



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:06 AM GMT

PDB ID : 2PGG  
Title : Crystal Structure of a Birnavirus (IBDV) RNA-dependent RNA Polymerase VP1  
Authors : Pan, J.; Vakharia, V.N.; Tao, Y.J.  
Deposited on : 2007-04-09  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<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

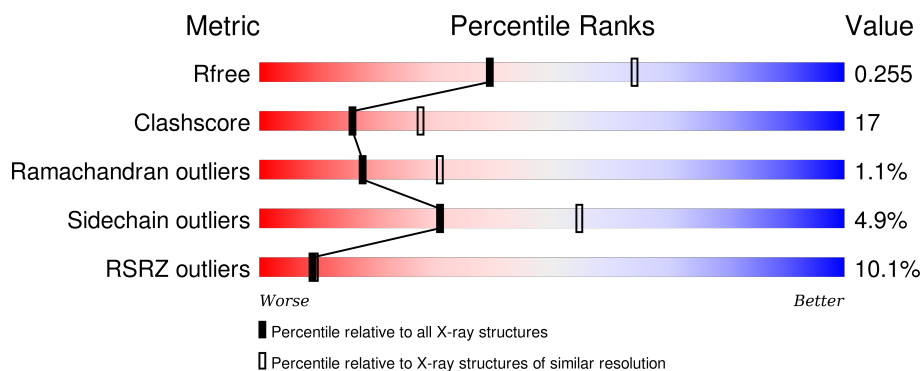
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	774	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6447 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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	765	Total	C	N	O	S	0	0	0
			6020	3848	1014	1136	22			

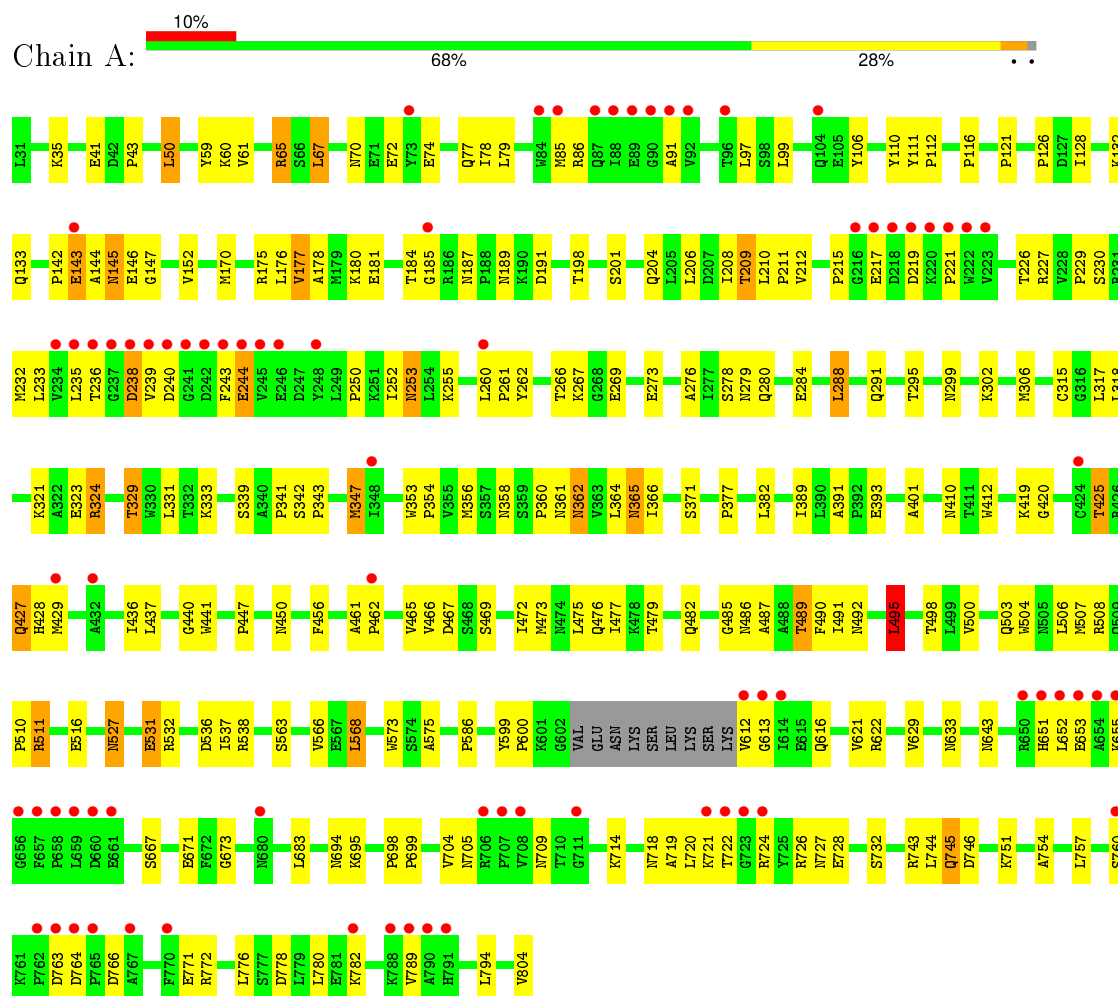
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	427	Total	O	0	0
			427	427		

### 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: RNA-directed RNA polymerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.10Å 122.10Å 359.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.97 – 2.50 39.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.3 (39.97-2.50) 96.4 (39.97-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.63 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.216 , 0.254 0.217 , 0.255	Depositor DCC
$R_{free}$ test set	3267 reflections (6.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.5	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 55.8	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	0 of 53744 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6447	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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	0.35	0/6164	0.61	1/8377 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	495	LEU	CA-CB-CG	6.22	129.62	115.30

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	6020	0	6033	205	1
2	A	427	0	0	17	0
