



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 10:32 AM EDT

PDB ID : 4M8D
Title : Crystal structure of an isatin hydrolase bound to product analogue thioisatinate
Authors : Bjerregaard-Andersen, K.; Sommer, T.; Jensen, J.K.; Jochimsen, B.; Etzerodt, M.; Morth, J.P.
Deposited on : 2013-08-13
Resolution : 1.90 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 : 2.35.1
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) : 2.35.1

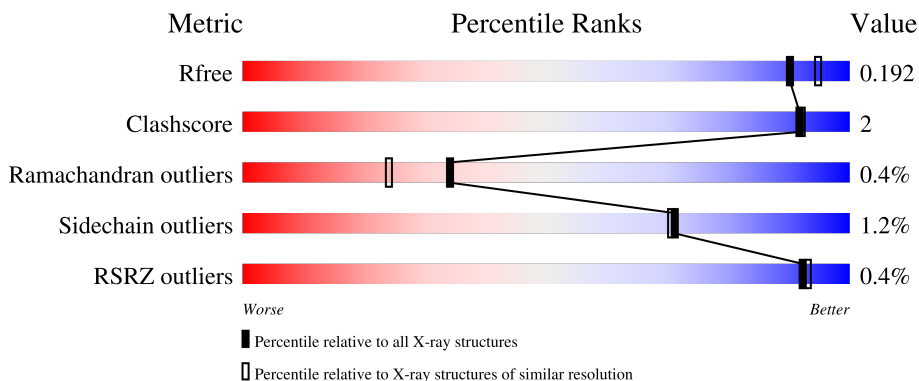
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	263	97%
1	B	263	97%
1	C	263	94% 5%
1	D	263	96%
1	E	263	94% 5%

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Mol	Chain	Length	Quality of chain
1	F	263	 97%
1	G	263	 95%
1	H	263	 94% 5%
1	I	263	 92% 7%
1	J	263	 92% 8%
1	K	263	 95%
1	L	263	 94% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27233 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	262	Total 1978	C 1257	N 333	O 380	S 8	0	1	0
1	B	262	Total 1973	C 1254	N 332	O 380	S 7	0	1	0
1	C	262	Total 1972	C 1254	N 332	O 378	S 8	0	0	0
1	D	263	Total 1978	C 1257	N 333	O 380	S 8	0	0	0
1	E	262	Total 1972	C 1254	N 332	O 378	S 8	0	0	0
1	F	263	Total 1977	C 1257	N 333	O 379	S 8	0	0	0
1	G	262	Total 1972	C 1254	N 332	O 378	S 8	0	0	0
1	H	263	Total 1978	C 1257	N 333	O 380	S 8	0	0	0
1	I	262	Total 1980	C 1259	N 335	O 378	S 8	0	1	0
1	J	262	Total 1972	C 1254	N 332	O 378	S 8	0	0	0
1	K	262	Total 1972	C 1254	N 332	O 378	S 8	0	0	0
1	L	262	Total 1972	C 1254	N 332	O 378	S 8	0	0	0

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

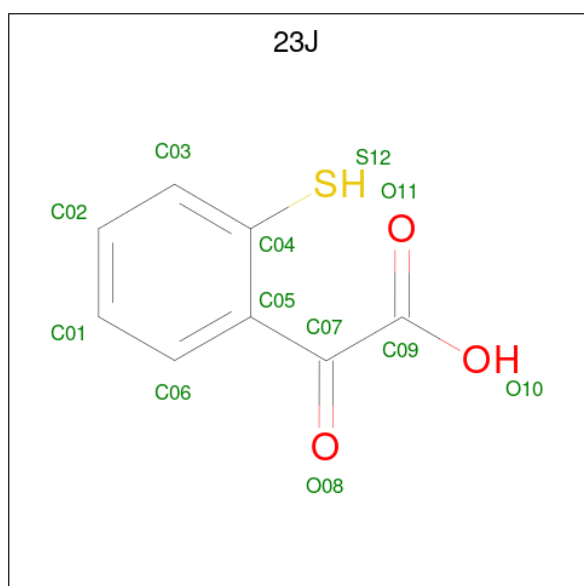
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mn 1	0	0
2	B	1	Total 1	Mn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		
2	G	1	Total	Mn	0	0
			1	1		
2	H	1	Total	Mn	0	0
			1	1		
2	I	1	Total	Mn	0	0
			1	1		
2	J	1	Total	Mn	0	0
			1	1		
2	K	1	Total	Mn	0	0
			1	1		
2	L	1	Total	Mn	0	0
			1	1		

