



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:51 PM GMT

PDB ID : 1CSJ  
Title : CRYSTAL STRUCTURE OF THE RNA-DEPENDENT RNA POLYMERASE OF HEPATITIS C VIRUS  
Authors : Bressanelli, S.; Tomei, L.; Roussel, A.; Incitti, I.; Vitale, R.L.; Mathieu, M.; De Francesco, R.; Rey, F.A.  
Deposited on : 1999-08-18  
Resolution : 2.80 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

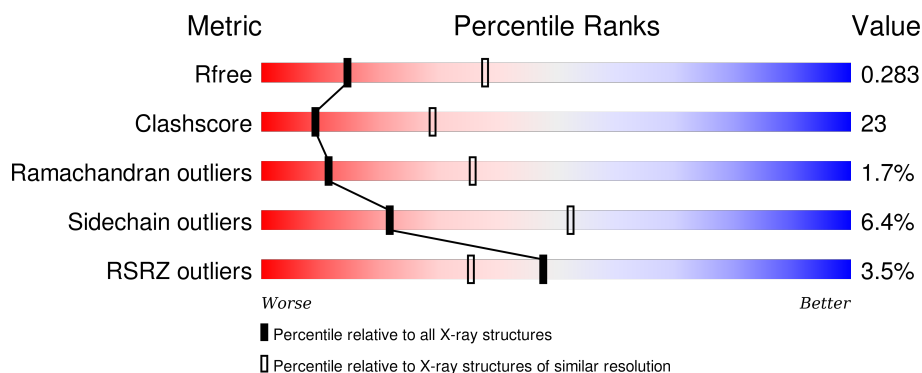
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	531	<div> <div>4%</div> <div>59%</div> <div>37%</div> <div>5%</div> </div>
1	B	531	<div> <div>3%</div> <div>56%</div> <div>39%</div> <div>.</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8428 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 HEPATITIS C VIRUS RNA POLYMERASE (NS5B).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	531	Total	C	N	O	S	Se	1	0	0
			4122	2595	727	769	19	12			
1	B	531	Total	C	N	O	S	Se	1	0	0
			4122	2595	727	769	19	12			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	94	Total	O	0	0
			94	94		
2	B	90	Total	O	0	0
			90	90		

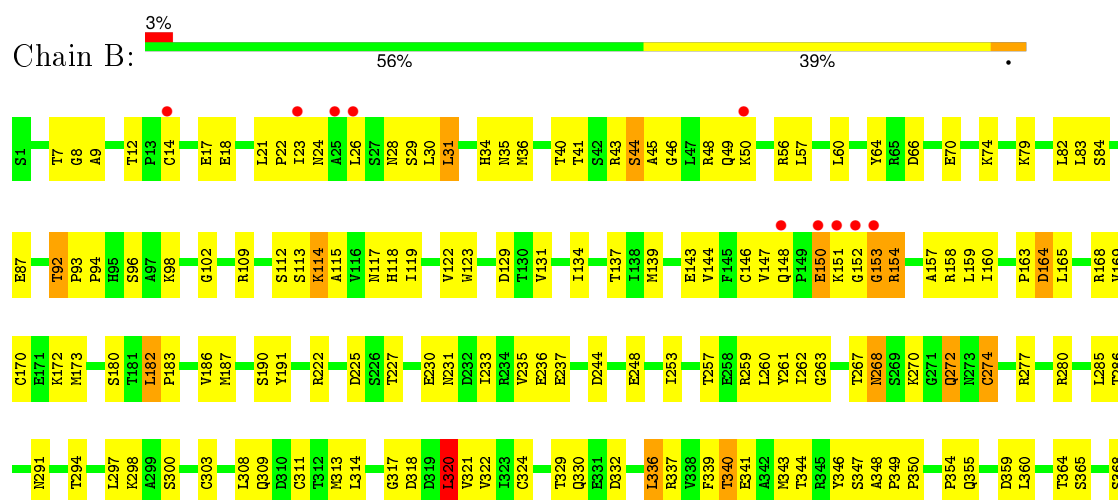
### 3 Residue-property plots

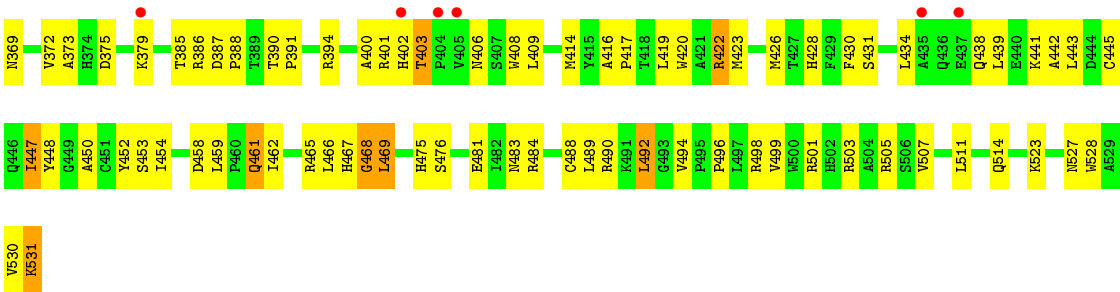
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: HEPATITIS C VIRUS RNA POLYMERASE (NS5B)



