Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 10:31 PM JST

PDB ID	:	6AH8
Title	:	Marine bacterial prolidase with promiscuous organophosphorus hydrolase activity
Authors	:	Jian, Y.
Deposited on	:	2018-08-17
Resolution	:	2.61 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:

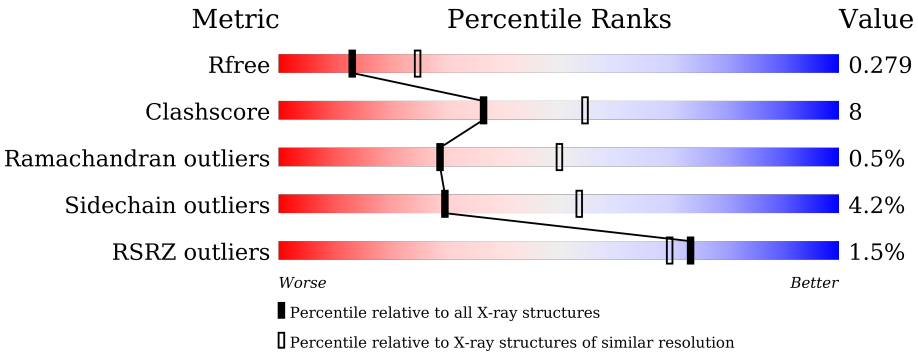
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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}	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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 <=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	448	83% 13%
1	B	448	80% 16%
1	C	448	81% 15%
1	D	448	3% 73% 23%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14361 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 Xaa-Pro dipeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3563	2288	606	655	14			
1	B	439	Total	C	N	O	S	0	0	0
			3563	2288	606	655	14			
1	C	439	Total	C	N	O	S	0	0	0
			3563	2288	606	655	14			
1	D	439	Total	C	N	O	S	0	0	0
			3563	2288	606	655	14			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	441	LEU	-	expression tag	UNP A0A1I7CHQ2
A	442	ASP	-	expression tag	UNP A0A1I7CHQ2
A	443	HIS	-	expression tag	UNP A0A1I7CHQ2
A	444	HIS	-	expression tag	UNP A0A1I7CHQ2
A	445	HIS	-	expression tag	UNP A0A1I7CHQ2
A	446	HIS	-	expression tag	UNP A0A1I7CHQ2
A	447	HIS	-	expression tag	UNP A0A1I7CHQ2
A	448	HIS	-	expression tag	UNP A0A1I7CHQ2
B	441	LEU	-	expression tag	UNP A0A1I7CHQ2
B	442	ASP	-	expression tag	UNP A0A1I7CHQ2
B	443	HIS	-	expression tag	UNP A0A1I7CHQ2
B	444	HIS	-	expression tag	UNP A0A1I7CHQ2
B	445	HIS	-	expression tag	UNP A0A1I7CHQ2
B	446	HIS	-	expression tag	UNP A0A1I7CHQ2
B	447	HIS	-	expression tag	UNP A0A1I7CHQ2
B	448	HIS	-	expression tag	UNP A0A1I7CHQ2
C	441	LEU	-	expression tag	UNP A0A1I7CHQ2
C	442	ASP	-	expression tag	UNP A0A1I7CHQ2
C	443	HIS	-	expression tag	UNP A0A1I7CHQ2
C	444	HIS	-	expression tag	UNP A0A1I7CHQ2
C	445	HIS	-	expression tag	UNP A0A1I7CHQ2

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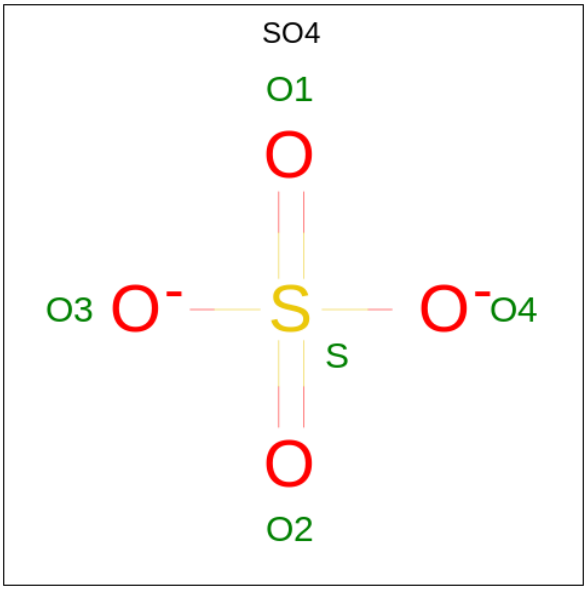
Chain	Residue	Modelled	Actual	Comment	Reference
C	446	HIS	-	expression tag	UNP A0A1I7CHQ2
C	447	HIS	-	expression tag	UNP A0A1I7CHQ2
C	448	HIS	-	expression tag	UNP A0A1I7CHQ2
D	441	LEU	-	expression tag	UNP A0A1I7CHQ2
D	442	ASP	-	expression tag	UNP A0A1I7CHQ2
D	443	HIS	-	expression tag	UNP A0A1I7CHQ2
D	444	HIS	-	expression tag	UNP A0A1I7CHQ2
D	445	HIS	-	expression tag	UNP A0A1I7CHQ2
D	446	HIS	-	expression tag	UNP A0A1I7CHQ2
D	447	HIS	-	expression tag	UNP A0A1I7CHQ2
D	448	HIS	-	expression tag	UNP A0A1I7CHQ2

