



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:05 am GMT

PDB ID : 4L0K  
Title : Crystal structure of a type II restriction endonuclease  
Authors : Zhuo, W.; Ge, J.; Yang, M.  
Deposited on : 2013-05-31  
Resolution : 2.33 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  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

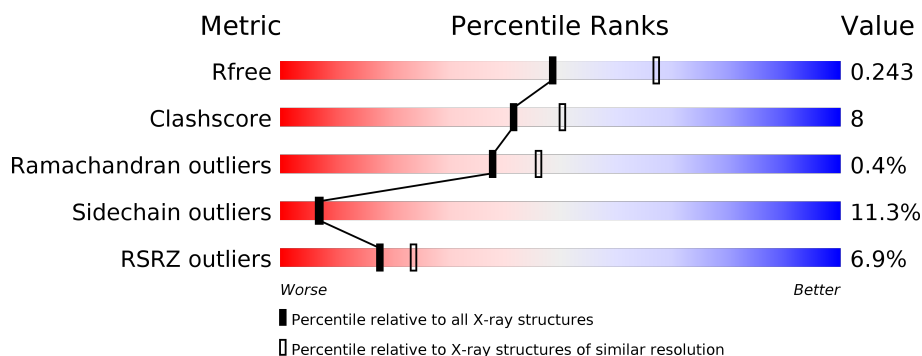
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.33 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))
$R_{free}$	100719	4787 (2.34-2.30)
Clashscore	112137	5439 (2.34-2.30)
Ramachandran outliers	110173	5386 (2.34-2.30)
Sidechain outliers	110143	5385 (2.34-2.30)
RSRZ outliers	101464	4814 (2.34-2.30)

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	227	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>16%</div> <div>• • 8%</div> </div> </div>
1	B	227	<div> <div>10%</div> <div> <div></div> <div>69%</div> <div>16%</div> <div>• 11%</div> </div> </div>
1	C	227	<div> <div>11%</div> <div> <div></div> <div>69%</div> <div>16%</div> <div>• • 10%</div> </div> </div>
1	D	227	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>14%</div> <div>5% • 9%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6903 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 DraIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1653	1059	283	297	14			
1	B	202	Total	C	N	O	S	0	0	0
			1595	1022	272	287	14			
1	C	204	Total	C	N	O	S	0	0	0
			1627	1045	279	290	13			
1	D	207	Total	C	N	O	S	0	0	0
			1656	1062	284	296	14			

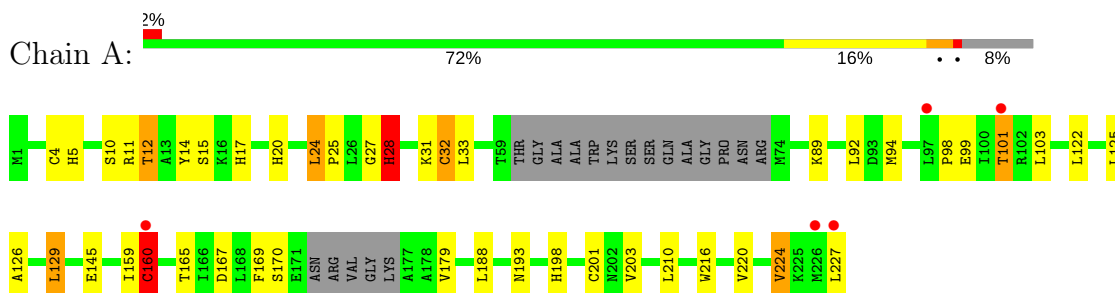
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	93	Total	O	0	0
			93	93		
2	B	92	Total	O	0	0
			92	92		
2	C	93	Total	O	0	0
			93	93		
2	D	94	Total	O	0	0
			94	94		