#### • Molecule 1: HEPATITIS C VIRUS RNA POLYMERASE (NS5B)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.06 Å 96.89 Å 194.43 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.00 – 2.80 19.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.5 (19.00-2.80) 92.5 (19.96-2.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.46 (at 2.79 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.237 , 0.286 0.236 , 0.283	Depositor DCC
$R_{free}$ test set	1983 reflections (6.73%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.2	Xtriage
Anisotropy	0.695	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	2 of 29492 reflections (0.007%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8428	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.96 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.8951e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [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	0.50	0/4198	0.68	3/5676 (0.1%)
1	B	0.49	0/4198	0.69	2/5676 (0.0%)
All	All	0.49	0/8396	0.68	5/11352 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	320	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	468	GLY	N-CA-C	5.30	126.35	113.10
1	A	320	LEU	CA-CB-CG	5.29	127.46	115.30
1	B	468	GLY	N-CA-C	5.28	126.29	113.10
1	A	163	PRO	N-CA-C	5.14	125.46	112.10

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	4122	0	4140	184	0
1	B	4122	0	4140	203	0
2	A	94	0	0	8	0
2	B	90	0	0	11	0
All	All	8428	0	8280	380	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 23.

All (380) 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:B:7:THR:O	1:B:9:ALA:N	1.89	1.04
1:A:170:CYS:HA	1:A:173:MSE:HE3	1.43	1.00
1:B:170:CYS:HA	1:B:173:MSE:HE3	1.44	0.99
1:B:344:THR:HG22	1:B:349:PRO:HA	1.43	0.98
1:A:344:THR:HG22	1:A:349:PRO:HA	1.46	0.97
1:A:7:THR:O	1:A:9:ALA:N	2.04	0.90
1:A:385:THR:HG22	1:A:386:ARG:H	1.37	0.89
1:A:48:ARG:HG2	1:A:159:LEU:HG	1.54	0.88
1:B:48:ARG:HG2	1:B:159:LEU:HG	1.53	0.88
1:B:148:GLN:HB3	1:B:150:GLU:HG2	1.56	0.87
1:A:96:SER:HB3	1:A:168:ARG:HH12	1.41	0.86
1:B:385:THR:HG22	1:B:386:ARG:H	1.40	0.85
1:B:7:THR:O	1:B:7:THR:HG23	1.76	0.84
1:B:96:SER:HB3	1:B:168:ARG:HH12	1.42	0.84
1:A:369:ASN:HD21	1:A:484:ARG:HH22	1.26	0.81
1:A:24:ASN:HD21	1:A:26:LEU:HB3	1.44	0.81
1:B:280:ARG:HE	1:B:291:ASN:HD21	1.25	0.81
1:B:385:THR:HG21	1:B:481:GLU:OE2	1.81	0.81
1:A:280:ARG:HE	1:A:291:ASN:HD21	1.29	0.80
1:B:369:ASN:HD21	1:B:484:ARG:HH22	1.29	0.80
1:A:79:LYS:HE2	1:B:79:LYS:HE2	1.63	0.79
1:B:253:ILE:O	1:B:257:THR:HG23	1.83	0.78
1:B:147:VAL:O	1:B:148:GLN:HG3	1.85	0.77
1:B:31:LEU:HD21	1:B:492:LEU:HD12	1.65	0.77
1:B:98:LYS:HD3	2:B:541:HOH:O	1.84	0.76
1:B:115:ALA:O	1:B:119:ILE:HG12	1.85	0.76
1:A:163:PRO:O	1:A:164:ASP:HB3	1.85	0.76
1:A:98:LYS:HD3	2:A:565:HOH:O	1.87	0.75
1:A:385:THR:HG21	1:A:481:GLU:OE2	1.87	0.75
1:A:31:LEU:HD21	1:A:492:LEU:HD12	1.68	0.74
1:A:498:ARG:HA	1:A:501:ARG:NH1	2.02	0.74
1:A:268:ASN:HB3	1:A:270:LYS:H	1.53	0.74
1:B:375:ASP:OD1	1:B:379:LYS:HG2	1.88	0.74
