



# Full wwPDB X-ray Structure Validation Report

May 29, 2020 – 06:14 am BST

PDB ID : 4WWX  
Title : Crystal structure of the core RAG1/2 recombinase  
Authors : Kim, M.S.; Lapkouski, M.; Yang, W.; Gellert, M.  
Deposited on : 2014-11-12  
Resolution : 3.20 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

<https://www.wwpdb.org/validation/2017/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  
Xtrriage (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

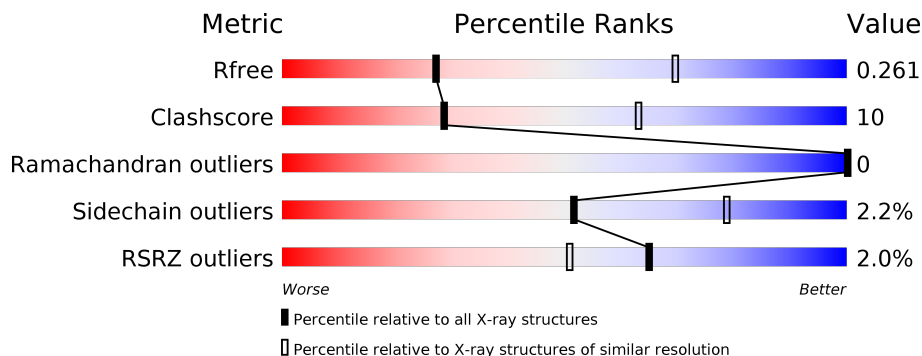
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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	B	618	<p>2% 77% 22% • 5%</p>
1	E	618	<p>2% 76% 20% • 5%</p>
2	X	349	<p>0% 70% 24% • 5%</p>
2	Y	349	<p>3% 67% 28% • 5%</p>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14978 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 V(D)J recombination-activating protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	612	Total	C	N	O	S	0	0	0
			4930	3103	877	916	34			
1	E	598	Total	C	N	O	S	0	0	0
			4815	3033	850	898	34			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	391	ALA	-	expression tag	UNP P15919
E	391	ALA	-	expression tag	UNP P15919

- Molecule 2 is a protein called V(D)J recombination-activating protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	X	333	Total	C	N	O	S	0	0	0
			2616	1674	442	481	19			
2	Y	333	Total	C	N	O	S	0	0	0
			2615	1674	442	480	19			

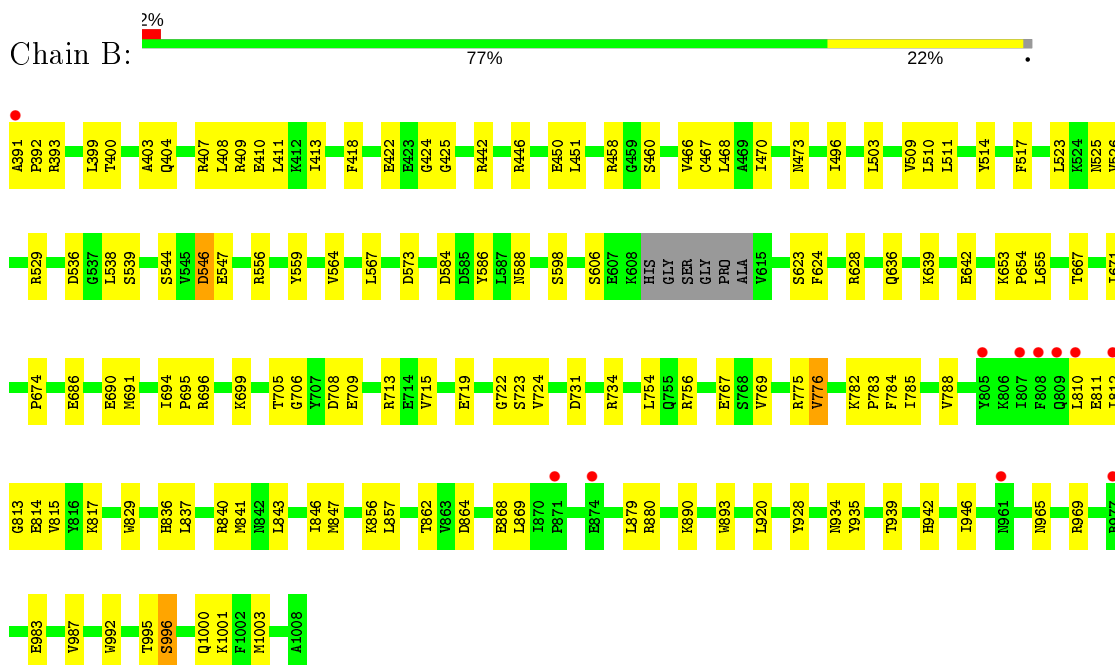
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		