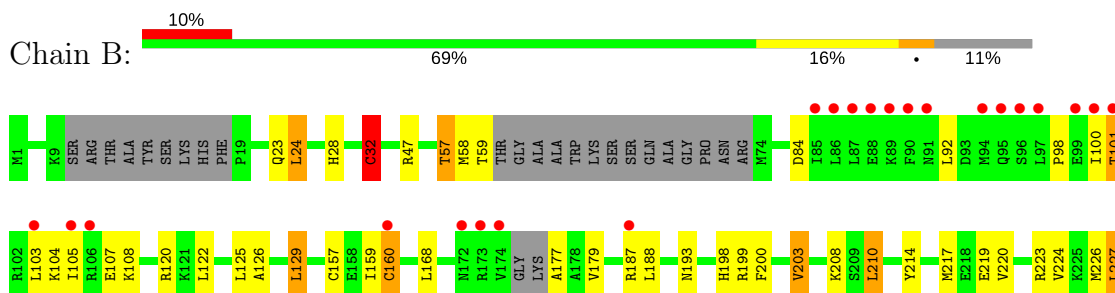
### 3 Residue-property plots [i](#)

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

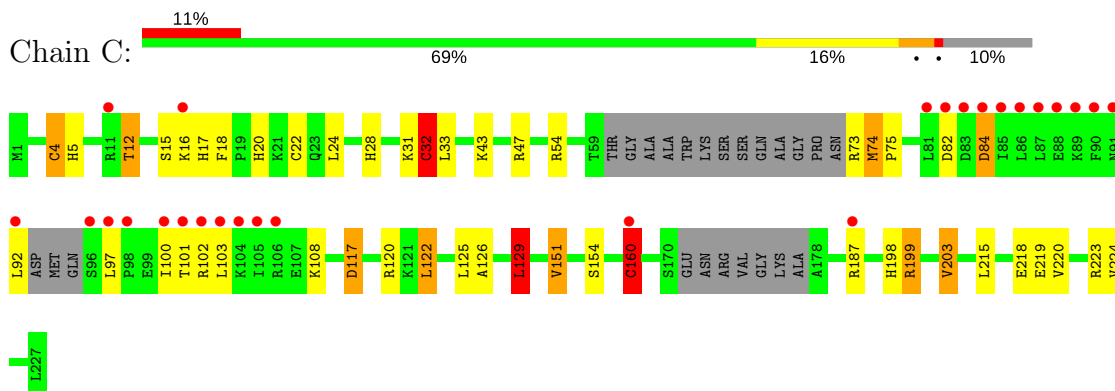
#### • Molecule 1: DraIII



#### • Molecule 1: DraIII

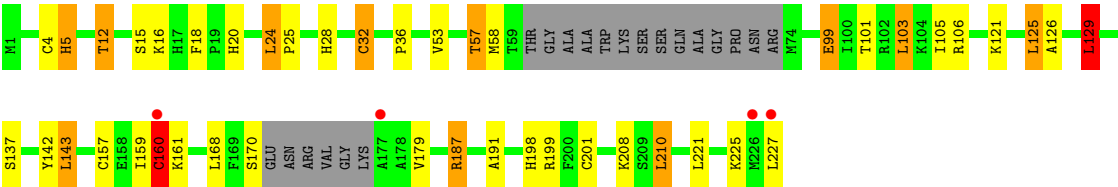


#### • Molecule 1: DraIII



#### • Molecule 1: DraIII





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.40Å 119.06Å 82.11Å 90.00° 92.89° 90.00°	Depositor
Resolution (Å)	35.72 – 2.33 35.72 – 2.33	Depositor EDS
% Data completeness (in resolution range)	98.3 (35.72-2.33) 98.3 (35.72-2.33)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.192 , 0.243 0.190 , 0.243	Depositor DCC
$R_{free}$ test set	2388 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.3	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 57.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6903	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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	0.69	1/1691 (0.1%)	0.60	0/2287
1	B	0.53	1/1629 (0.1%)	0.66	1/2201 (0.0%)
1	C	0.58	2/1664 (0.1%)	0.63	2/2248 (0.1%)
1	D	0.56	1/1694 (0.1%)	0.60	1/2288 (0.0%)
All	All	0.59	5/6678 (0.1%)	0.62	4/9024 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	CYS	CB-SG	15.30	2.08	1.82
1	D	160	CYS	CB-SG	13.40	2.05	1.82
1	C	160	CYS	CB-SG	10.30	1.99	1.82
1	B	32	CYS	CB-SG	9.97	1.99	1.82
1	C	32	CYS	CB-SG	6.90	1.94	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	227	LEU	CB-CG-CD2	-5.91	100.96	111.00
1	D	129	LEU	CA-CB-CG	5.42	127.76	115.30
1	C	129	LEU	CA-CB-CG	5.39	127.70	115.30
1	C	4	CYS	CA-CB-SG	5.18	123.33	114.00

