



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 05:09 AM EDT

PDB ID : 5F4P  
Title : HIV-1 gp120 complex with BNM-III-170  
Authors : Liang, S.; Hendrickson, W.A.  
Deposited on : 2015-12-03  
Resolution : 2.60 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35.1  
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) : 2.35.1

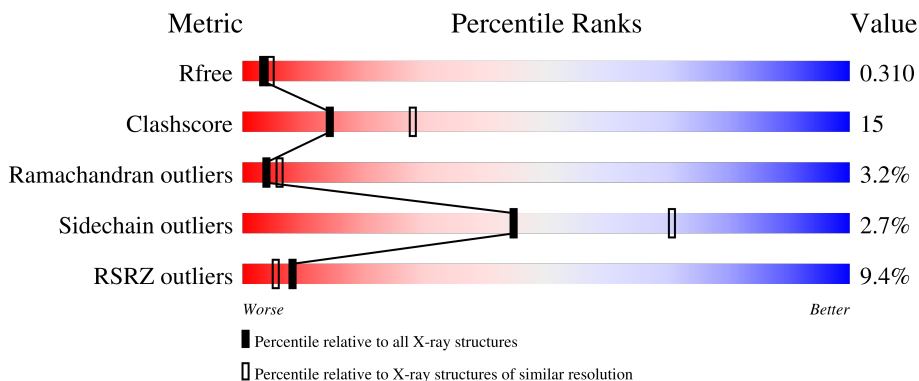
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 of 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	350	
1	D	350	

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	NAG	A	504	-	-	-	X
3	5VG	A	501	-	-	-	X

## 2 Entry composition [i](#)

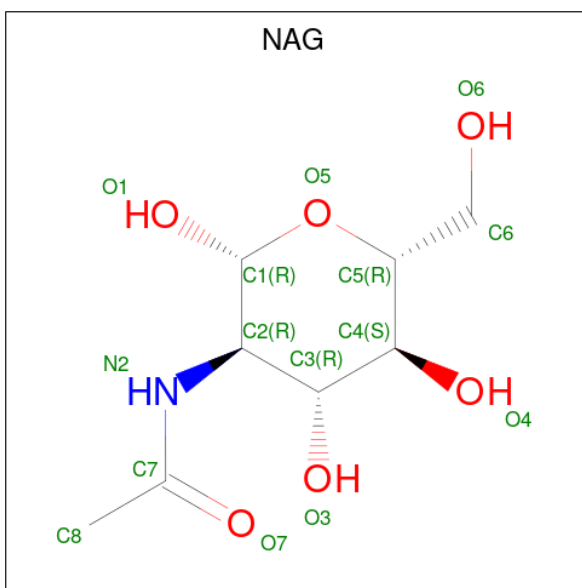
There are 4 unique types of molecules in this entry. The entry contains 5497 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ENVELOPE GLYCOPROTEIN GP120 of HIV-1 clade C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	335	Total 2627	C 1642	N 459	O 506	S 20	0	0	0
1	A	335	Total 2627	C 1642	N 459	O 506	S 20	0	0	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



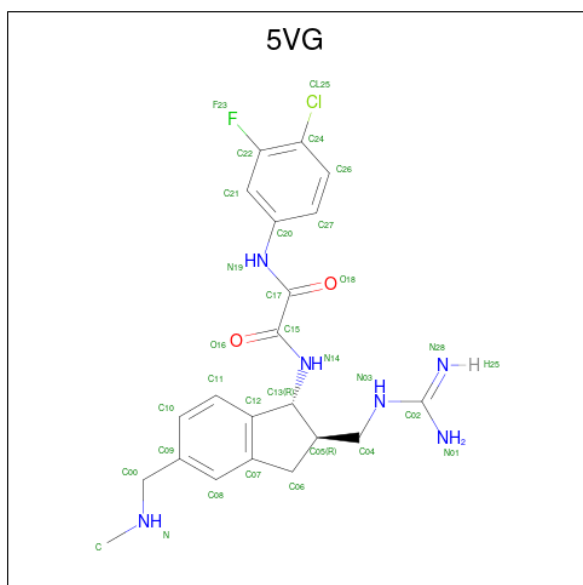
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	D	1	Total 14	C 8	N 1	O 5	0	0
2	D	1	Total 14	C 8	N 1	O 5	0	0
2	D	1	Total 14	C 8	N 1	O 5	0	0
2	D	1	Total 14	C 8	N 1	O 5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is {N}'-[(1 {R},2 {R})-2-(carbamimidamidomethyl)-5-(methylaminomethyl)-2,3-dihydro-1 {H}-inden-1-yl]- {N}-(4-chloranyl-3-fluoranyl-phenyl)ethanediamide (three-letter code: 5VG) (formula: C<sub>21</sub>H<sub>24</sub>ClFN<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	D	1	Total	C	Cl	F	N	O	0	0
			31	21	1	1	6	2		
3	A	1	Total	C	Cl	F	N	O	0	0
			31	21	1	1	6	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	6	Total O 6 6	0	0
4	A	7	Total O 7 7	0	0