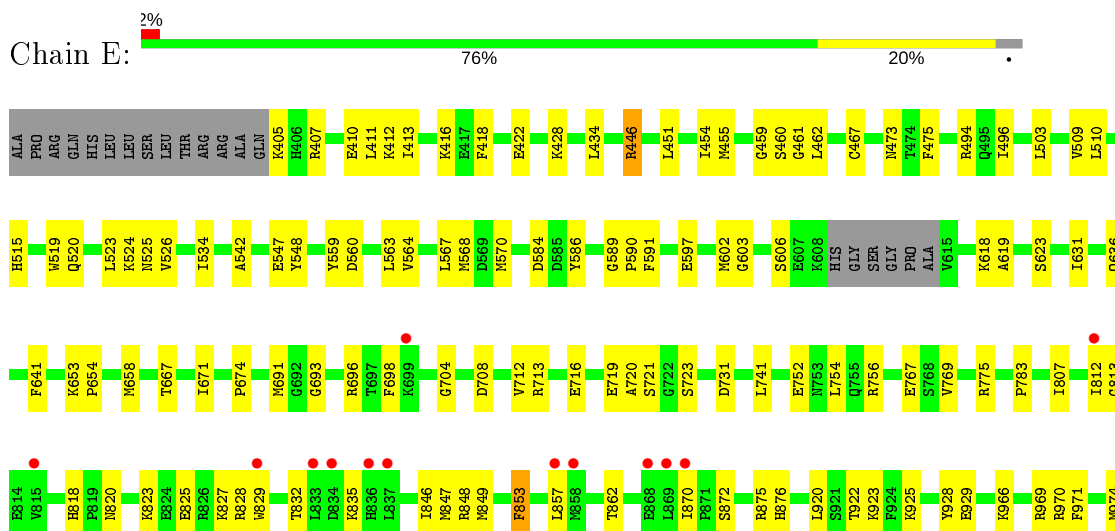
### 3 Residue-property plots

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: V(D)J recombination-activating protein 1

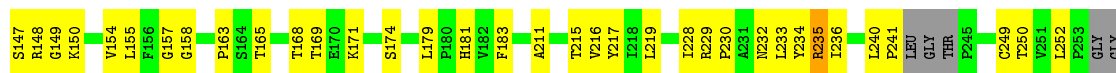
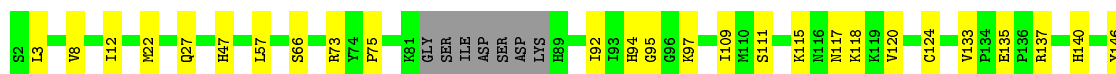


- Molecule 1: V(D)J recombination-activating protein 1

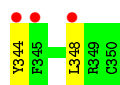
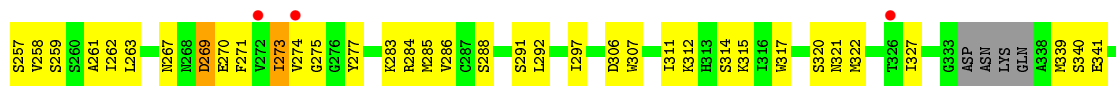
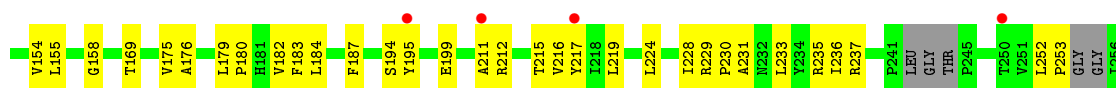
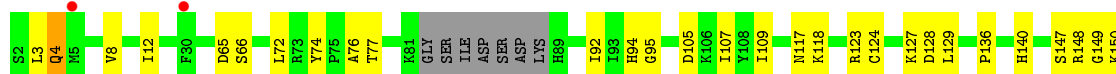




