



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:06 PM GMT

PDB ID : 1NHU  
Title : Hepatitis C virus RNA polymerase in complex with non-nucleoside analogue inhibitor  
Authors : Wang, M.; Ng, K.K.S.; Cherney, M.M.; Chan, L.; Yannopoulos, C.G.; Bedard, J.; Morin, N.; Nguyen-Ba, N.; Alaoui-Ismaili, M.H.; Bethell, R.C.; James, M.N.G.  
Deposited on : 2002-12-19  
Resolution : 2.00 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

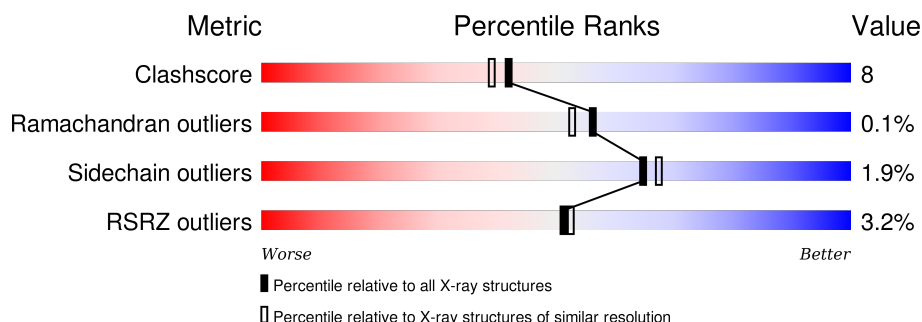
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


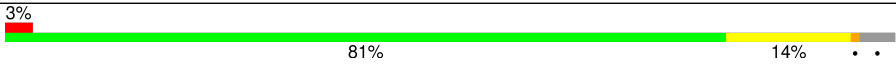
The reported resolution of this entry is 2.00 Å.

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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	578	
1	B	578	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	153	A	5001	-	-	-	X
2	153	B	6001	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9317 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.

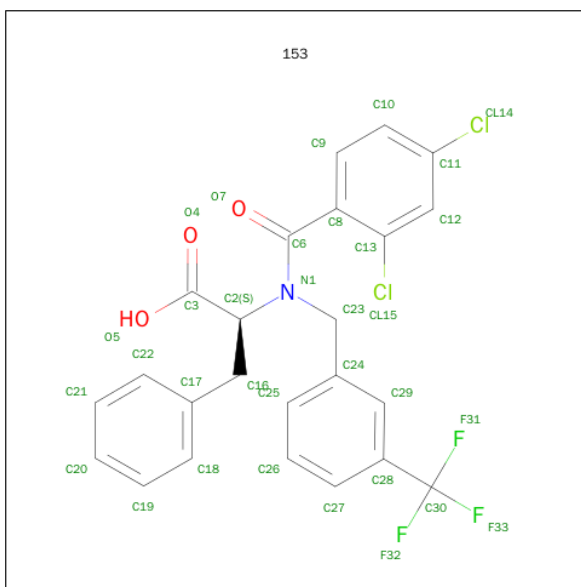
- Molecule 1 is a protein called HEPATITIS C VIRUS NS5B RNA-DEPENDENT RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	0
			4340	2738	765	806	31			
1	B	557	Total	C	N	O	S	0	0	0
			4334	2735	764	804	31			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ALA	-	EXPRESSION TAG	UNP P26663
A	-6	SER	-	EXPRESSION TAG	UNP P26663
A	-5	HIS	-	EXPRESSION TAG	UNP P26663
A	-4	HIS	-	EXPRESSION TAG	UNP P26663
A	-3	HIS	-	EXPRESSION TAG	UNP P26663
A	-2	HIS	-	EXPRESSION TAG	UNP P26663
A	-1	HIS	-	EXPRESSION TAG	UNP P26663
A	0	HIS	-	EXPRESSION TAG	UNP P26663
B	-7	ALA	-	EXPRESSION TAG	UNP P26663
B	-6	SER	-	EXPRESSION TAG	UNP P26663
B	-5	HIS	-	EXPRESSION TAG	UNP P26663
B	-4	HIS	-	EXPRESSION TAG	UNP P26663
B	-3	HIS	-	EXPRESSION TAG	UNP P26663
B	-2	HIS	-	EXPRESSION TAG	UNP P26663
B	-1	HIS	-	EXPRESSION TAG	UNP P26663
B	0	HIS	-	EXPRESSION TAG	UNP P26663

