



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:36 am GMT

PDB ID : 1ASM
Title : CRYSTAL STRUCTURES OF ESCHERICHIA COLI ASPARTATE AMINO-TRANSFERASE IN TWO CONFORMATIONS: COMPARISON OF AN UNLIGANDED OPEN AND TWO LIGANDED CLOSED FORMS
Authors : Jaeger, J.; Jansonius, J.N.
Deposited on : 1993-09-16
Resolution : 2.35 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

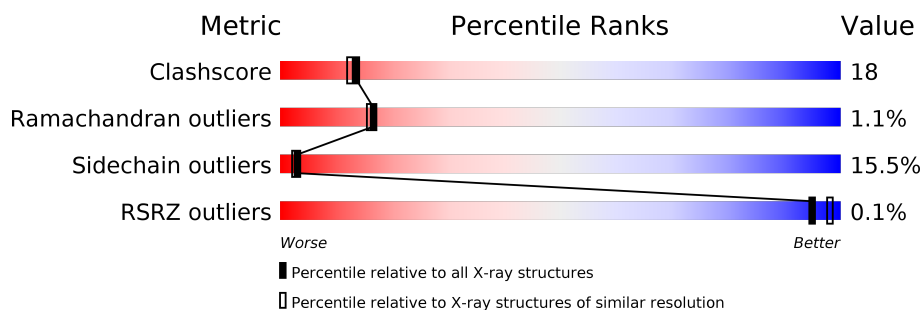
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	396	
1	B	396	

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
2	PLP	A	410	-	-	-	X
3	MAE	A	411	-	-	-	X

2 Entry composition [i](#)

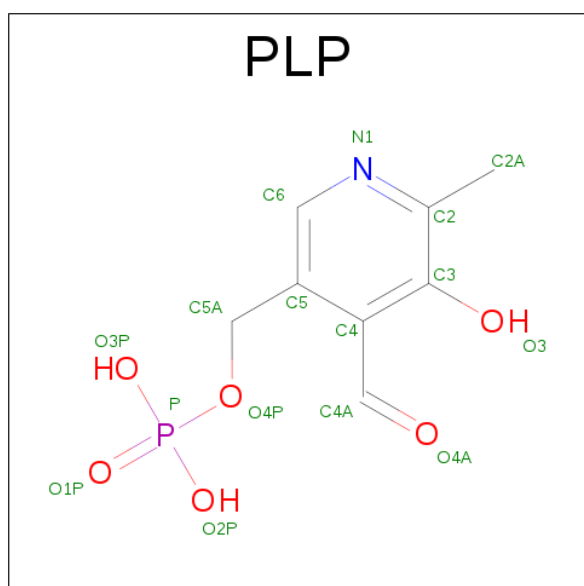
There are 4 unique types of molecules in this entry. The entry contains 6407 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ASPARTATE AMINOTRANSFERASE.

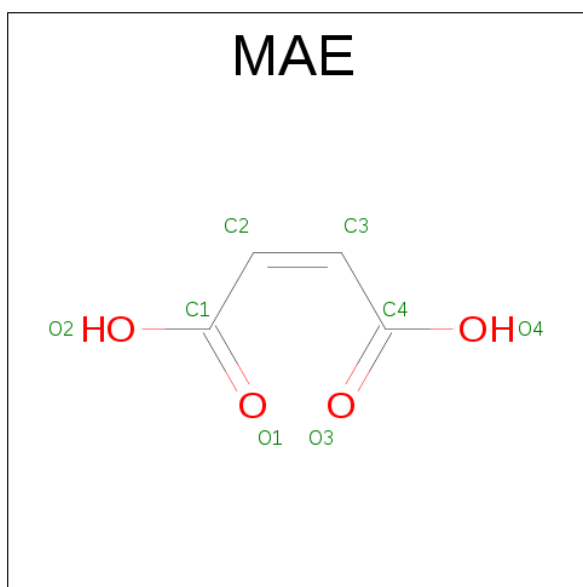
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3069	1936	536	584	13			
1	B	396	Total	C	N	O	S	2	0	0
			3069	1936	536	584	13			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: 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		

- Molecule 3 is MALEIC ACID (three-letter code: MAE) (formula: C₄H₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	4	4		
3	B	1	Total	C	O	0	0
			8	4	4		

