



# Full wwPDB X-ray Structure Validation Report

Nov 11, 2014 – 05:11 AM EST

PDB ID : 4R28  
Title : MspJI Restriction Endonuclease in Complex with 27-mer Oligonucleotide  
Authors : Horton, J.R.; Cheng, X.  
Deposited on : 2014-08-10  
Resolution : 3.06 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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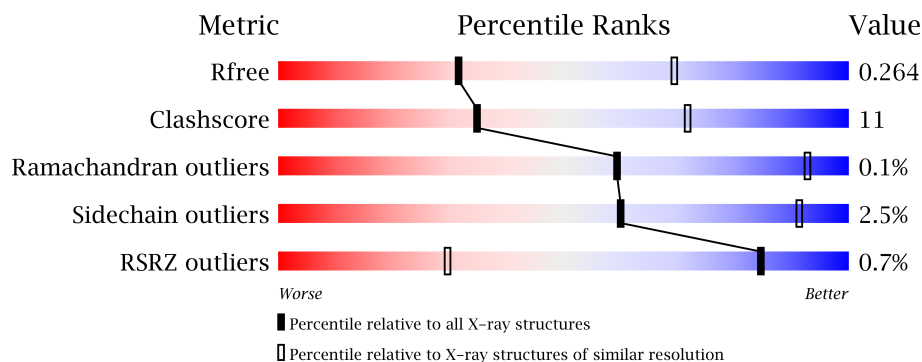
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable24103  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.1.3  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable24103

# 1 Overall quality at a glance

The reported resolution of this entry is 3.06 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))
$R_{free}$	66092	2079 (3.12-3.00)
Clashscore	79885	2629 (3.12-3.00)
Ramachandran outliers	78287	2536 (3.12-3.00)
Sidechain outliers	78261	2539 (3.12-3.00)
RSRZ outliers	66119	2081 (3.12-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	456	
1	B	456	
1	C	456	
1	D	456	
2	X	27	
3	Y	27	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14225 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Restriction endonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3263	2048	607	604	4			
1	B	447	Total	C	N	O	S	0	0	0
			3274	2051	612	606	5			
1	C	449	Total	C	N	O	S	0	0	0
			3318	2082	619	612	5			
1	D	449	Total	C	N	O	S	0	0	0
			3328	2088	625	610	5			

- Molecule 2 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	25	Total	C	N	O	P	0	0	0
			512	244	99	145	24			

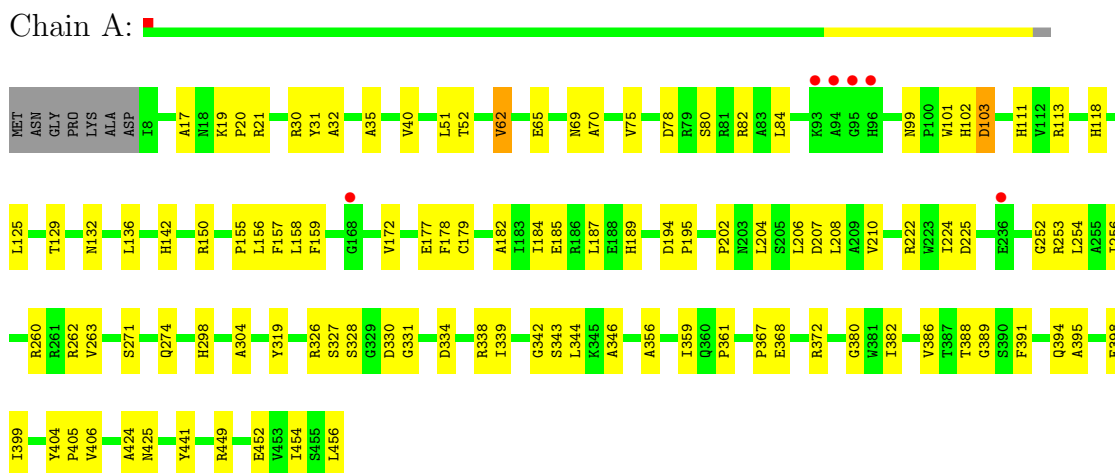
- Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	26	Total	C	N	O	P	0	0	0
			530	252	93	159	26			

