



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:46 PM GMT

PDB ID : 3UWX  
Title : Crystal structure of UvrA-UvrB complex  
Authors : Pakotiprapha, D.; Jeruzalmi, D.  
Deposited on : 2011-12-03  
Resolution : 4.40 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

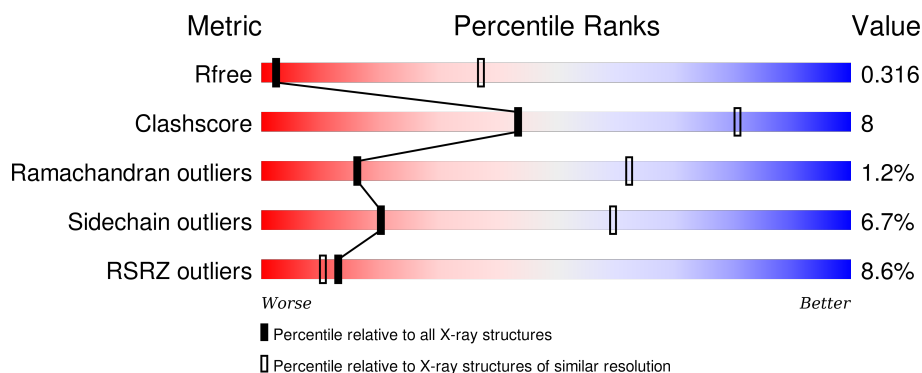
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.40 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))
$R_{free}$	91344	1067 (5.20-3.60)
Clashscore	102246	1175 (5.20-3.60)
Ramachandran outliers	100387	1114 (5.20-3.60)
Sidechain outliers	100360	1096 (5.20-3.60)
RSRZ outliers	91569	1071 (5.20-3.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	972	<div> <div>10%</div> <div>72%</div> <div>23%</div> <div>• •</div> </div>
2	B	683	<div> <div>6%</div> <div>66%</div> <div>19%</div> <div>• 13%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12193 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 Excinuclease ABC, A subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	945	Total	C	N	O	S	0	0	0
			7381	4646	1305	1402	28			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP E8SW61
A	-18	GLY	-	EXPRESSION TAG	UNP E8SW61
A	-17	SER	-	EXPRESSION TAG	UNP E8SW61
A	-16	SER	-	EXPRESSION TAG	UNP E8SW61
A	-15	HIS	-	EXPRESSION TAG	UNP E8SW61
A	-14	HIS	-	EXPRESSION TAG	UNP E8SW61
A	-13	HIS	-	EXPRESSION TAG	UNP E8SW61
A	-12	HIS	-	EXPRESSION TAG	UNP E8SW61
A	-11	HIS	-	EXPRESSION TAG	UNP E8SW61
A	-10	HIS	-	EXPRESSION TAG	UNP E8SW61
A	-9	SER	-	EXPRESSION TAG	UNP E8SW61
A	-8	SER	-	EXPRESSION TAG	UNP E8SW61
A	-7	GLY	-	EXPRESSION TAG	UNP E8SW61
A	-6	LEU	-	EXPRESSION TAG	UNP E8SW61
A	-5	VAL	-	EXPRESSION TAG	UNP E8SW61
A	-4	PRO	-	EXPRESSION TAG	UNP E8SW61
A	-3	ARG	-	EXPRESSION TAG	UNP E8SW61
A	-2	GLY	-	EXPRESSION TAG	UNP E8SW61
A	-1	SER	-	EXPRESSION TAG	UNP E8SW61
A	0	HIS	-	EXPRESSION TAG	UNP E8SW61

- Molecule 2 is a protein called UvrABC system protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	595	Total	C	N	O	S	0	0	0
			4809	3031	856	910	12			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-24	MET	-	EXPRESSION TAG	UNP E8SW62
B	-23	GLY	-	EXPRESSION TAG	UNP E8SW62
B	-22	SER	-	EXPRESSION TAG	UNP E8SW62
B	-21	SER	-	EXPRESSION TAG	UNP E8SW62
B	-20	HIS	-	EXPRESSION TAG	UNP E8SW62
B	-19	HIS	-	EXPRESSION TAG	UNP E8SW62
B	-18	HIS	-	EXPRESSION TAG	UNP E8SW62
B	-17	HIS	-	EXPRESSION TAG	UNP E8SW62
B	-16	HIS	-	EXPRESSION TAG	UNP E8SW62
B	-15	HIS	-	EXPRESSION TAG	UNP E8SW62
B	-14	SER	-	EXPRESSION TAG	UNP E8SW62
B	-13	SER	-	EXPRESSION TAG	UNP E8SW62
B	-12	GLY	-	EXPRESSION TAG	UNP E8SW62
B	-11	LEU	-	EXPRESSION TAG	UNP E8SW62
B	-10	VAL	-	EXPRESSION TAG	UNP E8SW62
B	-9	PRO	-	EXPRESSION TAG	UNP E8SW62
B	-8	ARG	-	EXPRESSION TAG	UNP E8SW62
B	-7	GLY	-	EXPRESSION TAG	UNP E8SW62
B	-6	SER	-	EXPRESSION TAG	UNP E8SW62
B	-5	HIS	-	EXPRESSION TAG	UNP E8SW62
B	-3	GLY	-	EXPRESSION TAG	UNP E8SW62
B	-2	PRO	-	EXPRESSION TAG	UNP E8SW62
B	-1	LYS	-	EXPRESSION TAG	UNP E8SW62
B	0	LYS	-	EXPRESSION TAG	UNP E8SW62
B	1	VAL	MET	SEE REMARK 999	UNP E8SW62
B	74	HIS	TYR	SEE REMARK 999	UNP E8SW62

