



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:35 PM UTC

PDB ID : 3UZO / pdb_00003uzo
Title : Crystal Structures of Branched-Chain Aminotransferase from *Deinococcus radiodurans* Complexes with alpha-Ketoisocaproate and L-Glutamate Suggest Its Radio-Resistance for Catalysis
Authors : Chen, C.D.; Huang, Y.C.; Chuankhayan, P.; Hsieh, Y.C.; Huang, T.F.; Lin, C.H.; Guan, H.H.; Liu, M.Y.; Chang, W.C.; Chen, C.J.
Deposited on : 2011-12-07
Resolution : 2.00 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

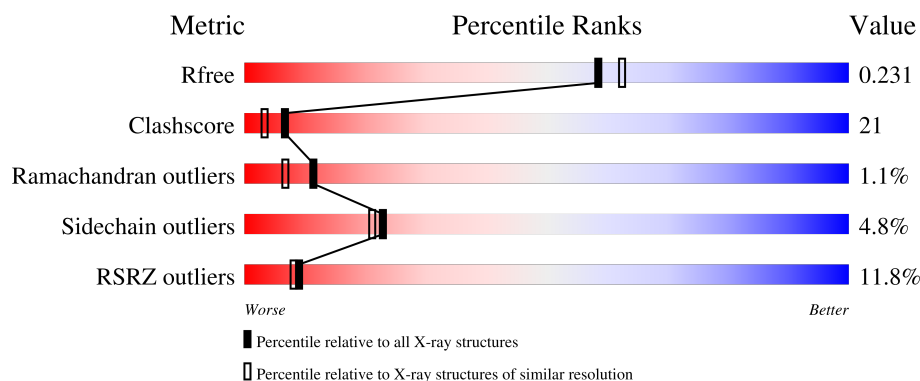
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	358	
1	B	358	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLU	A	600	-	-	X	-
3	GLU	B	500	-	-	X	-

2 Entry composition [i](#)

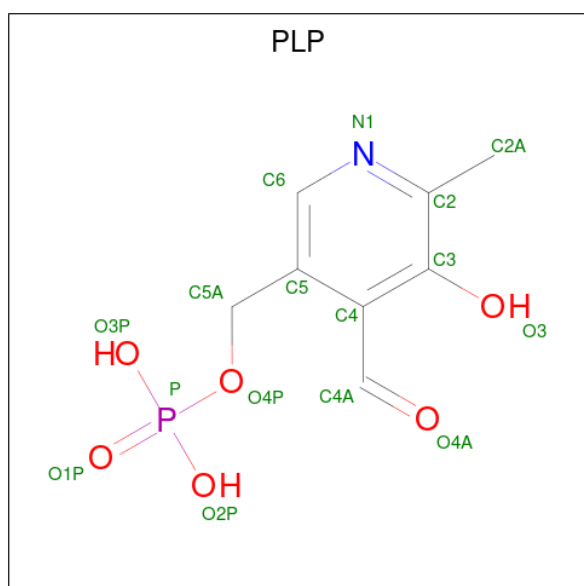
There are 4 unique types of molecules in this entry. The entry contains 5416 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

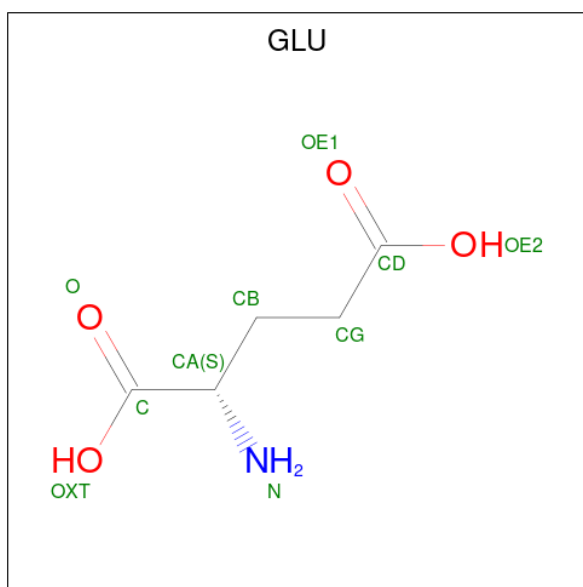
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2605	1662	439	495	9			
1	B	335	Total	C	N	O	S	0	0	0
			2605	1662	439	495	9			

- 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		

- Molecule 3 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	5	1	4		
3	B	1	Total	C	N	O	0	0
			10	5	1	4		

