



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:07 AM GMT

PDB ID : 2ZLF  
Title : The Structural Basis for Peptidomimetic Inhibition of Eukaryotic Ribonucleotide Reductase  
Authors : Xu, H.; Fairman, J.W.; Wijerathna, S.R.; LaMacchia, J.; Kreischer, N.R.; Helmbrecht, E.; Cooperman, B.S.; Dealwis, C.  
Deposited on : 2008-04-09  
Resolution : 2.59 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.

---

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

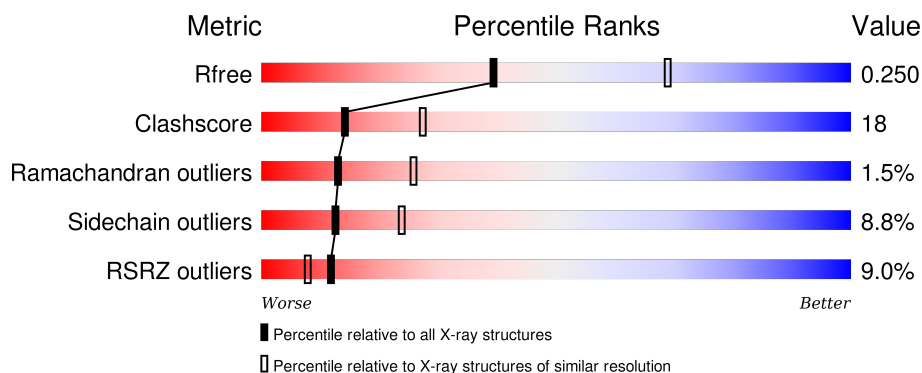
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	888	<div> <div>6%</div> <div>48%</div> <div>23%</div> <div>•</div> <div>25%</div> </div>
2	B	7	<div> <div>86%</div> <div>57%</div> <div>43%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5426 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 Ribonucleoside-diphosphate reductase large chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	663	Total	C	N	O	S	0	0	0
			5295	3370	902	992	31			

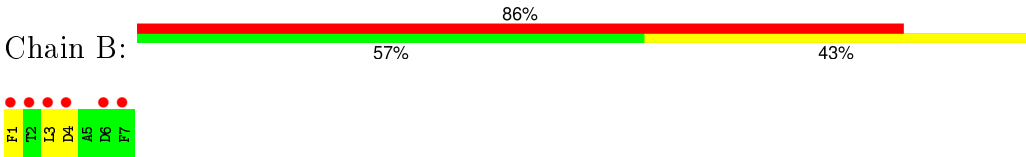
- Molecule 2 is a protein called FTLDADF.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	0	0	0
			59	39	7	13			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	71	Total	O	0	0
			71	71		
3	B	1	Total	O	0	0
			1	1		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.95Å 117.00Å 63.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.75 – 2.59 49.75 – 2.59	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.75-2.59) 96.1 (49.75-2.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.52 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.2.0007	Depositor
R, $R_{free}$	0.192 , 0.251 0.190 , 0.250	Depositor DCC
$R_{free}$ test set	1262 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.2	Xtriage
Anisotropy	0.716	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 24873 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5426	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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	0.48	0/5416	0.64	1/7332 (0.0%)
2	B	0.37	0/60	0.46	0/79
All	All	0.47	0/5476	0.64	1/7411 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	170	LEU	CA-CB-CG	5.26	127.40	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	458	GLU	Peptide

### 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	5295	0	5236	193	0
2	B	59	0	51	1	0
3	A	71	0	0	14	0
3	B	1	0	0	0	0
All	All	5426	0	5287	194	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 18.

