



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:55 am BST

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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

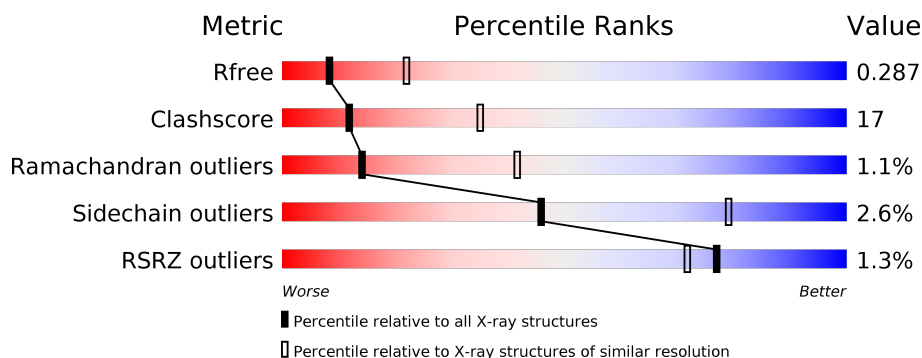
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 respectively. 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> <div></div> <div>68%</div> <div>28%</div> <div>..</div> </div> </div>
1	B	576	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>34%</div> <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
4	MG	B	604	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9200 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:

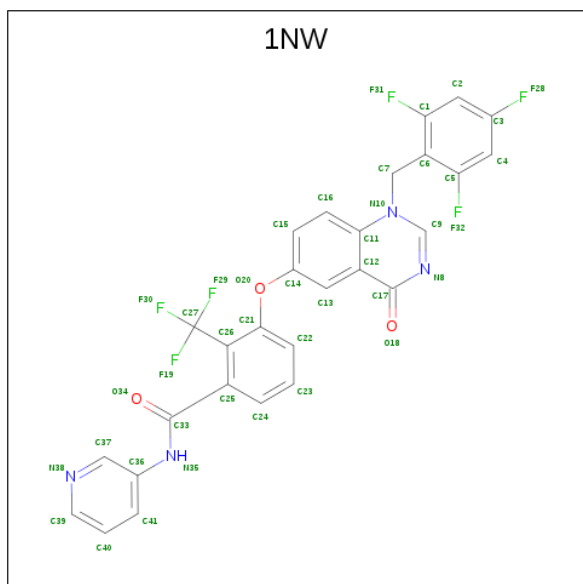
Chain	Residue	Modelled	Actual	Comment	Reference
A	571	HIS	-	EXPRESSION TAG	UNP O92972
A	572	HIS	-	EXPRESSION TAG	UNP O92972
A	573	HIS	-	EXPRESSION TAG	UNP O92972
A	574	HIS	-	EXPRESSION TAG	UNP O92972
A	575	HIS	-	EXPRESSION TAG	UNP O92972
A	576	HIS	-	EXPRESSION TAG	UNP O92972
B	571	HIS	-	EXPRESSION TAG	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 3-{[4-oxo-1-(2,4,6-trifluorobenzyl)-1,4-dihydroquinazolin-6-yl]oxy}-N-(pyridin-3-yl)-2-(trifluoromethyl)benzamide (three-letter code: 1NW) (formula: C<sub>28</sub>H<sub>16</sub>F<sub>6</sub>N<sub>4</sub>O<sub>3</sub>).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	0	0
			41	28	6	4	3		

- 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		

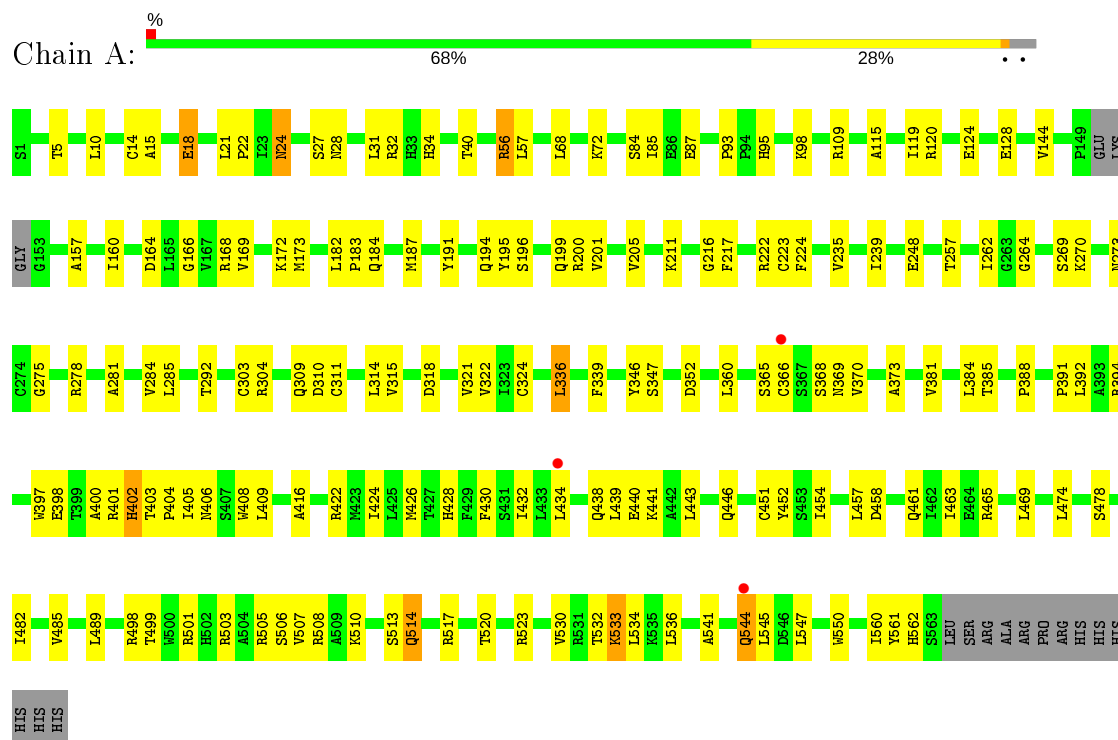
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	215	Total	O	0	0
			215	215		
5	B	163	Total	O	0	0
			163	163		