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mn 2 2	0	0
2	B	2	Total Mn 2 2	0	0
2	C	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

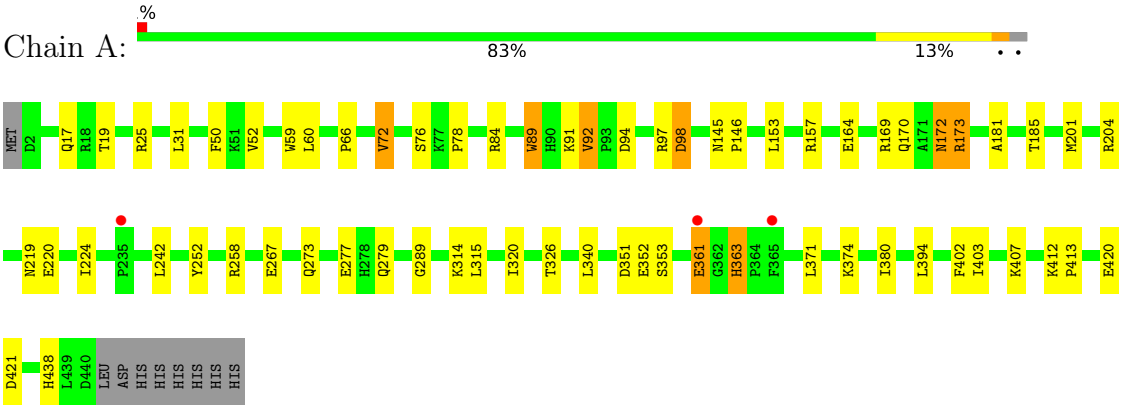
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	42	Total O 42 42	0	0
4	B	22	Total O 22 22	0	0
4	C	15	Total O 15 15	0	0
4	D	7	Total O 7 7	0	0

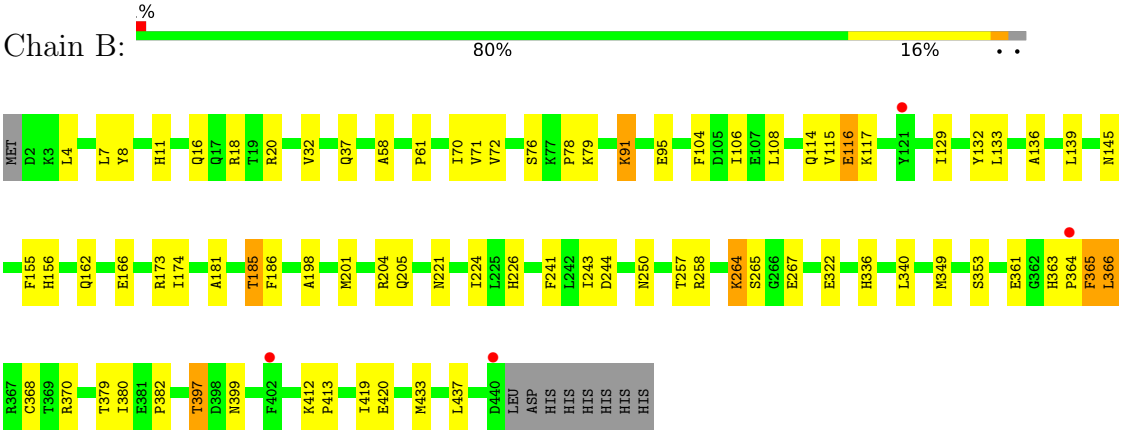
3 Residue-property plots (i)

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.