- Molecule 3 is oxo(2-sulfanylphenyl)acetic acid (three-letter code: 23J) (formula: C₈H₆O₃S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			12	8	3	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	S	0	1
			24	16	6	2		
3	C	1	Total	C	O	S	0	0
			12	8	3	1		
3	D	1	Total	C	O	S	0	0
			12	8	3	1		
3	E	1	Total	C	O	S	0	0
			12	8	3	1		
3	F	1	Total	C	O	S	0	1
			24	16	6	2		
3	G	1	Total	C	O	S	0	1
			24	16	6	2		
3	H	1	Total	C	O	S	0	0
			12	8	3	1		
3	I	1	Total	C	O	S	0	0
			12	8	3	1		
3	J	1	Total	C	O	S	0	0
			12	8	3	1		
3	K	1	Total	C	O	S	0	0
			12	8	3	1		
3	L	1	Total	C	O	S	0	0
			12	8	3	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Ca	0	0
			3	3		
4	B	3	Total	Ca	0	0
			3	3		
4	C	2	Total	Ca	0	0
			2	2		
4	D	1	Total	Ca	0	0
			1	1		
4	F	1	Total	Ca	0	0
			1	1		
4	I	1	Total	Ca	0	0
			1	1		
4	J	2	Total	Ca	0	0
			2	2		
4	L	3	Total	Ca	0	0
			3	3		

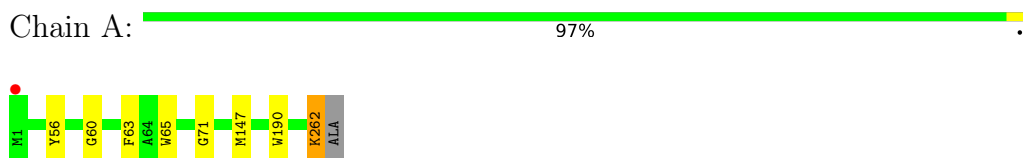
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	318	Total O 318 318	0	0
5	B	323	Total O 323 323	0	0
5	C	237	Total O 237 237	0	0
5	D	293	Total O 293 293	0	0
5	E	266	Total O 266 266	0	0
5	F	320	Total O 320 320	0	0
5	G	240	Total O 240 240	0	0
5	H	237	Total O 237 237	0	0
5	I	282	Total O 282 282	0	0
5	J	259	Total O 259 259	0	0
5	K	279	Total O 279 279	0	0
5	L	275	Total O 275 275	0	0

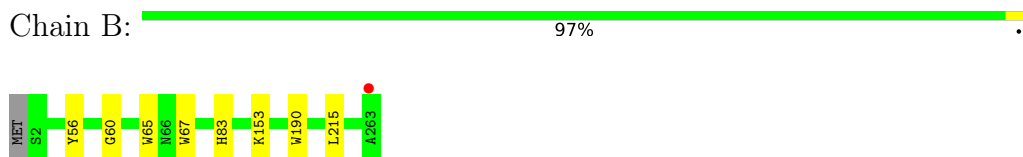
3 Residue-property plots [i](#)

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.

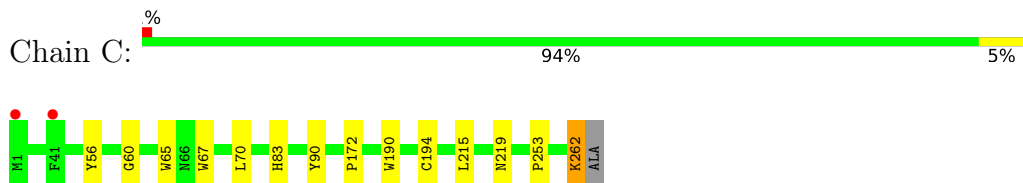
- Molecule 1: Putative uncharacterized protein



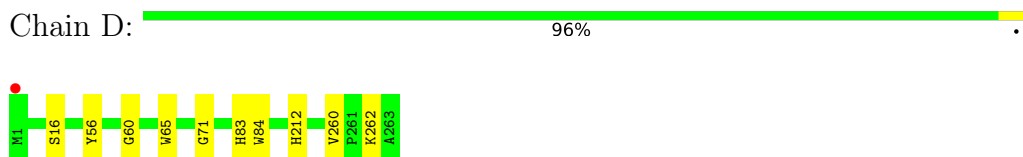
- Molecule 1: Putative uncharacterized protein