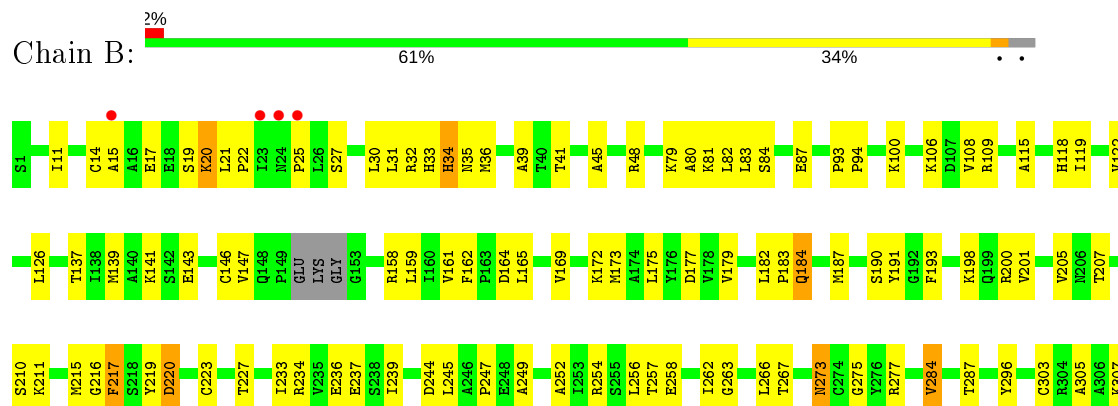
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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



HIS	S476	L308	P388
HIS	Y477	Q309	T389
HIS		D310	T390
HIS	E481	C311	P391
HIS		T312	I392
HIS	Y485	L313	
		L314	A395
L489		V315	A396
R490		N316	W397
Y491			
L492		L320	A400
G493		V321	R401
V494		V322	
P495		I323	M406
P496		C324	S407
		E325	W408
T499		S326	
			A416
R503		Q330	P417
		E331	T418
S506		D332	L419
V507		A333	W420
R508			A421
A509		L336	R422
K510		R337	M423
L511			I424
L512		T340	L425
		E341	M426
G515			T427
		R345	H428
C521			P429
		P350	F430
T524		G351	S431
L525		D352	I432
		P353	I433
A529			I434
		D359	A435
L534		L360	Q436
R535		E361	E437
L536		L362	Q438
T537		I363	I439
P538		T364	
I539		S365	
P540		C366	Y452
		S367	
I545		S368	D458
D546		N369	L459
L547		V370	P460
		S371	Q461
I560		V372	I462
Y561		A373	I463
H562		H374	E464
S563			R465
		R380	L466
LEU		V381	H467
SER		Y382	G468
ARG		Y383	I469
ALA			S470
ARG		R386	
PRO		D387	I474
ARG			H475



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.09Å 106.91Å 135.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 45.04 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.80) 96.3 (45.04-2.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.81Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, $R_{free}$	0.221 , 0.296 0.217 , 0.287	Depositor DCC
$R_{free}$ test set	3738 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.1	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 45.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9200	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 3.57% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, 1NW

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	0.38	0/4457	0.63	0/6049
1	B	0.34	0/4457	0.61	0/6049
All	All	0.36	0/8914	0.62	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	137	0
1	B	4362	0	4374	166	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
3	A	41	0	16	0	0
3	B	41	0	16	3	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	215	0	0	20	0
5	B	163	0	0	19	0
All	All	9200	0	8796	303	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 17.