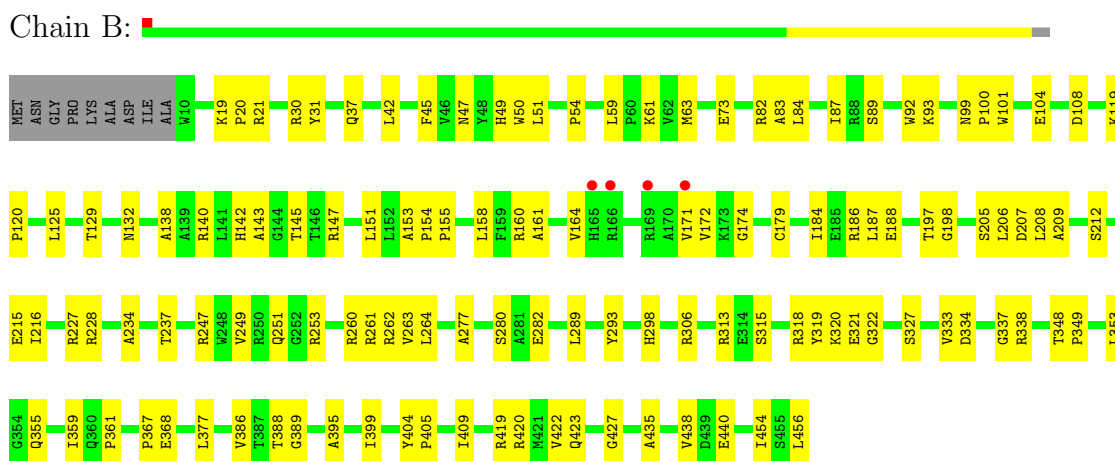
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Restriction endonuclease

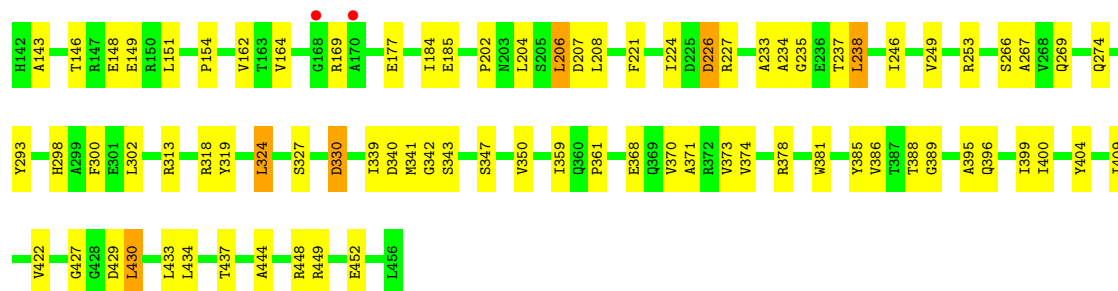


#### • Molecule 1: Restriction endonuclease



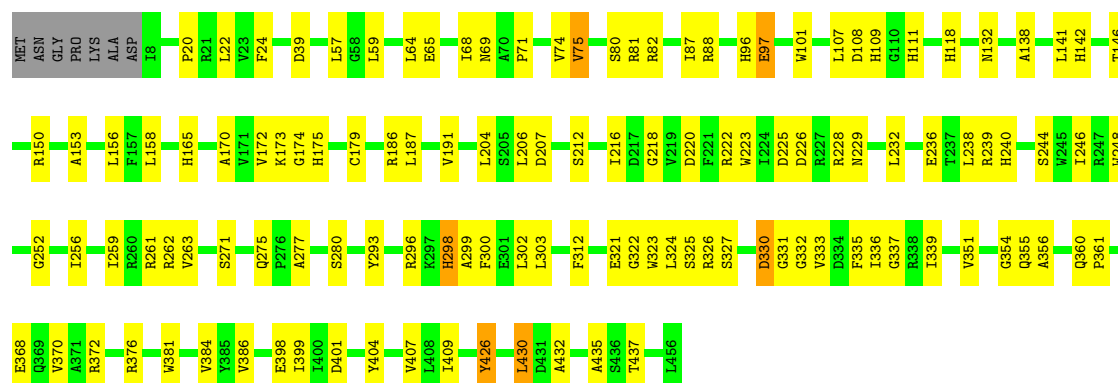
#### • Molecule 1: Restriction endonuclease





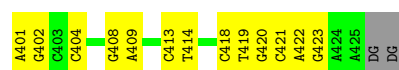
- Molecule 1: Restriction endonuclease

Chain D:



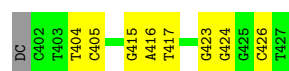
- Molecule 2: DNA (25-MER)

Chain X:



- Molecule 3: DNA (26-MER)

Chain Y:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.54Å 88.54Å 511.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.03 – 3.06 35.03 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (35.03-3.06) 98.0 (35.03-3.05)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.67 (at 3.06Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.227 , 0.258 0.234 , 0.264	Depositor DCC
$R_{free}$ test set	2091 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	79.8	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 31.5	EDS
Estimated twinning fraction	0.407 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 42615 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14225	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5CM

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	0.20	0/3332	0.37	0/4546
1	B	0.21	0/3342	0.38	0/4554
1	C	0.21	0/3386	0.38	0/4610
1	D	0.21	0/3398	0.39	0/4626
2	X	0.53	0/552	0.82	0/848
3	Y	0.51	0/592	0.88	0/911
All	All	0.25	0/14602	0.44	0/20095