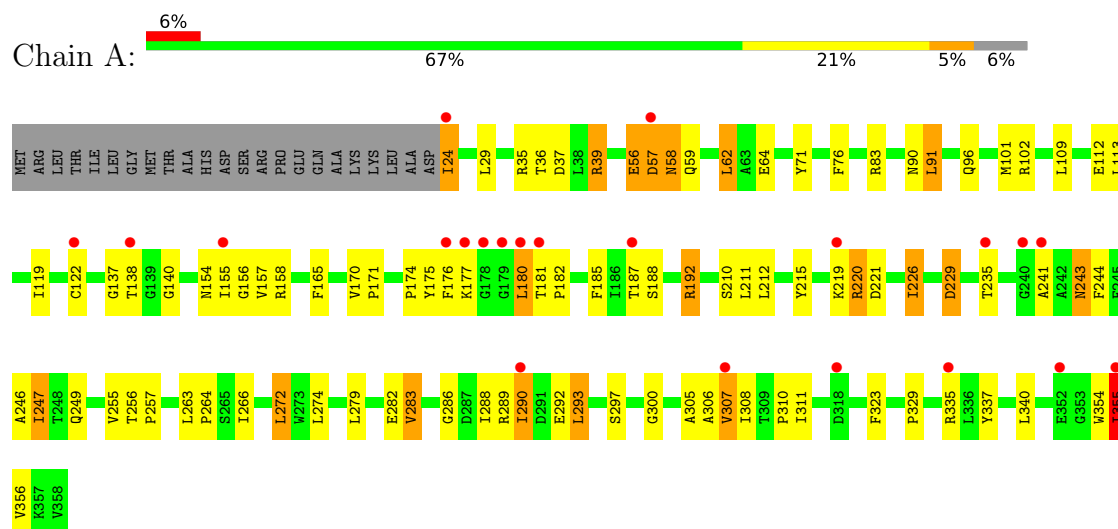
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	111	Total	O	0	0
			111	111		
4	B	45	Total	O	0	0
			45	45		

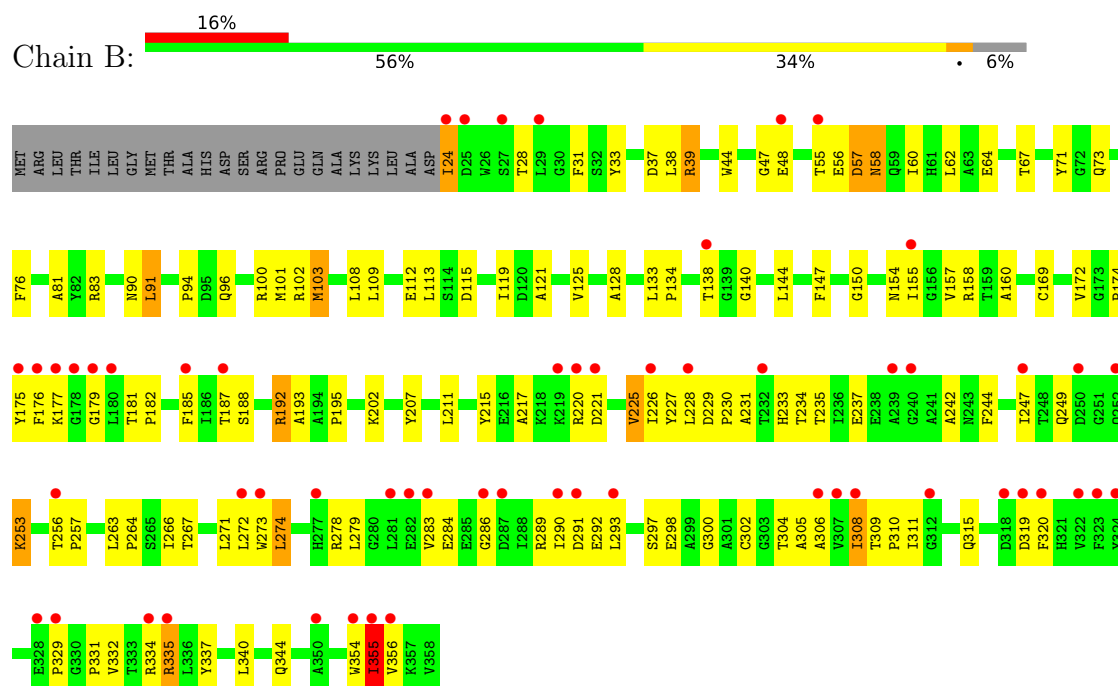
3 Residue-property plots [i](#)

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: Branched-chain-amino-acid aminotransferase