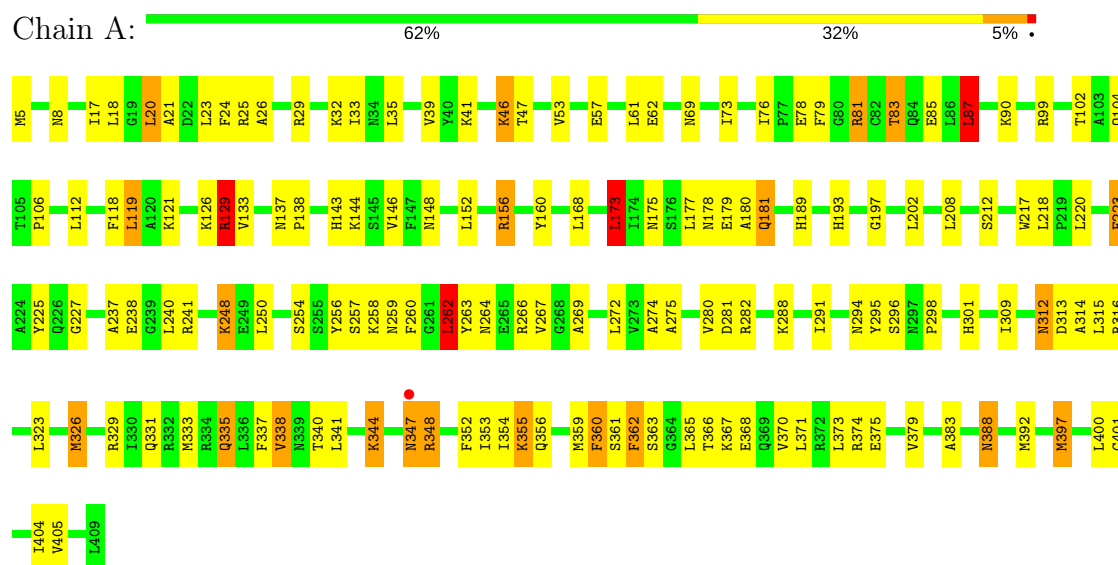
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	117	Total	O	0	0
			117	117		
4	B	106	Total	O	0	0
			106	106		

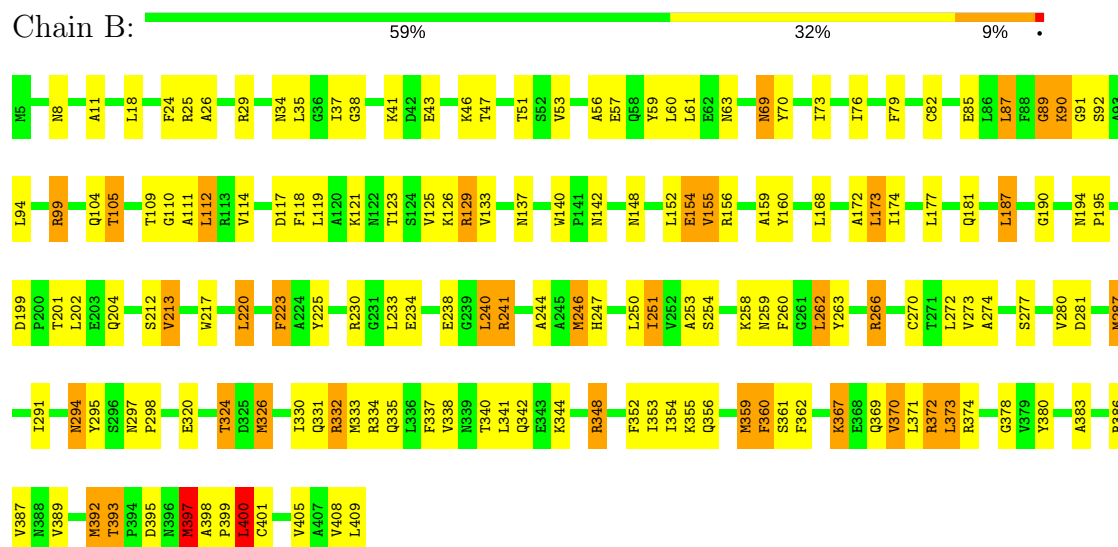
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: ASPARTATE AMINOTRANSFERASE



• Molecule 1: ASPARTATE AMINOTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.40Å 78.80Å 89.60Å 90.00° 118.60° 90.00°	Depositor
Resolution (Å)	10.00 – 2.35 15.03 – 2.24	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.35) 79.1 (15.03-2.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.24Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.188 , (Not available) 0.184 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.449 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6407	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: MAE, 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	0.87	1/3130 (0.0%)	1.06	13/4240 (0.3%)
1	B	0.89	0/3130	1.09	14/4240 (0.3%)
All	All	0.88	1/6260 (0.0%)	1.07	27/8480 (0.3%)

