



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:53 PM GMT

PDB ID : 4JU2  
Title : Crystal structure of hcv ns5b polymerase in complex with compound 12  
Authors : Coulombe, R.  
Deposited on : 2013-03-24  
Resolution : 2.70 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

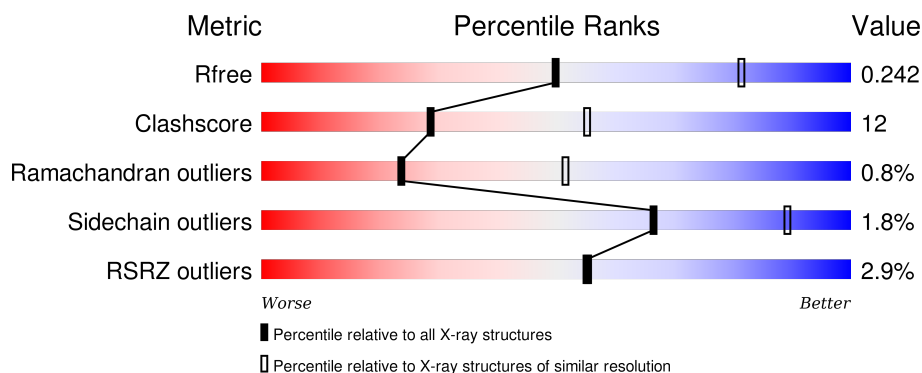
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	576	<div> <div></div> <div>72%</div> <div>25%</div> <div>• •</div> </div>
1	B	576	<div> <div>5%</div> <div>73%</div> <div>24%</div> <div>• •</div> </div>

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	GOL	B	601	-	-	-	X
4	MG	A	3003	-	-	-	X
4	MG	B	603	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9091 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	560	Total	C	N	O	S	0	0	0
			4362	2747	771	812	32			
1	B	560	Total	C	N	O	S	0	0	0
			4362	2747	771	812	32			

There are 12 discrepancies between the modelled and reference sequences:

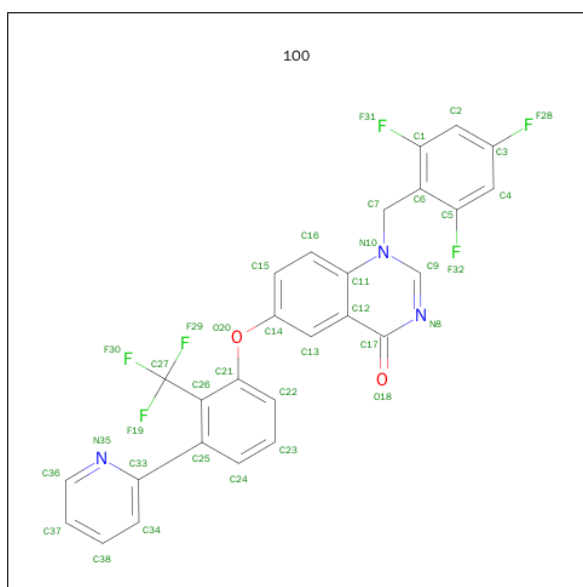
Chain	Residue	Modelled	Actual	Comment	Reference
A	571	HIS	-	EXPRESSION TAG	UNP O92972
A	572	HIS	-	EXPRESSION TAG	UNP O92972
A	573	HIS	-	EXPRESSION TAG	UNP O92972
A	574	HIS	-	EXPRESSION TAG	UNP O92972
A	575	HIS	-	EXPRESSION TAG	UNP O92972
A	576	HIS	-	EXPRESSION TAG	UNP O92972
B	571	HIS	-	EXPRESSION TAG	UNP O92972
B	572	HIS	-	EXPRESSION TAG	UNP O92972
B	573	HIS	-	EXPRESSION TAG	UNP O92972
B	574	HIS	-	EXPRESSION TAG	UNP O92972
B	575	HIS	-	EXPRESSION TAG	UNP O92972
B	576	HIS	-	EXPRESSION TAG	UNP O92972

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 6-[3-(PYRIDIN-2-YL)-2-(TRIFLUOROMETHYL)PHENOXY]-1-(2,4,6-TRIFLUOROBENZYL)QUINAZOLIN-4(1H)-ONE (three-letter code: 1O0) (formula: C<sub>27</sub>H<sub>15</sub>F<sub>6</sub>N<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			38	27	6	3	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	0	0
			38	27	6	3	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Mg	0	0
			2	2		
4	A	2	Total	Mg	0	0
			2	2		