1:A:498:ARG:HA	1:A:501:ARG:HH12	1.53	0.73
1:B:163:PRO:O	1:B:164:ASP:HB3	1.89	0.73
1:A:309:GLN:O	1:A:324:CYS:HB2	1.90	0.72
1:A:222:ARG:HD3	2:A:602:HOH:O	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ASN:HB3	1:B:270:LYS:H	1.55	0.72
1:B:498:ARG:HA	1:B:501:ARG:HH12	1.55	0.72
1:B:498:ARG:HA	1:B:501:ARG:NH1	2.06	0.71
1:B:23:ILE:HG22	1:B:24:ASN:N	2.05	0.71
1:A:428:HIS:O	1:A:431:SER:HB3	1.90	0.71
1:A:375:ASP:OD1	1:A:379:LYS:HG2	1.90	0.71
1:A:253:ILE:O	1:A:257:THR:HG23	1.91	0.71
1:A:280:ARG:HE	1:A:291:ASN:ND2	1.89	0.71
1:B:280:ARG:HE	1:B:291:ASN:ND2	1.87	0.70
1:A:26:LEU:O	1:A:29:SER:HB3	1.91	0.70
1:A:530:VAL:HG12	1:A:531:LYS:HZ2	1.57	0.70
1:A:414:MSE:HG2	1:A:448:TYR:OH	1.91	0.70
1:B:468:GLY:O	1:B:469:LEU:HB2	1.92	0.69
1:B:336:LEU:O	1:B:340:THR:HG22	1.91	0.69
1:A:163:PRO:O	1:A:164:ASP:CB	2.41	0.69
1:A:24:ASN:ND2	1:A:26:LEU:HB3	2.08	0.69
1:B:490:ARG:HG2	1:B:490:ARG:HH11	1.58	0.69
1:A:313:MSE:HG2	1:A:322:VAL:HG22	1.74	0.69
1:B:309:GLN:O	1:B:324:CYS:HB2	1.93	0.68
1:B:163:PRO:O	1:B:164:ASP:CB	2.41	0.68
1:A:340:THR:O	1:A:344:THR:HG23	1.94	0.68
1:B:313:MSE:HG2	1:B:322:VAL:HG22	1.76	0.68
1:B:14:CYS:HB2	1:B:139:MSE:HE1	1.76	0.68
1:A:385:THR:HG22	1:A:386:ARG:N	2.09	0.67
1:B:428:HIS:O	1:B:431:SER:HB3	1.94	0.67
1:B:439:LEU:O	1:B:439:LEU:HD23	1.95	0.67
1:B:530:VAL:HG12	1:B:531:LYS:HZ2	1.59	0.66
1:A:115:ALA:O	1:A:119:ILE:HG12	1.95	0.66
1:A:237:GLU:HG3	1:A:257:THR:HG21	1.78	0.66
1:B:151:LYS:HG2	1:B:152:GLY:H	1.60	0.66
1:B:7:THR:O	1:B:7:THR:CG2	2.44	0.66
1:A:19:SER:HB2	2:A:580:HOH:O	1.95	0.66
1:B:523:LYS:O	1:B:527:ASN:HB2	1.96	0.66
1:A:490:ARG:HH11	1:A:490:ARG:HG2	1.60	0.65
1:B:237:GLU:HG3	1:B:257:THR:HG21	1.77	0.65
1:B:26:LEU:O	1:B:29:SER:HB3	1.96	0.65
1:B:468:GLY:O	1:B:469:LEU:CB	2.45	0.65
1:B:231:ASN:O	1:B:235:VAL:HG23	1.97	0.65
1:A:523:LYS:O	1:A:527:ASN:HB2	1.97	0.65
1:A:439:LEU:HD23	1:A:439:LEU:O	1.96	0.64
1:A:468:GLY:O	1:A:469:LEU:HB2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ILE:HG13	1:A:259:ARG:HB3	1.77	0.64
1:B:340:THR:O	1:B:344:THR:HG23	1.98	0.64
1:B:414:MSE:HG2	1:B:448:TYR:OH	1.98	0.64
1:B:336:LEU:HD12	1:B:354:PRO:HG2	1.79	0.63
1:A:336:LEU:O	1:A:340:THR:HG22	1.98	0.63
1:A:336:LEU:HD12	1:A:354:PRO:HG2	1.79	0.63
1:B:409:LEU:HD23	1:B:445:CYS:HB2	1.80	0.63
1:A:93:PRO:HG2	1:A:96:SER:OG	1.98	0.63
1:A:400:ALA:O	1:A:401:ARG:HG2	1.99	0.63
1:B:530:VAL:HG12	1:B:531:LYS:NZ	2.14	0.63
1:A:308:LEU:HB2	1:A:311:CYS:SG	2.38	0.62
1:B:66:ASP:O	1:B:70:GLU:HG3	1.99	0.62
1:B:400:ALA:O	1:B:401:ARG:HG2	2.00	0.62
1:A:530:VAL:HG12	1:A:531:LYS:NZ	2.14	0.62
1:A:60:LEU:HD13	1:A:64:TYR:CE2	2.34	0.61
2:A:574:HOH:O	1:B:112:SER:HB2	2.00	0.61
1:B:23:ILE:HG22	1:B:24:ASN:H	1.64	0.61
1:B:423:MSE:HG2	1:B:528:TRP:CZ3	2.35	0.61
1:B:119:ILE:HG22	1:B:173:MSE:HE1	1.82	0.61
1:B:143:GLU:OE2	1:B:158:ARG:HD3	1.99	0.61
1:B:496:PRO:HG2	1:B:499:VAL:HG23	1.83	0.61
1:B:346:TYR:O	1:B:347:SER:HB3	1.98	0.61
1:B:423:MSE:HG2	1:B:528:TRP:CH2	2.36	0.61
1:A:66:ASP:O	1:A:70:GLU:HG3	2.00	0.61
1:B:330:GLN:HB2	2:B:538:HOH:O	2.01	0.61
1:A:496:PRO:HG2	1:A:499:VAL:HG23	1.84	0.60