• Molecule 2: V(D)J recombination-activating protein 2



• Molecule 2: V(D)J recombination-activating protein 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.76Å 180.05Å 200.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.74 – 3.20 49.23 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (43.74-3.20) 98.8 (49.23-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 3.19Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.205 , 0.259 0.209 , 0.261	Depositor DCC
$R_{free}$ test set	1980 reflections (3.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	108.5	Xtrriage
Anisotropy	0.261	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 56.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14978	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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, 0.333 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	B	0.41	0/5030	0.56	0/6774
1	E	0.40	0/4913	0.58	1/6616 (0.0%)
2	X	0.34	0/2681	0.56	0/3629
2	Y	0.34	0/2680	0.56	0/3629
All	All	0.38	0/15304	0.57	1/20648 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	520	GLN	C-N-CD	5.93	140.85	128.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4930	0	4905	88	0
1	E	4815	0	4781	80	0
2	X	2616	0	2569	61	0
2	Y	2615	0	2569	72	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14978	0	14824	290	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 (290) 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:767:GLU:OE2	1:E:775:ARG:NH1	2.14	0.81
2:X:327:ILE:HG22	2:X:348:LEU:HB3	1.67	0.76
2:X:292:LEU:HA	2:X:297:ILE:HG13	1.71	0.72
2:X:154:VAL:HG11	2:X:216:VAL:HG21	1.71	0.71
2:Y:273:ILE:HG23	2:Y:288:SER:HB2	1.74	0.69
2:Y:283:LYS:HE3	2:Y:315:LYS:HG2	1.74	0.69
2:Y:292:LEU:HA	2:Y:297:ILE:HG22	1.75	0.69
1:E:412:LYS:HE2	1:E:416:LYS:HD2	1.73	0.68
2:Y:283:LYS:NZ	2:Y:311:ILE:O	2.19	0.68
1:B:539:SER:OG	1:B:556:ARG:NH1	2.25	0.68
2:Y:285:MET:O	2:Y:307:TRP:NE1	2.27	0.68
2:Y:212:ARG:NH1	2:Y:269:ASP:OD2	2.28	0.67
1:B:864:ASP:OD1	1:B:880:ARG:NH2	2.29	0.66
1:E:832:THR:HA	1:E:835:LYS:HE2	1.77	0.65
1:E:691:MET:HG3	1:E:696:ARG:HG3	1.79	0.63
2:Y:229:ARG:HD3	2:Y:259:SER:HB2	1.79	0.63
2:Y:327:ILE:HG22	2:Y:348:LEU:HB3	1.79	0.63
1:B:731:ASP:OD2	1:B:756:ARG:NH1	2.27	0.63
1:E:428:LYS:HE2	1:E:455:MET:HE1	1.81	0.62
1:B:623:SER:HB3	1:B:654:PRO:HA	1.81	0.62
1:B:767:GLU:OE2	1:B:775:ARG:NH1	2.33	0.62
2:X:140:HIS:HD2	2:X:155:LEU:HD11	1.65	0.62
1:E:524:LYS:HE3	1:E:525:ASN:HD21	1.63	0.62
1:E:719:GLU:HB2	1:E:723:SER:HB2	1.82	0.61
2:Y:211:ALA:HB2	2:Y:216:VAL:HG13	1.82	0.61
1:E:713:ARG:HB2	1:E:720:ALA:HB2	1.82	0.61
1:B:496:ILE:HD13	1:E:496:ILE:HD13	1.82	0.61
1:B:511:LEU:HD23	1:B:992:TRP:CD1	2.36	0.60
2:Y:147:SER:OG	2:Y:148:ARG:N	2.33	0.60
2:Y:107:ILE:HD11	2:Y:129:LEU:HD21	1.82	0.60
2:X:168:THR:HG23	2:X:171:LYS:H	1.67	0.59
2:X:240:LEU:HD22	2:X:241:PRO:HD2	1.84	0.59