All (194) 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:456:THR:HA	1:A:462:THR:HA	1.37	1.04
1:A:481:LEU:HB3	1:A:505:ILE:HD12	1.40	0.99
1:A:720:THR:HG23	1:A:723:LYS:HD2	1.61	0.83
1:A:292:LYS:C	1:A:294:PRO:HD3	1.98	0.83
1:A:649:LEU:HB3	1:A:655:TRP:HB2	1.61	0.83
1:A:686:THR:HG22	1:A:689:GLU:HG3	1.62	0.81
1:A:630:SER:C	1:A:639:GLN:N	2.34	0.81
1:A:170:LEU:HD22	1:A:173:ARG:NH2	1.97	0.80
1:A:510:GLN:NE2	1:A:612:SER:HA	2.00	0.76
1:A:393:LEU:HD22	1:A:724:LEU:HD13	1.68	0.75
1:A:245:ALA:HA	3:A:894:HOH:O	1.86	0.75
1:A:510:GLN:HE22	1:A:612:SER:HA	1.51	0.74
1:A:106:ASN:HB3	1:A:109:THR:HG22	1.69	0.74
1:A:508:GLY:HA3	1:A:606:MET:CE	2.18	0.74
1:A:659:MET:CE	1:A:659:MET:HA	2.18	0.73
1:A:288:GLN:HB2	1:A:293:ARG:HD2	1.70	0.73
1:A:530:LEU:O	1:A:534:GLN:HG3	1.88	0.72
1:A:242:SER:HB3	1:A:286:VAL:HG11	1.70	0.72
1:A:508:GLY:HA3	1:A:606:MET:HE2	1.73	0.71
1:A:212:LYS:HD3	3:A:940:HOH:O	1.91	0.69
1:A:666:GLN:OE1	1:A:666:GLN:HA	1.93	0.69
1:A:220:LEU:HD21	1:A:426:ASN:HB3	1.77	0.67
1:A:564:PRO:HD3	3:A:949:HOH:O	1.94	0.67
1:A:109:THR:HG23	1:A:111:LYS:H	1.60	0.67
1:A:126:GLU:OE1	1:A:181:ARG:NH1	2.27	0.66
1:A:655:TRP:HA	1:A:659:MET:HG3	1.77	0.65
1:A:670:ILE:HD11	1:A:684:TYR:HB2	1.77	0.65
1:A:560:PHE:CZ	1:A:596:GLY:HA2	2.31	0.65
1:A:330:PRO:HB2	1:A:402:PRO:HB3	1.79	0.63
1:A:628:MET:HA	1:A:640:VAL:O	1.99	0.63