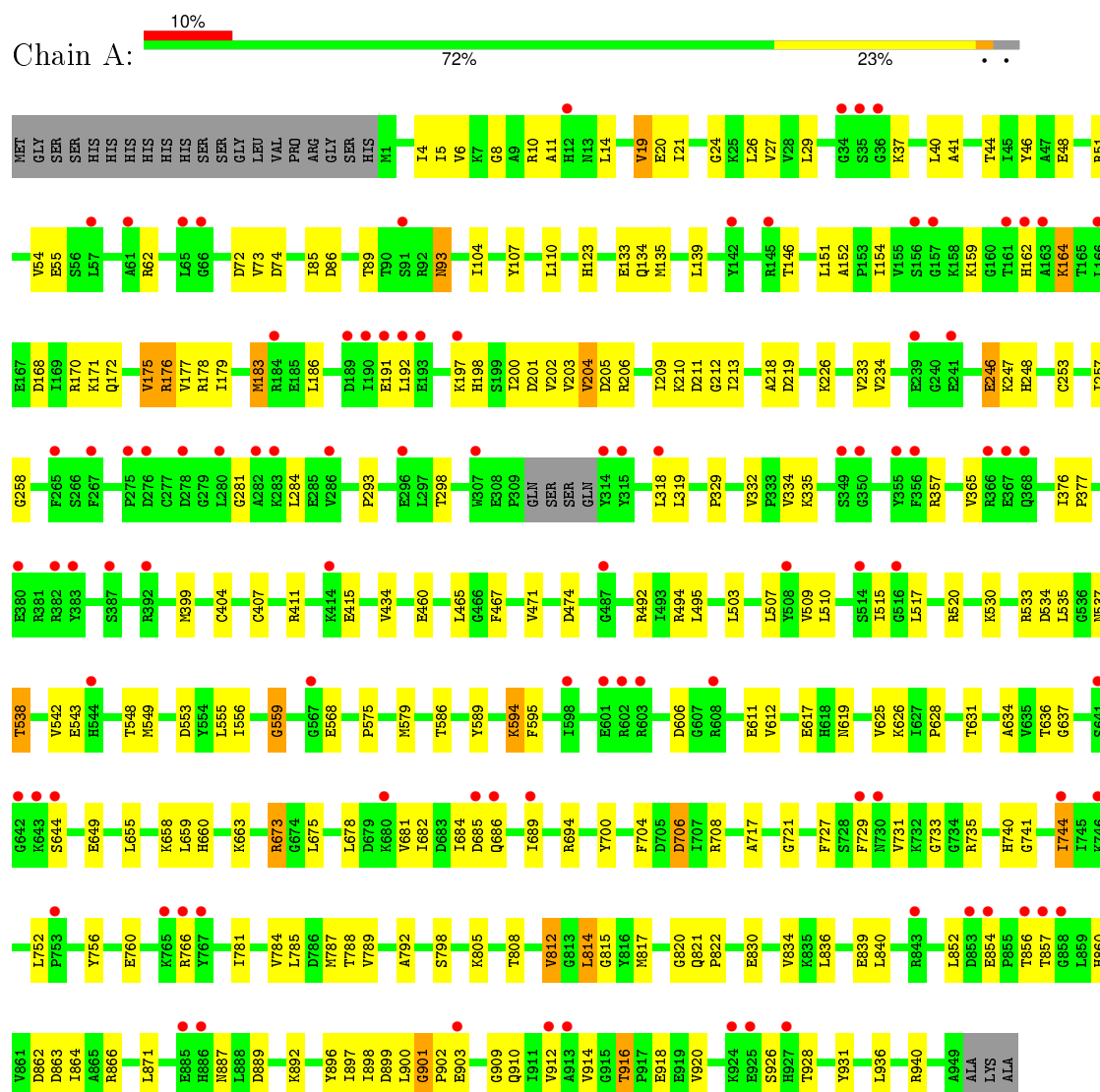
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Zn	0	0
			3	3		