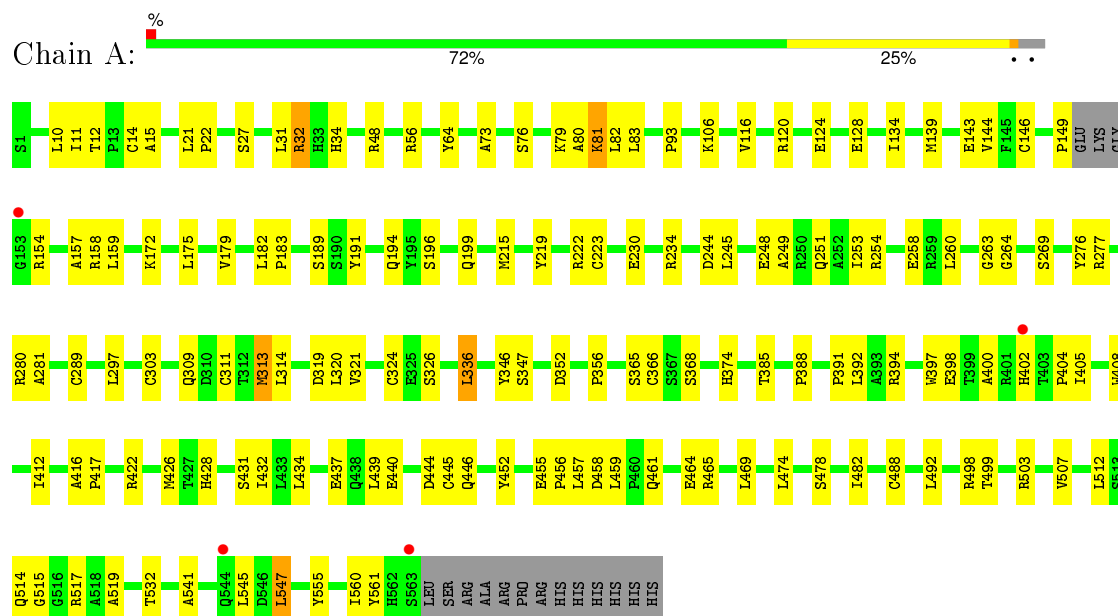
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	141	Total	O	0	0
			141	141		
5	B	134	Total	O	0	0
			134	134		

