



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:54 am BST

PDB ID : 5MFM
Title : Designed armadillo repeat protein peptide fusion YIIIM6AII_GS11_(KR)5
Authors : Hansen, S.; Ernst, P.; Reichen, C.; Ewald, C.; Mittl, P.; Plueckthun, A.
Deposited on : 2016-11-18
Resolution : 2.30 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 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 : 2.11
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) : 2.11

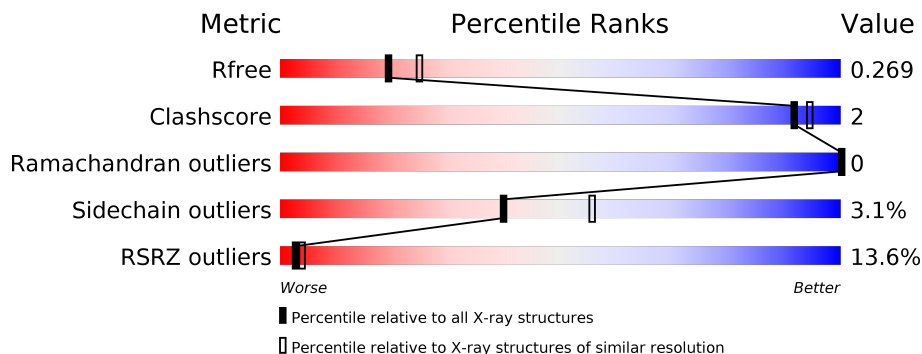
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	348	 4% 93% . .
1	B	348	 7% 93% . .
1	D	348	 15% 87% 8% .
1	E	348	 12% 88% 7% .
1	F	348	 12% 91% 5% .
1	P	348	 12% 9% . 88%

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Mol	Chain	Length	Quality of chain
1	Q	348	
2	C	350	

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
4	EDO	A	406	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 16466 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 YIIIM6AII_GS11_(KR)5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	335	Total 2589	C 1610	N 467	O 511	S 1	0	10	0
1	B	333	Total 2579	C 1605	N 465	O 508	S 1	0	10	0
1	D	333	Total 2585	C 1608	N 466	O 510	S 1	0	11	0
1	E	333	Total 2579	C 1605	N 465	O 508	S 1	0	10	0
1	F	334	Total 2492	C 1552	N 438	O 501	S 1	0	1	0
1	P	42	Total 321	C 194	N 58	O 69		0	0	0
1	Q	42	Total 321	C 194	N 58	O 69		0	0	0

- Molecule 2 is a protein called Importin subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	334	Total 2585	C 1608	N 466	O 510	S 1	0	10	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total 4	Ca 4	0	0
3	A	5	Total 5	Ca 5	0	0
3	D	7	Total 7	Ca 7	0	0
3	C	7	Total 7	Ca 7	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Mg 1 1	0	0
5	E	2	Total Mg 2 2	0	0
5	B	2	Total Mg 2 2	0	0
5	C	2	Total Mg 2 2	0	0
5	A	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	73	Total	O	0	0
			73	73		
6	B	57	Total	O	0	0
			57	57		
6	C	62	Total	O	0	0
			62	62		
6	D	38	Total	O	0	0
			38	38		
6	E	55	Total	O	0	0
			55	55		
6	F	64	Total	O	0	0
			64	64		
6	P	3	Total	O	0	0
			3	3		
6	Q	6	Total	O	0	0
			6	6		

3 Residue-property plots [i](#)

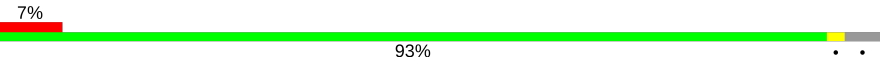
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

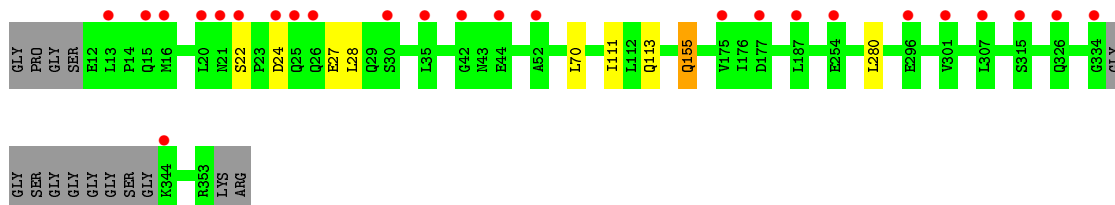
- Molecule 1: YIIIM6AII_GS11_(KR)5

Chain A: 




