



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:03 AM GMT

PDB ID : 3KQK  
Title : Three Conformational Snapshots of the Hepatitis C Virus NS3 Helicase Reveal a Ratchet Translocation Mechanism  
Authors : Gu, M.; Rice, C.M.  
Deposited on : 2009-11-17  
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

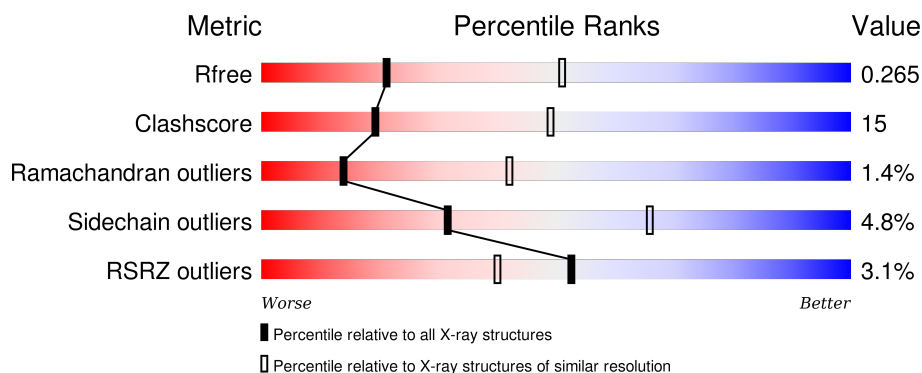
# 1 Overall quality at a glance

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	436	<div> <div>3%</div> <div>67%</div> <div>31%</div> <div>.</div> </div>
1	B	436	<div> <div>3%</div> <div>69%</div> <div>28%</div> <div>.</div> </div>
2	C	6	<div> <div>67%</div> <div>33%</div> </div>
2	D	6	<div> <div>67%</div> <div>33%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6922 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 Serine protease/NTPase/helicase NS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3275	2074	555	625	21			
1	B	436	Total	C	N	O	S	0	0	0
			3275	2074	555	625	21			

- Molecule 2 is a DNA chain called 5'-D(\*TP\*TP\*TP\*TP\*TP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	P	0	0	0
			117	60	12	40	5			
2	D	6	Total	C	N	O	P	0	0	0
			117	60	12	40	5			

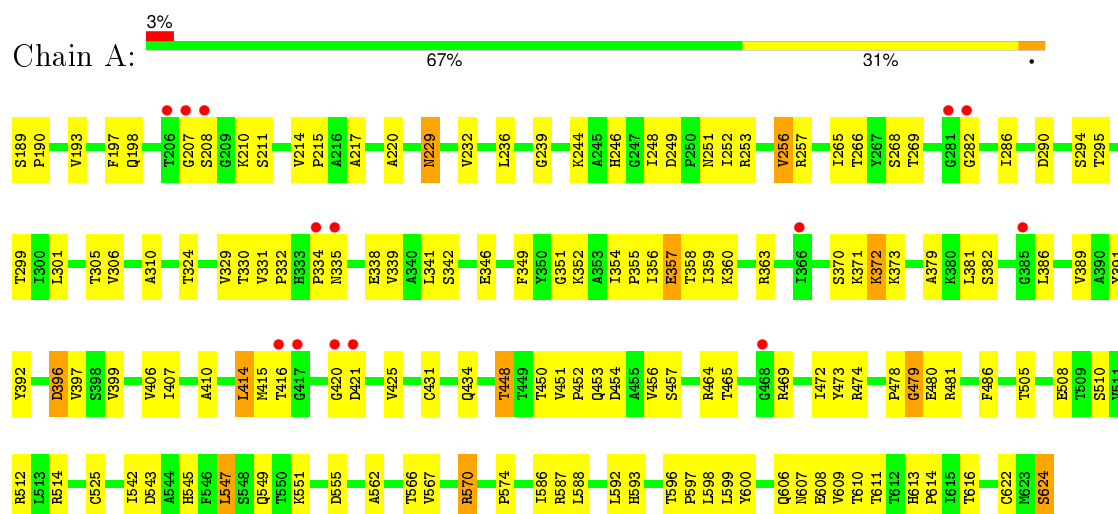
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total	O	0	0
			72	72		
3	B	61	Total	O	0	0
			61	61		
3	C	4	Total	O	0	0
			4	4		
3	D	1	Total	O	0	0
			1	1		