- Molecule 1: Branched-chain-amino-acid aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.88Å 75.98Å 79.12Å 90.00° 105.98° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 99.6 (30.00-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 1.85Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.263 0.228 , 0.231	Depositor DCC
R_{free} test set	2702 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 45.0	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	0.92	EDS
Total number of atoms	5416	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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	0.40	0/2675	0.92	11/3636 (0.3%)
1	B	0.34	0/2675	0.85	7/3636 (0.2%)
All	All	0.37	0/5350	0.88	18/7272 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ASP	N-CA-C	8.10	119.88	111.14
1	B	37	ASP	N-CA-C	7.75	119.64	111.03
1	A	137	GLY	N-CA-C	-6.45	106.24	113.79
1	A	229	ASP	CA-C-N	6.24	125.73	119.24
1	A	229	ASP	C-N-CA	6.24	125.73	119.24
1	B	48	GLU	N-CA-C	6.10	118.57	108.99
1	B	231	ALA	N-CA-C	5.91	117.72	111.28
1	A	91	LEU	N-CA-C	-5.73	99.07	108.41
1	B	229	ASP	CA-C-N	5.64	126.89	119.84
1	B	229	ASP	C-N-CA	5.64	126.89	119.84
1	A	192	ARG	N-CA-C	-5.61	106.60	113.50
1	A	282	GLU	N-CA-C	-5.47	102.38	110.48
1	A	241	ALA	N-CA-C	-5.43	106.13	114.16
1	A	226	ILE	N-CA-C	-5.19	100.27	107.80
1	B	91	LEU	N-CA-C	-5.17	99.99	108.41
1	A	243	ASN	N-CA-C	-5.15	103.88	110.53
1	A	57	ASP	N-CA-C	5.07	121.60	110.80
1	B	192	ARG	N-CA-C	-5.04	106.98	113.23

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	2605	0	2500	94	0
1	B	2605	0	2500	130	0
2	A	15	0	6	0	0
2	B	15	0	6	3	0
3	A	10	0	5	11	0
3	B	10	0	5	11	0
4	A	111	0	0	6	0
4	B	45	0	0	0	0
All	All	5416	0	5022	221	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 21.