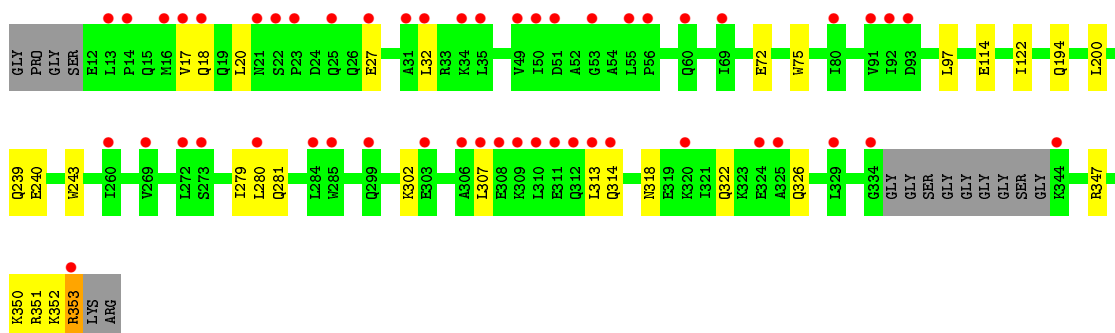
- Molecule 1: YIIIM6AII_GS11_(KR)5

Chain B: 




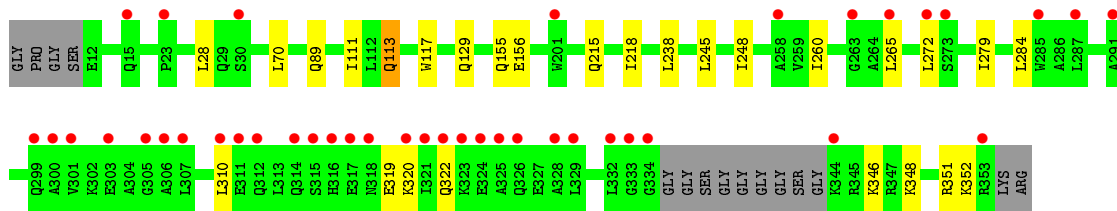
- Molecule 1: YIIIM6AII_GS11_(KR)5

Chain D: 

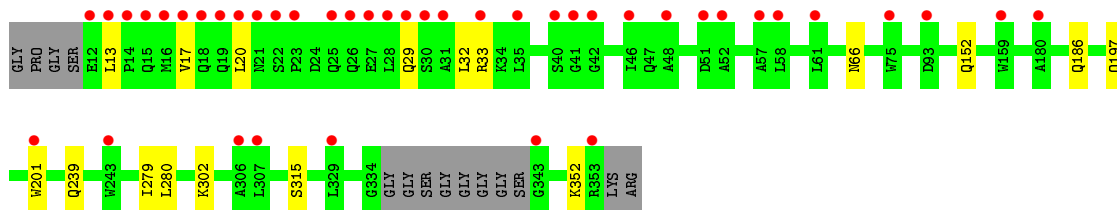
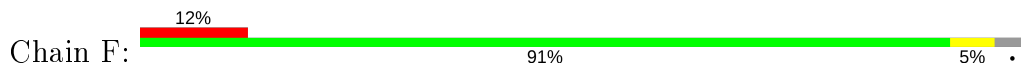


- Molecule 1: YIIIM6AII_GS11_(KR)5

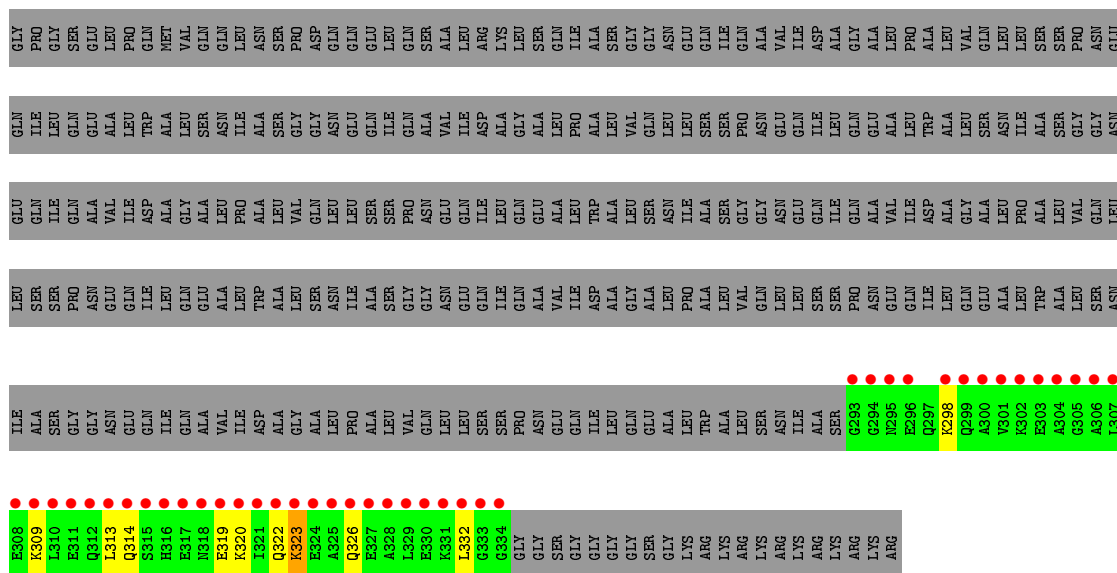
Chain E: 