- Molecule 2 is (2S)-2-[(2,4-DICHLORO-BENZOYL)-(3-TRIFLUOROMETHYL-BENZYL)-AMINO]-3-PHENYL-PROPIONIC ACID (three-letter code: 153) (formula: C<sub>24</sub>H<sub>18</sub>Cl<sub>2</sub>F<sub>3</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			33	24	2	3	1	3		
2	B	1	Total	C	Cl	F	N	O	0	0
			33	24	2	3	1	3		

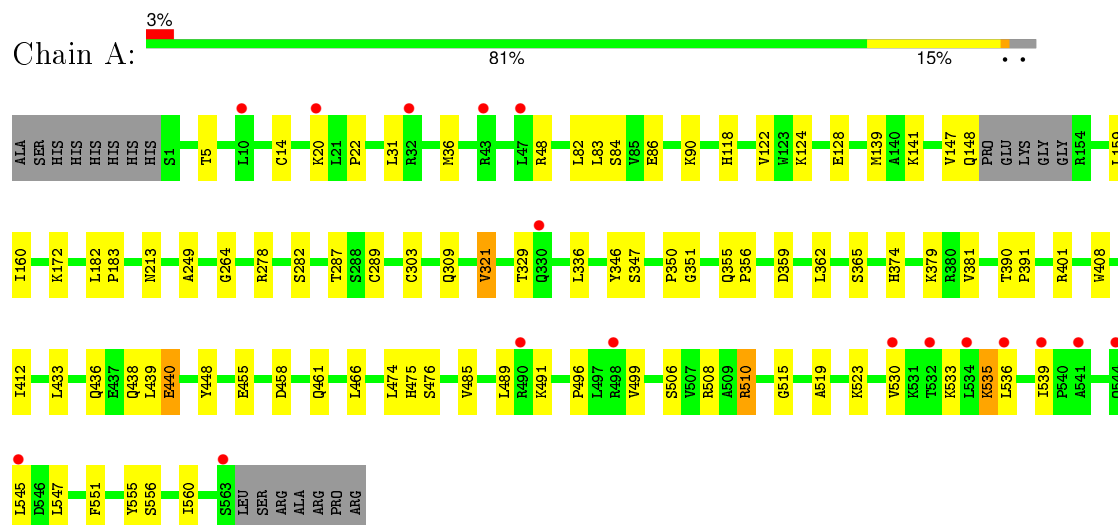
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	283	Total	O	0	0
			283	283		
3	B	294	Total	O	0	0
			294	294		