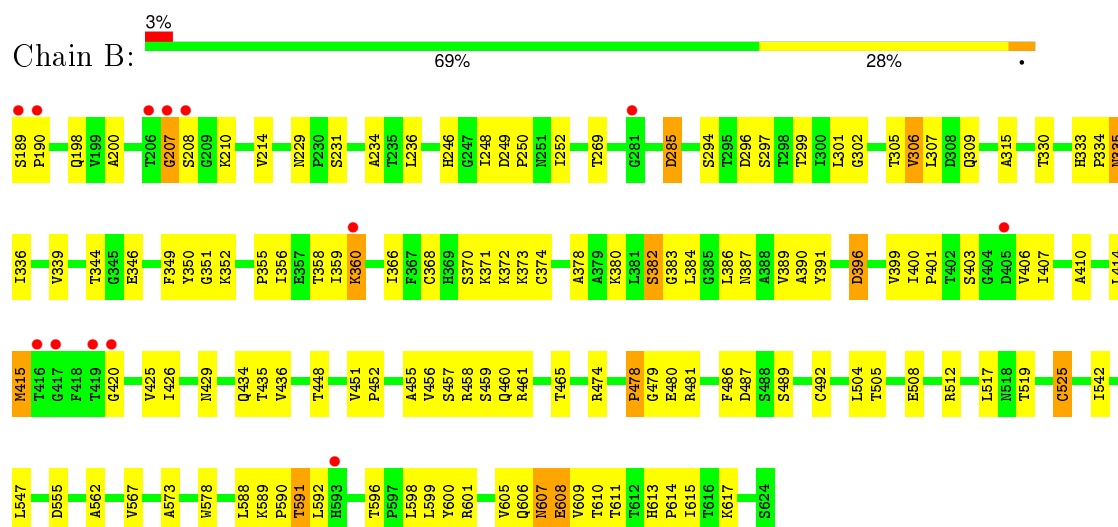
### 3 Residue-property plots

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: Serine protease/NTPase/helicase NS3



- Molecule 1: Serine protease/NTPase/helicase NS3



- Molecule 2: 5'-D(\*TP\*TP\*TP\*TP\*TP\*T)-3'





- Molecule 2: 5'-D(\*TP\*TP\*TP\*TP\*TP\*T)-3'



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.49Å 115.38Å 198.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.80 19.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.96-2.80) 93.8 (19.96-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.69 (at 2.79Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.210 , 0.265 0.207 , 0.265	Depositor DCC
$R_{free}$ test set	1243 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtriage
Anisotropy	0.623	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.2	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	1 of 24872 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6922	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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 [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	0.41	0/3356	0.60	0/4585
1	B	0.42	0/3356	0.58	0/4585
2	C	0.45	0/128	0.72	0/196
2	D	0.49	0/128	0.85	0/196
All	All	0.42	0/6968	0.60	0/9562

There are no bond length outliers.

There are no bond angle outliers.

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	3275	0	3236	109	0
1	B	3275	0	3236	96	0
2	C	117	0	74	2	0
2	D	117	0	74	4	0
3	A	72	0	0	4	0
3	B	61	0	0	7	0
3	C	4	0	0	0	0
3	D	1	0	0	0	0
All	All	6922	0	6620	203	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 15.