### 3 Residue-property plots [i](#)

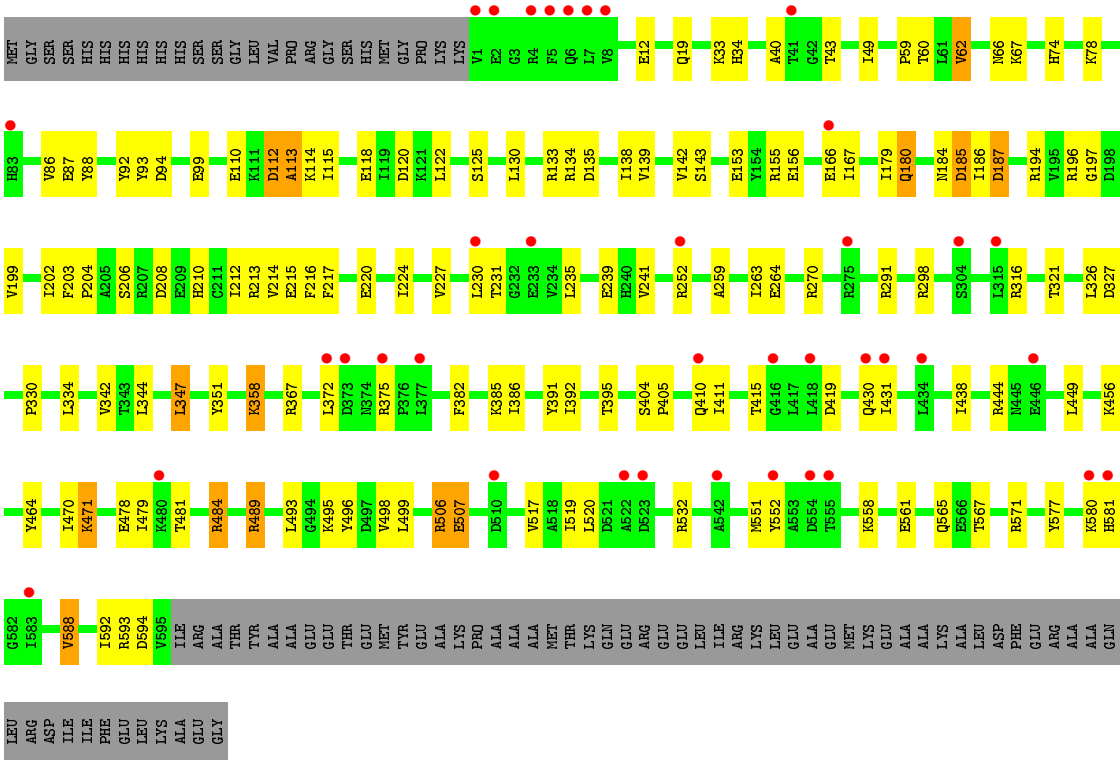
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Excinuclease ABC, A subunit



#### • Molecule 2: UvrABC system protein B





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	216.82Å 216.82Å 116.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.06 – 4.40 38.06 – 4.40	Depositor EDS
% Data completeness (in resolution range)	96.7 (38.06-4.40) 85.6 (38.06-4.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 4.44Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.288 , 0.349 0.260 , 0.316	Depositor DCC
$R_{free}$ test set	791 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	193.0	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 305.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 17613 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	12193	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	347.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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	0.24	0/7507	0.45	0/10143
2	B	0.26	0/4892	0.46	0/6612
All	All	0.25	0/12399	0.45	0/16755

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

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	7381	0	7458	140	0
2	B	4809	0	4839	66	0
3	A	3	0	0	0	0
All	All	12193	0	12297	199	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 8.