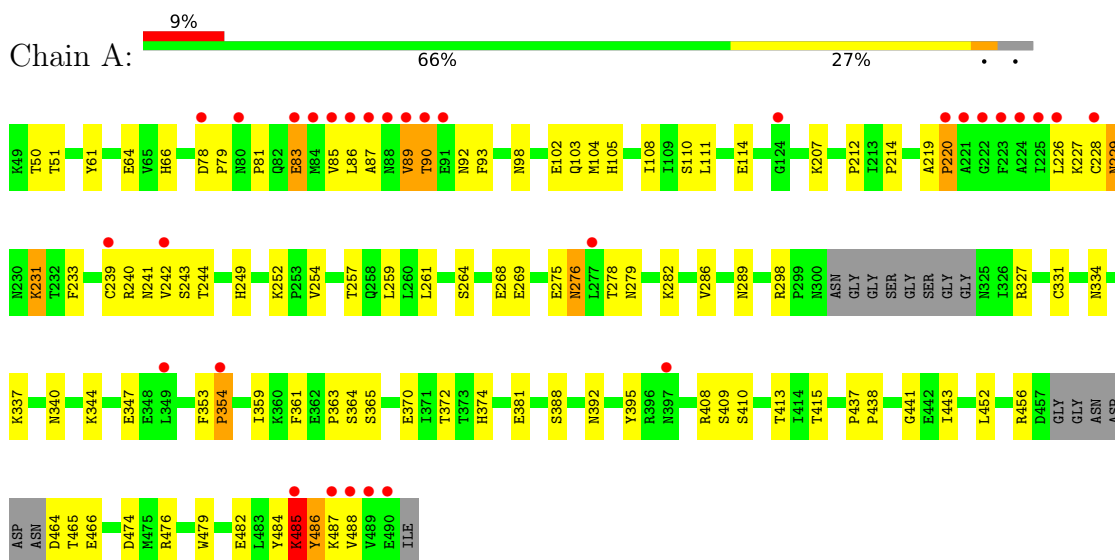
### 3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: ENVELOPE GLYCOPROTEIN GP120 of HIV-1 clade C



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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.38Å 127.52Å 192.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.24 – 2.60 48.24 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.24-2.60) 99.2 (48.24-2.59)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.12 (at 2.58Å)	Xtrriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, $R_{free}$	0.274 , 0.310 0.274 , 0.310	Depositor DCC
$R_{free}$ test set	1264 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.6	Xtrriage
Anisotropy	0.772	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5497	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: NAG, 5VG

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	0.34	0/2682	0.55	0/3640
1	D	0.29	0/2682	0.55	0/3640
All	All	0.32	0/5364	0.55	0/7280

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	D	0	4
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275	GLU	Peptide
1	A	484	TYR	Peptide
1	A	485	LYS	Peptide
1	D	353	PHE	Peptide
1	D	484	TYR	Peptide
1	D	485	LYS	Peptide
1	D	486	TYR	Peptide