All (203) 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:555:ASP:HB2	3:B:45:HOH:O	1.71	0.91
1:B:601:ARG:HH21	1:B:605:VAL:HG11	1.36	0.91
1:B:349:PHE:HB3	3:B:39:HOH:O	1.80	0.81
1:A:359:ILE:HD12	1:A:407:ILE:HD13	1.63	0.80
1:B:607:ASN:ND2	1:B:608:GLU:H	1.80	0.80
1:A:256:VAL:HG23	1:A:257:ARG:H	1.48	0.78
1:A:611:THR:HG22	1:A:611:THR:O	1.83	0.77
1:B:370:SER:OG	1:B:372:LYS:HG2	1.88	0.73
1:A:372:LYS:HE2	1:A:373:LYS:HG3	1.73	0.70
1:A:357:GLU:HA	1:A:360:LYS:HB2	1.73	0.70
1:B:207:GLY:HA2	1:B:210:LYS:HE3	1.72	0.70
1:A:547:LEU:O	1:A:551:LYS:HG3	1.92	0.69
1:B:415:MET:HB2	3:B:43:HOH:O	1.92	0.67
1:A:229:ASN:O	1:A:269:THR:HA	1.94	0.67
1:B:599:LEU:HD22	1:B:615:ILE:HG22	1.76	0.67
1:A:248:ILE:O	1:A:248:ILE:HG13	1.94	0.66
1:A:607:ASN:ND2	1:A:608:GLU:H	1.92	0.66
1:B:573:ALA:O	1:B:592:LEU:HD22	1.95	0.66
1:B:330:THR:HG22	1:B:459:SER:OG	1.96	0.66
1:B:478:PRO:HG2	1:B:479:GLY:H	1.61	0.66
1:B:429:ASN:HD22	1:B:458:ARG:NH1	1.95	0.65
1:B:451:VAL:HG23	1:B:452:PRO:HD2	1.78	0.65
1:B:350:TYR:N	3:B:39:HOH:O	2.28	0.64
1:B:346:GLU:OE2	1:B:355:PRO:HA	1.97	0.64
1:A:253:ARG:HB2	1:A:268:SER:HB2	1.80	0.64
1:B:372:LYS:NZ	1:B:373:LYS:HE3	2.12	0.64
1:A:542:ILE:HD13	1:A:547:LEU:HG	1.81	0.63
1:B:505:THR:OG1	1:B:508:GLU:HG3	1.99	0.62
1:A:379:ALA:HA	3:A:76:HOH:O	1.98	0.62
1:B:391:TYR:HB3	1:B:410:ALA:HB2	1.80	0.62
1:A:363:ARG:HG2	1:A:406:VAL:HG12	1.82	0.61
1:A:606:GLN:NE2	1:A:606:GLN:HA	2.14	0.61
1:A:434:GLN:HE21	1:A:448:THR:HG22	1.66	0.61
1:A:246:HIS:O	1:A:248:ILE:HG23	2.01	0.60
1:B:356:ILE:CD1	1:B:386:LEU:HD11	2.30	0.60
1:A:339:VAL:O	1:A:474:ARG:HA	2.02	0.60
1:B:429:ASN:HD22	1:B:458:ARG:HH12	1.50	0.60
1:A:542:ILE:HD11	1:A:562:ALA:HB3	1.83	0.59
1:A:207:GLY:HA2	1:A:210:LYS:HE3	1.83	0.59
1:A:294:SER:HB2	1:A:299:THR:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:PRO:HG2	1:A:479:GLY:H	1.67	0.58
1:A:586:ILE:HG23	1:A:587:ARG:N	2.18	0.58
1:B:486:PHE:O	1:B:525:CYS:HB2	2.03	0.58
1:A:355:PRO:O	1:A:358:THR:HB	2.05	0.57
1:A:505:THR:OG1	1:A:508:GLU:HG3	2.04	0.56
1:A:606:GLN:HE21	1:A:606:GLN:HA	1.68	0.56
1:A:588:LEU:O	1:A:592:LEU:HG	2.05	0.56
1:B:351:GLY:C	1:B:352:LYS:HD2	2.27	0.55
1:B:333:HIS:ND1	1:B:334:PRO:HD2	2.22	0.55
1:B:380:LYS:HB2	1:B:380:LYS:NZ	2.21	0.55
1:A:244:LYS:HZ1	1:B:360:LYS:HE2	1.71	0.55
1:A:211:SER:HB3	1:A:290:ASP:OD1	2.07	0.55
1:A:451:VAL:CG2	1:A:452:PRO:HD2	2.37	0.54
1:A:356:ILE:CD1	1:A:386:LEU:HD11	2.37	0.54
1:A:248:ILE:HD11	1:A:265:ILE:HD12	1.89	0.54
1:A:451:VAL:HG23	1:A:452:PRO:HD2	1.89	0.54
1:A:391:TYR:HB3	1:A:410:ALA:HB2	1.90	0.54
1:B:229:ASN:O	1:B:269:THR:HA	2.08	0.54
1:A:431:CYS:O	1:A:450:THR:HA	2.08	0.53
1:B:601:ARG:NH2	1:B:605:VAL:HG11	2.14	0.53
1:A:611:THR:HB	3:A:49:HOH:O	2.09	0.53
1:B:611:THR:O	1:B:617:LYS:HE2	2.08	0.53
1:B:346:GLU:CD	1:B:346:GLU:H	2.12	0.53
1:B:190:PRO:HG2	1:B:214:VAL:HG13	1.90	0.53
1:B:599:LEU:HD22	1:B:615:ILE:CG2	2.38	0.53
1:A:338:GLU:HG2	1:A:473:TYR:CD2	2.44	0.53
1:A:574:PRO:HG2	1:A:607:ASN:OD1	2.10	0.52
1:B:358:THR:HG23	1:B:474:ARG:CZ	2.38	0.52
1:A:338:GLU:HG2	1:A:473:TYR:HD2	1.75	0.52