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3263	0	3091	71	0
1	B	3274	0	3114	81	0
1	C	3318	0	3188	69	0
1	D	3328	0	3198	81	0
2	X	512	0	283	12	0
3	Y	530	0	294	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14225	0	13168	294	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (294) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:433:LEU:O	1:C:437:THR:HG23	1.75	0.86
1:D:322:GLY:H	1:D:337:GLY:HA2	1.53	0.72
1:B:59:LEU:HD22	1:B:228:ARG:HD3	1.72	0.72
1:C:63:MET:O	1:C:69:ASN:ND2	2.23	0.72
1:B:186:ARG:HB3	1:B:207:ASP:HB2	1.73	0.71
1:C:269:GLN:H	1:C:396:GLN:HE22	1.39	0.70
1:C:81:ARG:NH2	1:C:227:ARG:O	2.26	0.69
1:D:332:GLY:O	1:D:355:GLN:NE2	2.26	0.68
1:A:187:LEU:HD11	1:A:204:LEU:HB2	1.76	0.68
1:D:236:GLU:O	1:D:239:ARG:NH1	2.27	0.68
1:A:368:GLU:HG3	1:D:372:ARG:HD2	1.76	0.67
1:D:186:ARG:HB2	1:D:207:ASP:HB2	1.77	0.67
1:D:64:LEU:O	1:D:88:ARG:NH1	2.25	0.66
1:D:81:ARG:NH1	1:D:232:LEU:O	2.28	0.66
1:B:21:ARG:NH2	1:B:51:LEU:O	2.28	0.66
1:D:81:ARG:NH2	1:D:226:ASP:O	2.29	0.66
1:A:65:GLU:O	1:A:69:ASN:ND2	2.26	0.65
1:D:81:ARG:NH2	1:D:229:ASN:O	2.30	0.64
1:C:399:ILE:HG23	1:C:404:TYR:HB2	1.80	0.64
1:B:143:ALA:HB1	1:B:253:ARG:HH21	1.63	0.64
1:C:116:GLY:N	1:C:204:LEU:O	2.29	0.64
1:B:188:GLU:HB3	1:B:205:SER:HB3	1.79	0.64
1:C:318:ARG:NH1	1:C:342:GLY:O	2.31	0.63
1:B:37:GLN:NE2	1:B:54:PRO:O	2.32	0.63
1:D:223:TRP:HB3	1:D:240:HIS:HB2	1.81	0.62
1:D:138:ALA:O	1:D:142:HIS:ND1	2.32	0.62
1:D:74:VAL:HG21	1:D:228:ARG:HA	1.82	0.62
1:D:150:ARG:HH22	1:D:252:GLY:HA2	1.65	0.62
1:B:129:THR:OG1	1:B:132:ASN:ND2	2.32	0.62
1:A:334:ASP:OD2	1:A:356:ALA:N	2.25	0.61
1:B:99:ASN:ND2	1:B:101:TRP:O	2.33	0.61
1:B:89:SER:OG	1:B:161:ALA:N	2.27	0.60
1:B:399:ILE:HG23	1:B:404:TYR:HB2	1.81	0.60
1:C:64:LEU:HG	1:C:88:ARG:HD2	1.83	0.60
1:D:75:VAL:HA	1:D:80:SER:HA	1.82	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:103:ASP:N	1:A:103:ASP:OD1	2.34	0.60
1:A:187:LEU:HD13	1:A:206:LEU:HG	1.84	0.59
1:C:226:ASP:N	1:C:226:ASP:OD1	2.34	0.59
1:A:330:ASP:OD1	1:A:331:GLY:N	2.35	0.59
1:C:224:ILE:HA	1:C:227:ARG:HB2	1.85	0.59
1:A:319:TYR:O	1:B:260:ARG:NH2	2.33	0.59
1:B:37:GLN:HB2	1:B:61:LYS:HE2	1.83	0.59
1:A:21:ARG:NH2	1:A:51:LEU:O	2.33	0.59
1:D:324:LEU:HA	1:D:335:PHE:HA	1.84	0.59
1:D:430:LEU:H	1:D:430:LEU:HD22	1.68	0.59
1:A:368:GLU:OE2	1:D:372:ARG:NH1	2.36	0.58
1:A:75:VAL:HA	1:A:80:SER:HA	1.84	0.58
1:D:212:SER:N	1:D:259:ILE:O	2.36	0.58
1:D:20:PRO:HB3	1:D:222:ARG:HH21	1.68	0.58
1:D:354:GLY:HA2	1:D:384:VAL:HG13	1.86	0.58
1:B:320:LYS:NZ	1:B:456:LEU:O	2.31	0.57
1:C:146:THR:HB	1:C:149:GLU:HG2	1.85	0.57
1:A:449:ARG:HH22	1:D:111:HIS:HB3	1.69	0.57
1:A:359:ILE:O	1:A:388:THR:OG1	2.23	0.57
1:D:232:LEU:HD21	1:D:239:ARG:HH22	1.70	0.57
1:B:262:ARG:NH1	1:B:263:VAL:O	2.38	0.56
1:B:84:LEU:H	1:B:227:ARG:HH22	1.53	0.56
1:C:361:PRO:HA	1:C:389:GLY:HA2	1.87	0.56
1:C:302:LEU:HD23	1:C:437:THR:HB	1.86	0.56
1:C:448:ARG:NH1	1:C:452:GLU:OE2	2.38	0.56
1:D:57:LEU:HD11	1:D:225:ASP:HB3	1.86	0.56
1:D:24:PHE:HD1	1:D:218:GLY:HA3	1.70	0.56
1:A:254:LEU:O	1:B:306:ARG:NH1	2.38	0.56
1:A:202:PRO:HB3	1:B:140:ARG:HD3	1.88	0.56
1:B:89:SER:HB3	1:B:160:ARG:HA	1.87	0.56
1:A:32:ALA:HB3	1:A:35:ALA:HB2	1.88	0.56
1:C:169:ARG:NH1	3:Y:416:DA:OP2	2.38	0.56
1:B:158:LEU:HB2	1:B:179:CYS:HB2	1.87	0.56
1:D:262:ARG:NH2	1:D:401:ASP:OD2	2.39	0.56
1:B:100:PRO:HG3	1:B:423:GLN:HG3	1.87	0.56
