Full wwPDB X-ray Structure Validation Report (i)

Oct 22, 2023 – 07:14 AM EDT

PDB ID	:	2ZRT
Title	:	Crystal structure of Zn2+-bound form of des3-23ALG-2
Authors	:	Suzuki, H.; Kawasaki, M.; Kakiuchi, T.; Shibata, H.; Wakatsuki, S.; Maki, M.
Deposited on	:	2008-09-01
Resolution	:	3.30 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 (i) 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 (1)) were used in the production of this report:

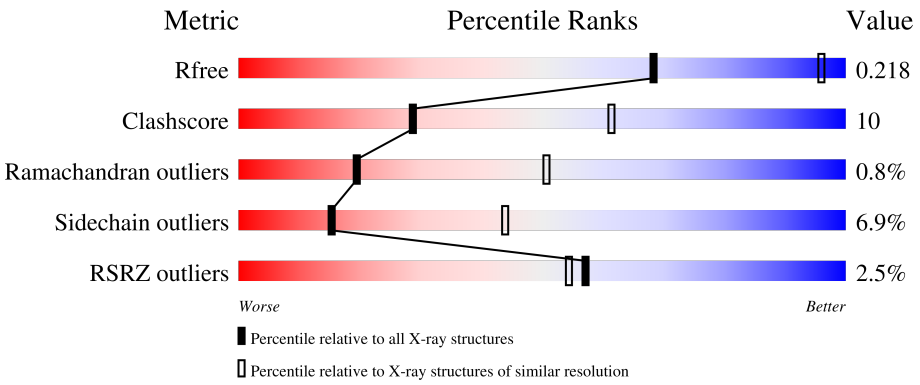
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	168	% 73% 20% • • •
1	B	168	65% 29% • •
1	C	168	73% 23% • •
1	D	168	76% 19% • •
1	E	168	67% 26% 5% • •

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Mol	Chain	Length	Quality of chain
1	F	168	73% 24%
1	G	168	7% 71% 23%
1	H	168	12% 72% 23%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11004 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 Programmed cell death protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	165	1376	874	239	259	4	0	0	0
1	B	165	1378	875	239	260	4	0	0	0
1	C	164	1370	871	238	257	4	0	0	0
1	D	163	1361	866	236	255	4	0	0	0
1	E	166	1384	878	240	262	4	0	0	0
1	F	165	1376	874	239	259	4	0	0	0
1	G	163	1361	866	236	255	4	0	0	0
1	H	163	1361	866	236	255	4	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	3	3	3	0	0
2	B	6	6	6	0	0
2	C	5	5	5	0	0
2	D	6	6	6	0	0
2	E	5	5	5	0	0
2	F	5	5	5	0	0

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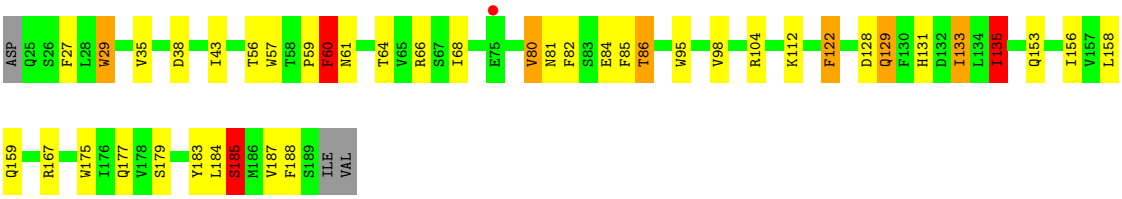
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	G	5	5	5	0	0
			Total	Zn		
2	H	2	2	2	0	0

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.

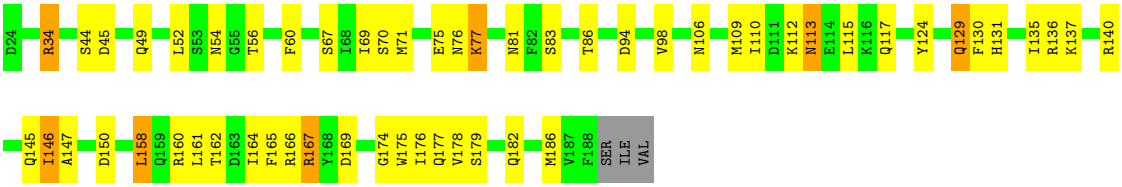
• Molecule 1: Programmed cell death protein 6

Chain A:



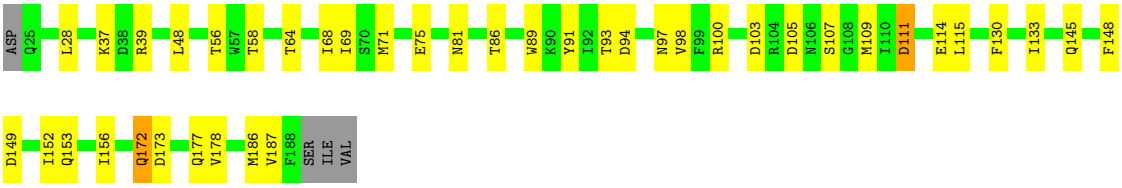
• Molecule 1: Programmed cell death protein 6

