



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:35 PM UTC

PDB ID : 1EKF / pdb_00001ekf
Title : CRYSTALLOGRAPHIC STRUCTURE OF HUMAN BRANCHED CHAIN AMINO ACID AMINOTRANSFERASE (MITOCHONDRIAL) COMPLEXED WITH PYRIDOXAL-5'-PHOSPHATE AT 1.95 ANGSTROMS (ORTHORHOMBIC FORM)
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Deposited on : 2000-03-08
Resolution : 1.95 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

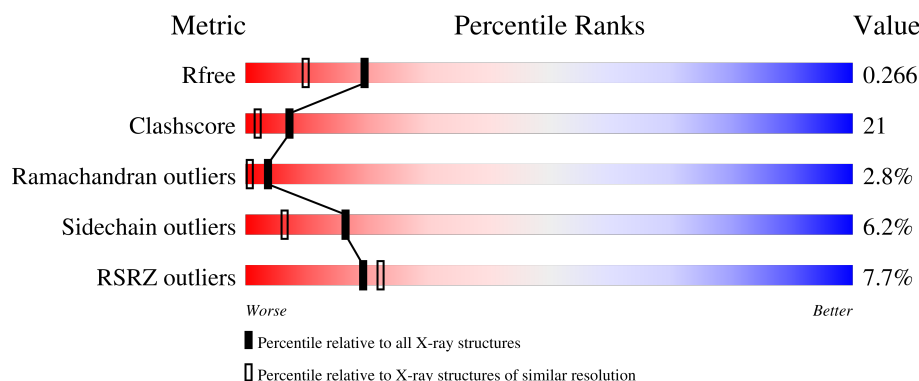
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	365	8% 66% 27% 7%
1	B	365	7% 65% 28% 7%

2 Entry composition [i](#)

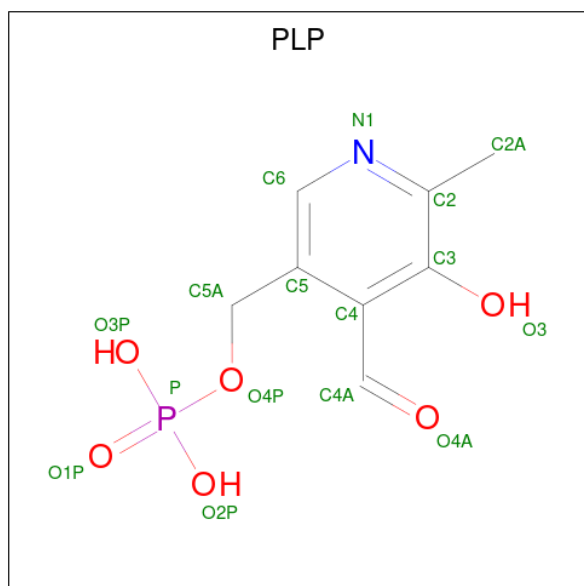
There are 3 unique types of molecules in this entry. The entry contains 6123 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (MITOCHONDRIAL).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2910	1875	507	510	18			
1	B	365	Total	C	N	O	S	0	0	0
			2910	1875	507	510	18			

- 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		

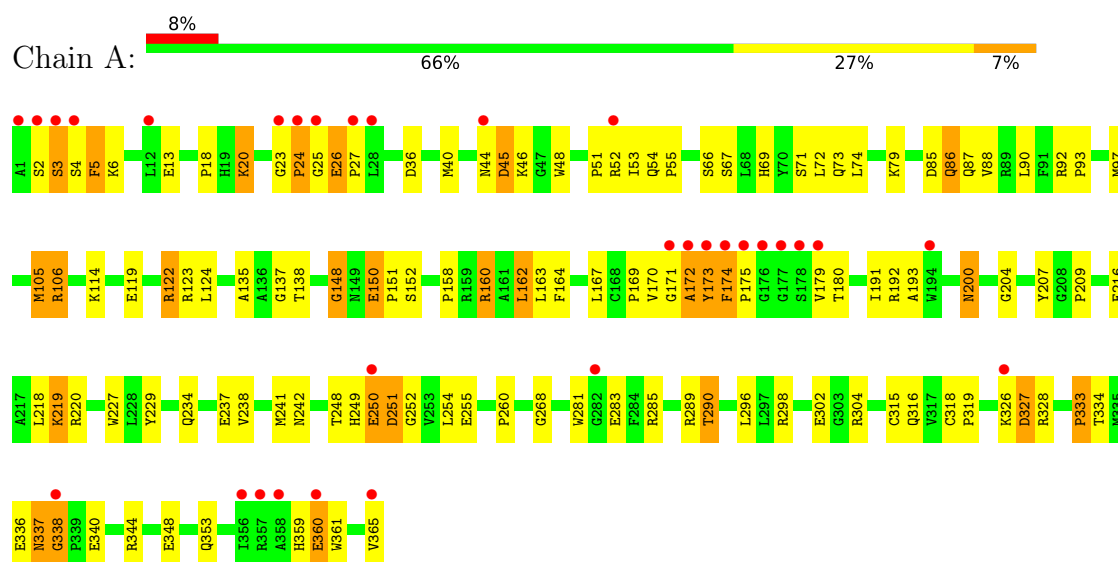
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	143	Total 143	O 143	0	0
3	B	130	Total 130	O 130	0	0

