



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:14 PM GMT

PDB ID : 4L0D
Title : Crystal structure of delta516-525 human cystathionine beta-synthase containing C-terminal 6xHis-tag
Authors : Ereno, J.; Majtan, T.; Oyenarte, I.; Kraus, J.P.; Martinez-Cruz, L.A.
Deposited on : 2013-05-31
Resolution : 2.97 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

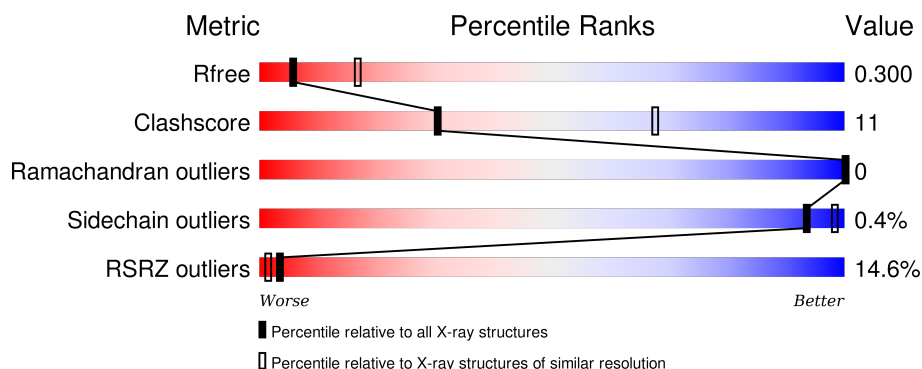
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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}	91344	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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 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	549	<div> <div>11%</div> <div> <div></div> <div>67%</div> <div>23%</div> <div>10%</div> </div> </div>
1	B	549	<div> <div>15%</div> <div> <div></div> <div>68%</div> <div>22%</div> <div>10%</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7728 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 Cystathionine beta-synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	1	0
			3807	2413	667	705	22			
1	B	496	Total	C	N	O	S	0	1	0
			3805	2412	666	705	22			

There are 38 discrepancies between the modelled and reference sequences:

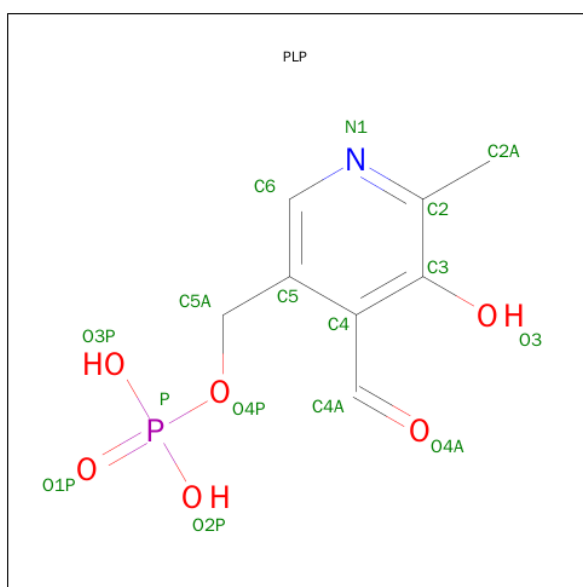
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	PRO	ENGINEERED MUTATION	UNP P35520
A	?	-	ILE	DELETION	UNP P35520
A	?	-	GLN	DELETION	UNP P35520
A	?	-	TYR	DELETION	UNP P35520
A	?	-	HIS	DELETION	UNP P35520
A	?	-	SER	DELETION	UNP P35520
A	?	-	THR	DELETION	UNP P35520
A	?	-	GLY	DELETION	UNP P35520
A	?	-	LYS	DELETION	UNP P35520
A	?	-	SER	DELETION	UNP P35520
A	?	-	SER	DELETION	UNP P35520
A	552	GLU	-	EXPRESSION TAG	UNP P35520
A	553	LEU	-	EXPRESSION TAG	UNP P35520
A	554	HIS	-	EXPRESSION TAG	UNP P35520
A	555	HIS	-	EXPRESSION TAG	UNP P35520
A	556	HIS	-	EXPRESSION TAG	UNP P35520
A	557	HIS	-	EXPRESSION TAG	UNP P35520
A	558	HIS	-	EXPRESSION TAG	UNP P35520
A	559	HIS	-	EXPRESSION TAG	UNP P35520
B	2	GLY	PRO	ENGINEERED MUTATION	UNP P35520
B	?	-	ILE	DELETION	UNP P35520
B	?	-	GLN	DELETION	UNP P35520
B	?	-	TYR	DELETION	UNP P35520
B	?	-	HIS	DELETION	UNP P35520
B	?	-	SER	DELETION	UNP P35520