## 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	2627	0	2548	81	0
1	D	2627	0	2548	83	0
2	A	84	0	78	7	0
2	D	84	0	78	6	0
3	A	31	0	0	1	0
3	D	31	0	0	1	0
4	A	7	0	0	0	0
4	D	6	0	0	2	0
All	All	5497	0	5252	166	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 (166) 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:D:90:THR:HG23	1:D:240:ARG:HD2	1.39	1.02
1:A:276:ASN:HD22	2:A:504:NAG:H82	1.30	0.95
1:A:268:GLU:HG3	1:A:269:GLU:H	1.37	0.91
1:D:100:MET:SD	1:D:485:LYS:NZ	2.45	0.90
1:D:485:LYS:HE3	1:D:487:LYS:HA	1.56	0.86
1:D:268:GLU:O	1:D:289:ASN:ND2	2.09	0.86
1:D:364:SER:HA	1:D:469:ARG:HG2	1.64	0.78
1:A:340:ASN:OD1	1:A:344:LYS:NZ	2.17	0.78
1:D:276:ASN:ND2	1:D:278:THR:OG1	2.23	0.72
1:D:84:MET:HG2	1:D:244:THR:HB	1.72	0.72
1:D:83:GLU:HG2	1:D:245:VAL:HG12	1.71	0.71
1:A:268:GLU:CG	1:A:269:GLU:H	1.99	0.71
1:A:89:VAL:HG21	1:A:242:VAL:HB	1.73	0.69
1:A:229:ASN:HB2	1:A:241:ASN:O	1.92	0.69
1:A:334:ASN:HB3	1:A:337:LYS:HE2	1.73	0.68
1:A:485:LYS:NZ	1:A:487:LYS:HA	2.07	0.68
1:D:457:ASP:OD1	1:D:469:ARG:NH2	2.28	0.67
1:D:358:THR:HG23	1:D:396:ARG:HG3	1.75	0.66
1:D:298:ARG:NH1	1:D:326:ILE:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ASN:O	1:A:487:LYS:NZ	2.21	0.66
1:A:98:ASN:HD21	1:A:485:LYS:HE3	1.62	0.65
1:A:485:LYS:HZ1	1:A:487:LYS:HA	1.60	0.65
1:A:276:ASN:OD1	1:A:278:THR:N	2.30	0.65
1:D:464:ASP:N	4:D:603:HOH:O	2.31	0.63
1:A:207:LYS:NZ	1:A:437:PRO:O	2.27	0.63
1:A:98:ASN:ND2	1:A:485:LYS:HE3	2.14	0.63
1:D:381:GLU:HG3	1:D:443:ILE:HD13	1.79	0.62
2:A:504:NAG:H3	2:A:504:NAG:H83	1.82	0.62
1:A:231:LYS:HB2	1:A:268:GLU:CD	2.20	0.61
1:D:476:ARG:O	1:D:480:ARG:HG3	2.01	0.61
1:A:289:ASN:HD21	2:A:505:NAG:H83	1.66	0.61
1:A:347:GLU:HG3	1:A:395:TYR:OH	2.01	0.60
1:D:89:VAL:HG21	1:D:240:ARG:O	2.02	0.60
1:D:49:LYS:HD2	1:D:50:THR:N	2.17	0.60
1:A:381:GLU:HG3	1:A:443:ILE:HD13	1.84	0.59
1:D:269:GLU:OE2	2:D:504:NAG:O6	2.20	0.59
1:D:89:VAL:HG23	1:D:240:ARG:HE	1.66	0.59
1:D:78:ASP:C	1:D:80:ASN:H	2.05	0.58
1:A:363:PRO:HG3	1:A:388:SER:HA	1.86	0.58
1:D:298:ARG:HD3	1:D:443:ILE:HD12	1.86	0.57
1:A:86:LEU:HD12	1:A:87:ALA:H	1.69	0.57
1:A:264:SER:N	1:A:482:GLU:OE2	2.38	0.57
1:A:86:LEU:HG	1:A:89:VAL:HG12	1.86	0.57
1:D:275:GLU:OE1	1:D:282:LYS:NZ	2.35	0.57
1:D:343:GLN:HG2	1:D:403:TYR:HB3	1.86	0.57
1:D:485:LYS:HD2	1:D:486:TYR:HB2	1.87	0.56
1:A:276:ASN:OD1	1:A:276:ASN:C	2.44	0.55
1:A:456:ARG:NH1	1:A:466:GLU:OE2	2.39	0.55
1:A:83:GLU:OE2	1:A:227:LYS:NZ	2.35	0.55
1:A:476:ARG:HA	1:A:479:TRP:CD1	2.41	0.55
1:D:216:HIS:ND1	1:D:248:THR:O	2.38	0.55
1:D:217:TYR:O	1:D:248:THR:HG23	2.06	0.54
1:D:84:MET:CG	1:D:244:THR:HB	2.38	0.54
1:A:286:VAL:HB	1:A:452:LEU:HB2	1.90	0.53
2:D:503:NAG:H83	2:D:503:NAG:H3	1.90	0.53
1:D:298:ARG:HH12	1:D:326:ILE:HA	1.74	0.53
1:A:226:LEU:HA	1:A:244:THR:HA	1.91	0.53
1:A:93:PHE:CE2	1:A:239:CYS:HB3	2.44	0.52
1:D:254:VAL:HG11	1:D:261:LEU:HB2	1.89	0.52
1:D:362:GLU:O	1:D:469:ARG:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:HIS:CD2	1:A:476:ARG:HH21	2.28	0.52
1:A:361:PHE:O	1:A:392:ASN:HA	2.09	0.52
1:D:392:ASN:HD21	2:D:506:NAG:C1	2.22	0.52
1:D:90:THR:CG2	1:D:240:ARG:HD2	2.24	0.52
1:D:351:LYS:HB3	1:D:352:HIS:ND1	2.25	0.52
1:A:298:ARG:NH1	1:A:441:GLY:O	2.42	0.52
1:D:64:GLU:OE1	1:D:67:ASN:ND2	2.43	0.51
1:D:476:ARG:HH21	1:D:480:ARG:NH2	2.09	0.51
1:A:231:LYS:HB2	1:A:268:GLU:OE2	2.09	0.51
1:A:93:PHE:HB2	1:A:233:PHE:HZ	1.75	0.51
1:D:289:ASN:HD21	2:D:504:NAG:H83	1.76	0.51
1:A:51:THR:HA	1:A:103:GLN:NE2	2.26	0.51
1:D:359:ILE:HB	1:D:395:TYR:HB3	1.91	0.51
1:A:268:GLU:CG	1:A:269:GLU:N	2.71	0.51
1:A:104:MET:O	1:A:108:ILE:HG12	2.12	0.50
1:D:93:PHE:CE1	1:D:487:LYS:HE2	2.46	0.49
1:A:485:LYS:HD2	1:A:486:TYR:HB2	1.93	0.49
1:D:86:LEU:CD2	1:D:88:ASN:H	2.24	0.49
1:D:392:ASN:OD1	1:D:406:THR:OG1	2.29	0.49
1:D:240:ARG:O	1:D:242:VAL:N	2.44	0.49
1:A:474:ASP:OD1	1:A:476:ARG:HG2	2.12	0.49
1:A:214:PRO:HG3	1:A:252:LYS:HE2	1.95	0.49
1:D:104:MET:O	1:D:108:ILE:HG12	2.13	0.48
1:A:268:GLU:O	2:A:505:NAG:H83	2.13	0.48
1:D:476:ARG:HA	1:D:479:TRP:CD1	2.48	0.48
1:A:254:VAL:HG11	1:A:261:LEU:HB2	1.95	0.48
1:A:50:THR:HG22	1:A:488:VAL:HG21	1.95	0.48
1:D:66:HIS:CD2	1:D:212:PRO:HA	2.48	0.48
1:D:248:THR:HG21	1:D:486:TYR:CE2	2.49	0.47
1:D:278:THR:O	1:D:456:ARG:NH2	2.48	0.47
1:A:344:LYS:N	1:A:344:LYS:HD2	2.29	0.47
1:A:89:VAL:HG22	1:A:90:THR:N	2.29	0.47
1:D:93:PHE:HE1	1:D:487:LYS:HE2	1.80	0.47
1:A:231:LYS:C	1:A:233:PHE:H	2.18	0.47
1:A:408:ARG:HG2	1:A:409:SER:N	2.29	0.47
1:D:478:ASN:O	1:D:481:SER:OG	2.29	0.47
1:D:441:GLY:O	4:D:601:HOH:O	2.21	0.46
1:A:464:ASP:OD1	1:A:465:THR:OG1	2.32	0.46
1:D:286:VAL:HB	1:D:452:LEU:HB2	1.97	0.46
1:A:485:LYS:CG	1:A:486:TYR:H	2.29	0.46
1:D:249:HIS:CD2	1:D:486:TYR:OH	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ARG:NH1	1:A:438:PRO:HD2	2.31	0.46
1:A:485:LYS:HG3	1:A:486:TYR:H	1.81	0.46
1:D:79:PRO:C	1:D:81:PRO:HD3	2.36	0.46
1:D:268:GLU:O	2:D:504:NAG:H83	2.16	0.46
1:A:228:CYS:C	1:A:229:ASN:HD22	2.19	0.46
1:A:51:THR:HA	1:A:103:GLN:HE22	1.80	0.45
1:A:64:GLU:OE2	1:A:66:HIS:ND1	2.45	0.45
1:A:50:THR:O	1:A:103:GLN:NE2	2.49	0.45
1:D:78:ASP:HA	1:D:79:PRO:HD2	1.73	0.45
1:D:86:LEU:HD22	1:D:89:VAL:HG13	1.98	0.45
1:D:89:VAL:HG23	1:D:90:THR:H	1.82	0.45
1:A:85:VAL:HA	1:A:243:SER:HA	1.98	0.45
1:A:279:ASN:HB3	1:A:282:LYS:HG3	1.99	0.45
2:A:504:NAG:H3	2:A:504:NAG:C8	2.46	0.45
1:D:364:SER:OG	1:D:372:THR:HA	2.17	0.45
1:A:85:VAL:HG13	1:A:243:SER:OG	2.17	0.45
1:D:64:GLU:HA	1:D:209:SER:HB3	1.99	0.44
1:A:410:SER:O	1:A:413:THR:HG22	2.17	0.44
1:D:272:ILE:HG12	1:D:348:GLU:HG2	1.98	0.44
1:D:357:LYS:HB3	1:D:464:ASP:O	2.17	0.44
1:A:219:ALA:HA	1:A:220:PRO:HD3	1.84	0.44
1:D:327:ARG:HG2	1:D:327:ARG:HH11	1.82	0.44
1:A:276:ASN:ND2	2:A:504:NAG:H82	2.14	0.44
1:A:227:LYS:HA	1:A:486:TYR:HA	2.00	0.43
1:A:485:LYS:HD2	1:A:486:TYR:N	2.33	0.43
1:D:207:LYS:NZ	1:D:437:PRO:O	2.34	0.43
1:D:276:ASN:OD1	1:D:277:LEU:N	2.50	0.43
1:A:259:LEU:HB2	1:A:374:HIS:CE1	2.53	0.43
1:A:66:HIS:CD2	1:A:212:PRO:HA	2.54	0.43
1:D:90:THR:HA	1:D:240:ARG:HG2	2.00	0.43
1:A:392:ASN:HD21	2:A:507:NAG:C1	2.32	0.43
1:D:96:TRP:HD1	1:D:236:THR:HG23	1.85	0.42
1:D:102:GLU:O	1:D:106:GLU:HG2	2.19	0.42
1:D:264:SER:N	1:D:482:GLU:OE2	2.52	0.42
1:A:249:HIS:CE1	1:A:482:GLU:HG3	2.54	0.42
1:A:344:LYS:HA	1:A:347:GLU:HB2	2.01	0.42
1:A:485:LYS:CG	1:A:486:TYR:N	2.82	0.42
1:D:69:TRP:HA	1:D:72:HIS:CD2	2.54	0.42
1:D:370:GLU:HG2	3:D:507:5VG:N19	2.33	0.42
1:A:66:HIS:CD2	1:A:111:LEU:HD21	2.54	0.42
1:D:64:GLU:OE2	1:D:66:HIS:ND1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:LEU:HG	1:D:451:GLY:HA2	2.01	0.42
1:D:230:ASN:HB3	1:D:233:PHE:HB2	2.02	0.42
1:D:393:GLY:HA3	1:D:403:TYR:CE1	2.55	0.42
1:A:93:PHE:HE2	1:A:239:CYS:HB3	1.84	0.42
1:A:257:THR:O	1:A:259:LEU:N	2.49	0.42
1:D:55:ALA:HA	1:D:75:VAL:O	2.20	0.41
1:D:226:LEU:HD23	1:D:244:THR:OG1	2.21	0.41
1:D:276:ASN:HD22	2:D:503:NAG:H82	1.85	0.41
1:D:363:PRO:HG3	1:D:388:SER:HA	2.03	0.41
1:A:89:VAL:CG2	1:A:90:THR:N	2.83	0.41
1:A:298:ARG:HH11	1:A:443:ILE:HG13	1.86	0.41
1:A:353:PHE:HA	1:A:354:PRO:HD2	1.91	0.41
1:A:364:SER:OG	1:A:372:THR:HA	2.20	0.41
1:D:294:ILE:HD12	1:D:333:ILE:HD11	2.03	0.41
1:A:359:ILE:HB	1:A:395:TYR:HB3	2.02	0.41
1:D:475:MET:O	1:D:478:ASN:HB2	2.20	0.41
1:A:370:GLU:HG2	3:A:501:5VG:N19	2.35	0.41
1:D:214:PRO:HG2	1:A:61:TYR:CE2	2.56	0.41
1:D:342:LEU:HD23	1:D:342:LEU:HA	1.84	0.41
1:D:257:THR:O	1:D:259:LEU:N	2.50	0.40
1:D:485:LYS:HD2	1:D:486:TYR:N	2.36	0.40
1:A:331:CYS:O	1:A:415:THR:HA	2.21	0.40
1:A:110:SER:O	1:A:114:GLU:HG3	2.20	0.40
1:D:219:ALA:HA	1:D:220:PRO:HD3	1.81	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	329/350 (94%)	294 (89%)	26 (8%)	9 (3%)	<b>5</b> <b>8</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	329/350 (94%)	292 (89%)	25 (8%)	12 (4%)	3	4
All	All	658/700 (94%)	586 (89%)	51 (8%)	21 (3%)	4	6

