



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 11:01 AM EDT

PDB ID : 5OKI  
Title : Crystal structure of the Ctf18-1-8 module from Ctf18-RFC in complex with a 63 kDa fragment of DNA Polymerase epsilon  
Authors : Grabarczyk, D.B.; Kisker, C.  
Deposited on : 2017-07-25  
Resolution : 4.50 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

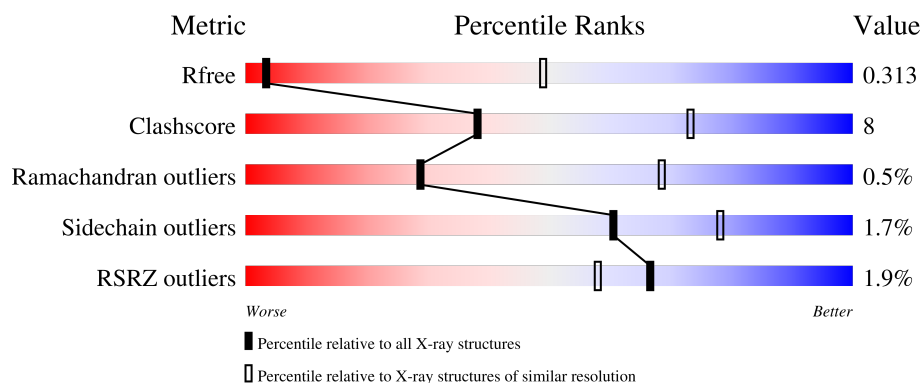
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

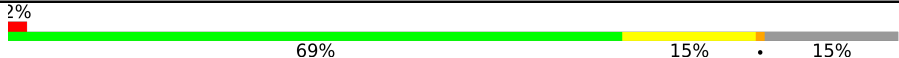

The reported resolution of this entry is 4.50 Å.

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	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	524	
1	B	524	
2	C	380	
2	G	380	
3	D	133	

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Mol	Chain	Length	Quality of chain
3	H	133	<div><div></div><div>2%82%17%•</div></div>
4	E	26	<div><div></div><div>92%8%</div></div>
4	I	26	<div><div></div><div>85%12%•</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15910 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 DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3575	2303	572	681	19			
1	B	468	Total	C	N	O	S	0	0	0
			3759	2417	610	713	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	ALA	ASP	engineered mutation	UNP P21951
A	292	ALA	GLU	engineered mutation	UNP P21951
B	290	ALA	ASP	engineered mutation	UNP P21951
B	292	ALA	GLU	engineered mutation	UNP P21951

- Molecule 2 is a protein called Sister chromatid cohesion protein DCC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	367	Total	C	N	O	S	0	0	0
			2995	1930	503	548	14			
2	G	373	Total	C	N	O	S	0	0	0
			3043	1960	510	559	14			

- Molecule 3 is a protein called Chromosome transmission fidelity protein 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	131	Total	C	N	O	S	0	0	0
			1044	661	181	196	6			
3	H	131	Total	C	N	O	S	0	0	0
			1044	661	181	196	6			

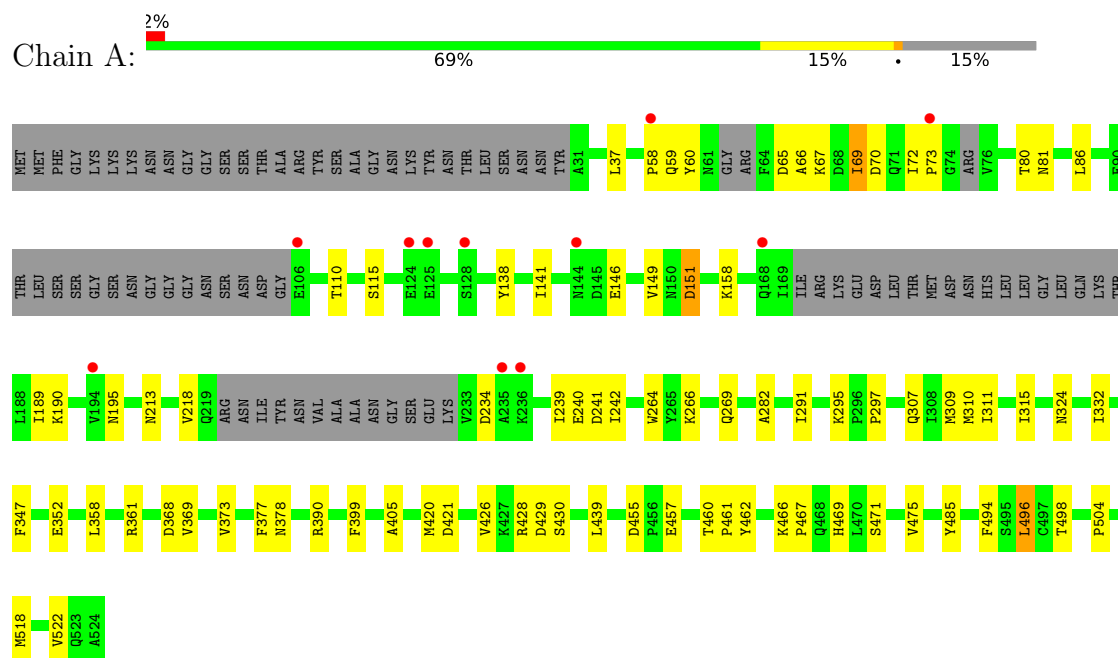
- Molecule 4 is a protein called Chromosome transmission fidelity protein 18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	26	Total	C	N	O	0	0	0
			225	148	40	37			
4	I	26	Total	C	N	O	0	0	0
			225	148	40	37			

