



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:39 AM GMT

PDB ID : 2NOV  
Title : Breakage-reunion domain of S.pneumoniae topo IV: crystal structure of a gram-positive quinolone target  
Authors : Laponogov, I.; Veselkov, D.A.; Sohi, M.K.; Pan, X.S.; Achari, A.; Yang, C.; Ferrara, J.D.; Fisher, L.M.; Sanderson, M.R.  
Deposited on : 2006-10-26  
Resolution : 2.67 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

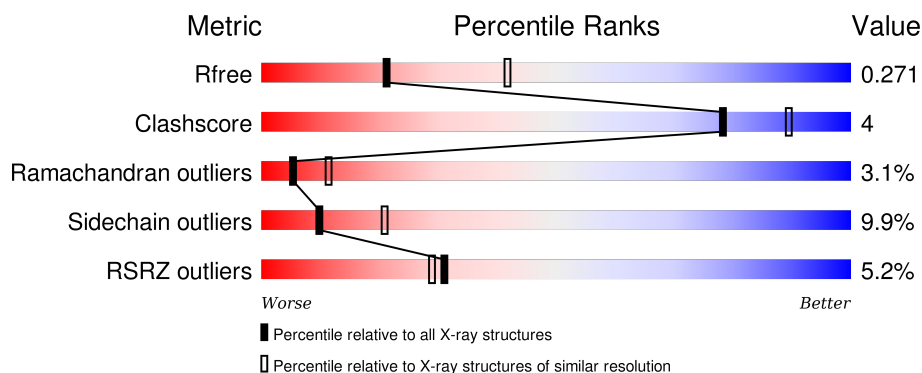
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.67 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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	496	<div> <div>2%</div> <div>73% 14% • 11%</div> </div>
1	B	496	<div> <div>3%</div> <div>73% 15% • 9%</div> </div>
1	C	496	<div> <div>2%</div> <div>75% 15% • 9%</div> </div>
1	D	496	<div> <div>12%</div> <div>73% 13% • 11%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13644 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 topoisomerase 4 subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3368	2128	576	652	12			
1	B	451	Total	C	N	O	S	0	0	0
			3458	2179	591	675	13			
1	C	451	Total	C	N	O	S	0	0	0
			3456	2180	592	671	13			
1	D	440	Total	C	N	O	S	0	0	0
			3338	2099	575	652	12			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	THR	ILE	CONFLICT	UNP P72525
A	489	LEU	ILE	CONFLICT	UNP P72525
A	491	HIS	-	EXPRESSION TAG	UNP P72525
A	492	HIS	-	EXPRESSION TAG	UNP P72525
A	493	HIS	-	EXPRESSION TAG	UNP P72525
A	494	HIS	-	EXPRESSION TAG	UNP P72525
A	495	HIS	-	EXPRESSION TAG	UNP P72525
A	496	HIS	-	EXPRESSION TAG	UNP P72525
B	257	THR	ILE	CONFLICT	UNP P72525
B	489	LEU	ILE	CONFLICT	UNP P72525
B	491	HIS	-	EXPRESSION TAG	UNP P72525
B	492	HIS	-	EXPRESSION TAG	UNP P72525
B	493	HIS	-	EXPRESSION TAG	UNP P72525
B	494	HIS	-	EXPRESSION TAG	UNP P72525
B	495	HIS	-	EXPRESSION TAG	UNP P72525
B	496	HIS	-	EXPRESSION TAG	UNP P72525
C	257	THR	ILE	CONFLICT	UNP P72525
C	489	LEU	ILE	CONFLICT	UNP P72525
C	491	HIS	-	EXPRESSION TAG	UNP P72525
C	492	HIS	-	EXPRESSION TAG	UNP P72525
C	493	HIS	-	EXPRESSION TAG	UNP P72525

