



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:38 PM UTC

PDB ID : 2ZSJ / pdb_00002zsj
Title : Crystal structure of threonine synthase from Aquifex aeolicus VF5
Authors : Mizutani, H.; Kunishima, N.
Deposited on : 2008-09-11
Resolution : 1.80 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

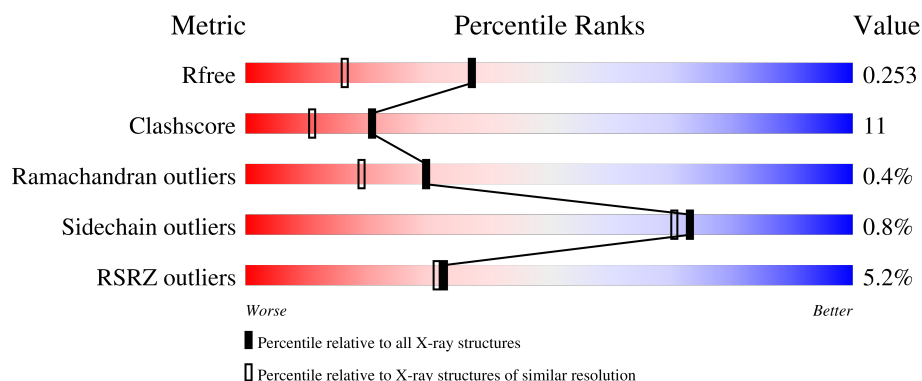
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	352	6% 76% 22% ..
1	B	352	5% 79% 20% ..
1	C	352	6% 79% 20% ..
1	D	352	4% 75% 24% .

2 Entry composition [i](#)

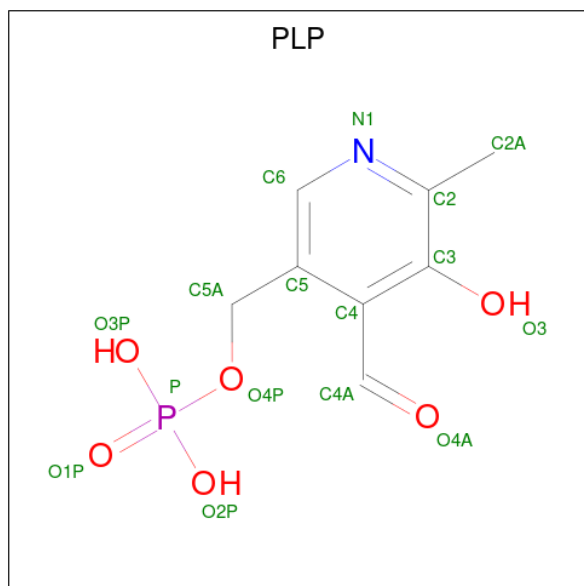
There are 3 unique types of molecules in this entry. The entry contains 11751 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Threonine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	1	0
			2655	1711	438	497	9			
1	B	350	Total	C	N	O	S	0	0	0
			2649	1707	438	495	9			
1	C	350	Total	C	N	O	S	0	1	0
			2652	1709	438	496	9			
1	D	348	Total	C	N	O	S	0	0	0
			2637	1699	436	493	9			

- 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		

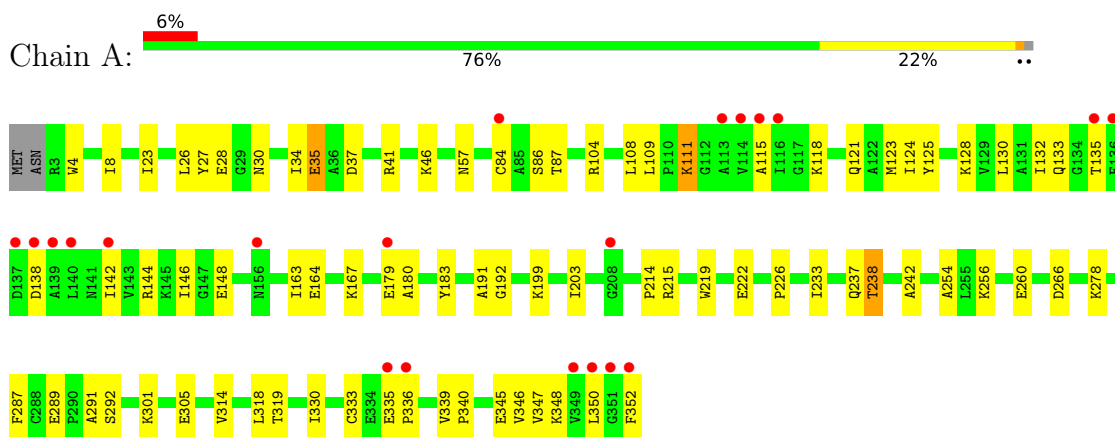
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	262	Total	O	0	0
			262	262		
3	B	290	Total	O	0	0
			290	290		
3	C	287	Total	O	0	0
			287	287		
3	D	259	Total	O	0	0
			259	259		