All (221) 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:305:ALA:CB	3:A:600:GLU:OE1	1.63	1.47
1:A:305:ALA:HB3	3:A:600:GLU:OE1	0.86	1.02
2:B:372:PLP:C4A	3:B:500:GLU:HG3	1.89	1.02
1:A:220:ARG:HH11	1:A:220:ARG:HB3	1.22	0.98
1:B:154:ASN:HD21	1:B:158:ARG:HH11	1.14	0.95
1:B:228:LEU:O	1:B:237:GLU:HG2	1.69	0.92
1:B:67:THR:HG21	1:B:73:GLN:OE1	1.70	0.91
1:B:304:THR:HB	3:B:500:GLU:OE2	1.72	0.90
1:A:244:PHE:O	1:A:256:THR:HG23	1.74	0.88
1:B:335:ARG:HH11	1:B:335:ARG:HB3	1.42	0.85
1:B:94:PRO:HB2	1:B:119:ILE:HD12	1.56	0.85
1:A:335:ARG:CZ	4:A:450:HOH:O	2.24	0.84
2:B:372:PLP:C4A	3:B:500:GLU:CG	2.56	0.84
1:A:180:LEU:O	1:A:329:PRO:HG3	1.77	0.84
1:B:247:ILE:HD13	1:B:332:VAL:HB	1.59	0.84
1:A:305:ALA:N	3:A:600:GLU:OE2	2.10	0.83
1:A:220:ARG:HB3	1:A:220:ARG:NH1	1.94	0.83
1:B:305:ALA:N	3:B:500:GLU:OE1	2.11	0.83
1:A:305:ALA:HB3	3:A:600:GLU:CD	2.02	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLN:HB3	1:A:266:ILE:HD12	1.60	0.82
1:B:217:ALA:HB2	1:B:225:VAL:HG12	1.63	0.80
1:B:91:LEU:HG	1:B:94:PRO:HG3	1.65	0.78
1:B:102:ARG:HG3	1:B:112:GLU:HB3	1.64	0.77
1:B:154:ASN:ND2	1:B:158:ARG:HH11	1.81	0.77
1:A:305:ALA:CB	3:A:600:GLU:CD	2.58	0.76
1:A:305:ALA:H	3:A:600:GLU:CD	1.93	0.75
1:B:304:THR:CB	3:B:500:GLU:OE2	2.36	0.74
1:A:305:ALA:HB2	3:A:600:GLU:OE1	1.83	0.74
1:B:115:ASP:O	1:B:119:ILE:HG12	1.88	0.73
1:B:257:PRO:HA	1:B:286:GLY:O	1.92	0.70
1:B:185:PHE:HB3	1:B:226:ILE:HG13	1.74	0.69
1:B:96:GLN:HB3	1:B:266:ILE:HD12	1.74	0.69
1:A:192:ARG:HB2	1:A:192:ARG:NH1	2.08	0.69
1:A:335:ARG:NH1	4:A:450:HOH:O	2.27	0.68
1:B:202:LYS:HZ1	3:B:500:GLU:N	1.91	0.68
1:B:267:THR:O	1:B:271:LEU:HD13	1.93	0.68
1:B:228:LEU:O	1:B:237:GLU:CG	2.41	0.68
1:A:289:ARG:HB2	1:A:292:GLU:HG2	1.76	0.67
1:A:354:TRP:O	1:A:355:ILE:HG22	1.94	0.67
1:A:192:ARG:HB2	1:A:192:ARG:HH11	1.60	0.65
1:B:263:LEU:HD12	1:B:264:PRO:HD2	1.79	0.65
1:B:24:ILE:N	1:B:24:ILE:HD13	2.12	0.64
1:A:39:ARG:HD3	1:B:64:GLU:OE1	1.97	0.64
3:A:600:GLU:O	1:B:157:VAL:HG23	1.96	0.64
1:B:228:LEU:HD12	1:B:233:HIS:HB3	1.78	0.64
1:A:24:ILE:HD13	1:A:24:ILE:N	2.13	0.64
1:B:329:PRO:HD2	1:B:334:ARG:HH12	1.63	0.64
1:A:185:PHE:HB3	1:A:226:ILE:HG13	1.80	0.64
1:B:67:THR:HG23	1:B:73:GLN:HB3	1.79	0.63
1:B:244:PHE:O	1:B:256:THR:HG23	1.98	0.63
1:A:180:LEU:HD11	1:A:337:TYR:CD2	2.34	0.62
1:A:247:ILE:HD12	1:A:247:ILE:N	2.15	0.61
1:B:340:LEU:O	1:B:344:GLN:HG3	2.00	0.61
1:A:90:ASN:OD1	1:A:355:ILE:HD11	2.00	0.61
1:B:304:THR:N	3:B:500:GLU:OE2	2.33	0.61
1:A:155:ILE:HG23	1:B:33:TYR:HB2	1.83	0.60
1:A:246:ALA:C	1:A:247:ILE:HD12	2.26	0.60
1:A:156:GLY:H	1:A:158:ARG:HH12	1.47	0.60
1:A:58:ASN:ND2	1:A:59:GLN:HE21	2.00	0.60
1:A:154:ASN:ND2	1:A:158:ARG:HH11	1.99	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ASN:CG	1:A:355:ILE:HD11	2.27	0.59
1:B:315:GLN:HE22	1:B:320:PHE:HB2	1.67	0.59
1:B:71:TYR:CE2	1:B:157:VAL:HG22	2.37	0.59
1:B:60:ILE:HD11	1:B:147:PHE:HZ	1.66	0.58
1:B:55:THR:HG22	1:B:57:ASP:H	1.66	0.58
1:A:101:MET:CE	1:A:113:LEU:HD12	2.34	0.58
1:A:180:LEU:HB3	1:A:329:PRO:CG	2.33	0.58
1:A:355:ILE:HD13	1:A:356:VAL:N	2.18	0.58
1:B:76:PHE:CE1	1:B:202:LYS:HE3	2.38	0.58
1:B:67:THR:CG2	1:B:160:ALA:HB2	2.34	0.57
1:B:289:ARG:HB3	1:B:289:ARG:NH1	2.20	0.57
1:B:60:ILE:HD11	1:B:147:PHE:CZ	2.40	0.57
1:B:329:PRO:HB2	1:B:334:ARG:NH1	2.20	0.57
1:B:28:THR:C	1:B:177:LYS:HZ1	2.13	0.57