All (303) 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:316:ASN:HA	5:B:1158:HOH:O	1.67	0.94
1:A:360:LEU:HD21	1:A:370:VAL:HB	1.50	0.93
1:A:541:ALA:O	1:A:544:GLN:HG2	1.76	0.86
1:B:386:ARG:HG3	5:B:1146:HOH:O	1.76	0.84
1:B:499:THR:HG22	1:B:503:ARG:HD2	1.57	0.84
1:B:314:LEU:HB3	1:B:321:VAL:HG13	1.59	0.84
1:A:120:ARG:O	1:A:124:GLU:HG2	1.82	0.80
1:A:68:LEU:O	1:A:72:LYS:HG3	1.83	0.78
1:B:187:MET:HG2	1:B:296:TYR:CD2	2.19	0.78
1:A:536:LEU:HA	5:A:3251:HOH:O	1.86	0.75
1:B:215:MET:HG3	1:B:332:ASP:OD2	1.87	0.75
1:A:409:LEU:HD21	1:A:454:ILE:HB	1.70	0.74
1:A:24:ASN:ND2	1:A:27:SER:H	1.86	0.74
1:A:40:THR:HB	1:A:157:ALA:HB2	1.71	0.73
1:B:284:VAL:HG13	5:B:1142:HOH:O	1.89	0.73
1:A:434:LEU:HD11	5:A:3229:HOH:O	1.89	0.73
1:B:303:CYS:HG	1:B:311:CYS:HG	1.37	0.72
1:A:503:ARG:O	1:A:507:VAL:HG23	1.90	0.71
1:A:434:LEU:HD23	1:A:439:LEU:HD11	1.72	0.71
1:A:508:ARG:CZ	1:A:530:VAL:HG21	2.20	0.71
1:B:175:LEU:O	1:B:179:VAL:HG22	1.90	0.71
1:A:360:LEU:CD2	1:A:370:VAL:HB	2.21	0.69
1:B:458:ASP:HA	1:B:461:GLN:NE2	2.08	0.69
1:A:530:VAL:HG12	1:A:532:THR:H	1.57	0.68
1:A:352:ASP:HA	5:A:3303:HOH:O	1.94	0.68
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.74	0.68
1:B:309:GLN:O	1:B:324:CYS:HB2	1.93	0.68
1:B:314:LEU:HB3	1:B:321:VAL:CG1	2.24	0.68
1:B:469:LEU:HD23	1:B:469:LEU:H	1.59	0.68
1:A:530:VAL:HG13	5:A:3113:HOH:O	1.93	0.67
1:B:80:ALA:HB3	1:B:245:LEU:HD23	1.77	0.67
1:B:215:MET:HB2	1:B:326:SER:HB2	1.76	0.67
1:A:394:ARG:O	1:A:398:GLU:HG3	1.96	0.66
1:A:406:ASN:ND2	1:A:443:LEU:HB3	2.11	0.66
1:A:373:ALA:HB3	1:A:474:LEU:HD22	1.78	0.66
1:B:499:THR:O	1:B:503:ARG:HG3	1.96	0.66
1:A:404:PRO:HB2	1:A:405:ILE:HD12	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ARG:HG2	1:A:426:MET:HE1	1.79	0.65
1:A:303:CYS:HG	1:A:311:CYS:HG	1.35	0.64
1:B:428:HIS:NE2	1:B:432:ILE:HD11	2.12	0.64
1:B:109:ARG:HG2	1:B:109:ARG:HH11	1.63	0.64
1:B:35:ASN:HB2	5:B:1022:HOH:O	1.98	0.63
1:B:503:ARG:O	1:B:507:VAL:HG23	1.96	0.63
1:B:390:THR:HB	1:B:391:PRO:HD3	1.80	0.63
1:A:248:GLU:HG3	5:A:3263:HOH:O	1.99	0.63
1:B:83:LEU:HB2	1:B:173:MET:HA	1.79	0.63
1:B:521:CYS:O	1:B:525:LEU:HB2	1.98	0.63
1:A:424:ILE:HD11	1:A:489:LEU:HD11	1.81	0.62
1:B:220:ASP:HB2	5:B:1134:HOH:O	1.99	0.62
1:A:360:LEU:C	1:A:360:LEU:HD23	2.20	0.62
1:B:392:LEU:O	1:B:395:ALA:HB3	2.00	0.61
1:A:24:ASN:HD22	1:A:400:ALA:HB2	1.63	0.61
1:A:120:ARG:HG2	1:A:120:ARG:HH11	1.66	0.61
1:A:223:CYS:HB3	5:A:3203:HOH:O	2.01	0.61
1:B:141:LYS:NZ	1:B:158:ARG:HH21	1.99	0.61
1:A:314:LEU:HB3	1:A:321:VAL:HG13	1.83	0.61
1:B:31:LEU:HD12	1:B:31:LEU:O	2.01	0.61
1:B:374:HIS:O	1:B:474:LEU:HA	2.01	0.60
1:A:523:ARG:HG3	1:A:534:LEU:HD12	1.82	0.60
1:B:20:LYS:HB2	1:B:20:LYS:NZ	2.15	0.60
1:B:273:ASN:ND2	1:B:275:GLY:H	2.00	0.60
1:A:124:GLU:O	1:A:128:GLU:HG3	2.00	0.59
1:B:359:ASP:HB3	1:B:362:LEU:HD12	1.83	0.59
1:A:514:GLN:HB2	5:A:3142:HOH:O	2.01	0.59
1:A:405:ILE:HD12	1:A:405:ILE:N	2.18	0.59
1:A:281:ALA:O	1:A:284:VAL:HG22	2.04	0.58
1:A:422:ARG:HA	1:A:426:MET:HE3	1.85	0.58
1:B:172:LYS:HE3	1:B:560:ILE:HD13	1.84	0.58
1:A:28:ASN:HB3	5:A:3149:HOH:O	2.04	0.58
1:A:18:GLU:HG2	1:A:401:ARG:CZ	2.33	0.58
1:B:485:VAL:O	1:B:489:LEU:HG	2.03	0.58
1:A:381:VAL:HB	1:A:474:LEU:HD21	1.85	0.58
1:B:459:LEU:O	1:B:463:ILE:HG13	2.04	0.58
1:B:198:LYS:HE3	5:B:1097:HOH:O	2.02	0.58
1:A:530:VAL:HG12	1:A:532:THR:N	2.19	0.57
1:B:14:CYS:HB2	1:B:139:MET:HE1	1.86	0.57
1:B:341:GLU:O	1:B:345:ARG:HG3	2.03	0.57
1:A:164:ASP:O	1:A:168:ARG:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:SER:O	1:B:474:LEU:HG	2.03	0.57
1:A:5:THR:O	1:A:275:GLY:HA3	2.03	0.57
1:A:201:VAL:O	1:A:205:VAL:HG13	2.04	0.57
1:A:388:PRO:C	1:A:391:PRO:HD2	2.24	0.57
1:B:201:VAL:O	1:B:205:VAL:HG23	2.05	0.57
1:A:68:LEU:HD12	1:A:68:LEU:O	2.04	0.57
1:B:108:VAL:HG21	1:B:165:LEU:HD21	1.87	0.57
1:B:100:LYS:HG2	1:B:164:ASP:OD1	2.04	0.56
1:A:533:LYS:O	1:A:534:LEU:HD23	2.05	0.56
1:B:100:LYS:HD3	5:B:1037:HOH:O	2.05	0.56
1:B:313:MET:SD	1:B:322:VAL:HG22	2.46	0.56
1:B:458:ASP:O	1:B:462:ILE:HG13	2.05	0.56
1:B:422:ARG:HG2	1:B:426:MET:HE1	1.85	0.56
1:A:196:SER:OG	1:A:199:GLN:HG3	2.05	0.56
1:B:353:PRO:HD3	5:B:1102:HOH:O	2.05	0.56
1:A:451:CYS:HB3	1:A:561:TYR:HD1	1.69	0.56
1:B:434:LEU:HD13	1:B:510:LYS:HD2	1.87	0.56
1:B:119:ILE:HD13	1:B:169:VAL:HG11	1.87	0.56
1:B:388:PRO:HB3	1:B:420:TRP:CD2	2.41	0.56
1:B:336:LEU:HD12	1:B:336:LEU:O	2.06	0.55
1:A:119:ILE:HD13	1:A:169:VAL:HG11	1.88	0.55
1:B:252:ALA:O	1:B:256:LEU:HG	2.06	0.55
1:B:418:THR:HG21	5:B:1124:HOH:O	2.07	0.55