1:A:396:ASP:O	1:A:399:VAL:HG23	2.10	0.52
1:B:425:VAL:HG23	1:B:465:THR:HB	1.91	0.52
1:A:452:PRO:HG2	1:A:481:ARG:HH12	1.75	0.51
1:B:372:LYS:HZ2	1:B:373:LYS:HE3	1.75	0.51
1:A:244:LYS:NZ	1:B:360:LYS:HE2	2.26	0.51
1:A:542:ILE:HD11	1:A:562:ALA:CB	2.40	0.51
1:B:378:ALA:O	1:B:382:SER:HB2	2.11	0.51
1:B:613:HIS:ND1	1:B:614:PRO:HD2	2.26	0.51
1:B:383:GLY:O	1:B:384:LEU:HD12	2.11	0.51
1:B:457:SER:O	1:B:461:ARG:HG2	2.10	0.50
1:A:397:VAL:HG21	1:A:416:THR:O	2.12	0.50
1:A:305:THR:OG1	1:A:512:ARG:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:GLY:O	1:B:306:VAL:HG12	2.11	0.50
1:A:189:SER:N	1:A:190:PRO:HD2	2.26	0.50
1:A:334:PRO:HA	3:B:73:HOH:O	2.12	0.50
1:A:611:THR:HG23	1:A:616:THR:HG21	1.93	0.50
1:B:436:VAL:HG12	1:B:487:ASP:OD2	2.11	0.50
1:B:294:SER:HB3	1:B:299:THR:HG21	1.94	0.50
1:A:510:SER:O	1:A:514:ARG:HB2	2.12	0.50
1:A:239:GLY:HA3	1:A:252:ILE:HD11	1.93	0.50
1:B:598:LEU:HB2	1:B:609:VAL:HG13	1.93	0.50
1:A:464:ARG:HG3	1:A:464:ARG:HH11	1.77	0.49
1:B:356:ILE:HD11	1:B:386:LEU:HD21	1.94	0.49
1:B:335:ASN:ND2	1:B:335:ASN:H	2.09	0.49
1:A:453:GLN:HB2	1:A:457:SER:HB3	1.94	0.49
1:A:414:LEU:HD23	1:A:415:MET:H	1.78	0.49
1:A:607:ASN:ND2	1:A:608:GLU:N	2.60	0.49
1:A:434:GLN:HG2	1:A:448:THR:HG22	1.94	0.48
1:A:593:HIS:HB3	3:A:10:HOH:O	2.11	0.48
1:A:371:LYS:HG3	1:A:392:TYR:CG	2.49	0.48
1:A:335:ASN:HB3	1:A:469:ARG:O	2.13	0.48
1:B:456:VAL:O	1:B:460:GLN:HG3	2.14	0.48
1:B:198:GLN:HE21	1:B:200:ALA:HB2	1.78	0.48
1:B:401:PRO:HG2	1:B:406:VAL:HG11	1.94	0.48
1:B:396:ASP:O	1:B:399:VAL:HG22	2.13	0.48
1:A:244:LYS:HZ3	1:B:360:LYS:HB3	1.78	0.48
1:B:434:GLN:HA	1:B:448:THR:HA	1.95	0.48
1:A:545:HIS:O	1:A:549:GLN:HG3	2.13	0.48
1:B:567:VAL:HG21	1:B:599:LEU:HD11	1.94	0.47
1:B:366:ILE:HD12	1:B:426:ILE:HD12	1.95	0.47
1:B:231:SER:HB3	1:B:234:ALA:HB3	1.97	0.47
1:B:307:LEU:HD13	1:B:519:THR:OG1	2.14	0.47
1:A:586:ILE:CG2	1:A:587:ARG:N	2.77	0.47
1:A:295:THR:HB	1:A:486:PHE:HB3	1.96	0.47
1:B:236:LEU:HD23	1:B:252:ILE:HG21	1.96	0.46
1:A:414:LEU:HD23	1:A:415:MET:N	2.30	0.46
1:A:248:ILE:CD1	1:A:265:ILE:HD12	2.45	0.46
1:A:371:LYS:HG3	1:A:392:TYR:CD2	2.50	0.46
1:A:351:GLY:C	1:A:352:LYS:HD2	2.35	0.46
1:B:246:HIS:HB2	1:B:248:ILE:HG22	1.98	0.46
1:A:611:THR:CG2	1:A:611:THR:O	2.55	0.46
1:B:380:LYS:O	1:B:384:LEU:HD13	2.16	0.46
1:B:606:GLN:HB2	3:B:112:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:LYS:HZ1	1:B:373:LYS:HE3	1.78	0.45
1:B:607:ASN:ND2	1:B:608:GLU:N	2.56	0.45
1:A:207:GLY:CA	1:A:210:LYS:HE3	2.43	0.45
1:A:214:VAL:N	1:A:215:PRO:HD2	2.31	0.45
1:A:567:VAL:HG21	1:A:599:LEU:HD11	1.97	0.45
1:B:455:ALA:HA	1:B:480:GLU:OE1	2.15	0.45
1:A:236:LEU:HD23	1:A:252:ILE:HG21	1.98	0.45
1:B:380:LYS:HZ3	1:B:380:LYS:HB2	1.82	0.45
1:B:368:CYS:HB2	1:B:374:CYS:SG	2.57	0.45
1:B:391:TYR:CE2	1:B:415:MET:HG2	2.52	0.45
1:B:429:ASN:ND2	1:B:458:ARG:HH12	2.13	0.45
1:A:330:THR:HB	1:A:480:GLU:OE1	2.16	0.45
1:B:596:THR:O	1:B:610:THR:HG22	2.17	0.45
1:A:253:ARG:HG2	1:A:253:ARG:HH11	1.82	0.44
1:A:598:LEU:HB2	1:A:609:VAL:HG13	1.99	0.44