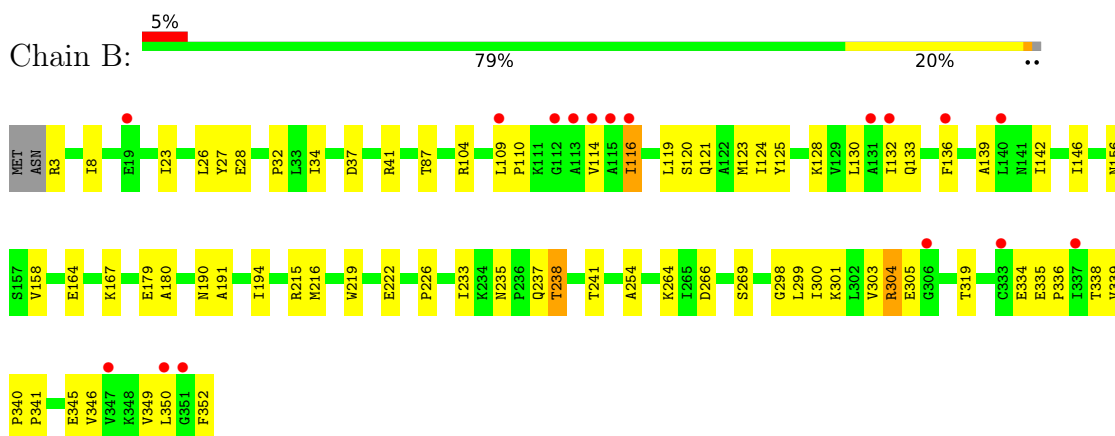
3 Residue-property plots [i](#)

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.

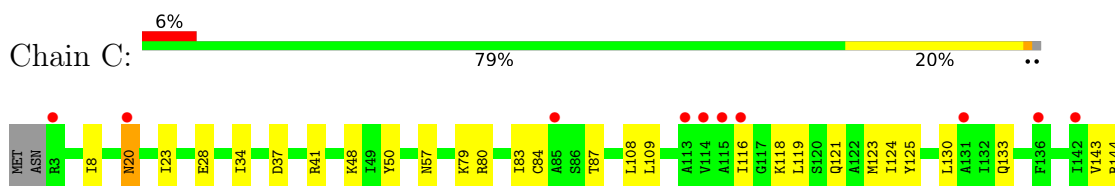
• Molecule 1: Threonine synthase

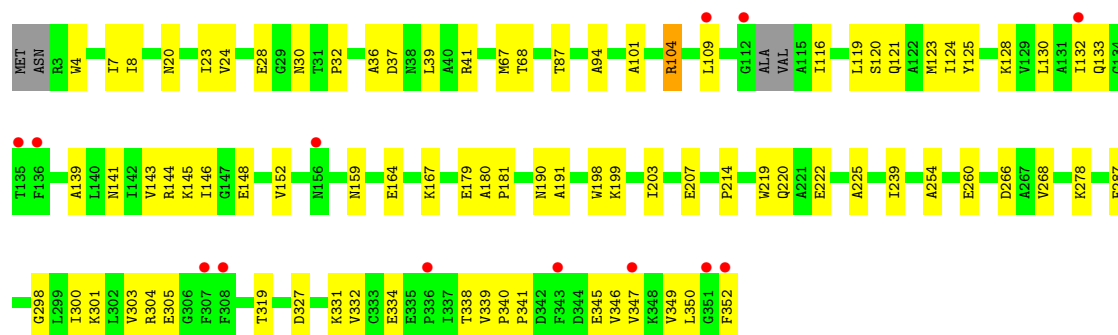


• Molecule 1: Threonine synthase



• Molecule 1: Threonine synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.09Å 71.86Å 99.46Å 75.44° 75.30° 89.99°	Depositor
Resolution (Å)	30.00 – 1.80 30.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	93.0 (30.00-1.80) 93.1 (30.00-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.254 0.223 , 0.253	Depositor DCC
R_{free} test set	6460 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.760	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.106 for h,-k,h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11751	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.87% 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	0.43	0/2714	0.91	4/3679 (0.1%)
1	B	0.43	0/2705	0.91	5/3667 (0.1%)
1	C	0.42	0/2711	0.91	6/3675 (0.2%)
1	D	0.42	0/2692	0.91	3/3647 (0.1%)
All	All	0.43	0/10822	0.91	18/14668 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	THR	N-CA-C	8.44	120.48	111.28
1	B	319	THR	N-CA-C	7.51	121.36	111.75
1	D	319	THR	N-CA-C	7.48	121.33	111.75
1	C	319	THR	N-CA-C	7.46	121.31	111.75
1	A	34	ILE	N-CA-C	6.46	118.09	108.54
1	B	241	THR	N-CA-C	6.22	118.85	111.33
1	C	34	ILE	N-CA-C	5.76	117.07	108.54
1	B	34	ILE	N-CA-C	5.25	116.27	108.23
1	C	241	THR	N-CA-C	5.24	117.67	111.33
1	C	57	ASN	CA-C-N	5.22	126.36	119.84
1	C	57	ASN	C-N-CA	5.22	126.36	119.84
1	B	215	ARG	N-CA-C	-5.19	101.50	109.76
1	D	159	ASN	CA-C-N	5.12	124.73	119.56
1	D	159	ASN	C-N-CA	5.12	124.73	119.56
1	A	57	ASN	CA-C-N	5.10	126.22	119.84
1	A	57	ASN	C-N-CA	5.10	126.22	119.84
1	C	304	ARG	CD-NE-CZ	-5.08	117.29	124.40
1	B	304	ARG	CD-NE-CZ	-5.00	117.40	124.40