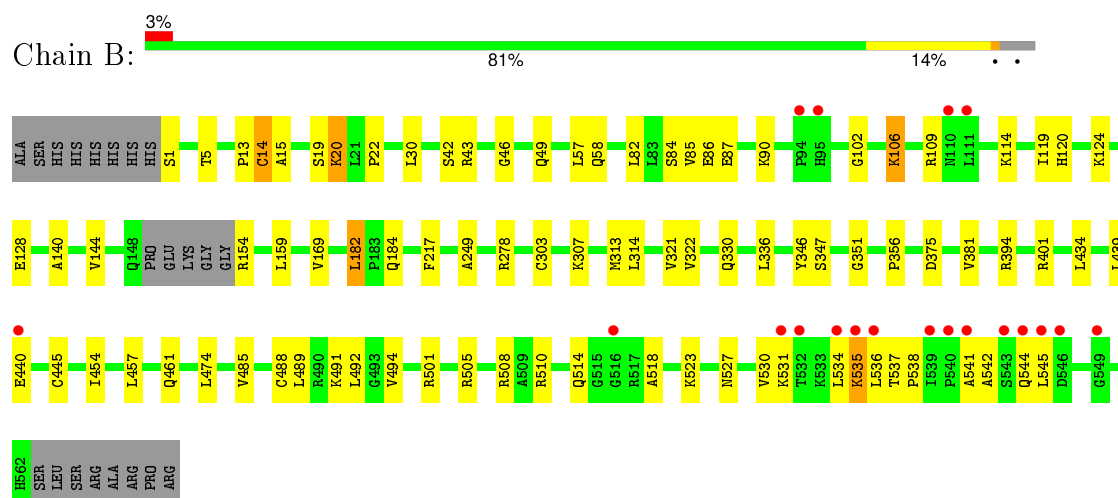
### 3 Residue-property plots

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 NS5B RNA-DEPENDENT RNA POLYMERASE



#### • Molecule 1: HEPATITIS C VIRUS NS5B RNA-DEPENDENT RNA POLYMERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.02Å 104.68Å 126.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.67 – 2.00 35.67 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.67-2.00) 99.8 (35.67-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.14 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.219 , 0.256 0.218 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	21.0	Xtriage
Anisotropy	0.941	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 55.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	2 of 77964 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9317	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	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 46.71 % 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 1.1015e-04. 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section:  
153

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	0.53	0/4434	0.71	2/6017 (0.0%)
1	B	0.56	0/4428	0.71	1/6009 (0.0%)
All	All	0.55	0/8862	0.71	3/12026 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	LEU	CA-CB-CG	5.99	129.07	115.30
1	B	351	GLY	N-CA-C	-5.30	99.86	113.10
1	A	351	GLY	N-CA-C	-5.23	100.02	113.10

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	4340	0	4357	69	0
1	B	4334	0	4352	77	0
2	A	33	0	17	1	0
2	B	33	0	17	1	0
3	A	283	0	0	11	0
3	B	294	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9317	0	8743	147	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 8.

