



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:47 am BST

PDB ID : 2W73
Title : High-resolution structure of the complex between calmodulin and a peptide from calcineurin A
Authors : Majava, V.; Kursula, P.
Deposited on : 2008-12-19
Resolution : 1.45 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
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

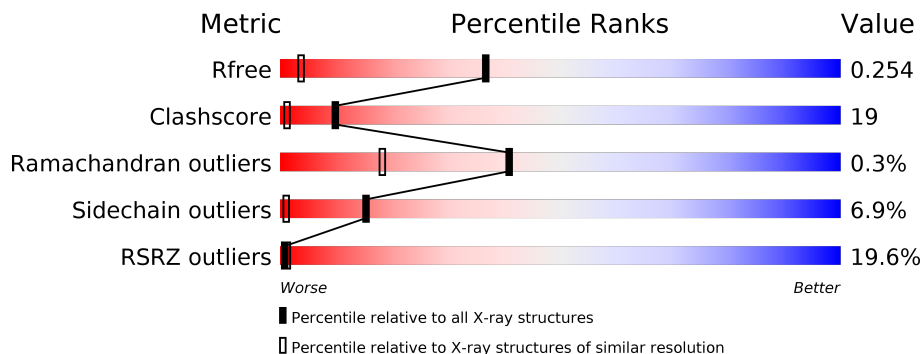
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	149	
1	B	149	
1	E	149	
1	F	149	
2	K	17	
2	L	17	

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Mol	Chain	Length	Quality of chain
2	M	17	
2	O	17	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6079 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 CALMODULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	145	Total 1297	C 819	N 199	O 261	S 18	0	22	0
1	B	145	Total 1306	C 819	N 202	O 268	S 17	0	22	0
1	E	145	Total 1221	C 763	N 189	O 255	S 14	5	11	0
1	F	146	Total 1264	C 781	N 201	O 269	S 13	0	14	0

- Molecule 2 is a protein called SERINE/THREONINE-PROTEIN PHOSPHATASE 2B CATALYTIC SUBUNIT ALPHA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	K	17	Total 167	C 107	N 35	O 23	S 2	0	3	0
2	L	17	Total 161	C 105	N 35	O 20	S 1	0	3	0
2	M	17	Total 158	C 105	N 33	O 19	S 1	0	3	0
2	O	17	Total 145	C 95	N 29	O 20	S 1	0	1	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	7	Total 7	Ca 7	0	0
3	A	4	Total 4	Ca 4	0	0
3	F	5	Total 5	Ca 5	0	0
3	E	4	Total 4	Ca 4	0	0

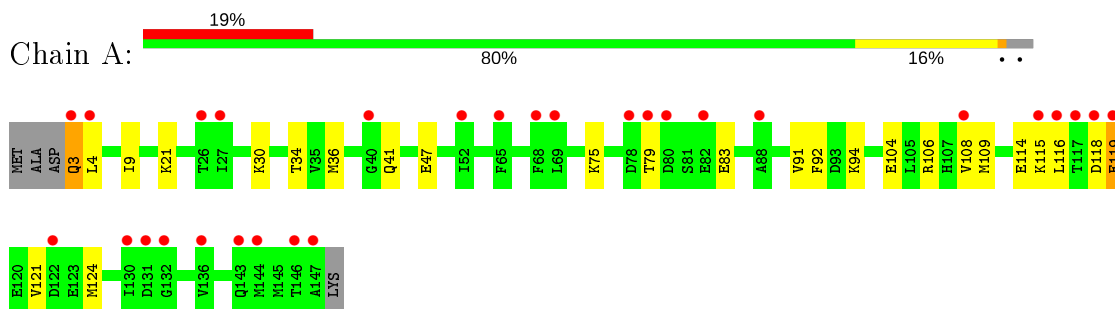
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	87	Total O 87 87	0	0
4	B	122	Total O 122 122	0	0
4	E	43	Total O 43 43	0	0
4	F	71	Total O 71 71	0	0
4	K	3	Total O 3 3	0	0
4	L	4	Total O 4 4	0	0
4	M	6	Total O 6 6	0	0
4	O	4	Total O 4 4	0	0

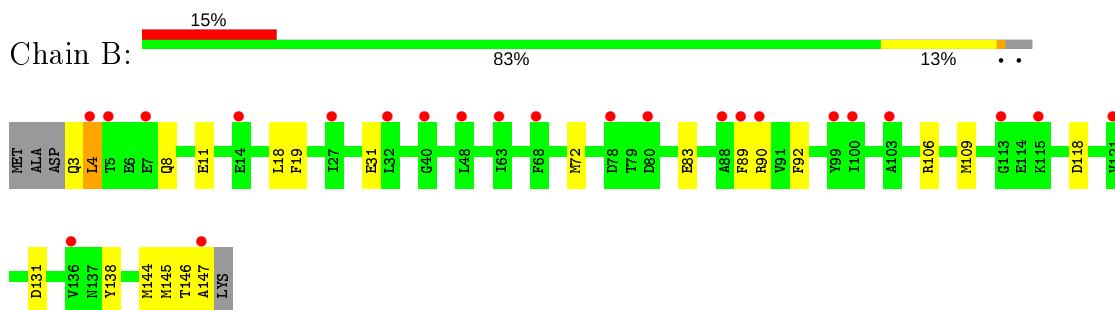
3 Residue-property plots [i](#)

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.