1:A:256:VAL:HG23	1:A:257:ARG:N	2.23	0.44
1:B:333:HIS:HB3	1:B:336:ILE:HB	1.99	0.44
1:B:248:ILE:O	1:B:250:PRO:HD3	2.16	0.44
1:B:285:ASP:HA	1:B:315:ALA:HA	1.99	0.44
1:B:578:TRP:CZ2	1:B:589:LYS:HG3	2.52	0.44
1:B:429:ASN:ND2	1:B:458:ARG:NH1	2.63	0.44
1:A:193:VAL:HG21	1:A:286:ILE:HD11	2.00	0.44
1:B:588:LEU:O	1:B:591:THR:HG23	2.16	0.44
1:A:217:ALA:O	1:A:220:ALA:HB3	2.18	0.44
1:B:382:SER:C	1:B:384:LEU:H	2.21	0.44
1:B:374:CYS:O	1:B:390:ALA:HB2	2.18	0.44
3:B:16:HOH:O	2:C:5:DT:H4'	2.17	0.44
1:A:425:VAL:HG23	1:A:465:THR:HB	2.00	0.44
1:A:370:SER:HA	2:D:2:DT:H5''	2.00	0.43
1:B:589:LYS:HB3	1:B:590:PRO:HD3	2.00	0.43
1:B:481:ARG:HH11	1:B:481:ARG:HG3	1.83	0.43
1:B:330:THR:HG21	1:B:458:ARG:HB3	2.00	0.43
1:A:346:GLU:OE2	1:A:355:PRO:HA	2.18	0.43
1:B:339:VAL:O	1:B:474:ARG:HA	2.18	0.43
1:B:189:SER:HB3	1:B:190:PRO:HD3	2.00	0.43
1:B:296:ASP:O	1:B:297:SER:C	2.56	0.43
1:A:596:THR:O	1:A:610:THR:HG22	2.18	0.43
1:B:189:SER:N	1:B:190:PRO:CD	2.81	0.43
1:A:389:VAL:O	1:A:389:VAL:HG23	2.18	0.43
1:A:342:SER:HB2	3:A:123:HOH:O	2.17	0.43
1:B:305:THR:OG1	1:B:512:ARG:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:SER:OG	1:A:372:LYS:HD3	2.18	0.43
1:A:351:GLY:O	1:A:352:LYS:HD2	2.19	0.43
1:A:356:ILE:HD12	1:A:386:LEU:HD11	2.00	0.42
1:A:371:LYS:HB3	2:D:2:DT:OP1	2.20	0.42
1:B:371:LYS:HE2	2:C:3:DT:OP2	2.19	0.42
1:A:372:LYS:CE	1:A:373:LYS:HG3	2.47	0.42
1:A:306:VAL:O	1:A:310:ALA:HB2	2.19	0.42
1:A:338:GLU:HG2	1:A:473:TYR:HB3	2.00	0.42
1:B:435:THR:HG22	1:B:436:VAL:N	2.33	0.42
1:B:359:ILE:HB	1:B:407:ILE:HD12	2.02	0.42
1:A:622:CYS:C	1:A:624:SER:H	2.23	0.42
1:A:542:ILE:HG12	1:A:543:ASP:N	2.35	0.42
1:A:549:GLN:HB3	1:A:549:GLN:HE21	1.60	0.42
1:A:197:PHE:O	1:A:198:GLN:NE2	2.52	0.42
1:B:382:SER:HA	1:B:386:LEU:O	2.20	0.42
1:A:232:VAL:HG23	2:D:5:DT:H5"	2.02	0.42
1:A:331:VAL:HG12	1:A:332:PRO:HD2	2.02	0.42
1:A:371:LYS:CB	2:D:2:DT:OP1	2.69	0.41
1:A:472:ILE:HG22	1:A:473:TYR:N	2.35	0.41
1:B:542:ILE:HD11	1:B:562:ALA:HB3	2.02	0.41
1:A:341:LEU:HD21	1:A:474:ARG:HB3	2.01	0.41
1:B:231:SER:HB3	1:B:234:ALA:CB	2.50	0.41
1:A:349:PHE:CD1	1:A:354:ILE:HD11	2.54	0.41
1:A:382:SER:HA	1:A:386:LEU:O	2.21	0.41
1:A:566:THR:O	1:A:570:ARG:HB2	2.20	0.41
1:A:379:ALA:C	1:A:381:LEU:N	2.73	0.41
1:B:360:LYS:HE2	1:B:360:LYS:HB3	1.85	0.41
1:A:379:ALA:O	1:A:381:LEU:N	2.53	0.41
1:B:356:ILE:HD11	1:B:386:LEU:HD11	2.00	0.41
1:B:504:LEU:HD21	1:B:512:ARG:NH2	2.36	0.41
1:B:305:THR:O	1:B:309:GLN:HG3	2.20	0.41
1:A:454:ASP:OD1	1:A:456:VAL:N	2.54	0.41
1:A:251:ASN:HB2	1:A:266:THR:HG23	2.01	0.41
1:B:489:SER:O	1:B:492:CYS:HB3	2.21	0.41
1:A:597:PRO:HA	1:A:610:THR:HG23	2.03	0.40
1:A:606:GLN:NE2	1:A:606:GLN:CA	2.82	0.40
1:B:389:VAL:O	1:B:389:VAL:HG23	2.20	0.40
1:A:613:HIS:HA	1:A:614:PRO:HD3	1.97	0.40
1:A:257:ARG:NH1	1:A:257:ARG:HB3	2.37	0.40
1:B:399:VAL:HG23	1:B:400:ILE:HG13	2.03	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	434/436 (100%)	398 (92%)	30 (7%)	6 (1%)	14	42
1	B	434/436 (100%)	395 (91%)	33 (8%)	6 (1%)	14	42
All	All	868/872 (100%)	793 (91%)	63 (7%)	12 (1%)	14	42