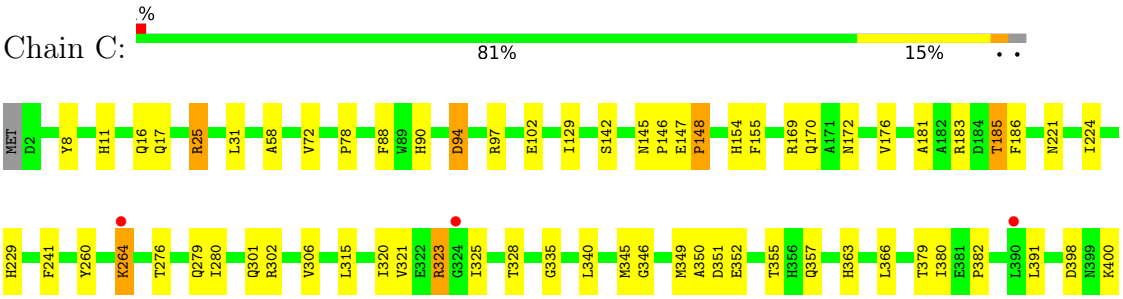
• Molecule 1: Xaa-Pro dipeptidase



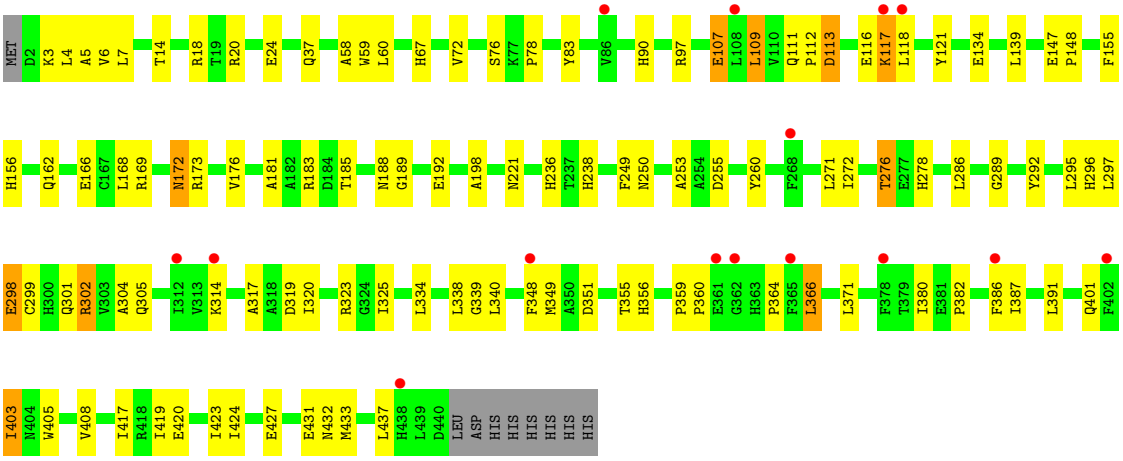
• Molecule 1: Xaa-Pro dipeptidase



• Molecule 1: Xaa-Pro dipeptidase



• Molecule 1: Xaa-Pro dipeptidase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	178.85Å 178.85Å 371.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.53 – 2.61 44.49 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.53-2.61) 99.8 (44.49-2.61)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.226 , 0.279 0.227 , 0.279	Depositor DCC
R_{free} test set	3493 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	54.8	Xtriage
Anisotropy	0.583	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 33.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14361	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MN, SO4

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	0/3665	0.58	0/4976
1	B	0.41	0/3665	0.57	0/4976
1	C	0.39	0/3665	0.57	0/4976
1	D	0.42	0/3665	0.59	0/4976
All	All	0.40	0/14660	0.58	0/19904

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	4
1	B	0	1
1	C	0	3
1	D	0	1
All	All	0	9

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	ARG	Sidechain
1	A	173	ARG	Sidechain
1	A	258	ARG	Sidechain
1	A	84	ARG	Sidechain
1	B	258	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	169	ARG	Sidechain
1	C	323	ARG	Sidechain
1	C	438	HIS	Peptide
1	D	173	ARG	Sidechain

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	3563	0	3421	45	0
1	B	3563	0	3421	59	0
1	C	3563	0	3421	43	0
1	D	3563	0	3421	82	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	5	0	0	0	0
3	C	10	0	0	0	0
4	A	42	0	0	3	0
4	B	22	0	0	0	0
4	C	15	0	0	0	0
4	D	7	0	0	0	0
All	All	14361	0	13684	220	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 8.