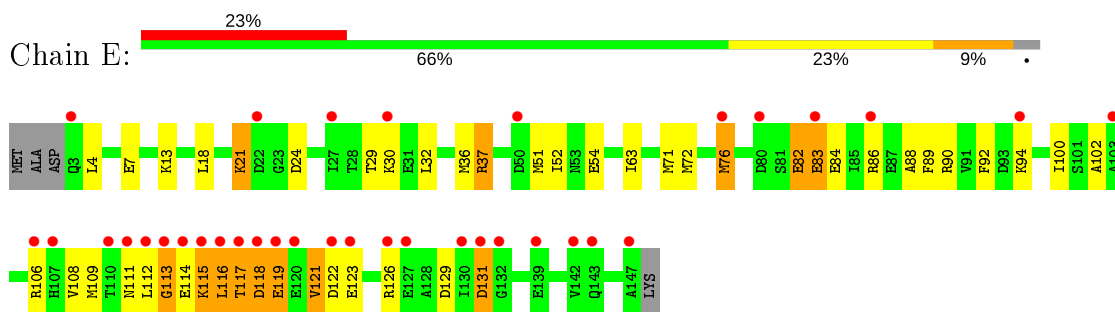
- Molecule 1: CALMODULIN



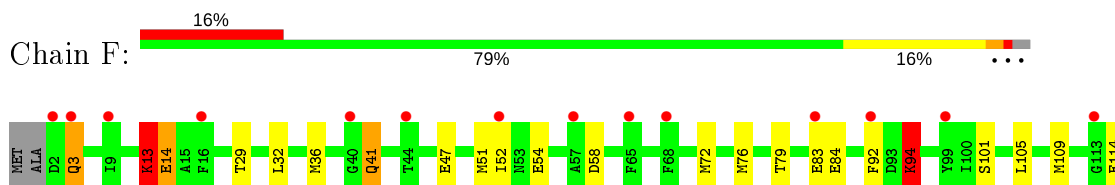
- Molecule 1: CALMODULIN

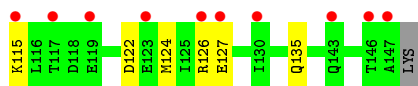


- Molecule 1: CALMODULIN

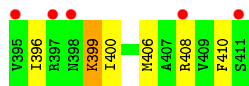


- Molecule 1: CALMODULIN

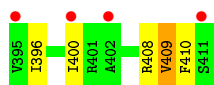




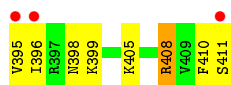
● Molecule 2: SERINE/THREONINE-PROTEIN PHOSPHATASE 2B CATALYTIC SUBUNIT ALPHA ISOFORM



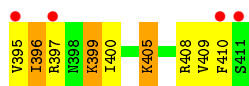
● Molecule 2: SERINE/THREONINE-PROTEIN PHOSPHATASE 2B CATALYTIC SUBUNIT ALPHA ISOFORM



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● Molecule 2: SERINE/THREONINE-PROTEIN PHOSPHATASE 2B CATALYTIC SUBUNIT ALPHA ISOFORM



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.31Å 81.32Å 71.19Å 90.00° 111.28° 90.00°	Depositor
Resolution (Å)	10.00 – 1.45 10.00 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.3 (10.00-1.45) 99.3 (10.00-1.45)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 1.45Å)	Xtrriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.186 , 0.217 0.226 , 0.254	Depositor DCC
R_{free} test set	6070 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtrriage
Anisotropy	0.153	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.51 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6079	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.91	0/1353	0.93	0/1809
1	B	1.01	2/1359 (0.1%)	1.02	3/1816 (0.2%)
1	E	0.83	0/1257	0.96	0/1683
1	F	0.98	5/1294 (0.4%)	1.02	1/1734 (0.1%)
2	K	0.72	0/168	0.96	0/218
2	L	1.32	1/171 (0.6%)	1.01	0/222
2	M	0.82	0/168	0.93	0/219
2	O	1.07	0/149	1.04	0/194
All	All	0.94	8/5919 (0.1%)	0.98	4/7895 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	89	PHE	CE1-CZ	-6.40	1.25	1.37
2	L	409	VAL	CB-CG2	-6.15	1.40	1.52
1	F	13	LYS	CB-CG	-5.85	1.36	1.52
1	F	13	LYS	CG-CD	-5.83	1.32	1.52
1	F	94	LYS	CB-CG	5.46	1.67	1.52
1	F	14	GLU	CG-CD	5.41	1.60	1.51
1	F	14	GLU	CB-CG	5.32	1.62	1.52
1	B	89	PHE	CD1-CE1	-5.13	1.28	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	89	PHE	CB-CG-CD2	6.28	125.19	120.80
1	B	131	ASP	CB-CG-OD1	5.75	123.48	118.30
1	F	58	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	89	PHE	CD1-CE1-CZ	5.33	126.49	120.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1297	0	1268	42	1
1	B	1306	0	1261	33	0
1	E	1221	0	1171	81	1
1	F	1264	0	1184	47	0
2	K	167	0	185	17	0
2	L	161	0	192	14	0
2	M	158	0	192	23	0
2	O	145	0	166	12	0
3	A	4	0	0	0	0
3	B	7	0	0	0	0
3	E	4	0	0	0	0
3	F	5	0	0	0	0
4	A	87	0	0	3	0
4	B	122	0	0	1	0
4	E	43	0	0	1	0
4	F	71	0	0	6	0
4	K	3	0	0	0	0
4	L	4	0	0	0	0
4	M	6	0	0	2	0
4	O	4	0	0	0	0
All	All	6079	0	5619	219	1

