.84	0.59
1:C:169:ASP:OD2	1:C:171:ALA:HB3	2.02	0.59
1:D:253:GLY:N	1:D:289:MET:HE3	2.17	0.58
1:C:148:SER:HB3	1:C:170:PRO:HG3	1.86	0.58
1:C:180:LYS:HZ3	1:C:184:LEU:CD1	2.17	0.58
1:C:134:MET:HA	1:C:134:MET:CE	2.30	0.58
1:C:135:ALA:HB2	1:C:142:MET:CE	2.33	0.58
1:D:147:PRO:HD3	1:D:177:THR:HG21	1.85	0.58
1:A:169:ASP:OD1	1:A:170:PRO:HD2	2.04	0.58
1:B:153:GLU:OE1	1:B:153:GLU:N	2.32	0.57
1:D:205:VAL:O	1:D:209:THR:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:SER:HB3	1:C:344:HIS:CD2	2.40	0.57
1:D:284:LEU:HD12	1:D:285:ASP:H	1.69	0.57
1:D:74:THR:HG22	1:D:327:LEU:HD21	1.87	0.56
1:B:109:LYS:HB2	1:B:111:LEU:CD1	2.35	0.56
1:C:166:ILE:HD12	1:C:184:LEU:HD21	1.88	0.56
1:D:253:GLY:H	1:D:289:MET:HE3	1.71	0.55
1:D:209:THR:OG1	1:D:210:THR:N	2.39	0.55
1:B:168:THR:OG1	1:B:177:THR:HG22	2.06	0.55
1:C:116:LYS:HG3	1:C:117:THR:N	2.22	0.55
1:A:62:ILE:HD11	1:A:134:MET:HE1	1.89	0.54
1:C:253:GLY:CA	1:C:289:MET:HE3	2.37	0.54
1:C:88:MET:O	1:D:88:MET:SD	2.66	0.54
1:A:91:THR:O	1:A:91:THR:CG2	2.54	0.54
1:C:113:THR:H	1:C:116:LYS:HE3	1.72	0.53
1:C:218:THR:HG22	1:D:54:ILE:HD11	1.91	0.53
1:D:211:GLY:O	1:D:212:PRO:C	2.51	0.53
1:C:180:LYS:NZ	1:C:184:LEU:HD11	2.24	0.53
1:D:95:LYS:HB3	1:D:130:SER:OG	2.07	0.53
1:D:79:ALA:HB1	1:D:338:LYS:O	2.09	0.53
1:D:126:ASN:HD22	2:D:401:PLP:H2A1	1.73	0.53
1:D:83:VAL:HG12	1:D:342:THR:HG23	1.91	0.53
1:C:113:THR:HG23	1:C:116:LYS:HE2	1.91	0.53
1:D:166:ILE:HD12	1:D:184:LEU:HD11	1.91	0.52
1:A:314:MET:CE	1:B:157:THR:HG23	2.39	0.52
1:B:134:MET:HA	1:B:134:MET:CE	2.35	0.52
1:B:279:PHE:O	1:B:281:PRO:HD3	2.09	0.52
1:C:135:ALA:HB2	1:C:142:MET:HE3	1.91	0.52
1:D:277:VAL:HG22	3:D:521:HOH:O	2.09	0.52
1:A:91:THR:O	1:A:91:THR:HG23	2.09	0.52
1:B:331:GLN:OE1	1:B:331:GLN:HA	2.09	0.51
1:A:125:GLY:O	1:A:126:ASN:CB	2.42	0.51
1:D:211:GLY:O	1:D:214:ILE:N	2.43	0.51
1:C:113:THR:HB	1:C:114:PRO:HD2	1.91	0.51
1:D:284:LEU:HD12	1:D:285:ASP:N	2.24	0.51
1:D:155:ARG:HA	1:D:158:MET:HE3	1.92	0.51
1:B:97:ARG:HB2	1:B:98:PRO:HD2	1.91	0.51
1:D:95:LYS:HB3	1:D:130:SER:CB	2.41	0.51
1:D:116:LYS:NZ	1:D:190:ASN:CG	2.69	0.50
1:D:147:PRO:CD	1:D:177:THR:HG21	2.42	0.50
1:A:133:PHE:CE2	1:A:134:MET:HE2	2.47	0.49
