



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 10:56 AM EDT

PDB ID : 7TJO  
Title : HIV-1 gp120 complex with CJF-II-197-S  
Authors : Gong, Z.; Hendrickson, W.A.  
Deposited on : 2022-01-16  
Resolution : 3.07 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 : 2.36  
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) : 2.36

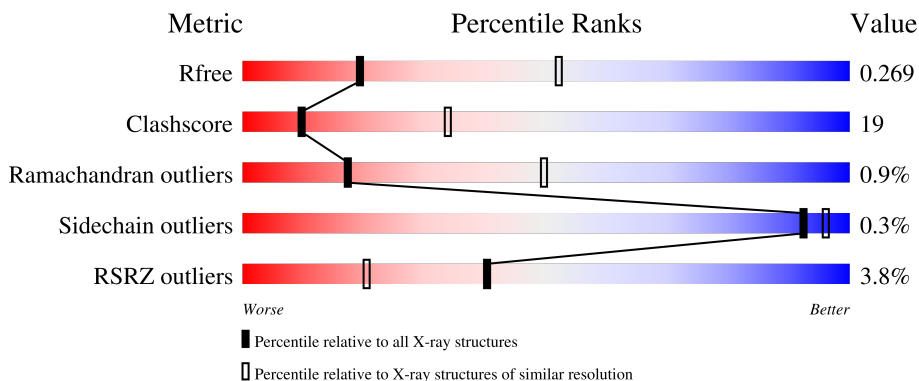
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.07 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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	358	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 61%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 32%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">2%      61%      32%      6%</p>
1	B	358	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 60%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 34%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">4%      60%      34%      6%</p>
1	C	358	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 34%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">4%      59%      34%      6%</p>
1	D	358	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 60%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">4%      60%      33%      6%</p>

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
3	NAG	A	505	-	-	-	X
3	NAG	A	510	-	-	-	X
3	NAG	B	505	-	-	-	X
3	NAG	B	506	-	-	-	X
3	NAG	B	510	-	-	-	X
3	NAG	C	510	-	-	-	X
3	NAG	D	505	-	-	-	X
3	NAG	D	506	-	-	-	X
3	NAG	D	510	-	-	-	X

## 2 Entry composition [i](#)

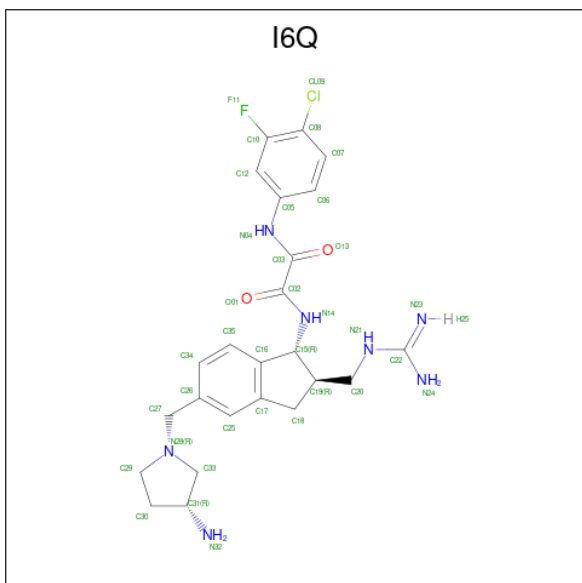
There are 5 unique types of molecules in this entry. The entry contains 11229 atoms, of which 5 are hydrogens and 0 are deuteriums.

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 Glycoprotein 120.

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
1	C	335	Total 2627	C 1642	N 459	O 506	S 20	0	0	0
1	B	335	Total 2627	C 1642	N 459	O 506	S 20	0	0	0

- Molecule 2 is N 1 -[(1R,2R)-5-[(3R)-3-aminopyrrolidin-1-yl]methyl]-2-(carbamimidamidomethyl)-2,3-dihydro-1H-inden-1-yl]-N 2 -(4-chloro-3-fluorophenyl)ethanediamide (three-letter code: I6Q) (formula: C<sub>24</sub>H<sub>29</sub>ClFN<sub>7</sub>O<sub>2</sub>).