1:A:468:GLY:O	1:A:469:LEU:CB	2.48	0.60
1:B:294:THR:CG2	1:B:298:LYS:HE3	2.31	0.60
1:B:23:ILE:HD12	1:B:23:ILE:N	2.16	0.60
1:B:92:THR:HG21	1:B:169:VAL:HG22	1.83	0.60
1:A:423:MSE:HG2	1:A:528:TRP:CH2	2.37	0.59
1:B:40:THR:HB	1:B:157:ALA:HB2	1.84	0.59
1:A:180:SER:O	1:A:183:PRO:HD2	2.01	0.59
1:A:531:LYS:HD3	1:A:531:LYS:N	2.17	0.59
1:B:308:LEU:HB2	1:B:311:CYS:SG	2.43	0.59
1:B:123:TRP:HZ2	1:B:248:GLU:HG2	1.67	0.59
1:B:257:THR:HA	1:B:261:TYR:HB2	1.85	0.59
1:B:332:ASP:HA	2:B:604:HOH:O	2.03	0.59
1:A:505:ARG:HG2	1:A:530:VAL:HG22	1.84	0.58
1:A:465:ARG:NH1	1:B:117:ASN:OD1	2.36	0.58
1:A:346:TYR:O	1:A:347:SER:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ILE:HG13	1:B:259:ARG:HB3	1.85	0.58
1:A:409:LEU:HD23	1:A:445:CYS:HB2	1.84	0.58
1:B:9:ALA:HB3	1:B:274:CYS:HA	1.85	0.58
1:B:257:THR:O	1:B:262:ILE:HB	2.03	0.58
1:B:31:LEU:HD21	1:B:492:LEU:CD1	2.31	0.58
1:B:531:LYS:HD3	1:B:531:LYS:N	2.18	0.58
1:A:423:MSE:HG2	1:A:528:TRP:CZ3	2.38	0.58
1:A:321:VAL:CG2	1:A:365:SER:HB2	2.34	0.58
1:A:489:LEU:HD22	1:A:494:VAL:CG2	2.33	0.57
1:A:321:VAL:HG21	1:A:365:SER:CB	2.34	0.57
1:A:141:LYS:HD3	1:A:158:ARG:NH2	2.18	0.57
1:A:237:GLU:CG	1:A:257:THR:HG21	2.35	0.57
1:A:406:ASN:ND2	1:A:443:LEU:HB3	2.19	0.57
1:A:294:THR:CG2	1:A:298:LYS:HE3	2.35	0.57
1:A:257:THR:HA	1:A:261:TYR:HB2	1.86	0.57
1:B:385:THR:HG22	1:B:386:ARG:N	2.15	0.57
1:B:505:ARG:HG2	1:B:530:VAL:HG22	1.86	0.57
1:A:123:TRP:HZ2	1:A:248:GLU:HG2	1.70	0.57
1:B:329:THR:HG23	2:B:580:HOH:O	2.04	0.57
1:A:40:THR:HB	1:A:157:ALA:HB2	1.87	0.56
1:B:180:SER:O	1:B:183:PRO:HD2	2.05	0.56
1:B:93:PRO:HG2	1:B:96:SER:OG	2.04	0.56
1:B:43:ARG:HH11	1:B:43:ARG:HG3	1.70	0.56
1:B:369:ASN:HD21	1:B:484:ARG:NH2	2.00	0.56
1:B:237:GLU:CG	1:B:257:THR:HG21	2.35	0.56
1:A:369:ASN:HD21	1:A:484:ARG:NH2	2.00	0.56
1:A:401:ARG:HH11	1:A:401:ARG:HG3	1.70	0.56
1:B:7:THR:HG22	1:B:274:CYS:C	2.26	0.56
1:B:43:ARG:NH1	1:B:43:ARG:HG3	2.21	0.56
1:B:83:LEU:HB2	1:B:173:MSE:HA	1.88	0.56
1:A:117:ASN:OD1	1:B:465:ARG:NH1	2.39	0.55
1:B:300:SER:OG	1:B:313:MSE:HE1	2.06	0.55
1:A:385:THR:CG2	1:A:420:TRP:HE1	2.20	0.55
1:A:388:PRO:HG2	1:A:488:CYS:SG	2.47	0.55
1:A:321:VAL:CG2	1:A:365:SER:CB	2.83	0.55
1:B:321:VAL:CG2	1:B:365:SER:HB2	2.37	0.55
1:B:321:VAL:HG21	1:B:365:SER:CB	2.37	0.55
1:A:489:LEU:HD22	1:A:494:VAL:HG21	1.87	0.55
1:B:402:HIS:CG	1:B:403:THR:N	2.75	0.55
1:A:109:ARG:HG3	1:A:109:ARG:HH11	1.72	0.54
1:A:9:ALA:HB3	1:A:274:CYS:HA	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:LEU:HD13	1:B:64:TYR:CE2	2.42	0.54
1:A:43:ARG:HH11	1:A:43:ARG:HG3	1.72	0.54
1:A:31:LEU:HD21	1:A:492:LEU:CD1	2.37	0.54
1:A:475:HIS:O	1:A:476:SER:HB2	2.08	0.54
1:B:257:THR:HG22	1:B:261:TYR:HD2	1.72	0.54
1:A:43:ARG:NH1	1:A:43:ARG:HG3	2.22	0.54
1:B:385:THR:CG2	1:B:420:TRP:HE1	2.20	0.54
1:A:119:ILE:HG22	1:A:173:MSE:HE1	1.88	0.54
1:B:337:ARG:HA	1:B:340:THR:HG23	1.90	0.54
1:A:336:LEU:HD12	1:A:354:PRO:CG	2.38	0.54
1:A:82:LEU:HD11	1:A:248:GLU:HB3	1.90	0.53
1:B:263:GLY:HA2	1:B:277:ARG:NH1	2.23	0.53
1:A:83:LEU:HB2	1:A:173:MSE:HA	1.90	0.53