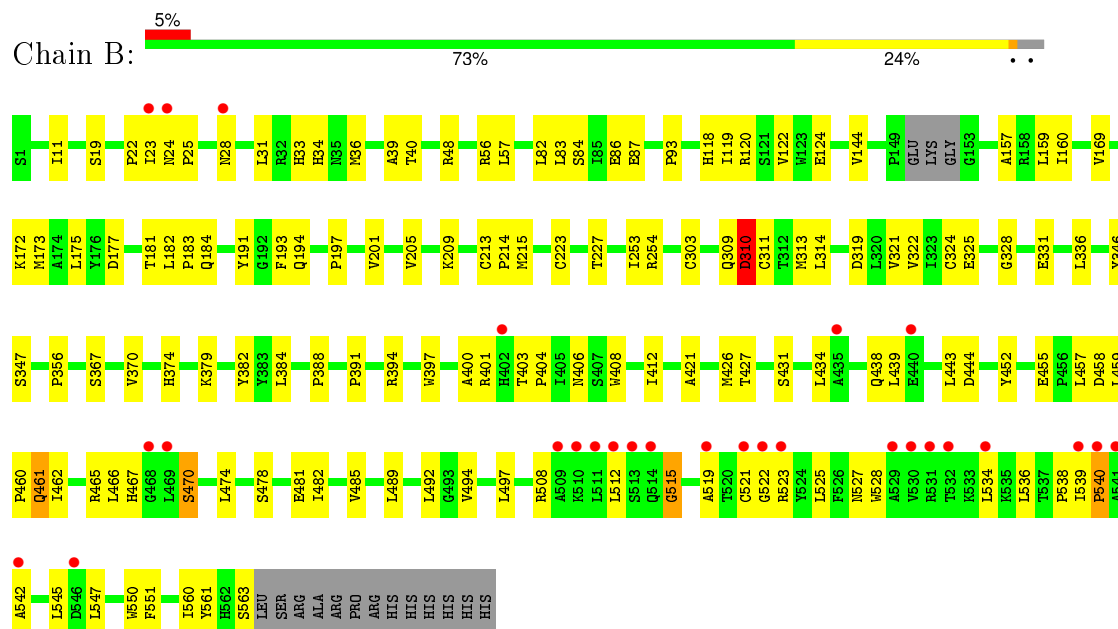
### 3 Residue-property plots

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: Genome polypeptide



#### • Molecule 1: Genome polypeptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.54Å 107.74Å 135.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 47.98 – 2.69	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.70) 99.6 (47.98-2.69)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 2.69Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, $R_{free}$	0.201 , 0.250 0.198 , 0.242	Depositor DCC
$R_{free}$ test set	2159 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.8	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.3	EDS
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 43399 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9091	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, 1O0

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	0.36	0/4457	0.62	0/6049
1	B	0.34	0/4457	0.60	0/6049
All	All	0.35	0/8914	0.61	0/12098

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

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	4362	0	4374	99	0
1	B	4362	0	4374	103	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
3	A	38	0	15	0	0
3	B	38	0	15	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	141	0	0	8	0
5	B	134	0	0	4	0
All	All	9091	0	8794	201	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 12.