All	All	6447	0	6033	205	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (205) 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:722:THR:HG23	1:A:724:ARG:H	1.11	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:TRP:HB2	1:A:537:ILE:HD12	1.43	0.99
1:A:612:VAL:HG13	1:A:613:GLY:H	1.32	0.92
1:A:209:THR:HG21	1:A:498:THR:OG1	1.75	0.84
1:A:191:ASP:CG	1:A:427:GLN:HG3	1.98	0.84
1:A:486:ASN:O	1:A:489:THR:HG22	1.77	0.84
1:A:78:ILE:HG22	1:A:79:LEU:HD22	1.63	0.81
1:A:329:THR:HG23	1:A:333:LYS:HB3	1.62	0.81
1:A:425:THR:HG22	1:A:428:HIS:H	1.47	0.79
1:A:722:THR:HG23	1:A:724:ARG:N	1.95	0.78
1:A:425:THR:HG23	1:A:427:GLN:HE21	1.50	0.76
1:A:425:THR:CG2	1:A:427:GLN:HG2	2.15	0.75
1:A:412:TRP:CB	1:A:537:ILE:HD12	2.17	0.75
1:A:425:THR:HB	1:A:428:HIS:HD2	1.50	0.75
1:A:323:GLU:HG3	2:A:1318:HOH:O	1.86	0.74
1:A:616:GLN:HB2	1:A:652:LEU:HD21	1.71	0.72
1:A:110:TYR:CE2	1:A:112:PRO:HG3	2.25	0.71
1:A:516:GLU:HG3	2:A:1104:HOH:O	1.91	0.71
1:A:86:ARG:HA	1:A:91:ALA:HB1	1.74	0.69
1:A:59:TYR:HE2	1:A:477:ILE:CG2	2.06	0.67
1:A:425:THR:HB	1:A:428:HIS:CD2	2.28	0.67
1:A:586:PRO:HD2	1:A:694:ASN:HD21	1.59	0.67
1:A:429:MET:HE3	1:A:465:VAL:HG23	1.74	0.67
1:A:719:ALA:O	1:A:722:THR:HG22	1.95	0.66
1:A:260:LEU:CD2	1:A:315:CYS:HB3	2.25	0.66
1:A:527:ASN:N	1:A:527:ASN:HD22	1.95	0.65
1:A:511:ARG:HB3	1:A:511:ARG:HH11	1.60	0.65
1:A:146:GLU:HG3	2:A:1344:HOH:O	1.96	0.65
1:A:266:THR:OG1	1:A:269:GLU:HG3	1.97	0.65
1:A:616:GLN:HG3	1:A:651:HIS:HD2	1.62	0.65
1:A:586:PRO:HD2	1:A:694:ASN:ND2	2.12	0.64
1:A:321:LYS:HE3	1:A:323:GLU:OE1	1.98	0.64
1:A:324:ARG:NH1	1:A:599:TYR:O	2.29	0.64
1:A:291:GLN:HE22	1:A:302:LYS:HD2	1.61	0.64
1:A:208:ILE:HD11	1:A:709:ASN:HB3	1.79	0.64
1:A:206:LEU:HD11	1:A:495:LEU:HD22	1.80	0.64
1:A:566:VAL:HG12	1:A:568:LEU:HD13	1.80	0.63
1:A:485:GLY:H	1:A:489:THR:HG21	1.64	0.62
1:A:425:THR:HG21	1:A:427:GLN:HG2	1.81	0.62
1:A:187:ASN:HD22	1:A:527:ASN:ND2	1.97	0.62
1:A:362:ASN:HD22	1:A:362:ASN:C	2.02	0.62
1:A:429:MET:CE	1:A:492:ASN:HD21	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:VAL:HG12	1:A:705:ASN:N	2.14	0.62