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	A	257	SER	C-N	-5.80	1.20	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	GLY	N-CA-C	-7.70	93.84	113.10
1	A	348	ARG	NE-CZ-NH2	7.68	124.14	120.30
1	A	156	ARG	NE-CZ-NH2	7.34	123.97	120.30
1	B	89	GLY	N-CA-C	7.30	131.35	113.10
1	B	266	ARG	NE-CZ-NH2	6.95	123.77	120.30
1	B	156	ARG	NE-CZ-NH2	6.93	123.76	120.30
1	A	81	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	B	400	LEU	CA-CB-CG	6.66	130.63	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	LYS	CB-CA-C	6.15	122.70	110.40
1	B	63	ASN	N-CA-C	6.08	127.43	111.00
1	A	262	LEU	CA-CB-CG	5.98	129.06	115.30
1	A	5	MET	CG-SD-CE	5.97	109.75	100.20
1	A	326	MET	CG-SD-CE	5.97	109.75	100.20
1	B	392	MET	CG-SD-CE	5.83	109.53	100.20
1	A	333	MET	CG-SD-CE	5.77	109.44	100.20
1	B	287	MET	CG-SD-CE	5.75	109.40	100.20
1	B	359	MET	CG-SD-CE	5.74	109.39	100.20
1	B	326	MET	CG-SD-CE	5.65	109.24	100.20
1	A	173	LEU	CA-CB-CG	5.64	128.28	115.30
1	B	246	MET	CG-SD-CE	5.64	109.22	100.20
1	B	397	MET	CG-SD-CE	5.60	109.16	100.20
1	A	360	PHE	CB-CA-C	-5.41	99.57	110.40
1	A	20	LEU	CB-CG-CD1	-5.39	101.84	111.00
1	A	87	LEU	CA-CB-CG	5.20	127.26	115.30
1	B	199	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	129	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	397	MET	CG-SD-CE	5.13	108.42	100.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	PHE	Mainchain
1	B	360	PHE	Mainchain

5.2 Too-close contacts [i](#)

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	3069	0	3015	104	0
1	B	3069	0	3016	125	0
2	A	15	0	6	3	0
2	B	15	0	6	4	0
3	A	8	0	2	1	0
3	B	8	0	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	117	0	0	6	0
4	B	106	0	0	5	0
All	All	6407	0	6047	219	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 18.