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Chain	Residue	Modelled	Actual	Comment	Reference
C	494	HIS	-	EXPRESSION TAG	UNP P72525
C	495	HIS	-	EXPRESSION TAG	UNP P72525
C	496	HIS	-	EXPRESSION TAG	UNP P72525
D	257	THR	ILE	CONFLICT	UNP P72525
D	489	LEU	ILE	CONFLICT	UNP P72525
D	491	HIS	-	EXPRESSION TAG	UNP P72525
D	492	HIS	-	EXPRESSION TAG	UNP P72525
D	493	HIS	-	EXPRESSION TAG	UNP P72525
D	494	HIS	-	EXPRESSION TAG	UNP P72525
D	495	HIS	-	EXPRESSION TAG	UNP P72525
D	496	HIS	-	EXPRESSION TAG	UNP P72525

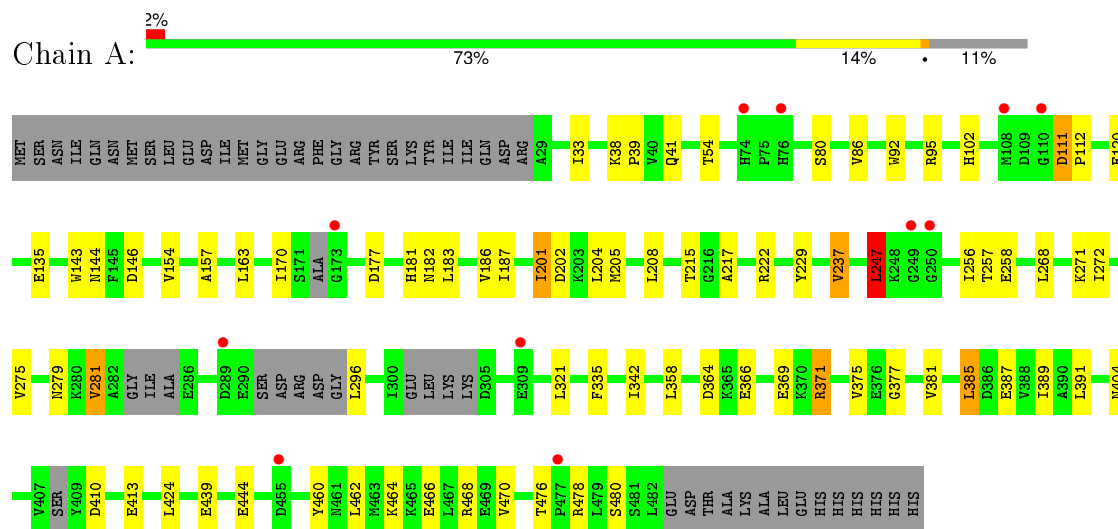
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total O 6 6	0	0
2	B	7	Total O 7 7	0	0
2	C	8	Total O 8 8	0	0
2	D	3	Total O 3 3	0	0

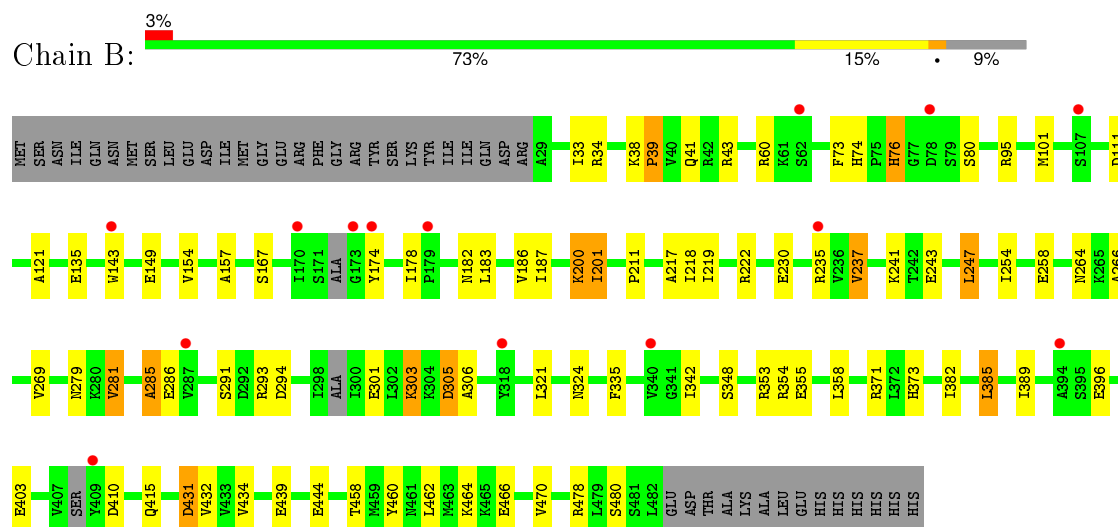
### 3 Residue-property plots [i](#)