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	1653	0	1644	25	0
1	B	1595	0	1588	29	0
1	C	1627	0	1628	27	0
1	D	1656	0	1664	27	0
2	A	93	0	0	2	0
2	B	92	0	0	5	0
2	C	93	0	0	5	0
2	D	94	0	0	1	0
All	All	6903	0	6524	105	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 (105) 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:D:160:CYS:CB	1:D:160:CYS:SG	2.05	1.45
1:A:160:CYS:CB	1:A:160:CYS:SG	2.08	1.39
1:D:160:CYS:SG	1:D:198:HIS:ND1	2.19	1.15
1:B:28:HIS:NE2	1:B:32:CYS:SG	2.19	1.14
1:A:160:CYS:SG	1:A:198:HIS:ND1	2.22	1.11
1:C:28:HIS:NE2	1:C:32:CYS:SG	2.28	1.05
1:B:160:CYS:SG	1:B:198:HIS:ND1	2.31	1.03
1:C:160:CYS:SG	1:C:198:HIS:ND1	2.34	1.01
1:D:28:HIS:NE2	1:D:32:CYS:SG	2.36	0.97
1:A:165:THR:OG1	1:A:167:ASP:OD1	1.87	0.92
1:B:177:ALA:N	2:B:360:HOH:O	2.02	0.91
1:B:223:ARG:NH2	2:B:340:HOH:O	2.08	0.85
1:C:120:ARG:NH1	2:C:335:HOH:O	2.08	0.85
1:A:28:HIS:NE2	1:A:32:CYS:SG	2.53	0.82
1:A:220:VAL:O	1:A:224:VAL:HG13	1.85	0.76
1:C:4:CYS:SG	1:C:28:HIS:NE2	2.60	0.74
1:A:12:THR:HG22	1:A:15:SER:H	1.52	0.74
1:D:12:THR:HG22	1:D:15:SER:H	1.54	0.72
1:C:218:GLU:OE1	2:C:363:HOH:O	2.08	0.71
1:C:28:HIS:CE1	1:C:32:CYS:SG	2.84	0.70
1:A:126:ALA:HA	1:A:129:LEU:HD22	1.75	0.68
1:B:47:ARG:NH2	1:C:219:GLU:OE2	2.27	0.67
1:B:23:GLN:OE1	1:B:120:ARG:NH2	2.28	0.67
1:C:126:ALA:HA	1:C:129:LEU:HD22	1.76	0.66
1:B:59:THR:O	1:B:108:LYS:NZ	2.25	0.66
1:A:28:HIS:CD2	1:A:32:CYS:SG	2.88	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:ARG:O	1:C:203:VAL:HG12	1.94	0.65
1:A:98:PRO:HG2	1:A:101:THR:HG23	1.80	0.63
1:B:126:ALA:HA	1:B:129:LEU:HD22	1.82	0.62
1:C:54:ARG:HD2	2:C:343:HOH:O	2.01	0.61
1:B:107:GLU:HG2	1:B:187:ARG:HE	1.65	0.61
1:D:57:THR:HG22	1:D:58:MET:HG2	1.83	0.61
1:D:53:VAL:O	1:D:57:THR:HB	2.01	0.61
1:C:12:THR:HG22	1:C:15:SER:H	1.66	0.60
1:C:22:CYS:SG	1:C:28:HIS:NE2	2.74	0.60
1:A:4:CYS:SG	1:A:28:HIS:HD2	2.25	0.59
1:C:151:VAL:HG22	1:C:154:SER:HB3	1.86	0.58
1:A:25:PRO:O	1:A:28:HIS:HB2	2.05	0.57
1:C:12:THR:HG21	1:C:20:HIS:NE2	2.20	0.56
1:A:28:HIS:HE2	1:A:32:CYS:HA	1.71	0.56
1:B:24:LEU:HB3	1:B:28:HIS:CD2	2.41	0.56
1:B:157:CYS:SG	1:B:160:CYS:N	2.76	0.55
1:D:12:THR:HG21	1:D:20:HIS:NE2	2.21	0.55
1:B:199:ARG:O	1:B:203:VAL:HG13	2.07	0.54
1:D:126:ALA:HA	1:D:129:LEU:HD22	1.90	0.54
1:C:15:SER:HA	1:C:18:PHE:O	2.08	0.54
1:B:159:ILE:HG12	1:B:210:LEU:HD11	1.90	0.54
1:D:24:LEU:HD13	1:D:36:PRO:HG3	1.90	0.53
1:B:200:PHE:CZ	1:D:208:LYS:HD2	2.44	0.53
1:A:188:LEU:HB3	1:A:193:ASN:ND2	2.24	0.52
1:D:159:ILE:HB	1:D:201:CYS:HB3	1.92	0.52
1:A:4:CYS:SG	1:A:28:HIS:CD2	3.02	0.51
1:C:31:LYS:HE3	1:C:33:LEU:HD21	1.91	0.51