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 19.

All (219) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:THR:HG22	1:E:118:ASP:CA	1.39	1.50
1:E:115:LYS:C	1:E:116:LEU:HD23	1.34	1.39
1:E:117:THR:CG2	1:E:118:ASP:HA	1.54	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71[A]:MET:HE3	1:E:72[A]:MET:CE	1.58	1.32
1:F:109[B]:MET:HA	1:F:109[B]:MET:CE	1.71	1.20
1:E:92[B]:PHE:CE1	1:E:108:VAL:HG11	1.82	1.15
1:E:114:GLU:HB3	1:E:116:LEU:HD21	1.16	1.12
1:E:92[B]:PHE:CD1	1:E:108:VAL:HG11	1.83	1.11
1:E:71[A]:MET:HE3	1:E:72[A]:MET:HE2	1.32	1.11
1:E:119:GLU:O	1:E:119:GLU:HG3	1.45	1.10
2:K:406[B]:MET:CE	2:K:410[B]:PHE:CE2	2.40	1.04
1:B:145[B]:MET:HE1	2:L:400:ILE:CD1	1.88	1.03
1:E:117:THR:HG22	1:E:118:ASP:C	1.79	1.03
1:E:92[B]:PHE:CE1	1:E:108:VAL:CG1	2.43	1.01
1:F:109[B]:MET:HA	1:F:109[B]:MET:HE3	1.04	1.00
1:E:115:LYS:C	1:E:116:LEU:CD2	2.30	0.99
2:K:406[B]:MET:HE1	2:K:410[B]:PHE:CE2	1.95	0.98
1:E:115:LYS:O	1:E:116:LEU:HD23	1.63	0.96
1:E:94:LYS:HZ1	1:E:108:VAL:CG2	1.80	0.94
1:E:71[A]:MET:HE3	1:E:72[A]:MET:HE3	1.49	0.93
1:A:75:LYS:O	1:A:79[B]:THR:HG23	1.69	0.92
2:K:406[B]:MET:HE3	2:K:410[B]:PHE:CD2	2.04	0.92
1:E:102:ALA:O	1:E:106:ARG:HG3	1.70	0.92
1:E:117:THR:CG2	1:E:118:ASP:CA	2.29	0.91
1:E:94:LYS:HZ1	1:E:108:VAL:HG23	1.36	0.91
1:E:71[A]:MET:CE	1:E:72[A]:MET:CE	2.49	0.88
1:E:106:ARG:HG2	1:E:121:VAL:HG21	1.56	0.88
2:K:406[B]:MET:HE1	2:K:410[B]:PHE:HE2	1.37	0.88
1:E:84:GLU:CD	2:M:405[A]:LYS:HG3	1.95	0.86
1:E:116:LEU:N	1:E:116:LEU:HD23	1.83	0.86
1:A:21[B]:LYS:HE2	4:A:2014:HOH:O	1.75	0.85
1:B:145[B]:MET:HE1	2:L:400:ILE:HD12	1.57	0.85
1:F:72[A]:MET:CE	2:M:410[A]:PHE:CE2	2.60	0.84
2:K:406[B]:MET:CE	2:K:410[B]:PHE:CD2	2.60	0.84
1:E:117:THR:CB	1:E:118:ASP:HA	2.06	0.83
1:A:106:ARG:NH2	1:A:116:LEU:O	2.11	0.83
1:E:123:GLU:OE2	1:E:126:ARG:NH1	2.11	0.82
1:F:29:THR:HG22	1:F:52:ILE:CD1	2.10	0.82
1:F:72[A]:MET:HE1	2:M:410[A]:PHE:CE2	2.15	0.82
1:F:109[B]:MET:CA	1:F:109[B]:MET:CE	2.53	0.81
1:B:145[B]:MET:HE1	2:L:400:ILE:HD13	1.62	0.81
1:E:114:GLU:CB	1:E:116:LEU:HD21	2.06	0.81
1:E:117:THR:HG22	1:E:118:ASP:HA	0.81	0.80
1:E:117:THR:CG2	1:E:118:ASP:O	2.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144[B]:MET:HE3	1:B:145[B]:MET:HE2	1.60	0.79
1:E:92[B]:PHE:HE1	1:E:108:VAL:CG1	1.92	0.78
1:A:119:GLU:HA	1:A:119:GLU:OE1	1.81	0.78
1:F:109[A]:MET:HE1	2:O:396:ILE:HG13	1.66	0.78
1:B:146:THR:O	1:B:147:ALA:HB2	1.83	0.77
1:E:71[A]:MET:CE	1:E:72[A]:MET:HE3	2.14	0.77
1:B:145[B]:MET:CE	2:L:400:ILE:CD1	2.62	0.76
1:E:115:LYS:O	1:E:116:LEU:CD2	2.31	0.76
1:E:119:GLU:CG	1:E:119:GLU:O	2.30	0.76
1:E:117:THR:CG2	1:E:118:ASP:C	2.52	0.75
1:F:32:LEU:O	1:F:36[B]:MET:HG3	1.86	0.75
1:E:113:GLY:HA2	1:E:114:GLU:O	1.87	0.75
1:A:3:GLN:OE1	1:A:3:GLN:HA	1.84	0.75
1:E:90:ARG:HG2	1:E:90:ARG:HH11	1.50	0.74
1:E:94:LYS:NZ	1:E:108:VAL:CG2	2.51	0.74
1:B:4:LEU:HG	1:B:8:GLN:HG2	1.70	0.73
1:E:52:ILE:HG12	1:E:63:ILE:HD11	1.71	0.72
1:E:82:GLU:CD	1:E:86:ARG:HH21	1.92	0.72
1:F:122[B]:ASP:OD1	4:F:2062:HOH:O	2.07	0.72
1:F:72[A]:MET:CE	2:M:410[A]:PHE:HE2	2.01	0.72
1:E:117:THR:HG22	1:E:118:ASP:O	1.89	0.72
1:E:92[B]:PHE:CD1	1:E:108:VAL:CG1	2.69	0.72
1:A:83:GLU:HB3	2:K:408[B]:ARG:NH2	2.07	0.70
1:B:144[B]:MET:HE3	1:B:145[B]:MET:CE	2.22	0.70
1:B:145[B]:MET:CE	2:L:400:ILE:HD12	2.21	0.70