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	485	LYS
1	A	81	PRO
1	A	354	PRO
1	A	365	SER
1	A	485	LYS
1	D	79	PRO
1	A	83	GLU
1	A	90	THR
1	A	486	TYR
1	D	84	MET
1	D	226	LEU
1	D	486	TYR
1	D	81	PRO
1	D	365	SER
1	D	487	LYS
1	A	79	PRO
1	D	89	VAL
1	D	270	ILE
1	A	220	PRO
1	D	354	PRO
1	D	220	PRO

### 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	297/305 (97%)	289 (97%)	8 (3%)	44	71
1	D	297/305 (97%)	289 (97%)	8 (3%)	44	71
All	All	594/610 (97%)	578 (97%)	16 (3%)	44	71

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	88	ASN
1	D	90	THR
1	D	249	HIS
1	D	328	GLN
1	D	347	GLU
1	D	352	HIS
1	D	397	ASN
1	D	469	ARG
1	A	78	ASP
1	A	89	VAL
1	A	102	GLU
1	A	229	ASN
1	A	231	LYS
1	A	240	ARG
1	A	276	ASN
1	A	485	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	234	ASN
1	D	249	HIS
1	D	289	ASN
1	A	98	ASN
1	A	229	ASN
1	A	234	ASN
1	A	249	HIS
1	A	289	ASN
1	A	293	ASN
1	A	392	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