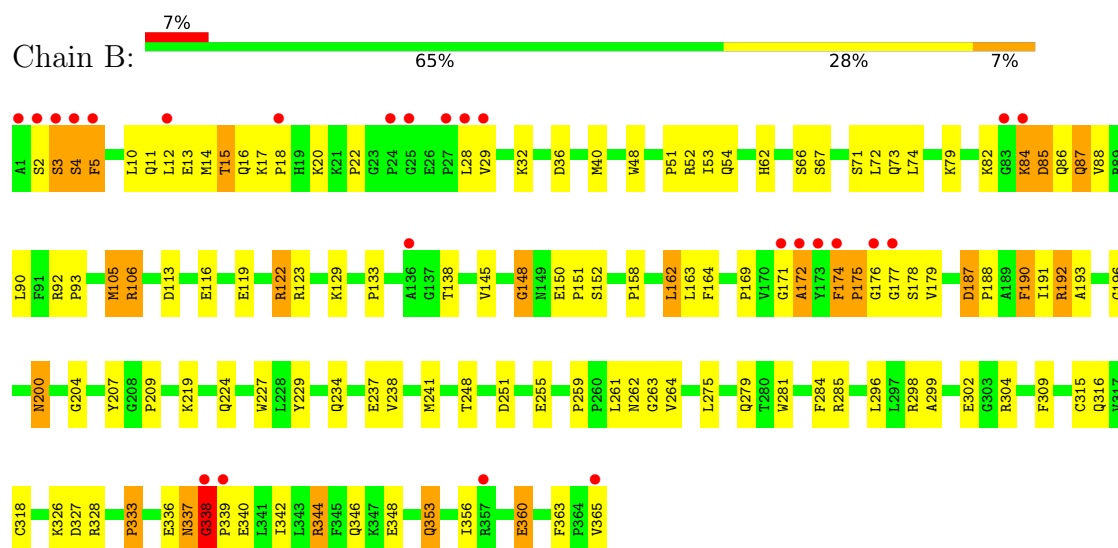
3 Residue-property plots [i](#)

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: BRANCHED CHAIN AMINO ACID AMINOTRANSFERASE (MITOCHONDRIAL)



- Molecule 1: BRANCHED CHAIN AMINO ACID AMINOTRANSFERASE (MITOCHONDRIAL)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.39Å 105.03Å 107.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.29 – 1.95 24.29 – 1.95	Depositor EDS
% Data completeness (in resolution range)	83.8 (24.29-1.95) 90.7 (24.29-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 1.89Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.222 , 0.260 0.231 , 0.266	Depositor DCC
R_{free} test set	4542 reflections (8.16%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6123	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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	0.55	0/2987	1.01	12/4053 (0.3%)
1	B	0.55	1/2987 (0.0%)	1.07	22/4053 (0.5%)
All	All	0.55	1/5974 (0.0%)	1.04	34/8106 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	259	PRO	CA-C	5.10	1.54	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	PHE	N-CA-C	8.38	122.05	111.24
1	B	11	GLN	N-CA-C	-7.87	97.49	110.17
1	A	45	ASP	N-CA-C	-7.67	103.72	113.23
1	B	262	ASN	N-CA-C	-7.59	98.53	109.31
1	B	174	PHE	CA-C-N	7.45	129.16	119.84
1	B	174	PHE	C-N-CA	7.45	129.16	119.84
1	A	148	GLY	N-CA-C	-7.25	102.78	112.14
1	B	259	PRO	CA-C-N	6.87	126.79	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	PRO	C-N-CA	6.87	126.79	119.85
1	B	337	ASN	N-CA-C	-6.83	96.25	110.80
1	B	148	GLY	N-CA-C	-6.65	103.56	112.14
1	A	46	LYS	N-CA-C	-6.59	105.21	113.18
1	B	338	GLY	N-CA-C	-6.46	99.15	112.34
1	A	5	PHE	N-CA-C	6.22	118.81	110.35
1	A	36	ASP	N-CA-C	6.17	118.97	111.82
1	B	36	ASP	N-CA-C	6.11	118.91	111.82
1	A	337	ASN	N-CA-C	-6.00	97.90	108.23
1	B	263	GLY	N-CA-C	5.96	121.38	114.16
1	B	177	GLY	N-CA-C	-5.74	106.06	114.61
1	B	53	ILE	N-CA-C	-5.56	99.87	107.99
1	A	173	TYR	N-CA-C	5.54	122.61	110.80
1	A	302	GLU	N-CA-C	-5.47	105.82	112.88
1	B	353	GLN	N-CA-C	5.45	117.22	111.28
1	A	79	LYS	N-CA-C	5.33	118.24	109.72
1	B	169	PRO	N-CA-C	-5.30	102.26	111.32
1	B	259	PRO	N-CA-C	5.28	115.54	110.47
1	A	53	ILE	N-CA-C	-5.21	100.39	107.99
1	B	187	ASP	CA-C-N	5.20	124.92	119.82
1	B	187	ASP	C-N-CA	5.20	124.92	119.82
1	B	79	LYS	N-CA-C	5.13	117.93	109.72
1	A	6	LYS	N-CA-C	5.13	117.76	109.40
1	A	169	PRO	N-CA-C	-5.09	102.62	111.32
1	B	363	PHE	CA-C-N	5.00	124.91	119.76
1	B	363	PHE	C-N-CA	5.00	124.91	119.76