All (220) 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:B:116:GLU:HG3	1:B:139:LEU:CD2	1.80	1.09
1:C:350:ALA:HB2	1:C:357:GLN:HG2	1.36	1.06
1:B:116:GLU:HG3	1:B:139:LEU:HD23	1.04	1.03
1:A:91:LYS:HG3	1:B:224:ILE:CD1	1.91	1.00
1:A:91:LYS:HG3	1:B:224:ILE:HD13	1.44	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:GLU:CG	1:B:139:LEU:HD23	1.95	0.96
1:C:351:ASP:OD2	1:C:355:THR:HG22	1.67	0.94
1:C:25:ARG:NH2	1:C:352:GLU:OE1	2.00	0.94
1:C:351:ASP:OD2	1:C:355:THR:CG2	2.22	0.86
1:B:366:LEU:CD1	1:B:368:CYS:O	2.28	0.82
1:D:299:CYS:HB2	1:D:334:LEU:HD13	1.64	0.79
1:D:297:LEU:O	1:D:301:GLN:HG2	1.85	0.76
1:B:264:LYS:HE2	1:B:264:LYS:O	1.87	0.74
1:D:302:ARG:HA	1:D:305:GLN:HG3	1.68	0.74
1:B:181:ALA:O	1:B:185:THR:HG23	1.87	0.74
1:D:113:ASP:OD1	1:D:113:ASP:N	2.18	0.73
1:D:59:TRP:CH2	1:D:72:VAL:HG21	2.22	0.73
1:C:279:GLN:OE1	1:C:435:ARG:NH1	2.22	0.73
1:D:391:LEU:HD21	1:D:408:VAL:HG21	1.72	0.71
1:B:433:MET:O	1:B:437:LEU:HD13	1.90	0.71
1:D:18:ARG:NH1	1:D:156:HIS:O	2.25	0.69
1:A:181:ALA:O	1:A:185:THR:HG23	1.93	0.68
1:C:72:VAL:HG12	1:C:78:PRO:HB3	1.75	0.68
1:D:296:HIS:CG	1:D:366:LEU:HD11	2.29	0.68
1:D:298:GLU:O	1:D:301:GLN:O	2.12	0.67
1:D:72:VAL:HG23	1:D:78:PRO:HB3	1.77	0.66
1:D:107:GLU:HG2	1:D:118:LEU:HD13	1.75	0.66
1:C:181:ALA:O	1:C:185:THR:HG23	1.95	0.66
1:D:338:LEU:HD23	1:D:339:GLY:N	2.11	0.66
1:A:315:LEU:HD21	1:A:402:PHE:CD1	2.30	0.65
1:B:16:GLN:NE2	1:B:78:PRO:HD3	2.11	0.65
1:D:278:HIS:ND1	1:D:302:ARG:HG2	2.12	0.64
1:A:91:LYS:HG3	1:B:224:ILE:HD11	1.76	0.64
1:C:351:ASP:CG	1:C:355:THR:HG22	2.16	0.64
1:A:201:MET:CE	1:A:204:ARG:HH12	2.10	0.64
1:B:181:ALA:O	1:B:185:THR:CG2	2.46	0.64
1:D:391:LEU:CD2	1:D:408:VAL:HG21	2.27	0.64
1:C:350:ALA:CB	1:C:357:GLN:HG2	2.21	0.63
1:A:201:MET:HE2	1:A:204:ARG:HH12	1.63	0.63
1:D:302:ARG:CA	1:D:305:GLN:HG3	2.28	0.63
1:A:98:ASP:OD1	4:A:601:HOH:O	2.16	0.61
1:D:172:ASN:O	1:D:176:VAL:HG23	2.00	0.61
1:D:116:GLU:HB2	1:D:139:LEU:HD22	1.84	0.60
1:C:323:ARG:HB2	1:C:325:ILE:HG13	1.83	0.59
1:A:72:VAL:HG23	1:A:78:PRO:HB3	1.83	0.59
1:A:320:ILE:HG22	1:A:326:THR:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:MET:O	1:D:437:LEU:HD12	2.03	0.59
1:D:109:LEU:CD2	1:D:111:GLN:H	2.15	0.59
1:A:394:LEU:CD2	1:A:403:ILE:HG13	2.33	0.59
1:A:201:MET:O	1:A:204:ARG:HD2	2.03	0.59
1:B:366:LEU:HD12	1:B:368:CYS:O	2.03	0.59
1:A:394:LEU:HD21	1:A:403:ILE:HG13	1.85	0.58
1:D:403:ILE:HD11	1:D:405:TRP:CZ3	2.40	0.57
1:C:346:GLY:HA2	1:C:349:MET:CE	2.33	0.56
1:D:3:LYS:O	1:D:6:VAL:HG22	2.05	0.56