14 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	NAG	A	502	-	14,14,15	0.42	0	17,19,21	0.39	0
2	NAG	A	506	-	14,14,15	0.28	0	17,19,21	0.44	0
2	NAG	A	504	-	14,14,15	0.29	0	17,19,21	1.44	1 (5%)
2	NAG	A	507	-	14,14,15	0.28	0	17,19,21	0.73	0
2	NAG	D	502	-	14,14,15	0.27	0	17,19,21	0.41	0
2	NAG	A	505	-	14,14,15	0.39	0	17,19,21	0.55	0
2	NAG	D	503	-	14,14,15	0.38	0	17,19,21	1.40	2 (11%)
2	NAG	D	501	-	14,14,15	0.32	0	17,19,21	0.37	0
2	NAG	A	503	-	14,14,15	0.43	0	17,19,21	0.47	0
2	NAG	D	506	-	14,14,15	0.35	0	17,19,21	0.56	0
2	NAG	D	504	-	14,14,15	0.38	0	17,19,21	0.71	0
3	5VG	A	501	-	33,33,33	2.43	12 (36%)	40,46,46	1.37	6 (15%)
2	NAG	D	505	-	14,14,15	0.14	0	17,19,21	0.48	0
3	5VG	D	507	-	33,33,33	2.41	11 (33%)	40,46,46	1.51	5 (12%)

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	NAG	A	502	-	-	1/6/23/26	0/1/1/1
2	NAG	A	506	-	-	2/6/23/26	0/1/1/1
2	NAG	A	504	-	-	5/6/23/26	0/1/1/1
2	NAG	A	507	-	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	502	-	-	0/6/23/26	0/1/1/1
2	NAG	A	505	-	-	3/6/23/26	0/1/1/1
2	NAG	D	503	-	-	3/6/23/26	0/1/1/1
2	NAG	D	501	-	-	0/6/23/26	0/1/1/1
2	NAG	A	503	-	-	0/6/23/26	0/1/1/1
2	NAG	D	506	-	-	4/6/23/26	0/1/1/1
2	NAG	D	504	-	-	4/6/23/26	0/1/1/1
3	5VG	A	501	-	-	2/19/32/32	0/3/3/3
2	NAG	D	505	-	-	2/6/23/26	0/1/1/1
3	5VG	D	507	-	-	4/19/32/32	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	507	5VG	C02-N03	7.12	1.47	1.33
3	A	501	5VG	C02-N03	7.08	1.47	1.33
3	A	501	5VG	C15-N14	5.18	1.44	1.34
3	D	507	5VG	C15-N14	5.09	1.44	1.34
3	A	501	5VG	C17-N19	4.79	1.46	1.35
3	D	507	5VG	C17-N19	4.68	1.45	1.35
3	D	507	5VG	C05-C13	-4.00	1.49	1.54
3	A	501	5VG	C05-C13	-3.92	1.49	1.54
3	A	501	5VG	C11-C10	3.58	1.45	1.38
3	D	507	5VG	C11-C10	3.51	1.45	1.38
3	D	507	5VG	C08-C09	3.32	1.45	1.39
3	A	501	5VG	C08-C09	3.22	1.44	1.39
3	A	501	5VG	C06-C05	-2.48	1.49	1.54
3	D	507	5VG	C06-C05	-2.44	1.49	1.54
3	A	501	5VG	C24-C22	2.36	1.42	1.38
3	A	501	5VG	C00-N	-2.36	1.43	1.46
3	A	501	5VG	C07-C12	2.33	1.43	1.39
3	D	507	5VG	C27-C26	2.32	1.43	1.38
3	D	507	5VG	C24-C22	2.31	1.41	1.38
3	D	507	5VG	C00-N	-2.27	1.43	1.46
3	A	501	5VG	C27-C26	2.26	1.42	1.38
3	D	507	5VG	C07-C12	2.24	1.43	1.39
3	A	501	5VG	C21-C22	2.05	1.41	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	504	NAG	C2-N2-C7	5.25	130.37	122.90
2	D	503	NAG	C2-N2-C7	4.55	129.39	122.90
3	D	507	5VG	C15-C17-N19	4.50	119.43	112.31
3	D	507	5VG	C12-C13-N14	-3.75	108.59	114.61
3	A	501	5VG	C15-C17-N19	3.63	118.05	112.31
3	D	507	5VG	C20-N19-C17	-3.05	122.24	127.53
3	A	501	5VG	C17-C15-N14	2.80	120.43	113.73
2	D	503	NAG	C1-C2-N2	2.77	115.22	110.49
3	A	501	5VG	C12-C13-N14	-2.68	110.32	114.61
3	D	507	5VG	C17-C15-N14	2.48	119.68	113.73
3	A	501	5VG	C06-C07-C12	-2.39	108.03	110.99
3	D	507	5VG	C06-C07-C12	-2.22	108.24	110.99
3	A	501	5VG	C07-C12-C13	-2.16	108.42	110.22
3	A	501	5VG	C20-N19-C17	-2.13	123.84	127.53

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	507	5VG	N03-C04-C05-C13
3	D	507	5VG	N03-C04-C05-C06
3	A	501	5VG	N03-C04-C05-C13
3	A	501	5VG	N03-C04-C05-C06
2	D	506	NAG	O5-C5-C6-O6
2	A	507	NAG	O5-C5-C6-O6
2	D	505	NAG	O5-C5-C6-O6
2	D	506	NAG	C4-C5-C6-O6
2	A	504	NAG	O5-C5-C6-O6
2	D	505	NAG	C4-C5-C6-O6
2	D	503	NAG	C8-C7-N2-C2
2	D	503	NAG	O7-C7-N2-C2
2	D	504	NAG	C8-C7-N2-C2
2	D	504	NAG	O7-C7-N2-C2
2	D	506	NAG	C8-C7-N2-C2
2	D	506	NAG	O7-C7-N2-C2
2	A	504	NAG	C8-C7-N2-C2
2	A	504	NAG	O7-C7-N2-C2
2	A	505	NAG	C8-C7-N2-C2
2	A	505	NAG	O7-C7-N2-C2
2	A	507	NAG	C8-C7-N2-C2
2	A	507	NAG	O7-C7-N2-C2
2	A	507	NAG	C4-C5-C6-O6
2	A	506	NAG	O5-C5-C6-O6