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	TYR	Sidechain
1	B	207	TYR	Sidechain

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	2910	0	2938	134	0
1	B	2910	0	2938	122	0
2	A	15	0	6	1	0
2	B	15	0	6	1	0
3	A	143	0	0	8	0
3	B	130	0	0	6	0
All	All	6123	0	5888	243	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 (243) 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:160:ARG:HG3	1:A:160:ARG:HH11	1.25	0.99
1:A:150:GLU:HG3	1:A:158:PRO:HA	1.45	0.98
1:A:122:ARG:HG3	1:A:365:VAL:O	1.66	0.96
1:B:200:ASN:H	1:B:200:ASN:HD22	1.11	0.95
1:A:200:ASN:H	1:A:200:ASN:HD22	1.11	0.94
1:B:122:ARG:HG3	1:B:365:VAL:O	1.67	0.93
1:A:26:GLU:N	1:A:27:PRO:HD3	1.91	0.85
1:B:337:ASN:O	1:B:338:GLY:C	2.19	0.84
1:A:338:GLY:O	1:A:340:GLU:N	2.12	0.83
1:B:90:LEU:HB3	1:B:93:PRO:HG3	1.61	0.81
1:A:337:ASN:O	1:A:338:GLY:C	2.23	0.81
1:A:23:GLY:H	1:A:24:PRO:HD3	1.45	0.81
1:A:71:SER:H	1:B:73:GLN:HE22	1.27	0.81
1:A:106:ARG:NH2	1:B:209:PRO:O	2.15	0.80
1:B:3:SER:O	1:B:4:SER:HB2	1.80	0.79
1:B:84:LYS:H	1:B:84:LYS:HD3	1.47	0.78
1:B:122:ARG:HB3	1:B:122:ARG:HH11	1.48	0.78
1:A:90:LEU:HB3	1:A:93:PRO:HG3	1.66	0.78
1:A:219:LYS:HB2	1:A:219:LYS:NZ	1.97	0.77
1:A:85:ASP:O	1:A:86:GLN:HB3	1.82	0.77
1:A:24:PRO:C	1:A:26:GLU:H	1.93	0.77
1:A:122:ARG:HH11	1:A:122:ARG:HB3	1.50	0.75
1:A:160:ARG:HG3	1:A:160:ARG:NH1	1.98	0.75
1:B:10:LEU:HD23	1:B:51:PRO:HB2	1.70	0.74
1:B:264:VAL:HG12	1:B:264:VAL:O	1.86	0.74
1:B:315:CYS:SG	1:B:318:CYS:HB2	2.29	0.72
1:A:20:LYS:NZ	1:A:20:LYS:HB3	2.05	0.71
1:A:365:VAL:HG12	3:A:474:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:LYS:C	1:A:328:ARG:H	1.99	0.70
1:B:84:LYS:HE3	1:B:356:ILE:HD13	1.73	0.70
1:B:73:GLN:HE21	1:B:204:GLY:HA3	1.57	0.69
1:B:20:LYS:HB3	1:B:20:LYS:NZ	2.08	0.69
1:A:52:ARG:NH1	1:A:54:GLN:NE2	2.40	0.69
1:B:52:ARG:NH1	1:B:54:GLN:NE2	2.41	0.68
1:A:73:GLN:HE21	1:A:204:GLY:HA3	1.60	0.67
1:A:315:CYS:SG	1:A:318:CYS:HB2	2.35	0.67
1:A:209:PRO:O	1:B:106:ARG:NH2	2.28	0.67
1:A:73:GLN:HE22	1:B:71:SER:H	1.41	0.66
1:A:152:SER:HB2	1:B:32:LYS:HD3	1.78	0.66
1:B:52:ARG:HH11	1:B:54:GLN:NE2	1.94	0.66
1:A:105:MET:HE3	1:A:105:MET:HA	1.77	0.66
1:A:52:ARG:HH11	1:A:54:GLN:NE2	1.94	0.65
1:B:20:LYS:HB3	1:B:20:LYS:HZ3	1.60	0.65
1:B:326:LYS:C	1:B:328:ARG:H	2.02	0.65
1:A:191:ILE:HD11	1:A:193:ALA:O	1.96	0.65
1:B:105:MET:HE3	1:B:105:MET:HA	1.78	0.65
1:B:298:ARG:HD3	1:B:302:GLU:OE2	1.97	0.64
1:B:192:ARG:HH12	1:B:193:ALA:HB3	1.62	0.64
1:B:122:ARG:CG	1:B:365:VAL:O	2.44	0.64
1:A:191:ILE:HG22	1:B:196:GLY:O	1.98	0.63
1:B:192:ARG:HH11	1:B:192:ARG:HB3	1.61	0.63
1:B:275:LEU:O	1:B:279:GLN:HG3	1.99	0.63
1:B:238:VAL:HG23	1:B:241:MET:HE3	1.81	0.63
1:A:359:HIS:HD2	1:A:361:TRP:H	1.46	0.62
1:B:200:ASN:HD22	1:B:200:ASN:N	1.89	0.62