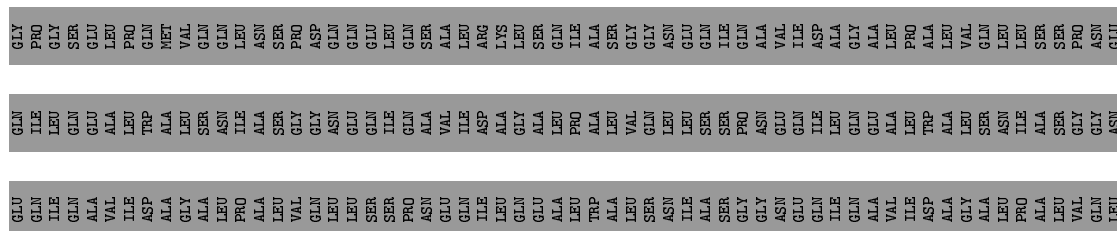
• Molecule 1: YIIIM6AII_GS11_(KR)5



• Molecule 1: YIIIM6AII_GS11_(KR)5



• Molecule 1: YIIIM6AII_GS11_(KR)5



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.76Å 89.39Å 123.85Å 90.00° 97.07° 90.00°	Depositor
Resolution (Å)	44.69 – 2.30 44.69 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (44.69-2.30) 98.6 (44.69-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.29Å)	Xtrriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.217 , 0.251 0.234 , 0.269	Depositor DCC
R_{free} test set	3887 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtrriage
Anisotropy	0.212	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16466	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4386e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MG, EDO

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	0.39	0/2613	0.55	0/3536
1	B	0.39	0/2603	0.56	0/3523
1	D	0.39	0/2609	0.54	0/3531
1	E	0.38	0/2603	0.55	0/3523
1	F	0.40	0/2517	0.55	0/3418
1	P	0.36	0/321	0.62	0/424
1	Q	0.41	0/321	0.60	0/424
2	C	0.39	0/2609	0.56	0/3531
All	All	0.39	0/16196	0.56	0/21910

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	2589	0	2658	6	0
1	B	2579	0	2650	3	0
1	D	2585	0	2654	13	0
1	E	2579	0	2650	13	0
1	F	2492	0	2531	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	321	0	318	3	0
1	Q	321	0	318	4	0
2	C	2585	0	2655	11	0
3	A	5	0	0	0	0
3	B	4	0	0	0	0
3	C	7	0	0	0	0
3	D	7	0	0	0	0
4	A	4	0	6	0	0
4	D	4	0	6	0	0
4	F	16	0	24	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
6	A	73	0	0	0	0
6	B	57	0	0	0	0
6	C	62	0	0	0	0
6	D	38	0	0	0	0
6	E	55	0	0	0	0
6	F	64	0	0	0	0
6	P	3	0	0	0	0
6	Q	6	0	0	0	0
All	All	16466	0	16470	52	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 2.