All (219) 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:397:MET:CE	1:A:400:LEU:HD23	1.89	1.03
1:B:38:GLY:C	1:B:359:MET:HE1	1.80	1.01
1:A:73:ILE:HD11	1:B:18:LEU:HD12	1.46	0.96
1:A:352:PHE:O	1:A:355:LYS:HG2	1.72	0.89
1:A:260:PHE:HB3	1:A:262:LEU:HD22	1.59	0.84
1:B:99:ARG:HG2	1:B:274:ALA:O	1.77	0.83
1:A:99:ARG:HD2	1:A:274:ALA:O	1.79	0.83
1:A:83:THR:HB	1:A:256:TYR:OH	1.80	0.81
1:B:393:THR:HG22	1:B:395:ASP:H	1.50	0.76
1:B:260:PHE:HB3	1:B:262:LEU:HD23	1.66	0.76
1:A:397:MET:HE3	1:A:400:LEU:HD23	1.68	0.75
1:B:129:ARG:HB3	1:B:154:GLU:HG2	1.69	0.74
1:B:277:SER:HA	1:B:280:VAL:HG12	1.69	0.74
1:A:73:ILE:CD1	1:B:18:LEU:HD12	2.18	0.73
1:A:29:ARG:HG3	4:A:457:HOH:O	1.87	0.73
1:A:225:TYR:HE2	2:A:410:PLP:O3	1.72	0.72
1:A:266:ARG:HH22	2:A:410:PLP:P	2.13	0.71
1:B:260:PHE:HB3	1:B:262:LEU:CD2	2.20	0.71
1:B:260:PHE:O	1:B:262:LEU:HD22	1.91	0.71
1:A:356:GLN:OE1	1:A:361:SER:HA	1.92	0.70
1:A:274:ALA:HB3	1:A:280:VAL:HB	1.73	0.69
1:B:159:ALA:O	1:B:173:LEU:HB2	1.93	0.69
1:B:99:ARG:HG2	1:B:99:ARG:HH11	1.57	0.69
1:A:99:ARG:HD3	1:A:275:ALA:O	1.92	0.68
1:A:266:ARG:HD2	1:B:297:ASN:O	1.93	0.68
1:B:374:ARG:HG2	1:B:374:ARG:O	1.94	0.68
1:A:41:LYS:O	1:A:329:ARG:NH1	2.27	0.67
1:B:332:ARG:HD2	1:B:333:MET:CE	2.25	0.67
1:A:144:LYS:NZ	1:A:148:ASN:HD21	1.93	0.67
1:A:294:ASN:HD21	1:B:294:ASN:HD21	1.43	0.67
1:B:38:GLY:C	1:B:359:MET:CE	2.60	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:GLY:O	1:B:359:MET:HE1	1.96	0.65
1:A:223:PHE:O	1:A:254:SER:HA	1.96	0.65
1:A:359:MET:HB3	1:A:388:ASN:HD21	1.61	0.65
1:A:237:ALA:O	1:A:241:ARG:HD3	1.98	0.64
1:B:195:PRO:HB3	1:B:386:ARG:HD3	1.80	0.64
1:B:266:ARG:HH22	2:B:410:PLP:P	2.21	0.63
1:A:212:SER:HB3	1:A:217:TRP:CE3	2.33	0.63
1:B:126:LYS:HB3	1:B:129:ARG:HH21	1.63	0.63
1:B:337:PHE:HB2	1:B:392:MET:CE	2.29	0.63
1:A:126:LYS:HD3	4:A:512:HOH:O	1.98	0.62
1:A:323:LEU:HD12	1:A:326:MET:HE3	1.81	0.62
1:A:212:SER:HB3	1:A:217:TRP:HE3	1.63	0.61
1:A:225:TYR:CE2	2:A:410:PLP:O3	2.53	0.61
1:B:76:ILE:O	1:B:79:PHE:HB3	2.00	0.61
1:A:312:ASN:ND2	1:A:314:ALA:H	1.99	0.61
1:A:79:PHE:O	1:A:83:THR:HG23	2.00	0.61
1:A:129:ARG:HH22	1:A:181:GLN:CD	2.04	0.61
1:B:393:THR:HG22	1:B:395:ASP:N	2.14	0.60
1:A:373:LEU:HD21	1:A:404:ILE:HA	1.83	0.60
1:B:337:PHE:HB2	1:B:392:MET:HE1	1.82	0.59
1:A:129:ARG:HH22	1:A:181:GLN:NE2	2.01	0.59
1:B:337:PHE:O	1:B:341:LEU:HB2	2.03	0.59
1:B:374:ARG:HG3	1:B:380:TYR:CE1	2.37	0.59
1:A:53:VAL:O	1:A:57:GLU:HG3	2.02	0.59
1:B:372:ARG:HG2	1:B:408:VAL:HG12	1.83	0.59
1:B:38:GLY:O	1:B:359:MET:CE	2.50	0.59
1:A:370:VAL:HG21	1:A:383:ALA:HA	1.86	0.57
1:A:21:ALA:O	1:A:25:ARG:HG2	2.04	0.57
1:B:274:ALA:HB3	1:B:280:VAL:HB	1.85	0.57
1:B:8:ASN:HB2	4:B:437:HOH:O	2.04	0.57
1:A:359:MET:HB3	1:A:388:ASN:ND2	2.20	0.56
1:A:87:LEU:O	1:A:241:ARG:HD2	2.04	0.56
1:B:338:VAL:HG21	1:B:354:ILE:HD11	1.87	0.56
1:B:148:ASN:ND2	1:B:155:VAL:HG13	2.21	0.56
1:A:76:ILE:O	1:A:79:PHE:HB3	2.06	0.56
1:B:117:ASP:O	1:B:121:LYS:HD3	2.06	0.56
1:A:85:GLU:CD	1:A:90:LYS:HG2	2.26	0.55
1:B:46:LYS:HG3	1:B:47:THR:H	1.71	0.55
1:B:38:GLY:CA	1:B:359:MET:HE1	2.35	0.55
1:A:99:ARG:O	1:A:280:VAL:HG21	2.07	0.55
1:B:38:GLY:CA	1:B:359:MET:CE	2.83	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:MET:HE2	1:B:400:LEU:HD22	1.89	0.55
1:A:177:LEU:O	1:A:180:ALA:HB3	2.05	0.55