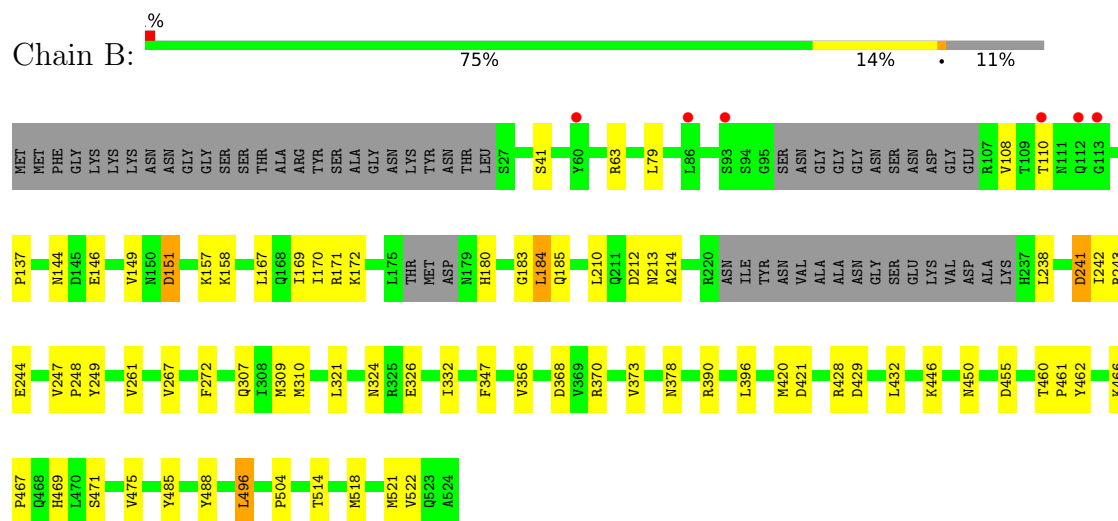
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

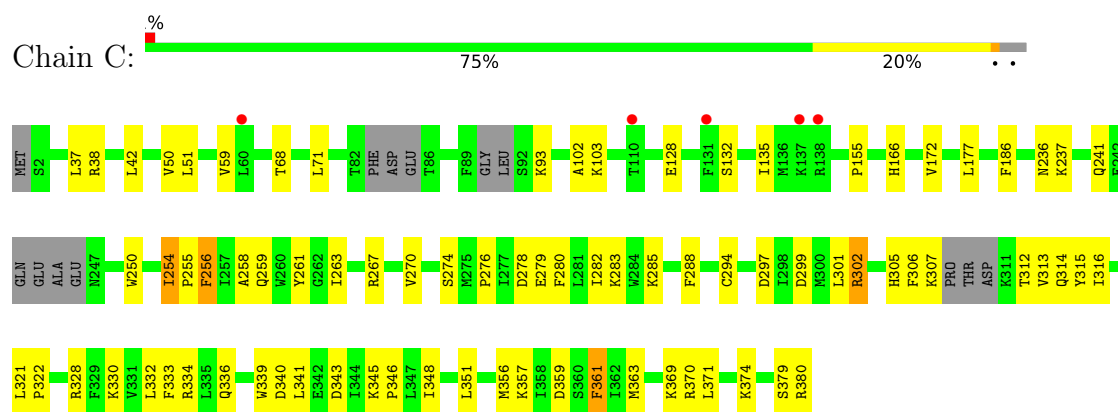
- Molecule 1: DNA polymerase epsilon catalytic subunit A



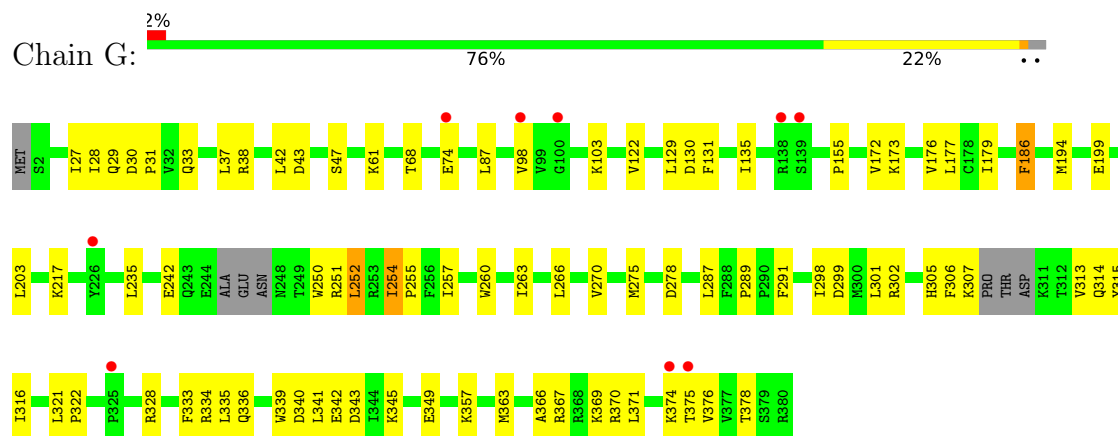
- Molecule 1: DNA polymerase epsilon catalytic subunit A