1:C:146:MET:O	1:C:167:LEU:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:ILE:HD11	1:D:134:MET:CE	2.42	0.49
1:C:335:ASN:O	1:C:338:LYS:HB2	2.13	0.49
1:A:157:THR:HG23	1:B:314:MET:HE3	1.94	0.49
1:D:205:VAL:O	1:D:209:THR:OG1	2.25	0.49
1:D:83:VAL:HG12	1:D:342:THR:CG2	2.43	0.48
1:D:227:MET:HE3	2:D:401:PLP:H5A2	1.95	0.48
1:C:202:ASN:O	1:C:205:VAL:HG12	2.13	0.48
1:A:147:PRO:CD	1:A:177:THR:HG21	2.42	0.48
1:D:319:SER:HB3	1:D:344:HIS:CD2	2.48	0.48
1:D:95:LYS:HG2	1:D:126:ASN:C	2.38	0.48
1:A:260:ASN:OD1	1:A:265:GLY:HA3	2.14	0.48
1:C:112:ILE:HD12	1:C:140:TYR:CE1	2.49	0.48
1:C:151:SER:OG	1:C:154:ARG:HB2	2.13	0.47
1:D:95:LYS:HG2	1:D:126:ASN:CB	2.45	0.47
1:D:335:ASN:OD1	1:D:338:LYS:NZ	2.40	0.47
1:A:86:GLU:O	1:A:89:GLN:HG3	2.15	0.47
1:C:113:THR:CB	1:C:114:PRO:HD2	2.45	0.47
1:C:180:LYS:HZ3	1:C:184:LEU:HD13	1.79	0.47
1:B:67:LEU:HD23	1:B:84:LYS:HA	1.96	0.47
1:B:131:MET:HE2	1:B:194:LEU:HD12	1.95	0.47
1:D:210:THR:O	1:D:211:GLY:C	2.58	0.47
1:A:91:THR:HB	1:A:96:ASP:CG	2.40	0.46
1:A:116:LYS:O	1:A:116:LYS:HG2	2.16	0.46
1:B:202:ASN:O	1:B:205:VAL:HG12	2.16	0.46
1:B:146:MET:O	1:B:167:LEU:HA	2.16	0.46
1:C:153:GLU:OE1	1:C:153:GLU:N	2.38	0.46
1:C:253:GLY:HA3	1:C:289:MET:HE3	1.97	0.46
1:D:246:ASN:OD1	1:D:246:ASN:C	2.57	0.46
1:A:62:ILE:CD1	1:A:134:MET:HE1	2.46	0.46
1:B:147:PRO:CD	1:B:177:THR:HG21	2.44	0.46
1:C:109:LYS:O	1:C:111:LEU:HD12	2.16	0.46
1:B:52:THR:CG2	1:B:53:ASN:N	2.79	0.46
1:C:113:THR:N	1:C:116:LYS:HE3	2.30	0.46
1:C:275:ASN:OD1	1:C:276:GLY:N	2.49	0.46
1:A:107:GLU:OE1	1:A:138:LYS:HE2	2.16	0.45
1:B:135:ALA:HB2	1:B:142:MET:HE2	1.98	0.45
1:D:210:THR:O	1:D:211:GLY:O	2.34	0.45
1:A:97:ARG:HB2	1:A:98:PRO:CD	2.47	0.45
1:A:154:ARG:HG3	1:A:154:ARG:HH11	1.80	0.45
1:D:95:LYS:HD2	1:D:95:LYS:HA	1.41	0.45
1:B:131:MET:CE	1:B:194:LEU:CD1	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:ALA:HB2	1:C:142:MET:HE2	1.98	0.45
1:D:168:THR:HG21	1:D:177:THR:HA	1.99	0.45
1:D:103:ILE:HD12	1:D:134:MET:HB3	1.99	0.45
1:A:62:ILE:CD1	1:A:134:MET:CE	2.95	0.44
1:D:335:ASN:HA	1:D:338:LYS:CE	2.47	0.44
1:A:95:LYS:CB	1:A:126:ASN:O	2.65	0.44
1:A:137:MET:HE2	1:A:137:MET:HB3	1.82	0.44
1:D:314:MET:HE3	1:D:314:MET:HB2	1.82	0.44
1:C:97:ARG:HB2	1:C:98:PRO:HD3	1.99	0.44
