



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:28 am BST

PDB ID : 5AJL
Title : Sdsa sulfatase tetragonal
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Deposited on : 2015-02-25
Resolution : 3.45 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

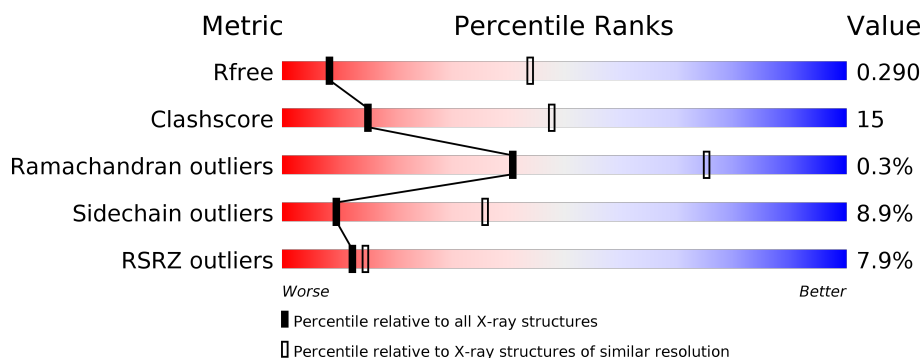
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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	658	<div> <div>9%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>• •</div> </div> </div>
1	B	658	<div> <div>7%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9846 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.

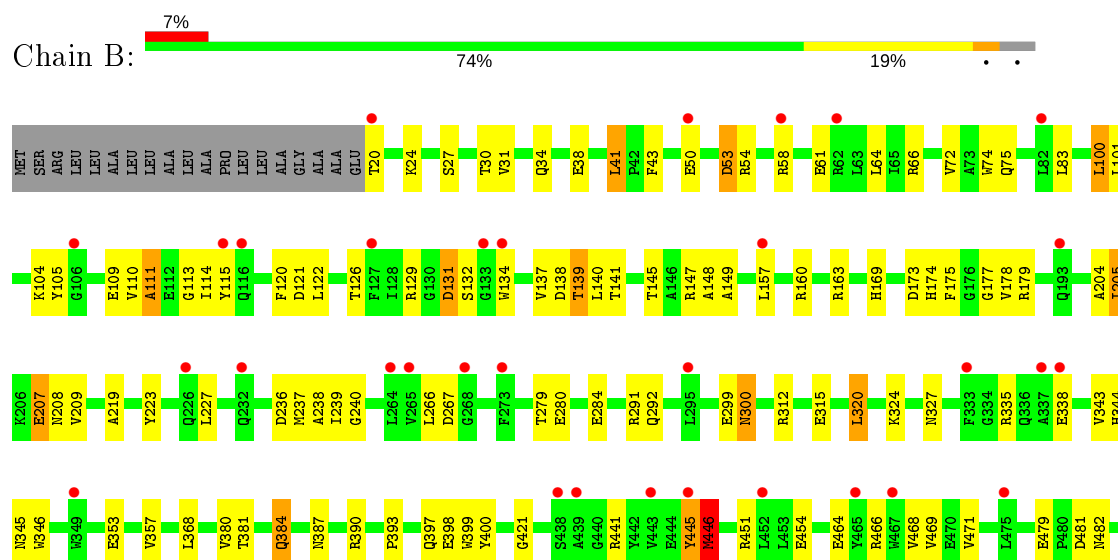
- Molecule 1 is a protein called ALKYL SULFATASE.

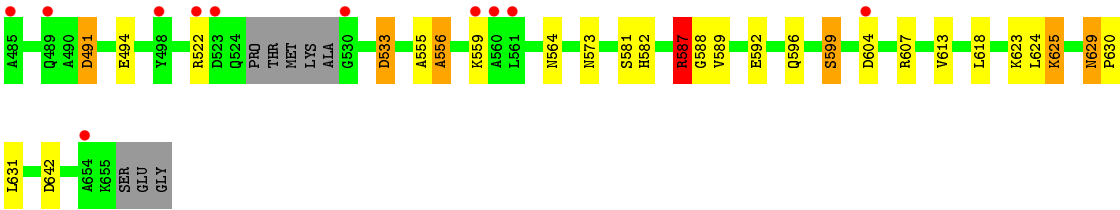
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	631	Total	C	N	O	S	0	0	1
			4921	3105	890	916	10			
1	B	631	Total	C	N	O	S	0	0	1
			4921	3105	890	916	10			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 1: ALKYL SULFATASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	88.58Å 88.58Å 193.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.61 – 3.45 52.61 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (52.61-3.45) 99.8 (52.61-3.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.244 , 0.289 0.248 , 0.290	Depositor DCC
R_{free} test set	1005 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	106.6	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9846	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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: 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	0.47	1/5028 (0.0%)	0.74	7/6829 (0.1%)
1	B	0.46	0/5028	0.73	4/6829 (0.1%)
All	All	0.47	1/10056 (0.0%)	0.73	11/13658 (0.1%)