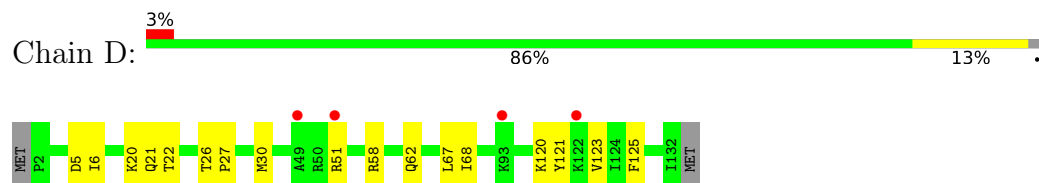
- Molecule 2: Sister chromatid cohesion protein DCC1



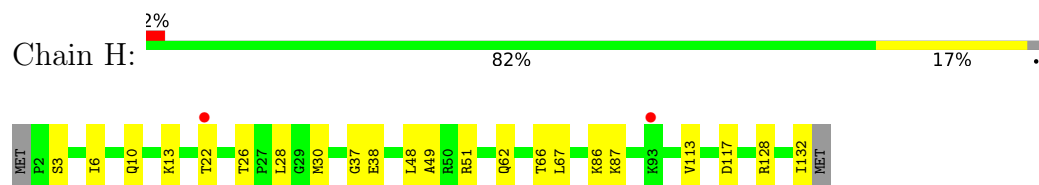
• Molecule 2: Sister chromatid cohesion protein DCC1



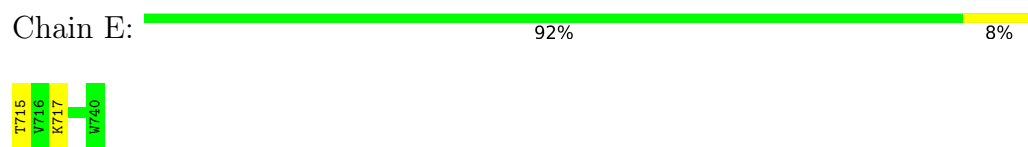
• Molecule 3: Chromosome transmission fidelity protein 8



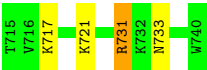
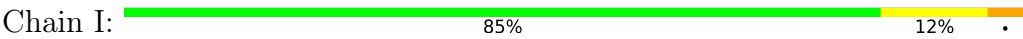
• Molecule 3: Chromosome transmission fidelity protein 8



• Molecule 4: Chromosome transmission fidelity protein 18



• Molecule 4: Chromosome transmission fidelity protein 18





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.68Å 145.83Å 378.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.72 – 4.50 47.72 – 4.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.72-4.50) 100.0 (47.72-4.50)	Depositor EDS
$R_{merge}$	0.67	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 4.45Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.293 , 0.312 0.294 , 0.313	Depositor DCC
$R_{free}$ test set	1012 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	130.3	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 82.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	15910	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	186.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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](#)

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	0.25	0/3661	0.54	0/4961
1	B	0.26	0/3849	0.53	0/5216
2	C	0.29	0/3060	0.52	0/4127
2	G	0.28	0/3111	0.53	0/4199
3	D	0.27	0/1060	0.55	0/1422
3	H	0.28	0/1060	0.54	0/1422
4	E	0.20	0/232	0.38	0/316
4	I	0.26	0/232	0.45	0/316
All	All	0.27	0/16265	0.53	0/21979

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3575	0	3441	48	0
1	B	3759	0	3623	44	1
2	C	2995	0	3027	66	0
2	G	3043	0	3068	66	1
3	D	1044	0	1078	12	0
3	H	1044	0	1078	16	0
4	E	225	0	220	1	0
4	I	225	0	220	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15910	0	15755	240	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 8.