1:A:185:GLY:HA2	2:A:1166:HOH:O	1.99	0.62
1:A:252:ILE:HD11	1:A:267:LYS:HD3	1.82	0.62
1:A:616:GLN:HG3	1:A:651:HIS:CD2	2.34	0.61
1:A:238:ASP:C	1:A:240:ASP:H	2.03	0.61
1:A:116:PRO:HB2	1:A:121:PRO:HA	1.83	0.61
1:A:181:GLU:O	1:A:184:THR:O	2.18	0.61
1:A:745:GLN:HG2	2:A:1256:HOH:O	2.01	0.61
1:A:600:PRO:HB3	1:A:622:ARG:HD2	1.82	0.60
1:A:714:LYS:HB2	2:A:1418:HOH:O	2.01	0.60
1:A:462:PRO:HB2	1:A:794:LEU:HD21	1.82	0.60
1:A:778:ASP:O	1:A:782:LYS:HG2	2.00	0.60
1:A:191:ASP:OD1	1:A:427:GLN:HG3	2.02	0.60
1:A:291:GLN:NE2	1:A:302:LYS:HD2	2.17	0.60
1:A:771:GLU:OE1	1:A:772:ARG:HD2	2.02	0.60
1:A:425:THR:HG23	1:A:427:GLN:HG2	1.85	0.59
1:A:236:THR:HB	1:A:244:GLU:HB3	1.85	0.58
1:A:65:ARG:HD3	1:A:476:GLN:OE1	2.01	0.58
1:A:667:SER:O	1:A:673:GLY:HA3	2.03	0.58
1:A:356:MET:HE3	1:A:436:ILE:HD11	1.85	0.58
1:A:722:THR:HA	2:A:1475:HOH:O	2.03	0.58
1:A:198:THR:H	1:A:201:SER:HB3	1.68	0.58
1:A:382:LEU:HD22	1:A:586:PRO:HA	1.85	0.58
1:A:41:GLU:O	1:A:43:PRO:HD3	2.03	0.58
1:A:226:THR:HA	1:A:450:ASN:ND2	2.19	0.57
1:A:145:ASN:ND2	1:A:147:GLY:H	2.02	0.57
1:A:362:ASN:H	1:A:365:ASN:HD21	1.50	0.57
1:A:429:MET:HE2	1:A:492:ASN:ND2	2.20	0.57
1:A:35:LYS:HG2	2:A:1121:HOH:O	2.05	0.57
1:A:531:GLU:OE1	1:A:532:ARG:HB2	2.05	0.57
1:A:482:GLN:OE1	1:A:489:THR:HA	2.05	0.56
1:A:425:THR:HG22	1:A:428:HIS:N	2.20	0.56
1:A:291:GLN:OE1	1:A:299:ASN:HB3	2.06	0.56
1:A:704:VAL:HG12	1:A:705:ASN:H	1.70	0.56
1:A:612:VAL:HG13	1:A:613:GLY:N	2.12	0.55
1:A:362:ASN:ND2	1:A:364:LEU:H	2.04	0.54
1:A:295:THR:HG21	2:A:1491:HOH:O	2.07	0.54
1:A:324:ARG:NH2	1:A:671:GLU:OE1	2.41	0.54
1:A:85:MET:SD	1:A:233:LEU:HD13	2.47	0.54
1:A:486:ASN:O	1:A:489:THR:CG2	2.53	0.53
1:A:427:GLN:NE2	1:A:427:GLN:H	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:TYR:CE2	1:A:477:ILE:CG2	2.91	0.53
1:A:511:ARG:HH11	1:A:511:ARG:CB	2.20	0.52
1:A:60:LYS:HE3	2:A:1270:HOH:O	2.09	0.52
1:A:59:TYR:HE2	1:A:477:ILE:HG23	1.74	0.52