1:E:84:GLU:OE2	2:M:405[A]:LYS:HE3	1.92	0.69
1:E:113:GLY:HA2	1:E:114:GLU:C	2.13	0.69
2:K:396:ILE:HD12	2:K:396:ILE:H	1.58	0.69
1:B:138[A]:TYR:OH	4:B:2118:HOH:O	2.09	0.68
1:E:71[A]:MET:CE	1:E:72[A]:MET:HE2	2.18	0.68
1:B:144[A]:MET:HE3	1:B:145[A]:MET:HG2	1.74	0.68
1:A:4:LEU:HD23	1:A:9:ILE:HG12	1.77	0.67
1:E:117:THR:HG23	1:E:118:ASP:O	1.94	0.67
1:B:145[B]:MET:CE	2:L:400:ILE:HD13	2.22	0.67
1:B:144[B]:MET:CE	1:B:145[B]:MET:CE	2.72	0.67
2:K:406[B]:MET:HE3	2:K:410[B]:PHE:CE2	2.19	0.67
1:F:29:THR:HG23	4:F:2025:HOH:O	1.95	0.66
1:B:83[A]:GLU:OE2	2:L:408[A]:ARG:NH2	2.28	0.66
1:B:145[B]:MET:HE1	2:L:400:ILE:HG21	1.77	0.66
1:E:90:ARG:HG2	1:E:90:ARG:NH1	2.09	0.66
1:A:4:LEU:HD23	1:A:9:ILE:CG1	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:LYS:CA	1:E:116:LEU:HD23	2.25	0.65
1:F:126:ARG:O	4:F:2064:HOH:O	2.15	0.65
1:A:106:ARG:HH22	1:A:116:LEU:C	2.00	0.65
1:E:82:GLU:OE1	1:E:86:ARG:NH2	2.30	0.65
2:K:406[B]:MET:HE3	2:K:410[B]:PHE:HD2	1.55	0.65
1:A:92[B]:PHE:HZ	2:K:400:ILE:HG12	1.62	0.65
1:B:146:THR:O	1:B:147:ALA:CB	2.47	0.64
1:E:82:GLU:OE1	1:E:86:ARG:NE	2.31	0.63
1:E:129:ASP:O	1:E:131:ASP:O	2.17	0.63
1:E:84:GLU:CD	2:M:405[A]:LYS:HE3	2.20	0.62
1:E:89[B]:PHE:CD1	1:E:100:ILE:HD11	2.36	0.61
1:A:106:ARG:NH2	1:A:116:LEU:HB2	2.16	0.61
1:F:72[A]:MET:HE3	2:M:410[A]:PHE:CE2	2.34	0.61
1:B:144[B]:MET:CE	1:B:145[B]:MET:HE3	2.32	0.60
1:B:83[A]:GLU:CD	2:L:408[A]:ARG:HD2	2.22	0.60
1:A:79[B]:THR:HG21	2:L:409:VAL:HA	1.83	0.60
1:E:84:GLU:OE1	2:M:405[A]:LYS:HE3	2.01	0.60
1:E:94:LYS:NZ	1:E:108:VAL:HB	2.17	0.59
1:F:79:THR:O	1:F:83[B]:GLU:HG2	2.01	0.59
1:F:84[A]:GLU:OE1	2:O:405:LYS:HD3	2.02	0.59
1:E:84:GLU:CD	2:M:405[A]:LYS:CG	2.70	0.59
1:F:51[A]:MET:HE1	2:M:410[A]:PHE:HE1	1.68	0.59
1:F:109[A]:MET:HE3	2:O:396:ILE:HG12	1.85	0.59
1:E:92[A]:PHE:CD1	1:E:108:VAL:HG11	2.37	0.58
1:F:92[B]:PHE:HE2	2:O:400:ILE:HG23	1.66	0.58
1:F:72[A]:MET:CE	2:M:410[A]:PHE:CZ	2.86	0.58
1:F:109[A]:MET:CE	2:O:396:ILE:HG13	2.34	0.58
1:E:29:THR:HG22	1:E:52:ILE:HD12	1.85	0.57
1:E:94:LYS:HZ1	1:E:108:VAL:CB	2.16	0.57
1:F:101:SER:HB3	1:F:135[B]:GLN:HE21	1.69	0.57
1:E:114:GLU:HB3	1:E:116:LEU:CD2	2.11	0.57
2:K:406[B]:MET:CE	2:K:410[B]:PHE:HE2	1.97	0.56
1:A:94:LYS:HE2	1:A:108:VAL:CG2	2.35	0.56
1:F:122[B]:ASP:O	1:F:126:ARG:HG3	2.06	0.56
1:B:145[B]:MET:CE	2:L:400:ILE:HG21	2.35	0.56
1:E:88:ALA:O	1:E:92[A]:PHE:HD2	1.89	0.55
1:F:83[B]:GLU:HG3	2:M:408[B]:ARG:HH22	1.71	0.55
1:A:21[B]:LYS:CE	4:A:2014:HOH:O	2.43	0.55
2:M:398:ASN:ND2	4:M:2002:HOH:O	2.39	0.55
1:B:72[A]:MET:CE	1:B:72[A]:MET:HA	2.37	0.55
1:F:41:GLN:NE2	2:M:411:SER:HB2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144[B]:MET:CE	1:B:145[B]:MET:HE2	2.28	0.55
1:A:114:GLU:OE2	2:K:399:LYS:CE	2.56	0.54
2:M:395:VAL:HG22	2:M:396:ILE:N	2.22	0.54
1:F:72[A]:MET:HE1	2:M:410[A]:PHE:CZ	2.42	0.54
1:E:76:MET:CE	2:O:408:ARG:NH1	2.71	0.54
1:F:72[A]:MET:HE3	2:M:410[A]:PHE:CZ	2.44	0.53
1:F:29:THR:HG22	1:F:52:ILE:HD12	1.90	0.53
1:A:94:LYS:CE	1:A:108:VAL:HG22	2.40	0.52
1:F:109[A]:MET:CE	2:O:396:ILE:CG1	2.87	0.52
1:E:118:ASP:OD1	1:E:118:ASP:N	2.40	0.52
1:F:127:GLU:O	4:F:2067:HOH:O	2.19	0.51
1:F:105:LEU:HD21	1:F:124:MET:HE2	1.92	0.51
1:E:94:LYS:NZ	1:E:108:VAL:HG23	2.18	0.51
1:E:108:VAL:CG1	1:E:109:MET:N	2.73	0.51
1:E:112:LEU:O	1:E:113:GLY:O	2.29	0.50
1:E:116:LEU:O	1:E:117:THR:O	2.30	0.50