Chain B:



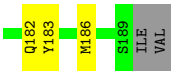
• Molecule 1: Programmed cell death protein 6

Chain C:



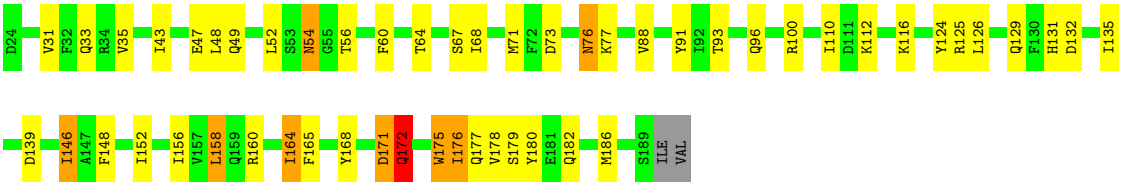
• Molecule 1: Programmed cell death protein 6

Chain D:



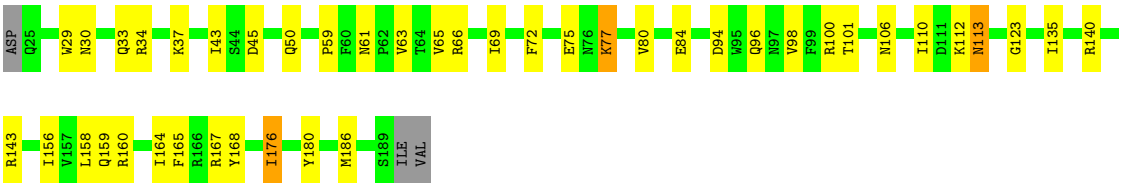
• Molecule 1: Programmed cell death protein 6

Chain E:



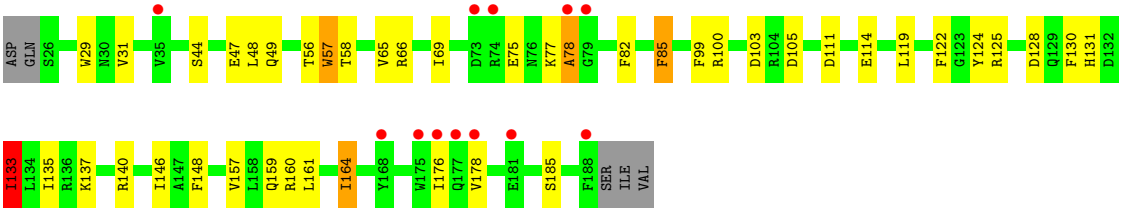
• Molecule 1: Programmed cell death protein 6

Chain F:



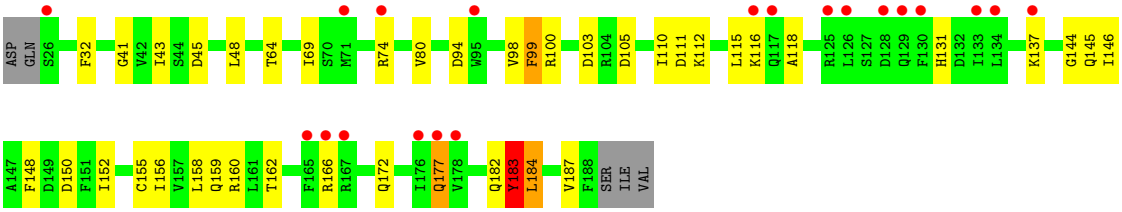
• Molecule 1: Programmed cell death protein 6

Chain G:



• Molecule 1: Programmed cell death protein 6

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.81Å 147.54Å 230.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	115.47 – 3.30 115.37 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (115.47-3.30) 100.0 (115.37-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	77.65 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.169 , 0.221 0.169 , 0.218	Depositor DCC
R_{free} test set	2785 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å^2)	95.0	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11004	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.35	0/1408	1.04	16/1901 (0.8%)
1	B	0.35	0/1410	0.53	0/1904
1	C	0.35	0/1402	0.60	2/1893 (0.1%)
1	D	0.33	0/1393	0.48	0/1881
1	E	0.34	0/1416	0.81	6/1912 (0.3%)
1	F	0.33	0/1408	0.50	1/1901 (0.1%)
1	G	0.35	0/1393	0.76	5/1881 (0.3%)
1	H	0.35	0/1393	0.54	3/1881 (0.2%)
All	All	0.34	0/11223	0.68	33/15154 (0.2%)

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	3
1	C	0	1
1	E	0	1
All	All	0	5