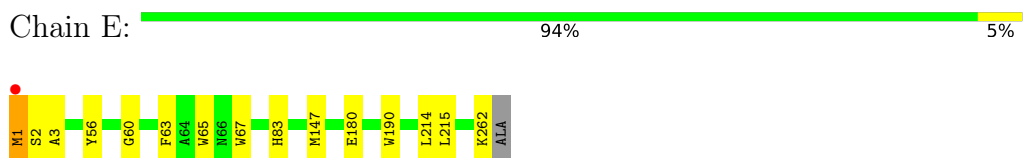
- Molecule 1: Putative uncharacterized protein



- Molecule 1: Putative uncharacterized protein



- Molecule 1: Putative uncharacterized protein



- Molecule 1: Putative uncharacterized protein

Chain F:  97%



● Molecule 1: Putative uncharacterized protein

Chain G:  95%



● Molecule 1: Putative uncharacterized protein

Chain H:  94% 5%



● Molecule 1: Putative uncharacterized protein

Chain I:  92% 7%



● Molecule 1: Putative uncharacterized protein

Chain J:  92% 8%



● Molecule 1: Putative uncharacterized protein

Chain K:  95%



● Molecule 1: Putative uncharacterized protein

Chain L:  94% 6%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.98Å 51.82Å 357.09Å 90.00° 91.92° 90.00°	Depositor
Resolution (Å)	29.98 – 1.90 49.51 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.98-1.90) 97.6 (49.51-1.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.79Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.152 , 0.192 0.153 , 0.192	Depositor DCC
R_{free} test set	14130 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtrriage
Anisotropy	0.495	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.015 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	27233	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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 26.76 % 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 2.4828e-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: MN, 23J, CA

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	0.42	0/2032	0.54	0/2772
1	B	0.40	0/2030	0.54	0/2769
1	C	0.33	0/2026	0.50	0/2764
1	D	0.39	0/2032	0.55	0/2771
1	E	0.39	0/2026	0.54	0/2764
1	F	0.39	0/2031	0.54	0/2771
1	G	0.36	0/2026	0.51	0/2764
1	H	0.35	0/2032	0.50	0/2771
1	I	0.37	0/2037	0.54	0/2778
1	J	0.38	0/2026	0.53	0/2764
1	K	0.37	0/2026	0.52	0/2764
1	L	0.38	0/2026	0.51	0/2764
All	All	0.38	0/24350	0.53	0/33216