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	DELETION	UNP P35520
B	?	-	GLY	DELETION	UNP P35520
B	?	-	LYS	DELETION	UNP P35520
B	?	-	SER	DELETION	UNP P35520
B	?	-	SER	DELETION	UNP P35520
B	552	GLU	-	EXPRESSION TAG	UNP P35520
B	553	LEU	-	EXPRESSION TAG	UNP P35520
B	554	HIS	-	EXPRESSION TAG	UNP P35520
B	555	HIS	-	EXPRESSION TAG	UNP P35520
B	556	HIS	-	EXPRESSION TAG	UNP P35520
B	557	HIS	-	EXPRESSION TAG	UNP P35520
B	558	HIS	-	EXPRESSION TAG	UNP P35520
B	559	HIS	-	EXPRESSION TAG	UNP P35520

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: 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 PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

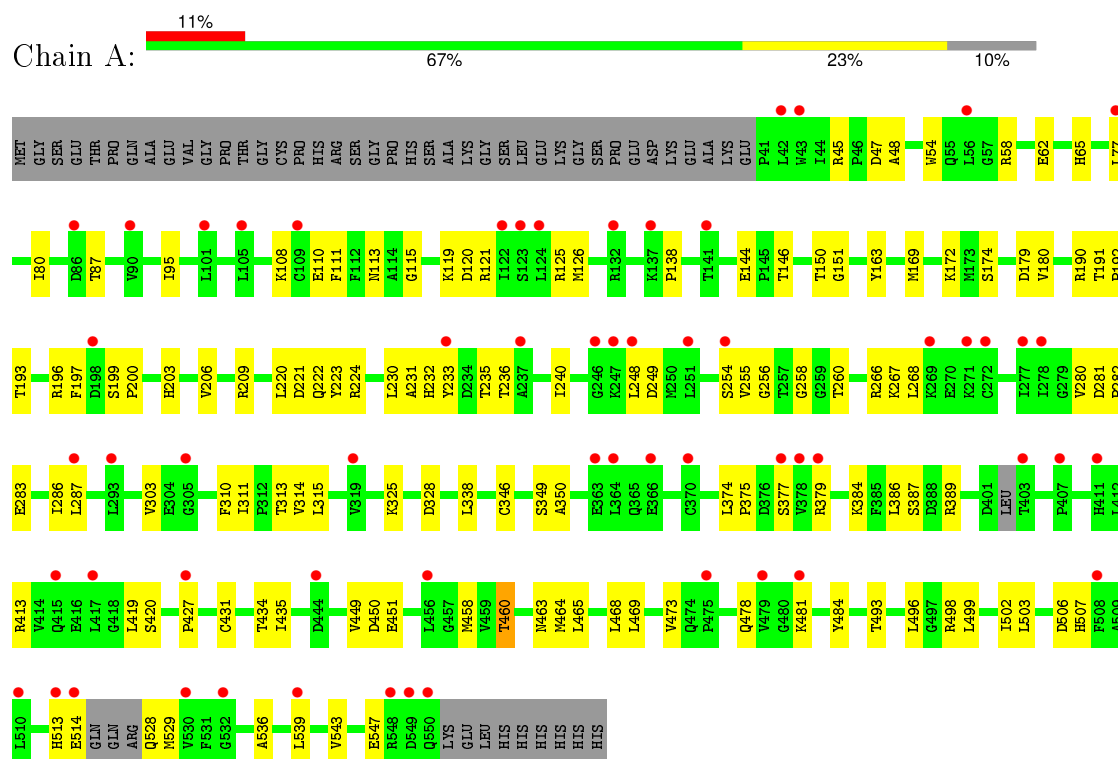


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

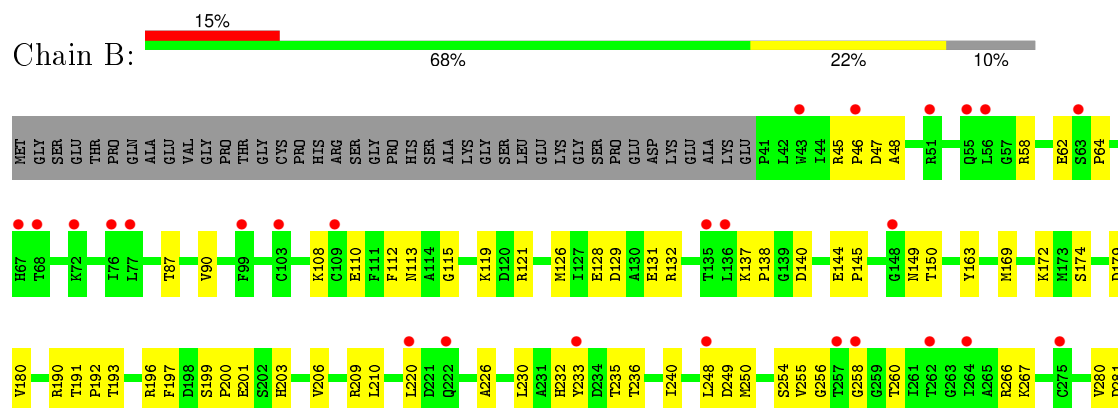
3 Residue-property plots

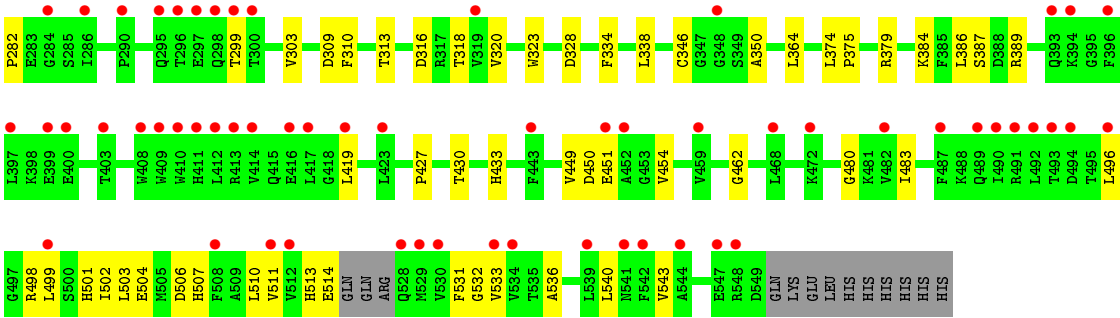
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Cystathionine beta-synthase



• Molecule 1: Cystathionine beta-synthase





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	124.36Å 136.20Å 169.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.06 – 2.97 53.65 – 2.97	Depositor EDS
% Data completeness (in resolution range)	95.6 (53.06-2.97) 97.8 (53.65-2.97)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.240 , 0.284 0.262 , 0.300	Depositor DCC
R_{free} test set	1498 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	70.6	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 72.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	3 of 29365 reflections (0.010%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7728	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, 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	0.37	0/3878	0.56	0/5253
1	B	0.39	0/3881	0.57	0/5261
All	All	0.38	0/7759	0.57	0/10514