All (240) 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:213:ASN:ND2	1:A:239:ILE:O	1.97	0.95
2:G:27:ILE:HA	2:G:33:GLN:HE22	1.40	0.84
2:G:369:LYS:HE2	2:G:378:THR:HG21	1.60	0.82
2:G:61:LYS:HB3	4:I:731:ARG:HB2	1.61	0.82
1:A:309:MET:HG3	1:A:310:MET:HG3	1.67	0.76
2:C:302:ARG:HB2	2:C:343:ASP:HA	1.67	0.76
1:B:309:MET:HG3	1:B:310:MET:HG3	1.69	0.75
3:D:21:GLN:HE21	3:D:120:LYS:HB2	1.53	0.73
3:D:21:GLN:HB3	3:D:27:PRO:HD3	1.70	0.73
2:G:302:ARG:HD3	2:G:342:GLU:HB3	1.70	0.73
1:A:426:VAL:O	1:A:430:SER:OG	2.07	0.72
2:C:341:LEU:HB3	2:C:374:LYS:HD3	1.70	0.72
2:G:194:MET:HG2	2:G:291:PHE:HE1	1.55	0.71
1:A:58:PRO:HG2	1:A:73:PRO:HB2	1.72	0.71
2:C:307:LYS:NZ	2:C:343:ASP:OD2	2.23	0.70
1:A:368:ASP:OD1	2:G:369:LYS:NZ	2.23	0.70
2:C:276:PRO:HA	2:C:312:THR:HA	1.73	0.69
2:C:186:PHE:HE1	2:C:261:TYR:CE1	2.09	0.69
2:G:298:ILE:HG23	2:G:302:ARG:NH1	2.07	0.69
1:B:370:ARG:NH1	2:C:370:ARG:O	2.27	0.68
2:C:302:ARG:HD3	2:C:346:PRO:HG3	1.76	0.66
2:G:302:ARG:HG2	2:G:343:ASP:OD1	1.95	0.66
1:A:60:TYR:N	1:A:269:GLN:OE1	2.26	0.66
2:C:254:ILE:H	2:C:255:PRO:HD2	1.59	0.66
2:G:203:LEU:HB3	2:G:252:LEU:HD21	1.78	0.66
2:C:328:ARG:HD3	2:C:351:LEU:HD13	1.77	0.66
2:G:333:PHE:HZ	2:G:366:ALA:HA	1.61	0.64
2:G:42:LEU:HD21	2:G:155:PRO:HD3	1.79	0.64
2:G:194:MET:HG2	2:G:291:PHE:CE1	2.33	0.64
3:H:48:LEU:HA	3:H:51:ARG:HG2	1.79	0.63
2:G:316:ILE:HD11	2:G:321:LEU:HD21	1.81	0.62
2:C:37:LEU:HB3	2:C:51:LEU:HD11	1.80	0.62
2:C:348:ILE:HA	2:C:351:LEU:HG	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ASN:HD21	1:A:240:GLU:HA	1.62	0.61
1:A:455:ASP:OD2	2:C:334:ARG:NH1	2.31	0.61
2:C:299:ASP:O	2:C:302:ARG:HG3	2.00	0.61
1:A:141:ILE:HG23	1:A:239:ILE:HG23	1.81	0.61
2:G:299:ASP:HA	2:G:302:ARG:HD2	1.83	0.61
2:G:68:THR:HG23	2:G:103:LYS:HE2	1.83	0.61
2:C:38:ARG:NH1	3:D:5:ASP:OD1	2.34	0.60
1:B:378:ASN:N	1:B:421:ASP:OD1	2.35	0.60
2:G:254:ILE:H	2:G:255:PRO:HD2	1.67	0.60
2:C:42:LEU:HD21	2:C:155:PRO:HD3	1.84	0.60
2:C:328:ARG:CZ	2:C:351:LEU:HD22	2.32	0.59
2:G:172:VAL:HB	2:G:177:LEU:HD23	1.85	0.58
2:G:129:LEU:HD23	2:G:130:ASP:HB2	1.85	0.58
3:D:21:GLN:NE2	3:D:121:TYR:HD1	2.02	0.58
1:A:37:LEU:HG	1:A:86:LEU:HD23	1.84	0.58
1:B:247:VAL:HG22	1:B:521:MET:HE1	1.85	0.58
2:C:306:PHE:HB2	2:C:336:GLN:OE1	2.04	0.58
2:G:336:GLN:NE2	2:G:339:TRP:HA	2.19	0.58
2:C:263:ILE:HG22	2:C:267:ARG:NH1	2.19	0.57
2:C:336:GLN:HB2	2:C:339:TRP:NE1	2.20	0.57
1:B:396:LEU:HD21	3:H:128:ARG:HH12	1.70	0.57
2:G:371:LEU:HD12	2:G:374:LYS:H	1.69	0.57
2:C:371:LEU:HD12	2:C:374:LYS:H	1.70	0.56
3:D:21:GLN:NE2	3:D:120:LYS:HB2	2.18	0.56
1:B:471:SER:O	1:B:475:VAL:HG13	2.06	0.56
2:C:302:ARG:CD	2:C:346:PRO:HG3	2.34	0.56
4:E:715:THR:OG1	4:E:717:LYS:NZ	2.37	0.56