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	122	PHE	CB-CA-C	-20.33	69.73	110.40
1	E	172	GLN	CB-CA-C	-18.09	74.23	110.40
1	G	122	PHE	CB-CA-C	-13.50	83.39	110.40
1	A	81	ASN	N-CA-C	13.35	147.05	111.00
1	G	78	ALA	N-CA-C	12.89	145.80	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	60	PHE	N-CA-C	-11.91	78.83	111.00
1	G	78	ALA	CB-CA-C	-11.18	93.33	110.10
1	E	171	ASP	CB-CA-C	10.79	131.99	110.40
1	A	81	ASN	CB-CA-C	-10.70	89.00	110.40
1	C	172	GLN	N-CA-C	10.39	139.05	111.00
1	E	76	ASN	N-CA-C	9.79	137.42	111.00
1	A	122	PHE	C-N-CA	9.77	142.81	122.30
1	E	172	GLN	N-CA-C	9.38	136.34	111.00
1	A	60	PHE	C-N-CA	9.16	144.61	121.70
1	A	29	TRP	CB-CA-C	8.48	127.37	110.40
1	A	80	VAL	CB-CA-C	-8.27	95.69	111.40
1	A	135	ILE	N-CA-C	7.99	132.56	111.00
1	E	172	GLN	C-N-CA	7.93	141.52	121.70
1	C	172	GLN	CB-CA-C	-6.89	96.61	110.40
1	H	99	PHE	CB-CA-C	-6.86	96.67	110.40
1	A	185	SER	CB-CA-C	6.45	122.36	110.10
1	A	129	GLN	N-CA-C	6.34	128.13	111.00
1	G	77	LYS	CB-CA-C	-6.03	98.34	110.40
1	H	182	GLN	CB-CA-C	-5.77	98.85	110.40
1	A	135	ILE	CB-CA-C	-5.51	100.59	111.60
1	E	175	TRP	CB-CA-C	-5.46	99.49	110.40
1	A	84	GLU	CB-CA-C	-5.45	99.50	110.40
1	G	57	TRP	CB-CA-C	-5.36	99.67	110.40
1	A	133	ILE	N-CA-C	5.24	125.14	111.00
1	H	183	TYR	N-CA-C	5.21	125.07	111.00
1	F	77	LYS	CB-CA-C	5.15	120.70	110.40
1	A	185	SER	C-N-CA	5.06	134.35	121.70
1	A	128	ASP	CB-CA-C	-5.06	100.28	110.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	PHE	Peptide
1	A	185	SER	Peptide
1	A	60	PHE	Peptide
1	C	172	GLN	Peptide
1	E	172	GLN	Peptide

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	1376	0	1309	25	0
1	B	1378	0	1308	36	0
1	C	1370	0	1303	24	0
1	D	1361	0	1296	22	0
1	E	1384	0	1312	38	0
1	F	1376	0	1309	24	0
1	G	1361	0	1296	23	0
1	H	1361	0	1296	29	0
2	A	3	0	0	0	0
2	B	6	0	0	0	0
2	C	5	0	0	0	0
2	D	6	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	2	0	0	0	0
All	All	11004	0	10429	207	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 10.