All (199) 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:A:176:ARG:HB3	1:A:203:VAL:HB	1.61	0.80
1:A:168:ASP:HA	1:A:171:LYS:HB3	1.69	0.75
2:B:74:HIS:CE1	2:B:88:TYR:HA	2.22	0.75
1:A:634:ALA:HB3	1:A:897:ILE:HG22	1.70	0.71
2:B:484:ARG:HB3	2:B:484:ARG:HH11	1.57	0.70
2:B:316:ARG:NH2	2:B:321:THR:O	2.25	0.69
1:A:151:LEU:HB2	1:A:233:VAL:HB	1.74	0.68
1:A:789:VAL:HB	1:A:815:GLY:HA2	1.77	0.67
1:A:146:THR:H	1:A:209:ILE:HB	1.60	0.67
2:B:74:HIS:CE1	2:B:139:VAL:HB	2.31	0.65
1:A:162:HIS:HA	1:A:164:LYS:HE2	1.79	0.65
1:A:812:VAL:HG22	1:A:836:LEU:HD12	1.79	0.65
2:B:66:ASN:ND2	2:B:507:GLU:OE2	2.29	0.65
2:B:484:ARG:HH21	2:B:506:ARG:HD3	1.61	0.65
1:A:682:ILE:HG21	1:A:839:GLU:HG2	1.77	0.64
1:A:85:ILE:HG23	1:A:494:ARG:HG2	1.79	0.64
1:A:248:HIS:ND1	1:A:258:GLY:O	2.26	0.64
2:B:264:GLU:OE2	2:B:298:ARG:NH1	2.30	0.62
1:A:729:PHE:HE1	1:A:766:ARG:HB3	1.64	0.62
2:B:74:HIS:HE1	2:B:88:TYR:HA	1.64	0.61
2:B:49:ILE:HG12	2:B:392:ILE:HD11	1.83	0.61
1:A:24:GLY:H	1:A:538:THR:HB	1.67	0.60
2:B:185:ASP:HA	2:B:194:ARG:HD3	1.83	0.60
1:A:54:VAL:HG11	1:A:752:LEU:HD11	1.82	0.60
1:A:123:HIS:HE1	1:A:253:CYS:HB3	1.67	0.59
2:B:419:ASP:O	2:B:571:ARG:NH1	2.28	0.58
1:A:139:LEU:HD22	1:A:234:VAL:HG11	1.85	0.58
1:A:329:PRO:HG2	1:A:332:VAL:HG21	1.86	0.58
2:B:112:ASP:OD1	2:B:113:ALA:N	2.37	0.57
2:B:60:THR:HG22	2:B:334:LEU:HB3	1.86	0.57
2:B:484:ARG:NH2	2:B:506:ARG:HB2	2.19	0.57
1:A:29:LEU:HD23	1:A:556:ILE:HB	1.85	0.57
2:B:87:GLU:HB2	2:B:138:ILE:HG12	1.87	0.57
2:B:489:ARG:NH1	2:B:593:ARG:O	2.37	0.57
1:A:179:ILE:HG23	1:A:200:ILE:HG12	1.86	0.57
1:A:10:ARG:NH2	1:A:72:ASP:OD1	2.38	0.56
1:A:852:LEU:HD11	1:A:871:LEU:HD11	1.86	0.56
1:A:660:HIS:HE1	1:A:681:VAL:H	1.52	0.56
1:A:8:GLY:O	1:A:10:ARG:NH1	2.38	0.56
1:A:694:ARG:HA	1:A:729:PHE:HE2	1.70	0.55
1:A:781:ILE:HA	1:A:784:VAL:HG12	1.88	0.55
1:A:636:THR:HG21	1:A:928:THR:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:214:VAL:HG23	2:B:224:ILE:HG12	1.89	0.54
2:B:184:ASN:ND2	2:B:187:ASP:O	2.40	0.54
1:A:55:GLU:HG2	1:A:62:ARG:HG3	1.89	0.54
1:A:549:MET:HE1	1:A:586:THR:HG21	1.90	0.54
1:A:520:ARG:HA	1:A:931:TYR:CZ	2.43	0.54
1:A:467:PHE:O	1:A:471:VAL:HG23	2.08	0.54
1:A:559:GLY:N	1:A:568:GLU:O	2.40	0.53
1:A:178:ARG:HA	1:A:183:MET:HA	1.90	0.53
2:B:156:GLU:OE1	2:B:252:ARG:NH2	2.40	0.53
1:A:404:CYS:HB3	1:A:407:CYS:SG	2.49	0.53
1:A:170:ARG:HB2	1:A:186:LEU:HD22	1.90	0.53
2:B:185:ASP:N	2:B:185:ASP:OD2	2.34	0.52
1:A:177:VAL:HG12	1:A:202:VAL:HG22	1.91	0.52
1:A:434:VAL:HB	1:A:474:ASP:HA	1.92	0.52
1:A:543:GLU:HG3	1:A:548:THR:HG21	1.90	0.52
1:A:731:VAL:O	1:A:735:ARG:HG2	2.09	0.52
2:B:78:LYS:HA	2:B:86:VAL:HG21	1.90	0.52
1:A:107:TYR:CZ	1:A:460:GLU:HG2	2.45	0.52
1:A:611:GLU:HB2	1:A:673:ARG:HB2	1.91	0.51
2:B:415:THR:HG21	2:B:588:VAL:HG13	1.92	0.51
1:A:636:THR:OG1	1:A:637:GLY:N	2.43	0.51
1:A:4:ILE:HG23	1:A:21:ILE:HB	1.92	0.51
1:A:204:VAL:HG12	2:B:197:GLY:HA3	1.92	0.51
1:A:863:ASP:OD2	1:A:866:ARG:NH2	2.44	0.51
1:A:44:THR:HG23	1:A:73:VAL:HG21	1.92	0.51