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3807	0	3832	90	0
1	B	3805	0	3834	84	0
2	A	15	0	7	3	0
2	B	15	0	7	3	0
3	A	43	0	30	5	0
3	B	43	0	30	6	0
All	All	7728	0	7740	170	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 (170) 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:413:ARG:NH1	1:A:493:THR:O	1.89	1.05
1:B:513:HIS:HB2	1:B:531:PHE:HE2	1.43	0.84
1:B:266:ARG:HD2	3:B:602:HEM:HBC2	1.63	0.81
1:B:110:GLU:OE2	1:B:121:ARG:NE	2.14	0.81
1:A:58:ARG:NE	1:A:62:GLU:OE1	2.16	0.78
1:B:513:HIS:HB2	1:B:531:PHE:CE2	2.26	0.71
1:A:191:THR:HG21	1:A:203:HIS:HA	1.73	0.70
1:B:180:VAL:HG21	1:B:379:ARG:NH1	2.07	0.68
1:B:303:VAL:HG23	1:B:328:ASP:OD2	1.93	0.68
1:B:350:ALA:HB1	1:B:374:LEU:HD22	1.76	0.65
1:A:303:VAL:HG23	1:A:328:ASP:OD2	1.97	0.65
1:A:110:GLU:OE2	1:A:121:ARG:NE	2.29	0.63
1:B:254:SER:HA	1:B:280:VAL:HB	1.80	0.62
1:B:191:THR:HG21	1:B:203:HIS:HA	1.81	0.62
1:A:255:VAL:HG13	1:A:258:GLY:HA2	1.82	0.61
1:A:179:ASP:HB3	1:B:386:LEU:HD22	1.80	0.61
1:B:58:ARG:NE	1:B:62:GLU:OE1	2.29	0.61
1:A:180:VAL:HG21	1:A:379:ARG:NH1	2.15	0.61
1:A:254:SER:HA	1:A:280:VAL:HB	1.82	0.61
1:B:255:VAL:HG13	1:B:258:GLY:HA2	1.82	0.61
1:A:281:ASP:OD2	1:A:282:PRO:HD2	2.00	0.61
1:B:129:ASP:OD2	1:B:132:ARG:NH1	2.33	0.61
1:B:172:LYS:HB2	1:B:193:THR:HG21	1.84	0.60
1:A:350:ALA:HB1	1:A:374:LEU:HD22	1.85	0.59
1:A:386:LEU:HD22	1:B:179:ASP:HB3	1.86	0.57
1:A:513:HIS:CG	1:A:514:GLU:N	2.72	0.57
1:B:200:PRO:HA	1:B:209[B]:ARG:HH12	1.69	0.57
1:B:232:HIS:CG	1:B:260:THR:HA	2.39	0.56
1:A:196:ARG:O	1:A:199:SER:OG	2.19	0.56
1:B:235:THR:OG1	1:B:236:THR:N	2.37	0.56
1:A:338:LEU:HD23	1:A:346:CYS:SG	2.46	0.56
1:A:200:PRO:O	1:A:209[B]:ARG:NH2	2.39	0.56
1:A:431:CYS:O	1:A:435:ILE:HD12	2.06	0.56
1:A:478:GLN:HB2	1:A:481:LYS:NZ	2.21	0.56
1:A:346:CYS:HA	1:A:377:SER:HA	1.88	0.55
1:B:540:LEU:HA	1:B:543:VAL:HG22	1.88	0.55
3:A:602:HEM:HBC2	3:A:602:HEM:HMC2	1.89	0.55
3:B:602:HEM:HBB2	3:B:602:HEM:HMB1	1.89	0.54
1:A:507:HIS:CG	1:B:192:PRO:HD3	2.42	0.54
1:B:513:HIS:CG	1:B:514:GLU:N	2.76	0.54
1:A:206:VAL:HG22	1:A:209[B]:ARG:HH21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:THR:O	1:B:240:ILE:HG13	2.08	0.54
1:B:119:LYS:HB3	1:B:150:THR:HA	1.89	0.53
1:B:138:PRO:HA	1:B:163:TYR:HE2	1.73	0.53
1:A:138:PRO:HA	1:A:163:TYR:HE2	1.74	0.53
1:A:111:PHE:HB2	1:A:377:SER:HB3	1.90	0.52
1:B:338:LEU:HD23	1:B:346:CYS:SG	2.49	0.52
1:A:258:GLY:HA3	1:A:315:LEU:HD13	1.92	0.52
1:B:196:ARG:O	1:B:199:SER:OG	2.20	0.52
1:B:256:GLY:H	2:B:601:PLP:H5A1	1.75	0.52
1:B:180:VAL:HG21	1:B:379:ARG:HH11	1.72	0.51
1:A:192:PRO:HD3	1:B:507:HIS:CG	2.44	0.51
1:B:316:ASP:OD2	1:B:318:THR:OG1	2.20	0.50
1:A:119:LYS:HB3	1:A:150:THR:HA	1.92	0.50
1:B:334:PHE:O	1:B:338:LEU:HB2	2.11	0.50
1:B:119:LYS:HG3	1:B:149:ASN:HB2	1.94	0.50
1:A:45:ARG:HD3	1:A:47:ASP:OD1	2.12	0.49
1:A:460:THR:HG23	1:A:463:ASN:HB3	1.94	0.49