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	6
1	B	0	11
All	All	0	17

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	524	GLN	C-O	5.98	1.34	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	LEU	CA-CB-CG	7.64	132.86	115.30
1	B	100	LEU	CA-CB-CG	7.54	132.65	115.30
1	A	618	LEU	CA-CB-CG	6.97	131.34	115.30
1	A	520	VAL	C-N-CD	6.68	142.42	128.40
1	B	629	ASN	C-N-CD	6.42	141.87	128.40
1	A	346	TRP	C-N-CD	5.87	140.74	128.40
1	A	100	LEU	CA-CB-CG	5.86	128.78	115.30
1	A	112	GLU	N-CA-C	-5.47	96.23	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	516	LEU	CA-CB-CG	5.09	127.01	115.30
1	B	451	ARG	NE-CZ-NH1	5.05	122.82	120.30

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	ILE	Peptide
1	A	345	ASN	Peptide
1	A	444	GLU	Peptide
1	A	445	TYR	Peptide
1	A	448	GLY	Peptide
1	A	556	ALA	Peptide
1	B	110	VAL	Peptide
1	B	111	ALA	Peptide
1	B	205	ILE	Peptide
1	B	207	GLU	Peptide
1	B	208	ASN	Peptide
1	B	345	ASN	Peptide
1	B	384	GLN	Peptide
1	B	446	MET	Peptide
1	B	53	ASP	Peptide
1	B	556	ALA	Peptide
1	B	587	ARG	Peptide

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	4921	0	4824	147	1
1	B	4921	0	4823	159	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
All	All	9846	0	9647	292	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 15.