1:A:94:LYS:CE	1:A:108:VAL:CG2	2.89	0.50
1:F:109[B]:MET:HE2	1:F:114:GLU:HB2	1.94	0.50
1:E:123:GLU:HG3	1:E:123:GLU:O	2.12	0.50
1:A:83:GLU:HB3	2:K:408[B]:ARG:HH21	1.77	0.49
1:A:94:LYS:NZ	4:A:2065:HOH:O	2.41	0.49
1:F:3:GLN:HG2	1:F:3:GLN:O	1.98	0.49
1:A:115:LYS:O	1:A:116:LEU:HD23	2.13	0.49
1:F:29:THR:HG22	1:F:52:ILE:HD11	1.94	0.49
1:A:94:LYS:HZ1	1:A:108:VAL:HG22	1.78	0.49
1:E:83:GLU:OE1	2:M:408[B]:ARG:NH1	2.45	0.49
1:A:114:GLU:OE2	2:K:399:LYS:HE3	2.12	0.49
1:E:108:VAL:HG13	1:E:109:MET:N	2.28	0.48
1:E:94:LYS:NZ	1:E:108:VAL:CB	2.74	0.48
1:A:75:LYS:HE3	2:L:410[A]:PHE:CE1	2.49	0.48
1:E:13[A]:LYS:CE	4:E:2011:HOH:O	2.61	0.48
1:B:109[B]:MET:CE	2:L:396:ILE:HD11	2.44	0.48
1:A:106:ARG:HD2	1:A:121:VAL:HG11	1.97	0.47
1:A:92[B]:PHE:CZ	2:K:400:ILE:HG12	2.45	0.47
1:B:92[A]:PHE:HE1	1:B:109[A]:MET:HE2	1.80	0.47
1:F:109[B]:MET:HE2	1:F:109[B]:MET:CA	2.42	0.47
1:E:94:LYS:HZ3	1:E:108:VAL:HB	1.80	0.47
1:E:106:ARG:CG	1:E:121:VAL:HG21	2.37	0.47
1:B:72[A]:MET:HE2	1:B:72[A]:MET:HA	1.96	0.47
1:F:41:GLN:CD	2:M:411:SER:HB2	2.35	0.46
1:F:109[A]:MET:HE3	2:O:396:ILE:CG1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:MET:CE	2:O:408:ARG:HH12	2.29	0.46
1:E:92[A]:PHE:CE1	1:E:108:VAL:HG11	2.49	0.46
1:A:36[B]:MET:CE	1:A:41:GLN:OE1	2.64	0.45
1:B:144[B]:MET:HE2	1:B:145[B]:MET:HE3	1.99	0.45
1:F:101:SER:CB	1:F:135[B]:GLN:HE21	2.29	0.45
1:E:82:GLU:OE1	1:E:86:ARG:CZ	2.64	0.45
1:B:144[B]:MET:HE2	1:B:145[B]:MET:CE	2.46	0.45
1:A:94:LYS:NZ	1:A:108:VAL:HG22	2.31	0.45
1:F:122[A]:ASP:O	1:F:126:ARG:HG3	2.15	0.45
1:B:144[A]:MET:CE	1:B:145[A]:MET:HG2	2.46	0.44
1:F:94:LYS:HD3	4:F:2052:HOH:O	2.16	0.44
1:B:72[A]:MET:CA	1:B:72[A]:MET:HE2	2.47	0.44
1:B:106[A]:ARG:HD2	1:B:118:ASP:OD1	2.18	0.44
1:B:109[A]:MET:HA	1:B:109[A]:MET:CE	2.48	0.44
1:F:114:GLU:OE2	2:O:399:LYS:NZ	2.32	0.44
1:F:14:GLU:HG3	4:F:2011:HOH:O	2.18	0.44
1:F:101:SER:HB3	1:F:135[B]:GLN:NE2	2.31	0.44
1:A:79[B]:THR:O	1:A:83:GLU:HG2	2.18	0.43
2:M:395:VAL:HG12	2:M:398:ASN:ND2	2.33	0.43
2:M:395:VAL:HG13	2:M:398:ASN:H	1.83	0.43
1:B:18:LEU:HD23	2:K:406[B]:MET:HG3	2.00	0.43
1:A:83:GLU:HB3	2:K:408[B]:ARG:CZ	2.49	0.43
2:M:405[A]:LYS:HD2	4:M:2004:HOH:O	2.17	0.42
1:A:91:VAL:O	1:A:94:LYS:NZ	2.52	0.42
1:F:3:GLN:CG	1:F:3:GLN:O	2.59	0.42
1:F:47:GLU:O	1:F:51[A]:MET:HG3	2.19	0.42
1:E:76:MET:SD	2:O:409:VAL:CG1	3.07	0.42
1:A:118:ASP:O	1:A:121:VAL:HG22	2.19	0.42
1:A:94:LYS:HG3	1:A:104:GLU:HG2	2.01	0.42
1:B:19:PHE:O	1:B:31:GLU:HB3	2.20	0.42
1:A:109[A]:MET:HG3	1:A:116:LEU:HD12	2.01	0.42
1:A:21[B]:LYS:HE3	1:A:34:THR:HG21	2.02	0.42
1:F:13:LYS:HG2	1:F:13:LYS:HZ3	1.34	0.42
1:A:124[B]:MET:HB2	1:A:124[B]:MET:HE2	1.83	0.41
1:E:112:LEU:O	1:E:113:GLY:C	2.59	0.41
1:E:123:GLU:CD	1:E:126:ARG:HD3	2.40	0.41
1:F:109[B]:MET:HE2	1:F:114:GLU:CB	2.51	0.41
1:E:63:ILE:HD13	1:E:71[B]:MET:HE3	2.03	0.41
1:A:94:LYS:HE2	1:A:108:VAL:HG23	2.02	0.41
1:A:79[A]:THR:O	1:A:83:GLU:HG2	2.21	0.41
1:E:51:MET:HA	1:E:54:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:LEU:O	1:E:21:LYS:HE3	2.21	0.41
1:A:30[B]:LYS:HA	1:A:30[B]:LYS:HD3	1.66	0.40
1:A:4:LEU:CD2	1:A:9:ILE:HG12	2.49	0.40
2:M:395:VAL:CG2	2:M:396:ILE:N	2.83	0.40
1:B:109[B]:MET:HE1	2:L:396:ILE:HD11	2.02	0.40
1:A:36[B]:MET:HE3	1:A:41:GLN:OE1	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLU:OE2	1:E:37:ARG:NH1[2_546]	2.06	0.14