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	2655	0	2702	69	0
1	B	2649	0	2696	69	0
1	C	2652	0	2701	62	0
1	D	2637	0	2681	68	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
2	C	15	0	6	0	0
2	D	15	0	6	0	0
3	A	262	0	0	5	0
3	B	290	0	0	3	0
3	C	287	0	0	7	0
3	D	259	0	0	3	0
All	All	11751	0	10804	239	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 (239) 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:C:350:LEU:HD11	1:D:130:LEU:HD11	1.47	0.97
1:D:278:LYS:HE2	1:D:332:VAL:HB	1.51	0.88
1:D:104:ARG:HB3	1:D:104:ARG:HH11	1.42	0.84
1:B:104:ARG:HH21	1:B:128:LYS:HE3	1.43	0.83
1:D:327:ASP:O	1:D:331:LYS:HG2	1.82	0.79
1:D:8:ILE:HG21	1:D:23:ILE:HD12	1.69	0.74
1:A:104:ARG:HH22	1:A:128:LYS:HE2	1.52	0.74
1:B:179:GLU:HG3	1:B:180:ALA:N	2.02	0.74
1:A:87:THR:HG22	1:A:109:LEU:HD13	1.70	0.73
1:B:104:ARG:NH2	1:B:128:LYS:HE3	2.03	0.73
1:A:111:LYS:HZ2	1:A:111:LYS:HB2	1.55	0.71
1:B:156:ASN:OD1	1:B:158:VAL:HG12	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ILE:HD11	1:B:216:MET:HB3	1.73	0.71
1:C:80:ARG:HG2	1:C:80:ARG:HH11	1.55	0.70
1:D:164:GLU:O	1:D:167:LYS:HG2	1.92	0.69
1:B:164:GLU:O	1:B:167:LYS:HG2	1.93	0.69
1:C:350:LEU:CD1	1:D:130:LEU:HD11	2.23	0.69
1:A:347:VAL:HG13	1:A:352:PHE:HB2	1.74	0.68
1:A:199:LYS:HG3	3:A:1190:HOH:O	1.94	0.68
1:B:104:ARG:HH21	1:B:128:LYS:CE	2.05	0.68
1:C:191:ALA:HB1	1:C:254:ALA:HB2	1.76	0.68
1:D:301:LYS:O	1:D:305:GLU:HG3	1.94	0.68
1:D:219:TRP:CZ3	1:D:266:ASP:HB3	2.29	0.68
1:A:350:LEU:HD11	1:B:130:LEU:HD11	1.76	0.68
1:C:346:VAL:O	1:C:350:LEU:HD13	1.94	0.68
1:B:222:GLU:HG2	1:B:269:SER:HA	1.74	0.67
1:A:191:ALA:HB1	1:A:254:ALA:HB2	1.75	0.67
1:A:164:GLU:O	1:A:167:LYS:HG2	1.94	0.67
1:A:301:LYS:O	1:A:305:GLU:HG3	1.95	0.66
1:B:8:ILE:HG21	1:B:23:ILE:HD12	1.77	0.65
1:D:346:VAL:O	1:D:350:LEU:HD13	1.96	0.65
1:A:8:ILE:HG21	1:A:23:ILE:HD12	1.77	0.65
1:B:300:ILE:O	1:B:303:VAL:HG22	1.98	0.64
1:C:130:LEU:HD22	1:D:350:LEU:HD11	1.80	0.63
1:B:190:ASN:O	1:B:191:ALA:HB3	1.99	0.63
1:A:130:LEU:CD2	1:B:350:LEU:HD11	2.29	0.63
1:B:109:LEU:O	1:B:132:ILE:HG22	1.98	0.63
1:B:219:TRP:CZ3	1:B:266:ASP:HB3	2.34	0.63
1:C:256:LYS:HD3	3:C:1293:HOH:O	1.98	0.63
1:A:135:THR:OG1	1:A:138:ASP:HB2	1.99	0.63
1:D:198:TRP:HZ2	1:D:260:GLU:HG2	1.63	0.63
1:B:301:LYS:O	1:B:305:GLU:HG3	1.99	0.62
1:B:191:ALA:HB1	1:B:254:ALA:HB2	1.81	0.62
1:A:278:LYS:HE2	3:A:1305:HOH:O	1.98	0.62
1:B:3:ARG:NH1	1:B:3:ARG:HB2	2.14	0.62
1:C:256:LYS:O	1:C:260:GLU:HG3	2.00	0.62
1:A:346:VAL:O	1:A:350:LEU:HD13	1.99	0.62
1:C:190:ASN:O	1:C:191:ALA:HB3	1.98	0.62
1:A:37:ASP:HB3	1:A:41:ARG:NH2	2.14	0.62
1:C:301:LYS:O	1:C:305:GLU:HG3	1.99	0.62
1:B:132:ILE:HG21	1:B:139:ALA:HB2	1.81	0.61
1:D:104:ARG:HB3	1:D:104:ARG:NH1	2.12	0.61
1:D:300:ILE:O	1:D:303:VAL:HG22	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:ASP:O	1:C:348:LYS:HG2	2.02	0.60