All (207) 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:G:69:ILE:HG21	1:G:78:ALA:O	1.39	1.19
1:A:135:ILE:HG22	1:A:135:ILE:O	1.46	1.11
1:A:135:ILE:O	1:A:135:ILE:CG2	2.21	0.87
1:B:75:GLU:HB2	1:B:77:LYS:HD2	1.57	0.86
1:A:59:PRO:C	1:A:60:PHE:O	2.01	0.85
1:A:129:GLN:HG3	1:A:129:GLN:O	1.76	0.85
1:D:56:THR:HB	1:D:58:THR:HG22	1.57	0.84
1:G:69:ILE:CG2	1:G:78:ALA:O	2.26	0.84
1:H:110:ILE:HB	1:H:146:ILE:HG22	1.60	0.83
1:G:157:VAL:O	1:G:161:LEU:HB2	1.81	0.80
1:E:76:ASN:O	1:E:76:ASN:CG	2.20	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ILE:HD12	1:B:146:ILE:HG12	1.66	0.77
1:H:99:PHE:O	1:H:99:PHE:CD2	2.41	0.73
1:H:48:LEU:HD13	1:H:69:ILE:HD11	1.70	0.72
1:E:176:ILE:HD12	1:E:177:GLN:H	1.55	0.70
1:F:96:GLN:HE21	1:F:100:ARG:NE	1.91	0.69
1:E:54:ASN:HD22	1:E:56:THR:H	1.40	0.68
1:D:64:THR:O	1:D:68:ILE:HG12	1.93	0.68
1:E:176:ILE:HD12	1:E:177:GLN:N	2.08	0.68
1:H:183:TYR:O	1:H:183:TYR:CD2	2.47	0.67
1:E:168:TYR:O	1:E:176:ILE:HD13	1.96	0.66
1:F:75:GLU:HG3	1:F:77:LYS:NZ	2.11	0.65
1:A:133:ILE:O	1:A:133:ILE:HG22	1.97	0.64
1:A:179:SER:HA	1:B:175:TRP:HA	1.80	0.63
1:B:135:ILE:CD1	1:B:146:ILE:HG12	2.28	0.62
1:F:112:LYS:HD3	1:F:135:ILE:HD12	1.82	0.62
1:H:156:ILE:O	1:H:160:ARG:HD2	2.00	0.62
1:F:96:GLN:HE21	1:F:100:ARG:HE	1.48	0.61
1:B:167:ARG:HH11	1:B:167:ARG:HG3	1.66	0.61
1:H:166:ARG:HG2	1:H:172:GLN:HE22	1.64	0.61
1:F:164:ILE:HA	1:F:167:ARG:HD3	1.82	0.61
1:G:82:PHE:HA	1:G:85:PHE:HB2	1.83	0.61
1:E:52:LEU:HB3	1:E:60:PHE:CD1	2.36	0.61
1:A:80:VAL:O	1:A:80:VAL:HG23	2.01	0.60
1:A:29:TRP:HD1	1:A:85:PHE:HB3	1.67	0.60
1:E:68:ILE:HD12	1:E:91:TYR:CE2	2.37	0.59
1:H:183:TYR:O	1:H:183:TYR:CG	2.55	0.59
1:B:178:VAL:HG12	1:B:182:GLN:HE21	1.68	0.58
1:E:179:SER:HB3	1:E:182:GLN:HG3	1.86	0.58
1:A:85:PHE:O	1:A:85:PHE:CD2	2.57	0.58
1:D:48:LEU:HD23	1:D:65:VAL:HG13	1.84	0.58
1:H:69:ILE:HG23	1:H:80:VAL:HG13	1.86	0.57
1:D:135:ILE:HG12	1:D:146:ILE:HD11	1.85	0.57
1:E:168:TYR:O	1:E:176:ILE:CD1	2.53	0.57
1:B:124:TYR:CE2	1:B:158:LEU:HD22	2.40	0.57
1:C:94:ASP:O	1:C:98:VAL:HG23	2.04	0.57
1:G:49:GLN:HB3	1:G:65:VAL:HG21	1.86	0.56
1:A:59:PRO:O	1:A:60:PHE:O	2.23	0.56
1:E:68:ILE:HD12	1:E:91:TYR:HE2	1.69	0.56
1:E:171:ASP:O	1:E:172:GLN:HB2	2.05	0.56
1:G:31:VAL:HG12	1:G:31:VAL:O	2.04	0.56
1:H:183:TYR:O	1:H:187:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:PHE:CE1	1:H:184:LEU:HD22	2.41	0.56
1:F:165:PHE:CD1	1:F:176:ILE:HD12	2.41	0.55
1:H:32:PHE:HZ	1:H:41:GLY:HA2	1.71	0.55
1:A:80:VAL:HG21	1:A:85:PHE:HD1	1.71	0.55
1:C:148:PHE:O	1:C:152:ILE:HG13	2.06	0.55
1:A:184:LEU:HB3	1:B:130:PHE:CE1	2.41	0.55
1:B:106:ASN:O	1:C:100:ARG:NH1	2.40	0.55
1:C:28:LEU:HD13	1:C:86:THR:HG22	1.89	0.54
1:H:146:ILE:HG13	1:H:150:ASP:HB2	1.89	0.54
1:C:68:ILE:HD12	1:C:91:TYR:HE2	1.73	0.54
1:F:98:VAL:HA	1:F:101:THR:HG22	1.89	0.54
1:B:109:MET:HG2	1:B:147:ALA:HA	1.89	0.54
1:B:112:LYS:HD3	1:B:131:HIS:HB2	1.89	0.54
1:A:95:TRP:HA	1:A:98:VAL:HB	1.88	0.54
1:F:43:ILE:HB	1:F:80:VAL:HG23	1.90	0.54
1:C:178:VAL:HG11	1:C:186:MET:HE1	1.89	0.54
1:A:29:TRP:O	1:A:85:PHE:CE2	2.62	0.53
1:C:187:VAL:HG11	1:D:161:LEU:HD21	1.90	0.53
1:G:135:ILE:HG12	1:G:146:ILE:HD11	1.91	0.53
1:E:116:LYS:HA	1:E:131:HIS:CE1	2.43	0.52
1:F:75:GLU:HG3	1:F:77:LYS:HZ1	1.75	0.52
1:D:111:ASP:H	1:D:114:GLU:HB2	1.75	0.52
1:E:43:ILE:HG21	1:E:48:LEU:HB2	1.90	0.52
1:B:124:TYR:HE2	1:B:158:LEU:HD22	1.73	0.52
1:F:37:LYS:HG3	1:F:50:GLN:HE22	1.76	0.51
1:G:185:SER:H	1:H:137:LYS:HB2	1.75	0.51
1:A:183:TYR:O	1:A:187:VAL:HG23	2.09	0.51
1:C:64:THR:O	1:C:68:ILE:HG12	2.10	0.50
1:E:43:ILE:CG2	1:E:48:LEU:HB2	2.42	0.50
1:G:48:LEU:HD23	1:G:65:VAL:HG13	1.94	0.50
1:C:177:GLN:HG3	1:D:177:GLN:HB3	1.94	0.50
1:D:124:TYR:HE2	1:D:158:LEU:HD22	1.76	0.50
1:H:100:ARG:HA	1:H:103:ASP:HB2	1.94	0.50
1:H:112:LYS:HG3	1:H:131:HIS:HB2	1.94	0.50
1:E:148:PHE:CE1	1:E:152:ILE:HD11	2.47	0.49
1:E:93:THR:HA	1:E:96:GLN:OE1	2.11	0.49
1:B:110:ILE:HB	1:B:146:ILE:HD12	1.95	0.49
1:E:73:ASP:OD1	1:E:77:LYS:NZ	2.45	0.49
1:E:176:ILE:HG13	1:E:178:VAL:HG13	1.94	0.49
1:F:72:PHE:O	1:F:84:GLU:HG2	2.13	0.49
1:C:48:LEU:HD22	1:C:69:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:ASP:HA	1:C:114:GLU:OE1	2.13	0.49
1:A:80:VAL:HG21	1:A:85:PHE:CD1	2.47	0.48
1:B:45:ASP:HB3	1:B:69:ILE:HD12	1.94	0.48
1:B:110:ILE:HB	1:B:146:ILE:CD1	2.42	0.48
1:B:182:GLN:O	1:B:186:MET:HG3	2.13	0.48
1:F:59:PRO:O	1:F:140:ARG:NH2	2.44	0.48
1:F:65:VAL:O	1:F:69:ILE:HG12	2.14	0.48
1:A:27:PHE:H	1:A:86:THR:HG22	1.79	0.48
1:A:156:ILE:HA	1:A:159:GLN:HG2	1.96	0.48
1:C:89:TRP:O	1:C:93:THR:OG1	2.22	0.48
1:F:106:ASN:O	1:G:100:ARG:HD2	2.14	0.48
1:D:68:ILE:HD12	1:D:91:TYR:CE2	2.48	0.48
1:E:76:ASN:O	1:E:76:ASN:ND2	2.46	0.47
1:F:113:ASN:OD1	1:F:113:ASN:N	2.47	0.47
1:H:111:ASP:HB3	1:H:145:GLN:HG2	1.97	0.47