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	1978	0	1922	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1973	0	1915	4	0
1	C	1972	0	1918	7	0
1	D	1978	0	1923	5	0
1	E	1972	0	1918	10	0
1	F	1977	0	1923	4	0
1	G	1972	0	1918	5	0
1	H	1978	0	1923	9	0
1	I	1980	0	1931	11	0
1	J	1972	0	1918	14	0
1	K	1972	0	1918	6	0
1	L	1972	0	1918	8	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	12	0	5	0	0
3	B	24	0	10	3	0
3	C	12	0	5	2	0
3	D	12	0	5	1	0
3	E	12	0	5	1	0
3	F	24	0	10	4	0
3	G	24	0	10	1	0
3	H	12	0	5	1	0
3	I	12	0	5	1	0
3	J	12	0	5	1	0
3	K	12	0	5	2	0
3	L	12	0	5	1	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	I	1	0	0	0	0
4	J	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	3	0	0	0	0
5	A	318	0	0	1	0
5	B	323	0	0	0	0
5	C	237	0	0	1	0
5	D	293	0	0	0	0
5	E	266	0	0	0	0
5	F	320	0	0	0	0
5	G	240	0	0	0	0
5	H	237	0	0	0	0
5	I	282	0	0	1	0
5	J	259	0	0	0	0
5	K	279	0	0	1	0
5	L	275	0	0	0	0
All	All	27233	0	23120	77	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 (77) 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:83:HIS:NE2	3:B:302[B]:23J:O10	2.14	0.79
1:A:262:LYS:O	5:A:711:HOH:O	2.12	0.67
1:F:83:HIS:NE2	3:F:302[A]:23J:O11	2.31	0.63
1:E:63:PHE:CE1	3:F:302[B]:23J:H1	2.35	0.62
1:C:83:HIS:NE2	3:C:302:23J:O11	2.33	0.61
1:K:83:HIS:NE2	3:K:302:23J:O10	2.34	0.60
1:G:67:TRP:HA	1:H:71:GLY:HA2	1.84	0.59
1:I:146:VAL:HG13	1:I:229:LEU:HD13	1.85	0.58
1:B:153:LYS:HD2	1:D:16:SER:HB2	1.86	0.58
1:L:83:HIS:NE2	3:L:302:23J:O11	2.36	0.58
1:K:138:GLU:OE1	1:K:185:LYS:NZ	2.32	0.56
3:C:302:23J:O10	5:C:469:HOH:O	2.18	0.56
1:H:180:GLU:HG2	1:H:214:LEU:HD13	1.88	0.56
1:I:67:TRP:HA	1:J:71:GLY:HA2	1.88	0.55
1:J:176:PRO:HD3	1:J:205:MET:HE2	1.90	0.54
1:E:1:MET:N	1:E:2:SER:HA	2.22	0.54
1:K:261:PRO:O	1:K:262:LYS:HB2	2.07	0.54
1:I:261:PRO:O	1:I:262:LYS:HB2	2.07	0.53
1:E:83:HIS:NE2	3:E:302:23J:O10	2.42	0.53
1:J:180:GLU:HG2	1:J:214:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:71:GLY:HA2	1:J:67:TRP:HA	1.92	0.52
1:D:83:HIS:NE2	3:D:302:23J:O10	2.43	0.52
1:J:202:ALA:HA	1:J:205:MET:SD	2.51	0.51
1:L:180:GLU:HG3	1:L:214:LEU:HD13	1.93	0.51
1:J:176:PRO:HD3	1:J:205:MET:CE	2.41	0.50
3:K:302:23J:O11	5:K:679:HOH:O	2.19	0.50
1:H:198:ASP:HB3	1:H:202:ALA:HB2	1.92	0.50
1:L:202:ALA:HA	1:L:205:MET:HG3	1.94	0.49
1:E:63:PHE:CD1	3:F:302[B]:23J:H1	2.46	0.49
1:C:70:LEU:HD21	1:C:253:PRO:HG3	1.93	0.49
1:A:63:PHE:CD1	3:B:302[A]:23J:H1	2.47	0.48
1:C:67:TRP:HA	1:D:71:GLY:HA2	1.95	0.48
1:I:13:LYS:HE2	1:J:1:MET:HG3	1.96	0.48
1:G:83:HIS:NE2	3:G:302[B]:23J:O11	2.46	0.47
1:H:83:HIS:NE2	3:H:302:23J:O10	2.47	0.47
1:I:1:MET:HA	1:I:2:SER:HA	1.58	0.47
1:E:67:TRP:HA	1:F:71:GLY:HA2	1.97	0.46
1:H:202:ALA:HB1	1:H:209:PHE:HA	1.97	0.46
1:L:172:PRO:HD2	1:L:194:CYS:SG	2.55	0.46
1:L:261:PRO:O	1:L:262:LYS:HB3	2.15	0.46
1:B:190:TRP:HB3	1:B:215:LEU:HD11	1.98	0.46
1:H:172:PRO:HD2	1:H:194:CYS:SG	2.56	0.46
1:I:83:HIS:NE2	3:I:302:23J:O11	2.49	0.45
1:C:172:PRO:HD2	1:C:194:CYS:SG	2.56	0.45
1:J:83:HIS:NE2	3:J:302:23J:O10	2.50	0.45
1:E:190:TRP:HB3	1:E:215:LEU:HD11	1.99	0.44
1:I:25:THR:HG23	1:I:76:THR:HB	1.97	0.44
1:K:71:GLY:HA2	1:L:67:TRP:HA	1.98	0.44
1:E:147:MET:HB2	1:E:190:TRP:CH2	2.52	0.44
1:C:262:LYS:HA	1:C:262:LYS:HD3	1.63	0.44
1:G:71:GLY:HA2	1:H:67:TRP:HA	2.00	0.44
1:A:63:PHE:CE1	3:B:302[A]:23J:H1	2.53	0.44
1:C:190:TRP:HB3	1:C:215:LEU:HD11	1.99	0.44
1:J:175:THR:OG1	1:J:177:ASP:OD1	2.26	0.44
1:E:3:ALA:HB2	1:F:18:GLU:HG2	1.99	0.44
5:I:533:HOH:O	1:J:1:MET:SD	2.62	0.44
1:J:261:PRO:O	1:J:262:LYS:HB2	2.17	0.44
1:D:260:VAL:HG23	1:D:262:LYS:HD3	2.01	0.43
1:G:180:GLU:HG2	1:G:214:LEU:HD13	1.99	0.43
1:J:15:LEU:HA	1:J:15:LEU:HD12	1.81	0.43
1:I:38:PRO:HA	1:I:39:PRO:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:147:MET:HB2	1:J:190:TRP:CH2	2.55	0.42
1:L:190:TRP:HB3	1:L:215:LEU:HD11	2.01	0.41
1:A:71:GLY:HA2	1:B:67:TRP:HA	2.03	0.41
1:G:38:PRO:HA	1:G:39:PRO:HD3	1.97	0.41
1:A:147:MET:HB2	1:A:190:TRP:CH2	2.55	0.41
1:D:84:TRP:CD2	1:D:212:HIS:HB3	2.56	0.41
1:K:70:LEU:HD21	1:K:253:PRO:HG2	2.03	0.41
1:C:90:TYR:CZ	1:C:219:ASN:HB2	2.56	0.41
1:H:20:GLU:OE1	1:H:262:LYS:HE3	2.21	0.41
1:I:10:LEU:HD22	1:J:10:LEU:HD22	2.02	0.41
1:F:149:THR:HG21	1:F:172:PRO:HG2	2.03	0.40
1:K:13:LYS:NZ	1:L:1:MET:O	2.47	0.40
1:E:63:PHE:CZ	3:F:302[B]:23J:H1	2.55	0.40
1:E:180:GLU:HG2	1:E:214:LEU:HD13	2.02	0.40
1:I:262:LYS:HE3	1:I:262:LYS:HB3	1.87	0.40
1:H:65:TRP:CD1	1:H:65:TRP:N	2.90	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	261/263 (99%)	256 (98%)	4 (2%)	1 (0%)	34 24
1	B	260/263 (99%)	255 (98%)	4 (2%)	1 (0%)	34 24
1	C	260/263 (99%)	252 (97%)	7 (3%)	1 (0%)	34 24
1	D	261/263 (99%)	256 (98%)	4 (2%)	1 (0%)	34 24
1	E	260/263 (99%)	256 (98%)	3 (1%)	1 (0%)	34 24
1	F	261/263 (99%)	256 (98%)	4 (2%)	1 (0%)	34 24
1	G	260/263 (99%)	255 (98%)	4 (2%)	1 (0%)	34 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	261/263 (99%)	256 (98%)	4 (2%)	1 (0%)	34	24
1	I	261/263 (99%)	255 (98%)	5 (2%)	1 (0%)	34	24
1	J	260/263 (99%)	255 (98%)	4 (2%)	1 (0%)	34	24
1	K	260/263 (99%)	254 (98%)	5 (2%)	1 (0%)	34	24
1	L	260/263 (99%)	254 (98%)	5 (2%)	1 (0%)	34	24
All	All	3125/3156 (99%)	3060 (98%)	53 (2%)	12 (0%)	34	24