1:B:316:GLN:HE22	1:B:353:GLN:HE22	1.46	0.62
1:B:2:SER:HB3	3:B:493:HOH:O	1.99	0.62
1:B:4:SER:HB3	1:B:48:TRP:HD1	1.63	0.62
1:B:238:VAL:HG23	1:B:238:VAL:O	1.99	0.62
1:A:200:ASN:HD22	1:A:200:ASN:N	1.89	0.61
1:A:249:HIS:CD2	1:A:250:GLU:H	2.18	0.61
1:A:337:ASN:O	1:A:338:GLY:O	2.18	0.61
1:A:179:VAL:HG12	1:A:179:VAL:O	2.00	0.61
1:A:344:ARG:HD2	3:A:479:HOH:O	2.00	0.61
1:B:200:ASN:H	1:B:200:ASN:ND2	1.91	0.61
1:B:255:GLU:OE1	1:B:285:ARG:HD2	2.00	0.61
1:A:175:PRO:HB3	1:A:180:THR:HG23	1.82	0.61
1:B:338:GLY:O	1:B:340:GLU:N	2.29	0.61
1:B:299:ALA:HA	1:B:304:ARG:NH1	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ARG:CG	1:A:365:VAL:O	2.44	0.60
1:A:71:SER:N	1:B:73:GLN:HE22	2.00	0.60
1:B:138:THR:HA	1:B:171:GLY:O	2.02	0.59
1:A:23:GLY:N	1:A:24:PRO:HD3	2.15	0.59
1:A:24:PRO:HB2	1:A:27:PRO:CD	2.33	0.59
1:A:238:VAL:HG23	1:A:241:MET:HE3	1.84	0.59
1:A:326:LYS:C	1:A:328:ARG:N	2.60	0.59
1:A:216:GLU:HA	1:A:219:LYS:HG2	1.84	0.58
1:A:122:ARG:HH11	1:A:122:ARG:CB	2.15	0.58
1:A:219:LYS:HB2	1:A:219:LYS:HZ3	1.67	0.58
1:B:12:LEU:HD21	1:B:14:MET:SD	2.44	0.58
1:B:251:ASP:OD2	1:B:285:ARG:NH2	2.35	0.58
1:B:122:ARG:HH11	1:B:122:ARG:CB	2.15	0.57
1:A:316:GLN:HE22	1:A:353:GLN:HE22	1.51	0.57
1:B:138:THR:HG22	1:B:171:GLY:O	2.03	0.57
1:B:82:LYS:HD3	1:B:86:GLN:NE2	2.19	0.57
1:A:26:GLU:N	1:A:27:PRO:CD	2.67	0.57
1:A:238:VAL:HG23	1:A:238:VAL:O	2.03	0.57
1:A:250:GLU:C	1:A:252:GLY:H	2.13	0.57
1:A:105:MET:HA	1:A:105:MET:CE	2.35	0.56
1:A:150:GLU:HG3	1:A:158:PRO:CA	2.29	0.56
1:A:137:GLY:O	1:A:172:ALA:HB2	2.04	0.56
1:B:174:PHE:HB3	1:B:178:SER:HB2	1.88	0.56
1:A:20:LYS:HB3	1:A:20:LYS:HZ3	1.70	0.56
1:A:163:LEU:HD23	1:A:163:LEU:C	2.31	0.55
1:B:15:THR:HG21	1:B:18:PRO:HG3	1.89	0.55
1:B:105:MET:HA	1:B:105:MET:CE	2.36	0.55
1:B:264:VAL:O	1:B:264:VAL:CG1	2.53	0.55
1:A:304:ARG:NH2	3:A:398:HOH:O	2.40	0.55
1:B:22:PRO:HB3	1:B:28:LEU:HD22	1.89	0.55
1:A:24:PRO:C	1:A:26:GLU:N	2.62	0.55
1:B:337:ASN:C	1:B:338:GLY:O	2.49	0.54
1:A:23:GLY:N	1:A:24:PRO:CD	2.71	0.54
1:B:326:LYS:C	1:B:328:ARG:N	2.64	0.54
1:A:86:GLN:C	1:A:86:GLN:CD	2.76	0.53
1:B:163:LEU:C	1:B:163:LEU:HD23	2.34	0.53
1:A:4:SER:HA	1:A:48:TRP:HD1	1.74	0.53
1:A:283:GLU:CD	1:A:344:ARG:HH22	2.17	0.53
1:B:3:SER:O	1:B:4:SER:CB	2.55	0.53
1:A:71:SER:H	1:B:73:GLN:NE2	2.03	0.52
1:A:180:THR:HG21	3:A:457:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LEU:HD13	1:B:158:PRO:HG3	1.91	0.52
1:A:333:PRO:HA	1:A:336:GLU:OE1	2.09	0.52
1:A:200:ASN:H	1:A:200:ASN:ND2	1.91	0.52
1:B:66:SER:HB2	1:B:72:LEU:HD12	1.92	0.52
1:B:192:ARG:HB2	1:B:227:TRP:CE3	2.45	0.51
1:A:179:VAL:HG12	1:A:319:PRO:HG2	1.92	0.51
1:B:333:PRO:HA	1:B:336:GLU:OE1	2.09	0.51
1:A:72:LEU:HD13	1:A:158:PRO:HG3	1.93	0.51
1:A:2:SER:O	1:A:3:SER:C	2.53	0.51