1:H:162:THR:O	1:H:166:ARG:HB2	2.14	0.47
1:A:61:ASN:HB3	1:A:64:THR:HB	1.96	0.47
1:C:37:LYS:H	1:C:37:LYS:HD2	1.78	0.47
1:H:148:PHE:O	1:H:152:ILE:HG12	2.14	0.47
1:B:160:ARG:O	1:B:164:ILE:HG12	2.14	0.47
1:E:132:ASP:HA	1:E:135:ILE:HG22	1.95	0.47
1:D:141:GLN:OE1	1:D:143:ARG:N	2.47	0.47
1:A:29:TRP:NE1	1:A:82:PHE:O	2.48	0.47
1:A:177:GLN:HB3	1:B:177:GLN:HG3	1.97	0.47
1:F:30:ASN:O	1:F:34:ARG:HB2	2.15	0.47
1:D:56:THR:C	1:D:58:THR:H	2.17	0.47
1:B:165:PHE:HZ	1:B:174:GLY:O	1.98	0.46
1:C:109:MET:HB3	1:C:145:GLN:HB3	1.96	0.46
1:E:124:TYR:CE2	1:E:158:LEU:HD22	2.50	0.46
1:E:64:THR:O	1:E:68:ILE:HG12	2.14	0.46
1:B:176:ILE:HD13	1:B:178:VAL:HG13	1.97	0.46
1:C:111:ASP:OD2	1:C:111:ASP:N	2.48	0.46
1:G:56:THR:O	1:G:57:TRP:HB2	2.16	0.46
1:G:99:PHE:CE1	1:G:148:PHE:HA	2.51	0.46
1:A:56:THR:O	1:A:57:TRP:HB2	2.16	0.46
1:C:56:THR:OG1	1:C:58:THR:OG1	2.32	0.46
1:H:155:CYS:HA	1:H:158:LEU:HB3	1.98	0.46
1:H:166:ARG:HG2	1:H:172:GLN:NE2	2.31	0.46
1:G:128:ASP:HA	1:G:131:HIS:ND1	2.30	0.45
1:C:148:PHE:CE2	1:C:152:ILE:HD11	2.51	0.45
1:D:109:MET:HG2	1:D:147:ALA:HA	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ILE:C	1:B:71:MET:H	2.20	0.45
1:D:110:ILE:HB	1:D:146:ILE:HB	1.97	0.45
1:D:115:LEU:HD23	1:D:131:HIS:HD2	1.81	0.45
1:E:43:ILE:HG23	1:E:47:GLU:HB3	1.97	0.45
1:E:31:VAL:O	1:E:35:VAL:HG23	2.17	0.45
1:C:97:ASN:ND2	1:C:100:ARG:HH12	2.15	0.45
1:E:48:LEU:HD11	1:E:88:VAL:HG11	1.98	0.45
1:G:130:PHE:CZ	1:H:184:LEU:HD22	2.52	0.45
1:D:131:HIS:HA	1:D:134:LEU:HD12	1.99	0.45
1:F:75:GLU:HG3	1:F:77:LYS:HZ2	1.78	0.45
1:F:168:TYR:CE2	1:F:186:MET:HG3	2.52	0.44
1:B:135:ILE:HD12	1:B:146:ILE:CG1	2.42	0.44
1:D:106:ASN:HB3	1:E:100:ARG:HB3	1.99	0.44
1:F:61:ASN:HD21	1:F:63:VAL:HB	1.82	0.44
1:H:99:PHE:O	1:H:99:PHE:CG	2.70	0.44
1:E:67:SER:O	1:E:71:MET:HG3	2.17	0.44
1:G:176:ILE:HG22	1:G:178:VAL:H	1.82	0.44
1:B:162:THR:HG22	1:B:166:ARG:HE	1.82	0.44
1:F:165:PHE:CE1	1:F:176:ILE:HD12	2.53	0.44
1:B:179:SER:OG	1:B:182:GLN:HB2	2.18	0.44
1:C:130:PHE:HA	1:C:133:ILE:HD12	1.99	0.43
1:C:75:GLU:OE2	1:C:81:ASN:ND2	2.51	0.43
1:H:98:VAL:O	1:H:99:PHE:HB3	2.17	0.43
1:B:67:SER:O	1:B:71:MET:HB2	2.18	0.43
1:D:68:ILE:HD12	1:D:91:TYR:HE2	1.83	0.43
1:D:179:SER:OG	1:D:182:GLN:HG3	2.17	0.43
1:E:110:ILE:O	1:E:146:ILE:HD12	2.19	0.43
1:G:119:LEU:HB3	1:G:124:TYR:HB2	2.01	0.43
1:G:44:SER:HB3	1:G:47:GLU:HB2	2.01	0.43
1:B:54:ASN:ND2	1:B:56:THR:OG1	2.49	0.43
1:H:177:GLN:O	1:H:177:GLN:HG2	2.19	0.43
1:E:165:PHE:CE2	1:F:180:TYR:HA	2.53	0.43
1:H:32:PHE:CE1	1:H:43:ILE:HD11	2.54	0.43
1:F:96:GLN:O	1:F:100:ARG:HG3	2.19	0.43
1:D:28:LEU:HD13	1:D:86:THR:HG22	2.01	0.42
1:E:164:ILE:HD13	1:E:186:MET:O	2.18	0.42
1:B:94:ASP:O	1:B:98:VAL:HG23	2.19	0.42
1:B:131:HIS:O	1:B:135:ILE:HG12	2.20	0.42
1:C:178:VAL:HG11	1:C:186:MET:CE	2.50	0.42
1:E:164:ILE:H	1:E:164:ILE:HG13	1.51	0.42
1:F:94:ASP:O	1:F:98:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:THR:O	1:A:68:ILE:HG12	2.20	0.42
1:B:34:ARG:HG2	1:B:34:ARG:HH11	1.83	0.42
1:C:91:TYR:OH	1:C:156:ILE:HD11	2.18	0.42
1:E:135:ILE:O	1:E:139:ASP:HB2	2.19	0.42
1:B:129:GLN:HE21	1:B:129:GLN:HB3	1.68	0.42
1:H:64:THR:CG2	1:H:152:ILE:HB	2.50	0.42
1:E:179:SER:OG	1:E:180:TYR:N	2.53	0.42
1:H:116:LYS:HG2	1:H:131:HIS:ND1	2.35	0.42
1:C:105:ASP:OD2	1:C:107:SER:HB3	2.19	0.42
1:G:103:ASP:HA	1:G:114:GLU:OE2	2.20	0.42
1:D:48:LEU:HD22	1:D:69:ILE:HD11	2.02	0.41
1:B:167:ARG:HG3	1:B:167:ARG:NH1	2.32	0.41
1:D:141:GLN:NE2	1:D:143:ARG:HB2	2.35	0.41
1:E:168:TYR:HB3	1:E:176:ILE:HD11	2.02	0.41
1:E:175:TRP:N	1:E:175:TRP:CD1	2.89	0.41
1:F:156:ILE:O	1:F:160:ARG:HG3	2.20	0.41
1:G:164:ILE:HD13	1:G:164:ILE:H	1.85	0.41
1:A:64:THR:HA	1:A:153:GLN:NE2	2.35	0.41
1:E:131:HIS:O	1:E:135:ILE:HB	2.21	0.41
1:G:161:LEU:HD21	1:H:187:VAL:HG11	2.02	0.41
1:C:149:ASP:OD1	1:C:149:ASP:N	2.54	0.41
1:B:52:LEU:HB3	1:B:60:PHE:CD1	2.56	0.41
1:B:140:ARG:HB2	1:B:150:ASP:OD2	2.21	0.41
1:H:115:LEU:HA	1:H:118:ALA:HB3	2.01	0.41
1:B:113:ASN:HD22	1:B:113:ASN:HA	1.59	0.41
1:E:156:ILE:O	1:E:160:ARG:HB2	2.21	0.41
1:E:171:ASP:O	1:E:172:GLN:CB	2.69	0.41
1:D:183:TYR:O	1:D:186:MET:HB3	2.21	0.40
1:G:133:ILE:HD13	1:G:133:ILE:H	1.85	0.40
1:A:188:PHE:CZ	1:B:161:LEU:HD12	2.56	0.40
1:B:115:LEU:HD22	1:B:135:ILE:HD11	2.02	0.40
1:G:56:THR:C	1:G:58:THR:H	2.25	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	163/168 (97%)	121 (74%)	40 (24%)	2 (1%)	13	42
1	B	163/168 (97%)	148 (91%)	12 (7%)	3 (2%)	8	35
1	C	162/168 (96%)	142 (88%)	20 (12%)	0	100	100
1	D	161/168 (96%)	152 (94%)	9 (6%)	0	100	100
1	E	164/168 (98%)	148 (90%)	16 (10%)	0	100	100
1	F	163/168 (97%)	148 (91%)	14 (9%)	1 (1%)	25	57
1	G	161/168 (96%)	142 (88%)	17 (11%)	2 (1%)	13	42
1	H	161/168 (96%)	145 (90%)	14 (9%)	2 (1%)	13	42
All	All	1298/1344 (97%)	1146 (88%)	142 (11%)	10 (1%)	19	51