All (147) 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:510:ARG:HH11	1:A:510:ARG:HG2	1.27	0.98
1:B:381:VAL:HG11	1:B:474:LEU:HD22	1.48	0.95
1:B:106:LYS:NZ	1:B:106:LYS:HA	1.83	0.92
1:A:5:THR:HG23	1:A:278:ARG:HH12	1.34	0.90
1:B:5:THR:HG23	1:B:278:ARG:HH12	1.41	0.85
1:B:46:GLY:HA2	1:B:49:GLN:HE21	1.41	0.85
1:B:541:ALA:O	1:B:544:GLN:HG2	1.77	0.84
1:B:313:MET:HG2	1:B:322:VAL:HG22	1.59	0.84
1:A:381:VAL:HG11	1:A:474:LEU:HD22	1.60	0.82
1:B:19:SER:H	1:B:20:LYS:NZ	1.79	0.80
1:A:455:GLU:HB3	3:A:5264:HOH:O	1.83	0.79
1:B:381:VAL:HG11	1:B:474:LEU:CD2	2.14	0.78
1:B:106:LYS:HZ2	1:B:106:LYS:HA	1.48	0.77
1:A:48:ARG:HG2	1:A:159:LEU:HD13	1.65	0.77
1:B:182:LEU:HD23	1:B:182:LEU:C	2.08	0.74
1:B:19:SER:H	1:B:20:LYS:HZ2	1.36	0.73
1:B:508:ARG:HE	1:B:530:VAL:HG11	1.52	0.73
1:A:510:ARG:NH1	1:A:510:ARG:HG2	2.01	0.72
1:B:535:LYS:HA	1:B:535:LYS:HE3	1.72	0.71
1:A:433:LEU:HB3	1:A:439:LEU:HD12	1.71	0.71
1:B:106:LYS:HZ3	1:B:106:LYS:HA	1.55	0.71
1:B:535:LYS:O	1:B:536:LEU:HB2	1.92	0.69
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.75	0.69
1:B:22:PRO:HG2	1:B:401:ARG:HG3	1.74	0.69
1:A:336:LEU:HD12	1:A:356:PRO:HD3	1.73	0.69
1:A:20:LYS:HG2	3:A:5121:HOH:O	1.91	0.68
1:B:314:LEU:HB3	1:B:321:VAL:CG1	2.24	0.67
1:B:336:LEU:HD12	1:B:356:PRO:HD3	1.76	0.67
1:B:488:CYS:HB2	3:B:6272:HOH:O	1.96	0.66
1:B:119:ILE:HD13	1:B:169:VAL:HG11	1.78	0.65
1:B:102:GLY:O	1:B:114:LYS:HE3	1.97	0.64
1:B:20:LYS:HE3	3:B:6157:HOH:O	1.98	0.64
1:B:434:LEU:HA	1:B:439:LEU:HD11	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.79	0.63
1:A:5:THR:HG23	1:A:278:ARG:NH1	2.13	0.60
1:A:510:ARG:NH1	3:A:5279:HOH:O	2.34	0.60
1:A:359:ASP:HB3	1:A:362:LEU:HD12	1.83	0.60
1:B:13:PRO:HD3	1:B:43:ARG:HH12	1.67	0.60
1:B:508:ARG:HE	1:B:530:VAL:CG1	2.16	0.59
1:A:213:ASN:HB2	3:A:5201:HOH:O	2.03	0.59
1:A:5:THR:HG21	1:A:278:ARG:HH22	1.69	0.58
1:B:84:SER:OG	1:B:87:GLU:HG3	2.05	0.56
1:B:510:ARG:O	1:B:514:GLN:HG2	2.05	0.56
1:B:491:LYS:HE3	1:B:492:LEU:HD11	1.88	0.56
1:A:560:ILE:HD13	3:A:5102:HOH:O	2.05	0.56
1:A:147:VAL:O	1:A:148:GLN:HB3	2.06	0.55
1:B:501:ARG:NE	2:B:6001:153:H26	2.21	0.55
1:A:86:GLU:O	1:A:90:LYS:HG2	2.06	0.54
1:A:508:ARG:HE	1:A:530:VAL:HG11	1.72	0.54
1:A:506:SER:O	1:A:510:ARG:HD3	2.06	0.54