1:A:337:ARG:HA	1:A:340:THR:HG23	1.90	0.53
1:A:257:THR:HG22	1:A:261:TYR:HD2	1.72	0.53
1:B:321:VAL:CG2	1:B:365:SER:CB	2.85	0.53
1:B:503:ARG:O	1:B:507:VAL:HG23	2.08	0.53
1:B:336:LEU:HD12	1:B:354:PRO:CG	2.39	0.53
1:B:23:ILE:CG2	1:B:24:ASN:N	2.71	0.53
1:B:489:LEU:HD22	1:B:494:VAL:CG2	2.39	0.53
1:B:82:LEU:HD11	1:B:248:GLU:HB3	1.91	0.53
1:A:92:THR:HG21	1:A:169:VAL:HG22	1.90	0.53
1:A:30:LEU:O	1:A:494:VAL:HB	2.10	0.52
1:A:257:THR:O	1:A:262:ILE:HB	2.08	0.52
1:A:336:LEU:O	1:A:339:PHE:HB3	2.09	0.52
1:A:12:THR:OG1	1:A:270:LYS:HG2	2.09	0.52
1:B:475:HIS:O	1:B:476:SER:HB2	2.09	0.52
1:B:12:THR:OG1	1:B:270:LYS:HG2	2.08	0.52
1:A:187:MSE:HB2	1:A:190:SER:HB2	1.91	0.52
1:B:483:ASN:HB2	2:B:596:HOH:O	2.08	0.52
1:B:337:ARG:O	1:B:341:GLU:HG3	2.09	0.52
1:A:96:SER:HB3	1:A:168:ARG:NH1	2.19	0.52
1:B:14:CYS:CB	1:B:139:MSE:HE1	2.40	0.52
1:B:434:LEU:HD11	1:B:511:LEU:HG	1.92	0.52
1:A:233:ILE:HD13	1:A:261:TYR:O	2.10	0.52
1:A:503:ARG:O	1:A:507:VAL:HG23	2.10	0.52
1:B:163:PRO:HG2	1:B:168:ARG:HG3	1.92	0.52
1:B:23:ILE:CG2	1:B:24:ASN:H	2.23	0.52
1:A:434:LEU:HD11	1:A:511:LEU:HG	1.92	0.52
1:A:231:ASN:O	1:A:235:VAL:HG23	2.10	0.52
1:B:385:THR:CG2	1:B:386:ARG:H	2.20	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:MSE:HB2	1:B:190:SER:HB2	1.92	0.51
1:B:233:ILE:HD13	1:B:261:TYR:O	2.11	0.51
1:B:30:LEU:O	1:B:494:VAL:HB	2.10	0.51
1:A:507:VAL:HG12	1:A:511:LEU:HD12	1.92	0.51
1:B:484:ARG:NE	2:B:568:HOH:O	2.38	0.51
1:A:7:THR:HG22	1:A:274:CYS:C	2.31	0.51
1:A:402:HIS:O	1:A:403:THR:C	2.49	0.51
1:B:430:PHE:HD2	1:B:511:LEU:HD11	1.76	0.51
1:A:385:THR:HG23	1:A:420:TRP:HE1	1.75	0.50
1:B:22:PRO:HG2	1:B:400:ALA:HB3	1.92	0.50
1:A:430:PHE:HD2	1:A:511:LEU:HD11	1.77	0.50
1:A:30:LEU:HB2	1:A:428:HIS:CD2	2.47	0.50
1:B:406:ASN:O	1:B:409:LEU:N	2.44	0.50
1:A:422:ARG:HA	1:A:426:MSE:HE3	1.94	0.50
1:B:109:ARG:HG3	1:B:109:ARG:HH11	1.77	0.50
1:A:118:HIS:O	1:A:122:VAL:HG23	2.13	0.49
1:A:300:SER:OG	1:A:313:MSE:HE1	2.12	0.49
1:B:489:LEU:HD22	1:B:494:VAL:HG21	1.94	0.49
1:A:230:GLU:HG2	1:A:262:ILE:HG13	1.94	0.49
1:B:507:VAL:HG12	1:B:511:LEU:HD12	1.93	0.49
1:B:317:GLY:HA3	2:B:539:HOH:O	2.13	0.49
1:A:514:GLN:O	1:A:514:GLN:HG2	2.13	0.49
1:B:36:MSE:O	1:B:146:CYS:HA	2.13	0.48
1:B:280:ARG:NE	1:B:291:ASN:ND2	2.60	0.48
1:B:170:CYS:CA	1:B:173:MSE:HE3	2.31	0.48
1:B:164:ASP:HA	2:B:590:HOH:O	2.13	0.48
1:A:320:LEU:HD22	1:A:321:VAL:N	2.28	0.48
1:A:21:LEU:HD23	1:A:34:HIS:HA	1.94	0.48
1:B:442:ALA:O	1:B:443:LEU:HD23	2.12	0.48
1:B:30:LEU:HB2	1:B:428:HIS:CD2	2.48	0.48
1:A:308:LEU:CB	1:A:311:CYS:SG	3.01	0.48
1:B:172:LYS:HE3	2:B:536:HOH:O	2.14	0.48
1:A:113:SER:OG	1:B:454:ILE:HA	2.14	0.48
1:A:403:THR:O	1:A:405:VAL:N	2.46	0.47
1:A:36:MSE:O	1:A:146:CYS:HA	2.13	0.47
1:A:164:ASP:HA	2:A:545:HOH:O	2.13	0.47
1:A:453:SER:O	1:B:112:SER:HA	2.14	0.47
1:B:385:THR:HG23	1:B:420:TRP:HE1	1.79	0.47
1:A:227:THR:HB	1:A:347:SER:O	2.15	0.47
1:A:416:ALA:HB3	1:A:417:PRO:HD3	1.96	0.47
1:B:152:GLY:O	1:B:153:GLY:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:ILE:HA	1:B:465:ARG:HH12	1.79	0.47