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	SER
1	G	66	ARG
1	H	183	TYR
1	B	76	ASN
1	B	169	ASP
1	B	70	SER
1	H	144	GLY
1	A	135	ILE
1	G	133	ILE
1	F	123	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	150/153 (98%)	139 (93%)	11 (7%)	14	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	150/153 (98%)	134 (89%)	16 (11%)	6	25
1	C	149/153 (97%)	143 (96%)	6 (4%)	31	61
1	D	148/153 (97%)	139 (94%)	9 (6%)	18	48
1	E	151/153 (99%)	140 (93%)	11 (7%)	14	41
1	F	150/153 (98%)	140 (93%)	10 (7%)	16	45
1	G	148/153 (97%)	136 (92%)	12 (8%)	11	36
1	H	148/153 (97%)	141 (95%)	7 (5%)	26	57
All	All	1194/1224 (98%)	1112 (93%)	82 (7%)	15	44

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	38	ASP
1	A	43	ILE
1	A	66	ARG
1	A	86	THR
1	A	104	ARG
1	A	112	LYS
1	A	131	HIS
1	A	158	LEU
1	A	167	ARG
1	A	175	TRP
1	B	34	ARG
1	B	44	SER
1	B	49	GLN
1	B	77	LYS
1	B	81	ASN
1	B	83	SER
1	B	86	THR
1	B	113	ASN
1	B	117	GLN
1	B	129	GLN
1	B	136	ARG
1	B	137	LYS
1	B	145	GLN
1	B	146	ILE
1	B	158	LEU
1	B	167	ARG
1	C	39	ARG