All (292) 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:111:ALA:CB	1:B:114:ILE:HB	1.46	1.45
1:B:223:TYR:CD1	1:B:237:MET:HE2	1.55	1.39
1:B:223:TYR:CD1	1:B:237:MET:CE	2.06	1.38
1:A:223:TYR:CD1	1:A:237:MET:HE2	1.58	1.37
1:B:174:HIS:CE1	1:B:344:HIS:CE1	2.16	1.34
1:B:174:HIS:CE1	1:B:344:HIS:HE1	1.48	1.29
1:B:126:THR:HB	1:B:137:VAL:CG2	1.63	1.28
1:B:111:ALA:HB2	1:B:114:ILE:CB	1.63	1.27
1:A:174:HIS:CE1	1:A:344:HIS:HE2	1.57	1.23
1:A:223:TYR:CD1	1:A:237:MET:CE	2.20	1.22
1:A:64:LEU:HD12	1:A:65:ILE:N	1.55	1.22
1:B:126:THR:HB	1:B:137:VAL:HG22	1.19	1.17
1:A:121:ASP:CG	1:A:141:THR:OG1	1.82	1.16
1:B:120:PHE:HE2	1:B:149:ALA:N	1.44	1.14
1:B:111:ALA:HB3	1:B:114:ILE:N	1.61	1.14
1:B:111:ALA:CB	1:B:114:ILE:CB	2.18	1.13
1:B:126:THR:CB	1:B:137:VAL:CG2	2.29	1.11
1:A:174:HIS:CE1	1:A:344:HIS:NE2	2.17	1.10
1:B:174:HIS:HE1	1:B:344:HIS:CE1	1.59	1.08
1:A:596:GLN:HG3	1:A:629:ASN:O	1.53	1.08
1:B:630:PRO:HD2	1:B:631:LEU:HG	1.23	1.08
1:B:111:ALA:HB3	1:B:114:ILE:H	0.99	1.07
1:A:293:LYS:HD3	1:A:336:GLN:O	1.53	1.07
1:B:139:THR:OG1	1:B:177:GLY:C	1.93	1.07
1:A:303:GLY:H	1:A:345:ASN:ND2	1.55	1.03
1:B:573:ASN:O	1:B:588:GLY:N	1.90	1.03
1:A:121:ASP:OD2	1:A:141:THR:CB	2.08	1.02
1:B:292:GLN:OE1	1:B:292:GLN:N	1.90	1.02
1:B:398:GLU:OE1	1:B:400:TYR:OH	1.75	1.02
1:B:163:ARG:NH1	1:B:267:ASP:OD2	1.92	1.00
1:B:120:PHE:CE2	1:B:149:ALA:N	2.31	0.98
1:B:139:THR:HG1	1:B:177:GLY:C	1.68	0.96
1:B:381:THR:H	1:B:384:GLN:HG3	1.28	0.96
1:B:111:ALA:CB	1:B:114:ILE:H	1.79	0.95
1:B:381:THR:OG1	1:B:384:GLN:HG2	1.67	0.95
1:A:586:LEU:HD13	1:B:327:ASN:ND2	1.79	0.95
1:B:140:LEU:O	1:B:173:ASP:O	1.84	0.94
1:B:239:ILE:HD12	1:B:344:HIS:CD2	2.02	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ILE:HD12	1:B:344:HIS:HD2	1.31	0.94
1:A:125:ILE:HB	1:A:140:LEU:HD11	1.49	0.93
1:A:121:ASP:OD1	1:A:122:LEU:N	2.03	0.92
1:B:122:LEU:HD12	1:B:240:GLY:HA3	1.51	0.92
1:B:223:TYR:CD1	1:B:237:MET:HE3	2.02	0.92
1:B:126:THR:CB	1:B:137:VAL:HG21	1.96	0.91
1:B:126:THR:HB	1:B:137:VAL:HG21	1.53	0.91
1:B:111:ALA:CB	1:B:114:ILE:N	2.32	0.91
1:A:286:ASN:ND2	1:A:297:MET:HE1	1.85	0.90
1:A:112:GLU:O	1:A:292:GLN:HG2	1.70	0.90
1:A:236:ASP:OD1	1:A:237:MET:N	2.05	0.89
1:B:223:TYR:CE1	1:B:237:MET:HE3	2.08	0.87
1:A:310:THR:OG1	1:A:312:ARG:HG2	1.74	0.87
1:A:239:ILE:HD12	1:A:344:HIS:ND1	1.89	0.86
1:B:121:ASP:OD1	1:B:122:LEU:N	2.09	0.86
1:A:223:TYR:HD1	1:A:237:MET:HE2	1.05	0.85
1:A:174:HIS:HE1	1:A:344:HIS:CD2	1.93	0.85
1:A:140:LEU:O	1:A:177:GLY:N	2.09	0.85
1:A:445:TYR:CD1	1:B:446:MET:HE1	2.11	0.85
1:B:126:THR:OG1	1:B:137:VAL:HG21	1.76	0.85
1:B:111:ALA:HB3	1:B:114:ILE:CA	2.07	0.85
1:A:280:GLU:HB2	1:A:299:GLU:HB3	1.58	0.84
1:B:140:LEU:O	1:B:173:ASP:C	2.15	0.84
1:B:111:ALA:CB	1:B:114:ILE:CA	2.56	0.82
1:B:223:TYR:HD1	1:B:237:MET:HE2	1.05	0.82
1:B:381:THR:OG1	1:B:384:GLN:CG	2.26	0.82
1:A:445:TYR:CD1	1:B:446:MET:CE	2.64	0.79
1:B:596:GLN:HG3	1:B:629:ASN:O	1.81	0.79
1:B:140:LEU:HD23	1:B:145:THR:HB	1.63	0.79
1:A:303:GLY:N	1:A:345:ASN:ND2	2.31	0.78
1:B:223:TYR:CE1	1:B:237:MET:CE	2.65	0.78
1:B:163:ARG:NH1	1:B:267:ASP:CG	2.38	0.77
1:A:236:ASP:OD1	1:A:240:GLY:O	2.01	0.77
1:A:223:TYR:CD1	1:A:237:MET:HE3	2.20	0.77
1:A:205:ILE:O	1:A:207:GLU:N	2.18	0.77