1:A:110:GLU:HG3	1:A:113:ASN:ND2	2.27	0.49
1:A:200:PRO:HA	1:A:209[A]:ARG:NH1	2.28	0.49
1:A:287:LEU:HD23	1:A:311:ILE:HD13	1.94	0.49
1:A:235:THR:OG1	1:A:236:THR:N	2.44	0.49
1:A:144:GLU:OE1	1:A:222:GLN:HG2	2.12	0.49
1:A:503:LEU:HD13	1:A:536:ALA:HA	1.95	0.49
1:A:233:TYR:O	1:A:267:LYS:HD2	2.13	0.49
1:A:465:LEU:O	1:A:469:LEU:HB2	2.13	0.49
1:A:174:SER:HB3	1:A:384:LYS:HD2	1.95	0.49
1:A:266:ARG:NH1	3:A:602:HEM:C2C	2.81	0.48
1:A:115:GLY:N	1:A:120:ASP:OD2	2.46	0.48
1:B:501:HIS:O	1:B:504:GLU:HB2	2.12	0.48
1:A:528:GLN:HG3	1:A:529:MET:H	1.78	0.48
1:A:232:HIS:CG	1:A:260:THR:HA	2.49	0.48
1:B:480:GLY:O	1:B:483:ILE:HG22	2.14	0.48
1:A:87:THR:OG1	1:A:108:LYS:HE3	2.14	0.48
1:A:125:ARG:HG2	1:A:231:ALA:HB2	1.94	0.48
1:B:137:LYS:HE2	1:B:140:ASP:OD2	2.14	0.48
1:A:387:SER:OG	1:A:389:ARG:HG3	2.14	0.48
1:B:233:TYR:O	1:B:267:LYS:HD2	2.13	0.48
1:A:543:VAL:O	1:A:547:GLU:HG2	2.14	0.48
1:B:430:THR:HG23	1:B:433:HIS:H	1.79	0.47
1:A:450:ASP:OD1	1:A:451:GLU:N	2.48	0.47
1:A:169:MET:O	1:A:190:ARG:HA	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:LEU:O	1:B:503:LEU:HG	2.13	0.47
1:A:126:MET:HE3	1:A:222:GLN:HA	1.96	0.47
1:A:54:TRP:HB2	3:A:602:HEM:C4B	2.50	0.47
1:B:427:PRO:HD3	1:B:449:VAL:O	2.15	0.47
1:B:266:ARG:HD2	3:B:602:HEM:CBC	2.39	0.47
1:A:197:PHE:CE2	1:A:310:PHE:HB3	2.50	0.46
1:B:64:PRO:HD3	3:B:602:HEM:HMB2	1.96	0.46
1:B:200:PRO:HA	1:B:209[B]:ARG:NH1	2.31	0.46
1:A:266:ARG:NH1	3:A:602:HEM:C3C	2.83	0.46
1:B:510:LEU:HD22	1:B:533:VAL:HG22	1.98	0.46
1:B:46:PRO:HB2	1:B:310:PHE:CE1	2.51	0.46
1:B:502:ILE:O	1:B:506:ASP:N	2.48	0.46
1:B:174:SER:HB3	1:B:384:LYS:HD2	1.96	0.46
1:B:144:GLU:HG3	1:B:145:PRO:O	2.15	0.46
1:B:206:VAL:O	1:B:210:LEU:HG	2.16	0.46
1:B:45:ARG:HD3	1:B:47:ASP:OD1	2.16	0.46
1:A:138:PRO:HA	1:A:163:TYR:CE2	2.52	0.45
1:B:169:MET:O	1:B:190:ARG:HA	2.15	0.45
1:B:115:GLY:O	1:B:379:ARG:NH2	2.49	0.45
1:B:110:GLU:OE2	1:B:121:ARG:NH2	2.50	0.45
1:A:191:THR:HG22	1:A:206:VAL:HG21	1.98	0.45
1:A:484:TYR:HE2	1:B:201:GLU:HG2	1.82	0.45
1:A:496:LEU:O	1:A:499:LEU:HB3	2.16	0.45
1:B:387:SER:OG	1:B:389:ARG:HG3	2.16	0.45
1:A:458:MET:HB2	1:A:484:TYR:HB2	1.98	0.45
1:B:230:LEU:HA	1:B:230:LEU:HD23	1.80	0.45
1:B:126:MET:HE2	1:B:220:LEU:HB3	1.98	0.45
1:A:283:GLU:HA	1:A:325:LYS:NZ	2.32	0.45
1:A:77:LEU:HB2	1:B:90:VAL:HG22	1.98	0.45
1:B:87:THR:OG1	1:B:108:LYS:HE3	2.17	0.45
1:A:427:PRO:HD3	1:A:449:VAL:O	2.17	0.44
1:A:180:VAL:HG21	1:A:379:ARG:HH11	1.80	0.44
1:B:48:ALA:O	1:B:313:THR:HG22	2.17	0.44
1:B:256:GLY:H	2:B:601:PLP:C5A	2.30	0.44
1:B:226:ALA:HA	3:B:602:HEM:HMD2	2.00	0.44
1:A:502:ILE:O	1:A:506:ASP:N	2.51	0.44
1:B:496:LEU:O	1:B:499:LEU:HB3	2.18	0.44
1:B:419:LEU:HD13	1:B:532:GLY:HA3	1.99	0.44
1:B:450:ASP:OD1	1:B:451:GLU:N	2.51	0.44
1:B:511:VAL:O	1:B:531:PHE:N	2.50	0.43
1:B:87:THR:HG21	1:B:110:GLU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:LEU:HD12	1:B:249:ASP:H	1.82	0.43