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	SER
1	A	420	GLY
1	B	360	LYS
1	B	478	PRO
1	A	479	GLY
1	B	420	GLY
1	B	607	ASN
1	B	208	SER
1	A	421	ASP
1	B	207	GLY
1	A	256	VAL
1	A	282	GLY

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	356/356 (100%)	340 (96%)	16 (4%)	34	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	356/356 (100%)	338 (95%)	18 (5%)	29	63
All	All	712/712 (100%)	678 (95%)	34 (5%)	31	66

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	ASN
1	A	249	ASP
1	A	301	LEU
1	A	324	THR
1	A	329	VAL
1	A	357	GLU
1	A	372	LYS
1	A	396	ASP
1	A	414	LEU
1	A	448	THR
1	A	525	CYS
1	A	547	LEU
1	A	555	ASP
1	A	570	ARG
1	A	600	TYR
1	A	624	SER
1	B	249	ASP
1	B	285	ASP
1	B	301	LEU
1	B	306	VAL
1	B	335	ASN
1	B	344	THR
1	B	382	SER
1	B	387	ASN
1	B	396	ASP
1	B	403	SER
1	B	414	LEU
1	B	415	MET
1	B	517	LEU
1	B	525	CYS
1	B	547	LEU
1	B	591	THR
1	B	600	TYR
1	B	608	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	GLN
1	A	201	HIS
1	A	387	ASN
1	A	434	GLN
1	A	453	GLN
1	A	460	GLN
1	A	518	ASN
1	A	549	GLN
1	A	556	ASN
1	A	580	GLN
1	A	606	GLN
1	A	607	ASN
1	B	198	GLN
1	B	335	ASN
1	B	387	ASN
1	B	453	GLN
1	B	460	GLN
1	B	518	ASN
1	B	552	GLN
1	B	556	ASN
1	B	606	GLN
1	B	607	ASN