1:B:88:VAL:O	1:B:365:VAL:N	2.44	0.51
1:B:187:ASP:HB3	1:B:190:PHE:CE1	2.46	0.51
1:B:85:ASP:CG	1:B:87:GLN:HB2	2.36	0.51
1:A:66:SER:HB2	1:A:72:LEU:HD12	1.93	0.50
1:A:92:ARG:N	1:A:93:PRO:HD3	2.26	0.50
1:A:249:HIS:HD2	3:A:398:HOH:O	1.93	0.50
1:A:337:ASN:C	1:A:338:GLY:O	2.53	0.50
1:A:238:VAL:HG23	1:A:241:MET:HB2	1.92	0.50
1:A:13:GLU:O	1:A:55:PRO:HD3	2.12	0.50
1:B:229:TYR:O	1:B:234:GLN:HG2	2.12	0.50
1:B:92:ARG:N	1:B:93:PRO:HD3	2.27	0.50
1:B:40:MET:SD	1:B:162:LEU:HD11	2.51	0.49
1:A:229:TYR:O	1:A:234:GLN:HG2	2.11	0.49
1:A:260:PRO:HD3	1:A:289:ARG:C	2.36	0.49
1:A:326:LYS:O	1:A:327:ASP:HB2	2.13	0.49
1:B:84:LYS:C	1:B:86:GLN:H	2.19	0.49
1:A:255:GLU:HB3	1:A:285:ARG:HD2	1.94	0.49
1:A:219:LYS:HB2	1:A:219:LYS:HZ2	1.75	0.49
1:B:105:MET:HE3	1:B:105:MET:CA	2.43	0.49
1:B:122:ARG:NH2	3:B:431:HOH:O	2.46	0.49
1:A:191:ILE:CG2	1:B:196:GLY:O	2.61	0.49
1:B:192:ARG:HB2	1:B:227:TRP:CD2	2.48	0.48
1:B:342:ILE:O	1:B:346:GLN:HG3	2.13	0.48
1:A:250:GLU:C	1:A:250:GLU:CD	2.80	0.48
1:B:192:ARG:HH11	1:B:192:ARG:CB	2.25	0.48
1:B:15:THR:CG2	1:B:18:PRO:HG3	2.42	0.48
1:B:150:GLU:HG3	1:B:152:SER:HB3	1.94	0.48
1:A:151:PRO:HD3	1:A:160:ARG:HD2	1.96	0.48
1:A:289:ARG:HG2	1:A:290:THR:N	2.27	0.48
1:A:250:GLU:HG2	1:A:298:ARG:HH12	1.78	0.48
1:B:309:PHE:HB3	1:B:342:ILE:HD11	1.95	0.48
1:A:40:MET:SD	1:A:162:LEU:HD11	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:MET:HE3	1:A:105:MET:CA	2.43	0.47
1:A:359:HIS:CD2	1:A:361:TRP:H	2.30	0.47
1:B:17:LYS:HD2	1:B:17:LYS:O	2.14	0.47
1:B:67:SER:HB3	1:B:148:GLY:O	2.15	0.47
1:B:337:ASN:O	1:B:338:GLY:O	2.31	0.47
1:B:171:GLY:O	1:B:172:ALA:HB2	2.13	0.47
1:B:22:PRO:HB3	1:B:28:LEU:CD2	2.44	0.47
1:A:174:PHE:H	1:A:175:PRO:HD2	1.79	0.47
1:A:281:TRP:CH2	1:A:344:ARG:HG2	2.50	0.47
1:B:90:LEU:CB	1:B:93:PRO:HG3	2.40	0.47
1:A:25:GLY:N	1:A:27:PRO:HD3	2.29	0.47
1:B:281:TRP:CH2	1:B:344:ARG:HG2	2.49	0.47
1:A:4:SER:HA	1:A:48:TRP:CD1	2.49	0.47
1:B:72:LEU:HD13	1:B:158:PRO:CG	2.44	0.47
1:A:124:LEU:HG	1:A:167:LEU:HD11	1.98	0.46
1:A:338:GLY:C	1:A:340:GLU:N	2.72	0.46
1:B:238:VAL:HG23	1:B:241:MET:HB2	1.97	0.46
1:A:135:ALA:HB3	1:A:138:THR:HG21	1.97	0.46
1:A:237:GLU:OE1	2:A:370:PLP:N1	2.48	0.46
1:B:192:ARG:HH12	1:B:193:ALA:CB	2.27	0.46
1:A:72:LEU:HD13	1:A:158:PRO:CG	2.46	0.46
1:A:85:ASP:O	1:A:86:GLN:CB	2.57	0.46
1:B:224:GLN:HE21	1:B:224:GLN:HB3	1.59	0.45
1:B:133:PRO:HB2	1:B:138:THR:OG1	2.16	0.45
1:A:334:THR:O	1:A:337:ASN:O	2.34	0.45
1:B:123:ARG:NH1	1:B:123:ARG:HB3	2.31	0.45
1:B:192:ARG:NH1	3:B:389:HOH:O	2.49	0.45
1:A:250:GLU:C	1:A:252:GLY:N	2.72	0.45
1:A:45:ASP:HA	3:A:507:HOH:O	2.17	0.45
1:B:29:VAL:HB	1:B:32:LYS:HG3	1.97	0.45
1:B:187:ASP:HA	1:B:188:PRO:HD3	1.85	0.45
1:A:69:HIS:CE1	1:B:145:VAL:HG21	2.52	0.44
1:A:365:VAL:O	1:A:365:VAL:HG23	2.17	0.44