1:A:154:ASN:HD21	1:A:158:ARG:HH11	1.53	0.56
1:B:247:ILE:HD13	1:B:332:VAL:CB	2.33	0.56
1:A:255:VAL:HG12	1:A:288:ILE:HD11	1.87	0.56
1:A:212:LEU:HD13	1:A:212:LEU:C	2.30	0.56
1:B:38:LEU:HD12	1:B:128:ALA:HB1	1.88	0.56
1:B:102:ARG:HG2	1:B:112:GLU:OE1	2.05	0.56
1:A:83:ARG:HD2	4:A:376:HOH:O	2.06	0.56
1:B:207:TYR:O	1:B:211:LEU:HD13	2.06	0.56
1:B:247:ILE:CD1	1:B:332:VAL:HB	2.33	0.55
1:B:304:THR:HB	3:B:500:GLU:CD	2.31	0.55
1:B:355:ILE:C	1:B:355:ILE:HD13	2.31	0.55
1:A:180:LEU:HB3	1:A:329:PRO:HG2	1.88	0.55
1:A:58:ASN:HD21	1:A:59:GLN:HE21	1.53	0.55
1:B:355:ILE:HD13	1:B:356:VAL:N	2.21	0.55
1:B:289:ARG:HB2	1:B:292:GLU:HG2	1.88	0.55
1:A:192:ARG:HH11	1:A:192:ARG:CB	2.20	0.54
1:A:257:PRO:HA	1:A:286:GLY:O	2.07	0.54
1:B:306:ALA:HB1	1:B:309:THR:OG1	2.07	0.54
1:A:176:PHE:O	1:A:177:LYS:HB2	2.08	0.54
1:A:102:ARG:HG3	1:A:112:GLU:HB3	1.90	0.53
1:A:306:ALA:O	1:A:307:VAL:C	2.52	0.53
1:B:220:ARG:O	1:B:221:ASP:HB2	2.09	0.53
1:A:71:TYR:CE2	1:A:157:VAL:HG22	2.44	0.53
1:B:179:GLY:O	1:B:181:THR:HG23	2.09	0.53
1:A:177:LYS:HB3	1:A:181:THR:HG21	1.92	0.52
1:B:67:THR:HG22	1:B:160:ALA:HB2	1.91	0.52
1:A:249:GLN:HA	1:A:297:SER:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:THR:O	1:A:39:ARG:NH2	2.32	0.52
1:A:290:ILE:HD12	4:A:411:HOH:O	2.09	0.52
1:B:138:THR:C	1:B:140:GLY:H	2.18	0.52
2:B:372:PLP:C4A	3:B:500:GLU:HG2	2.40	0.52
1:B:44:TRP:CZ2	1:B:47:GLY:HA2	2.45	0.51
1:B:101:MET:CE	1:B:113:LEU:HD12	2.39	0.51
1:B:290:ILE:HA	1:B:293:LEU:HD11	1.91	0.51
1:A:174:PRO:HB2	1:A:177:LYS:O	2.10	0.51
1:A:272:LEU:HD12	1:A:283:VAL:CG2	2.41	0.51
1:A:154:ASN:HD21	1:A:158:ARG:HG2	1.75	0.51
1:B:340:LEU:C	1:B:340:LEU:HD13	2.36	0.51
1:B:300:GLY:HA2	1:B:311:ILE:HG13	1.92	0.51
1:A:62:LEU:HD12	1:A:62:LEU:H	1.76	0.50
1:B:244:PHE:O	1:B:257:PRO:HD2	2.10	0.50
1:B:274:LEU:O	1:B:278:ARG:HB2	2.11	0.50
1:B:182:PRO:HA	1:B:310:PRO:O	2.10	0.50
1:B:100:ARG:O	1:B:103:MET:HG3	2.12	0.50
1:B:249:GLN:HA	1:B:297:SER:HB3	1.94	0.50
1:A:138:THR:C	1:A:140:GLY:H	2.20	0.50
1:B:121:ALA:O	1:B:125:VAL:HG23	2.12	0.50
1:A:62:LEU:HD12	1:A:62:LEU:N	2.27	0.49
1:B:308:ILE:N	1:B:308:ILE:HD12	2.27	0.49
1:B:94:PRO:HB2	1:B:119:ILE:CD1	2.36	0.49
1:A:119:ILE:HA	1:A:122:CYS:SG	2.53	0.49
1:A:256:THR:CG2	1:A:257:PRO:HD2	2.42	0.49
1:B:39:ARG:NH1	1:B:39:ARG:HB3	2.28	0.49
1:A:187:THR:HG22	1:A:188:SER:N	2.27	0.49
1:A:154:ASN:HD21	1:A:158:ARG:CG	2.26	0.48
1:B:192:ARG:NH1	1:B:192:ARG:HB2	2.28	0.48
1:B:185:PHE:CB	1:B:226:ILE:HG13	2.43	0.48
1:A:177:LYS:HB3	1:A:181:THR:CG2	2.43	0.48
1:B:83:ARG:HB2	1:B:133:LEU:HD22	1.94	0.48
1:B:242:ALA:HB1	1:B:302:CYS:O	2.14	0.48
1:A:101:MET:HE3	1:A:113:LEU:HD12	1.96	0.48
1:A:192:ARG:NH1	4:A:435:HOH:O	2.47	0.48
1:B:202:LYS:NZ	3:B:500:GLU:N	2.61	0.48
1:B:305:ALA:CB	3:B:500:GLU:OE1	2.62	0.48
1:B:253:LYS:HB2	1:B:253:LYS:NZ	2.29	0.47
1:A:215:TYR:CZ	1:A:219:LYS:HD3	2.50	0.47
1:A:279:LEU:N	1:A:279:LEU:HD12	2.30	0.47
1:A:64:GLU:OE1	1:B:39:ARG:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:TYR:OH	1:B:155:ILE:O	2.32	0.46
1:B:144:LEU:HD23	1:B:169:CYS:HB3	1.97	0.46
1:B:228:LEU:O	1:B:235:THR:O	2.33	0.46
1:B:290:ILE:C	1:B:290:ILE:HD12	2.39	0.46
1:B:39:ARG:HB3	1:B:39:ARG:CZ	2.46	0.46
1:B:228:LEU:CD2	1:B:290:ILE:HG21	2.44	0.46
1:B:298:GLU:OE1	1:B:331:PRO:HD2	2.16	0.46
1:A:192:ARG:NH1	1:A:210:SER:HB3	2.30	0.46
1:A:247:ILE:N	1:A:247:ILE:CD1	2.79	0.46