1:D:298:HIS:NE2	1:D:327:SER:O	2.39	0.56
1:A:262:ARG:NH1	1:A:263:VAL:O	2.39	0.55
1:B:30:ARG:NH1	1:B:31:TYR:O	2.39	0.55
1:A:343:SER:OG	1:A:344:LEU:N	2.40	0.55
1:C:313:ARG:NH1	1:C:319:TYR:O	2.40	0.55
1:C:81:ARG:HH22	1:C:227:ARG:HA	1.72	0.55
1:A:361:PRO:HA	1:A:389:GLY:HA2	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:57:LEU:HB3	1:C:59:LEU:HD23	1.90	0.54
3:Y:416:DA:H2"	3:Y:417:DT:H5"	1.89	0.54
1:A:398:GLU:OE2	1:D:376:ARG:NH1	2.40	0.54
1:A:111:HIS:CE1	1:B:318:ARG:HH12	2.26	0.54
1:B:338:ARG:NH1	1:B:454:ILE:O	2.41	0.54
1:B:197:THR:N	1:B:198:GLY:HA2	2.24	0.53
1:C:118:HIS:ND1	1:C:202:PRO:O	2.41	0.53
1:B:367:PRO:HB3	1:B:395:ALA:HA	1.89	0.53
1:B:277:ALA:HB3	1:B:280:SER:HB3	1.90	0.53
1:A:125:LEU:HD23	1:A:125:LEU:H	1.74	0.53
1:A:449:ARG:NH2	1:D:109:HIS:HB2	2.24	0.53
1:C:359:ILE:O	1:C:388:THR:OG1	2.24	0.53
1:D:293:TYR:HB3	1:D:300:PHE:HB2	1.90	0.53
1:A:326:ARG:CZ	1:A:331:GLY:HA3	2.38	0.53
1:B:87:ILE:HD13	1:B:158:LEU:HD23	1.89	0.53
1:D:107:LEU:HB3	1:D:261:ARG:HH21	1.74	0.53
1:D:172:VAL:O	1:D:173:LYS:HB2	2.08	0.53
1:A:184:ILE:HA	1:A:208:LEU:HB3	1.92	0.52
1:B:361:PRO:HA	1:B:389:GLY:HA2	1.91	0.52
1:C:238:LEU:HD21	1:C:249:VAL:HG21	1.90	0.52
2:X:413:DC:H2"	2:X:414:DT:O5'	2.09	0.52
2:X:418:DC:H2"	2:X:419:DT:C5	2.44	0.52
1:A:189:HIS:HB3	1:B:187:LEU:HD22	1.91	0.52
1:D:330:ASP:OD1	1:D:330:ASP:N	2.43	0.52
1:A:372:ARG:HD2	1:D:368:GLU:HB3	1.91	0.52
1:B:30:ARG:NH1	1:B:174:GLY:O	2.41	0.52
1:C:237:THR:HG23	1:C:238:LEU:HD13	1.92	0.52
1:A:425:ASN:OD1	1:B:253:ARG:N	2.43	0.52
1:C:71:PRO:O	1:C:82:ARG:NH1	2.38	0.52
1:D:68:ILE:HG22	1:D:87:ILE:HG23	1.92	0.52
1:C:430:LEU:O	1:C:434:LEU:HG	2.09	0.51
2:X:423:DG:H1	3:Y:405:DC:H42	1.57	0.51
1:D:244:SER:HB3	1:D:259:ILE:HB	1.92	0.51
1:D:426:TYR:HE1	1:D:430:LEU:HD13	1.76	0.51
1:B:104:GLU:OE2	1:B:420:ARG:NH2	2.42	0.51
1:C:340:ASP:HB3	1:C:347:SER:HB2	1.92	0.50
1:B:386:VAL:HG22	1:B:409:ILE:HD12	1.93	0.50
1:C:69:ASN:O	1:C:86:ALA:N	2.44	0.50
1:B:30:ARG:HG2	1:B:42:LEU:HB3	1.92	0.50
1:C:298:HIS:NE2	1:C:327:SER:O	2.44	0.50
1:C:206:LEU:HD13	1:C:208:LEU:HD21	1.94	0.50
1:C:422:VAL:O	1:C:427:GLY:N	2.41	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:233:ALA:O	1:C:235:GLY:N	2.45	0.50
1:C:396:GLN:O	1:C:400:ILE:HG12	2.12	0.50
2:X:404:DC:N4	3:Y:423:DG:O6	2.45	0.50
1:B:108:ASP:HA	1:B:263:VAL:HB	1.94	0.49
1:B:184:ILE:HG23	1:B:206:LEU:HD11	1.93	0.49
1:D:141:LEU:HD23	1:D:153:ALA:HA	1.93	0.49
1:D:22:LEU:HG	1:D:220:ASP:HB3	1.95	0.49
1:D:296:ARG:HG3	1:D:299:ALA:H	1.77	0.49
1:A:298:HIS:CD2	1:A:327:SER:HA	2.47	0.49
1:A:182:ALA:HB2	1:A:210:VAL:HG22	1.95	0.49
1:A:158:LEU:HB2	1:A:179:CYS:HB2	1.94	0.49
1:A:406:VAL:O	1:B:348:THR:OG1	2.24	0.48
1:C:185:GLU:N	1:C:207:ASP:O	2.42	0.48
1:A:21:ARG:NH1	1:A:225:ASP:OD2	2.46	0.48
1:A:338:ARG:HH11	1:A:454:ILE:HA	1.79	0.48
1:A:449:ARG:HB2	1:A:452:GLU:HG3	1.93	0.48
1:B:186:ARG:NH1	1:B:207:ASP:OD2	2.46	0.48
1:C:92:TRP:N	1:C:93:LYS:HA	2.28	0.48
1:A:150:ARG:HD3	1:A:252:GLY:HA2	1.94	0.48
1:C:30:ARG:NH2	1:C:43:ASP:OD2	2.46	0.48
1:B:298:HIS:NE2	1:B:327:SER:O	2.46	0.48
1:B:83:ALA:HA	1:B:227:ARG:HH12	1.79	0.48
1:D:325:SER:OG	1:D:333:VAL:O	2.31	0.48
1:A:380:GLY:HA3	1:B:405:PRO:HG3	1.95	0.48
1:D:398:GLU:HG2	1:D:404:TYR:HE2	1.78	0.48
1:D:238:LEU:HD23	1:D:246:ILE:HG22	1.95	0.48
1:A:84:LEU:HD11	1:A:224:ILE:HG23	1.96	0.48
1:A:382:ILE:HG22	1:A:405:PRO:HB2	1.96	0.48