1:B:7:LEU:HD22	1:B:162:GLN:HB3	1.86	0.56
1:D:189:GLY:HA2	1:D:238:HIS:NE2	2.21	0.56
1:D:192:GLU:OE2	1:D:221:ASN:ND2	2.34	0.56
1:C:315:LEU:HD11	1:C:402:PHE:CD2	2.41	0.56
1:D:386:PHE:HD2	1:D:408:VAL:HG23	1.71	0.56
1:D:168:LEU:HD21	1:D:339:GLY:HA2	1.88	0.56
1:B:37:GLN:HB2	1:B:132:TYR:CZ	2.41	0.56
1:B:366:LEU:HD11	1:B:368:CYS:O	2.03	0.56
1:D:155:PHE:HB2	1:D:349:MET:HE1	1.88	0.55
1:D:292:TYR:CZ	1:D:334:LEU:HD23	2.42	0.55
1:D:299:CYS:HB2	1:D:334:LEU:CD1	2.35	0.55
1:D:403:ILE:HD11	1:D:405:TRP:CE3	2.43	0.54
1:B:264:LYS:O	1:B:264:LYS:HG3	2.06	0.54
1:D:278:HIS:ND1	1:D:302:ARG:HD3	2.22	0.54
1:B:173:ARG:HA	1:B:437:LEU:HD23	1.89	0.54
1:C:186:PHE:CE1	1:C:241:PHE:HB2	2.42	0.54
1:D:380:ILE:HG22	1:D:382:PRO:HD3	1.90	0.54
1:D:271:LEU:HD22	1:D:417:ILE:HD12	1.90	0.53
1:D:83:TYR:CE1	1:D:112:PRO:HD3	2.44	0.53
1:C:346:GLY:HA2	1:C:349:MET:HE2	1.91	0.53
1:C:301:GLN:HA	1:C:321:VAL:HG21	1.91	0.53
1:A:224:ILE:HD13	1:B:91:LYS:HB3	1.90	0.53
1:D:58:ALA:HA	1:D:340:LEU:HD11	1.90	0.52
1:D:116:GLU:HB2	1:D:139:LEU:CD2	2.40	0.52
1:C:320:ILE:HA	1:C:325:ILE:HD12	1.90	0.52
1:C:58:ALA:HA	1:C:340:LEU:HD11	1.93	0.51
1:D:109:LEU:HD22	1:D:111:GLN:H	1.75	0.51
1:B:173:ARG:HA	1:B:437:LEU:CD2	2.40	0.51
1:A:89:TRP:CD1	1:A:89:TRP:N	2.79	0.51
1:D:286:LEU:HD23	1:D:295:LEU:HD11	1.92	0.51
1:A:412:LYS:N	1:A:413:PRO:HD2	2.26	0.51
1:B:380:ILE:O	1:B:420:GLU:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:LEU:HD23	1:D:295:LEU:CD1	2.40	0.51
1:D:278:HIS:ND1	1:D:302:ARG:CG	2.74	0.51
1:A:25:ARG:NH1	1:A:352:GLU:OE1	2.31	0.50
1:A:59:TRP:CH2	1:A:72:VAL:HG21	2.47	0.50
1:A:314:LYS:O	1:A:315:LEU:HD23	2.11	0.50
1:A:380:ILE:O	1:A:420:GLU:HA	2.12	0.50
1:D:278:HIS:CE1	1:D:302:ARG:HG2	2.47	0.50
1:A:289:GLY:HA2	1:A:371:LEU:HD11	1.94	0.50
1:B:104:PHE:HB2	1:B:106:ILE:HD11	1.93	0.50
1:D:3:LYS:O	1:D:7:LEU:HD12	2.11	0.50
1:B:58:ALA:HA	1:B:340:LEU:HD11	1.94	0.50
1:B:349:MET:O	1:B:370:ARG:HD2	2.12	0.50
1:A:91:LYS:CG	1:B:224:ILE:HD13	2.30	0.49
1:B:174:ILE:HG21	1:B:205:GLN:HE21	1.78	0.49
1:A:394:LEU:HD21	1:A:403:ILE:CG1	2.42	0.49
1:B:71:VAL:CG2	1:B:79:LYS:HB3	2.42	0.49
1:C:176:VAL:HG13	1:C:439:LEU:HB2	1.95	0.48
1:A:351:ASP:OD1	1:A:353:SER:OG	2.23	0.48
1:D:272:ILE:O	1:D:276:THR:HG22	2.14	0.48
1:C:186:PHE:CD1	1:C:241:PHE:HB2	2.48	0.48
1:B:185:THR:HG21	1:B:198:ALA:CB	2.43	0.48
1:A:89:TRP:HE3	1:B:226:HIS:HD1	1.62	0.48
1:A:50:PHE:CE1	1:A:66:PRO:HB3	2.49	0.48
1:C:351:ASP:OD2	1:C:355:THR:HG21	2.08	0.48
1:A:242:LEU:C	1:A:242:LEU:HD23	2.35	0.47