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	165/149 (111%)	165 (100%)	0	0	100	100
1	B	165/149 (111%)	165 (100%)	0	0	100	100
1	E	154/149 (103%)	148 (96%)	4 (3%)	2 (1%)	12	2
1	F	158/149 (106%)	157 (99%)	1 (1%)	0	100	100
2	K	18/17 (106%)	18 (100%)	0	0	100	100
2	L	18/17 (106%)	18 (100%)	0	0	100	100
2	M	18/17 (106%)	18 (100%)	0	0	100	100
2	O	16/17 (94%)	16 (100%)	0	0	100	100
All	All	712/664 (107%)	705 (99%)	5 (1%)	2 (0%)	41	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	117	THR
1	E	113	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	146/127 (115%)	144 (99%)	2 (1%)	67	37
1	B	146/127 (115%)	141 (97%)	5 (3%)	37	6
1	E	135/127 (106%)	116 (86%)	19 (14%)	3	0
1	F	139/127 (109%)	133 (96%)	6 (4%)	29	3
2	K	17/14 (121%)	16 (94%)	1 (6%)	19	1
2	L	17/14 (121%)	17 (100%)	0	100	100
2	M	17/14 (121%)	14 (82%)	3 (18%)	2	0
2	O	15/14 (107%)	10 (67%)	5 (33%)	0	0
All	All	632/564 (112%)	591 (94%)	41 (6%)	15	1