1:A:337:PHE:CD1	1:A:397:MET:HE1	2.42	0.54
1:A:46:LYS:HG3	1:A:47:THR:N	2.22	0.54
1:A:329:ARG:NH2	1:A:392:MET:O	2.40	0.54
1:B:46:LYS:CG	1:B:47:THR:H	2.19	0.54
1:B:372:ARG:HG2	1:B:408:VAL:CG1	2.37	0.54
1:B:123:THR:OG1	1:B:125:VAL:HG23	2.08	0.54
1:B:190:GLY:HA3	1:B:223:PHE:CD1	2.43	0.54
1:B:187:LEU:HD12	1:B:220:LEU:HG	1.89	0.54
1:B:393:THR:CG2	1:B:395:ASP:H	2.18	0.54
1:A:282:ARG:HG2	1:B:11:ALA:HB2	1.89	0.53
1:B:220:LEU:HD13	1:B:251:ILE:CG1	2.37	0.53
1:A:397:MET:HE2	1:A:400:LEU:HD23	1.84	0.53
1:A:102:THR:HG23	1:A:269:ALA:HB1	1.91	0.53
1:B:29:ARG:NH1	1:B:378:GLY:HA2	2.24	0.53
1:B:272:LEU:HD22	1:B:287:MET:CE	2.38	0.53
1:A:175:ASN:HB3	4:A:528:HOH:O	2.08	0.53
1:A:39:VAL:HG21	1:B:69:ASN:ND2	2.24	0.53
1:B:46:LYS:HG3	1:B:47:THR:N	2.24	0.53
1:B:190:GLY:HA3	1:B:223:PHE:CE1	2.45	0.52
1:A:340:THR:O	1:A:344:LYS:HB2	2.09	0.52
1:B:331:GLN:O	1:B:335:GLN:HG2	2.10	0.52
1:B:291:ILE:HG23	1:B:295:TYR:CZ	2.44	0.52
1:A:129:ARG:NH2	1:A:181:GLN:CD	2.62	0.52
1:B:401:CYS:O	1:B:405:VAL:HG23	2.09	0.51
1:B:99:ARG:HG2	1:B:99:ARG:NH1	2.23	0.51
1:B:148:ASN:HD21	1:B:155:VAL:HG13	1.74	0.51
1:B:367:LYS:HB2	1:B:367:LYS:NZ	2.24	0.51
1:B:266:ARG:NH2	2:B:410:PLP:P	2.84	0.51
1:B:220:LEU:HD13	1:B:251:ILE:HG13	1.92	0.50
1:B:201:THR:HB	1:B:204:GLN:HG3	1.93	0.50
1:A:173:LEU:HD11	1:A:208:LEU:HD21	1.94	0.50
1:B:370:VAL:HG21	1:B:383:ALA:HA	1.93	0.50
1:A:238:GLU:HB2	4:A:494:HOH:O	2.11	0.49
1:A:46:LYS:HZ1	1:A:47:THR:H	1.60	0.49
1:A:374:ARG:HA	1:A:379:VAL:O	2.12	0.49
1:A:248:LYS:HG3	1:A:275:ALA:HB2	1.95	0.49
1:B:53:VAL:O	1:B:57:GLU:HG3	2.12	0.49
1:A:20:LEU:HA	1:A:23:LEU:HD12	1.95	0.48
1:B:334:ARG:HB3	1:B:389:VAL:HG11	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:PHE:O	1:A:83:THR:CG2	2.60	0.48
1:A:81:ARG:HG3	1:A:81:ARG:HH11	1.77	0.48
1:A:347:ASN:N	1:A:347:ASN:HD22	2.11	0.48
1:A:78:GLU:HG3	4:A:484:HOH:O	2.12	0.48
1:B:332:ARG:HD2	1:B:333:MET:HE2	1.96	0.48
1:B:137:ASN:O	1:B:160:TYR:HB3	2.14	0.48
1:A:256:TYR:HB2	1:A:267:VAL:HB	1.95	0.48
1:A:291:ILE:HG23	1:A:295:TYR:CZ	2.49	0.48
1:A:309:ILE:O	1:A:316:ARG:HB2	2.12	0.48
1:B:177:LEU:HB3	1:B:217:TRP:CH2	2.49	0.48
1:A:312:ASN:ND2	1:A:315:LEU:H	2.12	0.48
1:A:337:PHE:O	1:A:341:LEU:HB2	2.13	0.48
1:A:338:VAL:HG21	1:A:354:ILE:HD11	1.96	0.47
1:B:87:LEU:O	1:B:241:ARG:NH1	2.46	0.47
1:A:363:SER:OG	1:A:365:LEU:HB2	2.14	0.47
1:B:140:TRP:CH2	1:B:142:ASN:HB3	2.50	0.47
1:B:99:ARG:NH1	1:B:274:ALA:O	2.44	0.47
1:B:69:ASN:HD22	1:B:70:TYR:H	1.62	0.47
1:A:323:LEU:HD12	1:A:326:MET:CE	2.44	0.47
1:B:112:LEU:HD13	1:B:253:ALA:CB	2.44	0.47
1:B:320:GLU:O	1:B:324:THR:CG2	2.62	0.47
1:B:35:LEU:HD13	1:B:387:VAL:HG13	1.95	0.47
1:B:225:TYR:HE2	2:B:410:PLP:O3	1.97	0.47
1:A:397:MET:HG3	1:A:397:MET:O	2.15	0.47
1:A:46:LYS:NZ	1:A:47:THR:H	2.12	0.46
1:B:320:GLU:O	1:B:324:THR:HG23	2.16	0.46
1:A:118:PHE:CD2	1:A:119:LEU:HD13	2.50	0.46
1:A:315:LEU:HD23	1:A:315:LEU:HA	1.62	0.46
1:B:338:VAL:O	1:B:342:GLN:HB2	2.15	0.46
1:B:195:PRO:HB2	1:B:386:ARG:HG3	1.98	0.46
1:A:401:CYS:O	1:A:405:VAL:HG23	2.15	0.46
1:A:18:LEU:HD23	1:B:73:ILE:HG13	1.98	0.46
1:A:312:ASN:ND2	1:A:314:ALA:N	2.62	0.46
1:A:331:GLN:O	1:A:335:GLN:HG2	2.15	0.46
1:B:105:THR:HG21	1:B:111:ALA:CA	2.46	0.46
1:B:85:GLU:CD	1:B:90:LYS:HG2	2.36	0.46
1:B:46:LYS:CG	1:B:47:THR:N	2.78	0.45