1:A:495:LEU:HD13	1:A:510:LEU:HD21	1.91	0.50
1:A:619:ASN:O	1:A:909:GLY:HA3	2.11	0.50
1:A:172:GLN:O	2:B:196:ARG:NH2	2.42	0.50
1:A:902:PRO:HD3	1:A:912:VAL:HG22	1.93	0.50
1:A:530:LYS:O	1:A:534:ASP:N	2.43	0.50
1:A:10:ARG:HA	1:A:14:LEU:HB2	1.94	0.49
2:B:449:LEU:HB2	2:B:517:VAL:HG22	1.93	0.49
1:A:735:ARG:NH1	1:A:740:HIS:HA	2.26	0.49
1:A:659:LEU:HD12	1:A:681:VAL:HG23	1.95	0.49
2:B:142:VAL:HG12	2:B:347:LEU:HD12	1.94	0.49
1:A:898:ILE:HG23	1:A:914:VAL:HG12	1.95	0.49
1:A:856:THR:HG21	1:A:887:ASN:HD22	1.77	0.49
2:B:196:ARG:HB2	2:B:199:VAL:HB	1.93	0.48
1:A:897:ILE:HG13	1:A:920:VAL:HG21	1.95	0.48
1:A:93:ASN:OD1	1:A:93:ASN:N	2.46	0.48
2:B:59:PRO:HG2	2:B:330:PRO:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:ILE:O	2:B:204:PRO:HD3	2.14	0.48
1:A:735:ARG:HD2	1:A:741:GLY:HA3	1.95	0.48
1:A:6:VAL:HG13	1:A:19:VAL:HG13	1.95	0.48
1:A:830:GLU:O	1:A:834:VAL:HG23	2.13	0.48
1:A:694:ARG:HA	1:A:729:PHE:CE2	2.48	0.47
1:A:293:PRO:HG3	1:A:663:LYS:NZ	2.29	0.47
1:A:37:LYS:HD2	1:A:542:VAL:HG13	1.96	0.47
1:A:814:LEU:HB3	1:A:815:GLY:H	1.55	0.47
1:A:594:LYS:HE3	1:A:595:PHE:H	1.79	0.47
2:B:99:GLU:OE2	2:B:367:ARG:NH2	2.45	0.47
2:B:110:GLU:HB3	2:B:112:ASP:H	1.80	0.47
1:A:293:PRO:HG3	1:A:663:LYS:HZ1	1.79	0.47
2:B:395:THR:HB	2:B:532:ARG:HG2	1.97	0.47
2:B:153:GLU:OE2	2:B:252:ARG:HG3	2.15	0.47
1:A:731:VAL:HG12	1:A:733:GLY:H	1.80	0.47
1:A:889:ASP:HA	1:A:892:LYS:HE2	1.96	0.47
1:A:171:LYS:HZ3	2:B:231:THR:HA	1.80	0.47
1:A:171:LYS:NZ	2:B:230:LEU:O	2.47	0.47
1:A:492:ARG:NH1	1:A:515:ILE:O	2.48	0.46
1:A:685:ASP:OD1	1:A:686:GLN:N	2.48	0.46
1:A:533:ARG:NH1	1:A:553:ASP:OD1	2.49	0.46
1:A:281:GLY:HA3	1:A:411:ARG:HG2	1.98	0.46
1:A:520:ARG:NH1	1:A:903:GLU:OE2	2.45	0.46
1:A:684:ILE:HD13	1:A:836:LEU:HA	1.96	0.46
1:A:104:ILE:HD13	1:A:465:LEU:HD12	1.97	0.46
1:A:628:PRO:HG3	1:A:896:TYR:CG	2.50	0.46
1:A:21:ILE:HG23	1:A:27:VAL:HG21	1.98	0.46
1:A:507:LEU:HA	1:A:538:THR:HG23	1.97	0.46
1:A:589:TYR:OH	1:A:862:ASP:OD1	2.31	0.46
2:B:382:PHE:O	2:B:386:ILE:HG13	2.15	0.46
1:A:660:HIS:CE1	1:A:681:VAL:H	2.33	0.45
1:A:5:ILE:HG12	1:A:20:GLU:HG2	1.98	0.45
2:B:88:TYR:HB3	2:B:122:LEU:HD13	1.98	0.45
1:A:357:ARG:HH21	1:A:365:VAL:HG21	1.81	0.45
1:A:655:LEU:HB3	1:A:681:VAL:HG21	1.98	0.45
2:B:438:ILE:HD13	2:B:498:VAL:HG21	1.97	0.45
1:A:612:VAL:HG23	1:A:625:VAL:H	1.82	0.45
1:A:916:THR:HG23	1:A:918:GLU:H	1.79	0.45
1:A:123:HIS:CE1	1:A:253:CYS:HB3	2.51	0.45
1:A:399:MET:HE3	1:A:399:MET:HB2	1.91	0.45
1:A:549:MET:HB3	1:A:555:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:PHE:O	1:A:708:ARG:HG3	2.17	0.45
1:A:689:ILE:HG23	1:A:700:TYR:CD2	2.52	0.45
1:A:48:GLU:CD	1:A:51:ARG:HH12	2.21	0.45
1:A:684:ILE:HB	1:A:852:LEU:HD22	2.00	0.44
2:B:212:ILE:HG12	2:B:241:VAL:HG21	2.00	0.44
2:B:484:ARG:HH11	2:B:484:ARG:CB	2.27	0.44
1:A:727:PHE:HB3	1:A:781:ILE:HD12	2.00	0.44
1:A:192:LEU:HB3	1:A:198:HIS:NE2	2.33	0.44
1:A:257:ILE:HD13	1:A:415:GLU:HB2	2.00	0.44
1:A:135:MET:O	1:A:139:LEU:HG	2.18	0.44
2:B:43:THR:HG21	2:B:410:GLN:HG2	2.00	0.44