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Mol	Chain	Res	Type
1	C	71	MET
1	C	111	ASP
1	C	115	LEU
1	C	153	GLN
1	C	173	ASP
1	D	38	ASP
1	D	54	ASN
1	D	56	THR
1	D	137	LYS
1	D	140	ARG
1	D	143	ARG
1	D	158	LEU
1	D	160	ARG
1	D	177	GLN
1	E	33	GLN
1	E	49	GLN
1	E	54	ASN
1	E	112	LYS
1	E	125	ARG
1	E	126	LEU
1	E	129	GLN
1	E	146	ILE
1	E	158	LEU
1	E	164	ILE
1	E	176	ILE
1	F	29	TRP
1	F	33	GLN
1	F	45	ASP
1	F	66	ARG
1	F	110	ILE
1	F	113	ASN
1	F	143	ARG
1	F	158	LEU
1	F	159	GLN
1	F	176	ILE
1	G	29	TRP
1	G	75	GLU
1	G	85	PHE
1	G	105	ASP
1	G	111	ASP
1	G	125	ARG
1	G	133	ILE

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Mol	Chain	Res	Type
1	G	137	LYS
1	G	140	ARG
1	G	159	GLN
1	G	160	ARG
1	G	164	ILE
1	H	45	ASP
1	H	74	ARG
1	H	94	ASP
1	H	105	ASP
1	H	159	GLN
1	H	177	GLN
1	H	184	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	177	GLN
1	B	49	GLN
1	B	81	ASN
1	B	113	ASN
1	B	129	GLN
1	B	159	GLN
1	B	177	GLN
1	B	182	GLN
1	C	30	ASN
1	C	49	GLN
1	C	76	ASN
1	C	97	ASN
1	C	141	GLN
1	C	153	GLN
1	C	182	GLN
1	D	33	GLN
1	D	49	GLN
1	D	54	ASN
1	D	61	ASN
1	D	76	ASN
1	D	129	GLN
1	D	131	HIS
1	D	153	GLN
1	E	49	GLN
1	E	50	GLN

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Mol	Chain	Res	Type
1	E	54	ASN
1	E	129	GLN
1	E	131	HIS
1	F	33	GLN
1	F	50	GLN
1	F	76	ASN
1	F	96	GLN
1	F	97	ASN
1	F	159	GLN
1	F	177	GLN
1	G	33	GLN
1	G	49	GLN
1	G	177	GLN
1	H	159	GLN
1	H	172	GLN