1:A:172:LYS:HB2	1:A:193:THR:HG21	2.00	0.43
1:A:47:ASP:HA	1:A:311:ILE:O	2.18	0.43
1:A:236:THR:O	1:A:240:ILE:HG13	2.19	0.43
1:A:224:ARG:HA	1:A:313:THR:OG1	2.18	0.43
1:B:197:PHE:HD2	1:B:309:ASP:OD2	2.01	0.43
1:A:431:CYS:O	1:A:434:THR:HB	2.19	0.43
1:A:468:LEU:HD23	1:A:473:VAL:O	2.19	0.43
1:A:349:SER:OG	2:A:601:PLP:N1	2.51	0.42
1:A:65:HIS:HB3	1:A:230:LEU:HD11	2.01	0.42
1:B:64:PRO:HD3	3:B:602:HEM:CMB	2.50	0.42
1:B:200:PRO:HB3	1:B:209[B]:ARG:NH2	2.34	0.42
1:A:256:GLY:H	2:A:601:PLP:H5A1	1.84	0.42
1:A:169:MET:HG3	1:A:190:ARG:NE	2.35	0.42
1:B:498:ARG:O	1:B:502:ILE:HG13	2.19	0.42
2:B:601:PLP:H2A1	2:B:601:PLP:HO3	1.71	0.42
1:A:498:ARG:O	1:A:502:ILE:HG13	2.20	0.42
1:B:110:GLU:HG3	1:B:113:ASN:ND2	2.35	0.42
1:B:232:HIS:CD2	1:B:260:THR:HA	2.54	0.42
1:A:431:CYS:HA	1:A:464:MET:HE3	2.02	0.42
1:A:221:ASP:OD1	1:A:224:ARG:NE	2.48	0.42
1:B:110:GLU:OE2	1:B:121:ARG:CZ	2.67	0.41
1:A:286:ILE:HG13	1:A:286:ILE:H	1.62	0.41
1:B:320:VAL:HG11	1:B:323:TRP:CE2	2.55	0.41
1:B:128:GLU:HA	1:B:131:GLU:OE2	2.19	0.41
1:B:250:MET:HE3	1:B:364:LEU:HD11	2.02	0.41
1:B:191:THR:HB	1:B:201:GLU:O	2.20	0.41
3:A:602:HEM:HMB1	3:A:602:HEM:HBB2	2.01	0.41
1:B:281:ASP:OD2	1:B:282:PRO:HD2	2.20	0.41
1:A:80:ILE:HD11	1:B:112:PHE:HZ	1.85	0.41
1:A:95:ILE:HD12	1:A:338:LEU:HD12	2.03	0.41
1:B:503:LEU:HD13	1:B:536:ALA:HA	2.03	0.41
1:A:48:ALA:O	1:A:313:THR:HG22	2.20	0.41
1:A:539:LEU:O	1:A:543:VAL:HG23	2.20	0.41
1:A:248:LEU:HD12	1:A:249:ASP:H	1.84	0.41
1:A:374:LEU:HA	1:A:375:PRO:HD3	1.82	0.41
1:A:223:TYR:O	1:A:314:VAL:HG22	2.21	0.41
1:A:419:LEU:HB3	1:A:420:SER:H	1.32	0.41
1:A:200:PRO:HD2	1:B:462:GLY:HA3	2.01	0.40
1:A:146:THR:HG21	1:A:151:GLY:HA3	2.02	0.40
1:A:256:GLY:H	2:A:601:PLP:C5A	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:LEU:HA	1:B:375:PRO:HD3	1.73	0.40
1:A:119:LYS:HD2	1:A:150:THR:OG1	2.21	0.40
1:A:126:MET:HB3	1:A:220:LEU:HD13	2.03	0.40
1:A:499:LEU:O	1:A:503:LEU:HG	2.21	0.40
1:B:126:MET:HB3	1:B:220:LEU:HD13	2.03	0.40
1:A:268:LEU:HA	1:A:268:LEU:HD12	1.85	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	489/549 (89%)	474 (97%)	15 (3%)	0	100	100
1	B	493/549 (90%)	479 (97%)	14 (3%)	0	100	100
All	All	982/1098 (89%)	953 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	407/463 (88%)	406 (100%)	1 (0%)	95	99
1	B	408/463 (88%)	406 (100%)	2 (0%)	92	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	815/926 (88%)	812 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	460	THR
1	B	299	THR
1	B	454	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	380	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLP	A	601	1	15,15,16	0.99	1 (6%)	21,22,23	1.26	2 (9%)
3	HEM	A	602	1	30,50,50	4.42	10 (33%)	24,82,82	3.10	10 (41%)
2	PLP	B	601	1	15,15,16	1.03	1 (6%)	21,22,23	1.29	3 (14%)
3	HEM	B	602	1	30,50,50	4.51	11 (36%)	24,82,82	3.01	9 (37%)