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	60	GLY
1	J	60	GLY
1	A	60	GLY
1	B	60	GLY
1	D	60	GLY
1	E	60	GLY
1	K	60	GLY
1	C	60	GLY
1	G	60	GLY
1	H	60	GLY
1	L	60	GLY
1	F	60	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/207 (100%)	205 (99%)	3 (1%)	67	65
1	B	207/207 (100%)	205 (99%)	2 (1%)	76	76
1	C	207/207 (100%)	204 (99%)	3 (1%)	67	65
1	D	207/207 (100%)	205 (99%)	2 (1%)	76	76
1	E	207/207 (100%)	203 (98%)	4 (2%)	57	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	207/207 (100%)	205 (99%)	2 (1%)	76	76
1	G	207/207 (100%)	204 (99%)	3 (1%)	67	65
1	H	207/207 (100%)	205 (99%)	2 (1%)	76	76
1	I	208/207 (100%)	203 (98%)	5 (2%)	49	43
1	J	207/207 (100%)	205 (99%)	2 (1%)	76	76
1	K	207/207 (100%)	206 (100%)	1 (0%)	88	89
1	L	207/207 (100%)	205 (99%)	2 (1%)	76	76
All	All	2486/2484 (100%)	2455 (99%)	31 (1%)	71	70

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	TYR
1	A	65	TRP
1	A	262	LYS
1	B	56	TYR
1	B	65	TRP
1	C	56	TYR
1	C	65	TRP
1	C	262	LYS
1	D	56	TYR
1	D	65	TRP
1	E	1	MET
1	E	56	TYR
1	E	65	TRP
1	E	262	LYS
1	F	56	TYR
1	F	65	TRP
1	G	56	TYR
1	G	65	TRP
1	G	262	LYS
1	H	56	TYR
1	H	65	TRP
1	I	56	TYR
1	I	65	TRP
1	I	146	VAL
1	I	248[A]	ARG
1	I	248[B]	ARG
1	J	40	ASP
1	J	65	TRP