1:D:189:GLY:HA2	1:D:238:HIS:CD2	2.48	0.47
1:C:412:LYS:N	1:C:413:PRO:CD	2.78	0.47
1:D:253:ALA:O	1:D:338:LEU:HD21	2.14	0.47
1:B:32:VAL:HG22	1:B:71:VAL:HG12	1.95	0.47
1:A:52:VAL:O	4:A:602:HOH:O	2.20	0.47
1:C:380:ILE:HG22	1:C:382:PRO:HD3	1.96	0.47
1:A:31:LEU:HD12	1:A:72:VAL:HG12	1.96	0.47
1:D:97:ARG:O	1:D:97:ARG:CG	2.62	0.47
1:A:273:GLN:O	1:A:277:GLU:HG2	2.15	0.47
1:B:382:PRO:HD2	1:B:419:ILE:O	2.15	0.46
1:A:363:HIS:ND1	1:A:363:HIS:N	2.62	0.46
1:D:7:LEU:HD23	1:D:162:GLN:HB3	1.96	0.46
1:A:219:ASN:HB3	1:A:413:PRO:O	2.15	0.46
1:B:366:LEU:HD13	1:B:368:CYS:N	2.30	0.46
1:D:181:ALA:O	1:D:185:THR:HG23	2.14	0.46
1:D:14:THR:HG22	1:D:18:ARG:HH21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:PHE:N	1:C:349:MET:HE1	2.31	0.46
1:C:276:THR:O	1:C:280:ILE:HG13	2.16	0.46
1:D:296:HIS:O	1:D:299:CYS:HB3	2.15	0.46
1:A:19:THR:HG21	1:A:72:VAL:HG13	1.98	0.46
1:B:18:ARG:NH1	1:B:156:HIS:O	2.50	0.45
1:B:186:PHE:CD1	1:B:241:PHE:HB2	2.52	0.45
1:A:172:ASN:ND2	4:A:606:HOH:O	2.49	0.45
1:C:221:ASN:HA	1:C:224:ILE:HD13	1.97	0.45
1:C:264:LYS:HD2	1:C:264:LYS:O	2.17	0.45
1:B:95:GLU:HG2	1:B:108:LEU:HD11	1.98	0.45
1:C:335:GLY:HA3	1:C:379:THR:O	2.16	0.45
1:D:271:LEU:O	1:D:271:LEU:HD23	2.17	0.45
1:D:292:TYR:CE1	1:D:334:LEU:HD23	2.51	0.45
1:D:320:ILE:HG12	1:D:325:ILE:HD11	1.98	0.45
1:B:201:MET:O	1:B:204:ARG:HD2	2.17	0.45
1:B:363:HIS:N	1:B:364:PRO:HD3	2.31	0.45
1:B:61:PRO:HB3	1:B:250:ASN:HB3	1.98	0.45
1:B:336:HIS:CE1	1:B:379:THR:HG21	2.52	0.45
1:A:220:GLU:OE2	1:A:413:PRO:HA	2.16	0.45
1:B:365:PHE:O	1:B:365:PHE:CG	2.70	0.45
1:A:91:LYS:HE3	1:B:221:ASN:OD1	2.17	0.44
1:A:157:ARG:NE	1:A:340:LEU:HD12	2.32	0.44
1:D:4:LEU:HD12	1:D:5:ALA:N	2.32	0.44
1:D:249:PHE:CE2	1:D:250:ASN:ND2	2.86	0.44
1:D:380:ILE:HD13	1:D:423:ILE:HD12	1.99	0.44
1:D:304:ALA:HA	1:D:320:ILE:HG21	2.00	0.44
1:A:92:VAL:HG22	1:A:92:VAL:O	2.16	0.44
1:A:145:ASN:N	1:A:146:PRO:CD	2.81	0.44
1:D:60:LEU:HD23	1:D:60:LEU:N	2.33	0.44
1:B:4:LEU:HD12	1:B:166:GLU:HB3	1.99	0.44
1:C:391:LEU:HD13	1:C:408:VAL:HG11	2.00	0.44
1:A:361:GLU:CD	1:A:361:GLU:N	2.70	0.44
1:D:37:GLN:HG2	1:D:67:HIS:NE2	2.33	0.44
1:B:412:LYS:N	1:B:413:PRO:CD	2.81	0.43
1:C:155:PHE:HA	1:C:349:MET:HE3	2.01	0.43
1:C:94:ASP:N	1:C:94:ASP:OD1	2.52	0.43
1:B:7:LEU:HD22	1:B:162:GLN:CB	2.48	0.43
1:B:129:ILE:HA	1:B:145:ASN:OD1	2.18	0.43
1:B:133:LEU:O	1:B:136:ALA:HB3	2.19	0.43
1:D:20:ARG:O	1:D:24:GLU:HB2	2.17	0.43
1:C:88:PHE:HB2	1:D:387:ILE:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:ARG:O	1:C:306:VAL:HG23	2.18	0.43