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 37 ligands modelled in this entry, 37 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 (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	165/168 (98%)	-0.09	1 (0%) 89 90	68, 139, 163, 166	0
1	B	165/168 (98%)	-0.16	0 100 100	52, 65, 84, 101	0
1	C	164/168 (97%)	-0.28	0 100 100	54, 68, 79, 82	0
1	D	163/168 (97%)	-0.28	0 100 100	58, 87, 101, 104	0
1	E	166/168 (98%)	-0.20	0 100 100	58, 76, 89, 97	0
1	F	165/168 (98%)	-0.08	0 100 100	61, 76, 105, 108	0
1	G	163/168 (97%)	0.26	12 (7%) 14 14	99, 120, 153, 159	0
1	H	163/168 (97%)	0.60	20 (12%) 4 3	138, 168, 174, 175	0
All	All	1314/1344 (97%)	-0.03	33 (2%) 57 54	52, 85, 169, 175	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	177	GLN	5.7
1	G	188	PHE	5.0
1	H	126	LEU	4.2
1	H	125	ARG	4.2
1	G	177	GLN	4.1
1	H	178	VAL	4.1
1	H	116	LYS	3.9
1	H	134	LEU	3.8
1	G	178	VAL	3.8
1	G	176	ILE	3.4
1	G	168	TYR	3.4
1	H	176	ILE	3.4
1	H	74	ARG	3.2
1	H	26	SER	3.1
1	H	129	GLN	3.0
1	G	181	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	74	ARG	2.7
1	H	117	GLN	2.6
1	H	128	ASP	2.6
1	G	35	VAL	2.5
1	A	75	GLU	2.5
1	H	130	PHE	2.4
1	G	73	ASP	2.4
1	H	71	MET	2.4
1	G	175	TRP	2.4
1	H	166	ARG	2.3
1	H	95	TRP	2.3
1	H	133	ILE	2.2
1	H	167	ARG	2.2
1	G	79	GLY	2.2
1	H	137	LYS	2.1
1	G	78	ALA	2.1
1	H	165	PHE	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, 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
2	ZN	G	993	1/1	0.70	0.11	219,219,219,219	0
2	ZN	H	990	1/1	0.83	0.07	162,162,162,162	0
2	ZN	E	990	1/1	0.89	0.14	142,142,142,142	0
2	ZN	A	992	1/1	0.89	0.15	117,117,117,117	0
2	ZN	G	994	1/1	0.89	0.09	169,169,169,169	0
2	ZN	D	990	1/1	0.89	0.09	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	D	992	1/1	0.91	0.09	176,176,176,176	0
2	ZN	F	994	1/1	0.92	0.18	178,178,178,178	0
2	ZN	D	994	1/1	0.93	0.18	96,96,96,96	0
2	ZN	B	992	1/1	0.95	0.14	95,95,95,95	0
2	ZN	G	991	1/1	0.96	0.10	109,109,109,109	0
2	ZN	G	992	1/1	0.96	0.08	137,137,137,137	0
2	ZN	B	2	1/1	0.96	0.15	87,87,87,87	0
2	ZN	D	1	1/1	0.96	0.17	119,119,119,119	0
2	ZN	G	990	1/1	0.96	0.08	155,155,155,155	0
2	ZN	H	992	1/1	0.96	0.06	169,169,169,169	0
2	ZN	C	990	1/1	0.97	0.17	86,86,86,86	0
2	ZN	C	994	1/1	0.97	0.16	99,99,99,99	0
2	ZN	A	991	1/1	0.97	0.12	103,103,103,103	0
2	ZN	E	993	1/1	0.97	0.16	102,102,102,102	0
2	ZN	E	994	1/1	0.97	0.14	87,87,87,87	0
2	ZN	F	993	1/1	0.97	0.11	125,125,125,125	0
2	ZN	A	990	1/1	0.97	0.17	124,124,124,124	0
2	ZN	E	991	1/1	0.98	0.16	104,104,104,104	0
2	ZN	E	992	1/1	0.98	0.14	81,81,81,81	0
2	ZN	D	993	1/1	0.98	0.14	115,115,115,115	0
2	ZN	B	993	1/1	0.98	0.12	118,118,118,118	0
2	ZN	F	991	1/1	0.98	0.11	98,98,98,98	0
2	ZN	B	994	1/1	0.98	0.19	103,103,103,103	0
2	ZN	C	992	1/1	0.98	0.15	103,103,103,103	0
2	ZN	B	990	1/1	0.99	0.11	95,95,95,95	0
2	ZN	C	991	1/1	0.99	0.15	80,80,80,80	0
2	ZN	F	990	1/1	0.99	0.11	125,125,125,125	0
2	ZN	D	991	1/1	0.99	0.16	111,111,111,111	0
2	ZN	F	992	1/1	0.99	0.14	90,90,90,90	0
2	ZN	B	991	1/1	0.99	0.17	75,75,75,75	0
2	ZN	C	993	1/1	0.99	0.10	108,108,108,108	0

6.5 Other polymers (i)

There are no such residues in this entry.