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	119	GLU
1	B	3	GLN
1	B	4	LEU
1	B	11	GLU
1	B	90[A]	ARG
1	B	90[B]	ARG
1	E	4	LEU
1	E	7	GLU
1	E	21	LYS
1	E	24	ASP
1	E	30	LYS
1	E	32[A]	LEU
1	E	32[B]	LEU

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Mol	Chain	Res	Type
1	E	37	ARG
1	E	76	MET
1	E	82	GLU
1	E	83	GLU
1	E	111	ASN
1	E	115	LYS
1	E	116	LEU
1	E	118	ASP
1	E	119	GLU
1	E	121	VAL
1	E	122	ASP
1	E	131	ASP
1	F	3	GLN
1	F	13	LYS
1	F	41	GLN
1	F	54	GLU
1	F	94	LYS
1	F	115	LYS
2	K	399	LYS
2	M	399	LYS
2	M	408[A]	ARG
2	M	408[B]	ARG
2	O	395	VAL
2	O	396	ILE
2	O	397	ARG
2	O	399	LYS
2	O	405	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	HIS
1	A	111	ASN
1	A	135	GLN
1	B	3	GLN
1	E	3	GLN
1	F	42	ASN
2	M	398	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 20 ligands modelled in this entry, 20 are monoatomic - leaving 0 for Mogul analysis.

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 [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

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	145/149 (97%)	1.28	29 (20%) 1 1	3, 9, 22, 27	0
1	B	145/149 (97%)	1.01	23 (15%) 1 2	3, 7, 17, 29	0
1	E	145/149 (97%)	1.49	35 (24%) 0 1	5, 16, 37, 53	1 (0%)
1	F	146/149 (97%)	1.12	24 (16%) 1 2	4, 12, 24, 34	1 (0%)
2	K	17/17 (100%)	2.27	5 (29%) 0 0	6, 12, 20, 29	0
2	L	17/17 (100%)	1.85	4 (23%) 0 1	7, 9, 27, 31	0
2	M	17/17 (100%)	1.61	3 (17%) 1 1	6, 11, 20, 26	0
2	O	17/17 (100%)	2.00	4 (23%) 0 1	6, 10, 26, 29	0
All	All	649/664 (97%)	1.30	127 (19%) 1 1	3, 11, 26, 53	2 (0%)

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	395	VAL	13.4
1	E	116	LEU	12.3
2	K	395	VAL	11.6
1	E	113	GLY	8.3
2	M	395	VAL	8.0
1	B	147	ALA	7.0
2	L	395	VAL	6.8
1	A	147	ALA	6.7
1	E	110	THR	6.3
1	E	119	GLU	5.9
2	K	411	SER	5.9
1	E	132	GLY	5.6
1	A	3	GLN	5.5
1	A	119	GLU	5.5
2	M	411	SER	5.4
1	E	106	ARG	5.3