1:C:172:LYS:HB3	1:C:176:GLY:HA3	2.00	0.44
1:C:198:SER:HA	1:C:283:ILE:HG23	1.99	0.44
1:D:255:GLU:HG2	1:D:292:VAL:HG12	2.00	0.43
1:D:95:LYS:O	1:D:98:PRO:HD2	2.18	0.43
1:A:142:MET:HE2	1:A:144:LEU:CD2	2.49	0.43
1:B:109:LYS:HB2	1:B:111:LEU:HD12	2.01	0.43
1:A:154:ARG:NH1	3:A:611:HOH:O	2.51	0.43
1:A:217:ASP:HA	1:B:52:THR:O	2.17	0.43
1:B:97:ARG:CB	1:B:98:PRO:CD	2.85	0.43
1:C:93:SER:OG	1:C:95:LYS:HB2	2.19	0.43
1:B:112:ILE:HD12	1:B:140:TYR:CZ	2.54	0.43
1:C:98:PRO:HB2	1:C:102:MET:HE2	2.00	0.43
1:C:133:PHE:CZ	1:C:134:MET:HE3	2.54	0.43
1:B:127:MET:O	1:B:131:MET:HG2	2.19	0.42
1:B:285:ASP:O	1:B:288:VAL:HG12	2.19	0.42
1:C:270:HIS:CE1	1:C:275:ASN:O	2.72	0.42
1:D:210:THR:HB	1:D:238:VAL:HG22	2.01	0.42
1:D:250:LYS:HZ2	1:D:250:LYS:HG2	1.65	0.42
1:B:86:GLU:HG3	1:B:94:ILE:HB	2.02	0.42
1:C:194:LEU:HA	1:C:194:LEU:HD23	1.71	0.42
1:B:112:ILE:HG22	1:B:117:THR:HG21	2.01	0.42
1:C:180:LYS:HZ3	1:C:184:LEU:HD11	1.79	0.42
1:A:314:MET:HE3	1:B:157:THR:HG23	2.00	0.42
1:B:94:ILE:O	1:B:94:ILE:CG1	2.60	0.42
1:B:319:SER:HB3	1:B:344:HIS:CD2	2.54	0.42
1:D:205:VAL:HG22	1:D:209:THR:HG21	2.00	0.42
1:B:137:MET:HE2	1:B:137:MET:HB3	1.87	0.42
1:A:246:ASN:OD1	1:A:246:ASN:C	2.60	0.41
1:D:188:THR:HA	1:D:189:PRO:HD3	1.86	0.41
1:D:199:ASN:HA	1:D:200:PRO:HD3	1.78	0.41
1:C:95:LYS:NZ	2:C:401:PLP:O3	2.45	0.41
1:D:126:ASN:ND2	2:D:401:PLP:H2A1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ILE:HD12	1:B:134:MET:HB3	2.01	0.41
1:C:120:ILE:HD13	1:C:184:LEU:HB3	2.01	0.41
1:C:206:HIS:CG	1:C:234:THR:HA	2.54	0.41
1:C:367:MET:HE2	1:C:367:MET:HB3	1.90	0.41
1:A:198:SER:HA	1:A:283:ILE:HG23	2.03	0.41
1:A:206:HIS:CG	1:A:234:THR:HA	2.56	0.41
1:D:97:ARG:HB2	1:D:98:PRO:CD	2.50	0.41
1:B:260:ASN:O	1:B:265:GLY:CA	2.69	0.41
1:C:154:ARG:NH2	3:C:526:HOH:O	2.54	0.41
1:C:209:THR:O	1:C:213:GLU:HG3	2.21	0.41
1:B:75:GLU:HA	1:B:76:GLY:HA2	1.84	0.41
1:A:206:HIS:CD2	1:A:234:THR:HA	2.56	0.41
1:B:236:SER:O	1:B:240:GLN:HG3	2.21	0.41
1:C:52:THR:HG23	1:C:53:ASN:N	2.36	0.41
1:C:67:LEU:HD23	1:C:84:LYS:HA	2.03	0.41
1:C:332:LEU:HA	1:C:333:PRO:HD3	1.79	0.41
1:D:332:LEU:HA	1:D:333:PRO:HD3	1.95	0.41
1:C:228:GLY:HA2	1:C:254:VAL:HB	2.03	0.41
1:D:210:THR:O	1:D:213:GLU:HB2	2.21	0.41