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

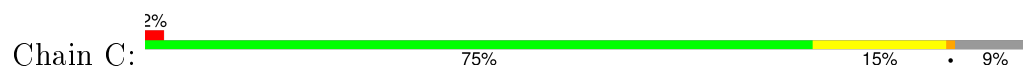
#### • Molecule 1: DNA topoisomerase 4 subunit A

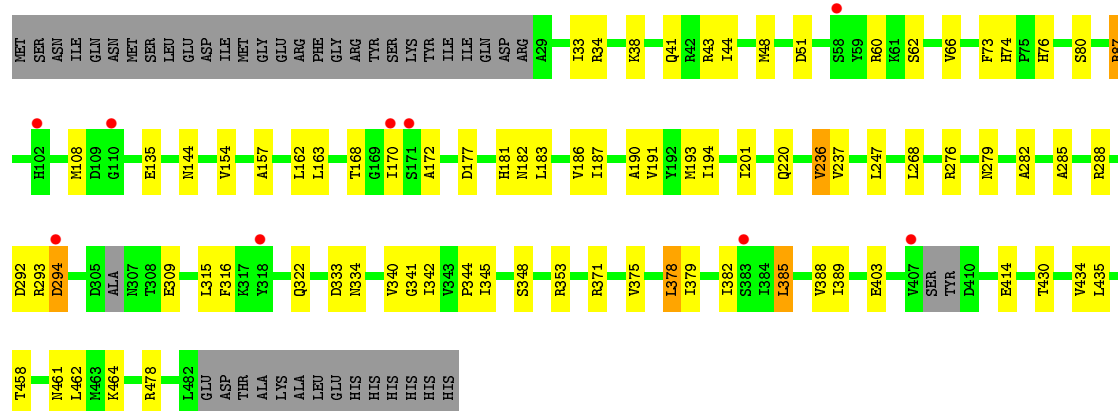


#### • Molecule 1: DNA topoisomerase 4 subunit A

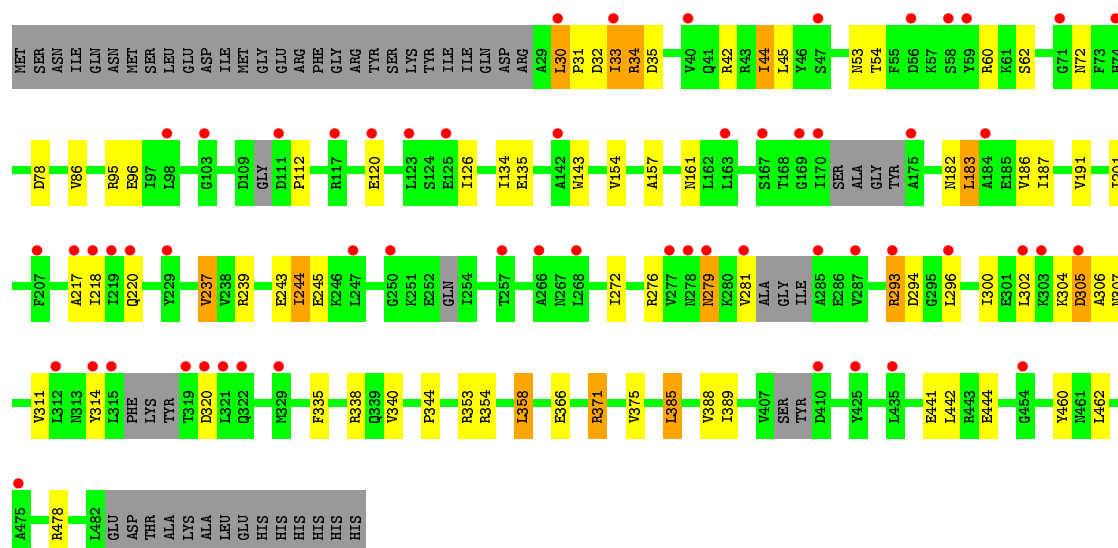
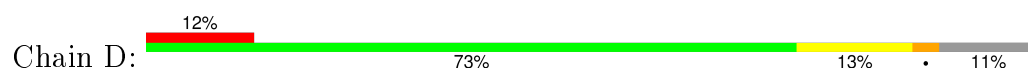