1:B:57:ASP:O	1:B:58:ASN:HB3	2.16	0.46
1:B:308:ILE:HB	1:B:337:TYR:HD1	1.80	0.46
1:A:256:THR:HG23	1:A:257:PRO:HD2	1.98	0.45
1:B:315:GLN:NE2	1:B:320:PHE:HB2	2.30	0.45
1:A:180:LEU:HD11	1:A:337:TYR:CE2	2.51	0.45
1:B:247:ILE:HD12	1:B:298:GLU:HG3	1.98	0.45
1:A:340:LEU:HD13	1:A:340:LEU:C	2.42	0.45
1:B:279:LEU:HD12	1:B:279:LEU:N	2.31	0.45
1:B:354:TRP:O	1:B:355:ILE:O	2.34	0.45
1:A:35:ARG:NH2	1:A:57:ASP:O	2.50	0.45
1:B:195:PRO:HG3	1:B:230:PRO:HB2	1.98	0.45
1:B:234:THR:O	1:B:290:ILE:HG13	2.16	0.45
1:A:355:ILE:O	1:A:355:ILE:CG2	2.65	0.44
1:B:175:TYR:HD2	1:B:176:PHE:CE1	2.35	0.44
1:B:289:ARG:HH12	1:B:291:ASP:HB2	1.83	0.44
1:B:91:LEU:O	1:B:355:ILE:HA	2.17	0.44
1:B:354:TRP:O	1:B:355:ILE:HG22	2.18	0.44
1:A:57:ASP:O	1:A:58:ASN:ND2	2.49	0.44
1:A:29:LEU:HD21	1:A:171:PRO:HB2	2.00	0.43
1:A:109:LEU:HD21	1:B:215:TYR:HB2	1.99	0.43
3:A:600:GLU:OXT	1:B:71:TYR:OH	2.30	0.43
1:B:94:PRO:CB	1:B:119:ILE:HD12	2.38	0.43
1:B:133:LEU:HD23	1:B:134:PRO:N	2.33	0.43
1:A:182:PRO:HB3	1:A:310:PRO:HB2	1.99	0.43
1:B:187:THR:HG22	1:B:188:SER:N	2.33	0.43
1:B:193:ALA:O	1:B:230:PRO:HG3	2.18	0.43
1:B:253:LYS:HD3	1:B:284:GLU:HB2	2.00	0.43
1:B:174:PRO:HG2	1:B:177:LYS:HG2	2.00	0.43
1:B:225:VAL:HG22	1:B:227:TYR:CE1	2.53	0.43
1:A:185:PHE:CB	1:A:226:ILE:HG13	2.48	0.43
1:B:24:ILE:N	1:B:24:ILE:CD1	2.82	0.43
1:B:90:ASN:ND2	1:B:355:ILE:HG13	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:GLU:CD	1:A:56:GLU:C	2.87	0.43
1:A:155:ILE:HD11	1:B:31:PHE:C	2.44	0.43
1:A:182:PRO:HA	1:A:310:PRO:O	2.19	0.43
1:A:293:LEU:HG	1:A:323:PHE:CZ	2.53	0.43
1:B:272:LEU:HG	1:B:283:VAL:HG21	2.01	0.43
1:A:220:ARG:O	1:A:221:ASP:HB2	2.19	0.42
1:A:229:ASP:OD1	1:A:235:THR:HG22	2.19	0.42
1:A:91:LEU:HD21	1:A:122:CYS:SG	2.59	0.42
1:B:67:THR:CG2	1:B:150:GLY:HA3	2.50	0.42
1:B:102:ARG:HG3	1:B:112:GLU:CB	2.43	0.42
1:B:228:LEU:C	1:B:235:THR:O	2.63	0.42
1:B:228:LEU:HD22	1:B:290:ILE:HG21	2.02	0.42
1:B:290:ILE:HD12	1:B:291:ASP:N	2.35	0.41
1:B:334:ARG:HG3	1:B:334:ARG:HH11	1.83	0.41
1:A:170:VAL:HG21	1:B:155:ILE:HG21	2.01	0.41
1:B:272:LEU:CD2	1:B:283:VAL:HG21	2.50	0.41
1:A:76:PHE:HE1	3:A:600:GLU:N	2.19	0.41
1:A:300:GLY:HA2	1:A:311:ILE:HG13	2.02	0.41
1:B:335:ARG:HH11	1:B:335:ARG:CB	2.23	0.41
1:A:113:LEU:HD11	1:A:165:PHE:CG	2.56	0.41
1:B:55:THR:HG22	1:B:56:GLU:N	2.35	0.41
1:B:256:THR:HG23	1:B:257:PRO:HD2	2.01	0.41
1:B:256:THR:CG2	1:B:257:PRO:HD2	2.51	0.41
1:B:315:GLN:HE21	1:B:315:GLN:HB2	1.69	0.41
1:A:175:TYR:CD1	1:A:305:ALA:HB1	2.55	0.41
1:B:81:ALA:HA	1:B:90:ASN:O	2.21	0.41
1:B:154:ASN:ND2	1:B:158:ARG:NH1	2.59	0.41
1:B:172:VAL:O	1:B:172:VAL:HG23	2.20	0.41
1:B:57:ASP:O	1:B:58:ASN:CB	2.67	0.41
1:A:263:LEU:HD12	1:A:264:PRO:HD2	2.03	0.41
1:B:108:LEU:O	1:B:109:LEU:HB2	2.20	0.41
1:B:273:TRP:CE3	1:B:274:LEU:HD12	2.56	0.41
1:A:257:PRO:HB3	4:A:365:HOH:O	2.21	0.40
1:A:305:ALA:N	3:A:600:GLU:CD	2.71	0.40
1:B:102:ARG:HD3	1:B:113:LEU:O	2.21	0.40
1:B:67:THR:HG21	1:B:160:ALA:HB2	2.03	0.40
1:A:24:ILE:N	1:A:24:ILE:CD1	2.81	0.40
1:A:355:ILE:O	1:A:355:ILE:HG23	2.20	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	333/358 (93%)	313 (94%)	16 (5%)	4 (1%)	10	6
1	B	333/358 (93%)	302 (91%)	28 (8%)	3 (1%)	14	9
All	All	666/716 (93%)	615 (92%)	44 (7%)	7 (1%)	11	7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	308	ILE
1	B	355	ILE
1	A	180	LEU
1	A	355	ILE
1	A	307	VAL
1	B	57	ASP
1	B	308	ILE