1:B:422:ARG:HA	1:B:426:MSE:HE3	1.96	0.47
1:A:179:VAL:HG21	1:A:285:LEU:HD22	1.96	0.47
1:B:461:GLN:H	1:B:461:GLN:NE2	2.12	0.47
1:B:372:VAL:HG12	1:B:373:ALA:N	2.30	0.47
1:B:46:GLY:O	1:B:50:LYS:HG3	2.15	0.47
1:A:263:GLY:HA2	1:A:277:ARG:NH1	2.30	0.47
1:B:364:THR:HA	1:B:368:SER:O	2.15	0.47
1:B:514:GLN:O	1:B:514:GLN:HG2	2.15	0.47
1:B:102:GLY:O	1:B:114:LYS:HD2	2.15	0.47
1:B:336:LEU:O	1:B:339:PHE:HB3	2.13	0.46
1:A:163:PRO:HG2	1:A:168:ARG:HG3	1.97	0.46
1:B:160:ILE:HG13	1:B:160:ILE:O	2.15	0.46
1:B:96:SER:HB3	1:B:168:ARG:NH1	2.21	0.46
1:B:466:LEU:HB3	1:B:467:HIS:CD2	2.50	0.46
1:A:385:THR:CG2	1:A:386:ARG:H	2.17	0.46
1:A:129:ASP:O	1:A:259:ARG:NH1	2.48	0.46
1:A:466:LEU:HB3	1:A:467:HIS:CD2	2.51	0.46
1:A:102:GLY:O	1:A:114:LYS:HD2	2.15	0.46
1:B:402:HIS:CG	1:B:403:THR:H	2.33	0.46
1:B:268:ASN:HB2	1:B:272:GLN:H	1.81	0.46
1:A:45:ALA:O	1:A:49:GLN:HG3	2.16	0.46
1:B:490:ARG:HG2	1:B:490:ARG:NH1	2.27	0.46
1:A:355:GLN:NE2	1:A:355:GLN:HA	2.31	0.46
1:A:268:ASN:HB2	1:A:272:GLN:H	1.80	0.46
1:A:321:VAL:HG21	1:A:365:SER:HB3	1.97	0.46
1:B:45:ALA:O	1:B:49:GLN:HG3	2.16	0.46
1:A:28:ASN:HA	1:A:31:LEU:O	2.15	0.46
1:A:515:GLY:O	1:A:519:ALA:HB2	2.15	0.46
1:A:151:LYS:HB3	1:A:152:GLY:H	1.60	0.46
1:B:79:LYS:HG2	1:B:244:ASP:HB3	1.98	0.46
1:B:40:THR:HB	1:B:157:ALA:CB	2.45	0.45
1:B:26:LEU:N	1:B:26:LEU:HD22	2.32	0.45
1:A:112:SER:HA	1:B:453:SER:O	2.16	0.45
1:A:143:GLU:CD	1:A:158:ARG:HH21	2.20	0.45
1:B:447:ILE:O	1:B:448:TYR:C	2.54	0.45
1:B:187:MSE:HG3	1:B:191:TYR:HB2	1.99	0.45
1:A:390:THR:HB	1:A:391:PRO:HD3	1.98	0.45
1:B:344:THR:HG22	1:B:350:PRO:HD3	1.99	0.45
1:A:280:ARG:NE	1:A:291:ASN:ND2	2.62	0.45
1:A:490:ARG:HG2	1:A:490:ARG:NH1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ARG:HB3	1:A:403:THR:HG23	1.98	0.45
1:A:150:GLU:N	1:A:150:GLU:OE1	2.48	0.45
1:A:360:LEU:O	1:A:360:LEU:HD23	2.17	0.45
1:A:79:LYS:HG2	1:A:244:ASP:HB3	1.99	0.44
1:B:466:LEU:HD23	1:B:467:HIS:NE2	2.32	0.44
1:A:454:ILE:HA	1:B:113:SER:OG	2.17	0.44
1:A:337:ARG:O	1:A:341:GLU:HG3	2.17	0.44
1:B:34:HIS:C	1:B:36:MSE:H	2.19	0.44
1:A:447:ILE:O	1:A:448:TYR:C	2.56	0.44
1:A:40:THR:HB	1:A:157:ALA:CB	2.47	0.44
1:A:24:ASN:HB3	1:A:27:SER:OG	2.18	0.44
1:A:314:LEU:HD23	1:A:314:LEU:HA	1.86	0.44
1:A:236:GLU:OE2	1:A:280:ARG:NH2	2.37	0.44
1:B:450:ALA:HB3	1:B:452:TYR:CE1	2.52	0.44
1:B:225:ASP:HB2	2:B:619:HOH:O	2.18	0.44
1:A:403:THR:C	1:A:405:VAL:H	2.22	0.44
1:B:227:THR:HB	1:B:347:SER:O	2.17	0.43
1:A:347:SER:OG	1:A:347:SER:O	2.36	0.43
1:B:321:VAL:HG21	1:B:365:SER:HB3	1.99	0.43
1:A:36:MSE:O	1:A:147:VAL:HG23	2.18	0.43
1:A:461:GLN:NE2	1:A:461:GLN:H	2.16	0.43
1:A:38:TYR:OH	1:A:155:LYS:HG2	2.18	0.43
1:A:280:ARG:HH21	1:A:291:ASN:HD22	1.65	0.43
1:A:372:VAL:HG12	1:A:373:ALA:N	2.33	0.43
1:B:21:LEU:HD12	1:B:22:PRO:HD2	2.00	0.43
1:B:343:MSE:HG3	1:B:348:ALA:HB3	2.00	0.43
1:B:303:CYS:SG	1:B:308:LEU:HD12	2.58	0.43
1:A:182:LEU:HD22	1:A:182:LEU:O	2.19	0.43
1:A:344:THR:HG22	1:A:350:PRO:HD3	2.00	0.43
1:B:36:MSE:O	1:B:147:VAL:HG23	2.19	0.43
1:B:320:LEU:HD22	1:B:321:VAL:N	2.34	0.43