1:B:321:VAL:HB	1:B:365:SER:OG	2.06	0.55
1:A:309:GLN:O	1:A:324:CYS:HB2	2.06	0.55
1:B:115:ALA:O	1:B:119:ILE:HG13	2.07	0.55
1:A:523:ARG:HD3	5:A:3188:HOH:O	2.06	0.55
1:A:84:SER:OG	1:A:87:GLU:HG3	2.07	0.55
1:A:32:ARG:NH1	5:A:3107:HOH:O	2.40	0.54
1:B:216:GLY:O	1:B:217:PHE:HB3	2.06	0.54
1:B:383:TYR:HH	1:B:477:TYR:HD2	1.55	0.54
1:B:27:SER:HA	5:B:1072:HOH:O	2.07	0.54
1:B:48:ARG:HG2	1:B:159:LEU:HG	1.89	0.54
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.90	0.53
1:A:56:ARG:HD3	1:A:56:ARG:N	2.23	0.53
1:A:438:GLN:NE2	1:A:441:LYS:HD2	2.23	0.53
1:B:266:LEU:HD21	1:B:277:ARG:HB2	1.91	0.53
1:B:458:ASP:HA	1:B:461:GLN:HE22	1.72	0.53
1:B:14:CYS:HB2	1:B:139:MET:CE	2.38	0.53
1:B:31:LEU:HA	1:B:493:GLY:O	2.08	0.53
1:A:406:ASN:HB3	1:A:408:TRP:NE1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:MET:HG2	1:B:296:TYR:CE2	2.42	0.53
1:B:469:LEU:N	1:B:469:LEU:HD23	2.24	0.52
1:A:461:GLN:HB3	1:A:545:LEU:HD11	1.91	0.52
1:B:489:LEU:HD22	1:B:494:VAL:HB	1.90	0.52
1:B:481:GLU:O	1:B:485:VAL:HG23	2.09	0.52
1:A:115:ALA:O	1:A:119:ILE:HG13	2.09	0.52
1:A:478:SER:O	1:A:482:ILE:HG13	2.08	0.52
1:B:81:LYS:HG2	1:B:177:ASP:OD2	2.10	0.52
1:A:264:GLY:HA3	5:A:3128:HOH:O	2.09	0.52
1:A:485:VAL:O	1:A:489:LEU:HG	2.10	0.51
1:B:109:ARG:HG2	1:B:109:ARG:NH1	2.25	0.51
1:B:19:SER:HB2	1:B:20:LYS:HD3	1.92	0.51
1:A:93:PRO:HG3	1:A:561:TYR:HB2	1.93	0.51
1:B:25:PRO:C	1:B:27:SER:H	2.14	0.51
1:A:517:ARG:HG3	1:A:517:ARG:HH11	1.76	0.51
1:A:405:ILE:HG21	1:A:446:GLN:HG3	1.92	0.51
1:B:17:GLU:OE1	1:B:41:THR:HB	2.10	0.51
1:B:187:MET:HG2	1:B:296:TYR:CG	2.46	0.51
1:A:24:ASN:ND2	1:A:27:SER:N	2.57	0.50
1:A:195:TYR:HB3	1:A:199:GLN:HB2	1.92	0.50
1:A:93:PRO:HB3	1:A:95:HIS:CE1	2.46	0.50
1:B:424:ILE:HD13	1:B:494:VAL:HG11	1.92	0.50
1:B:106:LYS:HG2	5:B:1083:HOH:O	2.12	0.50
1:B:422:ARG:HA	1:B:426:MET:CE	2.41	0.50
1:B:499:THR:CG2	1:B:503:ARG:HD2	2.38	0.50
1:B:452:TYR:CE1	1:B:562:HIS:HB2	2.47	0.50
1:A:303:CYS:CB	1:A:311:CYS:HG	2.25	0.50
1:A:314:LEU:HB3	1:A:321:VAL:CG1	2.41	0.50
1:A:336:LEU:O	1:A:339:PHE:HB3	2.12	0.50
1:A:428:HIS:O	1:A:432:ILE:HG13	2.12	0.50
1:A:401:ARG:HH11	1:A:401:ARG:HG3	1.77	0.49
1:B:475:HIS:HB2	3:B:602:1NW:H5	1.94	0.49
1:B:273:ASN:ND2	1:B:275:GLY:N	2.60	0.49
1:A:422:ARG:HG2	1:A:426:MET:CE	2.41	0.49
1:A:513:SER:O	1:A:514:GLN:HG3	2.12	0.49
1:A:406:ASN:HD21	1:A:443:LEU:HB3	1.78	0.49
1:B:184:GLN:HB2	5:B:1067:HOH:O	2.12	0.49
1:B:506:SER:O	1:B:510:LYS:HB2	2.12	0.49
1:A:434:LEU:C	1:A:434:LEU:HD13	2.32	0.49
1:B:257:THR:O	1:B:262:ILE:HG23	2.12	0.49
1:A:346:TYR:O	1:A:347:SER:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:HIS:O	1:B:432:ILE:HG13	2.13	0.49
1:B:254:ARG:NH2	1:B:258:GLU:HG2	2.27	0.49
1:B:422:ARG:HA	1:B:426:MET:HE3	1.94	0.49
1:B:508:ARG:NH1	1:B:512:LEU:HD11	2.28	0.49
1:A:217:PHE:HA	5:A:3146:HOH:O	2.11	0.48
1:A:452:TYR:CE1	1:A:562:HIS:HB2	2.48	0.48
1:A:24:ASN:ND2	1:A:400:ALA:HB2	2.28	0.48
1:A:416:ALA:HB1	1:A:463:ILE:HD13	1.94	0.48
1:A:172:LYS:HE3	1:A:560:ILE:HD13	1.95	0.48
1:A:440:GLU:HA	5:A:3232:HOH:O	2.12	0.48
1:A:507:VAL:O	1:A:510:LYS:HB2	2.13	0.48
1:B:207:THR:O	1:B:211:LYS:HG2	2.14	0.48
1:A:545:LEU:HD21	5:A:3173:HOH:O	2.14	0.48
1:B:499:THR:HG22	1:B:503:ARG:CD	2.36	0.48
1:B:39:ALA:HA	1:B:143:GLU:O	2.14	0.48
1:B:387:ASP:C	5:B:1146:HOH:O	2.52	0.47
1:A:200:ARG:HH21	1:A:365:SER:CB	2.27	0.47
1:A:452:TYR:OH	1:A:562:HIS:HD2	1.98	0.47
1:B:161:VAL:N	5:B:1127:HOH:O	2.34	0.47
1:A:182:LEU:N	1:A:183:PRO:HD2	2.29	0.47
1:A:21:LEU:HD23	1:A:34:HIS:CB	2.44	0.47
1:A:120:ARG:HG2	1:A:120:ARG:NH1	2.28	0.47
1:B:141:LYS:HZ2	1:B:158:ARG:HH21	1.62	0.47
1:B:182:LEU:HD21	1:B:239:ILE:HG22	1.95	0.47
1:B:489:LEU:HD22	1:B:494:VAL:CB	2.45	0.47
1:A:461:GLN:CB	1:A:545:LEU:HD11	2.45	0.47
1:B:223:CYS:O	1:B:227:THR:HG23	2.15	0.47
1:B:333:ALA:O	1:B:337:ARG:HG3	2.15	0.47
1:A:278:ARG:NH1	1:A:278:ARG:HG3	2.30	0.47
1:A:285:LEU:O	1:A:285:LEU:HD12	2.15	0.47
1:A:392:LEU:HA	1:A:392:LEU:HD23	1.77	0.46
1:B:118:HIS:O	1:B:122:VAL:HG23	2.15	0.46
1:B:233:ILE:O	1:B:236:GLU:HB3	2.16	0.46
1:B:436:GLN:O	1:B:437:GLU:HB2	2.14	0.46
1:A:222:ARG:HD2	5:A:3275:HOH:O	2.14	0.46
1:A:373:ALA:CB	1:A:474:LEU:HD22	2.43	0.46
1:B:33:HIS:HA	5:B:1161:HOH:O	2.16	0.46
1:A:506:SER:O	1:A:510:LYS:HG2	2.15	0.46
1:B:84:SER:OG	1:B:87:GLU:HG3	2.15	0.46
1:A:388:PRO:O	1:A:391:PRO:HD2	2.16	0.46
1:B:273:ASN:ND2	1:B:273:ASN:C	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:SER:HA	5:B:1152:HOH:O	2.16	0.46
1:B:434:LEU:CD1	1:B:507:VAL:HG13	2.46	0.46
1:B:439:LEU:N	1:B:439:LEU:HD12	2.30	0.46