1:B:174:PHE:CE1	1:B:179:VAL:HA	2.52	0.44
1:A:218:LEU:C	1:A:220:ARG:N	2.75	0.44
1:A:191:ILE:O	1:A:191:ILE:HG23	2.17	0.44
1:A:336:GLU:CD	1:A:336:GLU:H	2.26	0.44
1:A:67:SER:HB3	1:A:148:GLY:O	2.16	0.44
1:A:170:VAL:HG12	1:A:171:GLY:N	2.32	0.44
1:B:338:GLY:C	1:B:340:GLU:H	2.21	0.44
1:A:192:ARG:HB2	1:A:227:TRP:CE3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:GLU:HG3	3:A:479:HOH:O	2.18	0.43
1:B:174:PHE:CD1	1:B:179:VAL:HA	2.53	0.43
1:A:122:ARG:HH11	1:A:122:ARG:CG	2.31	0.43
1:B:237:GLU:OE1	2:B:370:PLP:N1	2.51	0.43
1:A:250:GLU:O	1:A:252:GLY:N	2.52	0.43
1:B:40:MET:HG2	1:B:52:ARG:HH12	1.83	0.43
1:B:316:GLN:NE2	1:B:353:GLN:HE22	2.14	0.43
1:A:218:LEU:HD12	3:A:492:HOH:O	2.19	0.43
1:A:251:ASP:OD1	1:A:285:ARG:NH2	2.39	0.43
1:B:336:GLU:CD	1:B:336:GLU:H	2.26	0.43
1:B:238:VAL:O	1:B:238:VAL:CG2	2.67	0.43
1:A:90:LEU:CB	1:A:93:PRO:HG3	2.44	0.42
1:A:191:ILE:CG2	1:B:196:GLY:C	2.92	0.42
1:A:360:GLU:O	1:A:360:GLU:OE1	2.37	0.42
1:A:163:LEU:HD23	1:A:164:PHE:N	2.34	0.42
1:B:163:LEU:HD23	1:B:164:PHE:N	2.33	0.42
1:B:304:ARG:NH2	3:B:489:HOH:O	2.52	0.42
1:B:326:LYS:O	1:B:328:ARG:N	2.52	0.42
1:A:123:ARG:NH1	1:A:123:ARG:HB3	2.34	0.42
1:A:336:GLU:CD	1:A:336:GLU:N	2.77	0.42
1:B:84:LYS:H	1:B:84:LYS:CD	2.20	0.42
1:A:25:GLY:C	1:A:27:PRO:HD3	2.42	0.42
1:B:360:GLU:OE1	1:B:360:GLU:O	2.38	0.42
1:A:44:ASN:HB3	1:A:45:ASP:H	1.67	0.41
1:A:71:SER:N	1:B:73:GLN:NE2	2.66	0.41
1:B:122:ARG:HH12	1:B:123:ARG:HG2	1.84	0.41
1:A:250:GLU:O	1:A:250:GLU:OE1	2.37	0.41
1:A:88:VAL:O	1:A:365:VAL:N	2.51	0.41
1:B:12:LEU:HD23	1:B:13:GLU:N	2.35	0.41
1:B:14:MET:O	1:B:15:THR:O	2.37	0.41
1:B:176:GLY:C	1:B:178:SER:N	2.75	0.41
1:B:284:PHE:HA	3:B:406:HOH:O	2.19	0.41
1:A:218:LEU:C	1:A:220:ARG:H	2.28	0.41
1:A:242:ASN:ND2	1:A:268:GLY:HA3	2.35	0.41
1:A:97:MET:HB3	1:A:114:LYS:HB3	2.02	0.41
1:A:122:ARG:HH12	1:A:123:ARG:HG2	1.85	0.41
1:A:248:THR:HA	1:A:254:LEU:HA	2.03	0.41
1:B:365:VAL:O	1:B:365:VAL:HG23	2.21	0.41
1:A:5:PHE:HB2	1:A:51:PRO:HG3	2.02	0.41
1:A:40:MET:HG2	1:A:52:ARG:HH12	1.86	0.41
1:A:73:GLN:NE2	1:B:71:SER:H	2.13	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:SER:O	1:B:3:SER:O	2.38	0.41
1:A:122:ARG:HH12	1:A:123:ARG:CD	2.34	0.40
1:B:62:HIS:CD2	1:B:151:PRO:HB3	2.57	0.40
1:B:336:GLU:CD	1:B:336:GLU:N	2.79	0.40
1:A:85:ASP:CG	1:A:87:GLN:HB2	2.47	0.40
1:A:283:GLU:OE1	1:A:344:ARG:NH2	2.55	0.40
1:B:122:ARG:HH12	1:B:123:ARG:CD	2.34	0.40
1:B:113:ASP:HB3	1:B:116:GLU:CG	2.52	0.40
1:B:264:VAL:HG12	3:B:389:HOH:O	2.21	0.40
1:B:281:TRP:NE1	1:B:348:GLU:OE2	2.53	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	363/365 (100%)	335 (92%)	19 (5%)	9 (2%)	4	1
1	B	363/365 (100%)	329 (91%)	23 (6%)	11 (3%)	3	0
All	All	726/730 (100%)	664 (92%)	42 (6%)	20 (3%)	4	1