2:X:3:LEU:HB3	2:X:348:LEU:HD23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:217:TYR:CZ	2:Y:297:ILE:HG12	2.38	0.59
1:B:584:ASP:OD1	1:B:586:TYR:HB2	2.03	0.59
2:Y:271:PHE:CD2	2:Y:292:LEU:HD11	2.38	0.59
1:E:523:LEU:HB2	1:E:526:VAL:HB	1.83	0.59
1:B:686:GLU:HG2	1:B:699:LYS:HG2	1.85	0.59
2:X:285:MET:O	2:X:307:TRP:NE1	2.36	0.58
2:X:292:LEU:HD23	2:X:297:ILE:HG12	1.86	0.57
1:B:705:THR:HG22	1:B:788:VAL:HB	1.86	0.57
1:B:857:LEU:HD12	1:B:862:THR:HG21	1.86	0.57
2:X:155:LEU:HB3	2:X:183:PHE:HB2	1.87	0.57
1:B:451:LEU:HD13	1:E:451:LEU:HD13	1.87	0.57
1:B:920:LEU:HD22	1:B:928:TYR:HD2	1.68	0.56
2:X:219:LEU:HD22	2:X:233:LEU:HD22	1.86	0.56
2:X:140:HIS:CD2	2:X:155:LEU:HD11	2.41	0.56
2:Y:277:TYR:HA	2:Y:283:LYS:HA	1.87	0.56
2:Y:252:LEU:HG	2:Y:253:PRO:HD2	1.86	0.56
2:Y:291:SER:O	2:Y:297:ILE:HA	2.06	0.56
1:B:606:SER:H	1:B:969:ARG:HH22	1.52	0.56
1:E:509:VAL:HG12	1:E:510:LEU:HD23	1.88	0.55
1:B:754:LEU:HD23	1:B:783:PRO:HD2	1.88	0.55
2:Y:274:VAL:HG12	2:Y:275:GLY:H	1.71	0.55
1:E:653:LYS:HE3	1:E:995:THR:O	2.07	0.55
2:Y:217:TYR:CE2	2:Y:297:ILE:HG21	2.42	0.55
1:E:980:LYS:NZ	1:E:983:GLU:OE1	2.39	0.55
2:Y:283:LYS:HE2	2:Y:314:SER:HB3	1.88	0.55
1:E:446:ARG:HD2	1:E:446:ARG:H	1.72	0.55
1:E:467:CYS:HB2	1:E:503:LEU:HD21	1.89	0.55
2:Y:140:HIS:HB3	2:Y:158:GLY:N	2.22	0.55
1:B:546:ASP:N	1:B:546:ASP:OD1	2.39	0.54
2:Y:199:GLU:OE1	2:Y:199:GLU:N	2.39	0.54
2:X:66:SER:HB3	2:X:124:CYS:H	1.72	0.54
2:Y:105:ASP:HB3	2:Y:136:PRO:HB3	1.90	0.54
2:Y:182:VAL:HG23	2:Y:195:TYR:HB2	1.89	0.54
2:Y:65:ASP:OD1	2:Y:123:ARG:NH1	2.41	0.54
2:Y:154:VAL:HG11	2:Y:216:VAL:HG21	1.90	0.54
2:X:217:TYR:HE1	2:X:235:ARG:HG2	1.73	0.54
1:B:544:SER:HB3	1:B:547:GLU:HG2	1.90	0.54
1:B:691:MET:HG3	1:B:696:ARG:HG3	1.90	0.54
1:E:671:ILE:O	1:E:674:PRO:HD2	2.08	0.54
1:E:754:LEU:HD23	1:E:783:PRO:HD2	1.90	0.54
1:B:836:HIS:NE2	1:B:868:GLU:OE1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:107:ILE:HG13	2:Y:129:LEU:HD11	1.90	0.53
1:B:836:HIS:CG	1:B:869:LEU:HD11	2.43	0.53
1:B:920:LEU:HD22	1:B:928:TYR:CD2	2.43	0.53
1:E:966:LYS:O	1:E:970:ARG:HG3	2.08	0.53
2:X:27:GLN:OE1	2:X:115:LYS:NZ	2.41	0.53
2:Y:217:TYR:HE2	2:Y:297:ILE:HG21	1.73	0.53
2:Y:277:TYR:HH	2:Y:317:TRP:H	1.54	0.53
2:Y:228:ILE:O	2:Y:230:PRO:HD3	2.09	0.53
1:B:811:GLU:HG2	1:B:879:LEU:HD11	1.90	0.53
1:E:606:SER:H	1:E:969:ARG:HH22	1.57	0.53
1:E:623:SER:HB3	1:E:654:PRO:HA	1.90	0.53
2:Y:140:HIS:CD2	2:Y:155:LEU:HD11	2.44	0.52
2:Y:267:ASN:HB2	2:Y:270:GLU:HB3	1.90	0.52
1:E:534:ILE:HG21	1:E:985:GLU:HG3	1.89	0.52
1:B:573:ASP:OD1	1:B:1001:LYS:NZ	2.42	0.52
2:X:275:GLY:HA3	2:X:317:TRP:CZ3	2.44	0.52
2:X:147:SER:OG	2:X:148:ARG:N	2.39	0.52
1:B:509:VAL:HG12	1:B:510:LEU:HD23	1.91	0.52
1:E:920:LEU:HD22	1:E:928:TYR:HD2	1.75	0.52
2:X:275:GLY:HA3	2:X:317:TRP:HZ3	1.74	0.52
1:E:752:GLU:O	1:E:756:ARG:HG3	2.10	0.52
2:Y:128:ASP:N	2:Y:128:ASP:OD1	2.41	0.52
2:Y:219:LEU:HD22	2:Y:233:LEU:HD22	1.90	0.52
1:B:598:SER:HB3	1:B:706:GLY:HA3	1.91	0.52