1:B:87:THR:HG22	1:B:109:LEU:HD13	1.83	0.60
1:C:8:ILE:HG21	1:C:23:ILE:HD12	1.83	0.60
1:C:309:LYS:HE2	3:C:1369:HOH:O	2.02	0.59
1:D:87:THR:HG22	1:D:109:LEU:HD13	1.82	0.59
1:D:191:ALA:HB1	1:D:254:ALA:HB2	1.83	0.59
1:A:111:LYS:NZ	1:B:338:THR:HG23	2.18	0.59
1:A:350:LEU:CD1	1:B:130:LEU:HD11	2.32	0.59
1:B:37:ASP:O	1:B:41:ARG:HG3	2.03	0.59
1:C:118:LYS:C	1:C:119:LEU:HD12	2.27	0.59
1:C:219:TRP:CZ3	1:C:266:ASP:HB3	2.38	0.59
1:C:87:THR:HG22	1:C:109:LEU:HD13	1.86	0.58
1:B:110:PRO:HG2	1:B:136:PHE:CD1	2.38	0.57
1:B:136:PHE:HD1	3:B:1286:HOH:O	1.85	0.57
1:D:139:ALA:O	1:D:143:VAL:HG23	2.04	0.57
1:D:141:ASN:O	1:D:145:LYS:HG2	2.05	0.57
1:A:115:ALA:HB3	1:A:118:LYS:NZ	2.19	0.56
1:A:350:LEU:HD11	1:B:130:LEU:CD1	2.35	0.56
1:C:28:GLU:CD	1:C:28:GLU:H	2.13	0.56
1:C:144:ARG:O	1:C:148:GLU:HG3	2.05	0.56
1:C:124:ILE:HD13	1:D:287:PHE:CE1	2.41	0.56
1:C:222:GLU:HG3	1:C:269:SER:HA	1.88	0.55
1:D:120:SER:HA	1:D:123:MET:HE3	1.88	0.55
1:D:144:ARG:HG2	1:D:148:GLU:OE2	2.06	0.55
1:A:335:GLU:OE2	1:A:336:PRO:HD2	2.07	0.55
1:C:350:LEU:HD11	1:D:130:LEU:CD1	2.30	0.55
1:B:226:PRO:HB3	1:B:233:ILE:HG12	1.89	0.55
1:D:119:LEU:HB2	1:D:123:MET:HE2	1.89	0.55
1:D:121:GLN:O	1:D:124:ILE:HG22	2.07	0.55
1:D:104:ARG:HH11	1:D:104:ARG:CB	2.17	0.54
1:D:28:GLU:CD	1:D:28:GLU:H	2.16	0.54
1:A:130:LEU:HD21	1:B:350:LEU:HD11	1.90	0.54
1:A:350:LEU:N	1:A:350:LEU:HD12	2.23	0.54
1:A:87:THR:HG22	1:A:109:LEU:CD1	2.38	0.54
1:D:104:ARG:NH2	1:D:128:LYS:HE3	2.22	0.54
1:C:352:PHE:CD1	1:C:352:PHE:N	2.75	0.54
1:C:163:ILE:HG12	3:C:1140:HOH:O	2.08	0.54
1:D:239:ILE:HD11	3:D:1247:HOH:O	2.08	0.53
1:A:123:MET:HE1	1:B:334:GLU:O	2.08	0.53
1:D:190:ASN:O	1:D:191:ALA:HB3	2.09	0.53
1:C:350:LEU:N	1:C:350:LEU:HD12	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:GLU:HG3	1:D:180:ALA:N	2.23	0.53
1:B:133:GLN:NE2	3:B:1269:HOH:O	2.40	0.53
1:D:222:GLU:HG3	1:D:268:VAL:C	2.33	0.53
1:A:121:GLN:O	1:A:124:ILE:HG22	2.09	0.53
1:C:339:VAL:HG13	1:D:132:ILE:HD13	1.91	0.53
1:A:179:GLU:HG3	1:A:180:ALA:N	2.23	0.52
1:B:179:GLU:CG	1:B:180:ALA:N	2.71	0.52
1:A:130:LEU:HD22	1:B:350:LEU:HD11	1.91	0.52
1:A:28:GLU:H	1:A:28:GLU:CD	2.16	0.52
1:B:235:ASN:ND2	1:B:237:GLN:HE21	2.08	0.52
1:C:130:LEU:CD2	1:D:350:LEU:HD11	2.40	0.52
1:A:242:ALA:HB3	1:A:291:ALA:CB	2.40	0.52
1:B:28:GLU:CD	1:B:28:GLU:H	2.18	0.52
1:C:121:GLN:O	1:C:124:ILE:HG22	2.10	0.52
1:C:352:PHE:HE2	1:D:146:ILE:HG23	1.75	0.52
1:B:3:ARG:HB2	1:B:3:ARG:HH11	1.75	0.52
1:C:20:ASN:C	1:C:20:ASN:HD22	2.18	0.52
1:C:215:ARG:NH1	3:C:1162:HOH:O	2.22	0.52
1:A:130:LEU:HD21	1:B:350:LEU:CD1	2.41	0.51
1:A:111:LYS:HZ3	1:B:338:THR:HG23	1.75	0.51
1:D:67:MET:HE3	1:D:94:ALA:HB2	1.92	0.51
1:A:219:TRP:CZ3	1:A:266:ASP:HB3	2.45	0.51
1:B:350:LEU:HD23	1:B:352:PHE:CZ	2.46	0.51
1:A:115:ALA:HB3	1:A:118:LYS:HZ2	1.75	0.51