1:A:260:LEU:HD22	1:A:315:CYS:HB3	1.89	0.52
1:A:382:LEU:HD22	1:A:586:PRO:CA	2.40	0.52
1:A:429:MET:CE	1:A:492:ASN:ND2	2.72	0.52
1:A:504:TRP:CD1	1:A:510:PRO:HD2	2.45	0.51
1:A:230:SER:CB	1:A:279:ASN:HD21	2.24	0.51
1:A:507:MET:O	1:A:508:ARG:HB2	2.11	0.51
1:A:280:GLN:O	1:A:284:GLU:HG3	2.10	0.51
1:A:467:ASP:HA	1:A:479:THR:O	2.11	0.51
1:A:126:PRO:HG3	1:A:599:TYR:CE2	2.46	0.50
1:A:243:PHE:O	1:A:244:GLU:HB2	2.10	0.50
1:A:425:THR:HG23	1:A:427:GLN:H	1.76	0.50
1:A:86:ARG:NH1	1:A:86:ARG:HB3	2.26	0.50
1:A:253:ASN:ND2	1:A:255:LYS:H	2.10	0.50
1:A:503:GLN:O	1:A:507:MET:HG3	2.11	0.50
1:A:145:ASN:HD22	1:A:145:ASN:C	2.13	0.50
1:A:170:MET:HG3	1:A:331:LEU:O	2.12	0.50
1:A:429:MET:HE3	1:A:465:VAL:CG2	2.42	0.49
1:A:429:MET:HE3	1:A:466:VAL:HG23	1.93	0.49
1:A:356:MET:HE3	1:A:436:ILE:CD1	2.42	0.49
1:A:178:ALA:HB1	1:A:419:LYS:HE2	1.95	0.49
1:A:612:VAL:CG1	1:A:613:GLY:H	2.15	0.49
1:A:79:LEU:HD23	1:A:97:LEU:HD11	1.95	0.49
1:A:230:SER:HB3	1:A:279:ASN:HD21	1.78	0.49
1:A:425:THR:HG23	1:A:427:GLN:NE2	2.24	0.48
1:A:472:ILE:O	1:A:473:MET:HB2	2.13	0.48
1:A:324:ARG:HH22	1:A:671:GLU:CD	2.16	0.48
1:A:437:LEU:HD23	1:A:441:TRP:CD1	2.48	0.48
1:A:329:THR:CG2	1:A:333:LYS:HB3	2.40	0.48
1:A:180:LYS:O	1:A:184:THR:HB	2.14	0.48
1:A:111:TYR:CE2	1:A:473:MET:HG2	2.48	0.48
1:A:133:GLN:NE2	1:A:643:ASN:HB2	2.28	0.48
1:A:362:ASN:HD22	1:A:364:LEU:H	1.60	0.48
1:A:238:ASP:C	1:A:240:ASP:N	2.67	0.48
1:A:361:ASN:HB3	1:A:366:ILE:HD12	1.95	0.48
1:A:250:PRO:HA	1:A:353:TRP:CE3	2.49	0.48
1:A:427:GLN:CD	1:A:427:GLN:H	2.16	0.48
1:A:362:ASN:H	1:A:365:ASN:ND2	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:PRO:HB2	1:A:262:TYR:CE1	2.50	0.47
1:A:128:ILE:HG22	1:A:132:LYS:HE3	1.96	0.47
1:A:358:ASN:ND2	2:A:1049:HOH:O	2.48	0.47
1:A:235:LEU:HD12	1:A:236:THR:H	1.78	0.47
1:A:743:ARG:HG2	1:A:743:ARG:HH11	1.80	0.47
1:A:79:LEU:HD21	1:A:276:ALA:HB2	1.97	0.47
1:A:187:ASN:HB3	1:A:527:ASN:HD21	1.79	0.46
1:A:776:LEU:O	1:A:780:LEU:HG	2.15	0.46