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Mol	Chain	Res	Type	RSRZ
1	E	122	ASP	5.2
1	E	118	ASP	5.2
1	A	118	ASP	5.0
1	A	130[A]	ILE	5.0
1	F	115	LYS	5.0
1	F	113	GLY	5.0
1	E	126	ARG	4.9
2	O	411	SER	4.7
2	L	411	SER	4.5
1	F	147	ALA	4.5
1	A	132	GLY	4.5
1	E	117	THR	4.2
1	E	3	GLN	4.2
1	E	114	GLU	4.2
2	K	398	ASN	4.1
1	F	68[A]	PHE	4.1
1	E	115	LYS	4.1
1	A	143	GLN	4.0
1	F	126	ARG	4.0
1	F	2	ASP	3.9
1	F	92[A]	PHE	3.9
1	A	131	ASP	3.8
1	E	147	ALA	3.8
2	K	397	ARG	3.7
1	E	120	GLU	3.7
1	E	123	GLU	3.7
1	B	48	LEU	3.6
1	B	4	LEU	3.5
1	E	22	ASP	3.5
1	F	143	GLN	3.4
1	F	99	TYR	3.4
1	E	139	GLU	3.4
1	E	130	ILE	3.3
1	A	115	LYS	3.3
1	F	117	THR	3.3
1	E	111	ASN	3.2
1	B	100	ILE	3.1
1	F	3	GLN	3.0
1	E	131	ASP	3.0
1	A	68	PHE	3.0
1	F	16	PHE	3.0
1	B	27	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	146	THR	3.0
1	E	142	VAL	2.9
1	E	127	GLU	2.9
1	E	50	ASP	2.9
1	A	40	GLY	2.8
1	A	69	LEU	2.8
1	E	107	HIS	2.7
1	B	136	VAL	2.7
1	A	4	LEU	2.7
1	A	79[A]	THR	2.6
1	B	7	GLU	2.6
2	O	397	ARG	2.6
2	M	396	ILE	2.6
1	B	5	THR	2.6
1	F	130	ILE	2.5
1	B	89	PHE	2.5
1	B	40	GLY	2.4
1	F	40	GLY	2.4
1	F	119	GLU	2.4
1	E	86	ARG	2.4
1	A	136	VAL	2.4
1	E	103	ALA	2.4
1	F	57	ALA	2.4
2	L	400	ILE	2.4
1	F	44	THR	2.4
2	K	408[A]	ARG	2.4
1	A	52	ILE	2.4
1	E	76	MET	2.4
1	E	143	GLN	2.3
1	A	65[A]	PHE	2.3
1	A	88	ALA	2.3
1	B	88	ALA	2.3
1	B	80	ASP	2.3
1	A	26	THR	2.3
1	F	123	GLU	2.3
1	A	117	THR	2.3
1	F	9	ILE	2.3
1	F	52	ILE	2.3
1	B	14	GLU	2.3
1	F	83[A]	GLU	2.3
1	B	121	VAL	2.3
1	A	78	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	127	GLU	2.2
1	F	65[A]	PHE	2.2
1	F	146	THR	2.2
1	A	108	VAL	2.2
1	B	113	GLY	2.2
1	A	144[A]	MET	2.2
1	B	103	ALA	2.2
1	E	80	ASP	2.2
1	B	115	LYS	2.2
1	B	63	ILE	2.2
1	B	90[A]	ARG	2.2
1	B	68	PHE	2.1
1	A	122	ASP	2.1
1	B	32	LEU	2.1
1	E	112	LEU	2.1
1	A	27	ILE	2.1
1	A	82	GLU	2.1
1	A	80	ASP	2.1
1	B	78	ASP	2.1
2	L	402	ALA	2.1
2	O	410[A]	PHE	2.1
1	B	99	TYR	2.1
1	E	83	GLU	2.1
1	E	94	LYS	2.1
1	E	30	LYS	2.1
1	A	116	LEU	2.0
1	E	27	ILE	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(\AA^2)	Q<0.9
3	CA	B	1154	1/1	0.95	0.31	23,23,23,23	0
3	CA	E	1151	1/1	0.95	0.05	14,14,14,14	0
3	CA	A	1151	1/1	0.96	0.06	11,11,11,11	0
3	CA	F	1151	1/1	0.96	0.08	10,10,10,10	0
3	CA	F	1152	1/1	0.97	0.10	8,8,8,8	0
3	CA	A	1150	1/1	0.98	0.09	9,9,9,9	0
3	CA	E	1150	1/1	0.98	0.04	16,16,16,16	0
3	CA	B	1152	1/1	0.98	0.04	11,11,11,11	0
3	CA	F	1149	1/1	0.98	0.07	10,10,10,10	0
3	CA	F	1150	1/1	0.98	0.10	7,7,7,7	0
3	CA	F	1148	1/1	0.99	0.10	4,4,4,4	0
3	CA	A	1149	1/1	0.99	0.18	3,3,3,3	0
3	CA	B	1149	1/1	0.99	0.10	4,4,4,4	0
3	CA	B	1151	1/1	0.99	0.12	4,4,4,4	0
3	CA	B	1150	1/1	0.99	0.09	4,4,4,4	0
3	CA	E	1148	1/1	0.99	0.05	11,11,11,11	0
3	CA	B	1153	1/1	0.99	0.08	8,8,8,8	0
3	CA	E	1149	1/1	0.99	0.06	8,8,8,8	0
3	CA	A	1148	1/1	0.99	0.13	4,4,4,4	0
3	CA	B	1148	1/1	0.99	0.12	4,4,4,4	0

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

There are no such residues in this entry.