All (201) 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:248:GLU:HG3	5:A:3114:HOH:O	1.79	0.81
1:B:303:CYS:HG	1:B:311:CYS:HG	1.29	0.80
1:A:303:CYS:HG	1:A:311:CYS:HG	1.27	0.79
1:B:119:ILE:HD13	1:B:169:VAL:HG11	1.64	0.78
1:B:515:GLY:HA2	1:B:519:ALA:HB2	1.64	0.77
1:A:175:LEU:O	1:A:179:VAL:HG13	1.85	0.76
1:B:201:VAL:HG13	1:B:370:VAL:HG13	1.68	0.76
1:A:439:LEU:HB3	1:A:457:LEU:HD21	1.70	0.73
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.72	0.72
1:A:314:LEU:HB3	1:A:321:VAL:HG13	1.71	0.72
1:A:22:PRO:HG2	1:A:400:ALA:HB1	1.74	0.70
1:A:503:ARG:O	1:A:507:VAL:HG23	1.92	0.70
1:B:439:LEU:HD23	1:B:457:LEU:HD21	1.73	0.70
1:A:394:ARG:O	1:A:398:GLU:HG3	1.91	0.69
1:B:33:HIS:HB2	1:B:492:LEU:O	1.92	0.69
1:A:314:LEU:HB3	1:A:321:VAL:CG1	2.23	0.68
1:A:440:GLU:HA	5:A:3143:HOH:O	1.92	0.68
1:A:499:THR:O	1:A:503:ARG:HG3	1.95	0.67
1:B:336:LEU:HD23	1:B:356:PRO:HD3	1.77	0.67
1:A:154:ARG:HH11	1:A:154:ARG:HG3	1.60	0.67
1:B:408:TRP:O	1:B:412:ILE:HG13	1.95	0.66
1:B:382:TYR:HB2	5:B:780:HOH:O	1.95	0.66
1:B:314:LEU:HB3	1:B:321:VAL:HG13	1.78	0.66
1:B:93:PRO:HG3	1:B:561:TYR:HB2	1.78	0.65
1:B:515:GLY:CA	1:B:519:ALA:HB2	2.25	0.65
1:B:33:HIS:HB3	1:B:36:MET:HG2	1.77	0.65
1:B:434:LEU:HD23	1:B:439:LEU:HD11	1.80	0.64
1:B:367:SER:HB2	5:B:707:HOH:O	1.98	0.64
1:A:405:ILE:HG12	1:A:446:GLN:HE21	1.62	0.64
1:B:313:MET:SD	1:B:322:VAL:HG22	2.38	0.62
1:B:508:ARG:HG3	1:B:522:GLY:O	1.99	0.62
1:B:175:LEU:HD21	1:B:253:ILE:HG12	1.82	0.62
1:B:24:ASN:N	1:B:25:PRO:HD3	2.16	0.61
1:A:455:GLU:HB3	5:A:3143:HOH:O	1.99	0.61
1:A:223:CYS:HB3	5:A:3220:HOH:O	2.01	0.60
1:A:336:LEU:HD12	1:A:356:PRO:HD3	1.82	0.60
1:A:116:VAL:O	1:A:120:ARG:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:GLN:O	1:B:324:CYS:HB2	2.03	0.58
1:A:21:LEU:HD12	1:A:22:PRO:HD2	1.84	0.58
1:B:22:PRO:O	1:B:25:PRO:HG3	2.04	0.58
1:A:48:ARG:HG2	1:A:159:LEU:HG	1.86	0.57
1:A:422:ARG:HA	1:A:426:MET:SD	2.44	0.57
1:A:461:GLN:HG2	1:A:541:ALA:HB3	1.86	0.57
1:A:263:GLY:HA2	1:A:277:ARG:NH1	2.20	0.57
1:A:515:GLY:HA2	1:A:519:ALA:HB2	1.87	0.56
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.86	0.56
1:A:388:PRO:HG2	1:A:488:CYS:SG	2.45	0.56
1:A:172:LYS:HE3	1:A:560:ILE:HD13	1.87	0.56
1:B:465:ARG:HD3	1:B:542:ALA:O	2.06	0.56
1:B:328:GLY:HA3	1:B:331:GLU:OE1	2.05	0.56
1:A:93:PRO:HG3	1:A:561:TYR:HB2	1.87	0.55
1:B:444:ASP:HA	1:B:452:TYR:O	2.06	0.55
1:B:534:LEU:HD12	1:B:534:LEU:H	1.72	0.54
1:B:421:ALA:O	1:B:426:MET:HG3	2.06	0.54
1:B:314:LEU:HB3	1:B:321:VAL:CG1	2.36	0.54
1:A:11:ILE:HD13	1:A:159:LEU:HD22	1.89	0.54
1:A:405:ILE:HG23	1:A:445:CYS:HA	1.90	0.54
1:B:439:LEU:HB3	1:B:457:LEU:HD21	1.89	0.54
1:B:460:PRO:HB2	1:B:461:GLN:HE21	1.73	0.54
1:A:309:GLN:O	1:A:324:CYS:HB2	2.07	0.54
1:B:489:LEU:HD22	1:B:494:VAL:HG11	1.89	0.53
1:A:14:CYS:HB2	1:A:139:MET:CE	2.38	0.53
1:A:532:THR:HG22	1:A:532:THR:O	2.09	0.53
1:A:21:LEU:HD23	1:A:34:HIS:HB2	1.91	0.53
1:A:80:ALA:HB3	1:A:245:LEU:HD23	1.90	0.53
1:A:478:SER:HB2	5:A:3188:HOH:O	2.09	0.52
1:B:48:ARG:HG2	1:B:159:LEU:HG	1.92	0.52