#### • Molecule 1: DNA topoisomerase 4 subunit A





• Molecule 1: DNA topoisomerase 4 subunit A



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.92Å 137.85Å 326.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	500.00 – 2.67 19.53 – 2.68	Depositor EDS
% Data completeness (in resolution range)	97.2 (500.00-2.67) 99.0 (19.53-2.68)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 2.67Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.224 , 0.276 0.215 , 0.271	Depositor DCC
$R_{free}$ test set	8219 reflections (10.61%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.1	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 59.5	EDS
Estimated twinning fraction	0.307 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	3 of 85700 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	13644	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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	0.65	0/3418	0.79	1/4621 (0.0%)
1	B	0.64	0/3510	0.80	1/4744 (0.0%)
1	C	0.65	0/3509	0.80	2/4747 (0.0%)
1	D	0.64	0/3385	0.78	0/4583
All	All	0.64	0/13822	0.79	4/18695 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	LEU	CA-CB-CG	6.73	130.77	115.30
1	B	247	LEU	CA-CB-CG	6.21	129.58	115.30
1	C	462	LEU	CA-CB-CG	5.71	128.43	115.30
1	C	236	VAL	N-CA-C	5.43	125.67	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3368	0	3260	25	0
1	B	3458	0	3349	23	0
1	C	3456	0	3358	28	0
1	D	3338	0	3184	21	0
2	A	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	7	0	0	0	0
2	C	8	0	0	0	0
2	D	3	0	0	0	0
All	All	13644	0	13151	97	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 4.