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	601	1	-	0/6/6/8	0/1/1/1
3	HEM	A	602	1	-	0/10/54/54	0/0/8/8
2	PLP	B	601	1	-	0/6/6/8	0/1/1/1
3	HEM	B	602	1	-	0/10/54/54	0/0/8/8

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	HEM	C3B-C4B	-14.34	1.39	1.51
3	A	602	HEM	C3B-C4B	-13.55	1.39	1.51
3	A	602	HEM	C2D-C3D	-12.38	1.17	1.54
3	B	602	HEM	C2D-C3D	-12.23	1.17	1.54
3	B	602	HEM	C3D-C4D	-9.97	1.38	1.51
3	A	602	HEM	C3D-C4D	-9.69	1.39	1.51
3	A	602	HEM	C2C-C1C	-7.53	1.38	1.52
3	B	602	HEM	C2C-C1C	-7.42	1.38	1.52
3	A	602	HEM	C2B-C1B	-3.55	1.40	1.51
3	A	602	HEM	C2D-C1D	-3.44	1.40	1.51
3	B	602	HEM	C2B-C1B	-3.38	1.40	1.51
3	B	602	HEM	C2D-C1D	-3.34	1.40	1.51
2	B	601	PLP	C3-C2	-2.25	1.39	1.40
2	A	601	PLP	C2-N1	2.04	1.38	1.34
3	B	602	HEM	C4A-CHB	2.38	1.46	1.39
3	A	602	HEM	CHD-C4C	3.00	1.43	1.36
3	B	602	HEM	CHD-C4C	3.05	1.43	1.36
3	A	602	HEM	CHC-C1C	3.11	1.43	1.36
3	B	602	HEM	CHC-C1C	3.33	1.44	1.36
3	B	602	HEM	CBB-CAB	3.61	1.50	1.29
3	A	602	HEM	CBB-CAB	3.66	1.50	1.29
3	A	602	HEM	FE-NC	4.41	2.13	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	HEM	FE-NC	4.53	2.13	1.95