1:B:74:LYS:HB3	1:B:74:LYS:HE2	1.87	0.43
1:B:236:GLU:OE2	1:B:280:ARG:NH2	2.37	0.43
1:B:308:LEU:CB	1:B:311:CYS:SG	3.06	0.43
1:A:516:GLY:O	1:A:519:ALA:HB3	2.19	0.43
1:B:182:LEU:HD22	1:B:186:VAL:HG23	1.99	0.43
1:B:390:THR:HB	1:B:391:PRO:HD3	2.00	0.42
1:B:347:SER:O	1:B:347:SER:OG	2.33	0.42
1:A:321:VAL:CG2	1:A:365:SER:HB3	2.49	0.42
1:B:94:PRO:HA	1:B:109:ARG:NH1	2.34	0.42
1:A:391:PRO:HG3	2:A:621:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:GLU:OE1	1:B:41:THR:HB	2.19	0.42
1:B:230:GLU:HG2	1:B:262:ILE:HG13	2.02	0.42
1:B:144:VAL:HB	1:B:394:ARG:HG2	2.00	0.42
1:A:40:THR:HB	1:A:157:ALA:CA	2.49	0.42
1:A:187:MSE:HG3	1:A:191:TYR:HB2	2.01	0.42
1:B:355:GLN:HA	1:B:355:GLN:NE2	2.35	0.42
1:A:469:LEU:O	1:A:470:SER:C	2.58	0.42
1:B:18:GLU:OE2	1:B:401:ARG:NE	2.53	0.42
1:B:21:LEU:HD12	1:B:22:PRO:CD	2.49	0.42
1:B:40:THR:HB	1:B:157:ALA:CA	2.48	0.42
1:B:462:ILE:HA	1:B:465:ARG:NH1	2.35	0.42
1:A:34:HIS:C	1:A:36:MSE:H	2.22	0.42
1:B:388:PRO:HG2	1:B:488:CYS:SG	2.60	0.42
1:B:406:ASN:HB3	1:B:408:TRP:NE1	2.35	0.42
1:A:462:ILE:HA	1:A:465:ARG:HH12	1.85	0.42
1:A:180:SER:HB3	2:A:551:HOH:O	2.20	0.42
1:B:318:ASP:OD2	1:B:318:ASP:N	2.43	0.42
1:A:44:SER:HB3	1:A:156:PRO:HA	2.02	0.42
1:A:318:ASP:OD2	1:A:318:ASP:N	2.47	0.41
1:B:416:ALA:HB3	1:B:417:PRO:HD3	2.02	0.41
1:B:222:ARG:HG2	1:B:222:ARG:HH11	1.85	0.41
1:B:118:HIS:O	1:B:122:VAL:HG23	2.20	0.41
1:B:154:ARG:HH11	1:B:154:ARG:HG3	1.84	0.41
1:B:84:SER:OG	1:B:87:GLU:HG3	2.20	0.41
1:B:44:SER:O	1:B:45:ALA:C	2.59	0.41
1:A:99:SER:C	1:A:101:PHE:H	2.23	0.41
1:B:344:THR:CG2	1:B:350:PRO:HD3	2.51	0.41
1:B:129:ASP:O	1:B:259:ARG:NH1	2.54	0.41
1:B:459:LEU:HD23	1:B:459:LEU:HA	1.88	0.41
1:B:490:ARG:NH1	1:B:490:ARG:CG	2.82	0.41
1:A:39:ALA:HB2	1:A:397:TRP:CH2	2.56	0.41
1:A:144:VAL:HB	1:A:394:ARG:HG2	2.02	0.41
1:B:406:ASN:HD22	1:B:408:TRP:HE1	1.68	0.41
1:A:303:CYS:SG	1:A:308:LEU:HD12	2.61	0.41
1:B:28:ASN:HA	1:B:31:LEU:O	2.21	0.41
1:A:466:LEU:HD23	1:A:467:HIS:NE2	2.36	0.41
1:A:342:ALA:HA	1:A:345:ARG:CZ	2.50	0.41
1:A:74:LYS:HE2	1:A:74:LYS:HB3	1.88	0.41
1:B:419:LEU:C	1:B:419:LEU:HD23	2.41	0.41
1:B:119:ILE:HG22	1:B:173:MSE:CE	2.51	0.41
1:A:331:GLU:N	1:A:331:GLU:OE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:THR:HG22	1:B:274:CYS:O	2.21	0.40
1:B:147:VAL:HG12	1:B:148:GLN:N	2.36	0.40
1:B:280:ARG:HH21	1:B:291:ASN:HD22	1.70	0.40
1:A:355:GLN:HA	1:A:356:PRO:HD3	1.96	0.40
1:B:119:ILE:H	1:B:119:ILE:HG12	1.72	0.40
1:A:7:THR:HG22	1:A:274:CYS:O	2.21	0.40
1:B:375:ASP:O	1:B:475:HIS:HE1	2.04	0.40
1:A:222:ARG:HH11	1:A:222:ARG:HG2	1.85	0.40
1:A:489:LEU:HD22	1:A:494:VAL:HG22	2.01	0.40
1:B:56:ARG:O	1:B:57:LEU:HD23	2.20	0.40
1:A:172:LYS:HE3	2:A:563:HOH:O	2.21	0.40
1:A:235:VAL:O	1:A:239:ILE:HG13	2.21	0.40
1:B:359:ASP:HA	2:B:595:HOH:O	2.22	0.40
1:A:7:THR:O	1:A:7:THR:HG23	2.21	0.40
1:A:468:GLY:O	1:A:469:LEU:HG	2.21	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	529/531 (100%)	480 (91%)	40 (8%)	9 (2%)	11	36
1	B	529/531 (100%)	476 (90%)	44 (8%)	9 (2%)	11	36
All	All	1058/1062 (100%)	956 (90%)	84 (8%)	18 (2%)	11	36