All (52) 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:D:352[A]:LYS:HB2	1:F:352:LYS:HB2	1.82	0.60
1:D:350[B]:LYS:HB2	1:F:352:LYS:HB2	1.83	0.60
1:E:113:GLN:HG2	1:E:156:GLU:HG3	1.86	0.57
1:D:32:LEU:HB3	1:D:72:GLU:HG2	1.87	0.55
2:C:302:LYS:HE3	1:Q:297:GLN:HG3	1.88	0.55
1:D:314:GLN:HE21	1:D:326:GLN:HG3	1.74	0.52
1:A:113:GLN:HG2	1:A:156:GLU:HG3	1.89	0.52
2:C:156:GLU:HA	2:C:349[B]:ARG:HH22	1.75	0.52
2:C:348[B]:LYS:HB2	1:E:352[B]:LYS:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:LYS:HG2	1:D:307:LEU:HD13	1.92	0.51
2:C:26:GLN:HA	1:E:320:LYS:HG3	1.93	0.51
2:C:352[B]:LYS:HB3	1:E:348[B]:LYS:HB2	1.95	0.49
1:F:17:VAL:HA	1:F:20:LEU:HD12	1.95	0.49
1:F:29:GLN:HG3	1:F:33:ARG:HH22	1.77	0.49
1:Q:316:HIS:HD2	1:Q:318:ASN:H	1.61	0.48
2:C:37:GLN:HE22	2:C:353[B]:ARG:HG3	1.80	0.47
1:Q:323:LYS:HA	1:Q:326:GLN:HB3	1.97	0.47
1:D:75:TRP:HA	1:D:353[A]:ARG:HH11	1.80	0.46
1:Q:316:HIS:CD2	1:Q:318:ASN:H	2.33	0.46
2:C:113:GLN:HG3	2:C:156:GLU:HG3	1.98	0.46
2:C:200:LEU:HB3	2:C:240:GLU:HB3	1.98	0.46
1:P:323:LYS:HA	1:P:326:GLN:HB2	1.97	0.46
1:D:318:ASN:HD21	1:F:66:ASN:HD21	1.63	0.46
1:B:24:ASP:HB3	1:B:27:GLU:HG2	1.98	0.45
1:D:17:VAL:HA	1:D:20:LEU:HD12	1.98	0.45
1:D:200:LEU:HB3	1:D:240:GLU:HB3	1.98	0.44
1:A:311:GLU:HA	1:A:314:GLN:HE21	1.81	0.44
1:P:314:GLN:HA	1:P:322:GLN:CG	2.48	0.44
1:D:114:GLU:HG2	1:D:353[A]:ARG:HH12	1.81	0.43
1:F:239:GLN:HG3	1:F:279:ILE:HD13	1.98	0.43
1:E:89:GLN:HB2	1:E:129:GLN:HE21	1.84	0.43
2:C:239:GLN:HG3	2:C:279:ILE:HD13	2.01	0.43
1:E:70:LEU:HG	1:E:111:ILE:HD12	2.01	0.43
1:E:215:GLN:HA	1:E:218:ILE:HD12	2.01	0.43
1:A:197:GLN:HG2	1:A:240:GLU:HG3	2.01	0.42
1:D:97:LEU:HD21	1:D:122:ILE:HG21	2.00	0.42
1:E:155:GLN:HE22	1:E:351[A]:ARG:HH22	1.67	0.42
1:E:238:LEU:HD23	1:E:279:ILE:HD12	2.00	0.42
1:E:245:LEU:HA	1:E:248:ILE:HD12	2.02	0.42
1:B:155:GLN:HB3	1:B:155:GLN:HE21	1.72	0.42
1:D:239:GLN:HG3	1:D:279:ILE:HD13	2.01	0.42
2:C:348[B]:LYS:HD2	1:E:352[B]:LYS:HD2	2.01	0.41
1:A:200:LEU:HB3	1:A:240:GLU:HB3	2.02	0.41
1:F:197:GLN:HE21	1:F:201:TRP:HE1	1.69	0.41
1:P:298:LYS:HB3	1:P:332:LEU:HD23	2.02	0.41
1:A:239:GLN:HG3	1:A:279:ILE:HD13	2.02	0.41
2:C:20:LEU:HB3	2:C:61:LEU:HD11	2.02	0.41
1:E:117:TRP:HE1	1:E:351[A]:ARG:HB3	1.86	0.41
1:E:260:ILE:HG12	1:E:265:LEU:HD11	2.04	0.40
1:B:70:LEU:HG	1:B:111:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:HG	1:A:111:ILE:HD12	2.03	0.40
1:D:114:GLU:HG2	1:D:351[B]:ARG:HH12	1.86	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	339/348 (97%)	337 (99%)	2 (1%)	0	100	100
1	B	337/348 (97%)	335 (99%)	2 (1%)	0	100	100
1	D	338/348 (97%)	337 (100%)	1 (0%)	0	100	100
1	E	337/348 (97%)	333 (99%)	4 (1%)	0	100	100
1	F	331/348 (95%)	330 (100%)	1 (0%)	0	100	100
1	P	40/348 (12%)	35 (88%)	5 (12%)	0	100	100
1	Q	40/348 (12%)	35 (88%)	5 (12%)	0	100	100
2	C	338/350 (97%)	333 (98%)	5 (2%)	0	100	100
All	All	2100/2786 (75%)	2075 (99%)	25 (1%)	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	272/267 (102%)	267 (98%)	5 (2%)	59	75
1	B	271/267 (102%)	266 (98%)	5 (2%)	59	75
1	D	272/267 (102%)	260 (96%)	12 (4%)	28	39
1	E	271/267 (102%)	262 (97%)	9 (3%)	38	53
1	F	262/267 (98%)	255 (97%)	7 (3%)	44	61
1	P	32/267 (12%)	27 (84%)	5 (16%)	2	2
1	Q	32/267 (12%)	27 (84%)	5 (16%)	2	2
2	C	272/269 (101%)	265 (97%)	7 (3%)	46	63
All	All	1684/2138 (79%)	1629 (97%)	55 (3%)	40	53