1:A:389:ILE:HG21	1:A:537:ILE:HD13	1.96	0.46
1:A:65:ARG:HG3	1:A:804:VAL:HG22	1.98	0.46
1:A:261:PRO:HB2	1:A:262:TYR:CD1	2.51	0.46
1:A:261:PRO:HD3	1:A:341:PRO:HB3	1.97	0.46
1:A:563:SER:H	1:A:633:ASN:HD21	1.63	0.46
1:A:253:ASN:C	1:A:253:ASN:HD22	2.19	0.46
1:A:142:PRO:O	1:A:143:GLU:HB3	2.16	0.46
1:A:429:MET:HE2	1:A:492:ASN:HD21	1.78	0.46
1:A:252:ILE:HD11	1:A:267:LYS:HB3	1.98	0.46
1:A:491:ILE:HG13	2:A:1044:HOH:O	2.14	0.45
1:A:510:PRO:HG3	2:A:1199:HOH:O	2.16	0.45
1:A:358:ASN:C	1:A:360:PRO:HD3	2.37	0.45
1:A:133:GLN:HE21	1:A:643:ASN:HB2	1.80	0.45
1:A:204:GLN:NE2	1:A:720:LEU:HD21	2.31	0.45
1:A:208:ILE:O	1:A:211:PRO:HD3	2.17	0.45
1:A:377:PRO:HG3	1:A:573:TRP:CE2	2.52	0.45
1:A:722:THR:CG2	1:A:724:ARG:H	2.04	0.45
1:A:353:TRP:HB3	1:A:354:PRO:HD3	1.98	0.45
1:A:189:ASN:ND2	2:A:1001:HOH:O	2.49	0.45
1:A:695:LYS:HE3	2:A:1371:HOH:O	2.15	0.45
1:A:425:THR:CB	1:A:428:HIS:HD2	2.24	0.44
1:A:59:TYR:CE2	1:A:477:ILE:HG23	2.51	0.44
1:A:229:PRO:HG2	1:A:279:ASN:OD1	2.18	0.44
1:A:757:LEU:O	1:A:760:SER:HB3	2.17	0.44
1:A:215:PRO:HD3	1:A:440:GLY:O	2.17	0.44
1:A:181:GLU:HB3	2:A:1056:HOH:O	2.18	0.44
1:A:447:PRO:HG3	1:A:732:SER:HA	2.00	0.43
1:A:209:THR:O	1:A:371:SER:HB2	2.18	0.43
1:A:175:ARG:O	1:A:178:ALA:HB3	2.17	0.43
1:A:763:ASP:CG	1:A:764:ASP:H	2.21	0.43
1:A:401:ALA:HB2	1:A:490:PHE:CD1	2.54	0.43
1:A:347:MET:HB3	1:A:456:PHE:CZ	2.54	0.43
1:A:217:GLU:O	1:A:217:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ILE:HD12	1:A:78:ILE:N	2.32	0.43
1:A:229:PRO:HG3	1:A:278:SER:HB2	1.99	0.43
1:A:743:ARG:HB2	1:A:746:ASP:OD2	2.19	0.43
1:A:527:ASN:N	1:A:527:ASN:ND2	2.66	0.43
1:A:317:LEU:HB2	1:A:339:SER:HB3	1.99	0.43
1:A:621:VAL:HA	1:A:683:LEU:HD21	2.01	0.43
1:A:50:LEU:HD13	1:A:475:LEU:HD12	2.01	0.42
1:A:653:GLU:C	1:A:655:LYS:H	2.22	0.42
1:A:461:ALA:HB3	1:A:462:PRO:HD3	2.00	0.42
1:A:704:VAL:CG1	1:A:705:ASN:N	2.81	0.42
1:A:726:ARG:NH1	1:A:728:GLU:OE2	2.50	0.42
1:A:227:ARG:HB2	1:A:232:MET:CE	2.50	0.42