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Mol	Chain	Res	Type
1	K	65	TRP
1	L	56	TYR
1	L	65	TRP

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 43 ligands modelled in this entry, 28 are monoatomic - leaving 15 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	23J	E	302	2	12,12,12	1.43	1 (8%)	14,16,16	1.59	2 (14%)
3	23J	A	302	2	12,12,12	1.23	1 (8%)	14,16,16	1.44	2 (14%)
3	23J	B	302[A]	-	12,12,12	0.83	1 (8%)	14,16,16	1.18	2 (14%)
3	23J	F	302[A]	2	12,12,12	1.33	2 (16%)	14,16,16	1.57	3 (21%)
3	23J	G	302[B]	2	12,12,12	0.81	1 (8%)	14,16,16	1.39	2 (14%)
3	23J	K	302	2	12,12,12	1.04	1 (8%)	14,16,16	1.41	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	23J	I	302	2	12,12,12	0.95	1 (8%)	14,16,16	1.35	2 (14%)
3	23J	C	302	2	12,12,12	0.83	1 (8%)	14,16,16	1.49	3 (21%)
3	23J	H	302	2	12,12,12	2.13	2 (16%)	14,16,16	1.41	2 (14%)
3	23J	J	302	2	12,12,12	1.72	1 (8%)	14,16,16	1.60	2 (14%)
3	23J	F	302[B]	-	12,12,12	0.91	0	14,16,16	1.43	3 (21%)
3	23J	D	302	2	12,12,12	0.86	0	14,16,16	1.43	2 (14%)
3	23J	B	302[B]	2	12,12,12	1.46	2 (16%)	14,16,16	1.45	2 (14%)
3	23J	G	302[A]	-	12,12,12	0.71	0	14,16,16	1.21	2 (14%)
3	23J	L	302	2	12,12,12	1.09	2 (16%)	14,16,16	1.55	3 (21%)

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
3	23J	E	302	2	-	0/8/8/8	0/1/1/1
3	23J	A	302	2	-	0/8/8/8	0/1/1/1
3	23J	B	302[A]	-	-	0/8/8/8	0/1/1/1
3	23J	F	302[A]	2	-	1/8/8/8	0/1/1/1
3	23J	G	302[B]	2	-	0/8/8/8	0/1/1/1
3	23J	K	302	2	-	2/8/8/8	0/1/1/1
3	23J	I	302	2	-	0/8/8/8	0/1/1/1
3	23J	C	302	2	-	0/8/8/8	0/1/1/1
3	23J	H	302	2	-	2/8/8/8	0/1/1/1
3	23J	J	302	2	-	2/8/8/8	0/1/1/1
3	23J	F	302[B]	-	-	2/8/8/8	0/1/1/1
3	23J	D	302	2	-	0/8/8/8	0/1/1/1
3	23J	B	302[B]	2	-	2/8/8/8	0/1/1/1
3	23J	G	302[A]	-	-	1/8/8/8	0/1/1/1
3	23J	L	302	2	-	0/8/8/8	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	302	23J	C09-C07	-6.88	1.47	1.54
3	J	302	23J	C09-C07	-5.45	1.49	1.54
3	E	302	23J	C09-C07	-4.36	1.50	1.54
3	B	302[B]	23J	C09-C07	-4.11	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	302[A]	23J	C09-C07	-3.61	1.51	1.54
3	A	302	23J	C09-C07	-3.42	1.51	1.54
3	L	302	23J	C09-C07	-2.71	1.52	1.54
3	K	302	23J	C09-C07	-2.63	1.52	1.54
3	B	302[B]	23J	O10-C09	-2.48	1.23	1.30
3	F	302[A]	23J	O10-C09	-2.40	1.23	1.30
3	I	302	23J	O10-C09	-2.22	1.24	1.30
3	H	302	23J	O10-C09	-2.11	1.24	1.30
3	L	302	23J	O10-C09	-2.09	1.24	1.30
3	B	302[A]	23J	O10-C09	-2.07	1.24	1.30
3	G	302[B]	23J	O10-C09	-2.07	1.24	1.30
3	C	302	23J	O10-C09	-2.04	1.24	1.30