1:A:267:GLU:OE2	1:A:407:LYS:NZ	2.51	0.43
1:C:147:GLU:N	1:C:148:PRO:HD2	2.34	0.43
1:B:155:PHE:N	1:B:349:MET:HE1	2.33	0.42
1:B:8:TYR:O	1:B:11:HIS:HB3	2.18	0.42
1:D:317:ALA:O	1:D:320:ILE:HB	2.18	0.42
1:B:397:THR:HG23	1:B:399:ASN:H	1.82	0.42
1:D:166:GLU:HG2	1:D:169:ARG:HH11	1.83	0.42
1:C:279:GLN:HE22	1:C:421:ASP:CG	2.22	0.42
1:C:407:LYS:O	1:C:410:GLU:HB2	2.18	0.42
1:D:380:ILE:O	1:D:420:GLU:HA	2.20	0.42
1:D:147:GLU:N	1:D:148:PRO:CD	2.83	0.42
1:D:424:ILE:HB	1:D:431:GLU:HB3	2.02	0.42
1:C:183:ARG:HG3	1:C:260:TYR:CE2	2.54	0.42
1:D:289:GLY:CA	1:D:371:LEU:HD11	2.50	0.42
1:D:183:ARG:HG3	1:D:260:TYR:CE2	2.55	0.42
1:D:351:ASP:OD2	1:D:355:THR:CG2	2.68	0.42
1:C:129:ILE:HA	1:C:145:ASN:OD1	2.20	0.42
1:D:185:THR:HG21	1:D:198:ALA:CB	2.50	0.42
1:A:438:HIS:NE2	1:C:438:HIS:NE2	2.69	0.41
1:C:154:HIS:CD2	1:C:345:MET:HG3	2.55	0.41
1:A:60:LEU:N	1:A:60:LEU:HD23	2.36	0.41
1:D:276:THR:HB	1:D:419:ILE:HD13	2.01	0.41
1:D:338:LEU:HD23	1:D:338:LEU:C	2.40	0.41
1:C:145:ASN:N	1:C:146:PRO:CD	2.83	0.41
1:D:289:GLY:HA2	1:D:371:LEU:HD11	2.02	0.41
1:B:244:ASP:CG	1:B:257:THR:OG1	2.59	0.41
1:C:16:GLN:NE2	1:C:78:PRO:HD3	2.36	0.41
1:D:271:LEU:HD22	1:D:417:ILE:CD1	2.49	0.41
1:B:32:VAL:HA	1:B:70:ILE:O	2.19	0.41
1:B:72:VAL:HG12	1:B:78:PRO:HB3	2.03	0.41
1:C:8:TYR:O	1:C:11:HIS:HB3	2.21	0.41
1:D:60:LEU:HD23	1:D:60:LEU:H	1.85	0.41
1:D:319:ASP:O	1:D:323:ARG:HG2	2.21	0.41
1:D:380:ILE:HD13	1:D:423:ILE:CD1	2.50	0.41
1:D:134:GLU:H	1:D:134:GLU:CD	2.24	0.41
1:B:115:VAL:C	1:B:117:LYS:H	2.24	0.41
1:B:155:PHE:CD1	1:B:370:ARG:NH1	2.89	0.41
1:B:241:PHE:CE1	1:B:243:ILE:HB	2.56	0.41
1:D:116:GLU:OE2	1:D:139:LEU:O	2.38	0.41
1:C:366:LEU:HD23	1:C:366:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:386:PHE:CD2	1:D:408:VAL:HG23	2.54	0.41
1:B:115:VAL:C	1:B:117:LYS:N	2.75	0.40
1:B:365:PHE:CD1	1:B:365:PHE:C	2.92	0.40
1:D:359:PRO:CG	1:D:364:PRO:HA	2.51	0.40
1:B:264:LYS:HE2	1:B:264:LYS:C	2.41	0.40
1:D:4:LEU:HD12	1:D:4:LEU:C	2.41	0.40
1:A:279:GLN:HE22	1:A:421:ASP:CG	2.25	0.40
1:A:164:GLU:HG2	1:A:252:TYR:CZ	2.57	0.40
1:B:264:LYS:O	1:B:264:LYS:CG	2.69	0.40
1:D:348:PHE:CE2	1:D:356:HIS:HB3	2.56	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	437/448 (98%)	417 (95%)	20 (5%)	0	100 100
1	B	437/448 (98%)	419 (96%)	16 (4%)	2 (0%)	29 50
1	C	437/448 (98%)	414 (95%)	23 (5%)	0	100 100
1	D	437/448 (98%)	403 (92%)	28 (6%)	6 (1%)	11 21
All	All	1748/1792 (98%)	1653 (95%)	87 (5%)	8 (0%)	29 50