2:X:211:ALA:HB2	2:X:216:VAL:HG13	1.92	0.52
1:E:418:PHE:CE1	1:E:422:GLU:HG3	2.46	0.51
1:E:719:GLU:O	1:E:721:SER:HA	2.11	0.51
2:X:135:GLU:H	2:X:137:ARG:HH21	1.58	0.51
2:X:274:VAL:HG12	2:X:275:GLY:H	1.74	0.51
2:Y:233:LEU:HD12	2:Y:252:LEU:HD22	1.93	0.51
2:X:217:TYR:HE2	2:X:297:ILE:HD13	1.75	0.51
1:B:523:LEU:HB2	1:B:526:VAL:HB	1.91	0.50
2:Y:8:VAL:HB	2:Y:12:ILE:HG12	1.93	0.50
1:B:467:CYS:HB2	1:B:503:LEU:HD21	1.93	0.50
1:B:450:GLU:HB3	1:E:454:ILE:HD13	1.92	0.50
1:E:459:GLY:HA3	1:E:461:GLY:H	1.75	0.50
2:X:115:LYS:HG3	2:X:120:VAL:HG12	1.93	0.50
2:X:283:LYS:HG3	2:X:285:MET:HG3	1.94	0.50
1:B:837:LEU:HD22	1:B:843:LEU:HD12	1.94	0.50
2:X:321:ASN:HA	2:X:327:ILE:HG13	1.93	0.50
1:E:857:LEU:HD12	1:E:862:THR:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:249:CYS:SG	2:X:250:THR:N	2.85	0.50
2:X:256:ILE:HG12	2:X:257:SER:H	1.77	0.49
1:B:756:ARG:HB3	1:B:776:VAL:HG22	1.94	0.49
1:E:716:GLU:HA	1:E:783:PRO:HB3	1.94	0.49
1:E:846:ILE:HG12	1:E:847:MET:O	2.12	0.49
1:E:410:GLU:O	1:E:413:ILE:HG12	2.12	0.49
1:B:473:ASN:CG	1:B:1003:MET:HG3	2.32	0.49
2:Y:66:SER:HB3	2:Y:124:CYS:H	1.76	0.49
1:B:810:LEU:HD22	1:B:815:VAL:HG21	1.95	0.49
1:E:636:GLN:OE1	1:E:636:GLN:N	2.46	0.49
1:E:547:GLU:OE2	1:E:548:TYR:N	2.46	0.49
1:B:812:ILE:HD11	1:B:829:TRP:HB3	1.94	0.49
1:E:591:PHE:HB2	1:E:698:PHE:CD1	2.48	0.49
1:E:691:MET:O	1:E:693:GLY:N	2.39	0.48
2:X:229:ARG:HH21	2:X:280:GLU:HA	1.78	0.48
1:E:708:ASP:O	1:E:712:VAL:HG23	2.12	0.48
2:X:217:TYR:CE2	2:X:297:ILE:HD13	2.48	0.48
1:B:466:VAL:O	1:B:470:ILE:HG13	2.14	0.48
2:X:148:ARG:HB2	2:X:240:LEU:HB3	1.96	0.48
2:Y:258:VAL:HG21	2:Y:261:ALA:HB2	1.96	0.47
1:B:422:GLU:OE2	1:E:407:ARG:HG3	2.15	0.47
2:Y:231:ALA:HB2	2:Y:257:SER:HB2	1.96	0.47
2:X:233:LEU:HB2	2:X:252:LEU:HB2	1.96	0.47
2:X:256:ILE:HG12	2:X:257:SER:N	2.29	0.47
1:B:754:LEU:HD23	1:B:754:LEU:HA	1.75	0.47
1:B:935:TYR:O	1:B:939:THR:OG1	2.28	0.47
2:Y:3:LEU:HD22	2:Y:348:LEU:HD12	1.96	0.47
1:B:708:ASP:OD1	1:B:709:GLU:N	2.47	0.47
1:B:509:VAL:HG22	1:B:514:TYR:CE2	2.49	0.47
1:B:713:ARG:NH1	1:B:719:GLU:O	2.48	0.47
1:E:812:ILE:HD11	1:E:829:TRP:O	2.15	0.47
1:E:584:ASP:C	1:E:586:TYR:H	2.18	0.47
1:E:597:GLU:HB2	1:E:704:GLY:HA2	1.96	0.47
2:X:228:ILE:O	2:X:230:PRO:HD3	2.14	0.47
1:E:825:GLU:HA	1:E:828:ARG:HD2	1.97	0.47
1:E:525:ASN:O	2:Y:169:THR:HG23	2.15	0.46
1:E:922:THR:OG1	1:E:923:LYS:N	2.47	0.46
2:Y:262:ILE:HG21	2:Y:320:SER:HA	1.97	0.46
1:B:408:LEU:HD13	1:E:434:LEU:HD23	1.96	0.46
1:B:667:THR:O	1:B:671:ILE:HG12	2.16	0.46
2:X:215:THR:HA	2:X:236:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:184:LEU:HD22	2:Y:195:TYR:HE2	1.80	0.46
1:B:723:SER:HA	1:B:724:VAL:HA	1.55	0.46
2:Y:277:TYR:OH	2:Y:317:TRP:N	2.25	0.46
1:B:410:GLU:O	1:B:413:ILE:HG12	2.16	0.46
2:X:149:GLY:HA2	2:X:150:LYS:HD3	1.97	0.46
1:B:392:PRO:HA	1:B:393:ARG:HA	1.62	0.46
2:Y:321:ASN:HA	2:Y:327:ILE:HG13	1.97	0.46
1:B:624:PHE:HD2	1:B:655:LEU:HD22	1.79	0.46