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
1	A	344[A]	LYS
1	A	344[B]	LYS
1	A	352[A]	LYS
1	A	352[B]	LYS
1	B	22	SER
1	B	28	LEU
1	B	113	GLN
1	B	155	GLN
1	B	280	LEU
2	C	11	SER
2	C	62	LEU
2	C	67	GLU
2	C	70	LEU
2	C	144	GLN
2	C	147	SER
2	C	288	SER
1	D	18	GLN
1	D	27	GLU
1	D	194	GLN
1	D	243	TRP
1	D	280	LEU
1	D	281	GLN
1	D	313	LEU
1	D	322	GLN
1	D	347[A]	ARG
1	D	347[B]	ARG

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Mol	Chain	Res	Type
1	D	353[A]	ARG
1	D	353[B]	ARG
1	E	28	LEU
1	E	113	GLN
1	E	272	LEU
1	E	284	LEU
1	E	310	LEU
1	E	319	GLU
1	E	322	GLN
1	E	346[A]	LYS
1	E	346[B]	LYS
1	F	13	LEU
1	F	32	LEU
1	F	152	GLN
1	F	186	GLN
1	F	280	LEU
1	F	302	LYS
1	F	315	SER
1	P	309	LYS
1	P	313	LEU
1	P	319	GLU
1	P	320	LYS
1	P	323	LYS
1	Q	318	ASN
1	Q	319	GLU
1	Q	322	GLN
1	Q	323	LYS
1	Q	329	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
1	A	314	GLN
1	B	194	GLN
2	C	37	GLN
2	C	326	GLN
1	D	26	GLN
1	D	110	GLN
1	D	171	GLN
1	D	281	GLN
1	D	314	GLN

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Mol	Chain	Res	Type
1	E	26	GLN
1	E	155	GLN
1	E	194	GLN
1	F	19	GLN
1	F	66	ASN
1	F	68	GLN
1	F	197	GLN
1	F	236	GLN
1	F	326	GLN
1	P	322	GLN
1	P	326	GLN
1	Q	316	HIS
1	Q	318	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](#)

Of 39 ligands modelled in this entry, 33 are monoatomic - leaving 6 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	$\# Z > 2$
4	EDO	F	401	-	3,3,3	0.65	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	F	402	-	3,3,3	0.60	0	2,2,2	0.23	0
4	EDO	A	406	-	3,3,3	0.49	0	2,2,2	0.26	0
4	EDO	F	403	-	3,3,3	0.75	0	2,2,2	0.07	0
4	EDO	F	404	-	3,3,3	0.58	0	2,2,2	0.32	0
4	EDO	D	405	-	3,3,3	0.58	0	2,2,2	0.19	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	F	401	-	-	0/1/1/1	-
4	EDO	F	402	-	-	0/1/1/1	-
4	EDO	A	406	-	-	0/1/1/1	-
4	EDO	F	403	-	-	1/1/1/1	-
4	EDO	F	404	-	-	0/1/1/1	-
4	EDO	D	405	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	403	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	335/348 (96%)	0.23	14 (4%) 36 43	38, 58, 99, 120	1 (0%)
1	B	333/348 (95%)	0.47	25 (7%) 14 19	47, 67, 111, 129	0
1	D	333/348 (95%)	0.87	51 (15%) 2 3	53, 75, 137, 158	0
1	E	333/348 (95%)	0.65	41 (12%) 4 6	39, 67, 208, 223	0
1	F	334/348 (95%)	0.68	42 (12%) 3 5	42, 69, 146, 188	10 (2%)
1	P	42/348 (12%)	7.19	41 (97%) 0 0	131, 174, 193, 196	16 (38%)
1	Q	42/348 (12%)	2.94	29 (69%) 0 0	85, 124, 148, 154	12 (28%)
2	C	334/350 (95%)	0.57	41 (12%) 4 6	39, 60, 148, 170	8 (2%)
All	All	2086/2786 (74%)	0.76	284 (13%) 3 4	38, 68, 152, 223	47 (2%)