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:ASN:HB3	1:A:645:LEU:HB3	1.81	0.63
1:A:483:ARG:NH2	1:A:487:ARG:HD2	2.13	0.62
1:A:660:LYS:O	1:A:664:ILE:HG13	2.00	0.61
1:A:717:ARG:O	1:A:746:GLN:HA	2.00	0.61
1:A:481:LEU:CB	1:A:505:ILE:HD12	2.25	0.61
1:A:166:ARG:HB2	1:A:169:HIS:ND1	2.16	0.60
1:A:520:ARG:HH22	1:A:648:ASP:CG	2.03	0.60
1:A:86:LEU:HD11	1:A:163:VAL:HG11	1.82	0.60
1:A:656:ASP:H	1:A:659:MET:HB2	1.65	0.60
1:A:109:THR:CG2	1:A:111:LYS:HB2	2.31	0.60
1:A:477:VAL:HG12	1:A:507:LEU:HD21	1.83	0.60
1:A:401:THR:HB	1:A:402:PRO:HA	1.84	0.60
1:A:167:PRO:O	1:A:171:ILE:HG13	2.00	0.60
1:A:140:ASP:OD2	1:A:167:PRO:HB2	2.02	0.60
1:A:306:ALA:HA	1:A:350:LEU:HB3	1.84	0.59
1:A:211:PRO:O	1:A:213:PRO:HD3	2.02	0.59
1:A:661:GLN:HE21	1:A:665:THR:HG21	1.66	0.59
1:A:105:VAL:HG22	1:A:112:PRO:HA	1.83	0.59
1:A:288:GLN:NE2	1:A:293:ARG:HH11	2.01	0.58
1:A:670:ILE:CD1	1:A:684:TYR:HB2	2.33	0.58
1:A:538:THR:HB	1:A:583:TRP:NE1	2.19	0.58
1:A:390:TYR:HB2	3:A:932:HOH:O	2.04	0.57
1:A:639:GLN:O	1:A:639:GLN:HG2	2.04	0.57
1:A:293:ARG:N	1:A:294:PRO:HD3	2.20	0.56
1:A:212:LYS:HA	3:A:940:HOH:O	2.05	0.56
1:A:483:ARG:HD3	3:A:891:HOH:O	2.05	0.56
1:A:183:ILE:HG23	1:A:187:LEU:HD13	1.87	0.56
1:A:582:MET:O	1:A:582:MET:HG2	2.05	0.56
1:A:140:ASP:OD2	1:A:168:GLN:HG2	2.05	0.55
1:A:699:ALA:HA	1:A:702:ARG:NH1	2.21	0.55
1:A:659:MET:HA	1:A:659:MET:HE1	1.88	0.55
1:A:273:ILE:HG21	1:A:323:ILE:HD12	1.89	0.55
1:A:481:LEU:HB3	1:A:505:ILE:CD1	2.27	0.55
1:A:454:ILE:HD13	1:A:518:LEU:HB3	1.89	0.55
1:A:313:ASP:O	1:A:316:LYS:HB2	2.07	0.54
1:A:482:ASN:ND2	1:A:599:ASN:OD1	2.41	0.54
1:A:294:PRO:HG3	3:A:923:HOH:O	2.07	0.53
1:A:606:MET:HE3	1:A:608:THR:CG2	2.38	0.53
1:A:618:ASN:ND2	1:A:624:VAL:HG12	2.24	0.53
1:A:534:GLN:O	1:A:538:THR:HG23	2.09	0.52
1:A:510:GLN:HA	1:A:620:CYS:HA	1.92	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:TYR:HB2	3:A:925:HOH:O	2.10	0.52
1:A:273:ILE:HD11	1:A:310:ASP:HB3	1.91	0.52
1:A:629:TYR:O	1:A:639:GLN:N	2.43	0.51
1:A:607:PRO:HD3	1:A:711:SER:OG	2.10	0.51
1:A:713:ASN:ND2	1:A:742:TYR:HB2	2.25	0.51
1:A:538:THR:HG22	1:A:583:TRP:HE1	1.75	0.51
1:A:326:ARG:HB3	1:A:326:ARG:NH1	2.26	0.51
1:A:251:HIS:HB3	1:A:424:SER:HB3	1.93	0.51
1:A:477:VAL:CG1	1:A:507:LEU:HD21	2.41	0.50
1:A:318:HIS:O	1:A:324:ARG:NH1	2.45	0.50
1:A:135:ILE:HG21	1:A:137:TYR:CZ	2.47	0.49
1:A:482:ASN:HD21	1:A:599:ASN:HD21	1.60	0.49
1:A:166:ARG:HB2	1:A:169:HIS:CE1	2.47	0.49
1:A:284:ARG:HD2	1:A:327:ASP:OD2	2.13	0.49