1:B:82:LEU:HD12	1:B:173:MET:O	2.09	0.52
1:B:120:ARG:NH1	1:B:124:GLU:HG3	2.25	0.52
1:A:79:LYS:HG3	1:A:244:ASP:HB3	1.91	0.52
1:B:461:GLN:H	1:B:461:GLN:NE2	2.09	0.51
1:B:201:VAL:HG13	1:B:370:VAL:CG1	2.40	0.51
1:A:368:SER:HB2	1:A:385:THR:O	2.10	0.51
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.91	0.51
1:B:346:TYR:O	1:B:347:SER:HB3	2.11	0.51
1:A:437:GLU:HA	5:A:3234:HOH:O	2.11	0.50
1:B:83:LEU:HD13	5:B:703:HOH:O	2.11	0.50
1:A:146:CYS:SG	1:A:492:LEU:HD21	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:GLU:O	1:B:485:VAL:HG23	2.12	0.50
1:B:84:SER:OG	1:B:87:GLU:HG3	2.12	0.50
1:B:40:THR:HB	1:B:157:ALA:HB2	1.94	0.50
1:B:561:TYR:CE2	1:B:563:SER:HB3	2.47	0.49
1:A:465:ARG:HG2	1:A:547:LEU:HD22	1.94	0.49
1:B:461:GLN:HG3	1:B:539:ILE:HG21	1.94	0.49
1:B:427:THR:O	1:B:431:SER:HB2	2.12	0.49
1:B:426:MET:HE2	1:B:525:LEU:HD22	1.94	0.49
1:B:397:TRP:CZ2	1:B:401:ARG:HD2	2.47	0.49
1:B:534:LEU:N	1:B:534:LEU:HD12	2.27	0.49
1:B:497:LEU:HD12	1:B:497:LEU:O	2.13	0.49
1:A:183:PRO:HG3	1:A:289:CYS:SG	2.52	0.49
1:A:465:ARG:NH1	1:A:545:LEU:O	2.46	0.49
1:A:515:GLY:CA	1:A:519:ALA:HB2	2.43	0.49
1:A:144:VAL:HB	1:A:394:ARG:HG2	1.95	0.49
1:A:144:VAL:HG21	1:A:397:TRP:CG	2.48	0.49
1:A:10:LEU:O	1:A:12:THR:HG23	2.13	0.49
1:A:249:ALA:O	1:A:253:ILE:HG13	2.13	0.48
1:A:14:CYS:HB2	1:A:139:MET:HE1	1.95	0.48
1:B:31:LEU:HD12	1:B:31:LEU:O	2.12	0.48
1:B:331:GLU:CD	1:B:331:GLU:H	2.16	0.48
1:B:56:ARG:O	1:B:57:LEU:HD23	2.14	0.48
1:B:182:LEU:HB3	1:B:183:PRO:HD3	1.96	0.48
1:B:527:ASN:ND2	1:B:536:LEU:HD11	2.28	0.47
1:A:191:TYR:O	1:A:194:GLN:HG2	2.13	0.47
1:A:313:MET:HG3	1:A:320:LEU:HD11	1.95	0.47
1:B:426:MET:CE	1:B:525:LEU:HD22	2.44	0.47
1:B:523:ARG:O	1:B:527:ASN:HB2	2.15	0.47
1:B:406:ASN:ND2	1:B:443:LEU:HB3	2.29	0.47
1:A:405:ILE:HG12	1:A:446:GLN:NE2	2.28	0.47
1:B:197:PRO:O	1:B:201:VAL:HG23	2.15	0.47
1:A:48:ARG:HD3	1:A:157:ALA:O	2.14	0.46
1:B:460:PRO:HD2	1:B:461:GLN:HE22	1.80	0.46
1:A:405:ILE:N	1:A:405:ILE:HD12	2.30	0.46
1:B:28:ASN:HA	1:B:34:HIS:NE2	2.29	0.46
1:B:11:ILE:HD13	1:B:159:LEU:HD22	1.98	0.46
1:B:374:HIS:HA	1:B:379:LYS:O	2.16	0.46
1:A:478:SER:O	1:A:482:ILE:HG13	2.16	0.46
1:A:196:SER:OG	1:A:199:GLN:HG3	2.15	0.46
1:B:191:TYR:CZ	1:B:193:PHE:HB2	2.50	0.46
1:B:191:TYR:CE2	1:B:193:PHE:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ARG:NH2	1:A:258:GLU:HG2	2.31	0.45
1:A:134:ILE:HD12	1:A:260:LEU:HB2	1.97	0.45
1:B:309:GLN:HB3	1:B:325:GLU:HB3	1.98	0.45
1:A:428:HIS:O	1:A:432:ILE:HG13	2.16	0.45
1:A:12:THR:OG1	1:A:269:SER:OG	2.32	0.45
1:A:81:LYS:HE2	1:A:83:LEU:CD1	2.46	0.45
1:B:201:VAL:CG2	1:B:384:LEU:HB2	2.47	0.45
1:A:189:SER:HA	1:A:194:GLN:HE22	1.82	0.45
1:B:374:HIS:O	1:B:474:LEU:HA	2.16	0.45
1:A:455:GLU:HB2	1:A:458:ASP:OD2	2.17	0.45
1:A:321:VAL:HB	1:A:365:SER:HB3	1.99	0.44
1:A:388:PRO:C	1:A:391:PRO:HD2	2.37	0.44
1:A:81:LYS:HE2	1:A:83:LEU:HD12	2.00	0.44
1:A:222:ARG:HH11	1:A:222:ARG:HG2	1.82	0.44
1:A:251:GLN:NE2	1:B:254:ARG:HG2	2.33	0.44
1:B:160:ILE:HG13	1:B:160:ILE:O	2.17	0.44