1:A:169:HIS:NE2	1:A:299:GLU:OE1	2.18	0.76
1:A:303:GLY:H	1:A:345:ASN:HD22	1.32	0.76
1:A:310:THR:HG23	1:A:312:ARG:HG3	1.66	0.76
1:A:140:LEU:N	1:A:140:LEU:HD12	2.00	0.76
1:B:398:GLU:OE1	1:B:400:TYR:CZ	2.38	0.75
1:A:445:TYR:HD1	1:B:446:MET:HE1	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:HIS:CE1	1:A:344:HIS:CD2	2.72	0.73
1:B:132:SER:OG	1:B:163:ARG:NH1	2.22	0.72
1:B:205:ILE:HD13	1:B:205:ILE:N	2.04	0.72
1:A:286:ASN:CG	1:A:297:MET:HE3	2.11	0.72
1:A:286:ASN:ND2	1:A:297:MET:CE	2.53	0.71
1:A:303:GLY:N	1:A:345:ASN:HD22	1.88	0.71
1:A:64:LEU:CD1	1:A:65:ILE:N	2.46	0.71
1:A:445:TYR:CE1	1:B:446:MET:HE3	2.26	0.70
1:A:64:LEU:HD12	1:A:65:ILE:CA	2.20	0.70
1:A:223:TYR:HA	1:A:237:MET:HE1	1.73	0.70
1:B:120:PHE:CE2	1:B:149:ALA:CA	2.75	0.70
1:A:174:HIS:NE2	1:A:344:HIS:NE2	2.32	0.70
1:A:64:LEU:HD12	1:A:65:ILE:C	2.11	0.69
1:B:126:THR:CB	1:B:137:VAL:HG22	2.05	0.69
1:A:280:GLU:CB	1:A:299:GLU:HB3	2.21	0.69
1:A:310:THR:CG2	1:A:312:ARG:HG3	2.22	0.69
1:A:286:ASN:CG	1:A:297:MET:CE	2.61	0.69
1:A:586:LEU:CD1	1:B:327:ASN:ND2	2.55	0.68
1:B:464:GLU:O	1:B:468:VAL:HG23	1.94	0.67
1:A:279:THR:HG22	1:A:322:TRP:CG	2.30	0.67
1:B:174:HIS:NE2	1:B:299:GLU:OE2	2.21	0.67
1:A:611:LYS:HD2	1:A:611:LYS:C	2.14	0.67
1:B:132:SER:OG	1:B:163:ARG:NH2	2.24	0.67
1:A:464:GLU:O	1:A:468:VAL:HG23	1.94	0.66
1:A:64:LEU:C	1:A:64:LEU:HD12	2.16	0.66
1:A:200:PHE:HD2	1:A:201:MET:HG2	1.60	0.66
1:B:280:GLU:HB3	1:B:284:GLU:OE1	1.95	0.66
1:A:223:TYR:CE1	1:A:237:MET:HE3	2.31	0.65
1:A:48:ASP:HB3	1:A:346:TRP:CZ2	2.31	0.65
1:A:124:ASN:ND2	1:A:345:ASN:O	2.28	0.65
1:A:293:LYS:CD	1:A:336:GLN:O	2.39	0.65
1:B:573:ASN:O	1:B:588:GLY:CA	2.45	0.64
1:B:174:HIS:NE2	1:B:344:HIS:CE1	2.64	0.64
1:B:126:THR:H	1:B:137:VAL:HG23	1.61	0.64
1:A:205:ILE:O	1:A:206:LYS:C	2.35	0.64
1:A:223:TYR:HA	1:A:237:MET:CE	2.27	0.64
1:B:74:TRP:CE2	1:B:120:PHE:O	2.51	0.64
1:A:139:THR:OG1	1:A:178:VAL:N	2.30	0.64
1:B:139:THR:OG1	1:B:178:VAL:N	2.29	0.64
1:A:121:ASP:OD2	1:A:141:THR:OG1	0.65	0.63
1:A:201:MET:O	1:A:204:ALA:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:GLY:H	1:A:345:ASN:HD21	1.44	0.63
1:A:310:THR:OG1	1:A:312:ARG:CG	2.47	0.63
1:B:204:ALA:HB3	1:B:205:ILE:HD13	1.80	0.62
1:A:443:VAL:O	1:A:448:GLY:N	2.33	0.62
1:B:111:ALA:HB2	1:B:114:ILE:HB	0.68	0.62
1:B:343:VAL:O	1:B:344:HIS:ND1	2.23	0.61
1:B:380:VAL:HG13	1:B:384:GLN:HB2	1.81	0.61
1:B:630:PRO:HD2	1:B:631:LEU:CG	2.15	0.61
1:A:397:GLN:O	1:A:398:GLU:HG2	2.01	0.61
1:A:343:VAL:O	1:A:344:HIS:HD2	1.84	0.60
1:B:126:THR:OG1	1:B:137:VAL:CG2	2.41	0.60
1:B:163:ARG:HH12	1:B:267:ASP:CG	2.04	0.59
1:B:381:THR:N	1:B:384:GLN:HG3	2.09	0.59
1:B:223:TYR:CG	1:B:237:MET:HE2	2.29	0.59
1:A:205:ILE:HD13	1:A:205:ILE:N	2.17	0.59
1:A:200:PHE:CD2	1:A:201:MET:HG2	2.37	0.59
1:B:132:SER:OG	1:B:163:ARG:CZ	2.51	0.58
1:A:611:LYS:HD2	1:A:611:LYS:O	2.02	0.58
1:B:111:ALA:CB	1:B:114:ILE:CG1	2.82	0.58
1:A:445:TYR:CE1	1:B:446:MET:CE	2.88	0.57
1:A:237:MET:O	1:A:238:ALA:HB3	2.05	0.56
1:B:120:PHE:HE2	1:B:148:ALA:C	2.06	0.56
1:B:111:ALA:HB1	1:B:114:ILE:HG13	1.87	0.56
1:A:137:VAL:O	1:A:138:ASP:HB2	2.06	0.56
1:A:279:THR:CG2	1:A:322:TRP:HA	2.36	0.56
1:A:586:LEU:CD1	1:B:327:ASN:HD22	2.18	0.56
1:B:109:GLU:OE2	1:B:111:ALA:O	2.24	0.56