2:G:242:GLU:OE1	2:G:251:ARG:NH2	2.39	0.56
2:C:302:ARG:HD2	2:C:302:ARG:O	2.06	0.56
1:A:471:SER:O	1:A:475:VAL:HG13	2.06	0.56
1:A:295:LYS:NZ	1:A:457:GLU:OE2	2.36	0.56
1:B:460:THR:HB	1:B:461:PRO:HD3	1.88	0.56
1:A:378:ASN:N	1:A:421:ASP:OD1	2.38	0.55
2:C:278:ASP:OD1	2:C:278:ASP:N	2.40	0.55
2:C:186:PHE:CE1	2:C:261:TYR:CE1	2.93	0.55
2:G:339:TRP:O	2:G:376:VAL:HB	2.07	0.54
2:C:270:VAL:HG23	2:C:315:TYR:HB2	1.90	0.54
2:C:322:PRO:O	2:C:328:ARG:HD2	2.08	0.54
1:B:466:LYS:HD3	1:B:469:HIS:HB2	1.90	0.54
2:G:27:ILE:HA	2:G:33:GLN:NE2	2.18	0.53
1:A:460:THR:HB	1:A:461:PRO:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:322:PRO:O	2:G:328:ARG:NH1	2.38	0.53
3:H:38:GLU:HB2	4:I:721:LYS:HB3	1.90	0.53
1:A:466:LYS:HD3	1:A:469:HIS:HB2	1.90	0.53
3:D:20:LYS:HD3	3:D:120:LYS:NZ	2.23	0.53
1:B:446:LYS:O	1:B:488:TYR:OH	2.23	0.53
2:C:316:ILE:HD11	2:C:321:LEU:HD21	1.90	0.53
2:G:278:ASP:OD1	2:G:278:ASP:N	2.42	0.52
1:B:184:LEU:HD23	1:B:185:GLN:H	1.74	0.52
2:C:37:LEU:HB2	3:D:6:ILE:HD12	1.91	0.52
2:G:135:ILE:HD13	2:G:176:VAL:HG21	1.90	0.52
2:C:166:HIS:CG	2:C:236:ASN:HB3	2.45	0.52
3:D:62:GLN:HB2	3:D:67:LEU:HD11	1.91	0.52
1:A:59:GLN:CD	1:A:59:GLN:H	2.13	0.52
2:C:68:THR:HG23	2:C:103:LYS:HE2	1.92	0.52
1:B:368:ASP:OD1	2:C:369:LYS:HG3	2.10	0.51
2:G:68:THR:OG1	3:H:37:GLY:O	2.19	0.51
1:B:241:ASP:OD1	1:B:242:ILE:N	2.37	0.51
2:G:74:GLU:HA	2:G:98:VAL:HG12	1.91	0.51
2:G:307:LYS:NZ	2:G:343:ASP:OD2	2.43	0.51
1:B:146:GLU:HA	1:B:149:VAL:HG23	1.92	0.51
2:G:27:ILE:HG22	2:G:37:LEU:HD21	1.90	0.51
2:C:172:VAL:HB	2:C:177:LEU:HD23	1.93	0.51
1:B:356:VAL:HG21	3:H:128:ARG:HD3	1.93	0.51
2:C:258:ALA:HB1	2:C:294:CYS:SG	2.51	0.51
2:C:330:LYS:O	2:C:334:ARG:HG3	2.11	0.51
2:C:332:LEU:HD22	2:C:339:TRP:CH2	2.46	0.51
1:B:518:MET:O	1:B:522:VAL:HG23	2.10	0.50
1:A:70:ASP:HA	1:A:266:LYS:HZ2	1.76	0.50
1:A:377:PHE:CD2	1:A:439:LEU:HD13	2.46	0.50
2:C:302:ARG:HD2	2:C:302:ARG:C	2.31	0.50
2:C:341:LEU:HB3	2:C:374:LYS:CD	2.39	0.50
2:G:266:LEU:HB3	2:G:315:TYR:CD1	2.46	0.50
1:B:420:MET:HE3	1:B:504:PRO:HB2	1.94	0.50
2:C:285:LYS:O	2:C:288:PHE:CE1	2.65	0.50
2:G:305:HIS:ND1	2:G:313:VAL:HG23	2.27	0.50
1:B:243:ARG:HE	1:B:243:ARG:HA	1.77	0.49
1:B:247:VAL:HG22	1:B:521:MET:CE	2.41	0.49
2:C:328:ARG:CD	2:C:351:LEU:HD13	2.42	0.49
1:A:399:PHE:HD2	1:A:405:ALA:HB2	1.77	0.49
1:B:144:ASN:OD1	1:B:238:LEU:HB3	2.13	0.49
1:B:307:GLN:HG2	1:B:390:ARG:NH2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:HIS:O	1:B:180:HIS:ND1	2.46	0.49
1:A:213:ASN:ND2	1:A:240:GLU:HA	2.27	0.49
1:A:462:TYR:O	1:A:466:LYS:N	2.39	0.49
2:G:341:LEU:HB2	2:G:375:THR:O	2.13	0.49
3:H:86:LYS:HB2	3:H:87:LYS:HD2	1.94	0.48
2:C:301:LEU:O	2:C:305:HIS:HD2	1.96	0.48