1:A:144:ARG:O	1:A:148:GLU:HG3	2.11	0.51
1:D:119:LEU:C	1:D:123:MET:HE2	2.36	0.51
1:B:345:GLU:O	1:B:349:VAL:HG23	2.11	0.50
1:C:80:ARG:HG2	1:C:80:ARG:NH1	2.20	0.50
1:D:104:ARG:HH22	1:D:128:LYS:HG3	1.75	0.50
1:C:83:ILE:CG2	1:C:154:ILE:HD13	2.41	0.50
1:B:194:ILE:HD12	1:B:216:MET:HE3	1.94	0.50
1:B:299:LEU:O	1:B:303:VAL:HG13	2.12	0.50
1:C:119:LEU:O	1:C:123:MET:HG3	2.12	0.50
1:A:132:ILE:HD13	1:B:339:VAL:CG1	2.42	0.49
1:C:203:ILE:O	1:C:207:GLU:HG3	2.11	0.49
1:A:84:CYS:SG	1:A:86:SER:HB3	2.53	0.49
1:A:121:GLN:HG2	1:A:125:TYR:CE2	2.48	0.49
1:B:335:GLU:OE2	1:B:336:PRO:HD2	2.13	0.48
1:C:133:GLN:O	1:D:341:PRO:HD3	2.13	0.48
1:B:339:VAL:HG23	1:B:340:PRO:HD2	1.94	0.48
1:D:350:LEU:HD23	1:D:352:PHE:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LYS:NZ	1:A:118:LYS:HB2	2.29	0.48
1:D:203:ILE:O	1:D:207:GLU:HG3	2.13	0.48
1:A:132:ILE:HD13	1:B:339:VAL:HG13	1.95	0.48
1:A:4:TRP:CE2	1:A:30:ASN:HB2	2.49	0.47
1:C:123:MET:HE1	1:D:334:GLU:O	2.14	0.47
1:D:37:ASP:O	1:D:41:ARG:HG3	2.14	0.47
1:B:340:PRO:CG	1:B:345:GLU:HG2	2.44	0.47
1:B:41:ARG:HG2	1:B:41:ARG:HH11	1.79	0.47
1:C:108:LEU:HD23	1:C:130:LEU:HB2	1.96	0.47
1:C:179:GLU:HG3	1:C:180:ALA:N	2.28	0.47
1:C:339:VAL:CG1	1:D:132:ILE:HD13	2.45	0.47
1:D:347:VAL:HG13	1:D:352:PHE:HB2	1.97	0.47
1:A:215:ARG:NH1	3:A:1176:HOH:O	2.48	0.47
3:A:1301:HOH:O	1:B:32:PRO:HG3	2.14	0.47
1:C:37:ASP:HB3	1:C:41:ARG:HH12	1.80	0.47
1:C:108:LEU:HD12	1:C:143:VAL:HG22	1.97	0.46
1:D:121:GLN:HG2	1:D:125:TYR:CE2	2.50	0.46
1:A:339:VAL:HG23	1:A:340:PRO:HD2	1.96	0.46
1:D:4:TRP:CE2	1:D:30:ASN:HB2	2.50	0.46
1:A:118:LYS:HZ2	1:A:118:LYS:HB2	1.81	0.46
1:C:87:THR:HG22	1:C:109:LEU:CD1	2.45	0.46
1:C:181:PRO:O	1:C:214:PRO:HB3	2.15	0.46
1:D:104:ARG:HH12	1:D:128:LYS:HG2	1.81	0.46
1:D:345:GLU:O	1:D:349:VAL:HG23	2.15	0.46
1:A:183:TYR:HB2	1:A:314:VAL:HG22	1.98	0.46
1:C:256:LYS:NZ	3:C:1179:HOH:O	2.48	0.46
1:C:342:ASP:OD2	1:C:345:GLU:HG2	2.15	0.46
1:D:199:LYS:O	1:D:203:ILE:HG12	2.16	0.46
1:A:142:ILE:O	1:A:146:ILE:HG13	2.14	0.45
1:D:303:VAL:HG23	1:D:304:ARG:N	2.30	0.45
1:A:104:ARG:NH2	1:A:128:LYS:HE2	2.27	0.45
1:B:142:ILE:O	1:B:146:ILE:HG13	2.16	0.45
1:B:303:VAL:HG23	1:B:304:ARG:N	2.30	0.45
1:A:111:LYS:HB2	1:A:111:LYS:NZ	2.26	0.45
1:C:37:ASP:HB3	1:C:41:ARG:NH1	2.30	0.45
1:C:259:GLN:HE21	1:C:259:GLN:HB3	1.63	0.45
1:B:264:LYS:HD2	3:B:1308:HOH:O	2.16	0.45
1:C:121:GLN:HG2	1:C:125:TYR:CE2	2.52	0.45
1:B:41:ARG:HG2	1:B:41:ARG:NH1	2.31	0.45
1:A:199:LYS:O	1:A:203:ILE:HG12	2.17	0.44
1:A:108:LEU:HD23	1:A:130:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ALA:HB1	1:A:214:PRO:HD3	1.98	0.44
1:A:133:GLN:O	1:B:341:PRO:HD3	2.17	0.44
1:A:179:GLU:CG	1:A:180:ALA:N	2.81	0.44
1:B:109:LEU:C	1:B:132:ILE:HG22	2.42	0.44
1:B:237:GLN:O	1:B:238:THR:HB	2.18	0.44
1:A:26:LEU:O	1:A:27:TYR:HB2	2.16	0.44