1:D:212:PRO:HA	1:D:241:TYR:CE2	2.55	0.41
1:D:322:ASN:HB3	1:D:342:THR:OG1	2.21	0.41
1:A:159:ARG:HA	1:A:159:ARG:HD2	1.88	0.40
1:B:95:LYS:HD2	1:B:127:MET:HE2	2.03	0.40
1:C:206:HIS:CD2	1:C:234:THR:HA	2.56	0.40
1:C:253:GLY:HA3	1:C:289:MET:CE	2.51	0.40
1:D:166:ILE:HD12	1:D:184:LEU:CD1	2.51	0.40
1:A:242:LEU:HD23	1:A:242:LEU:HA	1.93	0.40
1:B:95:LYS:HA	1:B:95:LYS:HD3	1.74	0.40
1:D:206:HIS:CG	1:D:234:THR:HA	2.57	0.40
1:A:314:MET:HE2	1:B:161:PHE:CE2	2.56	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	315/344 (92%)	307 (98%)	8 (2%)	0	100	100
1	B	319/344 (93%)	310 (97%)	9 (3%)	0	100	100
1	C	327/344 (95%)	321 (98%)	6 (2%)	0	100	100
1	D	315/344 (92%)	301 (96%)	12 (4%)	2 (1%)	21	38
All	All	1276/1376 (93%)	1239 (97%)	35 (3%)	2 (0%)	43	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	211	GLY
1	D	210	THR

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	263/285 (92%)	258 (98%)	5 (2%)	50	76
1	B	266/285 (93%)	261 (98%)	5 (2%)	50	76
1	C	272/285 (95%)	259 (95%)	13 (5%)	23	46
1	D	263/285 (92%)	257 (98%)	6 (2%)	44	72
All	All	1064/1140 (93%)	1035 (97%)	29 (3%)	39	67

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	THR
1	A	93	SER
1	A	95	LYS
1	A	116	LYS
1	A	291	LYS
1	B	93	SER

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Mol	Chain	Res	Type
1	B	113	THR
1	B	137	MET
1	B	150	THR
1	B	210	THR
1	C	49	HIS
1	C	52	THR
1	C	93	SER
1	C	95	LYS
1	C	113	THR
1	C	117	THR
1	C	151	SER
1	C	154	ARG
1	C	164	GLU
1	C	226	VAL
1	C	288	VAL
1	C	336	LYS
1	C	372	VAL
1	D	95	LYS
1	D	165	LEU
1	D	210	THR
1	D	275	ASN
1	D	314	MET
1	D	331	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	192	HIS
1	B	248	ASN
1	C	196	GLN
1	D	85	GLN
1	D	126	ASN
1	D	219	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	500	1	15,15,16	1.28	2 (13%)	21,22,23	1.54	4 (19%)
2	PLP	D	401	1	15,15,16	1.04	1 (6%)	21,22,23	7.73	3 (14%)
2	PLP	C	401	1	15,15,16	2.85	2 (13%)	21,22,23	5.40	3 (14%)
2	PLP	B	501	1	15,15,16	0.96	1 (6%)	21,22,23	5.99	5 (23%)

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	500	1	-	0/6/6/8	0/1/1/1
2	PLP	D	401	1	-	2/6/6/8	0/1/1/1
2	PLP	C	401	1	-	0/6/6/8	0/1/1/1