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	HEM	C3B-C4B-NB	-4.11	103.77	111.63
3	B	602	HEM	C3B-C4B-NB	-4.05	103.89	111.63
3	A	602	HEM	CBA-CAA-C2A	-2.84	107.44	112.53
3	B	602	HEM	CBA-CAA-C2A	-2.81	107.50	112.53
3	A	602	HEM	C1D-CHD-C4C	-2.79	121.16	125.82
3	B	602	HEM	C1D-CHD-C4C	-2.71	121.29	125.82
3	A	602	HEM	CAA-CBA-CGA	-2.49	108.19	112.75
2	B	601	PLP	C5-C6-N1	-2.09	120.22	123.86
2	A	601	PLP	C6-C5-C4	2.05	119.89	118.15
2	B	601	PLP	C6-C5-C4	2.64	120.39	118.15
3	A	602	HEM	CMD-C2D-C3D	2.72	126.37	114.35
3	B	602	HEM	CMD-C2D-C3D	2.78	126.67	114.35
2	A	601	PLP	O4P-C5A-C5	3.79	115.26	108.99
2	B	601	PLP	O4P-C5A-C5	3.80	115.27	108.99
3	B	602	HEM	C3B-C4B-CHC	4.09	128.92	123.16
3	A	602	HEM	C3B-C4B-CHC	4.66	129.72	123.16
3	A	602	HEM	CAD-C3D-C2D	4.69	126.72	113.22
3	B	602	HEM	CMC-C2C-C3C	4.71	128.28	116.53
3	B	602	HEM	CAD-C3D-C2D	5.05	127.74	113.22
3	A	602	HEM	CMC-C2C-C3C	5.21	129.54	116.53
3	B	602	HEM	CMB-C2B-C3B	5.86	131.16	116.53
3	A	602	HEM	CMB-C2B-C3B	5.96	131.41	116.53
3	B	602	HEM	C2D-C3D-C4D	7.80	114.72	101.50
3	A	602	HEM	C2D-C3D-C4D	7.81	114.73	101.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	PLP	3	0
3	A	602	HEM	5	0
2	B	601	PLP	3	0
3	B	602	HEM	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	496/549 (90%)	1.00	60 (12%) 6 3	53, 93, 150, 202	0
1	B	496/549 (90%)	1.10	85 (17%) 2 1	46, 88, 142, 184	0
All	All	992/1098 (90%)	1.05	145 (14%) 3 1	46, 90, 147, 202	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	397	LEU	6.0
1	A	403	THR	5.7
1	B	403	THR	5.2
1	B	411	HIS	5.2
1	B	416	GLU	4.8
1	A	233	TYR	4.7
1	A	548	ARG	4.5
1	B	528	GLN	4.4
1	B	534	VAL	4.3
1	A	550	GLN	4.1
1	B	136	LEU	4.1
1	A	407	PRO	4.0
1	A	248	LEU	3.9
1	B	533	VAL	3.9
1	B	413	ARG	3.9
1	B	496	LEU	3.6
1	B	539	LEU	3.6
1	A	137	LYS	3.5
1	A	271	LYS	3.5
1	A	269	LYS	3.4
1	A	549	ASP	3.4
1	B	68	THR	3.3
1	A	56	LEU	3.3
1	B	262	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	417	LEU	3.3
1	B	451	GLU	3.3
1	A	251	LEU	3.2
1	B	542	PHE	3.1
1	B	409	TRP	3.1
1	B	417	LEU	3.1
1	B	412	LEU	3.1
1	A	305	GLY	3.0
1	B	410	TRP	3.0
1	A	278	ILE	3.0
1	B	529	MET	3.0
1	B	530	VAL	3.0
1	A	246	GLY	3.0
1	A	122	ILE	2.9
1	A	530	VAL	2.9
1	A	532	GLY	2.9