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	24	PRO
1	A	173	TYR
1	B	3	SER
1	B	4	SER
1	B	15	THR
1	A	338	GLY
1	B	172	ALA

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Mol	Chain	Res	Type
1	A	174	PHE
1	A	251	ASP
1	B	5	PHE
1	B	175	PRO
1	B	85	ASP
1	A	18	PRO
1	A	172	ALA
1	B	191	ILE
1	A	333	PRO
1	B	333	PRO
1	B	339	PRO
1	B	338	GLY

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	316/316 (100%)	298 (94%)	18 (6%)	18	8
1	B	316/316 (100%)	295 (93%)	21 (7%)	15	5
All	All	632/632 (100%)	593 (94%)	39 (6%)	16	6

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	26	GLU
1	A	74	LEU
1	A	86	GLN
1	A	105	MET
1	A	106	ARG
1	A	119	GLU
1	A	122	ARG
1	A	150	GLU
1	A	160	ARG
1	A	162	LEU

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Mol	Chain	Res	Type
1	A	200	ASN
1	A	219	LYS
1	A	250	GLU
1	A	290	THR
1	A	296	LEU
1	A	327	ASP
1	A	360	GLU
1	B	5	PHE
1	B	16	GLN
1	B	74	LEU
1	B	84	LYS
1	B	87	GLN
1	B	105	MET
1	B	106	ARG
1	B	119	GLU
1	B	122	ARG
1	B	129	LYS
1	B	162	LEU
1	B	175	PRO
1	B	192	ARG
1	B	200	ASN
1	B	219	LYS
1	B	248	THR
1	B	261	LEU
1	B	296	LEU
1	B	327	ASP
1	B	344	ARG
1	B	360	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	50	GLN
1	A	54	GLN
1	A	57	GLN
1	A	73	GLN
1	A	86	GLN
1	A	200	ASN
1	A	206	ASN
1	A	215	GLN
1	A	224	GLN