1:A:46:TYR:HB2	1:A:509:VAL:HG21	2.00	0.44
1:A:717:ALA:O	1:A:721:GLY:N	2.50	0.44
1:A:376:ILE:HB	1:A:377:PRO:HD3	2.00	0.44
1:A:784:VAL:HA	1:A:787:MET:HG3	1.98	0.44
1:A:575:PRO:O	1:A:579:MET:HB2	2.17	0.44
1:A:319:LEU:HD23	1:A:319:LEU:HA	1.85	0.44
1:A:936:LEU:O	1:A:940:ARG:HB2	2.17	0.44
1:A:175:VAL:HG21	2:B:215:GLU:CD	2.38	0.44
2:B:520:LEU:HA	2:B:552:TYR:HB2	2.00	0.43
1:A:744:ILE:HG21	1:A:756:TYR:HB3	2.01	0.43
2:B:471:LYS:HB3	2:B:496:TYR:HA	2.01	0.43
1:A:29:LEU:HD12	1:A:41:ALA:HB2	2.00	0.43
2:B:438:ILE:HG21	2:B:470:ILE:HD13	2.01	0.43
1:A:175:VAL:HG22	2:B:213:ARG:NH2	2.34	0.43
2:B:40:ALA:O	2:B:43:THR:HG22	2.19	0.43
1:A:146:THR:HB	1:A:209:ILE:HG13	2.00	0.43
2:B:62:VAL:HG13	2:B:139:VAL:HG22	2.01	0.43
2:B:130:LEU:HA	2:B:130:LEU:HD23	1.90	0.43
1:A:503:LEU:O	1:A:537:ASN:ND2	2.34	0.43
1:A:805:LYS:O	1:A:808:THR:OG1	2.28	0.43
1:A:171:LYS:HE2	1:A:171:LYS:HB2	1.82	0.43
2:B:358:LYS:HB3	2:B:372:LEU:HD23	2.01	0.43
1:A:788:THR:O	1:A:792:ALA:N	2.46	0.43
1:A:159:LYS:HG3	1:A:197:LYS:HG2	2.01	0.43
1:A:298:THR:HA	1:A:332:VAL:O	2.19	0.42
1:A:86:ASP:OD2	1:A:89:THR:HG22	2.19	0.42
2:B:507:GLU:H	2:B:507:GLU:CD	2.21	0.42
1:A:706:ASP:OD1	1:A:706:ASP:N	2.52	0.42
1:A:152:ALA:O	1:A:154:ILE:N	2.53	0.42
2:B:351:TYR:HE1	2:B:375:ARG:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:HIS:O	1:A:864:ILE:HG12	2.20	0.42
2:B:404:SER:HA	2:B:405:PRO:HD3	1.92	0.42
2:B:430:GLN:HG3	2:B:431:ILE:HD12	2.02	0.42
2:B:259:ALA:O	2:B:263:ILE:HG13	2.18	0.42
1:A:785:LEU:HG	1:A:820:GLY:HA3	2.00	0.42
1:A:899:ASP:OD1	1:A:926:SER:OG	2.28	0.42
2:B:419:ASP:HB3	2:B:567:THR:HG23	2.01	0.42
1:A:471:VAL:HG12	1:A:492:ARG:HD2	2.02	0.42
1:A:151:LEU:HB3	1:A:201:ASP:HB3	2.02	0.42
1:A:206:ARG:NH2	2:B:216:PHE:O	2.53	0.41
1:A:535:LEU:HA	1:A:535:LEU:HD12	1.83	0.41
2:B:125:SER:HA	2:B:206:SER:HB2	2.02	0.41
1:A:854:GLU:O	1:A:857:THR:HG22	2.20	0.41
2:B:495:LYS:HB3	2:B:495:LYS:HE2	1.75	0.41
1:A:689:ILE:HD11	1:A:834:VAL:HB	2.02	0.41
1:A:808:THR:HG22	1:A:840:LEU:HD12	2.01	0.41
2:B:33:LYS:HE3	2:B:34:HIS:HE2	1.86	0.41
1:A:133:GLU:HG2	1:A:134:GLN:N	2.35	0.41
1:A:589:TYR:HA	1:A:594:LYS:O	2.20	0.41
1:A:901:GLY:N	1:A:910:GLN:O	2.54	0.41
1:A:821:GLN:HA	1:A:822:PRO:HD3	1.90	0.41
1:A:6:VAL:CG1	1:A:19:VAL:HG13	2.50	0.41
2:B:344:LEU:HD11	2:B:391:TYR:CE2	2.56	0.41
2:B:519:ILE:HB	2:B:551:MET:HG2	2.03	0.41
1:A:658:LYS:HB3	1:A:675:LEU:HD21	2.02	0.41
1:A:248:HIS:HB3	1:A:257:ILE:HG22	2.02	0.41
2:B:62:VAL:HG22	2:B:139:VAL:HG13	2.02	0.41
1:A:164:LYS:H	1:A:164:LYS:HG3	1.53	0.41
1:A:329:PRO:HG2	1:A:332:VAL:CG2	2.49	0.40
2:B:135:ASP:N	2:B:135:ASP:OD1	2.53	0.40
1:A:211:ASP:O	1:A:213:ILE:N	2.54	0.40
1:A:205:ASP:OD1	1:A:206:ARG:N	2.55	0.40
2:B:327:ASP:OD1	2:B:385:LYS:HE3	2.22	0.40
2:B:577:TYR:CZ	2:B:581:HIS:CE1	3.10	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	941/972 (97%)	855 (91%)	72 (8%)	14 (2%)	13	58
2	B	593/683 (87%)	557 (94%)	32 (5%)	4 (1%)	26	71
All	All	1534/1655 (93%)	1412 (92%)	104 (7%)	18 (1%)	16	62