2:C:340:ASP:OD1	2:C:374:LYS:HD2	2.14	0.48
2:G:287:LEU:O	2:G:287:LEU:HD23	2.14	0.48
1:B:79:LEU:HG	1:B:261:VAL:HG22	1.96	0.47
1:A:291:ILE:HG22	1:A:311:ILE:HG12	1.95	0.47
1:A:146:GLU:O	1:A:149:VAL:HG23	2.15	0.47
2:G:61:LYS:NZ	4:I:733:ASN:OD1	2.48	0.47
3:H:87:LYS:HD3	4:I:717:LYS:HG2	1.97	0.47
1:B:514:THR:O	1:B:518:MET:HG2	2.14	0.47
1:A:373:VAL:HG11	1:A:485:TYR:CZ	2.50	0.47
2:C:71:LEU:HB2	2:C:102:ALA:HB3	1.96	0.47
2:G:199:GLU:OE2	2:G:217:LYS:HE2	2.15	0.47
3:H:48:LEU:HD23	3:H:51:ARG:HD3	1.97	0.47
1:B:332:ILE:HD11	1:B:467:PRO:HB2	1.96	0.47
1:A:352:GLU:OE2	1:A:361:ARG:NE	2.47	0.46
1:B:347:PHE:CE2	1:B:475:VAL:HB	2.50	0.46
2:C:297:ASP:O	2:C:301:LEU:HG	2.16	0.46
2:C:278:ASP:O	2:C:282:ILE:HG13	2.16	0.46
2:G:336:GLN:HB3	2:G:339:TRP:CE2	2.50	0.46
1:A:297:PRO:HD3	2:C:314:GLN:HE22	1.81	0.46
2:C:259:GLN:O	2:C:263:ILE:HG13	2.16	0.46
2:G:301:LEU:O	2:G:302:ARG:HG3	2.16	0.46
1:A:65:ASP:OD1	1:A:66:ALA:N	2.49	0.45
1:A:332:ILE:HD11	1:A:467:PRO:HB2	1.97	0.45
3:H:62:GLN:HB2	3:H:67:LEU:HD11	1.97	0.45
2:G:186:PHE:CE1	2:G:260:TRP:CD1	3.05	0.45
1:A:151:ASP:OD1	1:A:151:ASP:N	2.50	0.45
1:A:428:ARG:NH2	1:A:429:ASP:OD2	2.39	0.45
3:H:49:ALA:HB2	3:H:66:THR:HG21	1.98	0.45
1:A:297:PRO:HA	1:A:457:GLU:OE1	2.16	0.45
1:B:247:VAL:HA	1:B:248:PRO:HD3	1.68	0.45
1:B:267:VAL:HG13	1:B:272:PHE:CE1	2.52	0.45
2:G:257:ILE:HD12	2:G:257:ILE:H	1.82	0.45
2:G:270:VAL:CG1	2:G:314:GLN:HA	2.46	0.45
1:A:72:ILE:O	1:A:266:LYS:NZ	2.41	0.45
2:C:276:PRO:HA	2:C:312:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:359:ASP:O	2:C:363:MET:HG2	2.16	0.45
1:B:324:ASN:OD1	1:B:326:GLU:HB2	2.17	0.45
1:A:264:TRP:CZ2	1:A:282:ALA:HB2	2.51	0.45
2:G:341:LEU:HB3	2:G:374:LYS:HD3	1.98	0.45
1:B:462:TYR:O	1:B:466:LYS:N	2.47	0.44
2:G:131:PHE:O	2:G:135:ILE:HG13	2.17	0.44
1:A:361:ARG:NH1	2:G:367:ARG:HH21	2.15	0.44
1:A:496:LEU:HD12	1:A:496:LEU:HA	1.81	0.44
1:B:151:ASP:N	1:B:151:ASP:OD1	2.50	0.44
1:B:180:HIS:CE1	1:B:183:GLY:HA3	2.53	0.44
1:B:428:ARG:NH2	1:B:429:ASP:OD2	2.43	0.44
2:G:38:ARG:HE	3:H:3:SER:HB3	1.82	0.44
2:G:87:LEU:HD13	3:H:132:ILE:HD11	2.00	0.44
1:A:315:ILE:HD13	1:A:369:VAL:HG11	2.00	0.44
1:B:496:LEU:HD12	1:B:496:LEU:HA	1.86	0.44
1:A:347:PHE:CE2	1:A:475:VAL:HB	2.52	0.44
1:B:137:PRO:HG3	1:B:249:TYR:CE1	2.53	0.44
1:B:146:GLU:O	1:B:149:VAL:HG23	2.18	0.44
3:D:58:ARG:O	3:D:68:ILE:HA	2.18	0.44
1:A:420:MET:HE3	1:A:504:PRO:HB2	1.99	0.43
1:B:108:VAL:O	1:B:110:THR:HG23	2.17	0.43
3:D:26:THR:HG23	3:D:30:MET:O	2.19	0.43
1:A:115:SER:OG	1:A:195:ASN:HA	2.17	0.43
1:B:210:LEU:HD22	1:B:241:ASP:HA	1.99	0.43
2:C:186:PHE:CE1	2:C:261:TYR:HE1	2.36	0.43
2:C:237:LYS:HE3	2:C:256:PHE:HE2	1.83	0.43