1:B:388:PRO:C	1:B:391:PRO:HD2	2.38	0.44
1:A:154:ARG:HG3	1:A:154:ARG:NH1	2.29	0.44
1:A:541:ALA:O	1:A:545:LEU:HG	2.18	0.43
1:B:508:ARG:NH1	1:B:512:LEU:HD11	2.33	0.43
1:B:466:LEU:HD22	1:B:551:PHE:HE2	1.83	0.43
1:B:172:LYS:HE3	1:B:560:ILE:HD13	2.00	0.43
1:B:455:GLU:HB2	1:B:458:ASP:OD2	2.18	0.43
1:A:374:HIS:O	1:A:474:LEU:HA	2.19	0.43
1:B:536:LEU:HD12	1:B:536:LEU:N	2.33	0.43
1:B:177:ASP:O	1:B:181:THR:HG23	2.18	0.43
1:A:280:ARG:HG3	1:A:281:ALA:O	2.18	0.43
1:B:118:HIS:O	1:B:122:VAL:HG23	2.19	0.43
1:A:555:TYR:CD1	1:A:560:ILE:HG13	2.54	0.43
1:A:456:PRO:O	1:A:459:LEU:HG	2.19	0.43
1:A:434:LEU:CD2	1:A:439:LEU:HD11	2.48	0.42
1:B:215:MET:SD	1:B:215:MET:C	2.97	0.42
1:A:416:ALA:N	1:A:417:PRO:CD	2.82	0.42
1:B:478:SER:O	1:B:482:ILE:HG13	2.19	0.42
1:A:457:LEU:HD12	1:A:517:ARG:NH2	2.35	0.42
1:A:143:GLU:OE2	1:A:158:ARG:NH2	2.53	0.42
1:B:184:GLN:HB2	5:B:803:HOH:O	2.19	0.42
1:B:539:ILE:HG23	1:B:540:PRO:HD2	2.01	0.42
1:A:222:ARG:HD3	5:A:3140:HOH:O	2.19	0.42
1:B:33:HIS:HB3	1:B:36:MET:CG	2.46	0.42
1:B:23:ILE:O	1:B:24:ASN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:GLY:HA3	1:A:277:ARG:O	2.20	0.42
1:B:86:GLU:OE1	1:B:86:GLU:N	2.52	0.42
1:A:392:LEU:HA	1:A:392:LEU:HD23	1.87	0.42
1:A:264:GLY:HA2	1:A:276:TYR:CZ	2.55	0.42
1:A:444:ASP:HA	1:A:452:TYR:O	2.19	0.42
1:B:397:TRP:CE2	1:B:401:ARG:HD2	2.55	0.41
1:A:56:ARG:HD3	1:A:56:ARG:N	2.35	0.41
1:A:402:HIS:CD2	5:A:3157:HOH:O	2.72	0.41
1:A:230:GLU:O	1:A:234:ARG:HG3	2.20	0.41
1:A:404:PRO:HB2	1:A:405:ILE:HD12	2.01	0.41
1:A:215:MET:HB2	1:A:326:SER:HB2	2.01	0.41
1:B:403:THR:HA	1:B:404:PRO:HD3	1.94	0.41
1:B:223:CYS:O	1:B:227:THR:HG23	2.20	0.41
1:A:464:GLU:OE1	1:A:469:LEU:HD21	2.20	0.41
1:B:547:LEU:O	1:B:550:TRP:HB2	2.20	0.41
1:B:521:CYS:O	1:B:525:LEU:HB2	2.20	0.41
1:A:73:ALA:O	1:A:76:SER:HB2	2.21	0.41
1:B:11:ILE:O	1:B:11:ILE:HG22	2.20	0.41
1:A:346:TYR:O	1:A:347:SER:HB3	2.20	0.41
1:A:31:LEU:HB2	1:A:492:LEU:O	2.21	0.41
1:B:197:PRO:HB2	1:B:467:HIS:HE1	1.86	0.41
1:B:470:SER:O	1:B:474:LEU:HG	2.19	0.41
1:B:19:SER:HA	1:B:39:ALA:HB3	2.01	0.41
1:A:124:GLU:O	1:A:128:GLU:HG3	2.20	0.41
1:A:64:TYR:CZ	1:A:297:LEU:HD21	2.56	0.41
1:A:32:ARG:HD2	1:A:32:ARG:N	2.36	0.41
1:A:431:SER:HB2	1:A:507:VAL:HG21	2.03	0.41
1:B:459:LEU:N	1:B:460:PRO:CD	2.83	0.41
1:B:191:TYR:O	1:B:194:GLN:HG2	2.21	0.41
1:B:205:VAL:HG13	1:B:209:LYS:HE3	2.02	0.41
1:B:213:CYS:HA	1:B:214:PRO:HD2	1.92	0.41
1:B:458:ASP:O	1:B:462:ILE:HG13	2.21	0.41
1:A:440:GLU:CD	1:A:440:GLU:H	2.23	0.41
1:A:408:TRP:O	1:A:412:ILE:HG13	2.22	0.40
1:B:197:PRO:HB2	1:B:467:HIS:CE1	2.56	0.40
1:B:83:LEU:HB2	1:B:173:MET:HA	2.04	0.40
1:B:314:LEU:HA	1:B:314:LEU:HD12	1.75	0.40
1:B:310:ASP:O	1:B:324:CYS:HA	2.22	0.40
1:B:331:GLU:N	1:B:331:GLU:CD	2.75	0.40
1:B:523:ARG:HH11	1:B:523:ARG:HG3	1.85	0.40
1:A:512:LEU:C	1:A:514:GLN:H	2.25	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	556/576 (96%)	526 (95%)	29 (5%)	1 (0%)	52 80
1	B	556/576 (96%)	513 (92%)	35 (6%)	8 (1%)	14 35
All	All	1112/1152 (96%)	1039 (93%)	64 (6%)	9 (1%)	24 51