1:A:556:ALA:O	1:A:559:LYS:HG3	2.06	0.56
1:B:111:ALA:HB1	1:B:114:ILE:CB	2.30	0.56
1:A:443:VAL:O	1:A:448:GLY:HA2	2.06	0.56
1:B:111:ALA:HB1	1:B:114:ILE:CG1	2.36	0.56
1:B:137:VAL:O	1:B:138:ASP:HB2	2.06	0.55
1:B:205:ILE:HG22	1:B:209:VAL:HG21	1.89	0.55
1:B:139:THR:HG21	1:B:178:VAL:HB	1.87	0.55
1:A:462:ARG:HB2	1:A:464:GLU:HG2	1.87	0.55
1:A:443:VAL:HG12	1:A:448:GLY:HA2	1.88	0.55
1:B:121:ASP:OD2	1:B:141:THR:OG1	2.18	0.55
1:B:280:GLU:HB2	1:B:299:GLU:HB3	1.88	0.55
1:A:111:ALA:O	1:A:112:GLU:C	2.44	0.55
1:A:201:MET:O	1:A:204:ALA:HB3	2.06	0.54
1:A:236:ASP:CG	1:A:238:ALA:H	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:GLY:O	1:A:629:ASN:C	2.43	0.54
1:A:57:ILE:O	1:A:58:ARG:HG3	2.07	0.54
1:B:120:PHE:HE2	1:B:149:ALA:H	1.46	0.54
1:B:204:ALA:CB	1:B:205:ILE:HD13	2.37	0.54
1:B:381:THR:OG1	1:B:384:GLN:HG3	2.08	0.54
1:A:112:GLU:O	1:A:292:GLN:CG	2.51	0.54
1:A:64:LEU:CD1	1:A:65:ILE:C	2.76	0.54
1:B:169:HIS:NE2	1:B:280:GLU:OE1	2.40	0.54
1:A:139:THR:C	1:A:140:LEU:HD12	2.29	0.54
1:B:219:ALA:HB2	1:B:312:ARG:HG3	1.89	0.54
1:A:164:THR:HG21	1:A:266:LEU:HD13	1.91	0.53
1:B:74:TRP:CD2	1:B:120:PHE:O	2.61	0.53
1:B:381:THR:H	1:B:384:GLN:CG	2.13	0.53
1:A:170:ALA:HB1	1:A:204:ALA:HA	1.91	0.53
1:B:223:TYR:HA	1:B:237:MET:CE	2.38	0.53
1:B:387:ASN:OD1	1:B:466:ARG:NH2	2.42	0.53
1:A:446:MET:HA	1:B:446:MET:HA	1.89	0.52
1:B:120:PHE:CE2	1:B:148:ALA:C	2.83	0.52
1:A:279:THR:HG22	1:A:322:TRP:CD2	2.44	0.52
1:B:223:TYR:CG	1:B:237:MET:CE	2.86	0.52
1:A:341:PHE:HB3	1:A:347:PRO:HB3	1.91	0.52
1:B:291:ARG:C	1:B:292:GLN:OE1	2.48	0.52
1:A:64:LEU:HD21	1:A:66:ARG:HH11	1.74	0.52
1:A:64:LEU:CD1	1:A:65:ILE:O	2.58	0.52
1:B:113:GLY:HA2	1:B:129:ARG:HD2	1.92	0.52
1:B:137:VAL:O	1:B:137:VAL:HG23	2.10	0.52
1:A:471:VAL:HG21	1:B:445:TYR:CE2	2.45	0.52
1:A:205:ILE:HG22	1:A:209:VAL:HG21	1.92	0.52
1:B:479:GLU:HB3	1:B:482:ASN:HB2	1.92	0.52
1:B:380:VAL:CG1	1:B:384:GLN:HB2	2.40	0.51
1:B:120:PHE:CD2	1:B:149:ALA:HB2	2.46	0.51
1:A:443:VAL:O	1:A:448:GLY:CA	2.59	0.51
1:A:64:LEU:HD12	1:A:65:ILE:H	1.60	0.51
1:B:380:VAL:HG13	1:B:384:GLN:CB	2.40	0.51
1:A:293:LYS:O	1:A:293:LYS:HG2	2.10	0.51
1:B:236:ASP:OD2	1:B:238:ALA:N	2.43	0.51
1:A:521:PRO:HD2	1:A:646:TRP:CE3	2.46	0.50
1:B:393:PRO:O	1:B:397:GLN:HB2	2.12	0.50
1:A:279:THR:HG21	1:A:322:TRP:HA	1.94	0.50
1:A:169:HIS:CE1	1:A:299:GLU:HB2	2.47	0.50
1:A:169:HIS:HE2	1:A:299:GLU:CD	2.13	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:MET:HB2	1:A:242:GLY:HA2	1.94	0.50
1:B:204:ALA:C	1:B:205:ILE:HD13	2.32	0.50
1:B:169:HIS:CD2	1:B:280:GLU:OE1	2.64	0.49
1:B:204:ALA:HB3	1:B:205:ILE:CD1	2.42	0.49
1:A:64:LEU:HD21	1:A:66:ARG:NH1	2.27	0.49
1:B:74:TRP:CD1	1:B:120:PHE:O	2.65	0.49
1:B:53:ASP:OD1	1:B:104:LYS:HE3	2.12	0.49
1:B:140:LEU:CD2	1:B:145:THR:HB	2.37	0.49
1:A:596:GLN:CG	1:A:629:ASN:O	2.42	0.49
1:A:303:GLY:CA	1:A:345:ASN:HD22	2.24	0.49
1:A:303:GLY:CA	1:A:345:ASN:ND2	2.76	0.49
1:A:139:THR:N	1:A:174:HIS:O	2.29	0.49
1:A:279:THR:CG2	1:A:322:TRP:CG	2.95	0.49
1:A:239:ILE:HD12	1:A:344:HIS:CE1	2.48	0.49
1:B:139:THR:OG1	1:B:177:GLY:CA	2.61	0.48
1:B:139:THR:OG1	1:B:139:THR:O	2.29	0.48
1:B:139:THR:HG21	1:B:178:VAL:CB	2.44	0.48
1:B:27:SER:O	1:B:31:VAL:HG23	2.14	0.47