2:C:285:LYS:O	2:C:288:PHE:HE1	2.01	0.43
2:C:279:GLU:HG2	2:C:283:LYS:HE2	1.99	0.43
2:G:260:TRP:O	2:G:263:ILE:HB	2.18	0.43
2:C:261:TYR:CD2	2:C:261:TYR:C	2.92	0.43
2:G:260:TRP:HA	2:G:263:ILE:HD12	2.00	0.43
2:C:241:GLN:HB3	2:C:250:TRP:NE1	2.33	0.43
1:A:324:ASN:HB2	1:A:358:LEU:HD13	2.00	0.43
3:H:26:THR:HG23	3:H:30:MET:O	2.19	0.43
1:A:138:TYR:CG	1:A:190:LYS:HE3	2.54	0.43
2:G:321:LEU:HB2	2:G:328:ARG:NH2	2.34	0.43
2:G:122:VAL:HG11	2:G:179:ILE:HG13	2.01	0.42
2:C:333:PHE:HB3	2:C:379:SER:OG	2.19	0.42
1:A:80:THR:O	1:A:81:ASN:ND2	2.53	0.42
1:B:212:ASP:O	1:B:214:ALA:N	2.49	0.42
2:C:93:LYS:HE3	2:C:93:LYS:HB2	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:380:ARG:H	2:C:380:ARG:CZ	2.33	0.42
1:A:518:MET:O	1:A:522:VAL:HG23	2.20	0.42
1:B:242:ILE:O	1:B:242:ILE:HG13	2.20	0.42
2:C:50:VAL:HG12	2:C:59:VAL:HA	2.01	0.42
2:G:340:ASP:HB3	2:G:343:ASP:OD2	2.20	0.42
1:A:58:PRO:HG2	1:A:73:PRO:CB	2.46	0.42
3:D:62:GLN:HB2	3:D:67:LEU:CD1	2.50	0.42
2:C:274:SER:HB3	2:C:314:GLN:OE1	2.19	0.42
3:D:123:VAL:HG22	3:D:125:PHE:CE1	2.55	0.42
2:G:263:ILE:HA	2:G:266:LEU:HD12	2.00	0.42
2:G:345:LYS:O	2:G:349:GLU:HG3	2.20	0.42
2:G:30:ASP:OD1	2:G:31:PRO:HD2	2.19	0.42
1:A:241:ASP:OD1	1:A:242:ILE:N	2.50	0.41
1:B:373:VAL:HG11	1:B:485:TYR:CZ	2.56	0.41
2:G:336:GLN:HB3	2:G:339:TRP:NE1	2.36	0.41
1:A:307:GLN:HG2	1:A:390:ARG:NH2	2.34	0.41
2:G:43:ASP:OD1	2:G:47:SER:N	2.49	0.41
2:G:270:VAL:HG11	2:G:314:GLN:HA	2.02	0.41
2:C:356:MET:HB2	2:C:361:PHE:CE1	2.55	0.41
2:G:306:PHE:CE2	2:G:335:LEU:HD22	2.54	0.41
2:G:370:ARG:HB3	2:G:375:THR:HA	2.02	0.41
2:C:357:LYS:HB3	2:C:357:LYS:NZ	2.35	0.41
1:A:494:PHE:O	1:A:498:THR:HG23	2.20	0.41
1:B:169:ILE:HG21	1:B:171:ARG:NH1	2.36	0.41
2:G:287:LEU:HG	2:G:289:PRO:HD3	2.03	0.41
2:C:280:PHE:CD2	2:C:313:VAL:HG11	2.56	0.41
2:G:28:ILE:HD13	2:G:37:LEU:HD23	2.03	0.41
2:G:291:PHE:CD1	2:G:291:PHE:N	2.87	0.41
2:G:302:ARG:HD3	2:G:342:GLU:CB	2.45	0.41
3:H:6:ILE:HA	3:H:113:VAL:HG13	2.03	0.41
1:B:310:MET:HE2	1:B:321:LEU:HD11	2.03	0.41
2:C:186:PHE:HE1	2:C:261:TYR:CD1	2.39	0.41
2:G:340:ASP:HB3	2:G:343:ASP:CG	2.41	0.41
1:B:157:LYS:HG3	1:B:167:LEU:HD11	2.03	0.40
2:C:132:SER:HA	2:C:135:ILE:HD12	2.04	0.40
2:G:235:LEU:HD13	2:G:250:TRP:CD1	2.56	0.40
2:G:266:LEU:HB3	2:G:315:TYR:HD1	1.86	0.40
3:H:10:GLN:O	3:H:13:LYS:HG2	2.20	0.40
2:C:356:MET:HB2	2:C:361:PHE:CD1	2.56	0.40
1:A:149:VAL:HG13	1:A:189:ILE:HD11	2.04	0.40
1:B:432:LEU:HD11	1:B:446:LYS:HE2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:321:LEU:HB2	2:C:328:ARG:NH2	2.36	0.40
3:H:28:LEU:HB2	3:H:117:ASP:OD2	2.22	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:B:455:ASP:OD2	2:G:334:ARG:NH2[5_555]	2.14	0.06