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	270/289 (93%)	255 (94%)	15 (6%)	19	16
1	B	270/289 (93%)	259 (96%)	11 (4%)	27	26
All	All	540/578 (93%)	514 (95%)	26 (5%)	23	21

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ILE
1	A	39	ARG
1	A	56	GLU
1	A	58	ASN
1	A	62	LEU
1	A	211	LEU
1	A	220	ARG
1	A	243	ASN
1	A	247	ILE
1	A	272	LEU
1	A	274	LEU
1	A	283	VAL
1	A	290	ILE
1	A	293	LEU
1	A	355	ILE
1	B	24	ILE
1	B	39	ARG
1	B	58	ASN
1	B	62	LEU
1	B	103	MET
1	B	225	VAL
1	B	253	LYS
1	B	274	LEU
1	B	319	ASP
1	B	335	ARG
1	B	355	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	59	GLN
1	A	154	ASN
1	A	277	HIS
1	A	315	GLN
1	A	321	HIS
1	B	154	ASN
1	B	196	HIS
1	B	277	HIS
1	B	315	GLN
1	B	321	HIS
1	B	344	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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$
3	GLU	A	600	-	8,9,9	1.01	0	8,11,11	0.76	0
2	PLP	A	371	-	15,15,16	2.73	6 (40%)	21,22,23	1.74	9 (42%)
2	PLP	B	372	-	15,15,16	2.85	7 (46%)	21,22,23	1.81	8 (38%)
3	GLU	B	500	-	8,9,9	1.02	0	8,11,11	0.76	0