1:A:456:THR:CG2	1:A:459:ASP:HB3	2.42	0.49
1:A:482:ASN:HD21	1:A:599:ASN:ND2	2.10	0.49
1:A:253:HIS:CE1	1:A:302:GLU:HG3	2.48	0.48
1:A:456:THR:HG21	1:A:459:ASP:HB3	1.95	0.48
1:A:294:PRO:HD2	3:A:894:HOH:O	2.13	0.48
1:A:447:SER:HB3	1:A:606:MET:HE1	1.95	0.48
1:A:109:THR:HG23	1:A:111:LYS:N	2.28	0.48
1:A:257:SER:HA	1:A:307:ASP:OD2	2.13	0.48
1:A:679:GLU:HG3	1:A:680:LEU:N	2.27	0.48
1:A:477:VAL:CG1	1:A:507:LEU:CD2	2.92	0.48
1:A:109:THR:CG2	1:A:111:LYS:H	2.24	0.48
1:A:472:GLU:O	1:A:475:LYS:HB2	2.14	0.48
1:A:475:LYS:HD2	1:A:546:ALA:HB2	1.96	0.48
1:A:719:PRO:HG3	1:A:745:THR:OG1	2.14	0.48
1:A:509:VAL:O	1:A:620:CYS:HA	2.15	0.47
1:A:506:ALA:HB1	1:A:604:ALA:HB3	1.96	0.47
1:A:657:GLU:C	1:A:659:MET:H	2.17	0.47
1:A:94:PHE:HD1	1:A:169:HIS:HD2	1.62	0.47
1:A:459:ASP:N	1:A:459:ASP:OD2	2.47	0.47
1:A:288:GLN:H	1:A:293:ARG:CD	2.26	0.47
1:A:538:THR:HB	1:A:583:TRP:CE2	2.49	0.47
1:A:142:GLN:NE2	1:A:142:GLN:N	2.63	0.47
1:A:326:ARG:HB3	1:A:326:ARG:HH11	1.79	0.47
1:A:652:LEU:C	1:A:654:ILE:H	2.18	0.47
1:A:314:ILE:HD12	1:A:314:ILE:HA	1.75	0.47
1:A:656:ASP:OD1	1:A:659:MET:HG2	2.15	0.47
1:A:482:ASN:ND2	1:A:599:ASN:HD21	2.12	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:LYS:C	1:A:463:SER:N	2.66	0.46
1:A:94:PHE:O	1:A:97:VAL:HG22	2.15	0.46
1:A:724:LEU:HD22	1:A:728:HIS:NE2	2.30	0.46
1:A:251:HIS:HE1	1:A:435:SER:OG	1.97	0.46
1:A:519:LEU:O	1:A:520:ARG:HB2	2.16	0.46
1:A:244:THR:HG21	1:A:491:PRO:HB3	1.97	0.46
1:A:538:THR:CG2	1:A:583:TRP:HE1	2.29	0.46
1:A:693:LYS:HG3	1:A:730:TYR:CE2	2.50	0.46
1:A:300:TYR:OH	1:A:425:SER:HB3	2.16	0.46
1:A:443:CYS:HA	3:A:939:HOH:O	2.15	0.46
1:A:389:TRP:NE1	1:A:393:LEU:HD11	2.30	0.46
1:A:702:ARG:HH11	1:A:710:HIS:HE1	1.64	0.46
1:A:453:PHE:HD2	1:A:469:LYS:HB3	1.81	0.45
1:A:606:MET:HB2	1:A:607:PRO:HD2	1.98	0.45
1:A:477:VAL:HG12	1:A:507:LEU:CD2	2.47	0.45
1:A:486:ASP:OD2	1:A:503:ARG:NH2	2.48	0.45
1:A:656:ASP:H	1:A:659:MET:CB	2.28	0.45
1:A:724:LEU:HD22	1:A:728:HIS:CD2	2.51	0.45
1:A:588:LEU:O	1:A:588:LEU:HD12	2.16	0.45
1:A:650:VAL:C	1:A:652:LEU:H	2.20	0.45
1:A:255:ILE:HB	1:A:272:LEU:HD21	1.99	0.45
1:A:170:LEU:O	1:A:174:VAL:HG23	2.17	0.45
1:A:746:GLN:HB2	3:A:904:HOH:O	2.17	0.45
1:A:661:GLN:O	1:A:665:THR:HG23	2.17	0.45
1:A:96:LYS:HA	1:A:96:LYS:HD2	1.84	0.44
1:A:557:TYR:HB3	1:A:598:ARG:O	2.18	0.44
1:A:428:CYS:HB2	1:A:430:GLU:OE2	2.18	0.44
1:A:308:ILE:O	1:A:312:ILE:HG23	2.16	0.44
1:A:338:PHE:O	1:A:342:VAL:HG23	2.18	0.44
2:B:1:PHE:CZ	2:B:3:LEU:HD21	2.53	0.44