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	901	GLY
1	A	212	GLY
1	A	559	GLY
1	A	617	GLU
1	A	798	SER
2	B	112	ASP
1	A	74	ASP
1	A	204	VAL
1	A	606	ASP
2	B	143	SER
2	B	180	GLN
1	A	11	ALA
1	A	218	ALA
1	A	814	LEU
2	B	113	ALA
1	A	246	GLU
1	A	247	LYS
1	A	334	VAL

### 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	796/818 (97%)	763 (96%)	33 (4%)	37	72
2	B	523/592 (88%)	467 (89%)	56 (11%)	8	39
All	All	1319/1410 (94%)	1230 (93%)	89 (7%)	20	59

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

Mol	Chain	Res	Type
1	A	19	VAL
1	A	26	LEU
1	A	40	LEU
1	A	93	ASN
1	A	110	LEU
1	A	164	LYS
1	A	175	VAL
1	A	176	ARG
1	A	183	MET
1	A	191	GLU
1	A	210	LYS
1	A	219	ASP
1	A	226	LYS
1	A	246	GLU
1	A	284	LEU
1	A	318	LEU
1	A	335	LYS
1	A	517	LEU
1	A	538	THR
1	A	594	LYS
1	A	626	LYS
1	A	631	THR
1	A	644	SER
1	A	649	GLU
1	A	673	ARG
1	A	678	LEU
1	A	706	ASP
1	A	744	ILE
1	A	760	GLU
1	A	812	VAL
1	A	817	MET
1	A	900	LEU
1	A	916	THR

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Mol	Chain	Res	Type
2	B	12	GLU
2	B	19	GLN
2	B	62	VAL
2	B	67	LYS
2	B	92	TYR
2	B	93	TYR
2	B	94	ASP
2	B	114	LYS
2	B	115	ILE
2	B	118	GLU
2	B	120	ASP
2	B	133	ARG
2	B	134	ARG
2	B	155	ARG
2	B	166	GLU
2	B	167	ILE
2	B	179	ILE
2	B	180	GLN
2	B	185	ASP
2	B	186	ILE
2	B	187	ASP
2	B	203	PHE
2	B	208	ASP
2	B	210	HIS
2	B	217	PHE
2	B	220	GLU
2	B	227	VAL
2	B	235	LEU
2	B	239	GLU
2	B	270	ARG
2	B	291	ARG
2	B	326	LEU
2	B	342	VAL
2	B	347	LEU
2	B	358	LYS
2	B	411	ILE
2	B	444	ARG
2	B	456	LYS
2	B	464	TYR
2	B	471	LYS
2	B	478	GLU
2	B	479	ILE