1:A:273:GLU:CD	1:A:273:GLU:H	2.22	0.42
1:A:410:ASN:OD1	1:A:538:ARG:HG3	2.19	0.42
1:A:698:PRO:HA	1:A:699:PRO:HD3	1.85	0.42
1:A:67:LEU:HD12	1:A:67:LEU:H	1.85	0.42
1:A:362:ASN:HB2	1:A:371:SER:O	2.20	0.42
1:A:469:SER:HB2	1:A:477:ILE:O	2.20	0.42
1:A:382:LEU:HD21	1:A:575:ALA:HA	2.02	0.42
1:A:176:LEU:HD11	1:A:318:LEU:CD2	2.50	0.41
1:A:184:THR:HG22	1:A:185:GLY:N	2.34	0.41
1:A:74:GLU:O	1:A:77:GLN:HB2	2.20	0.41
1:A:70:ASN:HA	1:A:99:LEU:O	2.20	0.41
1:A:61:VAL:HG22	1:A:477:ILE:CD1	2.51	0.41
1:A:342:SER:HB2	1:A:343:PRO:HD3	2.02	0.41
1:A:284:GLU:O	1:A:288:LEU:HD22	2.20	0.41
1:A:391:ALA:HB1	1:A:393:GLU:OE1	2.21	0.41
1:A:184:THR:CG2	1:A:185:GLY:N	2.84	0.41
1:A:229:PRO:HG3	1:A:278:SER:CB	2.50	0.41
1:A:727:ASN:O	1:A:766:ASP:HB3	2.20	0.41
1:A:191:ASP:OD2	1:A:427:GLN:HG3	2.19	0.41
1:A:506:LEU:CD1	1:A:721:LYS:HD3	2.51	0.40
1:A:61:VAL:HA	1:A:477:ILE:HD13	2.02	0.40
1:A:177:VAL:HG22	2:A:1101:HOH:O	2.21	0.40
1:A:751:LYS:O	1:A:754:ALA:HB3	2.21	0.40
1:A:145:ASN:HD22	1:A:147:GLY:H	1.69	0.40
1:A:329:THR:O	1:A:329:THR:CG2	2.68	0.40
1:A:504:TRP:HD1	1:A:510:PRO:HD2	1.84	0.40
1:A:410:ASN:ND2	1:A:536:ASP:HA	2.37	0.40
1:A:67:LEU:HD13	1:A:106:TYR:CE2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ALA:CB	1:A:144:ALA:CB[10_666]	2.16	0.04

## 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	761/774 (98%)	709 (93%)	44 (6%)	8 (1%)	17 31

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	VAL
1	A	221	PRO
1	A	238	ASP
1	A	244	GLU
1	A	420	GLY
1	A	789	VAL
1	A	143	GLU
1	A	487	ALA

### 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	657/666 (99%)	625 (95%)	32 (5%)	31 55

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LEU
1	A	65	ARG
1	A	67	LEU
1	A	72	GLU
1	A	145	ASN
1	A	152	VAL
1	A	177	VAL
1	A	209	THR
1	A	210	LEU
1	A	212	VAL
1	A	219	ASP
1	A	253	ASN
1	A	288	LEU
1	A	306	MET
1	A	324	ARG
1	A	329	THR
1	A	347	MET
1	A	362	ASN
1	A	365	ASN
1	A	425	THR
1	A	427	GLN
1	A	489	THR
1	A	495	LEU
1	A	500	VAL
1	A	511	ARG