1:D:121:LYS:HG3	1:D:191:ALA:O	2.11	0.51
1:A:24:LEU:HD21	1:A:33:LEU:HD12	1.91	0.51
1:A:12:THR:O	1:A:15:SER:OG	2.18	0.51
1:D:15:SER:HA	1:D:18:PHE:O	2.11	0.50
1:B:226:MET:O	1:B:227:LEU:HB2	2.12	0.49
1:D:221:LEU:O	1:D:225:LYS:HD3	2.11	0.49
1:B:208:LYS:O	2:B:314:HOH:O	2.20	0.49
1:B:220:VAL:O	1:B:224:VAL:HG13	2.13	0.49
1:D:101:THR:O	1:D:105:ILE:HG13	2.12	0.49
1:D:168:LEU:HB3	1:D:179:VAL:HG23	1.95	0.49
1:A:169:PHE:CD1	1:A:169:PHE:N	2.81	0.48
1:C:16:LYS:HG2	1:C:17:HIS:CD2	2.48	0.48
1:B:193:ASN:OD1	2:B:342:HOH:O	2.20	0.47
1:A:94:MET:HE2	2:A:315:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:PRO:HG2	1:B:101:THR:HG23	1.97	0.47
1:D:121:LYS:HD2	1:D:125:LEU:HD22	1.95	0.47
1:A:169:PHE:CZ	1:A:179:VAL:HG11	2.50	0.47
1:D:159:ILE:HG13	1:D:210:LEU:HD11	1.97	0.47
1:C:73:ARG:N	2:C:370:HOH:O	2.48	0.47
1:A:159:ILE:HB	1:A:201:CYS:HB3	1.96	0.46
1:B:59:THR:HG23	1:B:108:LYS:HD2	1.98	0.46
1:D:24:LEU:HD12	1:D:25:PRO:HD2	1.97	0.45
1:B:214:TYR:HA	1:B:217:MET:HE2	1.99	0.45
1:D:142:TYR:HD2	1:D:143:LEU:HD13	1.81	0.45
1:D:210:LEU:HD12	1:D:210:LEU:HA	1.87	0.45
1:C:220:VAL:O	1:C:224:VAL:HG13	2.18	0.44
1:B:126:ALA:O	1:B:129:LEU:HB2	2.18	0.44
1:B:168:LEU:HB3	1:B:179:VAL:CG2	2.48	0.44
1:C:215:LEU:O	1:C:219:GLU:HG3	2.18	0.44
1:C:117:ASP:HA	1:C:120:ARG:NH1	2.33	0.43
1:A:17:HIS:NE2	1:A:89:LYS:O	2.51	0.43
1:B:217:MET:HE3	1:D:221:LEU:HG	2.01	0.43
1:A:12:THR:HG22	1:A:15:SER:N	2.29	0.43
1:B:101:THR:HA	1:B:104:LYS:HB2	2.01	0.43
1:C:84:ASP:N	1:C:84:ASP:OD2	2.50	0.42
1:D:161:LYS:NZ	2:D:338:HOH:O	2.49	0.42
1:A:14:TYR:OH	2:A:322:HOH:O	2.14	0.42
1:B:214:TYR:HD1	1:B:217:MET:HE1	1.84	0.42
1:D:12:THR:HG22	1:D:15:SER:N	2.28	0.42
1:A:216:TRP:O	1:A:220:VAL:HG23	2.19	0.42
1:B:101:THR:O	1:B:105:ILE:HG12	2.19	0.42
1:D:157:CYS:SG	1:D:160:CYS:N	2.87	0.42
1:D:99:GLU:HG3	1:D:103:LEU:HD22	2.03	0.41
1:C:122:LEU:HD12	1:C:122:LEU:HA	1.89	0.41
1:C:12:THR:HG22	1:C:15:SER:HB3	2.02	0.41
1:D:187:ARG:O	1:D:187:ARG:NH2	2.53	0.41
1:A:12:THR:HG21	1:A:20:HIS:NE2	2.35	0.41
1:C:100:ILE:HD12	1:C:100:ILE:HA	1.84	0.41
1:B:57:THR:HG22	1:B:58:MET:HG2	2.03	0.41
1:B:219:GLU:OE1	2:B:339:HOH:O	2.22	0.40
1:C:223:ARG:NH2	2:C:320:HOH:O	2.50	0.40
1:C:74:MET:HA	1:C:75:PRO:HD3	1.95	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	202/227 (89%)	194 (96%)	6 (3%)	2 (1%)	18	19
1	B	194/227 (86%)	187 (96%)	7 (4%)	0	100	100
1	C	196/227 (86%)	192 (98%)	4 (2%)	0	100	100
1	D	201/227 (88%)	196 (98%)	4 (2%)	1 (0%)	32	39
All	All	793/908 (87%)	769 (97%)	21 (3%)	3 (0%)	38	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	5	HIS
1	A	28	HIS
1	A	27	GLY