1:A:319:TYR:HD1	1:A:339:ILE:HG12	1.77	0.48
1:B:92:TRP:N	1:B:93:LYS:HA	2.29	0.47
1:C:339:ILE:HB	1:C:350:VAL:HB	1.95	0.47
1:D:277:ALA:O	1:D:280:SER:OG	2.22	0.47
1:A:84:LEU:HD11	1:A:224:ILE:HD12	1.96	0.47
1:A:99:ASN:O	1:A:102:HIS:ND1	2.34	0.47
1:B:322:GLY:H	1:B:337:GLY:HA2	1.79	0.47
1:D:158:LEU:HB2	1:D:179:CYS:HB2	1.96	0.47
1:D:187:LEU:HD12	1:D:206:LEU:HD11	1.95	0.47
1:D:71:PRO:O	1:D:82:ARG:NH1	2.46	0.47
1:B:154:PRO:HA	1:B:155:PRO:HD3	1.82	0.47
1:C:141:LEU:HD12	1:C:154:PRO:HD3	1.95	0.47
1:D:312:PHE:HB3	1:D:339:ILE:HD11	1.96	0.47
2:X:419:DT:H2'	2:X:420:DG:C8	2.48	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:342:GLY:O	1:B:315:SER:OG	2.26	0.47
1:D:432:ALA:HA	1:D:435:ALA:HB3	1.96	0.47
1:B:99:ASN:HD21	1:B:101:TRP:HB2	1.80	0.47
1:C:371:ALA:HA	1:C:374:VAL:HG22	1.97	0.47
1:D:335:PHE:CE2	1:D:354:GLY:HA3	2.50	0.47
1:A:424:ALA:HA	1:B:145:THR:HG22	1.96	0.47
1:B:138:ALA:O	1:B:142:HIS:ND1	2.29	0.46
1:D:312:PHE:HE1	1:D:407:VAL:HG21	1.80	0.46
1:C:37:GLN:NE2	1:C:53:SER:O	2.45	0.46
1:A:30:ARG:NH1	1:A:31:TYR:O	2.47	0.46
1:B:349:PRO:HG3	1:B:454:ILE:HG23	1.96	0.46
2:X:421:DC:H2'	2:X:422:DA:C8	2.51	0.46
2:X:414:DT:O2	3:Y:415:DG:N2	2.48	0.46
1:C:72:ALA:HB2	3:Y:426:DC:H5'	1.96	0.46
1:C:274:GLN:NE2	1:C:396:GLN:OE1	2.48	0.46
1:D:271:SER:O	1:D:275:GLN:NE2	2.48	0.46
1:C:293:TYR:HB3	1:C:300:PHE:HD2	1.81	0.46
1:B:359:ILE:O	1:B:388:THR:OG1	2.21	0.46
1:A:17:ALA:O	1:A:222:ARG:NH1	2.49	0.46
1:C:70:ALA:HB3	1:C:134:LEU:HD13	1.98	0.46
1:B:264:LEU:N	1:D:191:VAL:O	2.48	0.46
1:D:323:TRP:O	1:D:335:PHE:HB2	2.16	0.46
1:B:184:ILE:HA	1:B:208:LEU:HD23	1.98	0.45
1:C:324:LEU:HB3	1:C:444:ALA:HB2	1.98	0.45
1:B:247:ARG:HE	1:B:251:GLN:NE2	2.14	0.45
1:B:353:LEU:HD13	1:B:377:LEU:HD23	1.99	0.45
1:C:126:PRO:HA	1:C:127:GLY:HA2	1.69	0.45
1:C:64:LEU:HD11	1:C:88:ARG:HB2	1.98	0.45
1:D:108:ASP:HA	1:D:263:VAL:HB	1.99	0.45
1:D:336:ILE:HD11	1:D:351:VAL:HG13	1.99	0.45
2:X:423:DG:H1	3:Y:405:DC:N4	2.13	0.45
2:X:413:DC:H4'	2:X:414:DT:OP1	2.16	0.45
1:D:370:VAL:HG11	1:D:399:ILE:HD11	1.97	0.45
1:C:378:ARG:H	1:C:381:TRP:HB2	1.81	0.45
1:A:136:LEU:HD12	1:B:125:LEU:HD13	1.99	0.45
1:B:368:GLU:HB3	1:C:368:GLU:HB3	1.99	0.45
1:C:47:ASN:OD1	1:C:50:TRP:N	2.45	0.45
1:A:274:GLN:HE22	1:A:391:PHE:HD2	1.65	0.44
1:D:24:PHE:CD1	1:D:218:GLY:HA3	2.52	0.44
1:D:256:ILE:HA	1:D:259:ILE:HG12	2.00	0.44
1:B:212:SER:HB2	1:B:261:ARG:HA	2.00	0.44
1:C:422:VAL:HG22	1:C:433:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:303:LEU:HB2	1:D:437:THR:HG21	2.00	0.44
1:D:87:ILE:HD11	1:D:156:LEU:HD23	1.98	0.44
1:B:333:VAL:HG21	1:B:353:LEU:HD23	1.99	0.44
1:C:330:ASP:OD1	1:C:330:ASP:N	2.51	0.44
1:A:298:HIS:CG	1:A:327:SER:HA	2.53	0.44
1:A:118:HIS:HB2	1:A:132:ASN:HD21	1.81	0.44
1:D:226:ASP:OD2	1:D:239:ARG:NH2	2.51	0.44
1:D:300:PHE:CE2	1:D:356:ALA:HB1	2.53	0.44
1:A:142:HIS:CE1	1:A:156:LEU:HD13	2.53	0.43
1:C:395:ALA:O	1:C:399:ILE:HG13	2.17	0.43
1:C:370:VAL:HG11	1:C:399:ILE:HD11	2.00	0.43
1:B:313:ARG:NH2	1:B:319:TYR:O	2.51	0.43
1:C:449:ARG:HG2	1:C:449:ARG:H	1.59	0.43
1:C:96:HIS:HA	1:C:102:HIS:CB	2.48	0.43
1:B:422:VAL:O	1:B:427:GLY:N	2.52	0.43
1:B:30:ARG:HB2	1:B:45:PHE:HB2	2.00	0.43
1:C:234:ALA:O	1:C:237:THR:HG22	2.18	0.43
1:D:165:HIS:HA	1:D:170:ALA:HA	2.01	0.43
1:C:429:ASP:N	1:C:429:ASP:OD1	2.52	0.43
1:D:65:GLU:H	1:D:69:ASN:ND2	2.16	0.43
1:A:70:ALA:HB1	1:A:82:ARG:HH21	1.83	0.43