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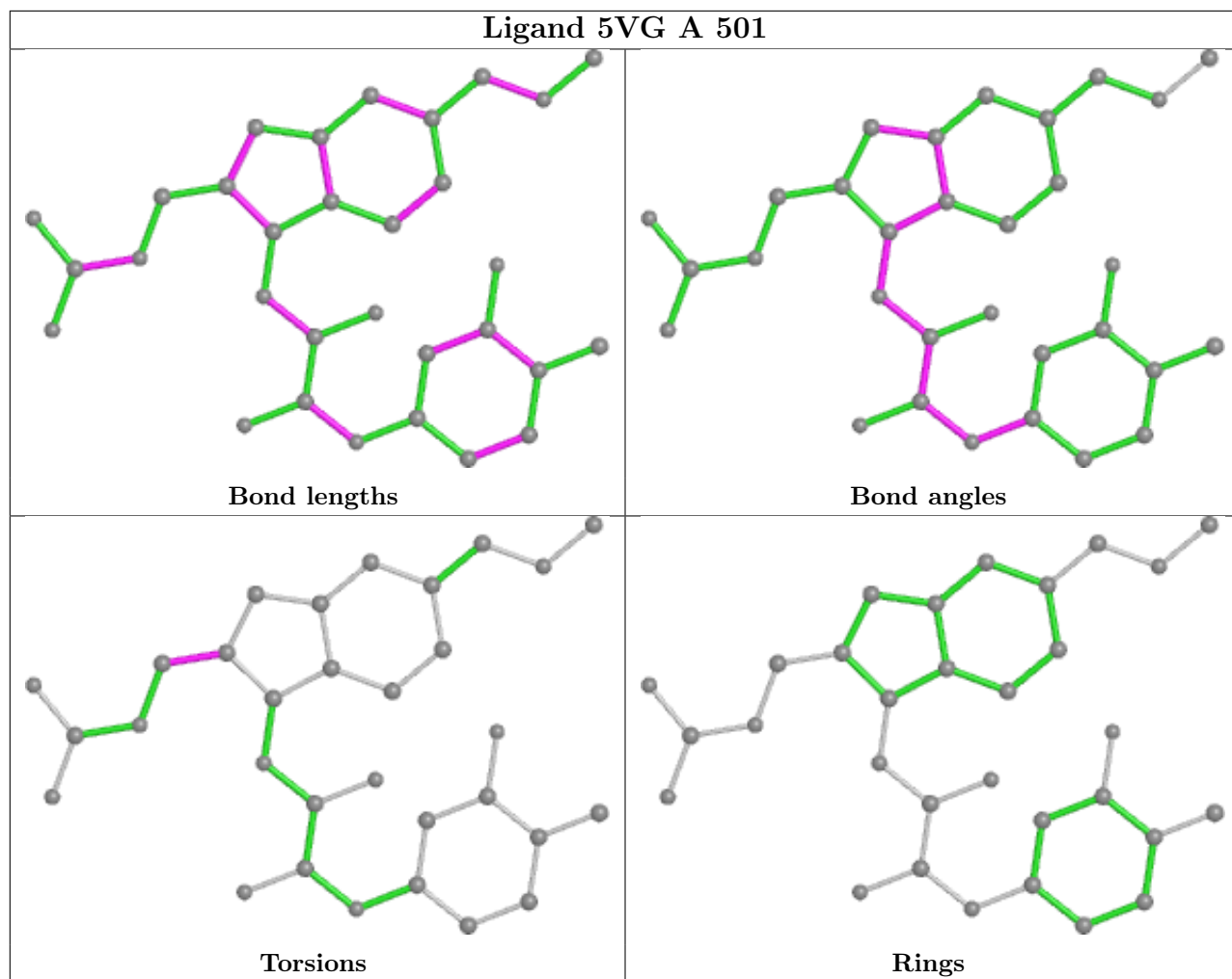
Mol	Chain	Res	Type	Atoms
2	A	506	NAG	C4-C5-C6-O6
2	A	504	NAG	C4-C5-C6-O6
2	D	504	NAG	O5-C5-C6-O6
2	A	505	NAG	O5-C5-C6-O6
2	D	503	NAG	C3-C2-N2-C7
2	A	502	NAG	C3-C2-N2-C7
2	A	504	NAG	C3-C2-N2-C7
2	D	504	NAG	C4-C5-C6-O6
3	D	507	5VG	C27-C20-N19-C17
3	D	507	5VG	C21-C20-N19-C17