1:B:89:GLY:O	1:B:90:LYS:O	2.34	0.45
1:A:99:ARG:NH2	4:A:477:HOH:O	2.50	0.45
1:B:348:ARG:HH11	1:B:348:ARG:HB2	1.81	0.45
1:B:82:CYS:SG	4:B:469:HOH:O	2.39	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LEU:O	1:B:240:LEU:HD22	2.17	0.45
1:B:356:GLN:OE1	1:B:361:SER:HA	2.17	0.45
1:B:230:ARG:HD3	4:B:453:HOH:O	2.16	0.45
1:B:277:SER:HA	1:B:280:VAL:CG1	2.44	0.45
1:A:352:PHE:HA	1:A:355:LYS:HD3	1.99	0.44
1:A:118:PHE:HD2	1:A:119:LEU:HD13	1.83	0.44
1:B:129:ARG:HG3	4:B:492:HOH:O	2.17	0.44
1:B:251:ILE:CD1	1:B:270:CYS:SG	3.06	0.44
1:B:337:PHE:HB2	1:B:392:MET:HE3	1.98	0.44
1:B:105:THR:HG21	1:B:111:ALA:N	2.33	0.44
1:B:225:TYR:CE2	2:B:410:PLP:O3	2.71	0.44
1:A:137:ASN:HA	1:A:138:PRO:HA	1.82	0.44
1:B:202:LEU:HD13	1:B:238:GLU:HB3	2.00	0.44
1:B:24:PHE:CE1	1:B:34:ASN:HB2	2.53	0.44
1:A:39:VAL:HG21	1:B:69:ASN:HD21	1.82	0.44
1:A:104:GLN:O	1:A:298:PRO:HG3	2.17	0.44
1:B:105:THR:HG21	1:B:111:ALA:HB2	2.00	0.44
1:A:35:LEU:HD11	1:A:400:LEU:CD1	2.48	0.43
1:A:57:GLU:OE2	1:A:301:HIS:HE1	2.01	0.43
1:B:220:LEU:HD13	1:B:251:ILE:HG12	2.00	0.43
1:B:374:ARG:HG3	1:B:380:TYR:CZ	2.52	0.43
1:B:104:GLN:O	1:B:298:PRO:HG3	2.18	0.43
1:B:177:LEU:HA	1:B:177:LEU:HD23	1.61	0.43
1:B:374:ARG:NH2	4:B:419:HOH:O	2.48	0.43
1:A:366:THR:HG22	1:A:368:GLU:H	1.83	0.43
1:B:340:THR:O	1:B:344:LYS:HG2	2.18	0.43
1:A:312:ASN:HD22	1:A:314:ALA:N	2.16	0.43
1:A:85:GLU:OE2	1:A:90:LYS:HG2	2.18	0.43
1:B:367:LYS:HB2	1:B:367:LYS:HZ2	1.83	0.43
1:A:338:VAL:HG21	1:A:354:ILE:CD1	2.48	0.43
1:A:193:HIS:O	1:A:197:GLY:N	2.50	0.42
1:B:109:THR:O	1:B:109:THR:HG22	2.19	0.42
1:B:110:GLY:O	1:B:114:VAL:HG13	2.20	0.42
1:A:17:ILE:HG21	3:A:411:MAE:O3	2.20	0.42
1:B:223:PHE:HD1	1:B:223:PHE:HA	1.65	0.42
1:B:94:LEU:HD11	1:B:244:ALA:HB1	2.01	0.42
1:A:312:ASN:HD22	1:A:312:ASN:C	2.23	0.42
1:B:352:PHE:O	1:B:355:LYS:HB3	2.20	0.42
1:A:99:ARG:O	1:A:280:VAL:HG11	2.20	0.42
1:A:227:GLY:HA3	1:A:323:LEU:HD21	2.02	0.42
1:B:112:LEU:HD13	1:B:253:ALA:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:THR:CG2	1:A:269:ALA:HB1	2.49	0.41
1:B:393:THR:CG2	1:B:395:ASP:HB2	2.50	0.41
1:B:43:GLU:CD	1:B:43:GLU:H	2.23	0.41
1:A:143:HIS:HE1	1:A:189:HIS:CE1	2.38	0.41
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.75	0.41
1:A:129:ARG:NH2	1:A:181:GLN:OE1	2.53	0.41
1:A:295:TYR:O	1:B:266:ARG:NH1	2.53	0.41
1:B:213:VAL:HG23	1:B:247:HIS:CD2	2.55	0.41
1:B:34:ASN:HA	1:B:380:TYR:HB2	2.02	0.41
1:A:106:PRO:HD3	1:A:295:TYR:CZ	2.55	0.41
1:A:137:ASN:O	1:A:160:TYR:HB3	2.21	0.41
1:A:288:LYS:HE2	1:A:288:LYS:HB3	1.90	0.41
1:B:326:MET:O	1:B:330:ILE:HG13	2.21	0.41
1:B:369:GLN:O	1:B:373:LEU:HB2	2.19	0.41
1:A:266:ARG:NH1	1:B:295:TYR:O	2.54	0.41
1:B:380:TYR:CD1	1:B:380:TYR:N	2.88	0.41
1:A:24:PHE:CE2	1:A:32:LYS:HE3	2.56	0.41
1:A:362:PHE:HA	1:A:362:PHE:HD1	1.79	0.41
1:B:212:SER:HA	1:B:217:TRP:CE3	2.56	0.41
1:B:159:ALA:HB3	1:B:172:ALA:O	2.21	0.40
1:B:223:PHE:O	1:B:254:SER:HA	2.21	0.40
1:B:56:ALA:O	1:B:59:TYR:HB3	2.21	0.40
1:B:194:ASN:HA	1:B:195:PRO:HA	1.84	0.40
1:B:398:ALA:HB3	1:B:399:PRO:CD	2.51	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	394/396 (100%)	371 (94%)	20 (5%)	3 (1%)	22 24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	394/396 (100%)	369 (94%)	19 (5%)	6 (2%)	12	10
All	All	788/792 (100%)	740 (94%)	39 (5%)	9 (1%)	17	16