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Mol	Chain	Res	Type
2	B	481	THR
2	B	484	ARG
2	B	489	ARG
2	B	493	LEU
2	B	499	LEU
2	B	506	ARG
2	B	507	GLU
2	B	558	LYS
2	B	561	GLU
2	B	565	GLN
2	B	580	LYS
2	B	588	VAL
2	B	592	ILE
2	B	594	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	660	HIS
2	B	19	GLN
2	B	72	GLN
2	B	74	HIS
2	B	116	ASN
2	B	288	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	945/972 (97%)	0.55	94 (9%)	9 8	250, 336, 486, 771	0
2	B	595/683 (87%)	0.35	38 (6%)	23 16	252, 325, 437, 576	0
All	All	1540/1655 (93%)	0.47	132 (8%)	13 10	250, 332, 468, 771	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	GLU	7.6
1	A	192	LEU	7.3
1	A	162	HIS	7.0
1	A	161	THR	6.6
1	A	367	GLU	6.1
1	A	276	ASP	5.7
1	A	644	SER	5.5
1	A	355	TYR	5.4
1	A	315	TYR	5.4
2	B	6	GLN	4.9
1	A	368	GLN	4.4
1	A	924	LYS	4.3
1	A	314	TYR	4.1
1	A	603	ARG	4.0
2	B	304	SER	4.0
1	A	858	GLY	4.0
1	A	925	GLU	3.9
1	A	387	SER	3.8
1	A	767	TYR	3.8
1	A	567	GLY	3.8
1	A	913	ALA	3.8
1	A	166	LEU	3.8
1	A	65	LEU	3.8
1	A	383	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	5	PHE	3.7
2	B	7	LEU	3.7
1	A	275	PRO	3.6
1	A	414	LYS	3.6
2	B	4	ARG	3.6
1	A	382	ARG	3.6
1	A	641	SER	3.6
1	A	853	ASP	3.5
1	A	66	GLY	3.5
2	B	552	TYR	3.5
2	B	480	LYS	3.4
1	A	350	GLY	3.4
1	A	601	GLU	3.4
1	A	157	GLY	3.2
1	A	598	ILE	3.2
1	A	857	THR	3.2
1	A	283	LYS	3.1
1	A	193	GLU	3.1
1	A	197	LYS	3.1
2	B	430	GLN	3.1
2	B	1	VAL	3.1
1	A	843	ARG	3.1
1	A	642	GLY	3.1
1	A	163	ALA	3.1
1	A	927	HIS	3.1
1	A	349	SER	3.0
2	B	233	GLU	3.0
1	A	516	GLY	3.0
1	A	34	GLY	3.0
1	A	885	GLU	3.0
1	A	190	ILE	2.9
1	A	380	GLU	2.9
2	B	377	LEU	2.9
1	A	184	ARG	2.9
2	B	373	ASP	2.9
2	B	581	HIS	2.8
1	A	145	ARG	2.8
2	B	8	VAL	2.8
1	A	514	SER	2.8
2	B	555	THR	2.8
1	A	286	VAL	2.8
2	B	522	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	230	LEU	2.7
1	A	854	GLU	2.7
1	A	318	LEU	2.7
1	A	57	LEU	2.7
1	A	91	SER	2.7
1	A	36	GLY	2.7
1	A	296	GLU	2.6
2	B	510	ASP	2.6
1	A	356	PHE	2.6
1	A	685	ASP	2.6
2	B	315	LEU	2.6
2	B	372	LEU	2.6
1	A	689	ILE	2.6
1	A	608	ARG	2.6
2	B	554	ASP	2.5
1	A	686	GLN	2.5
1	A	602	ARG	2.5
1	A	744	ILE	2.5
1	A	856	THR	2.5
1	A	746	LYS	2.5
1	A	508	TYR	2.4
1	A	643	LYS	2.4
2	B	2	GLU	2.4
2	B	542	ALA	2.4
1	A	265	PHE	2.3
1	A	886	HIS	2.3
2	B	41	THR	2.3
1	A	267	PHE	2.3
2	B	416	GLY	2.3
1	A	753	PRO	2.3
1	A	12	HIS	2.3
1	A	61	ALA	2.3
2	B	166	GLU	2.3
1	A	35	SER	2.2
1	A	156	SER	2.2
1	A	307	TRP	2.2
2	B	580	LYS	2.2
1	A	282	ALA	2.2
1	A	730	ASN	2.2
1	A	729	PHE	2.2
1	A	366	ARG	2.1
1	A	912	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	523	ASP	2.1
2	B	252	ARG	2.1
1	A	142	TYR	2.1
1	A	392	ARG	2.1
1	A	487	GLY	2.1
1	A	766	ARG	2.1
2	B	434	LEU	2.1
1	A	903	GLU	2.1
2	B	431	ILE	2.1
1	A	189	ASP	2.1
1	A	239	GLU	2.1
1	A	765	LYS	2.1
1	A	280	LEU	2.1
1	A	544	HIS	2.1
1	A	680	LYS	2.1
2	B	583	ILE	2.1
2	B	83	HIS	2.1
1	A	278	ASP	2.0
2	B	275	ARG	2.0
2	B	418	LEU	2.0
2	B	446	GLU	2.0
2	B	410	GLN	2.0
1	A	241	GLU	2.0
2	B	375	ARG	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	A	1006	1/1	0.99	0.10	-0.89	550,550,550,550	0
3	ZN	A	1004	1/1	0.92	0.07	-1.90	550,550,550,550	0
3	ZN	A	1005	1/1	0.91	0.07	-2.12	550,550,550,550	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.