All (284) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	322	GLN	19.0
1	P	323	LYS	14.2
1	P	329	LEU	13.9
1	P	319	GLU	13.2
1	P	325	ALA	12.7
1	P	321	ILE	11.3
1	P	315	SER	11.0
1	P	300	ALA	10.2
1	P	318	ASN	9.8
1	P	302	LYS	9.3
1	P	301	VAL	8.9
1	P	334	GLY	8.9
1	F	16	MET	8.8
1	P	304	ALA	8.8
1	P	313	LEU	8.6
1	F	52	ALA	7.9

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Mol	Chain	Res	Type	RSRZ
1	P	307	LEU	7.7
1	E	312	GLN	7.7
1	Q	321	ILE	7.6
1	P	317	GLU	7.5
2	C	23	PRO	7.4
1	F	22	SER	7.4
1	E	307	LEU	7.3
1	P	332	LEU	7.2
1	P	314	GLN	7.0
1	F	46	ILE	6.9
1	P	293	GLY	6.9
1	P	306	ALA	6.7
1	Q	330	GLU	6.7
1	D	311	GLU	6.7
1	P	320	LYS	6.6
1	Q	334	GLY	6.4
1	F	12	GLU	6.3
1	F	31	ALA	6.3
2	C	17	VAL	6.2
1	P	316	HIS	6.2
2	C	31	ALA	6.2
1	F	51	ASP	6.2
1	F	28	LEU	6.1
1	P	295	ASN	6.0
1	F	21	ASN	5.9
1	E	311	GLU	5.9
1	E	315	SER	5.9
2	C	22	SER	5.8
1	P	303	GLU	5.8
1	P	331	LYS	5.7
1	D	23	PRO	5.7
1	Q	317	GLU	5.7
1	E	334	GLY	5.7
1	D	307	LEU	5.7
1	D	49	VAL	5.6
1	E	329	LEU	5.6
1	P	327	GLU	5.5
1	P	305	GLY	5.5
1	Q	319	GLU	5.5
1	F	29	GLN	5.5
1	B	307	LEU	5.4
1	D	80	ILE	5.4