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	37	ILE
1	B	92	SER
1	A	69	ASN
1	B	90	LYS
1	B	373	LEU
1	B	26	ALA
1	A	26	ALA
1	B	263	TYR
1	A	263	TYR

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	320/320 (100%)	272 (85%)	48 (15%)	3	3
1	B	320/320 (100%)	269 (84%)	51 (16%)	3	2
All	All	640/640 (100%)	541 (84%)	99 (16%)	3	2

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	33	ILE
1	A	46	LYS
1	A	61	LEU
1	A	62	GLU
1	A	83	THR
1	A	87	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	112	LEU
1	A	119	LEU
1	A	121	LYS
1	A	129	ARG
1	A	133	VAL
1	A	146	VAL
1	A	152	LEU
1	A	156	ARG
1	A	168	LEU
1	A	173	LEU
1	A	178	ASN
1	A	179	GLU
1	A	181	GLN
1	A	202	LEU
1	A	218	LEU
1	A	220	LEU
1	A	223	PHE
1	A	240	LEU
1	A	248	LYS
1	A	250	LEU
1	A	258	LYS
1	A	259	ASN
1	A	262	LEU
1	A	264	ASN
1	A	272	LEU
1	A	281	ASP
1	A	296	SER
1	A	312	ASN
1	A	313	ASP
1	A	335	GLN
1	A	338	VAL
1	A	344	LYS
1	A	347	ASN
1	A	348	ARG
1	A	353	ILE
1	A	355	LYS
1	A	362	PHE
1	A	367	LYS
1	A	371	LEU
1	A	375	GLU
1	A	388	ASN
1	B	25	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	41	LYS
1	B	51	THR
1	B	60	LEU
1	B	61	LEU
1	B	69	ASN
1	B	87	LEU
1	B	99	ARG
1	B	105	THR
1	B	112	LEU
1	B	118	PHE
1	B	119	LEU
1	B	129	ARG
1	B	133	VAL
1	B	152	LEU
1	B	154	GLU
1	B	155	VAL
1	B	168	LEU
1	B	173	LEU
1	B	174	ILE
1	B	181	GLN
1	B	187	LEU
1	B	213	VAL
1	B	220	LEU
1	B	223	PHE
1	B	233	LEU
1	B	234	GLU
1	B	240	LEU
1	B	241	ARG
1	B	246	MET
1	B	250	LEU
1	B	251	ILE
1	B	259	ASN
1	B	262	LEU
1	B	273	VAL
1	B	281	ASP
1	B	294	ASN
1	B	324	THR
1	B	332	ARG
1	B	348	ARG
1	B	353	ILE
1	B	360	PHE
1	B	362	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	367	LYS
1	B	370	VAL
1	B	371	LEU
1	B	372	ARG
1	B	393	THR
1	B	397	MET
1	B	400	LEU
1	B	409	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	84	GLN
1	A	148	ASN
1	A	175	ASN
1	A	189	HIS
1	A	206	GLN
1	A	226	GLN
1	A	259	ASN
1	A	264	ASN
1	A	301	HIS
1	A	312	ASN
1	A	331	GLN
1	A	339	ASN
1	A	347	ASN
1	A	388	ASN
1	B	63	ASN
1	B	69	ASN
1	B	96	ASN
1	B	175	ASN
1	B	226	GLN
1	B	247	HIS
1	B	259	ASN
1	B	294	ASN
1	B	331	GLN
1	B	339	ASN
1	B	342	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 carbohydrates 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	$\# Z > 2$
2	PLP	A	410	1	15,15,16	1.86	3 (20%)	20,22,23	1.71	5 (25%)
3	MAE	A	411	-	1,7,7	1.65	0	0,8,8	0.00	-
2	PLP	B	410	1	15,15,16	2.27	4 (26%)	20,22,23	1.72	3 (15%)
3	MAE	B	411	-	1,7,7	3.49	1 (100%)	0,8,8	0.00	-