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	538	PRO
1	B	540	PRO
1	A	15	ALA
1	B	400	ALA
1	B	528	TRP
1	B	438	GLN
1	B	470	SER
1	B	310	ASP
1	B	515	GLY

### 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	477/491 (97%)	464 (97%)	13 (3%)	52 82
1	B	477/491 (97%)	473 (99%)	4 (1%)	86 96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	954/982 (97%)	937 (98%)	17 (2%)	66 89

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	SER
1	A	32	ARG
1	A	81	LYS
1	A	106	LYS
1	A	149	PRO
1	A	182	LEU
1	A	313	MET
1	A	319	ASP
1	A	336	LEU
1	A	352	ASP
1	A	366	CYS
1	A	498	ARG
1	A	547	LEU
1	B	310	ASP
1	B	319	ASP
1	B	461	GLN
1	B	545	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	273	ASN
1	A	436	GLN
1	A	438	GLN
1	A	446	GLN
1	A	514	GLN
1	A	544	GLN
1	A	562	HIS
1	B	184	GLN
1	B	206	ASN
1	B	273	ASN
1	B	330	GLN
1	B	406	ASN
1	B	438	GLN
1	B	461	GLN

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Mol	Chain	Res	Type
1	B	467	HIS

### 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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	GOL	A	3001	-	5,5,5	0.46	0	5,5,5	0.24	0
3	1O0	A	3002	-	42,42,42	2.42	16 (38%)	53,62,62	1.35	9 (16%)
2	GOL	B	601	-	5,5,5	0.30	0	5,5,5	0.21	0
3	1O0	B	602	-	42,42,42	2.69	19 (45%)	53,62,62	1.40	10 (18%)