1:B:314:LEU:HB3	1:B:321:VAL:HG12	1.89	0.54
1:A:535:LYS:HG3	1:A:536:LEU:H	1.73	0.54
1:B:510:ARG:HG2	3:B:6291:HOH:O	2.07	0.54
1:A:508:ARG:HG3	1:A:508:ARG:HH11	1.71	0.54
1:A:560:ILE:CD1	3:A:5102:HOH:O	2.56	0.53
1:A:183:PRO:HG3	1:A:289:CYS:SG	2.49	0.53
1:A:182:LEU:HD23	1:A:182:LEU:C	2.29	0.52
1:A:124:LYS:O	1:A:128:GLU:HG3	2.08	0.52
1:B:154:ARG:N	3:B:6206:HOH:O	2.43	0.52
1:A:381:VAL:HG11	1:A:474:LEU:CD2	2.35	0.51
1:B:217:PHE:CE2	1:B:336:LEU:HD21	2.46	0.51
1:A:510:ARG:NH1	1:A:510:ARG:CG	2.72	0.50
1:B:84:SER:OG	1:B:86:GLU:HG2	2.11	0.50
1:A:172:LYS:NZ	3:A:5102:HOH:O	2.44	0.50
1:A:556:SER:HB3	3:A:5225:HOH:O	2.11	0.50
1:B:439:LEU:O	1:B:457:LEU:HG	2.12	0.50
1:A:523:LYS:HZ1	1:A:535:LYS:HG3	1.77	0.49
1:B:124:LYS:O	1:B:128:GLU:HG3	2.11	0.49
1:A:287:THR:HG21	3:A:5226:HOH:O	2.12	0.49
1:B:5:THR:CG2	1:B:278:ARG:HH12	2.21	0.49
1:A:523:LYS:NZ	1:A:536:LEU:H	2.11	0.48
1:B:527:ASN:HA	3:B:6294:HOH:O	2.13	0.48
2:A:5001:153:H162	2:A:5001:153:H231	1.75	0.48
1:A:22:PRO:HG2	1:A:401:ARG:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:LEU:HD23	1:B:182:LEU:O	2.14	0.48
1:B:508:ARG:HH11	1:B:508:ARG:HG3	1.79	0.47
1:A:535:LYS:O	1:A:536:LEU:HB2	2.14	0.47
1:B:182:LEU:CD2	1:B:182:LEU:C	2.81	0.47
1:A:390:THR:HB	1:A:391:PRO:HD3	1.97	0.47
1:B:491:LYS:HE3	1:B:492:LEU:CD1	2.44	0.47
1:A:515:GLY:HA2	1:A:519:ALA:HB2	1.97	0.47
1:B:485:VAL:O	1:B:489:LEU:HG	2.15	0.47
1:B:13:PRO:HD3	1:B:43:ARG:NH1	2.30	0.46
1:B:85:VAL:HG21	1:B:120:HIS:CE1	2.51	0.46
1:A:5:THR:CG2	1:A:278:ARG:HH22	2.27	0.46
1:B:1:SER:CB	3:B:6145:HOH:O	2.63	0.46
1:A:458:ASP:HA	1:A:461:GLN:NE2	2.30	0.46
1:B:375:ASP:HB2	3:B:6076:HOH:O	2.16	0.46
1:A:118:HIS:O	1:A:122:VAL:HG23	2.16	0.46
1:B:439:LEU:HD12	1:B:439:LEU:N	2.31	0.45
1:A:408:TRP:O	1:A:412:ILE:HG13	2.16	0.45
1:B:535:LYS:CA	1:B:535:LYS:HE3	2.46	0.45
1:B:445:CYS:SG	1:B:454:ILE:HD12	2.57	0.45
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.98	0.45
1:B:14:CYS:O	1:B:15:ALA:HB2	2.17	0.44
1:A:374:HIS:HA	1:A:379:LYS:O	2.17	0.44
1:B:461:GLN:HB3	1:B:542:ALA:HA	1.98	0.44
1:A:160:ILE:HA	1:A:282:SER:OG	2.18	0.44
1:A:545:LEU:HB3	1:A:547:LEU:CD1	2.47	0.44
1:A:124:LYS:HE2	1:A:128:GLU:OE2	2.18	0.44
1:A:496:PRO:HG2	1:A:499:VAL:HG23	2.00	0.43