1:A:211:LYS:NZ	1:A:310:ASP:OD2	2.46	0.46
1:B:372:VAL:HG11	1:B:380:ARG:HH21	1.80	0.46
1:B:381:VAL:HG11	1:B:474:LEU:HD21	1.98	0.46
1:A:109:ARG:HG2	1:A:109:ARG:HH11	1.81	0.45
1:A:303:CYS:HB3	1:A:311:CYS:HG	1.80	0.45
1:A:517:ARG:O	1:A:520:THR:HB	2.15	0.45
1:B:79:LYS:HG3	1:B:244:ASP:HB3	1.99	0.45
1:B:31:LEU:HD22	1:B:492:LEU:HD22	1.98	0.45
1:B:93:PRO:HG3	1:B:561:TYR:HB2	1.98	0.45
1:B:495:PRO:HA	1:B:496:PRO:HD3	1.81	0.45
1:A:438:GLN:HE22	1:A:441:LYS:HD2	1.81	0.45
1:B:30:LEU:O	1:B:494:VAL:HA	2.16	0.45
1:A:200:ARG:NH1	5:A:3264:HOH:O	2.38	0.44
1:A:187:MET:SD	1:A:292:THR:HG22	2.56	0.44
1:A:22:PRO:HG3	1:A:401:ARG:NH2	2.32	0.44
1:A:257:THR:O	1:A:262:ILE:HG23	2.18	0.44
1:B:182:LEU:HB3	1:B:183:PRO:HD3	1.98	0.44
1:B:506:SER:O	1:B:510:LYS:HE3	2.17	0.44
1:A:428:HIS:CE1	1:A:432:ILE:HD11	2.52	0.44
1:B:439:LEU:HD12	1:B:439:LEU:H	1.81	0.44
1:B:462:ILE:O	1:B:466:LEU:HG	2.18	0.44
1:A:216:GLY:HA2	1:A:322:VAL:O	2.18	0.44
1:B:22:PRO:HD2	1:B:400:ALA:HB1	2.00	0.44
1:B:496:PRO:HA	3:B:602:1NW:H16	2.00	0.44
1:B:162:PHE:HA	5:B:1142:HOH:O	2.18	0.44
1:B:263:GLY:HA3	1:B:277:ARG:O	2.18	0.44
1:B:374:HIS:O	1:B:475:HIS:N	2.51	0.44
1:A:360:LEU:HD21	1:A:370:VAL:CB	2.36	0.44
1:B:45:ALA:O	1:B:48:ARG:HB3	2.17	0.44
1:A:124:GLU:HB3	5:A:3234:HOH:O	2.17	0.43
1:A:278:ARG:HG3	1:A:278:ARG:HH11	1.83	0.43
1:A:166:GLY:HA3	5:A:3310:HOH:O	2.18	0.43
1:A:57:LEU:HD23	1:A:57:LEU:O	2.18	0.43
1:B:93:PRO:HA	1:B:94:PRO:HD3	1.87	0.43
1:A:498:ARG:HG3	1:A:498:ARG:HH11	1.84	0.43
1:A:31:LEU:O	1:A:31:LEU:HD12	2.19	0.43
1:B:137:THR:HA	1:B:267:THR:O	2.18	0.43
1:B:21:LEU:HD12	1:B:34:HIS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ILE:O	1:B:11:ILE:HG22	2.18	0.43
1:B:141:LYS:HE3	1:B:141:LYS:HB2	1.85	0.43
1:B:237:GLU:HG3	1:B:257:THR:OG1	2.18	0.43
1:A:545:LEU:HB3	1:A:547:LEU:HD21	2.01	0.43
1:B:126:LEU:HD11	1:B:256:LEU:HD21	1.99	0.43
1:B:416:ALA:HB3	1:B:417:PRO:HD3	2.00	0.43
1:B:539:ILE:HA	1:B:540:PRO:HD3	1.84	0.43
1:A:368:SER:HB2	1:A:385:THR:O	2.19	0.43
1:B:425:LEU:HD23	1:B:425:LEU:HA	1.78	0.43
1:B:465:ARG:HD2	1:B:547:LEU:HD12	2.01	0.43
1:A:14:CYS:HB3	1:A:269:SER:HB2	2.01	0.42
1:A:191:TYR:O	1:A:194:GLN:HG2	2.19	0.42
1:A:304:ARG:HA	5:A:3286:HOH:O	2.18	0.42
1:B:216:GLY:HA2	1:B:322:VAL:O	2.19	0.42
1:B:36:MET:O	1:B:146:CYS:HA	2.19	0.42
1:B:381:VAL:CG1	1:B:474:LEU:HD21	2.49	0.42
1:A:85:ILE:HG12	1:A:173:MET:SD	2.59	0.42
1:B:234:ARG:NH1	5:B:1043:HOH:O	2.52	0.42
1:A:21:LEU:HA	1:A:22:PRO:HD3	1.87	0.42
1:B:352:ASP:O	1:B:353:PRO:C	2.56	0.42
1:B:361:GLU:HG3	1:B:370:VAL:O	2.19	0.42
1:A:144:VAL:HG21	1:A:397:TRP:CD2	2.54	0.42
1:B:428:HIS:CE1	1:B:432:ILE:HD11	2.54	0.42
1:B:468:GLY:O	1:B:470:SER:N	2.53	0.42
1:B:305:ALA:C	1:B:307:LYS:H	2.23	0.42
1:B:545:LEU:HD13	1:B:547:LEU:HD21	2.00	0.42
1:B:364:THR:HA	1:B:368:SER:O	2.20	0.42
1:A:160:ILE:O	1:A:160:ILE:HG13	2.20	0.42
1:B:340:THR:CG2	1:B:350:PRO:HG3	2.50	0.42
1:A:18:GLU:HG2	1:A:401:ARG:NH2	2.35	0.41
1:A:458:ASP:HA	1:A:461:GLN:HE22	1.84	0.41
1:B:406:ASN:HB3	1:B:408:TRP:NE1	2.35	0.41
1:B:420:TRP:HB3	1:B:485:VAL:HG13	2.02	0.41
1:A:224:PHE:CG	1:A:318:ASP:HB2	2.55	0.41
1:B:48:ARG:NH1	5:B:1151:HOH:O	2.53	0.41
1:A:403:THR:HA	1:A:404:PRO:HD3	1.81	0.41
1:B:284:VAL:HG23	1:B:287:THR:OG1	2.21	0.41
1:A:501:ARG:O	1:A:505:ARG:HB2	2.21	0.41
1:B:303:CYS:HG	1:B:311:CYS:CB	2.33	0.41
1:A:235:VAL:O	1:A:239:ILE:HG13	2.21	0.41
1:A:498:ARG:NH1	1:A:498:ARG:HG3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:TRP:CE2	1:B:401:ARG:HD2	2.55	0.41
1:B:490:ARG:HD2	3:B:602:1NW:N38	2.36	0.41
1:B:20:LYS:HD3	1:B:20:LYS:N	2.36	0.41
1:A:499:THR:HG22	1:A:503:ARG:HE	1.86	0.41
1:B:372:VAL:HG11	1:B:380:ARG:NH2	2.35	0.41
1:B:30:LEU:O	1:B:495:PRO:HD3	2.21	0.41
1:A:270:LYS:HA	1:A:270:LYS:HD3	1.81	0.41
1:A:369:ASN:O	1:A:384:LEU:HD12	2.20	0.41
1:A:402:HIS:HB2	5:A:3291:HOH:O	2.20	0.41
1:B:434:LEU:HD11	1:B:507:VAL:HG13	2.03	0.41
1:A:440:GLU:HG2	1:A:457:LEU:HD12	2.03	0.40
1:B:383:TYR:HE2	1:B:418:THR:HA	1.86	0.40
1:B:426:MET:O	1:B:430:PHE:HB2	2.21	0.40
1:B:534:LEU:HD12	1:B:534:LEU:N	2.36	0.40
1:B:207:THR:HA	1:B:210:SER:OG	2.21	0.40
1:B:32:ARG:CZ	1:B:32:ARG:HB3	2.51	0.40
1:B:172:LYS:HE3	1:B:560:ILE:CD1	2.51	0.40
1:B:191:TYR:CZ	1:B:193:PHE:HB2	2.57	0.40
1:B:314:LEU:HA	1:B:314:LEU:HD12	1.86	0.40
1:A:547:LEU:O	1:A:550:TRP:HB2	2.22	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%)	513 (92%)	38 (7%)	5 (1%)	17	46
1	B	556/576 (96%)	500 (90%)	49 (9%)	7 (1%)	12	36
All	All	1112/1152 (96%)	1013 (91%)	87 (8%)	12 (1%)	14	41