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	302	23J	C04-C05-C07	3.74	126.90	121.19
3	B	302[B]	23J	C04-C05-C07	3.49	126.51	121.19
3	F	302[A]	23J	C04-C05-C07	3.49	126.50	121.19
3	J	302	23J	C04-C05-C07	3.49	126.50	121.19
3	C	302	23J	C04-C05-C07	3.39	126.36	121.19
3	K	302	23J	C04-C05-C07	3.32	126.25	121.19
3	L	302	23J	C04-C05-C07	3.28	126.19	121.19
3	D	302	23J	C04-C05-C07	3.22	126.10	121.19
3	A	302	23J	C04-C05-C07	3.20	126.07	121.19
3	J	302	23J	O10-C09-O11	3.20	130.92	123.61
3	G	302[B]	23J	C04-C05-C07	3.14	125.97	121.19
3	A	302	23J	O10-C09-O11	3.03	130.55	123.61
3	H	302	23J	O10-C09-O11	3.01	130.50	123.61
3	I	302	23J	C04-C05-C07	3.00	125.76	121.19
3	E	302	23J	O10-C09-O11	2.99	130.45	123.61
3	H	302	23J	C04-C05-C07	2.90	125.62	121.19
3	L	302	23J	O10-C09-O11	2.87	130.18	123.61
3	F	302[B]	23J	C04-C05-C07	2.74	125.37	121.19
3	B	302[A]	23J	C04-C05-C07	2.66	125.24	121.19
3	G	302[A]	23J	C04-C05-C07	2.65	125.23	121.19
3	B	302[B]	23J	O10-C09-O11	2.64	129.64	123.61
3	F	302[A]	23J	O10-C09-O11	2.59	129.53	123.61
3	K	302	23J	O10-C09-O11	2.57	129.49	123.61
3	D	302	23J	O10-C09-O11	2.55	129.45	123.61
3	C	302	23J	O10-C09-O11	2.39	129.07	123.61
3	G	302[B]	23J	O10-C09-O11	2.36	129.02	123.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	302	23J	O11-C09-C07	-2.26	113.42	120.99
3	F	302[B]	23J	O11-C09-C07	-2.23	113.51	120.99
3	F	302[A]	23J	O11-C09-C07	-2.21	113.59	120.99
3	I	302	23J	O10-C09-O11	2.19	128.62	123.61
3	F	302[B]	23J	O10-C09-O11	2.17	128.57	123.61
3	B	302[A]	23J	O10-C09-O11	2.13	128.49	123.61
3	G	302[A]	23J	O10-C09-O11	2.12	128.45	123.61
3	C	302	23J	O11-C09-C07	-2.04	114.13	120.99

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302[B]	23J	O08-C07-C09-O10
3	F	302[B]	23J	O08-C07-C09-O10
3	G	302[A]	23J	O08-C07-C09-O10
3	H	302	23J	O08-C07-C09-O10
3	J	302	23J	O08-C07-C09-O10
3	K	302	23J	O08-C07-C09-O10
3	H	302	23J	C05-C07-C09-O10
3	B	302[B]	23J	C05-C07-C09-O10
3	F	302[A]	23J	C05-C07-C09-O10
3	F	302[B]	23J	C05-C07-C09-O10
3	J	302	23J	C05-C07-C09-O10
3	K	302	23J	C05-C07-C09-O10

There are no ring outliers.

13 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	302	23J	1	0
3	B	302[A]	23J	2	0
3	F	302[A]	23J	1	0
3	G	302[B]	23J	1	0
3	K	302	23J	2	0
3	I	302	23J	1	0
3	C	302	23J	2	0
3	H	302	23J	1	0
3	J	302	23J	1	0
3	F	302[B]	23J	3	0
3	D	302	23J	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302[B]	23J	1	0
3	L	302	23J	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	262/263 (99%)	-0.68	1 (0%) 92 93	10, 18, 33, 65	0
1	B	262/263 (99%)	-0.67	1 (0%) 92 93	9, 20, 34, 57	0
1	C	262/263 (99%)	-0.46	2 (0%) 86 87	16, 29, 45, 92	0
1	D	263/263 (100%)	-0.57	1 (0%) 92 93	13, 21, 40, 99	0
1	E	262/263 (99%)	-0.65	1 (0%) 92 93	11, 21, 37, 119	0
1	F	263/263 (100%)	-0.65	1 (0%) 92 93	11, 19, 36, 71	0
1	G	262/263 (99%)	-0.57	1 (0%) 92 93	14, 25, 41, 86	0
1	H	263/263 (100%)	-0.42	2 (0%) 86 87	15, 28, 44, 94	0
1	I	262/263 (99%)	-0.64	1 (0%) 92 93	13, 22, 36, 88	0
1	J	262/263 (99%)	-0.65	0 100 100	13, 22, 36, 54	0
1	K	262/263 (99%)	-0.62	1 (0%) 92 93	14, 23, 38, 104	0
1	L	262/263 (99%)	-0.68	1 (0%) 92 93	13, 21, 35, 67	0
All	All	3147/3156 (99%)	-0.60	13 (0%) 92 93	9, 22, 40, 119	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	1	MET	8.9
1	K	1	MET	8.9
1	E	1	MET	8.3
1	F	1	MET	6.9
1	D	1	MET	6.6
1	I	1	MET	6.5
1	C	1	MET	4.9
1	H	1	MET	4.8
1	H	263	ALA	4.7
1	A	1	MET	4.0
1	L	1	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	41	PHE	2.1
1	B	263	ALA	2.1