2	PLP	B	501	1	-	3/6/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	PLP	C4A-C4	-10.33	1.31	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	PLP	C3-C2	-2.68	1.38	1.41
2	A	500	PLP	C2-N1	2.63	1.38	1.33
2	C	401	PLP	C2-N1	2.41	1.38	1.33
2	D	401	PLP	C2-N1	2.29	1.37	1.33
2	B	501	PLP	C2-N1	2.18	1.37	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	PLP	C4A-C4-C5	29.94	151.80	120.94
2	B	501	PLP	C4A-C4-C5	23.06	144.70	120.94
2	C	401	PLP	C4A-C4-C5	20.39	141.96	120.94
2	D	401	PLP	C4A-C4-C3	-18.46	89.73	120.52
2	B	501	PLP	C4A-C4-C3	-13.93	97.30	120.52
2	C	401	PLP	C4A-C4-C3	-13.23	98.47	120.52
2	A	500	PLP	C3-C4-C5	3.16	122.38	118.59
2	B	501	PLP	C6-C5-C4	3.15	120.68	118.10
2	A	500	PLP	O4P-C5A-C5	3.08	115.13	109.36
2	A	500	PLP	C5-C6-N1	-2.57	119.64	123.83
2	C	401	PLP	C6-C5-C4	2.45	120.11	118.10
2	D	401	PLP	C6-C5-C4	2.29	119.97	118.10
2	A	500	PLP	O3P-P-O4P	2.21	112.44	106.67
2	B	501	PLP	O3P-P-O4P	2.08	112.08	106.67
2	B	501	PLP	C5-C6-N1	-2.02	120.54	123.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	PLP	C4-C5-C5A-O4P
2	B	501	PLP	C6-C5-C5A-O4P
2	D	401	PLP	C4-C5-C5A-O4P
2	D	401	PLP	C6-C5-C5A-O4P
2	B	501	PLP	C5A-O4P-P-O3P

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	PLP	3	0
2	C	401	PLP	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	317/344 (92%)	-0.21	5 (1%) 70 67	30, 47, 78, 109	0
1	B	321/344 (93%)	-0.13	6 (1%) 66 62	28, 50, 79, 115	0
1	C	329/344 (95%)	-0.05	7 (2%) 63 59	27, 52, 92, 128	0
1	D	317/344 (92%)	-0.14	2 (0%) 85 83	29, 50, 84, 109	0
All	All	1284/1376 (93%)	-0.13	20 (1%) 70 67	27, 50, 84, 128	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	50	ALA	6.7
1	B	52	THR	4.6
1	D	209	THR	3.8
1	A	51	SER	3.1
1	B	278	GLY	3.1
1	C	51	SER	2.9
1	B	271	HIS	2.7
1	C	172	LYS	2.6
1	B	172	LYS	2.6
1	A	367	MET	2.5
1	C	44	LEU	2.5
1	B	53	ASN	2.4
1	A	95	LYS	2.3
1	B	124	SER	2.3
1	C	113	THR	2.2
1	D	367	MET	2.2
1	C	49	HIS	2.2
1	A	126	ASN	2.1
1	A	125	GLY	2.1
1	C	180	LYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PLP	B	501	15/16	0.97	0.06	31,44,48,51	0
2	PLP	C	401	15/16	0.97	0.07	38,46,53,55	0
2	PLP	D	401	15/16	0.97	0.07	35,41,51,53	0
2	PLP	A	500	15/16	0.98	0.05	26,36,46,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.