### 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	181/197 (92%)	159 (88%)	22 (12%)	6	5
1	B	174/197 (88%)	159 (91%)	15 (9%)	12	14
1	C	179/197 (91%)	155 (87%)	24 (13%)	4	4
1	D	183/197 (93%)	163 (89%)	20 (11%)	7	8
All	All	717/788 (91%)	636 (89%)	81 (11%)	7	7

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	10	SER
1	A	11	ARG
1	A	12	THR
1	A	24	LEU
1	A	28	HIS
1	A	31	LYS
1	A	32	CYS
1	A	92	LEU
1	A	99	GLU
1	A	101	THR
1	A	103	LEU
1	A	122	LEU
1	A	125	LEU
1	A	129	LEU
1	A	145	GLU
1	A	160	CYS
1	A	170	SER
1	A	203	VAL
1	A	210	LEU
1	A	224	VAL
1	A	227	LEU
1	B	24	LEU
1	B	32	CYS
1	B	57	THR
1	B	84	ASP
1	B	92	LEU
1	B	100	ILE
1	B	101	THR
1	B	103	LEU
1	B	122	LEU
1	B	125	LEU
1	B	129	LEU
1	B	160	CYS
1	B	188	LEU
1	B	203	VAL
1	B	210	LEU
1	C	5	HIS
1	C	12	THR
1	C	24	LEU
1	C	32	CYS
1	C	43	LYS
1	C	47	ARG