1:B:147:ARG:HG3	1:B:249:VAL:HG12	2.00	0.43
1:C:318:ARG:NH1	1:C:347:SER:HB3	2.33	0.43
1:C:386:VAL:HA	1:C:409:ILE:HB	2.01	0.43
1:A:253:ARG:HA	1:A:256:ILE:HG13	2.00	0.43
1:B:334:ASP:HB2	1:B:355:GLN:HA	2.01	0.43
1:B:49:HIS:NE2	1:B:63:MET:SD	2.87	0.43
1:A:113:ARG:HH21	1:B:318:ARG:HH21	1.67	0.42
3:Y:404:DT:H4'	3:Y:405:DC:OP1	2.19	0.42
1:B:47:ASN:HB3	1:B:50:TRP:HB3	2.00	0.42
1:C:143:ALA:HA	1:C:253:ARG:HD2	2.00	0.42
1:C:266:SER:OG	1:C:267:ALA:N	2.53	0.42
1:C:36:ASN:OD1	1:C:37:GLN:N	2.52	0.42
1:D:248:TRP:HB2	1:D:259:ILE:HD13	2.00	0.42
1:D:59:LEU:HB3	1:D:228:ARG:HH21	1.84	0.42
1:D:187:LEU:HD11	1:D:204:LEU:HD23	2.02	0.42
1:A:367:PRO:HB3	1:A:395:ALA:HA	2.01	0.42
1:B:215:GLU:HG2	1:B:216:ILE:HG23	2.01	0.42
1:B:19:LYS:HA	1:B:20:PRO:HD3	1.79	0.42
1:A:159:PHE:HA	1:A:177:GLU:O	2.20	0.42
1:A:52:THR:HG21	1:A:62:VAL:HG11	2.02	0.42
1:B:234:ALA:O	1:B:237:THR:HG22	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:174:GLY:C	1:D:175:HIS:ND1	2.73	0.42
2:X:404:DC:H42	3:Y:424:DG:H1	1.68	0.42
1:B:151:LEU:HB3	1:B:249:VAL:HG11	2.02	0.42
1:C:341:MET:O	1:C:347:SER:HA	2.20	0.42
1:B:73:GLU:HG3	1:B:82:ARG:CZ	2.50	0.42
1:B:84:LEU:HB3	1:B:227:ARG:NH2	2.35	0.42
1:D:326:ARG:NH1	1:D:331:GLY:HA3	2.35	0.42
1:A:343:SER:N	1:A:346:ALA:O	2.53	0.41
1:B:171:VAL:HA	1:B:172:VAL:HA	1.64	0.41
1:C:238:LEU:HG	1:C:246:ILE:HG22	2.02	0.41
1:A:404:TYR:OH	1:D:376:ARG:HD3	2.19	0.41
1:A:101:TRP:CZ2	1:A:424:ALA:HB2	2.55	0.41
1:A:101:TRP:HZ2	1:A:424:ALA:HB2	1.86	0.41
1:B:142:HIS:CE1	1:B:153:ALA:HB1	2.55	0.41
1:D:107:LEU:HD21	1:D:179:CYS:HB3	2.02	0.41
1:D:386:VAL:HA	1:D:409:ILE:HB	2.02	0.41
3:Y:423:DG:H2'	3:Y:424:DG:C8	2.55	0.41
1:A:19:LYS:HA	1:A:20:PRO:HD3	1.88	0.41
1:B:209:ALA:HB1	1:B:260:ARG:HG2	2.01	0.41
1:A:456:LEU:HA	1:B:262:ARG:HG2	2.02	0.41
1:B:282:GLU:HG3	1:B:419:ARG:HH11	1.85	0.41
1:B:289:LEU:HD22	1:B:293:TYR:HE2	1.86	0.41
1:A:394:GLN:NE2	1:A:398:GLU:OE1	2.53	0.41
1:D:39:ASP:OD1	1:D:39:ASP:N	2.53	0.41
1:A:157:PHE:HD2	1:A:178:PHE:HE1	1.68	0.41
1:C:148:GLU:HA	1:C:151:LEU:HD12	2.02	0.41
1:A:344:LEU:HD22	1:B:104:GLU:HB3	2.03	0.41
1:B:119:LYS:HA	1:B:120:PRO:HD3	1.94	0.41
1:B:435:ALA:HA	1:B:438:VAL:HG22	2.03	0.41
1:C:184:ILE:HA	1:C:208:LEU:HD23	2.02	0.41
1:A:399:ILE:HG23	1:A:404:TYR:HB2	2.02	0.41
1:D:229:ASN:HB3	1:D:232:LEU:HB2	2.02	0.41
1:D:96:HIS:HA	1:D:97:GLU:HA	1.67	0.41
1:D:118:HIS:HB2	1:D:132:ASN:HD21	1.86	0.41
1:D:351:VAL:HB	1:D:381:TRP:CD1	2.56	0.41
2:X:401:DA:H2''	2:X:402:DG:C8	2.56	0.41
1:A:84:LEU:HD23	1:A:155:PRO:HD2	2.02	0.40
1:C:373:VAL:HG21	1:C:385:TYR:HD2	1.87	0.40
1:D:302:LEU:HD23	1:D:437:THR:HA	2.02	0.40
1:A:185:GLU:OE1	1:A:260:ARG:NH1	2.52	0.40
1:A:304:ALA:HB1	1:A:386:VAL:HB	2.03	0.40
1:D:325:SER:OG	1:D:326:ARG:N	2.54	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:360:GLN:HA	1:D:361:PRO:HD3	1.93	0.40
1:C:111:HIS:HE1	1:C:207:ASP:HB3	1.85	0.40
1:C:162:VAL:HG12	1:C:177:GLU:HB2	2.04	0.40
1:C:70:ALA:HA	1:C:71:PRO:HD3	1.91	0.40
1:D:271:SER:OG	1:D:275:GLN:NE2	2.54	0.40
2:X:408:DG:H2'	2:X:409:DA:C8	2.56	0.40
1:A:194:ASP:HA	1:A:195:PRO:HD3	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	447/456 (98%)	437 (98%)	10 (2%)	0	100	100
1	B	445/456 (98%)	428 (96%)	16 (4%)	1 (0%)	56	91
1	C	447/456 (98%)	427 (96%)	19 (4%)	1 (0%)	56	91
1	D	447/456 (98%)	431 (96%)	16 (4%)	0	100	100
All	All	1786/1824 (98%)	1723 (96%)	61 (3%)	2 (0%)	59	93