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	GOL	A	3001	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	100	A	3002	-	-	0/18/18/18	0/5/5/5
2	GOL	B	601	-	-	0/4/4/4	0/0/0/0
3	100	B	602	-	-	0/18/18/18	0/5/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	100	C36-N35	2.04	1.39	1.34
3	A	3002	100	C13-C14	2.06	1.40	1.37
3	A	3002	100	C9-N10	2.07	1.40	1.35
3	B	602	100	C9-N10	2.08	1.40	1.35
3	A	3002	100	C4-C5	2.10	1.41	1.37
3	B	602	100	C33-N35	2.13	1.39	1.35
3	A	3002	100	C6-C1	2.30	1.42	1.38
3	A	3002	100	C15-C14	2.36	1.43	1.38
3	A	3002	100	C2-C3	2.46	1.41	1.37
3	B	602	100	C13-C14	2.50	1.41	1.37
3	A	3002	100	C24-C25	2.54	1.44	1.39
3	A	3002	100	C2-C1	2.55	1.42	1.37
3	A	3002	100	C16-C15	2.61	1.42	1.36
3	B	602	100	C24-C25	2.61	1.44	1.39
3	B	602	100	C4-C5	2.62	1.42	1.37
3	B	602	100	C15-C14	2.66	1.44	1.38
3	A	3002	100	C6-C5	2.77	1.43	1.38
3	B	602	100	C4-C3	2.82	1.42	1.37
3	B	602	100	C2-C1	2.84	1.42	1.37
3	B	602	100	C16-C15	2.87	1.42	1.36
3	B	602	100	C2-C3	2.99	1.42	1.37
3	B	602	100	C6-C1	3.03	1.43	1.38
3	B	602	100	C6-C5	3.35	1.44	1.38
3	A	3002	100	C17-N8	3.74	1.40	1.33
3	B	602	100	C17-N8	4.00	1.40	1.33
3	A	3002	100	C21-C26	4.60	1.46	1.39
3	A	3002	100	C25-C26	4.67	1.47	1.40
3	B	602	100	C21-C26	4.91	1.47	1.39
3	A	3002	100	C11-N10	4.97	1.45	1.39
3	B	602	100	C25-C26	5.54	1.49	1.40
3	A	3002	100	C17-C12	5.65	1.50	1.41
3	B	602	100	C17-C12	5.66	1.50	1.41
3	B	602	100	C11-N10	5.75	1.46	1.39
3	A	3002	100	C12-C11	6.08	1.46	1.41
3	B	602	100	C12-C11	6.31	1.46	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	100	C16-C11-C12	-3.32	115.30	119.97
3	A	3002	100	C16-C11-C12	-3.10	115.60	119.97
3	A	3002	100	C6-C7-N10	-2.47	111.43	114.29
3	B	602	100	C4-C3-C2	-2.08	120.77	123.52
3	B	602	100	C13-C12-C17	-2.01	119.74	122.22
3	A	3002	100	C9-N8-C17	2.10	119.21	116.04
3	A	3002	100	F32-C5-C6	2.10	120.03	117.45
3	A	3002	100	C5-C4-C3	2.16	118.88	116.63
3	B	602	100	F31-C1-C6	2.17	120.12	117.45
3	A	3002	100	C1-C2-C3	2.32	119.06	116.63
3	B	602	100	C1-C2-C3	2.32	119.06	116.63
3	A	3002	100	C13-C12-C11	2.44	122.36	118.49
3	B	602	100	F32-C5-C6	2.53	120.56	117.45
3	A	3002	100	C7-N10-C11	2.53	123.56	120.38
3	B	602	100	C13-C12-C11	2.59	122.59	118.49
3	B	602	100	C5-C4-C3	2.63	119.37	116.63
3	B	602	100	C7-N10-C11	3.00	124.14	120.38
3	A	3002	100	C16-C11-N10	3.43	125.42	121.47
3	B	602	100	C16-C11-N10	3.86	125.91	121.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	560/576 (97%)	-0.24	4 (0%) 89 90	33, 50, 78, 98	0
1	B	560/576 (97%)	0.12	28 (5%) 32 31	32, 63, 102, 117	0
All	All	1120/1152 (97%)	-0.06	32 (2%) 55 55	32, 55, 94, 117	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	541	ALA	5.3
1	B	23	ILE	4.8
1	B	24	ASN	4.7
1	B	469	LEU	4.6
1	B	531	ARG	4.1
1	B	530	VAL	4.1
1	B	511	LEU	4.0
1	B	539	ILE	3.6
1	B	542	ALA	3.6
1	B	402	HIS	3.2
1	B	534	LEU	3.1
1	B	523	ARG	3.0
1	B	468	GLY	3.0
1	A	153	GLY	2.5
1	B	509	ALA	2.5
1	B	519	ALA	2.5
1	A	402	HIS	2.5
1	B	522	GLY	2.5
1	B	440	GLU	2.4
1	B	435	ALA	2.4
1	A	544	GLN	2.3
1	B	510	LYS	2.2
1	B	513	SER	2.2
1	B	540	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	532	THR	2.2
1	B	514	GLN	2.2
1	B	512	LEU	2.2
1	B	529	ALA	2.2
1	B	521	CYS	2.1
1	B	546	ASP	2.1
1	A	563	SER	2.0
1	B	28	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
4	MG	A	3003	1/1	0.95	0.23	3.33	65,65,65,65	0
4	MG	B	603	1/1	0.76	0.24	3.33	77,77,77,77	0
2	GOL	B	601	6/6	0.94	0.24	2.68	80,80,81,81	0
4	MG	A	3004	1/1	0.92	0.28	1.99	66,66,66,66	0
2	GOL	A	3001	6/6	0.94	0.16	0.59	60,65,67,68	0
3	1O0	A	3002	38/38	0.94	0.17	0.58	50,53,57,57	0
3	1O0	B	602	38/38	0.92	0.20	0.22	62,68,78,78	0
4	MG	B	604	1/1	0.46	0.49	-	83,83,83,83	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.