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	533	LYS
1	A	15	ALA
1	A	544	GLN
1	B	15	ALA
1	B	469	LEU
1	B	217	PHE
1	B	310	ASP
1	A	514	GLN
1	B	538	PRO
1	A	469	LEU
1	B	247	PRO
1	B	147	VAL

### 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	477/491 (97%)	464 (97%)	13 (3%)	44	78
1	B	477/491 (97%)	465 (98%)	12 (2%)	47	80
All	All	954/982 (97%)	929 (97%)	25 (3%)	46	79

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	18	GLU
1	A	24	ASN
1	A	56	ARG
1	A	98	LYS
1	A	184	GLN
1	A	273	ASN
1	A	315	VAL
1	A	336	LEU
1	A	366	CYS
1	A	402	HIS
1	A	430	PHE

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Mol	Chain	Res	Type
1	A	465	ARG
1	B	20	LYS
1	B	34	HIS
1	B	184	GLN
1	B	190	SER
1	B	200	ARG
1	B	220	ASP
1	B	273	ASN
1	B	284	VAL
1	B	430	PHE
1	B	465	ARG
1	B	469	LEU
1	B	545	LEU

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	35	ASN
1	A	148	GLN
1	A	273	ASN
1	A	406	ASN
1	A	438	GLN
1	A	514	GLN
1	A	562	HIS
1	B	33	HIS
1	B	148	GLN
1	B	199	GLN
1	B	206	ASN
1	B	273	ASN
1	B	461	GLN
1	B	514	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 [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	B	601	-	5,5,5	0.43	0	5,5,5	0.32	0
2	GOL	A	3001	-	5,5,5	0.34	0	5,5,5	0.28	0
3	1NW	A	3002	-	44,45,45	2.27	16 (36%)	60,66,66	1.74	16 (26%)
3	1NW	B	602	-	44,45,45	2.44	19 (43%)	60,66,66	1.74	17 (28%)

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	B	601	-	-	2/4/4/4	-
2	GOL	A	3001	-	-	1/4/4/4	-
3	1NW	A	3002	-	-	3/22/22/22	0/5/5/5
3	1NW	B	602	-	-	0/22/22/22	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	1NW	C25-C26	7.48	1.49	1.39
3	A	3002	1NW	C25-C26	6.48	1.48	1.39
3	B	602	1NW	C12-C11	5.68	1.45	1.41
3	A	3002	1NW	C12-C11	5.27	1.45	1.41
3	A	3002	1NW	C11-N10	4.63	1.45	1.39
3	B	602	1NW	C11-N10	4.02	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	1NW	C17-N8	4.01	1.40	1.33
3	A	3002	1NW	C17-N8	3.65	1.39	1.33
3	A	3002	1NW	C21-C26	3.60	1.46	1.40
3	B	602	1NW	C21-C26	3.34	1.45	1.40
3	B	602	1NW	C16-C15	3.19	1.43	1.36
3	B	602	1NW	C6-C5	3.07	1.43	1.38
3	B	602	1NW	C13-C14	3.06	1.42	1.37
3	A	3002	1NW	C16-C15	3.06	1.43	1.36
3	A	3002	1NW	C2-C1	2.92	1.42	1.37
3	B	602	1NW	C41-C36	2.82	1.44	1.39
3	B	602	1NW	C6-C1	2.81	1.42	1.38
3	A	3002	1NW	C13-C14	2.77	1.42	1.37
3	B	602	1NW	C4-C3	2.66	1.42	1.37
3	A	3002	1NW	C41-C36	2.63	1.43	1.39
3	A	3002	1NW	C33-N35	2.60	1.42	1.35
3	B	602	1NW	C2-C1	2.45	1.41	1.37
3	B	602	1NW	C33-N35	2.43	1.42	1.35
3	A	3002	1NW	C6-C1	2.42	1.42	1.38
3	A	3002	1NW	C2-C3	2.41	1.41	1.37
3	B	602	1NW	C22-C21	2.34	1.44	1.39
3	B	602	1NW	C4-C5	2.32	1.41	1.37
3	B	602	1NW	C2-C3	2.27	1.41	1.37
3	B	602	1NW	C24-C25	2.26	1.43	1.39
3	A	3002	1NW	C37-N38	2.25	1.39	1.34
3	B	602	1NW	C27-C26	2.21	1.56	1.51
3	B	602	1NW	C37-N38	2.15	1.38	1.34
3	A	3002	1NW	C22-C21	2.12	1.44	1.39
3	A	3002	1NW	C4-C3	2.09	1.41	1.37
3	A	3002	1NW	C37-C36	2.00	1.42	1.39