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	117	LYS
1	D	302	ARG
1	B	361	GLU
1	B	116	GLU
1	D	255	ASP

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Mol	Chain	Res	Type
1	D	401	GLN
1	D	432	ASN
1	D	360	PRO

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	378/387 (98%)	363 (96%)	15 (4%)	31	55
1	B	378/387 (98%)	365 (97%)	13 (3%)	37	61
1	C	378/387 (98%)	358 (95%)	20 (5%)	22	43
1	D	378/387 (98%)	362 (96%)	16 (4%)	30	53
All	All	1512/1548 (98%)	1448 (96%)	64 (4%)	30	53

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	72	VAL
1	A	76	SER
1	A	89	TRP
1	A	92	VAL
1	A	94	ASP
1	A	97	ARG
1	A	98	ASP
1	A	153	LEU
1	A	170	GLN
1	A	172	ASN
1	A	173	ARG
1	A	361	GLU
1	A	363	HIS
1	A	374	LYS
1	B	20	ARG
1	B	76	SER
1	B	91	LYS

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Mol	Chain	Res	Type
1	B	114	GLN
1	B	185	THR
1	B	264	LYS
1	B	265	SER
1	B	267	GLU
1	B	322	GLU
1	B	353	SER
1	B	365	PHE
1	B	366	LEU
1	B	397	THR
1	C	17	GLN
1	C	25	ARG
1	C	31	LEU
1	C	90	HIS
1	C	94	ASP
1	C	97	ARG
1	C	102	GLU
1	C	142	SER
1	C	148	PRO
1	C	170	GLN
1	C	172	ASN
1	C	185	THR
1	C	229	HIS
1	C	264	LYS
1	C	328	THR
1	C	363	HIS
1	C	398	ASP
1	C	400	LYS
1	C	435	ARG
1	C	439	LEU
1	D	76	SER
1	D	90	HIS
1	D	107	GLU
1	D	109	LEU
1	D	113	ASP
1	D	117	LYS
1	D	121	TYR
1	D	172	ASN
1	D	188	ASN
1	D	236	HIS
1	D	276	THR
1	D	298	GLU

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Mol	Chain	Res	Type
1	D	314	LYS
1	D	366	LEU
1	D	403	ILE
1	D	427	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 for Mogul analysis.

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	SO4	C	504	-	4,4,4	0.38	0	6,6,6	0.32	0
3	SO4	A	503	-	4,4,4	0.34	0	6,6,6	0.18	0
3	SO4	C	503	-	4,4,4	0.36	0	6,6,6	0.30	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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, 95^{th} 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	439/448 (97%)	-0.34	3 (0%)	87	85	42, 60, 89, 121	0
1	B	439/448 (97%)	-0.17	4 (0%)	84	82	43, 70, 100, 127	0
1	C	439/448 (97%)	-0.14	4 (0%)	84	82	42, 70, 115, 139	0
1	D	439/448 (97%)	0.11	15 (3%)	45	38	53, 86, 118, 153	0
All	All	1756/1792 (97%)	-0.13	26 (1%)	73	70	42, 71, 110, 153	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	314	LYS	4.6
1	A	365	PHE	4.5
1	D	402	PHE	4.2
1	B	121	TYR	3.7
1	D	438	HIS	3.5
1	D	118	LEU	3.3
1	C	324	GLY	3.1
1	B	440	ASP	2.8
1	D	361	GLU	2.8
1	D	86	VAL	2.7
1	D	312	ILE	2.7
1	D	108	LEU	2.6
1	A	361	GLU	2.5
1	C	264	LYS	2.5
1	D	348	PHE	2.4
1	D	386	PHE	2.4
1	B	402	PHE	2.3
1	D	117	LYS	2.3
1	D	365	PHE	2.3
1	D	268	PHE	2.2
1	C	390	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	378	PHE	2.2
1	D	362	GLY	2.1
1	C	439	LEU	2.1
1	A	235	PRO	2.1
1	B	364	PRO	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 monosaccharides 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, 95^{th} 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
3	SO4	A	503	5/5	0.90	0.12	83,92,99,105	0
3	SO4	C	504	5/5	0.95	0.11	107,108,110,111	0
2	MN	D	501	1/1	0.96	0.14	99,99,99,99	0
3	SO4	C	503	5/5	0.97	0.09	72,78,84,85	0
2	MN	A	502	1/1	0.97	0.14	80,80,80,80	0
2	MN	C	502	1/1	0.98	0.16	92,92,92,92	0
2	MN	A	501	1/1	0.98	0.13	64,64,64,64	0
2	MN	D	502	1/1	0.98	0.15	80,80,80,80	0
2	MN	B	501	1/1	0.98	0.18	85,85,85,85	0
2	MN	B	502	1/1	0.98	0.13	80,80,80,80	0
2	MN	C	501	1/1	0.98	0.15	70,70,70,70	0

6.5 Other polymers (i)

There are no such residues in this entry.