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	164	VAL
1	B	164	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	305/358 (85%)	295 (97%)	10 (3%)	50	88
1	B	308/358 (86%)	306 (99%)	2 (1%)	92	98
1	C	316/358 (88%)	307 (97%)	9 (3%)	56	90
1	D	317/358 (88%)	307 (97%)	10 (3%)	51	88
All	All	1246/1432 (87%)	1215 (98%)	31 (2%)	60	91

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	VAL
1	A	62	VAL
1	A	78	ASP
1	A	103	ASP
1	A	129	THR
1	A	172	VAL
1	A	207	ASP
1	A	271	SER
1	A	328	SER
1	A	441	TYR
1	B	321	GLU
1	B	440	GLU
1	C	81	ARG
1	C	206	LEU
1	C	221	PHE
1	C	226	ASP
1	C	238	LEU
1	C	324	LEU
1	C	330	ASP
1	C	343	SER
1	C	430	LEU
1	D	75	VAL
1	D	97	GLU
1	D	101	TRP
1	D	146	THR
1	D	216	ILE
1	D	298	HIS
1	D	321	GLU
1	D	330	ASP
1	D	426	TYR
1	D	430	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such



sidechains are listed below:

Mol	Chain	Res	Type
1	C	274	GLN
1	C	396	GLN
1	D	192	GLN
1	D	275	GLN
1	D	355	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	5CM	X	405	2	19,21,22	1.79	4 (21%)	24,30,33	1.67	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5CM	X	405	2	-	0/5/21/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	405	5CM	C5-C4	4.63	1.48	1.41
2	X	405	5CM	P-OP1	4.03	1.51	1.46
2	X	405	5CM	C2-N1	3.31	1.42	1.38
2	X	405	5CM	O2-C2	2.80	1.25	1.21