### 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	436/436 (100%)	-0.11	14 (3%)	51	39	8, 41, 70, 78	0
1	B	436/436 (100%)	-0.02	13 (2%)	54	41	15, 43, 71, 80	0
2	C	6/6 (100%)	-0.10	0	100	100	33, 43, 45, 49	0
2	D	6/6 (100%)	-0.15	0	100	100	32, 43, 45, 49	0
All	All	884/884 (100%)	-0.06	27 (3%)	52	40	8, 42, 71, 80	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	207	GLY	7.4
1	B	416	THR	4.9
1	A	208	SER	4.2
1	A	421	ASP	4.0
1	B	189	SER	3.7
1	A	206	THR	3.5
1	B	417	GLY	3.4
1	A	207	GLY	3.3
1	B	281	GLY	3.3
1	B	405	ASP	3.2
1	B	420	GLY	3.2
1	B	190	PRO	3.1
1	A	416	THR	3.1
1	A	366	ILE	2.7
1	A	335	ASN	2.7
1	A	281	GLY	2.7
1	A	334	PRO	2.4
1	B	419	THR	2.4
1	A	417	GLY	2.3
1	A	468	GLY	2.3
1	B	593	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	282	GLY	2.3
1	B	208	SER	2.3
1	B	206	THR	2.2
1	A	385	GLY	2.2
1	A	420	GLY	2.1
1	B	360	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.