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Mol	Chain	Res	Type
1	A	234	GLN
1	A	249	HIS
1	A	279	GLN
1	A	321	HIS
1	A	353	GLN
1	A	359	HIS
1	B	19	HIS
1	B	54	GLN
1	B	57	GLN
1	B	73	GLN
1	B	86	GLN
1	B	87	GLN
1	B	200	ASN
1	B	206	ASN
1	B	215	GLN
1	B	224	GLN
1	B	234	GLN
1	B	331	HIS
1	B	337	ASN
1	B	353	GLN

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 [i](#)

2 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	B	370	1	15,15,16	1.60	2 (13%)	21,22,23	1.79	6 (28%)
2	PLP	A	370	1	15,15,16	1.67	2 (13%)	21,22,23	1.87	8 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	B	370	1	-	0/6/6/8	0/1/1/1
2	PLP	A	370	1	-	0/6/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	370	PLP	C5-C4	3.44	1.44	1.40
2	A	370	PLP	C4A-C4	3.00	1.57	1.51
2	B	370	PLP	C5-C4	2.95	1.43	1.40
2	B	370	PLP	C4A-C4	2.65	1.56	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	370	PLP	O2P-P-O4P	-3.52	97.48	106.67
2	A	370	PLP	O4P-C5A-C5	3.42	115.76	109.36
2	A	370	PLP	O2P-P-O4P	-3.28	98.12	106.67
2	B	370	PLP	O4P-C5A-C5	3.27	115.48	109.36
2	A	370	PLP	C4A-C4-C5	3.16	124.20	120.94
2	B	370	PLP	C4A-C4-C5	2.85	123.88	120.94
2	A	370	PLP	C5A-C5-C6	-2.66	115.02	119.36
2	B	370	PLP	O3P-P-O1P	2.27	119.68	110.83
2	A	370	PLP	O4P-P-O1P	2.25	112.52	106.44
2	B	370	PLP	O4P-P-O1P	2.19	112.35	106.44
2	A	370	PLP	O3P-P-O1P	2.17	119.29	110.83
2	A	370	PLP	C5-C6-N1	-2.15	120.34	123.83
2	B	370	PLP	C5A-C5-C6	-2.09	115.96	119.36
2	A	370	PLP	C6-N1-C2	2.06	122.93	119.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	370	PLP	1	0
2	A	370	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	365/365 (100%)	0.47	31 (8%)	16 19	18, 30, 53, 73	0
1	B	365/365 (100%)	0.55	25 (6%)	23 27	17, 33, 55, 69	0
All	All	730/730 (100%)	0.51	56 (7%)	19 22	17, 32, 54, 73	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	PRO	8.3
1	A	173	TYR	6.2
1	A	174	PHE	5.9
1	A	177	GLY	5.6
1	A	24	PRO	5.4
1	B	338	GLY	5.2
1	B	3	SER	4.8
1	B	24	PRO	4.7
1	A	338	GLY	4.5
1	A	358	ALA	4.5
1	A	178	SER	4.3
1	B	84	LYS	4.3
1	B	173	TYR	4.1
1	A	179	VAL	4.0
1	B	25	GLY	4.0
1	B	1	ALA	3.9
1	A	172	ALA	3.7
1	B	83	GLY	3.7
1	B	171	GLY	3.5
1	B	27	PRO	3.5
1	B	28	LEU	3.3
1	A	2	SER	3.3
1	A	365	VAL	3.1
1	A	23	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1	ALA	3.0
1	A	25	GLY	3.0
1	B	339	PRO	3.0
1	B	365	VAL	2.9
1	B	5	PHE	2.9
1	A	3	SER	2.8
1	B	174	PHE	2.8
1	A	28	LEU	2.7
1	B	12	LEU	2.7
1	A	357	ARG	2.7
1	A	52	ARG	2.6
1	A	250	GLU	2.6
1	A	4	SER	2.6
1	A	27	PRO	2.4
1	A	176	GLY	2.4
1	B	172	ALA	2.3
1	A	44	ASN	2.3
1	B	2	SER	2.2
1	B	4	SER	2.2
1	B	29	VAL	2.2
1	A	12	LEU	2.2
1	A	171	GLY	2.2
1	B	136	ALA	2.2
1	A	282	GLY	2.1
1	A	356	ILE	2.1
1	B	177	GLY	2.1
1	A	326	LYS	2.1
1	B	176	GLY	2.1
1	A	360	GLU	2.0
1	A	194	TRP	2.0
1	B	18	PRO	2.0
1	B	357	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	PLP	A	370	15/16	0.97	0.06	17,24,32,33	0
2	PLP	B	370	15/16	0.98	0.06	17,25,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.