1:B:596:GLN:CG	1:B:629:ASN:O	2.58	0.47
1:B:205:ILE:O	1:B:207:GLU:N	2.47	0.47
1:A:140:LEU:CD1	1:A:140:LEU:N	2.73	0.47
1:B:121:ASP:O	1:B:122:LEU:C	2.53	0.47
1:B:24:LYS:NZ	1:B:491:ASP:OD2	2.48	0.47
1:B:604:ASP:HA	1:B:607:ARG:HB2	1.96	0.47
1:A:280:GLU:HB3	1:A:284:GLU:OE1	2.15	0.47
1:A:604:ASP:HA	1:A:607:ARG:HG3	1.96	0.46
1:A:63:LEU:HD12	1:A:63:LEU:HA	1.75	0.46
1:A:169:HIS:NE2	1:A:280:GLU:OE2	2.48	0.46
1:A:310:THR:CG2	1:A:312:ARG:CG	2.94	0.46
1:A:343:VAL:O	1:A:344:HIS:CD2	2.67	0.46
1:A:288:TRP:HH2	1:A:293:LYS:HG3	1.79	0.46
1:B:599:SER:HB3	1:B:625:LYS:HG3	1.96	0.45
1:A:76:LEU:HD13	1:A:105:TYR:CD2	2.51	0.45
1:A:223:TYR:CE1	1:A:237:MET:CE	2.83	0.45
1:A:139:THR:C	1:A:140:LEU:CD1	2.86	0.45
1:A:141:THR:CG2	1:A:243:LEU:HD11	2.47	0.45
1:B:120:PHE:CE2	1:B:148:ALA:HB3	2.52	0.45
1:B:346:TRP:CD1	1:B:346:TRP:O	2.70	0.45
1:B:205:ILE:HG22	1:B:209:VAL:CG2	2.47	0.44
1:B:74:TRP:CG	1:B:120:PHE:O	2.71	0.44
1:A:48:ASP:CG	1:A:346:TRP:HZ2	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:PHE:HB3	1:B:399:TRP:CZ2	2.52	0.44
1:A:140:LEU:O	1:A:176:GLY:CA	2.65	0.44
1:A:48:ASP:HB3	1:A:346:TRP:HZ2	1.78	0.44
1:A:564:ASN:HB3	1:A:597:THR:HA	1.99	0.44
1:B:140:LEU:HD23	1:B:145:THR:CB	2.40	0.44
1:A:303:GLY:HA3	1:A:345:ASN:HD22	1.80	0.44
1:A:345:ASN:N	1:A:345:ASN:OD1	2.51	0.44
1:B:236:ASP:OD2	1:B:238:ALA:HA	2.18	0.44
1:B:300:ASN:OD1	1:B:300:ASN:N	2.51	0.43
1:B:353:GLU:O	1:B:357:VAL:HG23	2.18	0.43
1:B:587:ARG:O	1:B:589:VAL:N	2.51	0.43
1:B:139:THR:HG23	1:B:175:PHE:HA	2.00	0.43
1:A:397:GLN:O	1:A:398:GLU:CG	2.66	0.43
1:A:141:THR:HG21	1:A:243:LEU:CD1	2.49	0.43
1:A:303:GLY:HA3	1:A:345:ASN:ND2	2.33	0.43
1:A:286:ASN:OD1	1:A:297:MET:HE3	2.19	0.43
1:B:320:LEU:HD11	1:B:324:LYS:HE2	2.00	0.43
1:A:309:TYR:CE1	1:B:421:GLY:HA3	2.54	0.43
1:A:574:TYR:CE1	1:A:587:ARG:HB2	2.54	0.43
1:B:120:PHE:CE2	1:B:149:ALA:HA	2.51	0.42
1:B:134:TRP:NE1	1:B:160:ARG:HB2	2.34	0.42
1:A:443:VAL:CG1	1:A:448:GLY:HA2	2.48	0.42
1:B:573:ASN:O	1:B:588:GLY:HA2	2.19	0.42
1:A:346:TRP:C	1:A:346:TRP:CD1	2.93	0.42
1:A:199:GLY:O	1:A:203:ALA:HB2	2.20	0.42
1:B:564:ASN:N	1:B:564:ASN:HD22	2.16	0.42
1:B:629:ASN:OD1	1:B:631:LEU:N	2.33	0.42
1:B:139:THR:N	1:B:174:HIS:O	2.26	0.42
1:B:555:ALA:O	1:B:559:LYS:HE3	2.20	0.42
1:A:48:ASP:CB	1:A:346:TRP:HZ2	2.32	0.42
1:B:223:TYR:HD1	1:B:237:MET:CE	1.79	0.42
1:A:139:THR:OG1	1:A:178:VAL:CA	2.68	0.42
1:A:236:ASP:CG	1:A:237:MET:N	2.72	0.42
1:B:533:ASP:N	1:B:533:ASP:OD1	2.45	0.41
1:B:556:ALA:HB1	1:B:581:SER:HA	2.02	0.41
1:B:120:PHE:CE2	1:B:149:ALA:HB2	2.56	0.41
1:A:63:LEU:HD21	1:A:65:ILE:HD11	2.02	0.41
1:A:297:MET:HE3	1:A:297:MET:HA	2.02	0.41
1:A:345:ASN:HB2	1:A:346:TRP:H	1.60	0.41
1:A:445:TYR:CE1	1:B:471:VAL:HG21	2.56	0.41
1:B:30:THR:O	1:B:34:GLN:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:GLY:HA3	1:B:582:HIS:CE1	2.56	0.41
1:B:126:THR:N	1:B:137:VAL:HG23	2.34	0.40
1:A:446:MET:HA	1:B:446:MET:SD	2.62	0.40
1:B:115:TYR:CE2	1:B:157:LEU:HD13	2.56	0.40
1:B:121:ASP:OD2	1:B:141:THR:CB	2.69	0.40
1:A:520:VAL:HG23	1:A:520:VAL:O	2.21	0.40
1:B:74:TRP:NE1	1:B:120:PHE:O	2.54	0.40
1:B:466:ARG:HA	1:B:469:VAL:HG22	2.04	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:62:ARG:NH1	1:B:587:ARG:NH1[3_554]	2.16	0.04