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	410	1	-	0/6/6/8	0/1/1/1
3	MAE	A	411	-	-	0/0/5/5	0/0/0/0
2	PLP	B	410	1	-	0/6/6/8	0/1/1/1
3	MAE	B	411	-	-	0/0/5/5	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	410	PLP	C3-C2	-6.29	1.36	1.40
2	A	410	PLP	C3-C2	-4.56	1.37	1.40
2	B	410	PLP	C5A-C5	-3.47	1.41	1.50
2	A	410	PLP	P-O2P	-2.36	1.45	1.54
2	B	410	PLP	P-O1P	-2.33	1.42	1.50
2	B	410	PLP	C5-C4	-2.31	1.37	1.40
2	A	410	PLP	C5A-C5	3.32	1.60	1.50
3	B	411	MAE	C3-C2	3.49	1.49	1.31

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	410	PLP	C5-C6-N1	-2.62	119.43	123.87
2	A	410	PLP	C5-C6-N1	-2.56	119.54	123.87
2	A	410	PLP	O2P-P-O4P	-2.17	100.95	106.73
2	B	410	PLP	C6-C5-C4	2.62	120.37	118.18
2	A	410	PLP	C5A-C5-C6	2.93	124.36	119.33
2	A	410	PLP	O3P-P-O4P	3.22	115.30	106.73
2	A	410	PLP	O4P-C5A-C5	3.63	116.62	109.32
2	B	410	PLP	O4P-C5A-C5	5.83	121.04	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	410	PLP	3	0
3	A	411	MAE	1	0
2	B	410	PLP	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	396/396 (100%)	-0.83	1 (0%) 93 97	11, 29, 64, 103	0
1	B	396/396 (100%)	-0.82	0 100 100	12, 30, 67, 98	1 (0%)
All	All	792/792 (100%)	-0.83	1 (0%) 95 98	11, 30, 64, 103	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	347	ASN	2.3

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	MAE	A	411	8/8	0.85	0.24	11.19	28,34,42,43	0
2	PLP	A	410	15/16	0.94	0.10	2.13	13,17,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	PLP	B	410	15/16	0.96	0.10	1.56	10,18,26,27	0
3	MAE	B	411	8/8	0.94	0.10	0.28	31,35,40,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.