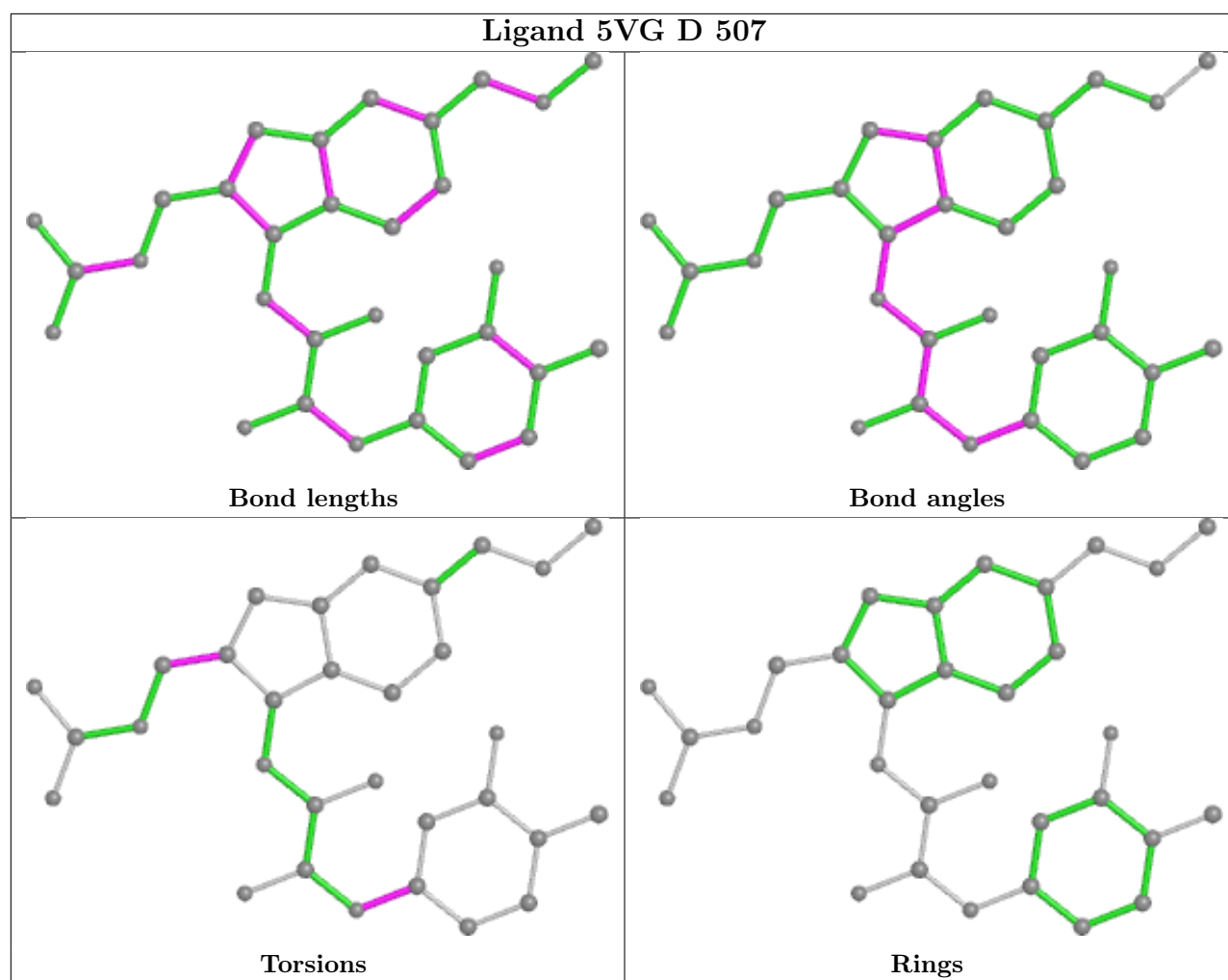
There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	504	NAG	4	0
2	A	507	NAG	1	0
2	A	505	NAG	2	0
2	D	503	NAG	2	0
2	D	506	NAG	1	0
2	D	504	NAG	3	0
3	A	501	5VG	1	0
3	D	507	5VG	1	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 [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	335/350 (95%)	0.69	31 (9%) <b>8</b> <b>6</b>	38, 71, 106, 123	0
1	D	335/350 (95%)	0.76	32 (9%) <b>8</b> <b>5</b>	54, 81, 101, 125	0
All	All	670/700 (95%)	0.73	63 (9%) <b>8</b> <b>5</b>	38, 77, 103, 125	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	VAL	6.9
1	D	88	ASN	6.0
1	D	486	TYR	5.9
1	A	87	ALA	5.5
1	D	87	ALA	5.3
1	A	221	ALA	5.2
1	D	90	THR	5.0
1	D	239	CYS	4.8
1	D	89	VAL	4.3
1	D	86	LEU	4.3
1	D	223	PHE	4.2
1	A	223	PHE	4.2
1	A	88	ASN	4.1
1	D	85	VAL	4.1
1	A	489	VAL	4.0
1	A	84	MET	3.6
1	D	93	PHE	3.5
1	D	240	ARG	3.5
1	D	226	LEU	3.4
1	A	225	ILE	3.4
1	A	124	GLY	3.3
1	D	345	VAL	3.3
1	D	91	GLU	3.3
1	D	224	ALA	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	78	ASP	3.1
1	A	85	VAL	3.1
1	A	222	GLY	3.1
1	D	483	LEU	3.0
1	A	86	LEU	3.0
1	A	80	ASN	3.0
1	A	485	LYS	2.9
1	A	242	VAL	2.8
1	D	487	LYS	2.7
1	D	272	ILE	2.7
1	A	226	LEU	2.7
1	D	92	ASN	2.6
1	A	90	THR	2.6
1	A	490	GLU	2.6
1	D	484	TYR	2.6
1	D	248	THR	2.5
1	A	228	CYS	2.5
1	A	91	GLU	2.4
1	D	228	CYS	2.4
1	D	300	ASN	2.4
1	D	215	LEU	2.3
1	A	224	ALA	2.3
1	D	242	VAL	2.3
1	A	277	LEU	2.2
1	A	354	PRO	2.2
1	D	404	ASN	2.2
1	D	241	ASN	2.1
1	D	342	LEU	2.1
1	A	349	LEU	2.1
1	D	225	ILE	2.1
1	A	239	CYS	2.1
1	D	49	LYS	2.1
1	A	397	ASN	2.1
1	D	265	LEU	2.1
1	A	488	VAL	2.1
1	A	83	GLU	2.0
1	A	487	LYS	2.0
1	A	220	PRO	2.0
1	D	289	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