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	627/658 (95%)	592 (94%)	32 (5%)	3 (0%)	29	66
1	B	627/658 (95%)	586 (94%)	40 (6%)	1 (0%)	47	80
All	All	1254/1316 (95%)	1178 (94%)	72 (6%)	4 (0%)	41	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	GLU
1	B	131	ASP
1	A	138	ASP
1	A	385	VAL

5.3.2 Protein sidechains ⓘ

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	499/521 (96%)	457 (92%)	42 (8%)	11	38
1	B	499/521 (96%)	452 (91%)	47 (9%)	8	33
All	All	998/1042 (96%)	909 (91%)	89 (9%)	9	36

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	21	THR
1	A	31	VAL
1	A	45	ASP
1	A	64	LEU
1	A	66	ARG
1	A	83	LEU
1	A	100	LEU
1	A	103	LEU
1	A	129	ARG
1	A	131	ASP
1	A	139	THR
1	A	141	THR
1	A	160	ARG
1	A	163	ARG
1	A	279	THR
1	A	297	MET
1	A	317	ARG
1	A	324	LYS
1	A	331	HIS
1	A	345	ASN
1	A	346	TRP
1	A	351	ASN
1	A	356	GLU
1	A	368	LEU
1	A	445	TYR
1	A	454	GLU

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Mol	Chain	Res	Type
1	A	457	ARG
1	A	464	GLU
1	A	481	ASP
1	A	483	ARG
1	A	486	ARG
1	A	499	GLN
1	A	516	LEU
1	A	522	ARG
1	A	586	LEU
1	A	587	ARG
1	A	592	GLU
1	A	611	LYS
1	A	613	VAL
1	A	618	LEU
1	A	624	LEU
1	B	20	THR
1	B	38	GLU
1	B	41	LEU
1	B	50	GLU
1	B	54	ARG
1	B	58	ARG
1	B	61	GLU
1	B	64	LEU
1	B	66	ARG
1	B	72	VAL
1	B	75	GLN
1	B	83	LEU
1	B	100	LEU
1	B	101	LEU
1	B	105	TYR
1	B	131	ASP
1	B	139	THR
1	B	147	ARG
1	B	179	ARG
1	B	227	LEU
1	B	266	LEU
1	B	279	THR
1	B	300	ASN
1	B	315	GLU
1	B	320	LEU
1	B	335	ARG
1	B	338	GLU