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	405	5CM	C2-N3-C4	5.49	120.76	115.50
2	X	405	5CM	C6-N1-C2	2.83	120.89	118.86
2	X	405	5CM	N4-C4-N3	2.67	120.80	116.99
2	X	405	5CM	C5-C6-N1	-2.34	119.91	122.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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(Å²)	Q<0.9
1	A	449/456 (98%)	-0.17	6 (1%)	74	19	47, 91, 154, 281	0
1	B	447/456 (98%)	-0.20	4 (0%)	81	24	43, 92, 147, 189	0
1	C	449/456 (98%)	-0.18	2 (0%)	90	42	58, 93, 148, 243	0
1	D	449/456 (98%)	-0.21	0	100	100	58, 92, 135, 200	0
2	X	25/27 (92%)	-0.73	0	100	100	77, 95, 113, 127	0
3	Y	26/27 (96%)	-0.76	0	100	100	72, 94, 123, 140	0
All	All	1845/1878 (98%)	-0.21	12 (0%)	84	30	43, 92, 149, 281	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	93	LYS	5.0
1	C	168	GLY	4.7
1	A	96	HIS	4.4
1	A	168	GLY	3.5
1	A	95	GLY	3.5
1	B	165	HIS	3.4
1	B	169	ARG	2.9
1	C	170	ALA	2.8
1	A	94	ALA	2.7
1	A	236	GLU	2.5
1	B	171	VAL	2.2
1	B	166	ARG	2.2

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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	5CM	X	405	20/21	0.14	-1.48	69,83,87,88	0

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

There are no ligands in this entry.

### 6.5 Other polymers

There are no such residues in this entry.