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Mol	Chain	Res	Type	RSRZ
1	P	326	GLN	5.4
1	Q	325	ALA	5.3
1	A	16	MET	5.3
1	E	322	GLN	5.2
1	P	330	GLU	5.2
2	C	32	LEU	5.2
1	F	40	SER	5.1
1	A	353[A]	ARG	5.1
2	C	26	GLN	5.1
1	D	334	GLY	5.1
1	D	17	VAL	5.0
1	D	310	LEU	5.0
1	F	18	GLN	4.9
1	E	306	ALA	4.9
1	E	258	ALA	4.9
1	P	294	GLY	4.8
1	F	35	LEU	4.8
1	D	324	GLU	4.8
1	F	27	GLU	4.8
1	F	19	GLN	4.8
1	D	16	MET	4.8
1	E	303	GLU	4.8
1	E	326	GLN	4.7
1	A	41	GLY	4.7
2	C	21	ASN	4.7
1	D	325	ALA	4.7
2	C	34	LYS	4.6
1	A	21	ASN	4.6
1	P	324	GLU	4.5
1	Q	328	ALA	4.5
1	E	332	LEU	4.4
1	D	308	GLU	4.3
1	E	15	GLN	4.3
1	E	316	HIS	4.3
1	E	285	TRP	4.3
1	P	333	GLY	4.3
1	B	16	MET	4.3
1	P	298	LYS	4.3
1	E	301	VAL	4.2
1	P	312	GLN	4.2
1	E	201	TRP	4.2
1	P	299	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
2	C	70	LEU	4.1
1	E	310	LEU	4.1
1	P	308	GLU	4.1
2	C	46	ILE	4.1
1	D	55	LEU	4.1
2	C	201	TRP	4.1
1	D	329	LEU	4.1
1	F	306	ALA	4.0
1	D	306	ALA	4.0
1	Q	331	LYS	4.0
1	A	35	LEU	4.0
1	P	309	LYS	4.0
1	Q	316	HIS	4.0
1	D	353[A]	ARG	3.9
2	C	33	ARG	3.9
1	Q	296	GLU	3.9
1	D	34	LYS	3.9
1	D	56	PRO	3.8
1	Q	332	LEU	3.8
1	Q	323	LYS	3.8
1	D	314	GLN	3.8
2	C	353[A]	ARG	3.8
1	F	26	GLN	3.8
1	B	44	GLU	3.7
1	E	328	ALA	3.7
1	F	14	PRO	3.7
1	E	273	SER	3.6
1	Q	333	GLY	3.6
1	Q	322	GLN	3.6
1	D	303	GLU	3.6
2	C	11	SER	3.5
2	C	24	ASP	3.5
2	C	19	GLN	3.5
1	B	24	ASP	3.5
1	D	13	LEU	3.4
1	Q	318	ASN	3.4
1	E	272	LEU	3.4
1	F	20	LEU	3.3
1	E	299	GLN	3.3
1	F	13	LEU	3.3
1	F	17	VAL	3.3
1	B	35	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	C	27	GLU	3.3
1	B	26	GLN	3.2
2	C	16	MET	3.2
1	F	61	LEU	3.2
1	Q	320	LYS	3.2
2	C	28	LEU	3.2
1	F	201	TRP	3.2
1	F	15	GLN	3.2
1	F	25	GLN	3.1
1	P	311	GLU	3.1
1	B	315	SER	3.1
1	D	344[A]	LYS	3.1
1	E	314	GLN	3.1
1	Q	324	GLU	3.1
2	C	68	GLN	3.1
1	D	14	PRO	3.1
1	B	15	GLN	3.0
1	D	50	ILE	3.0
1	Q	312	GLN	3.0
1	Q	326	GLN	3.0
1	D	272	LEU	3.0
1	D	313	LEU	3.0
1	D	269	VAL	3.0
1	B	20	LEU	3.0
1	Q	315	SER	3.0
1	B	21	ASN	3.0
1	D	32	LEU	2.9
2	C	35	LEU	2.9
1	Q	309	LYS	2.9
1	P	310	LEU	2.9
1	B	52	ALA	2.9
2	C	44	GLU	2.9
1	D	309	LYS	2.9
1	F	58	LEU	2.9
1	D	285	TRP	2.9
1	F	329	LEU	2.8
1	E	317	GLU	2.8
2	C	62	LEU	2.8
2	C	53	GLY	2.8
2	C	117	TRP	2.8
2	C	81	ALA	2.8
1	F	30	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	325	ALA	2.8
1	A	28	LEU	2.8
1	E	265	LEU	2.8
1	Q	305	GLY	2.8
1	F	353	ARG	2.8
1	F	42	GLY	2.7
2	C	29	GLN	2.7
1	E	321	ILE	2.7
1	B	254	GLU	2.7
2	C	51	ASP	2.7
1	A	11	SER	2.7
1	P	328	ALA	2.6
1	E	305	GLY	2.6
2	C	61	LEU	2.6
1	D	53	GLY	2.6
1	D	22	SER	2.6
1	E	324	GLU	2.6
1	E	344[A]	LYS	2.6
1	B	177	ASP	2.6
1	D	312	GLN	2.6
1	E	291	ALA	2.6
1	B	22	SER	2.5
1	F	75	TRP	2.5
1	D	35	LEU	2.5
1	A	352[A]	LYS	2.5
1	E	320	LYS	2.5
2	C	15	GLN	2.5
1	D	69	ILE	2.5
1	E	263	GLY	2.5
1	D	60	GLN	2.5
1	Q	299	GLN	2.5
1	E	323	LYS	2.5
1	Q	297	GLN	2.5
2	C	20	LEU	2.5
1	D	21	ASN	2.4
1	Q	310	LEU	2.4
1	Q	329	LEU	2.4
1	F	23	PRO	2.4
1	E	333	GLY	2.4
2	C	69	ILE	2.4
1	E	287	LEU	2.4