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	GLY
1	A	164	ASP
1	A	268	ASN

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Mol	Chain	Res	Type
1	B	8	GLY
1	B	154	ARG
1	B	164	ASP
1	B	268	ASN
1	B	403	THR
1	A	404	PRO
1	A	438	GLN
1	A	469	LEU
1	B	153	GLY
1	B	438	GLN
1	B	469	LEU
1	B	35	ASN
1	A	35	ASN
1	A	403	THR
1	A	448	TYR

### 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	452/440 (103%)	423 (94%)	29 (6%)	22	52	
1	B	452/440 (103%)	423 (94%)	29 (6%)	22	52	
All	All	904/880 (103%)	846 (94%)	58 (6%)	22	52	

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	CYS
1	A	31	LEU
1	A	44	SER
1	A	83	LEU
1	A	92	THR
1	A	114	LYS
1	A	131	VAL
1	A	137	THR

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Mol	Chain	Res	Type
1	A	155	LYS
1	A	165	LEU
1	A	260	LEU
1	A	267	THR
1	A	272	GLN
1	A	274	CYS
1	A	285	LEU
1	A	286	THR
1	A	297	LEU
1	A	314	LEU
1	A	320	LEU
1	A	340	THR
1	A	360	LEU
1	A	387	ASP
1	A	422	ARG
1	A	441	LYS
1	A	447	ILE
1	A	458	ASP
1	A	461	GLN
1	A	492	LEU
1	A	531	LYS
1	B	31	LEU
1	B	44	SER
1	B	92	THR
1	B	114	LYS
1	B	131	VAL
1	B	137	THR
1	B	150	GLU
1	B	165	LEU
1	B	182	LEU
1	B	260	LEU
1	B	267	THR
1	B	272	GLN
1	B	274	CYS
1	B	285	LEU
1	B	286	THR
1	B	297	LEU
1	B	314	LEU
1	B	320	LEU
1	B	336	LEU
1	B	340	THR
1	B	360	LEU

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Mol	Chain	Res	Type
1	B	387	ASP
1	B	422	ARG
1	B	441	LYS
1	B	447	ILE
1	B	458	ASP
1	B	461	GLN
1	B	492	LEU
1	B	531	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	35	ASN
1	A	58	GLN
1	A	63	HIS
1	A	142	ASN
1	A	194	GLN
1	A	206	ASN
1	A	272	GLN
1	A	291	ASN
1	A	355	GLN
1	A	369	ASN
1	A	374	HIS
1	A	406	ASN
1	A	461	GLN
1	A	475	HIS
1	A	514	GLN
1	B	35	ASN
1	B	58	GLN
1	B	120	HIS
1	B	142	ASN
1	B	194	GLN
1	B	206	ASN
1	B	272	GLN
1	B	291	ASN
1	B	355	GLN
1	B	369	ASN
1	B	374	HIS
1	B	406	ASN
1	B	461	GLN
1	B	475	HIS

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Mol	Chain	Res	Type
1	B	514	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	519/531 (97%)	-0.01	20 (3%) 43 31	8, 26, 68, 89	0
1	B	519/531 (97%)	0.01	16 (3%) 52 40	9, 26, 67, 88	0
All	All	1038/1062 (97%)	-0.00	36 (3%) 48 35	8, 26, 67, 89	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	25	ALA	5.1
1	A	27	SER	3.9
1	A	151	LYS	3.9
1	B	405	VAL	3.8
1	B	25	ALA	3.7
1	B	402	HIS	3.6
1	B	151	LYS	3.5
1	B	152	GLY	3.4
1	A	23	ILE	3.3
1	A	148	GLN	3.2
1	A	513	SER	3.2
1	A	26	LEU	3.0
1	B	150	GLU	2.6
1	B	153	GLY	2.6
1	B	26	LEU	2.6
1	A	402	HIS	2.4
1	B	23	ILE	2.4
1	A	405	VAL	2.4
1	A	514	GLN	2.4
1	B	148	GLN	2.4
1	A	435	ALA	2.3
1	A	150	GLU	2.3
1	A	152	GLY	2.3
1	A	149	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	502	HIS	2.2
1	B	437	GLU	2.2
1	A	436	GLN	2.2
1	B	379	LYS	2.1
1	B	404	PRO	2.1
1	B	435	ALA	2.1
1	A	28	ASN	2.1
1	A	95	HIS	2.1
1	A	351	GLY	2.0
1	A	352	ASP	2.0
1	B	14	CYS	2.0
1	B	50	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 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.