1:E:870:ILE:HB	1:E:876:HIS:NE2	2.31	0.46
2:X:146:TYR:HA	2:X:150:LYS:O	2.16	0.46
2:Y:109:ILE:CD1	2:Y:127:LYS:HB2	2.46	0.46
1:B:536:ASP:OD2	1:B:538:LEU:HB2	2.15	0.45
1:B:813:GLY:HA3	1:B:829:TRP:CH2	2.51	0.45
1:B:983:GLU:O	1:B:987:VAL:HG23	2.17	0.45
1:E:560:ASP:O	1:E:564:VAL:HG23	2.15	0.45
1:E:570:MET:HE1	1:E:641:PHE:CD2	2.51	0.45
1:B:418:PHE:CD2	1:E:411:LEU:HD22	2.52	0.45
2:X:217:TYR:CE1	2:X:235:ARG:HG2	2.52	0.45
1:E:872:SER:HB3	1:E:875:ARG:HG2	1.98	0.45
1:B:400:THR:O	1:B:404:GLN:HG3	2.17	0.45
1:E:418:PHE:CZ	1:E:422:GLU:HG3	2.52	0.45
1:E:667:THR:O	1:E:671:ILE:HG12	2.17	0.45
2:X:277:TYR:HH	2:X:317:TRP:H	1.58	0.45
2:Y:149:GLY:HA2	2:Y:150:LYS:HA	1.66	0.45
2:Y:284:ARG:NH1	2:Y:286:VAL:HG23	2.32	0.45
1:B:841:MET:HB2	1:B:843:LEU:HG	1.99	0.45
1:E:524:LYS:HG2	1:E:525:ASN:CG	2.37	0.45
1:E:563:LEU:O	1:E:567:LEU:HB2	2.17	0.45
2:Y:183:PHE:CE1	2:Y:194:SER:HB3	2.51	0.45
2:Y:285:MET:HB3	2:Y:285:MET:HE3	1.89	0.45
1:B:636:GLN:N	1:B:636:GLN:OE1	2.50	0.44
1:B:639:LYS:HD3	1:B:642:GLU:HB2	1.98	0.44
2:X:279:LEU:HB2	2:X:282:GLN:HB2	1.99	0.44
1:B:814:GLU:HB3	1:B:817:LYS:HB2	2.00	0.44
1:E:459:GLY:CA	1:E:460:SER:HB2	2.48	0.44
2:X:267:ASN:HB2	2:X:270:GLU:HB3	1.98	0.44
1:B:628:ARG:HD2	1:B:639:LYS:HE2	1.99	0.44
1:B:424:GLY:HA2	1:B:425:GLY:HA2	1.65	0.44
1:B:473:ASN:ND2	1:B:1003:MET:HG3	2.33	0.44
1:B:722:GLY:HA3	1:B:734:ARG:HH21	1.82	0.44
2:X:117:ASN:HB2	2:X:118:LYS:H	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:137:ARG:HH11	2:X:157:GLY:HA2	1.83	0.44
1:B:715:VAL:HB	1:B:785:ILE:HB	2.00	0.44
1:B:965:ASN:O	1:B:969:ARG:HG3	2.18	0.44
1:E:920:LEU:HD22	1:E:928:TYR:CD2	2.52	0.44
1:E:603:GLY:O	1:E:618:LYS:HA	2.17	0.43
1:B:671:ILE:O	1:B:674:PRO:HD2	2.19	0.43
1:B:715:VAL:HG12	1:B:784:PHE:HE1	1.83	0.43
1:B:843:LEU:HD21	1:B:856:LYS:HB3	2.00	0.43
1:E:818:HIS:C	1:E:820:ASN:H	2.22	0.43
2:X:216:VAL:HB	2:X:236:ILE:HD12	2.00	0.43
2:X:285:MET:HA	2:X:317:TRP:HH2	1.83	0.43
2:Y:314:SER:HB3	2:Y:315:LYS:HA	1.99	0.43
2:X:171:LYS:HB3	2:X:174:SER:OG	2.18	0.43
1:B:840:ARG:HA	1:B:840:ARG:CZ	2.48	0.43
2:X:140:HIS:HB3	2:X:158:GLY:N	2.33	0.43
1:E:823:LYS:HG3	1:E:827:LYS:HE2	2.01	0.43
1:B:690:GLU:HA	1:B:695:PRO:HA	2.00	0.43
1:E:925:LYS:HE2	1:E:929:GLU:OE2	2.19	0.42
1:B:846:ILE:HG22	1:B:847:MET:O	2.19	0.42
1:E:807:ILE:HD13	1:E:807:ILE:HA	1.88	0.42
2:X:296:THR:C	2:X:297:ILE:HD12	2.39	0.42
2:X:57:LEU:HD23	2:X:57:LEU:HA	1.83	0.42
1:B:767:GLU:OE2	1:B:775:ARG:HD2	2.19	0.42
1:E:570:MET:HE1	1:E:641:PHE:CE2	2.54	0.42
2:X:8:VAL:HB	2:X:12:ILE:HG12	2.01	0.42
2:Y:184:LEU:HD12	2:Y:184:LEU:HA	1.92	0.42
2:Y:235:ARG:HH11	2:Y:237:ARG:HH21	1.66	0.42
2:Y:261:ALA:HA	2:Y:275:GLY:O	2.20	0.42
1:B:391:ALA:HA	1:B:392:PRO:HD3	1.95	0.42
1:B:509:VAL:HG22	1:B:514:TYR:CZ	2.54	0.42
1:B:517:PHE:CD2	1:B:564:VAL:HG21	2.54	0.42
1:E:515:HIS:ND1	1:E:568:MET:HG3	2.35	0.42
2:X:304:THR:HA	2:X:305:PRO:HD3	1.87	0.42
2:Y:117:ASN:OD1	2:Y:118:LYS:HG3	2.19	0.42