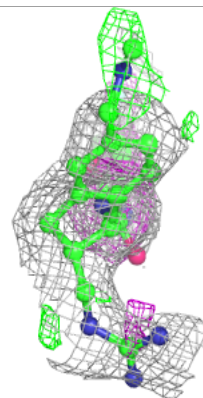
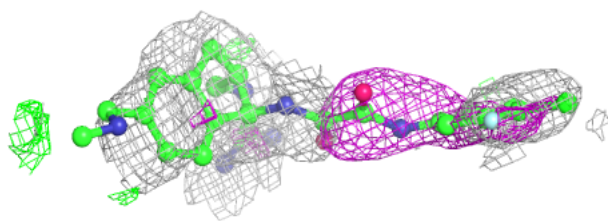
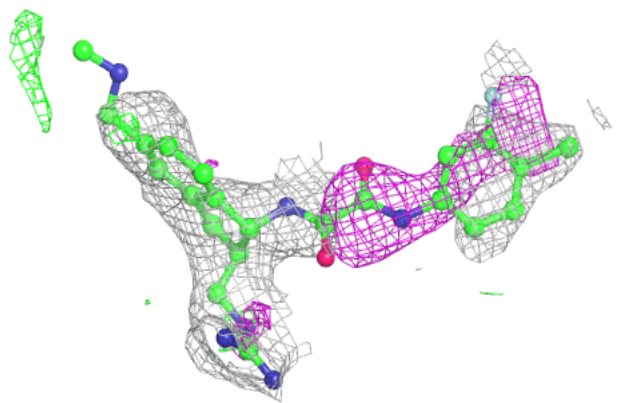
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

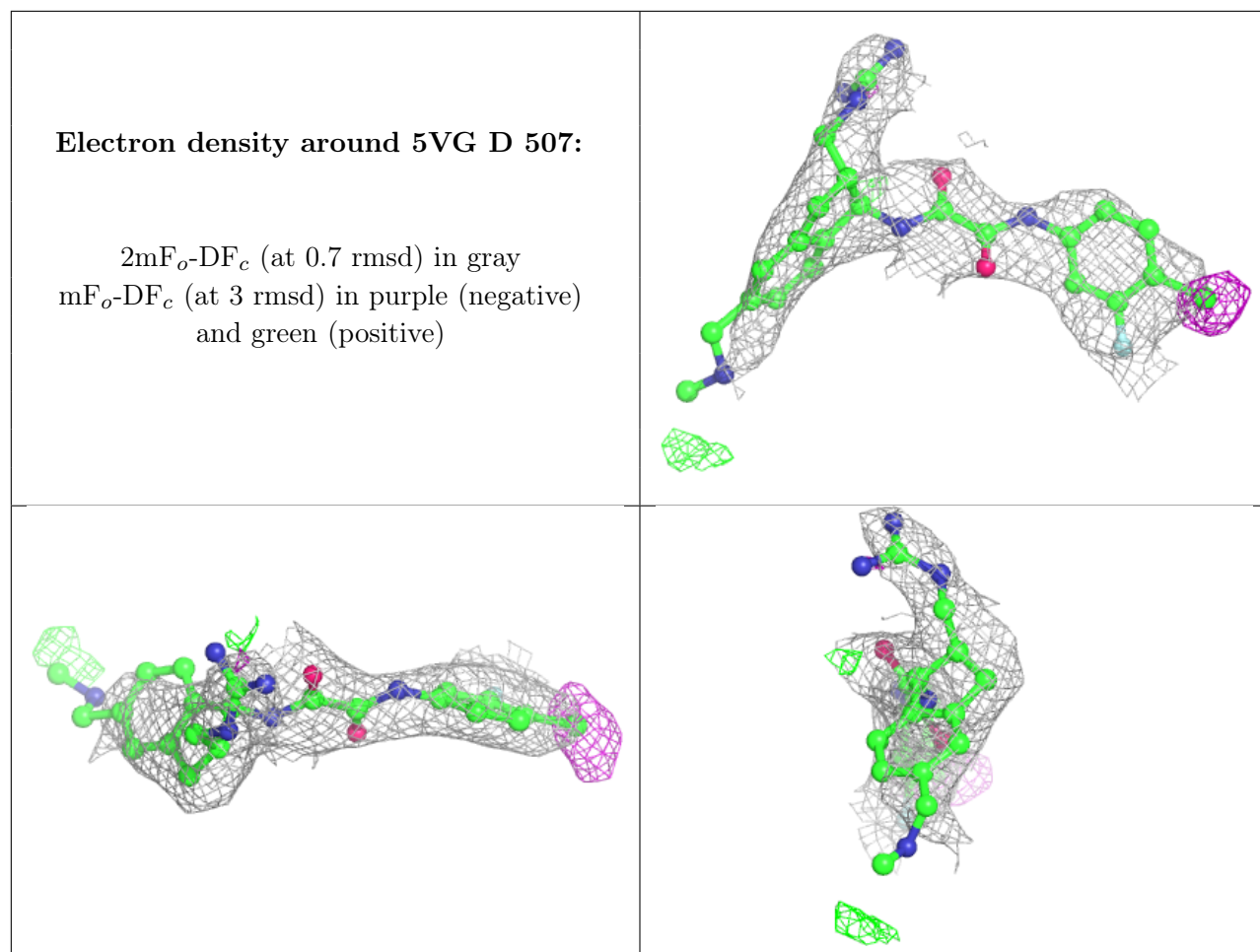
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	D	503	14/15	0.65	0.26	88,96,101,101	0
3	5VG	A	501	31/31	0.66	0.44	64,72,87,96	0
2	NAG	A	502	14/15	0.70	0.29	88,103,110,113	0
2	NAG	D	506	14/15	0.70	0.33	88,100,112,114	0
2	NAG	A	504	14/15	0.72	0.44	85,92,102,110	0
2	NAG	A	505	14/15	0.76	0.33	86,92,104,106	0
2	NAG	D	504	14/15	0.77	0.20	88,94,100,109	0
2	NAG	A	503	14/15	0.78	0.30	46,60,70,75	0
3	5VG	D	507	31/31	0.81	0.30	64,76,90,95	0
2	NAG	D	505	14/15	0.81	0.25	69,88,94,95	0
2	NAG	A	506	14/15	0.83	0.28	71,81,88,89	0
2	NAG	D	502	14/15	0.84	0.28	66,78,86,93	0
2	NAG	D	501	14/15	0.85	0.33	83,93,99,103	0
2	NAG	A	507	14/15	0.85	0.31	65,72,85,95	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 5VG A 501:**

$2mF_o-DF_c$  (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.