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Mol	Chain	Res	Type
1	B	368	LEU
1	B	390	ARG
1	B	441	ARG
1	B	445	TYR
1	B	446	MET
1	B	454	GLU
1	B	481	ASP
1	B	491	ASP
1	B	494	GLU
1	B	522	ARG
1	B	533	ASP
1	B	587	ARG
1	B	592	GLU
1	B	599	SER
1	B	613	VAL
1	B	618	LEU
1	B	623	LYS
1	B	624	LEU
1	B	625	LYS
1	B	642	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	345	ASN
1	A	473	ASN
1	B	455	GLN
1	B	473	ASN
1	B	564	ASN
1	B	590	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 4 ligands modelled in this entry, 4 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	631/658 (95%)	0.62	57 (9%)  	77, 128, 168, 197	0
1	B	631/658 (95%)	0.57	43 (6%)  	81, 128, 176, 204	0
All	All	1262/1316 (95%)	0.60	100 (7%)  	77, 128, 172, 204	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	654	ALA	6.0
1	A	655	LYS	5.0
1	A	524	GLN	4.5
1	B	530	GLY	4.0
1	B	133	GLY	3.8
1	A	610	LEU	3.7
1	A	57	ILE	3.6
1	A	134	TRP	3.6
1	A	162	ILE	3.4
1	A	136	VAL	3.4
1	A	164	THR	3.4
1	A	195	ILE	3.3
1	A	623	LYS	3.3
1	A	82	LEU	3.3
1	B	452	LEU	3.2
1	A	107	LEU	3.2
1	A	522	ARG	3.2
1	A	129	ARG	3.1
1	B	445	TYR	3.1
1	A	135	ILE	3.1
1	A	271	PHE	3.0
1	A	563	ILE	3.0
1	A	192	VAL	2.9
1	B	106	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	578	LEU	2.8
1	A	460	TYR	2.8
1	B	58	ARG	2.8
1	A	163	ARG	2.8
1	B	338	GLU	2.8
1	A	622	GLY	2.8
1	A	266	LEU	2.7
1	B	443	VAL	2.7
1	B	560	ALA	2.7
1	B	82	LEU	2.7
1	A	561	LEU	2.7
1	B	265	VAL	2.6
1	B	485	ALA	2.6
1	B	232	GLN	2.6
1	B	62	ARG	2.6
1	B	561	LEU	2.6
1	A	516	LEU	2.6
1	B	475	LEU	2.6
1	A	456	ALA	2.5
1	B	349	TRP	2.5
1	A	589	VAL	2.5
1	B	193	GLN	2.5
1	A	127	PHE	2.5
1	B	522	ARG	2.5
1	A	150	TYR	2.5
1	A	620	PHE	2.5
1	B	295	LEU	2.5
1	B	226	GLN	2.5
1	A	633	LEU	2.4
1	A	116	GLN	2.4
1	A	618	LEU	2.4
1	B	115	TYR	2.4
1	B	489	GLN	2.4
1	A	636	LEU	2.4
1	A	194	ILE	2.4
1	B	134	TRP	2.3
1	A	133	GLY	2.3
1	B	273	PHE	2.3
1	A	43	PHE	2.3
1	A	33	ALA	2.3
1	B	438	SER	2.3
1	B	50	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	445	TYR	2.3
1	A	153	VAL	2.2
1	B	467	TRP	2.2
1	A	485	ALA	2.2
1	A	49	PHE	2.2
1	B	654	ALA	2.2
1	A	62	ARG	2.2
1	A	115	TYR	2.2
1	B	604	ASP	2.2
1	B	264	LEU	2.1
1	B	333	PHE	2.1
1	B	439	ALA	2.1
1	A	31	VAL	2.1
1	B	116	GLN	2.1
1	A	189	SER	2.1
1	A	32	GLU	2.1
1	A	556	ALA	2.1
1	A	166	ILE	2.1
1	A	255	ARG	2.1
1	A	110	VAL	2.1
1	B	127	PHE	2.1
1	B	498	TYR	2.1
1	A	574	TYR	2.1
1	B	465	TYR	2.1
1	A	467	TRP	2.0
1	A	126	THR	2.0
1	B	20	THR	2.0
1	B	157	LEU	2.0
1	B	337	ALA	2.0
1	B	559	LYS	2.0
1	B	523	ASP	2.0
1	B	268	GLY	2.0
1	A	446	MET	2.0
1	A	576	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
2	ZN	A	1001	1/1	0.88	0.13	90,90,90,90	1
2	ZN	B	1001	1/1	0.97	0.16	96,96,96,96	1
2	ZN	A	1002	1/1	0.99	0.06	106,106,106,106	1
2	ZN	B	1002	1/1	0.99	0.04	102,102,102,102	1

6.5 Other polymers [i](#)

There are no such residues in this entry.