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, 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	CA	C	304	1/1	0.63	0.18	81,81,81,81	0
3	23J	F	302[B]	12/12	0.81	0.19	16,29,31,39	12
3	23J	F	302[A]	12/12	0.81	0.19	21,29,31,42	12
3	23J	G	302[B]	12/12	0.84	0.25	37,45,45,156	12
3	23J	H	302	12/12	0.84	0.21	36,39,43,158	12
3	23J	G	302[A]	12/12	0.84	0.25	43,45,47,156	12
3	23J	C	302	12/12	0.85	0.17	39,40,52,83	12
3	23J	I	302	12/12	0.86	0.21	35,37,42,117	12
3	23J	B	302[A]	12/12	0.88	0.22	31,33,35,112	12
3	23J	B	302[B]	12/12	0.88	0.22	24,32,33,112	12
3	23J	E	302	12/12	0.90	0.16	32,36,40,103	12
3	23J	K	302	12/12	0.90	0.15	26,29,36,67	12
3	23J	D	302	12/12	0.90	0.16	28,31,42,101	12
3	23J	L	302	12/12	0.91	0.12	31,35,41,152	0
3	23J	J	302	12/12	0.91	0.14	32,35,40,140	12
4	CA	A	303	1/1	0.94	0.08	36,36,36,36	0
4	CA	A	305	1/1	0.94	0.10	52,52,52,52	0
4	CA	B	303	1/1	0.94	0.06	34,34,34,34	0
4	CA	B	305	1/1	0.94	0.06	43,43,43,43	0
3	23J	A	302	12/12	0.94	0.16	33,34,45,136	0
4	CA	L	305	1/1	0.95	0.07	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MN	H	301	1/1	0.96	0.05	24,24,24,24	0
2	MN	C	301	1/1	0.96	0.06	22,22,22,22	0
4	CA	D	303	1/1	0.97	0.08	46,46,46,46	0
4	CA	J	304	1/1	0.97	0.05	50,50,50,50	0
4	CA	C	303	1/1	0.97	0.05	31,31,31,31	0
2	MN	K	301	1/1	0.98	0.07	20,20,20,20	0
4	CA	L	304	1/1	0.98	0.05	35,35,35,35	0
4	CA	I	303	1/1	0.98	0.07	21,21,21,21	0
2	MN	A	301	1/1	0.99	0.06	14,14,14,14	0
2	MN	L	301	1/1	0.99	0.05	17,17,17,17	0
4	CA	B	304	1/1	0.99	0.06	23,23,23,23	0
2	MN	D	301	1/1	0.99	0.06	18,18,18,18	0
2	MN	E	301	1/1	0.99	0.05	15,15,15,15	0
2	MN	F	301	1/1	0.99	0.06	16,16,16,16	0
2	MN	G	301	1/1	0.99	0.04	22,22,22,22	0
4	CA	F	303	1/1	0.99	0.06	21,21,21,21	0
2	MN	B	301	1/1	0.99	0.05	17,17,17,17	0
4	CA	J	303	1/1	0.99	0.05	26,26,26,26	0
2	MN	I	301	1/1	0.99	0.05	16,16,16,16	0
4	CA	L	303	1/1	0.99	0.03	23,23,23,23	0
2	MN	J	301	1/1	0.99	0.04	18,18,18,18	0
4	CA	A	304	1/1	0.99	0.04	22,22,22,22	0

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

There are no such residues in this entry.