1:D:339:VAL:HG23	1:D:340:PRO:HD2	2.00	0.44
1:A:163:ILE:HD12	1:A:192:GLY:O	2.18	0.44
1:B:346:VAL:O	1:B:350:LEU:HD13	2.17	0.44
1:C:222:GLU:HG3	1:C:268:VAL:C	2.42	0.44
3:C:1232:HOH:O	1:D:32:PRO:HG3	2.17	0.44
1:D:339:VAL:CG2	1:D:340:PRO:HD2	2.47	0.44
1:A:226:PRO:HB3	1:A:233:ILE:HG12	2.00	0.44
1:B:190:ASN:O	1:B:191:ALA:CB	2.66	0.44
1:A:333:CYS:SG	1:B:120:SER:HA	2.58	0.43
1:A:347:VAL:CG1	1:A:352:PHE:HB2	2.45	0.43
1:C:190:ASN:O	1:C:191:ALA:CB	2.66	0.43
1:B:121:GLN:O	1:B:124:ILE:HG22	2.18	0.43
1:C:350:LEU:CD1	1:C:350:LEU:N	2.82	0.43
1:A:339:VAL:CG2	1:A:340:PRO:HD2	2.49	0.43
1:D:133:GLN:NE2	3:D:1269:HOH:O	2.50	0.43
1:C:352:PHE:CE2	1:D:152:VAL:HG21	2.53	0.43
1:D:7:ILE:HD11	1:D:68:THR:CG2	2.48	0.43
1:A:352:PHE:N	1:A:352:PHE:CD1	2.81	0.43
1:C:352:PHE:N	1:C:352:PHE:HD1	2.16	0.43
1:A:330:ILE:HG23	1:B:116:ILE:HD13	2.01	0.43
1:B:110:PRO:HA	1:B:132:ILE:HG23	2.01	0.42
1:A:256:LYS:O	1:A:260:GLU:HG3	2.19	0.42
1:A:287:PHE:CE1	1:B:124:ILE:HD13	2.54	0.42
1:C:269:SER:OG	1:C:272:GLU:HG3	2.19	0.42
1:C:79:LYS:HG3	1:C:153:GLU:HB2	2.00	0.42
1:D:350:LEU:HD23	1:D:352:PHE:CE2	2.54	0.42
1:A:35[A]:GLU:CD	1:A:35[A]:GLU:H	2.28	0.42
1:C:133:GLN:HG3	1:D:338:THR:HG23	2.02	0.42
1:B:121:GLN:HG2	1:B:125:TYR:CE2	2.55	0.42
1:B:179:GLU:HG3	1:B:180:ALA:H	1.80	0.42
1:D:219:TRP:CE2	1:D:298:GLY:HA3	2.55	0.42
1:A:222:GLU:OE2	3:A:1362:HOH:O	2.22	0.42
1:C:242:ALA:HB3	1:C:291:ALA:CB	2.50	0.41
1:A:345:GLU:O	1:A:348:LYS:HB3	2.18	0.41
1:D:116:ILE:HG13	1:D:123:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ARG:HG2	1:A:144:ARG:HH11	1.85	0.41
1:D:198:TRP:CZ2	1:D:260:GLU:HG2	2.48	0.41
1:C:84:CYS:HB3	1:C:155:VAL:HG23	2.02	0.41
1:C:50:TYR:HB2	1:C:315:THR:HG22	2.03	0.41
1:A:237:GLN:O	1:A:238:THR:HB	2.21	0.41
1:D:36:ALA:HB1	1:D:39:LEU:HB3	2.03	0.41
1:A:292:SER:HB3	1:A:318:LEU:HA	2.03	0.41
1:B:26:LEU:O	1:B:27:TYR:HB2	2.21	0.41
1:B:219:TRP:CE2	1:B:298:GLY:HA3	2.56	0.41
1:C:48:LYS:HD3	3:C:1276:HOH:O	2.20	0.41
1:C:222:GLU:HG3	1:C:268:VAL:O	2.21	0.41
1:D:181:PRO:O	1:D:214:PRO:HG3	2.20	0.41
1:D:220:GLN:OE1	1:D:225:ALA:HA	2.21	0.41
1:B:119:LEU:O	1:B:123:MET:HG3	2.20	0.40
1:D:24:VAL:HG11	1:D:101:ALA:HB2	2.01	0.40
1:B:340:PRO:HG2	1:B:345:GLU:HG2	2.03	0.40
1:A:350:LEU:CD1	1:A:350:LEU:N	2.85	0.40
1:B:350:LEU:N	1:B:350:LEU:HD12	2.36	0.40
1:C:219:TRP:CE2	1:C:298:GLY:HA3	2.56	0.40
1:D:20:ASN:HB2	3:D:1207:HOH:O	2.20	0.40
1:D:41:ARG:NH1	1:D:41:ARG:HG2	2.36	0.40
1:D:119:LEU:O	1:D:123:MET:HG3	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	349/352 (99%)	339 (97%)	9 (3%)	1 (0%)	36 25
1	B	348/352 (99%)	335 (96%)	10 (3%)	3 (1%)	14 5
1	C	349/352 (99%)	337 (97%)	10 (3%)	2 (1%)	21 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	344/352 (98%)	336 (98%)	8 (2%)	0	100	100
All	All	1390/1408 (99%)	1347 (97%)	37 (3%)	6 (0%)	30	19