1	B	492	LEU	2.9
1	A	277	ILE	2.9
1	A	105	LEU	2.9
1	B	452	ALA	2.8
1	B	135	THR	2.8
1	A	514	GLU	2.8
1	B	408	TRP	2.8
1	A	42	LEU	2.7
1	B	222	GLN	2.7
1	A	293	LEU	2.7
1	B	284	GLY	2.7
1	B	348	GLY	2.7
1	B	414	VAL	2.7
1	A	43	TRP	2.7
1	A	427	PRO	2.6
1	B	248	LEU	2.6
1	B	67	HIS	2.6
1	A	109	CYS	2.6
1	A	481	LYS	2.6
1	B	77	LEU	2.6
1	B	541	ASN	2.6
1	A	124	LEU	2.6
1	B	400	GLU	2.6
1	A	319	VAL	2.6
1	B	298	GLN	2.5
1	A	479	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	46	PRO	2.5
1	B	51	ARG	2.5
1	B	394	LYS	2.5
1	A	539	LEU	2.5
1	A	254	SER	2.5
1	B	423	LEU	2.5
1	B	275	CYS	2.5
1	B	548	ARG	2.5
1	B	511	VAL	2.5
1	B	419	LEU	2.5
1	A	379	ARG	2.5
1	A	363	GLU	2.5
1	A	90	VAL	2.5
1	A	377	SER	2.4
1	B	443	PHE	2.4
1	B	63	SER	2.4
1	B	490	ILE	2.4
1	A	132	ARG	2.4
1	A	415	GLN	2.4
1	A	247	LYS	2.4
1	A	513	HIS	2.4
1	B	297	GLU	2.4
1	B	295	GLN	2.4
1	B	72	LYS	2.4
1	A	364	LEU	2.4
1	B	43	TRP	2.4
1	B	233	TYR	2.3
1	A	287	LEU	2.3
1	B	468	LEU	2.3
1	B	547	GLU	2.3
1	A	237	ALA	2.3
1	B	109	CYS	2.3
1	A	86	ASP	2.3
1	A	411	HIS	2.3
1	B	508	PHE	2.3
1	B	56	LEU	2.3
1	B	220	LEU	2.3
1	B	148	GLY	2.3
1	B	290	PRO	2.3
1	A	141	THR	2.2
1	B	299	THR	2.2
1	B	300	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	491	ARG	2.2
1	A	508	PHE	2.2
1	B	296	THR	2.2
1	B	258	GLY	2.2
1	A	366	GLU	2.2
1	B	393	GLN	2.2
1	B	487	PHE	2.2
1	B	493	THR	2.2
1	A	198	ASP	2.1
1	B	489	GLN	2.1
1	A	370	CYS	2.1
1	B	286	ILE	2.1
1	B	472	LYS	2.1
1	B	459	VAL	2.1
1	B	99	PHE	2.1
1	B	399	GLU	2.1
1	B	103	CYS	2.1
1	B	499	LEU	2.1
1	B	55	GLN	2.1
1	A	77	LEU	2.1
1	A	101	LEU	2.1
1	A	510	LEU	2.1
1	A	444	ASP	2.1
1	B	76	ILE	2.1
1	B	257	THR	2.1
1	A	456	LEU	2.1
1	B	482	VAL	2.1
1	B	544	ALA	2.1
1	A	272	CYS	2.0
1	B	494	ASP	2.0
1	B	319	VAL	2.0
1	A	123	SER	2.0
1	A	475	PRO	2.0
1	B	264	ILE	2.0
1	A	378	VAL	2.0
1	B	396	PHE	2.0
1	B	512	VAL	2.0

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

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(\AA^2)	Q<0.9
3	HEM	B	602	43/43	0.92	0.34	0.77	101,104,104,104	0
3	HEM	A	602	43/43	0.93	0.29	0.61	107,108,109,109	0
2	PLP	B	601	15/16	0.90	0.22	-0.70	53,66,75,76	0
2	PLP	A	601	15/16	0.92	0.20	-1.23	58,75,85,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.