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	GLU	A	600	-	-	0/9/9/9	-
2	PLP	A	371	-	-	0/6/6/8	0/1/1/1
2	PLP	B	372	-	-	0/6/6/8	0/1/1/1
3	GLU	B	500	-	-	0/9/9/9	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	372	PLP	C5-C4	7.06	1.48	1.40
2	A	371	PLP	C5-C4	6.62	1.48	1.40
2	B	372	PLP	C6-N1	3.79	1.42	1.34
2	A	371	PLP	C4A-C4	3.68	1.59	1.51
2	B	372	PLP	C2-N1	3.61	1.40	1.33
2	A	371	PLP	C2-N1	3.55	1.40	1.33
2	A	371	PLP	C3-C2	3.51	1.44	1.41
2	B	372	PLP	C3-C4	3.50	1.46	1.40
2	A	371	PLP	C6-N1	3.47	1.41	1.34
2	B	372	PLP	C4A-C4	3.42	1.58	1.51
2	B	372	PLP	C3-C2	3.12	1.44	1.41
2	A	371	PLP	C3-C4	2.82	1.45	1.40
2	B	372	PLP	C2A-C2	2.28	1.54	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	372	PLP	O4P-C5A-C5	2.94	114.88	109.36
2	B	372	PLP	C6-N1-C2	2.74	124.17	119.20
2	B	372	PLP	C5A-C5-C6	-2.65	115.04	119.36
2	A	371	PLP	C5-C6-N1	-2.61	119.58	123.83
2	B	372	PLP	C2A-C2-C3	2.60	123.84	120.80
2	A	371	PLP	C6-N1-C2	2.60	123.91	119.20
2	B	372	PLP	C4A-C4-C5	2.59	123.61	120.94
2	B	372	PLP	C5-C6-N1	-2.57	119.65	123.83
2	A	371	PLP	C4A-C4-C5	2.51	123.53	120.94
2	A	371	PLP	C5A-C5-C6	-2.46	115.35	119.36
2	A	371	PLP	C2A-C2-C3	2.46	123.67	120.80
2	B	372	PLP	C3-C2-N1	-2.41	117.92	120.96
2	A	371	PLP	O4P-C5A-C5	2.37	113.80	109.36
2	A	371	PLP	C3-C2-N1	-2.33	118.02	120.96
2	A	371	PLP	O4P-P-O1P	2.19	112.35	106.44
2	A	371	PLP	C6-C5-C4	2.13	119.84	118.10
2	B	372	PLP	O4P-P-O1P	2.04	111.96	106.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	GLU	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	372	PLP	3	0
3	B	500	GLU	11	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	335/358 (93%)	0.19	22 (6%) 24 23	7, 16, 33, 114	0
1	B	335/358 (93%)	0.97	57 (17%) 4 4	9, 28, 55, 105	0
All	All	670/716 (93%)	0.58	79 (11%) 9 8	7, 21, 50, 114	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	176	PHE	8.5
1	B	307	VAL	7.9
1	B	24	ILE	7.4
1	A	178	GLY	6.6
1	A	155	ILE	6.3
1	A	122	CYS	6.1
1	B	178	GLY	5.8
1	B	228	LEU	5.6
1	B	306	ALA	5.3
1	B	355	ILE	5.3
1	B	291	ASP	5.1
1	B	155	ILE	5.0
1	B	318	ASP	4.8
1	A	177	LYS	4.8
1	B	175	TYR	4.6
1	A	240	GLY	4.6
1	B	290	ILE	4.4
1	A	307	VAL	4.2
1	B	308	ILE	4.2
1	B	232	THR	3.9
1	B	29	LEU	3.9
1	B	320	PHE	3.8
1	A	180	LEU	3.8
1	B	220	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	138	THR	3.7
1	B	27	SER	3.6
1	B	283	VAL	3.6
1	A	355	ILE	3.6
1	B	177	LYS	3.6
1	A	24	ILE	3.6
1	B	176	PHE	3.6
1	A	318	ASP	3.5
1	A	290	ILE	3.4
1	B	221	ASP	3.4
1	A	179	GLY	3.4
1	B	272	LEU	3.4
1	A	138	THR	3.4
1	B	179	GLY	3.3
1	B	180	LEU	3.3
1	B	240	GLY	3.3
1	B	256	THR	3.2
1	A	352	GLU	3.2
1	B	329	PRO	3.1
1	A	335	ARG	3.0
1	B	239	ALA	2.9
1	B	226	ILE	2.9
1	B	252	GLN	2.8
1	B	287	ASP	2.8
1	B	334	ARG	2.7
1	B	55	THR	2.7
1	A	187	THR	2.7
1	B	328	GLU	2.6
1	B	187	THR	2.5
1	B	322	VAL	2.5
1	B	219	LYS	2.5
1	A	181	THR	2.5
1	A	219	LYS	2.4
1	B	286	GLY	2.4
1	B	324	TYR	2.4
1	B	247	ILE	2.4
1	B	354	TRP	2.4
1	B	282	GLU	2.4
1	B	185	PHE	2.4
1	B	335	ARG	2.3
1	B	293	LEU	2.3
1	A	235	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	277	HIS	2.3
1	A	241	ALA	2.3
1	B	25	ASP	2.3
1	B	319	ASP	2.3
1	B	323	PHE	2.2
1	B	250	ASP	2.2
1	B	281	LEU	2.1
1	B	48	GLU	2.1
1	A	57	ASP	2.1
1	B	356	VAL	2.1
1	B	312	GLY	2.0
1	B	273	TRP	2.0
1	B	350	ALA	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
3	GLU	B	500	10/10	0.49	0.34	42,80,80,80	0
3	GLU	A	600	10/10	0.65	0.30	25,66,66,66	0
2	PLP	B	372	15/16	0.90	0.12	28,31,34,36	0
2	PLP	A	371	15/16	0.96	0.08	13,16,20,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.