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	114	VAL
1	B	116	ILE
1	B	238	THR
1	C	238	THR
1	A	238	THR
1	C	116	ILE

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	273/274 (100%)	268 (98%)	5 (2%)	51	43
1	B	272/274 (99%)	272 (100%)	0	100	100
1	C	273/274 (100%)	269 (98%)	4 (2%)	57	49
1	D	271/274 (99%)	270 (100%)	1 (0%)	84	83
All	All	1089/1096 (99%)	1079 (99%)	10 (1%)	73	67

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35[A]	GLU
1	A	35[B]	GLU
1	A	46	LYS
1	A	111	LYS
1	A	289	GLU
1	C	20	ASN
1	C	167	LYS
1	C	259	GLN

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Mol	Chain	Res	Type
1	C	352	PHE
1	D	104	ARG

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

Mol	Chain	Res	Type
1	A	5	GLN
1	A	10	GLN
1	A	30	ASN
1	A	141	ASN
1	A	166	GLN
1	B	5	GLN
1	B	10	GLN
1	B	20	ASN
1	B	133	GLN
1	B	235	ASN
1	B	237	GLN
1	B	247	ASN
1	C	10	GLN
1	C	20	ASN
1	C	247	ASN
1	C	259	GLN
1	D	10	GLN
1	D	20	ASN
1	D	89	ASN
1	D	133	GLN
1	D	166	GLN
1	D	193	ASN
1	D	237	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 [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	C	1103	1	15,15,16	1.44	1 (6%)	21,22,23	1.19	3 (14%)
2	PLP	B	1102	1	15,15,16	1.36	2 (13%)	21,22,23	1.28	4 (19%)
2	PLP	A	1101	1	15,15,16	1.45	1 (6%)	21,22,23	1.19	3 (14%)
2	PLP	D	1104	1	15,15,16	1.50	1 (6%)	21,22,23	1.27	4 (19%)