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3002	1NW	C2-C1-C6	-4.30	121.57	124.59
3	B	602	1NW	C4-C5-C6	-4.27	121.59	124.59
3	B	602	1NW	C27-C26-C25	4.11	125.89	120.33
3	B	602	1NW	C2-C1-C6	-4.08	121.73	124.59
3	A	3002	1NW	C16-C11-N10	4.04	126.10	121.55
3	A	3002	1NW	C4-C5-C6	-3.93	121.83	124.59
3	A	3002	1NW	C16-C11-C12	-3.51	115.40	120.01
3	B	602	1NW	C16-C11-N10	3.38	125.35	121.55
3	B	602	1NW	C16-C11-C12	-3.20	115.81	120.01

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3002	1NW	C7-N10-C11	3.13	124.06	120.32
3	A	3002	1NW	C5-C4-C3	2.95	119.72	116.62
3	A	3002	1NW	C6-C7-N10	-2.87	110.51	114.13
3	A	3002	1NW	C13-C12-C11	2.72	122.03	118.51
3	A	3002	1NW	C25-C26-C21	-2.72	116.01	118.77
3	B	602	1NW	C25-C26-C21	-2.70	116.03	118.77
3	B	602	1NW	C13-C12-C11	2.59	121.86	118.51
3	B	602	1NW	C7-N10-C11	2.52	123.33	120.32
3	A	3002	1NW	C4-C3-C2	-2.47	120.39	123.52
3	A	3002	1NW	O34-C33-N35	2.46	129.34	123.71
3	A	3002	1NW	C5-C6-C1	2.38	117.83	114.51
3	B	602	1NW	F32-C5-C6	2.33	120.41	117.63
3	B	602	1NW	O34-C33-N35	2.29	128.94	123.71
3	B	602	1NW	O34-C33-C25	-2.28	116.85	121.01
3	B	602	1NW	C1-C2-C3	2.26	119.00	116.62
3	B	602	1NW	C5-C4-C3	2.26	118.99	116.62
3	B	602	1NW	C5-C6-C1	2.22	117.61	114.51
3	B	602	1NW	C41-C36-C37	-2.20	115.61	117.80
3	B	602	1NW	F30-C27-C26	2.19	117.52	112.34
3	A	3002	1NW	C15-C16-C11	2.10	122.92	119.70
3	B	602	1NW	F31-C1-C6	2.09	120.12	117.63
3	A	3002	1NW	O34-C33-C25	-2.08	117.21	121.01
3	A	3002	1NW	C9-N8-C17	2.04	119.30	115.88
3	A	3002	1NW	C27-C26-C25	2.04	123.08	120.33

There are no chirality outliers.

All (6) torsion outliers are listed below:

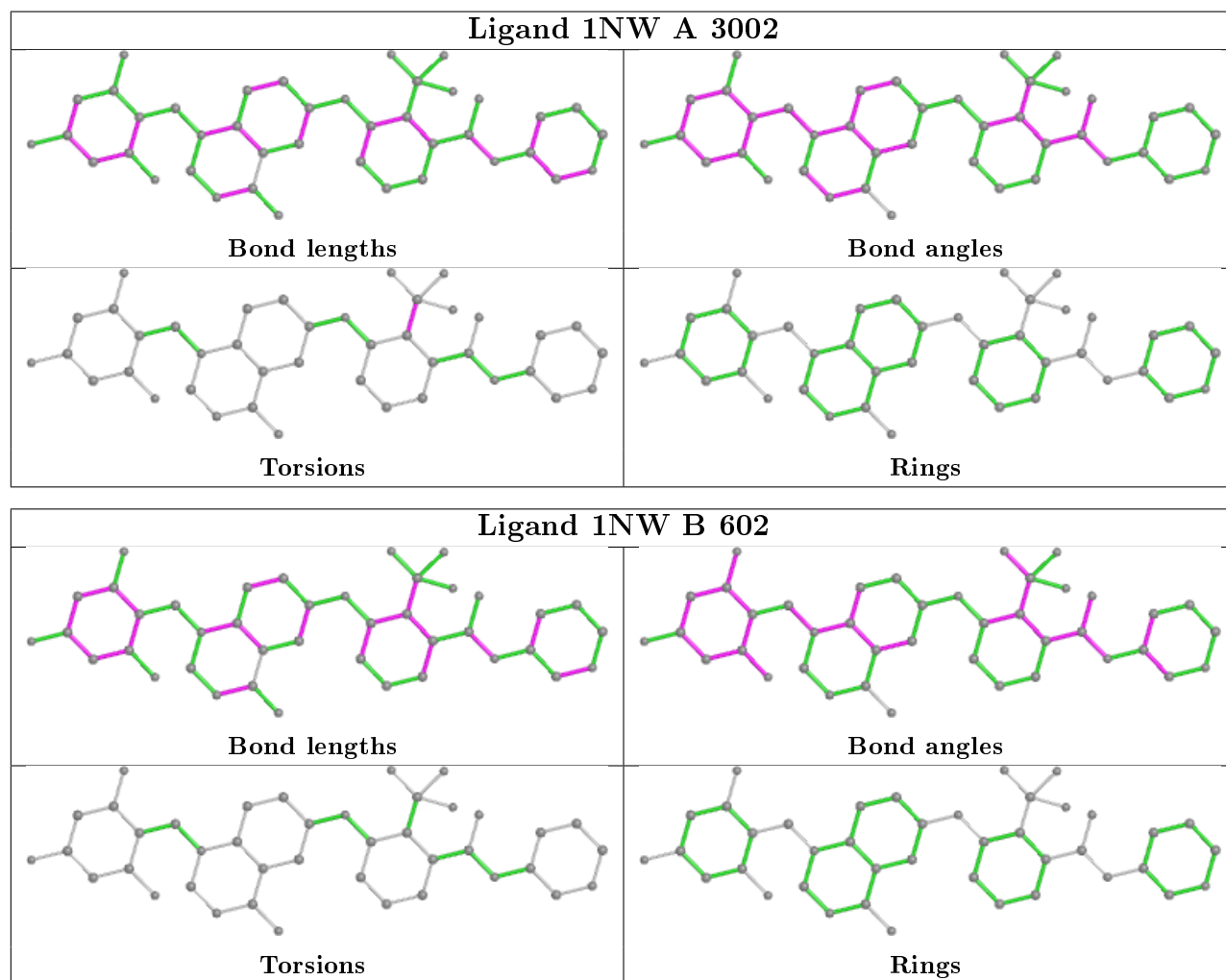
Mol	Chain	Res	Type	Atoms
2	A	3001	GOL	O1-C1-C2-C3
2	B	601	GOL	O1-C1-C2-C3
3	A	3002	1NW	C25-C26-C27-F29
3	A	3002	1NW	C25-C26-C27-F30
3	A	3002	1NW	C25-C26-C27-F19
2	B	601	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	1NW	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.35	3 (0%) 91 88	17, 41, 75, 96	0
1	B	560/576 (97%)	-0.08	12 (2%) 63 54	20, 53, 94, 112	0
All	All	1120/1152 (97%)	-0.21	15 (1%) 77 72	17, 45, 86, 112	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	24	ASN	4.0
1	A	544	GLN	3.1
1	B	515	GLY	3.1
1	B	15	ALA	2.9
1	B	524	TYR	2.8
1	B	511	LEU	2.6
1	B	529	ALA	2.5
1	B	536	LEU	2.5
1	B	23	ILE	2.3
1	B	25	PRO	2.3
1	A	434	LEU	2.3
1	B	366	CYS	2.2
1	A	366	CYS	2.2
1	B	367	SER	2.2
1	B	330	GLN	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](#)