All (97) 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:38:LYS:H	1:A:41:GLN:HE21	1.05	0.98
1:C:33:ILE:HD11	1:C:333:ASP:HB3	1.68	0.76
1:C:38:LYS:H	1:C:41:GLN:HE21	1.30	0.76
1:A:38:LYS:H	1:A:41:GLN:NE2	1.85	0.74
1:B:264:ASN:HD22	1:B:266:ALA:HB3	1.52	0.74
1:C:201:ILE:H	1:C:201:ILE:HD12	1.57	0.69
1:B:200:LYS:HD3	1:B:200:LYS:H	1.62	0.64
1:D:354:ARG:HH21	1:D:358:LEU:HD21	1.61	0.64
1:D:220:GLN:HB2	1:D:237:VAL:HG13	1.80	0.63
1:B:43:ARG:HE	1:B:73:PHE:HB3	1.64	0.61
1:A:201:ILE:HD12	1:A:201:ILE:H	1.68	0.59
1:C:51:ASP:HB3	1:C:60:ARG:HH22	1.66	0.59
1:D:244:ILE:HD13	1:D:244:ILE:H	1.67	0.59
1:A:466:GLU:O	1:A:470:VAL:HG23	2.04	0.58
1:D:201:ILE:HD12	1:D:201:ILE:H	1.69	0.58
1:C:190:ALA:O	1:C:194:ILE:HG13	2.05	0.57
1:B:235:ARG:HB3	1:B:324:ASN:HD22	1.69	0.57
1:D:53:ASN:HD22	1:D:60:ARG:HH21	1.53	0.56
1:B:183:LEU:O	1:B:187:ILE:HG12	2.06	0.56
1:C:62:SER:O	1:C:66:VAL:HG23	2.08	0.54
1:D:218:ILE:HG23	1:D:239:ARG:HB3	1.90	0.53
1:C:182:ASN:O	1:C:186:VAL:HG23	2.09	0.53
1:C:293:ARG:HG2	1:C:294:ASP:H	1.73	0.53
1:A:182:ASN:O	1:A:186:VAL:HG23	2.10	0.51
1:B:39:PRO:O	1:B:43:ARG:HG2	2.11	0.51
1:A:38:LYS:N	1:A:41:GLN:HE21	1.90	0.51
1:D:272:ILE:HG21	1:D:300:ILE:HD12	1.93	0.51
1:D:182:ASN:O	1:D:186:VAL:HG23	2.09	0.51
1:D:281:VAL:HG21	1:D:311:VAL:HG23	1.93	0.50
1:D:32:ASP:HB2	1:D:34:ARG:HH21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ARG:HG2	1:C:87:ARG:HH11	1.76	0.50
1:B:285:ALA:HB3	1:B:301:GLU:O	2.12	0.50
1:C:33:ILE:HD13	1:C:348:SER:HB3	1.94	0.49
1:B:303:LYS:C	1:B:305:ASP:H	2.15	0.49
1:B:201:ILE:HD12	1:B:201:ILE:H	1.78	0.49
1:C:43:ARG:NH2	1:C:74:HIS:H	2.11	0.49
1:A:371:ARG:O	1:A:375:VAL:HG23	2.13	0.48
1:A:102:HIS:HB3	1:A:120:GLU:HG3	1.94	0.48
1:D:96:GLU:HB3	1:D:126:ILE:HD13	1.94	0.48
1:B:200:LYS:H	1:B:200:LYS:CD	2.22	0.48
1:B:101:MET:HG3	1:B:121:ALA:HB2	1.95	0.48
1:D:385:LEU:O	1:D:389:ILE:HG12	2.14	0.48
1:C:44:ILE:O	1:C:48:MET:HB2	2.13	0.48
1:B:38:LYS:H	1:B:41:GLN:HE21	1.62	0.47
1:A:163:LEU:HD22	1:A:163:LEU:N	2.30	0.47
1:C:33:ILE:HA	1:C:162:LEU:HD22	1.96	0.46
1:A:247:LEU:H	1:A:247:LEU:HD13	1.79	0.46
1:A:256:ILE:HD13	1:A:321:LEU:HD21	1.97	0.46
1:C:385:LEU:O	1:C:388:VAL:HG12	2.15	0.46
1:A:181:HIS:HE1	1:A:229:TYR:OH	1.97	0.46
1:C:385:LEU:O	1:C:389:ILE:HG12	2.16	0.46
1:C:340:VAL:HG23	1:C:344:PRO:HG2	1.98	0.46
1:A:202:ASP:HA	1:A:205:MET:HE2	1.97	0.45
1:D:44:ILE:HG22	1:D:45:LEU:HD23	1.98	0.45
1:A:385:LEU:O	1:A:389:ILE:HG12	2.17	0.45
1:B:382:ILE:HD13	1:B:432:VAL:HG13	1.99	0.45
1:C:187:ILE:O	1:C:191:VAL:HG23	2.16	0.45
1:D:35:ASP:O	1:D:161:ASN:HB3	2.17	0.44
1:B:241:LYS:HB3	1:B:258:GLU:HG2	1.99	0.44
1:B:211:PRO:HG2	1:B:219:ILE:HD13	1.98	0.44
1:A:377:GLY:O	1:A:381:VAL:HG13	2.17	0.44
1:D:338:ARG:HH12	1:D:344:PRO:HB2	1.83	0.44
1:B:167:SER:HB3	1:B:178:ILE:HD13	1.99	0.43
1:B:466:GLU:O	1:B:470:VAL:HG23	2.18	0.43
1:A:272:ILE:O	1:A:272:ILE:HG22	2.17	0.43
1:C:33:ILE:HD12	1:C:34:ARG:HG3	2.00	0.43
1:C:333:ASP:O	1:C:334:ASN:HB2	2.19	0.43
1:C:461:ASN:HA	1:C:464:LYS:HE3	2.01	0.43
1:D:30:LEU:HD23	1:D:31:PRO:HD2	2.00	0.43
1:C:375:VAL:O	1:C:379:ILE:HG12	2.19	0.42
1:D:187:ILE:O	1:D:191:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:LEU:O	1:C:181:HIS:HD2	2.02	0.42
1:D:371:ARG:O	1:D:375:VAL:HG23	2.19	0.42
1:D:183:LEU:O	1:D:187:ILE:HG12	2.20	0.42
1:D:42:ARG:C	1:D:44:ILE:H	2.23	0.42
1:A:464:LYS:NZ	1:A:468:ARG:HH22	2.17	0.42
1:A:183:LEU:O	1:A:187:ILE:HG12	2.20	0.41
1:A:208:LEU:HD23	1:A:342:ILE:HD11	2.02	0.41
1:C:316:PHE:O	1:C:322:GLN:HB3	2.19	0.41
1:A:271:LYS:O	1:A:275:VAL:HG23	2.20	0.41
1:B:460:TYR:O	1:B:464:LYS:HG3	2.21	0.41
1:B:385:LEU:O	1:B:389:ILE:HG12	2.20	0.41
1:A:215:THR:O	1:A:258:GLU:HB2	2.21	0.41
1:C:201:ILE:H	1:C:201:ILE:CD1	2.25	0.41
1:A:460:TYR:O	1:A:464:LYS:HG3	2.20	0.41
1:A:257:THR:O	1:A:296:LEU:HB3	2.21	0.41
1:A:111:ASP:HA	1:A:112:PRO:HD2	1.91	0.41
1:C:220:GLN:O	1:C:236:VAL:O	2.39	0.41
1:C:378:LEU:HB3	1:C:435:LEU:HD21	2.03	0.41
1:B:431:ASP:HA	1:B:434:VAL:HG12	2.03	0.40
1:A:146:ASP:OD1	1:A:146:ASP:N	2.53	0.40
1:D:33:ILE:HG13	1:D:33:ILE:H	1.65	0.40
1:C:341:GLY:O	1:C:345:ILE:HG13	2.21	0.40
1:C:168:THR:HG22	1:C:177:ASP:OD2	2.21	0.40
1:B:373:HIS:O	1:B:415:GLN:NE2	2.53	0.40
1:B:266:ALA:O	1:B:269:VAL:HG12	2.22	0.40
1:B:182:ASN:O	1:B:186:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	428/496 (86%)	386 (90%)	31 (7%)	11 (3%)	7	15
1	B	443/496 (89%)	400 (90%)	26 (6%)	17 (4%)	4	8
1	C	445/496 (90%)	392 (88%)	43 (10%)	10 (2%)	8	20
1	D	426/496 (86%)	357 (84%)	53 (12%)	16 (4%)	4	8
All	All	1742/1984 (88%)	1535 (88%)	153 (9%)	54 (3%)	5	11