2:Y:341:GLU:HB2	2:Y:344:TYR:OH	2.20	0.42
1:B:399:LEU:HB3	1:B:403:ALA:HB3	2.02	0.42
2:Y:284:ARG:HG2	2:Y:286:VAL:HG22	2.02	0.42
1:E:618:LYS:NZ	1:E:848:ARG:HH22	2.17	0.42
1:E:475:PHE:HE1	1:E:971:PHE:CE1	2.38	0.42
2:Y:215:THR:HA	2:Y:236:ILE:O	2.19	0.42
1:E:473:ASN:ND2	1:E:1003:MET:HG3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:77:THR:HA	2:Y:92:ILE:O	2.19	0.42
2:Y:339:MET:HB3	2:Y:340:SER:H	1.55	0.41
2:Y:94:HIS:HA	2:Y:95:GLY:HA2	1.79	0.41
1:B:942:HIS:O	1:B:946:ILE:HG13	2.20	0.41
1:E:591:PHE:CE1	1:E:631:ILE:HD12	2.55	0.41
2:X:163:PRO:C	2:X:165:THR:H	2.24	0.41
2:X:179:LEU:H	2:X:179:LEU:HD22	1.85	0.41
1:E:548:TYR:HB2	2:Y:74:TYR:HE2	1.86	0.41
1:B:408:LEU:HD23	1:B:408:LEU:HA	1.85	0.41
1:B:890:LYS:HA	1:B:893:TRP:CE2	2.56	0.41
2:X:92:ILE:HD13	2:X:109:ILE:HG12	2.01	0.41
2:X:94:HIS:HA	2:X:95:GLY:HA2	1.76	0.41
2:X:73:ARG:HB2	2:X:97:LYS:O	2.21	0.41
2:Y:4:GLN:HB3	2:Y:4:GLN:HE21	1.66	0.41
1:B:715:VAL:HG12	1:B:784:PHE:CE1	2.56	0.41
1:E:407:ARG:O	1:E:410:GLU:HB3	2.20	0.41
2:X:47:HIS:CE1	2:X:120:VAL:H	2.39	0.41
1:B:468:LEU:HA	1:B:503:LEU:HD13	2.03	0.41
1:E:589:GLY:HA3	1:E:590:PRO:HA	1.87	0.41
2:X:232:ASN:ND2	2:X:234:TYR:HE1	2.17	0.41
2:Y:217:TYR:CE2	2:Y:297:ILE:HG12	2.54	0.41
2:Y:72:LEU:HA	2:Y:72:LEU:HD23	1.75	0.41
1:B:567:LEU:HD12	1:B:567:LEU:HA	1.97	0.41
1:B:694:ILE:HA	1:B:695:PRO:HD3	1.81	0.41
1:B:879:LEU:HD23	1:B:879:LEU:HA	1.94	0.41
1:B:996:SER:O	1:B:1000:GLN:HG3	2.21	0.41
1:E:519:TRP:HE1	1:E:560:ASP:HB2	1.85	0.41
1:E:475:PHE:HA	1:E:974:MET:SD	2.61	0.41
2:X:22:MET:HB3	2:X:22:MET:HE2	1.69	0.41
2:Y:76:ALA:HB3	2:Y:94:HIS:O	2.21	0.41
1:E:542:ALA:HB2	2:Y:175:VAL:HG22	2.01	0.41
1:E:849:MET:HG3	1:E:853:PHE:HB3	2.03	0.41
2:X:12:ILE:H	2:X:12:ILE:HG13	1.74	0.41
2:Y:155:LEU:HB3	2:Y:183:PHE:HB2	2.03	0.41
2:Y:92:ILE:HD13	2:Y:187:PHE:CE1	2.56	0.41
1:B:653:LYS:HE3	1:B:995:THR:O	2.21	0.41
1:B:442:ARG:NH1	1:E:428:LYS:HD2	2.36	0.41
1:E:461:GLY:HA3	1:E:462:LEU:HD12	2.02	0.41
1:E:567:LEU:HD12	1:E:567:LEU:HA	1.93	0.41
2:X:75:PRO:HB3	2:X:95:GLY:O	2.21	0.41
2:Y:285:MET:HE1	2:Y:312:LYS:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:216:VAL:HB	2:Y:236:ILE:HD12	2.03	0.40
1:B:525:ASN:O	2:X:169:THR:HG23	2.21	0.40
1:E:658:MET:HE2	1:E:671:ILE:HG21	2.04	0.40
1:E:813:GLY:HA3	1:E:829:TRP:CD2	2.57	0.40
2:Y:176:ALA:HA	2:Y:224:LEU:HD12	2.04	0.40
1:B:836:HIS:HE2	1:B:840:ARG:HG3	1.86	0.40
1:B:934:ASN:OD1	1:B:934:ASN:N	2.54	0.40
1:E:602:MET:HB2	1:E:619:ALA:HB3	2.04	0.40
1:B:408:LEU:O	1:B:411:LEU:N	2.54	0.40
1:B:782:LYS:HA	1:B:783:PRO:HD3	1.97	0.40
2:Y:179:LEU:HA	2:Y:180:PRO:HD3	1.82	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	B	608/618 (98%)	563 (93%)	45 (7%)	0	100	100
1	E	594/618 (96%)	554 (93%)	40 (7%)	0	100	100
2	X	323/349 (93%)	280 (87%)	43 (13%)	0	100	100
2	Y	323/349 (93%)	279 (86%)	44 (14%)	0	100	100
All	All	1848/1934 (96%)	1676 (91%)	172 (9%)	0	100	100