1:A:288:GLN:HB2	1:A:293:ARG:CD	2.42	0.44
1:A:482:ASN:HD21	1:A:599:ASN:CG	2.21	0.44
1:A:702:ARG:HH11	1:A:710:HIS:CE1	2.36	0.44
1:A:95:SER:HB3	1:A:128:LYS:HB2	1.99	0.44
1:A:396:GLN:HA	1:A:401:THR:O	2.18	0.44
1:A:575:TRP:CZ2	1:A:703:SER:HB3	2.52	0.43
1:A:183:ILE:O	1:A:187:LEU:HD13	2.18	0.43
1:A:120:VAL:O	1:A:124:VAL:HG23	2.18	0.43
1:A:534:GLN:O	1:A:538:THR:CG2	2.66	0.43
1:A:518:LEU:HA	1:A:518:LEU:HD12	1.81	0.43
1:A:436:ALA:HB1	1:A:437:PRO:HD2	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:GLY:O	1:A:291:ASN:N	2.51	0.42
1:A:649:LEU:HD23	1:A:649:LEU:HA	1.84	0.42
1:A:675:ASN:HB3	3:A:937:HOH:O	2.19	0.42
1:A:213:PRO:HD2	1:A:489:TYR:HB2	2.00	0.42
1:A:384:LYS:HD2	3:A:918:HOH:O	2.19	0.42
1:A:718:ALA:HA	1:A:746:GLN:NE2	2.35	0.42
1:A:454:ILE:HG12	1:A:519:LEU:HD21	2.01	0.42
1:A:288:GLN:HB3	1:A:289:GLY:H	1.58	0.42
1:A:179:HIS:CE1	1:A:480:ASN:OD1	2.73	0.42
1:A:451:PRO:HG3	1:A:514:ASP:HB2	1.99	0.42
1:A:363:TYR:HB2	1:A:408:ASP:OD1	2.19	0.42
1:A:244:THR:OG1	1:A:245:ALA:N	2.52	0.42
1:A:109:THR:HG23	1:A:111:LYS:HG3	2.01	0.42
1:A:119:ASP:O	1:A:123:ILE:HD12	2.20	0.42
1:A:109:THR:HG23	1:A:111:LYS:CB	2.50	0.42
1:A:473:ILE:O	1:A:477:VAL:HG23	2.19	0.42
1:A:251:HIS:HD2	3:A:892:HOH:O	2.02	0.42
1:A:142:GLN:HE21	1:A:142:GLN:N	2.16	0.42
1:A:471:HIS:HE1	1:A:545:GLU:OE2	2.02	0.42
1:A:508:GLY:HA3	1:A:606:MET:HE1	1.98	0.41
1:A:717:ARG:HD2	1:A:717:ARG:HA	1.84	0.41
1:A:294:PRO:HB2	1:A:295:GLY:H	1.59	0.41
1:A:273:ILE:HB	1:A:274:PRO:HD3	2.03	0.41
1:A:512:LEU:HD23	1:A:512:LEU:HA	1.88	0.41
1:A:260:SER:O	1:A:268:THR:HB	2.20	0.41
1:A:292:LYS:HA	1:A:292:LYS:HD2	1.78	0.41
1:A:131:LEU:HD12	1:A:131:LEU:HA	1.82	0.41
1:A:170:LEU:HD22	1:A:173:ARG:HH22	1.83	0.41
1:A:174:VAL:O	1:A:178:ILE:HG13	2.21	0.41
1:A:486:ASP:CG	1:A:503:ARG:HH22	2.24	0.41
1:A:199:THR:HG21	1:A:611:THR:HB	2.02	0.41
1:A:656:ASP:HB2	1:A:657:GLU:H	1.60	0.41
1:A:657:GLU:OE2	1:A:660:LYS:HD3	2.21	0.40
1:A:510:GLN:HE22	1:A:615:LEU:HB2	1.85	0.40
1:A:602:THR:N	1:A:707:ASP:OD2	2.54	0.40
1:A:666:GLN:O	1:A:668:GLY:N	2.54	0.40
1:A:557:TYR:CE1	1:A:600:SER:HB3	2.57	0.40
1:A:487:ARG:HG2	1:A:487:ARG:HH11	1.86	0.40
1:A:716:LEU:HD13	1:A:719:PRO:HA	2.03	0.40
1:A:651:ASP:O	1:A:652:LEU:HD23	2.20	0.40
1:A:172:MET:HE2	1:A:190:TYR:CD1	2.56	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	659/888 (74%)	605 (92%)	44 (7%)	10 (2%)	13	26
2	B	5/7 (71%)	5 (100%)	0	0	100	100
All	All	664/895 (74%)	610 (92%)	44 (7%)	10 (2%)	13	26