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	C	1103	1	-	0/6/6/8	0/1/1/1
2	PLP	B	1102	1	-	0/6/6/8	0/1/1/1
2	PLP	A	1101	1	-	0/6/6/8	0/1/1/1
2	PLP	D	1104	1	-	0/6/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	PLP	C5-C4	4.22	1.45	1.40
2	C	1103	PLP	C5-C4	4.18	1.45	1.40
2	D	1104	PLP	C5-C4	4.12	1.45	1.40
2	B	1102	PLP	C5-C4	3.59	1.44	1.40
2	B	1102	PLP	C3-C4	2.02	1.44	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	PLP	C6-N1-C2	2.37	123.50	119.20
2	B	1102	PLP	C6-N1-C2	2.31	123.40	119.20
2	A	1101	PLP	O3P-P-O4P	2.28	112.62	106.67
2	D	1104	PLP	C6-N1-C2	2.22	123.23	119.20
2	D	1104	PLP	O3P-P-O4P	2.22	112.46	106.67
2	B	1102	PLP	C5-C6-N1	-2.21	120.24	123.83
2	C	1103	PLP	C6-N1-C2	2.18	123.15	119.20
2	D	1104	PLP	C5-C6-N1	-2.14	120.34	123.83
2	A	1101	PLP	C5-C6-N1	-2.09	120.42	123.83
2	C	1103	PLP	C5-C6-N1	-2.09	120.43	123.83
2	C	1103	PLP	O3P-P-O4P	2.04	112.00	106.67
2	B	1102	PLP	C5A-C5-C4	-2.03	118.63	122.64
2	B	1102	PLP	C5A-C5-C6	2.03	122.66	119.36
2	D	1104	PLP	C5A-C5-C6	2.00	122.63	119.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	350/352 (99%)	0.53	21 (6%)	27 26	12, 25, 45, 65	1 (0%)
1	B	350/352 (99%)	0.39	17 (4%)	35 33	14, 25, 45, 53	0
1	C	350/352 (99%)	0.48	21 (6%)	27 26	13, 24, 48, 58	1 (0%)
1	D	348/352 (98%)	0.56	13 (3%)	45 45	14, 26, 46, 57	0
All	All	1398/1408 (99%)	0.49	72 (5%)	33 31	12, 25, 46, 65	2 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	352	PHE	4.9
1	B	114	VAL	4.9
1	C	115	ALA	4.6
1	A	352	PHE	4.5
1	D	136	PHE	4.4
1	C	350	LEU	4.0
1	B	115	ALA	3.9
1	B	136	PHE	3.9
1	A	115	ALA	3.5
1	A	351	GLY	3.3
1	C	351	GLY	3.2
1	A	136	PHE	3.2
1	A	336	PRO	3.1
1	C	136	PHE	3.1
1	A	84	CYS	3.1
1	C	333	CYS	3.1
1	A	156	ASN	3.0
1	C	113	ALA	3.0
1	D	352	PHE	2.9
1	A	139	ALA	2.9
1	A	113	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	337	ILE	2.9
1	D	156	ASN	2.8
1	D	343	PHE	2.8
1	A	349	VAL	2.7
1	B	333	CYS	2.7
1	A	114	VAL	2.7
1	B	112	GLY	2.6
1	D	132	ILE	2.6
1	C	131	ALA	2.6
1	A	138	ASP	2.6
1	A	335	GLU	2.6
1	A	350	LEU	2.6
1	C	347	VAL	2.6
1	D	347	VAL	2.6
1	B	109	LEU	2.5
1	B	140	LEU	2.5
1	D	109	LEU	2.5
1	C	20	ASN	2.4
1	D	308	PHE	2.4
1	B	113	ALA	2.4
1	D	307	PHE	2.4
1	C	334	GLU	2.4
1	B	350	LEU	2.4
1	A	179	GLU	2.4
1	C	335	GLU	2.3
1	B	116	ILE	2.3
1	A	142	ILE	2.3
1	C	349	VAL	2.3
1	A	135	THR	2.2
1	D	112	GLY	2.2
1	C	116	ILE	2.2
1	C	114	VAL	2.2
1	B	19	GLU	2.2
1	D	135	THR	2.2
1	D	351	GLY	2.2
1	C	336	PRO	2.2
1	B	132	ILE	2.2
1	B	347	VAL	2.2
1	B	131	ALA	2.2
1	B	306	GLY	2.1
1	A	140	LEU	2.1
1	C	85	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	137	ASP	2.1
1	B	337	ILE	2.1
1	D	336	PRO	2.1
1	A	116	ILE	2.0
1	C	142	ILE	2.0
1	A	208	GLY	2.0
1	B	351	GLY	2.0
1	C	3	ARG	2.0
1	C	156	ASN	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($\text{\AA}^2$)	Q<0.9
2	PLP	A	1101	15/16	0.96	0.07	19,21,23,24	0
2	PLP	B	1102	15/16	0.96	0.07	15,19,21,24	0
2	PLP	D	1104	15/16	0.96	0.07	18,20,23,24	0
2	PLP	C	1103	15/16	0.97	0.06	17,18,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.