## 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	433/524 (83%)	418 (96%)	12 (3%)	3 (1%)	22	62
1	B	460/524 (88%)	438 (95%)	19 (4%)	3 (1%)	22	62
2	C	357/380 (94%)	338 (95%)	18 (5%)	1 (0%)	41	76
2	G	367/380 (97%)	347 (95%)	18 (5%)	2 (0%)	29	68
3	D	129/133 (97%)	128 (99%)	1 (1%)	0	100	100
3	H	129/133 (97%)	128 (99%)	1 (1%)	0	100	100
4	E	24/26 (92%)	22 (92%)	2 (8%)	0	100	100
4	I	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
All	All	1923/2126 (90%)	1840 (96%)	74 (4%)	9 (0%)	29	68

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	241	ASP
1	A	69	ILE
1	B	213	ASN

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Mol	Chain	Res	Type
2	G	357	LYS
1	B	244	GLU
1	A	110	THR
1	A	218	VAL
2	C	254	ILE
2	G	254	ILE

### 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	392/464 (84%)	386 (98%)	6 (2%)	65	80
1	B	410/464 (88%)	401 (98%)	9 (2%)	52	71
2	C	339/352 (96%)	334 (98%)	5 (2%)	65	80
2	G	344/352 (98%)	338 (98%)	6 (2%)	60	78
3	D	118/120 (98%)	116 (98%)	2 (2%)	60	78
3	H	118/120 (98%)	117 (99%)	1 (1%)	81	89
4	E	24/24 (100%)	24 (100%)	0	100	100
4	I	24/24 (100%)	23 (96%)	1 (4%)	30	55
All	All	1769/1920 (92%)	1739 (98%)	30 (2%)	60	78

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LYS
1	A	69	ILE
1	A	151	ASP
1	A	158	LYS
1	A	234	ASP
1	A	496	LEU
1	B	41	SER
1	B	63	ARG
1	B	151	ASP

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Mol	Chain	Res	Type
1	B	158	LYS
1	B	170	ILE
1	B	172	LYS
1	B	184	LEU
1	B	450	ASN
1	B	496	LEU
2	C	128	GLU
2	C	256	PHE
2	C	302	ARG
2	C	345	LYS
2	C	361	PHE
3	D	22	THR
3	D	51	ARG
2	G	29	GLN
2	G	173	LYS
2	G	186	PHE
2	G	252	LEU
2	G	275	MET
2	G	363	MET
3	H	22	THR
4	I	731	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	ASN
1	B	83	HIS
2	C	305	HIS
3	D	21	GLN
2	G	33	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	A	445/524 (84%)	-0.02	11 (2%) 57 48	150, 187, 274, 337	0
1	B	468/524 (89%)	-0.15	6 (1%) 77 68	100, 163, 239, 286	0
2	C	367/380 (96%)	-0.15	5 (1%) 75 66	138, 181, 243, 305	0
2	G	373/380 (98%)	-0.12	9 (2%) 59 49	119, 185, 247, 331	0
3	D	131/133 (98%)	0.12	4 (3%) 49 39	139, 184, 275, 288	0
3	H	131/133 (98%)	0.00	2 (1%) 73 64	106, 190, 262, 289	0
4	E	26/26 (100%)	-0.18	0 100 100	90, 189, 204, 219	0
4	I	26/26 (100%)	-0.27	0 100 100	111, 161, 193, 234	0
All	All	1967/2126 (92%)	-0.09	37 (1%) 66 58	90, 180, 254, 337	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	93	LYS	4.2
1	A	124	GLU	3.8
1	A	235	ALA	3.0
1	A	144	ASN	3.0
1	A	194	VAL	2.9
2	G	139	SER	2.8
3	H	22	THR	2.8
2	G	74	GLU	2.8
1	A	236	LYS	2.8
3	D	49	ALA	2.7
1	B	112	GLN	2.7
2	C	110	THR	2.7
1	A	128	SER	2.7
1	A	106	GLU	2.6
2	G	375	THR	2.6
1	A	168	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	93	SER	2.5
2	G	98	VAL	2.5
1	A	58	PRO	2.4
2	C	131	PHE	2.4
1	B	113	GLY	2.4
1	B	86	LEU	2.4
3	D	93	LYS	2.4
2	G	138	ARG	2.3
3	D	122	LYS	2.3
2	G	100	GLY	2.3
1	B	60	TYR	2.2
1	A	73	PRO	2.2
2	G	374	LYS	2.2
1	B	110	THR	2.2
2	G	226	TYR	2.2
1	A	125	GLU	2.2
2	G	325	PRO	2.2
2	C	138	ARG	2.1
3	D	51	ARG	2.1
2	C	60	LEU	2.1
2	C	137	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.