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	LYS
1	A	457	SER
1	A	459	ASP
1	A	717	ARG
1	A	289	GLY
1	A	290	GLY
1	A	294	PRO
1	A	629	TYR
1	A	667	ASN
1	A	321	GLU

### 5.3.2 Protein sidechains [i](#)

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	574/761 (75%)	524 (91%)	50 (9%)	13	24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	6/6 (100%)	5 (83%)	1 (17%)	3	4
All	All	580/767 (76%)	529 (91%)	51 (9%)	12	24

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	ASP
1	A	125	MET
1	A	131	LEU
1	A	138	ASP
1	A	142	GLN
1	A	159	ILE
1	A	162	GLN
1	A	170	LEU
1	A	176	LEU
1	A	214	GLN
1	A	242	SER
1	A	244	THR
1	A	265	THR
1	A	287	ASP
1	A	288	GLN
1	A	292	LYS
1	A	293	ARG
1	A	301	LEU
1	A	314	ILE
1	A	326	ARG
1	A	337	LEU
1	A	359	LEU
1	A	361	ASP
1	A	388	LEU
1	A	443	CYS
1	A	444	ASN
1	A	445	LEU
1	A	462	THR
1	A	482	ASN
1	A	503	ARG
1	A	505	ILE
1	A	512	LEU
1	A	514	ASP
1	A	518	LEU
1	A	530	LEU
1	A	538	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	606	MET
1	A	629	TYR
1	A	656	ASP
1	A	659	MET
1	A	667	ASN
1	A	679	GLU
1	A	686	THR
1	A	707	ASP
1	A	712	LEU
1	A	714	LEU
1	A	721	MET
1	A	724	LEU
1	A	743	LEU
1	A	745	THR
2	B	4	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
1	A	142	GLN
1	A	168	GLN
1	A	251	HIS
1	A	266	ASN
1	A	288	GLN
1	A	317	ASN
1	A	482	ASN
1	A	510	GLN
1	A	567	GLN
1	A	599	ASN
1	A	618	ASN
1	A	661	GLN
1	A	667	ASN
1	A	692	GLN
1	A	710	HIS
1	A	713	ASN
1	A	746	GLN

### 5.3.3 RNA ⓘ

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	663/888 (74%)	0.40	54 (8%) 15 10	15, 31, 76, 94	0
2	B	7/7 (100%)	3.35	6 (85%) 0 0	44, 57, 70, 70	0
All	All	670/895 (74%)	0.43	60 (8%) 12 8	15, 32, 76, 94	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	289	GLY	7.5
1	A	640	VAL	7.1
1	A	663	LEU	6.6
1	A	639	GLN	6.5
1	A	290	GLY	6.5
1	A	629	TYR	5.5
1	A	318	HIS	5.5
1	A	80	ARG	5.2
2	B	3	LEU	5.1
1	A	78	ALA	4.9
1	A	145	TYR	4.8
1	A	655	TRP	4.8
1	A	146	PHE	4.7
1	A	77	LEU	4.6
2	B	2	THR	4.5
1	A	323	ILE	4.5
1	A	81	ILE	4.2
1	A	79	ALA	4.1
1	A	662	TYR	4.0
1	A	319	GLY	4.0
1	A	292	LYS	3.9
1	A	459	ASP	3.9
1	A	320	LYS	3.8
1	A	661	GLN	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	4	ASP	3.7
1	A	660	LYS	3.5
2	B	6	ASP	3.5
1	A	321	GLU	3.5
2	B	1	PHE	3.3
1	A	462	THR	3.2
1	A	317	ASN	3.1
2	B	7	PHE	2.9
1	A	654	ILE	2.9
1	A	630	SER	2.8
1	A	83	ILE	2.8
1	A	656	ASP	2.8
1	A	659	MET	2.6
1	A	665	THR	2.6
1	A	390	TYR	2.5
1	A	293	ARG	2.5
1	A	652	LEU	2.5
1	A	88	LYS	2.4
1	A	82	ALA	2.4
1	A	428	CYS	2.4
1	A	670	ILE	2.4
1	A	628	MET	2.4
1	A	87	HIS	2.4
1	A	84	SER	2.4
1	A	641	VAL	2.3
1	A	429	CYS	2.3
1	A	142	GLN	2.3
1	A	657	GLU	2.2
1	A	322	GLU	2.2
1	A	427	LEU	2.2
1	A	181	ARG	2.2
1	A	294	PRO	2.1
1	A	460	GLY	2.1
1	A	672	GLY	2.1
1	A	288	GLN	2.1
1	A	746	GLN	2.1

## 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.