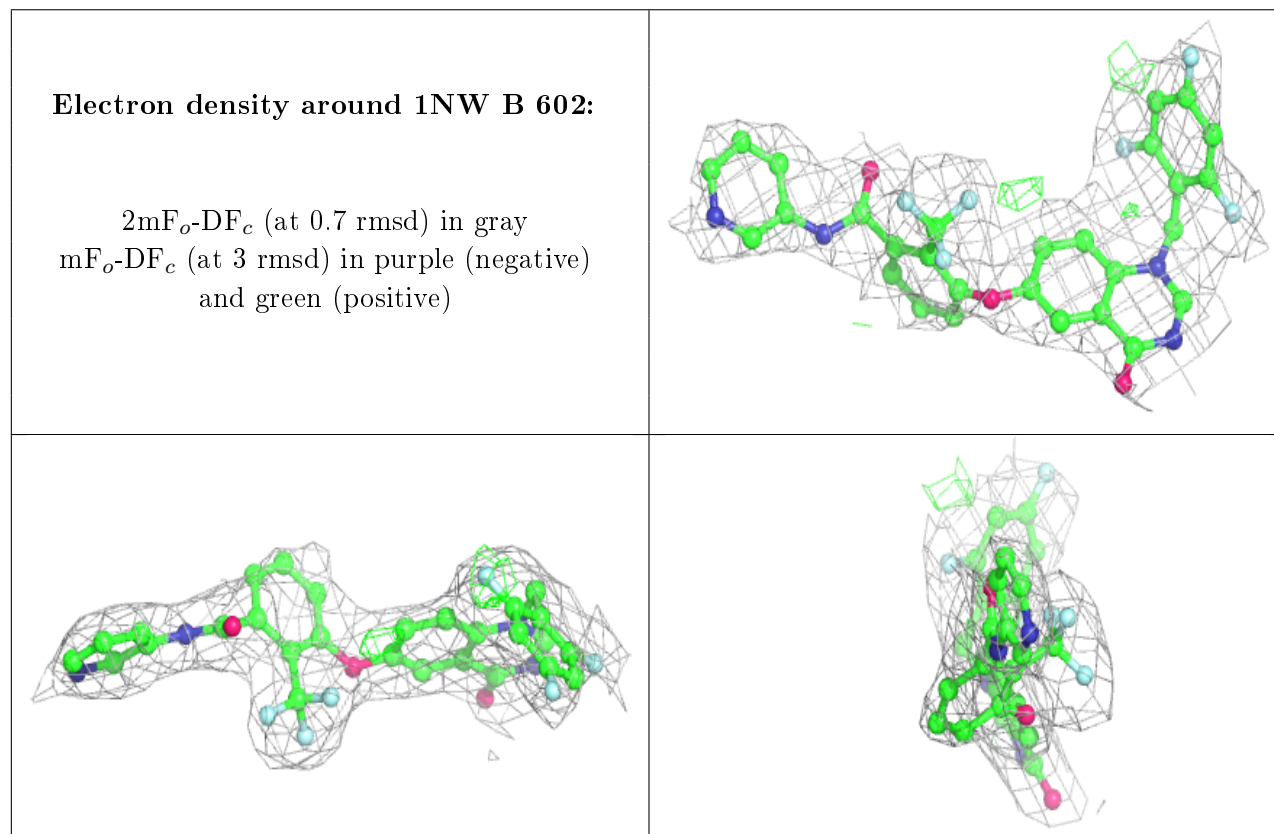
There are no carbohydrates in this entry.

## 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. 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.

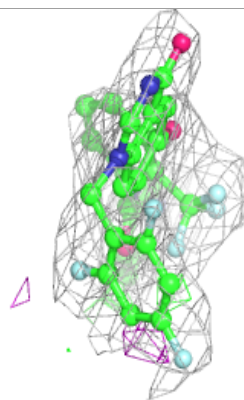
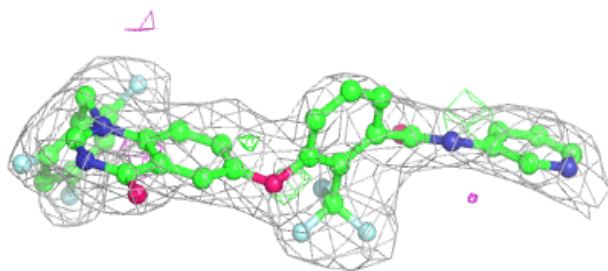
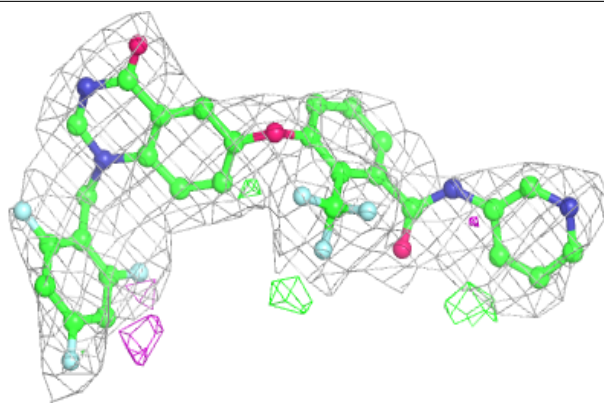
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	B	603	1/1	0.59	0.26	73,73,73,73	0
4	MG	B	604	1/1	0.72	0.60	69,69,69,69	0
3	1NW	B	602	41/41	0.85	0.20	61,68,71,74	0
2	GOL	B	601	6/6	0.89	0.32	62,62,63,63	0
3	1NW	A	3002	41/41	0.91	0.22	43,56,58,59	0
4	MG	A	3003	1/1	0.91	0.24	44,44,44,44	0
2	GOL	A	3001	6/6	0.93	0.19	56,57,57,57	0
4	MG	A	3004	1/1	0.93	0.43	57,57,57,57	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around 1NW A 3002:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.