1	A	527	ASN
1	A	531	GLU
1	A	568	LEU
1	A	629	VAL
1	A	718	ASN
1	A	744	LEU
1	A	745	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	145	ASN
1	A	189	ASN
1	A	204	GLN
1	A	253	ASN

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Mol	Chain	Res	Type
1	A	291	GLN
1	A	362	ASN
1	A	365	ASN
1	A	427	GLN
1	A	428	HIS
1	A	492	ASN
1	A	493	ASN
1	A	527	ASN
1	A	633	ASN
1	A	651	HIS
1	A	694	ASN
1	A	745	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	765/774 (98%)	0.46	77 (10%) 9 9	27, 42, 89, 126	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	ASP	7.3
1	A	242	ASP	7.1
1	A	217	GLU	6.9
1	A	92	VAL	6.8
1	A	243	PHE	6.8
1	A	91	ALA	6.6
1	A	654	ALA	6.5
1	A	236	THR	5.9
1	A	220	LYS	5.8
1	A	612	VAL	5.7
1	A	245	VAL	5.5
1	A	241	GLY	5.4
1	A	237	GLY	5.4
1	A	789	VAL	5.3
1	A	218	ASP	5.2
1	A	87	GLN	5.1
1	A	90	GLY	5.1
1	A	88	ILE	5.1
1	A	89	GLU	5.0
1	A	143	GLU	5.0
1	A	763	ASP	5.0
1	A	765	PRO	5.0
1	A	238	ASP	4.9
1	A	240	ASP	4.7
1	A	239	VAL	4.6
1	A	762	PRO	4.4
1	A	764	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	221	PRO	4.1
1	A	235	LEU	3.9
1	A	706	ARG	3.9
1	A	614	ILE	3.8
1	A	657	PHE	3.8
1	A	724	ARG	3.6
1	A	723	GLY	3.6
1	A	244	GLU	3.6
1	A	661	GLU	3.6
1	A	722	THR	3.4
1	A	658	PRO	3.3
1	A	659	LEU	3.2
1	A	653	GLU	3.2
1	A	790	ALA	3.1
1	A	234	VAL	3.1
1	A	680	ASN	3.0
1	A	462	PRO	2.9
1	A	707	PRO	2.9
1	A	248	TYR	2.8
1	A	656	GLY	2.8
1	A	260	LEU	2.8
1	A	73	TYR	2.8
1	A	655	LYS	2.7
1	A	246	GLU	2.7
1	A	104	GLN	2.5
1	A	711	GLY	2.5
1	A	429	MET	2.5
1	A	791	HIS	2.5
1	A	782	LYS	2.4
1	A	760	SER	2.4
1	A	432	ALA	2.3
1	A	767	ALA	2.3
1	A	770	PHE	2.3
1	A	185	GLY	2.3
1	A	613	GLY	2.3
1	A	651	HIS	2.3
1	A	223	VAL	2.3
1	A	222	TRP	2.2
1	A	721	LYS	2.2
1	A	650	ARG	2.2
1	A	652	LEU	2.2
1	A	424	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	788	LYS	2.1
1	A	85	MET	2.1
1	A	660	ASP	2.1
1	A	708	VAL	2.1
1	A	84	TRP	2.0
1	A	216	GLY	2.0
1	A	96	THR	2.0
1	A	348	ILE	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.