1:A:530:VAL:O	1:A:533:LYS:HD2	2.18	0.43
1:B:461:GLN:HB2	1:B:545:LEU:HD11	2.00	0.43
1:A:84:SER:OG	1:A:86:GLU:HG2	2.19	0.43
1:A:36:MET:HE1	1:A:491:LYS:HG3	2.00	0.43
1:B:307:LYS:HE3	1:B:307:LYS:HB2	1.88	0.43
1:A:346:TYR:O	1:A:347:SER:HB3	2.18	0.43
1:B:109:ARG:HH11	1:B:109:ARG:HG2	1.83	0.43
1:B:523:LYS:HG3	1:B:534:LEU:CD2	2.48	0.43
1:A:461:GLN:HG2	1:A:539:ILE:HG21	2.00	0.43
1:A:523:LYS:HE3	3:A:5281:HOH:O	2.19	0.42
1:A:508:ARG:HH11	1:A:508:ARG:CG	2.32	0.42
1:B:537:THR:HB	1:B:538:PRO:HD2	2.01	0.42
1:A:485:VAL:O	1:A:489:LEU:HG	2.19	0.42
1:A:141:LYS:CE	1:A:160:ILE:HB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:SER:HA	1:B:140:ALA:CB	2.49	0.42
1:A:466:LEU:HD22	1:A:551:PHE:HE2	1.85	0.42
1:B:20:LYS:H	1:B:20:LYS:NZ	2.18	0.42
1:A:458:ASP:HA	1:A:461:GLN:HE21	1.84	0.42
1:A:475:HIS:O	1:A:476:SER:HB2	2.19	0.42
1:B:86:GLU:O	1:B:90:LYS:HG2	2.18	0.42
1:A:264:GLY:HA3	3:A:5097:HOH:O	2.18	0.42
1:A:440:GLU:OE1	1:A:440:GLU:N	2.40	0.42
1:B:106:LYS:CA	1:B:106:LYS:NZ	2.70	0.42
1:B:501:ARG:NH2	1:B:505:ARG:HH21	2.18	0.42
1:A:436:GLN:O	1:A:438:GLN:HG3	2.20	0.42
1:B:217:PHE:CD2	1:B:336:LEU:HD21	2.55	0.41
1:B:514:GLN:HB2	1:B:518:ALA:HB3	2.03	0.41
1:A:515:GLY:CA	1:A:519:ALA:HB2	2.50	0.41
1:B:537:THR:HB	1:B:538:PRO:CD	2.51	0.41
1:A:141:LYS:HE2	1:A:160:ILE:HB	2.02	0.41
1:B:439:LEU:N	1:B:439:LEU:CD1	2.83	0.41
1:B:440:GLU:OE1	1:B:440:GLU:N	2.49	0.41
1:B:20:LYS:CE	3:B:6157:HOH:O	2.64	0.41
1:A:555:TYR:CD1	1:A:560:ILE:HG13	2.56	0.41
1:B:346:TYR:O	1:B:347:SER:HB3	2.20	0.41
1:B:58:GLN:HG2	1:B:347:SER:HB2	2.02	0.41
1:A:321:VAL:CG2	1:A:365:SER:HB3	2.51	0.41
1:B:102:GLY:O	1:B:114:LYS:CE	2.68	0.41
1:B:510:ARG:NH1	3:B:6291:HOH:O	2.54	0.41
1:A:523:LYS:HZ2	1:A:536:LEU:HD12	1.86	0.41
1:A:14:CYS:HB2	1:A:139:MET:CE	2.50	0.41
1:A:355:GLN:O	1:A:355:GLN:HG3	2.19	0.41
1:B:336:LEU:CD1	1:B:356:PRO:HD3	2.46	0.40
1:B:30:LEU:O	1:B:494:VAL:HG22	2.21	0.40
1:A:448:TYR:CE2	1:A:551:PHE:HD1	2.39	0.40
1:B:531:LYS:HE3	1:B:531:LYS:HB2	1.91	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	554/578 (96%)	535 (97%)	18 (3%)	1 (0%)	52	48
1	B	553/578 (96%)	535 (97%)	18 (3%)	0	100	100
All	All	1107/1156 (96%)	1070 (97%)	36 (3%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	535	LYS