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Mol	Chain	Res	Type
1	C	74	MET
1	C	82	ASP
1	C	84	ASP
1	C	92	LEU
1	C	97	LEU
1	C	101	THR
1	C	102	ARG
1	C	103	LEU
1	C	108	LYS
1	C	117	ASP
1	C	122	LEU
1	C	125	LEU
1	C	129	LEU
1	C	151	VAL
1	C	160	CYS
1	C	187	ARG
1	C	199	ARG
1	C	203	VAL
1	D	4	CYS
1	D	5	HIS
1	D	12	THR
1	D	16	LYS
1	D	24	LEU
1	D	32	CYS
1	D	57	THR
1	D	99	GLU
1	D	103	LEU
1	D	106	ARG
1	D	125	LEU
1	D	129	LEU
1	D	137	SER
1	D	143	LEU
1	D	160	CYS
1	D	170	SER
1	D	187	ARG
1	D	199	ARG
1	D	210	LEU
1	D	227	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

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	208/227 (91%)	-0.11	5 (2%) 59 66	24, 39, 73, 80	0
1	B	202/227 (88%)	0.40	22 (10%) 6 9	24, 39, 87, 98	0
1	C	204/227 (89%)	0.54	26 (12%) 4 6	24, 39, 109, 119	0
1	D	207/227 (91%)	-0.14	4 (1%) 67 73	23, 41, 69, 93	0
All	All	821/908 (90%)	0.17	57 (6%) 18 24	23, 40, 85, 119	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	92	LEU	10.1
1	C	87	LEU	9.6
1	C	101	THR	8.4
1	C	105	ILE	6.9
1	B	100	ILE	6.4
1	B	103	LEU	6.3
1	C	97	LEU	6.2
1	A	227	LEU	5.8
1	C	100	ILE	5.6
1	C	98	PRO	5.4
1	D	227	LEU	5.3
1	B	90	PHE	5.2
1	C	96	SER	4.7
1	B	105	ILE	4.4
1	B	95	GLN	4.3
1	C	90	PHE	4.3
1	C	187	ARG	4.2
1	B	96	SER	4.2
1	C	86	LEU	4.2
1	C	102	ARG	4.2
1	B	101	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	97	LEU	4.0
1	D	226	MET	3.9
1	B	85	ILE	3.9
1	C	84	ASP	3.6
1	C	104	LYS	3.5
1	C	82	ASP	3.4
1	B	174	VAL	3.3
1	B	187	ARG	3.3
1	B	88	GLU	3.2
1	B	173	ARG	3.2
1	C	106	ARG	3.2
1	C	89	LYS	3.2
1	B	87	LEU	3.0
1	A	226	MET	2.9
1	D	177	ALA	2.9
1	D	160	CYS	2.8
1	B	86	LEU	2.8
1	C	83	ASP	2.8
1	C	91	ASN	2.8
1	B	99	GLU	2.8
1	A	160	CYS	2.7
1	C	16	LYS	2.7
1	B	160	CYS	2.7
1	A	101	THR	2.7
1	B	106	ARG	2.6
1	B	94	MET	2.6
1	C	103	LEU	2.6
1	C	11	ARG	2.5
1	B	89	LYS	2.5
1	C	85	ILE	2.5
1	B	172	ASN	2.5
1	B	91	ASN	2.4
1	C	160	CYS	2.4
1	C	88	GLU	2.1
1	C	81	LEU	2.1
1	A	97	LEU	2.0

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

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



### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.