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	ALA
1	A	279	ASN
1	A	335	PHE
1	B	76	HIS
1	B	174	TYR
1	B	217	ALA
1	B	303	LYS
1	C	285	ALA
1	D	78	ASP
1	D	293	ARG
1	D	304	LYS
1	A	80	SER
1	A	144	ASN
1	A	217	ALA
1	B	157	ALA
1	B	285	ALA
1	B	291	SER
1	B	335	PHE
1	B	480	SER
1	C	80	SER
1	C	279	ASN
1	C	309	GLU
1	D	157	ALA
1	D	217	ALA
1	D	335	PHE
1	A	391	LEU
1	B	34	ARG
1	B	237	VAL
1	B	279	ASN
1	B	281	VAL
1	B	305	ASP
1	C	157	ALA
1	D	243	GLU

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Mol	Chain	Res	Type
1	D	307	ASN
1	D	320	ASP
1	A	237	VAL
1	B	80	SER
1	B	306	ALA
1	C	144	ASN
1	C	172	ALA
1	D	34	ARG
1	D	279	ASN
1	D	294	ASP
1	D	305	ASP
1	D	306	ALA
1	B	74	HIS
1	C	237	VAL
1	C	282	ALA
1	A	480	SER
1	D	62	SER
1	A	281	VAL
1	A	170	ILE
1	D	112	PRO
1	C	170	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	346/431 (80%)	312 (90%)	34 (10%)	10	21
1	B	357/431 (83%)	316 (88%)	41 (12%)	7	15
1	C	358/431 (83%)	331 (92%)	27 (8%)	17	36
1	D	337/431 (78%)	301 (89%)	36 (11%)	8	17
All	All	1398/1724 (81%)	1260 (90%)	138 (10%)	10	21