1	D	299	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	48	ALA	2.4
2	C	47	GLN	2.4
1	B	334	GLY	2.4
1	D	91	VAL	2.4
1	E	353[A]	ARG	2.4
1	F	93	ASP	2.4
1	D	260	ILE	2.4
1	A	344[A]	LYS	2.4
1	B	42	GLY	2.4
1	E	300	ALA	2.4
1	A	296	GLU	2.4
1	A	335	GLY	2.4
1	F	243	TRP	2.3
1	Q	327	GLU	2.3
1	D	18	GLN	2.3
1	B	30	SER	2.3
2	C	326	GLN	2.3
1	F	57	ALA	2.3
1	F	159	TRP	2.3
1	B	175	VAL	2.3
1	D	320	LYS	2.3
1	D	280	LEU	2.3
1	D	93	ASP	2.3
1	B	344[A]	LYS	2.3
1	P	296	GLU	2.3
1	D	25	GLN	2.3
1	E	30	SER	2.3
1	B	13	LEU	2.2
1	B	25	GLN	2.2
1	E	23	PRO	2.2
2	C	50	ILE	2.2
1	B	301	VAL	2.2
1	A	15	GLN	2.2
1	B	326	GLN	2.2
1	F	180	ALA	2.2
1	D	284	LEU	2.2
1	D	27	GLU	2.2
2	C	36	SER	2.2
1	F	33	ARG	2.1
1	D	273	SER	2.1
1	E	318	ASN	2.1
1	Q	303	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	350[A]	LYS	2.1
1	B	187	LEU	2.1
1	F	307	LEU	2.1
1	F	343	GLY	2.1
2	C	65	PRO	2.1
1	F	41	GLY	2.1
1	D	92	ILE	2.1
1	A	13	LEU	2.1
1	Q	307	LEU	2.1
2	C	75	TRP	2.1
1	B	296	GLU	2.0
2	C	14	PRO	2.0
1	D	51	ASP	2.0
1	D	31	ALA	2.0
2	C	37	GLN	2.0
1	A	77	LEU	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 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. 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
4	EDO	F	404	4/4	0.47	0.37	110,111,111,111	0
4	EDO	A	406	4/4	0.64	0.45	96,96,97,97	0
4	EDO	D	405	4/4	0.74	0.36	95,95,95,95	0
3	CA	C	404	1/1	0.77	0.11	123,123,123,123	0
3	CA	D	407	1/1	0.77	0.17	86,86,86,86	0
3	CA	B	404	1/1	0.80	0.39	105,105,105,105	0
3	CA	C	408	1/1	0.81	0.05	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	F	402	4/4	0.81	0.17	59,59,59,60	0
4	EDO	F	403	4/4	0.81	0.28	50,51,52,52	0
4	EDO	F	401	4/4	0.83	0.30	63,63,63,63	0
3	CA	C	401	1/1	0.84	0.22	67,67,67,67	0
3	CA	C	409	1/1	0.85	0.04	125,125,125,125	0
3	CA	B	402	1/1	0.85	0.10	80,80,80,80	0
5	MG	D	406	1/1	0.88	0.18	77,77,77,77	0
3	CA	D	404	1/1	0.90	0.09	109,109,109,109	0
3	CA	B	403	1/1	0.90	0.21	117,117,117,117	0
3	CA	D	409	1/1	0.91	0.06	100,100,100,100	0
3	CA	A	403	1/1	0.91	0.20	74,74,74,74	0
5	MG	C	405	1/1	0.92	0.15	79,79,79,79	0
3	CA	A	404	1/1	0.92	0.07	62,62,62,62	0
3	CA	D	402	1/1	0.92	0.19	74,74,74,74	0
5	MG	C	406	1/1	0.93	0.23	52,52,52,52	0
5	MG	A	408	1/1	0.93	0.20	55,55,55,55	0
3	CA	D	403	1/1	0.93	0.13	56,56,56,56	0
3	CA	A	402	1/1	0.94	0.16	56,56,56,56	0
3	CA	C	403	1/1	0.94	0.14	53,53,53,53	0
3	CA	D	401	1/1	0.95	0.12	71,71,71,71	0
3	CA	A	401	1/1	0.96	0.07	55,55,55,55	0
5	MG	B	406	1/1	0.96	0.14	70,70,70,70	0
3	CA	D	408	1/1	0.96	0.15	62,62,62,62	0
3	CA	A	405	1/1	0.97	0.06	113,113,113,113	0
3	CA	B	401	1/1	0.97	0.09	61,61,61,61	0
5	MG	B	405	1/1	0.97	0.15	62,62,62,62	0
5	MG	A	407	1/1	0.97	0.12	58,58,58,58	0
3	CA	C	402	1/1	0.97	0.14	60,60,60,60	0
5	MG	E	401	1/1	0.98	0.23	62,62,62,62	0
5	MG	E	402	1/1	0.98	0.11	56,56,56,56	0
3	CA	C	407	1/1	0.98	0.08	50,50,50,50	0
5	MG	F	405	1/1	0.98	0.19	68,68,68,68	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.