There are no Ramachandran outliers to report.

### 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	B	539/543 (99%)	527 (98%)	12 (2%)	52	79
1	E	527/543 (97%)	518 (98%)	9 (2%)	60	83
2	X	293/306 (96%)	284 (97%)	9 (3%)	40	72
2	Y	293/306 (96%)	287 (98%)	6 (2%)	55	80
All	All	1652/1698 (97%)	1616 (98%)	36 (2%)	52	79

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	407	ARG
1	B	409	ARG
1	B	446	ARG
1	B	458	ARG
1	B	460	SER
1	B	529	ARG
1	B	546	ASP
1	B	559	TYR
1	B	588	ASN
1	B	769	VAL
1	B	776	VAL
1	B	996	SER
2	X	111	SER
2	X	133	VAL
2	X	181	HIS
2	X	235	ARG
2	X	256	ILE
2	X	264	THR
2	X	269	ASP
2	X	291	SER
2	X	322	MET
1	E	405	LYS
1	E	446	ARG
1	E	494	ARG
1	E	559	TYR
1	E	731	ASP
1	E	741	LEU
1	E	769	VAL
1	E	853	PHE
1	E	996	SER

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Mol	Chain	Res	Type
2	Y	4	GLN
2	Y	263	LEU
2	Y	269	ASP
2	Y	273	ILE
2	Y	306	ASP
2	Y	322	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	525	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 2 ligands modelled in this entry, 2 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, 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	B	612/618 (99%)	-0.01	11 (1%) 68 55	54, 84, 151, 179	0
1	E	598/618 (96%)	0.03	13 (2%) 62 48	59, 92, 147, 173	0
2	X	333/349 (95%)	0.01	2 (0%) 89 83	68, 123, 154, 162	0
2	Y	333/349 (95%)	0.23	12 (3%) 42 27	77, 130, 157, 168	0
All	All	1876/1934 (97%)	0.05	38 (2%) 65 51	54, 103, 154, 179	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	X	299	ILE	3.5
1	E	833	LEU	3.5
1	B	810	LEU	3.0
1	E	836	HIS	3.0
2	Y	195	TYR	3.0
2	Y	5	MET	3.0
1	B	812	ILE	2.9
2	Y	274	VAL	2.9
2	Y	217	TYR	2.9
2	Y	348	LEU	2.8
1	E	837	LEU	2.8
2	Y	272	VAL	2.7
2	Y	326	THR	2.7
1	E	857	LEU	2.6
1	B	977	ARG	2.6
2	Y	345	PHE	2.6
1	E	869	LEU	2.5
1	E	812	ILE	2.4
1	E	815	VAL	2.4
1	E	834	ASP	2.4
1	E	699	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	X	272	VAL	2.3
1	B	805	TYR	2.3
1	B	391	ALA	2.2
1	B	871	PRO	2.2
2	Y	30	PHE	2.2
1	E	868	GLU	2.1
1	E	870	ILE	2.1
1	B	807	ILE	2.1
1	E	858	MET	2.1
2	Y	211	ALA	2.1
1	B	809	GLN	2.1
2	Y	250	THR	2.1
1	B	808	PHE	2.0
1	B	961	ASN	2.0
1	B	874	GLU	2.0
1	E	829	TRP	2.0
2	Y	344	TYR	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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	E	1101	1/1	0.99	0.23	86,86,86,86	0
3	ZN	B	1101	1/1	1.00	0.22	83,83,83,83	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.