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ILE
1	A	39	PRO
1	A	54	THR
1	A	86	VAL
1	A	92	TRP
1	A	95	ARG
1	A	111	ASP
1	A	135	GLU
1	A	143	TRP
1	A	154	VAL
1	A	177	ASP
1	A	201	ILE
1	A	204	LEU
1	A	222	ARG
1	A	237	VAL
1	A	247	LEU
1	A	268	LEU
1	A	281	VAL
1	A	358	LEU
1	A	364	ASP
1	A	366	GLU
1	A	369	GLU
1	A	371	ARG
1	A	385	LEU
1	A	387	GLU
1	A	404	ASN
1	A	410	ASP
1	A	413	GLU
1	A	424	LEU
1	A	439	GLU
1	A	444	GLU
1	A	462	LEU
1	A	476	THR
1	A	478	ARG
1	B	33	ILE
1	B	39	PRO
1	B	60	ARG
1	B	76	HIS
1	B	95	ARG
1	B	111	ASP
1	B	135	GLU
1	B	143	TRP
1	B	149	GLU

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Mol	Chain	Res	Type
1	B	154	VAL
1	B	200	LYS
1	B	201	ILE
1	B	218	ILE
1	B	222	ARG
1	B	230	GLU
1	B	237	VAL
1	B	243	GLU
1	B	247	LEU
1	B	254	ILE
1	B	281	VAL
1	B	286	GLU
1	B	293	ARG
1	B	294	ASP
1	B	321	LEU
1	B	342	ILE
1	B	348	SER
1	B	353	ARG
1	B	354	ARG
1	B	355	GLU
1	B	358	LEU
1	B	371	ARG
1	B	385	LEU
1	B	396	GLU
1	B	403	GLU
1	B	410	ASP
1	B	431	ASP
1	B	439	GLU
1	B	444	GLU
1	B	458	THR
1	B	462	LEU
1	B	478	ARG
1	C	73	PHE
1	C	76	HIS
1	C	87	ARG
1	C	108	MET
1	C	135	GLU
1	C	154	VAL
1	C	183	LEU
1	C	193	MET
1	C	247	LEU
1	C	268	LEU

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Mol	Chain	Res	Type
1	C	276	ARG
1	C	288	ARG
1	C	292	ASP
1	C	294	ASP
1	C	315	LEU
1	C	342	ILE
1	C	353	ARG
1	C	371	ARG
1	C	378	LEU
1	C	382	ILE
1	C	385	LEU
1	C	403	GLU
1	C	414	GLU
1	C	430	THR
1	C	434	VAL
1	C	458	THR
1	C	478	ARG
1	D	30	LEU
1	D	33	ILE
1	D	44	ILE
1	D	54	THR
1	D	72	ASN
1	D	86	VAL
1	D	95	ARG
1	D	120	GLU
1	D	134	ILE
1	D	135	GLU
1	D	143	TRP
1	D	154	VAL
1	D	183	LEU
1	D	237	VAL
1	D	244	ILE
1	D	245	GLU
1	D	276	ARG
1	D	279	ASN
1	D	293	ARG
1	D	296	LEU
1	D	302	LEU
1	D	305	ASP
1	D	314	TYR
1	D	340	VAL
1	D	353	ARG

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Mol	Chain	Res	Type
1	D	358	LEU
1	D	366	GLU
1	D	371	ARG
1	D	385	LEU
1	D	388	VAL
1	D	441	GLU
1	D	442	LEU
1	D	444	GLU
1	D	460	TYR
1	D	462	LEU
1	D	478	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	68	ASN
1	A	72	ASN
1	A	181	HIS
1	A	267	ASN
1	A	324	ASN
1	A	339	GLN
1	A	461	ASN
1	B	41	GLN
1	B	104	ASN
1	B	264	ASN
1	B	324	ASN
1	B	326	ASN
1	B	423	GLN
1	C	41	GLN
1	C	72	ASN
1	C	94	ASN
1	C	181	HIS
1	C	307	ASN
1	C	313	ASN
1	C	324	ASN
1	C	415	GLN
1	C	461	ASN
1	D	53	ASN
1	D	68	ASN
1	D	72	ASN
1	D	334	ASN