### 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	476/492 (97%)	468 (98%)	8 (2%)	68	71
1	B	475/492 (96%)	465 (98%)	10 (2%)	61	63
All	All	951/984 (97%)	933 (98%)	18 (2%)	65	67

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	LEU
1	A	303	CYS
1	A	309	GLN
1	A	321	VAL
1	A	329	THR
1	A	350	PRO
1	A	440	GLU
1	A	510	ARG
1	B	14	CYS
1	B	20	LYS
1	B	57	LEU

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Mol	Chain	Res	Type
1	B	106	LYS
1	B	159	LEU
1	B	182	LEU
1	B	184	GLN
1	B	303	CYS
1	B	330	GLN
1	B	535	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	34	HIS
1	A	49	GLN
1	A	273	ASN
1	A	309	GLN
1	A	374	HIS
1	A	446	GLN
1	A	544	GLN
1	B	49	GLN
1	B	184	GLN
1	B	273	ASN
1	B	374	HIS
1	B	475	HIS
1	B	544	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	153	A	5001	-	32,35,35	2.32	14 (43%)	44,50,50	1.24	6 (13%)
2	153	B	6001	-	32,35,35	2.25	13 (40%)	44,50,50	1.22	6 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	153	A	5001	-	-	0/26/30/30	0/3/3/3
2	153	B	6001	-	-	0/26/30/30	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5001	153	C22-C17	2.14	1.43	1.38
2	A	5001	153	C27-C28	2.15	1.42	1.39
2	B	6001	153	C12-C13	2.15	1.42	1.38
2	B	6001	153	C12-C11	2.18	1.42	1.38
2	A	5001	153	C30-C28	2.18	1.54	1.49
2	B	6001	153	C22-C17	2.22	1.43	1.38
2	A	5001	153	C12-C11	2.38	1.42	1.38
2	A	5001	153	C10-C11	2.41	1.42	1.38
2	A	5001	153	C29-C24	2.44	1.43	1.39
2	B	6001	153	C10-C11	2.45	1.42	1.38
2	A	5001	153	C25-C24	2.48	1.44	1.38
2	B	6001	153	C8-C13	2.50	1.43	1.39
2	B	6001	153	C25-C24	2.60	1.44	1.38
2	A	5001	153	C18-C17	2.66	1.44	1.38
2	B	6001	153	C18-C17	2.70	1.44	1.38
2	B	6001	153	C23-C24	2.73	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6001	153	C29-C24	2.85	1.44	1.39
2	A	5001	153	C23-C24	2.85	1.56	1.51
2	A	5001	153	C8-C13	2.88	1.43	1.39
2	A	5001	153	C29-C28	3.38	1.45	1.39
2	B	6001	153	C29-C28	3.58	1.45	1.39
2	B	6001	153	C6-N1	3.94	1.41	1.35
2	B	6001	153	C2-N1	4.23	1.53	1.47
2	A	5001	153	C23-N1	4.35	1.54	1.46
2	B	6001	153	C23-N1	4.45	1.54	1.46
2	A	5001	153	C6-N1	4.62	1.42	1.35
2	A	5001	153	C2-N1	4.82	1.54	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6001	153	C12-C13-C8	-3.30	119.39	121.59
2	A	5001	153	C12-C13-C8	-3.26	119.42	121.59
2	B	6001	153	C26-C27-C28	-2.77	117.71	120.76
2	A	5001	153	C26-C27-C28	-2.77	117.71	120.76
2	A	5001	153	O7-C6-C8	-2.20	115.65	120.14
2	A	5001	153	C24-C23-N1	2.07	117.32	113.46
2	B	6001	153	C27-C28-C29	2.07	121.62	117.63
2	B	6001	153	C9-C8-C13	2.09	120.28	117.77
2	A	5001	153	C9-C8-C13	2.13	120.34	117.77
2	B	6001	153	C24-C23-N1	2.52	118.15	113.46
2	B	6001	153	C8-C6-N1	2.66	121.56	117.78
2	A	5001	153	C8-C6-N1	2.86	121.85	117.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5001	153	1	0
2	B	6001	153	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	558/578 (96%)	0.12	17 (3%)	54 55	13, 26, 47, 68	0
1	B	557/578 (96%)	0.04	19 (3%)	49 50	12, 23, 47, 68	0
All	All	1115/1156 (96%)	0.08	36 (3%)	51 52	12, 25, 47, 68	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	544	GLN	4.8
1	B	545	LEU	4.4
1	A	541	ALA	4.3
1	A	532	THR	4.0
1	B	543	SER	3.9
1	A	563	SER	3.8
1	B	541	ALA	3.6
1	A	534	LEU	3.5
1	B	536	LEU	3.2
1	A	544	GLN	3.0
1	B	549	GLY	3.0
1	A	545	LEU	2.9
1	B	532	THR	2.8
1	B	534	LEU	2.7
1	A	490	ARG	2.5
1	A	43	ARG	2.5
1	B	531	LYS	2.4
1	B	546	ASP	2.4
1	B	539	ILE	2.4
1	A	498	ARG	2.3
1	B	516	GLY	2.3
1	A	47	LEU	2.3
1	A	536	LEU	2.3
1	A	20	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	535	LYS	2.2
1	A	32	ARG	2.2
1	A	330	GLN	2.2
1	A	10	LEU	2.2
1	B	540	PRO	2.2
1	A	530	VAL	2.1
1	B	111	LEU	2.1
1	B	440	GLU	2.1
1	A	539	ILE	2.0
1	B	94	PRO	2.0
1	B	95	HIS	2.0
1	B	110	ASN	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	153	A	5001	33/33	0.75	0.28	2.74	38,45,54,55	0
2	153	B	6001	33/33	0.73	0.26	2.57	33,44,55,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.