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Mol	Chain	Res	Type
1	D	339	GLN

### 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	440/496 (88%)	0.24	11 (2%) 61 59	33, 60, 88, 105	0
1	B	451/496 (90%)	0.25	14 (3%) 52 51	30, 60, 93, 104	0
1	C	451/496 (90%)	0.04	9 (1%) 68 68	21, 52, 83, 97	0
1	D	440/496 (88%)	0.84	58 (13%) 4 3	54, 81, 109, 123	0
All	All	1782/1984 (89%)	0.34	92 (5%) 31 29	21, 65, 96, 123	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	322	GLN	7.6
1	D	315	LEU	5.8
1	D	475	ALA	4.8
1	D	142	ALA	4.7
1	D	321	LEU	4.6
1	D	314	TYR	4.3
1	B	170	ILE	4.3
1	D	285	ALA	4.3
1	B	174	TYR	4.2
1	B	394	ALA	4.1
1	D	40	VAL	4.1
1	D	279	ASN	4.0
1	D	250	GLY	4.0
1	D	302	LEU	3.9
1	D	278	ASN	3.9
1	D	175	ALA	3.8
1	A	173	GLY	3.7
1	C	294	ASP	3.7
1	A	249	GLY	3.6
1	D	277	VAL	3.5
1	B	287	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	217	ALA	3.3
1	C	102	HIS	3.3
1	D	163	LEU	3.2
1	D	219	ILE	3.1
1	D	120	GLU	3.0
1	D	58	SER	2.9
1	D	184	ALA	2.9
1	D	303	LYS	2.9
1	C	110	GLY	2.9
1	B	179	PRO	2.9
1	D	293	ARG	2.8
1	D	220	GLN	2.8
1	D	281	VAL	2.8
1	A	110	GLY	2.8
1	B	235	ARG	2.8
1	B	409	TYR	2.8
1	D	74	HIS	2.8
1	C	318	TYR	2.7
1	B	78	ASP	2.7
1	B	318	TYR	2.7
1	B	107	SER	2.7
1	D	207	PHE	2.7
1	C	383	SER	2.6
1	B	143	TRP	2.6
1	D	59	TYR	2.6
1	A	289	ASP	2.6
1	D	33	ILE	2.5
1	C	407	VAL	2.5
1	D	247	LEU	2.5
1	A	455	ASP	2.5
1	D	454	GLY	2.4
1	D	268	LEU	2.4
1	D	296	LEU	2.4
1	D	170	ILE	2.4
1	D	257	THR	2.4
1	D	410	ASP	2.4
1	A	108	MET	2.4
1	A	250	GLY	2.3
1	A	74	HIS	2.3
1	D	117	ARG	2.3
1	D	123	LEU	2.3
1	D	329	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	309	GLU	2.2
1	D	425	TYR	2.2
1	C	58	SER	2.2
1	D	229	TYR	2.2
1	B	173	GLY	2.2
1	D	287	VAL	2.2
1	C	170	ILE	2.2
1	C	171	SER	2.2
1	D	71	GLY	2.2
1	D	167	SER	2.2
1	D	169	GLY	2.1
1	D	56	ASP	2.1
1	D	320	ASP	2.1
1	D	319	THR	2.1
1	D	218	ILE	2.1
1	B	62	SER	2.1
1	D	103	GLY	2.1
1	D	435	LEU	2.1
1	A	477	PRO	2.1
1	D	30	LEU	2.1
1	B	340	VAL	2.1
1	D	98	LEU	2.0
1	D	312	LEU	2.0
1	A	76	HIS	2.0
1	D	47	SER	2.0
1	D	125	GLU	2.0
1	D	305	ASP	2.0
1	D	266	ALA	2.0
1	D	111	ASP	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 ⓘ

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.