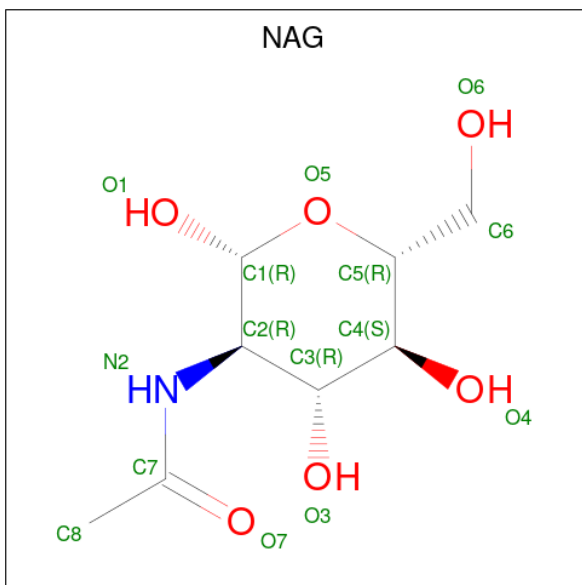
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	F	N			O
2	D	1	Total 35	C 24	Cl 1	F 1	N 7	O 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total	C	Cl	F	N	O	0	0
			35	24	1	1	7	2		
2	C	1	Total	C	Cl	F	N	O	0	0
			35	24	1	1	7	2		
2	B	1	Total	C	Cl	F	N	O	0	0
			35	24	1	1	7	2		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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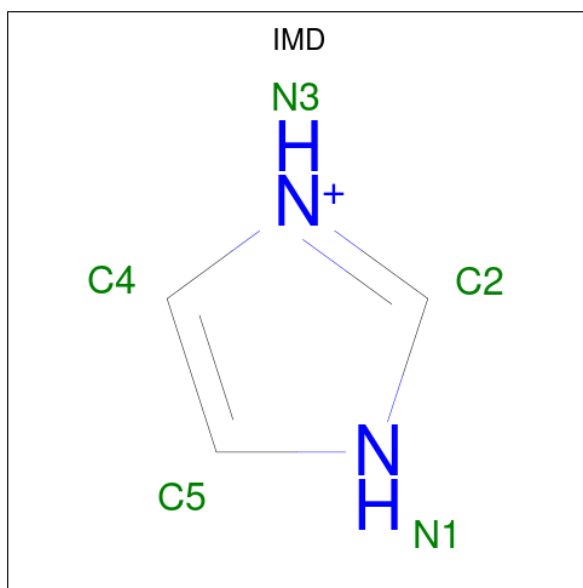
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	N		
4	A	1	Total 10	C 3	H 5	N 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	18	Total 18	O 18	0

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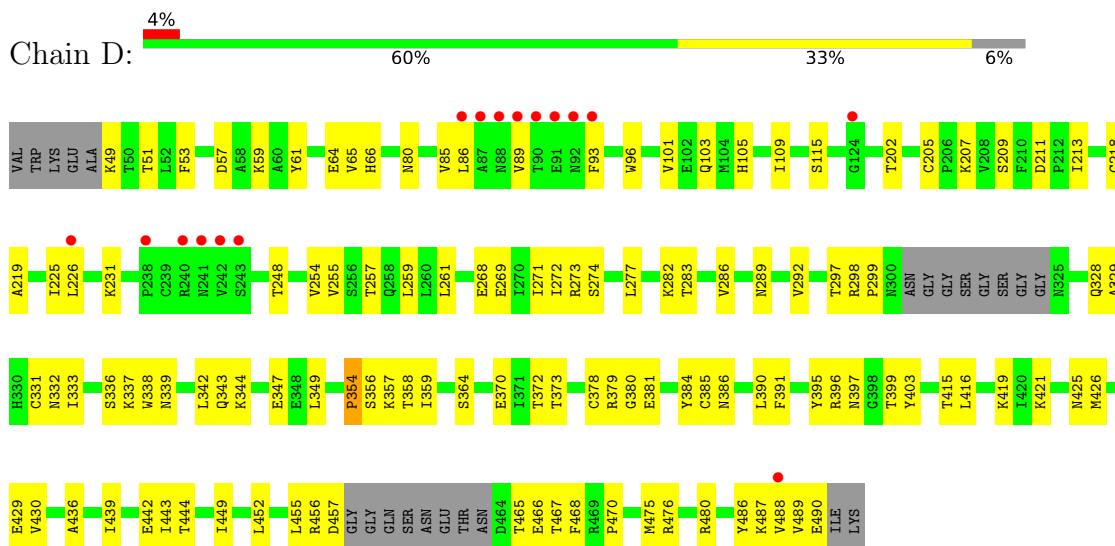
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
5	A	15	Total O 15 15	0	0
5	C	19	Total O 19 19	0	0
5	B	15	Total O 15 15	0	0



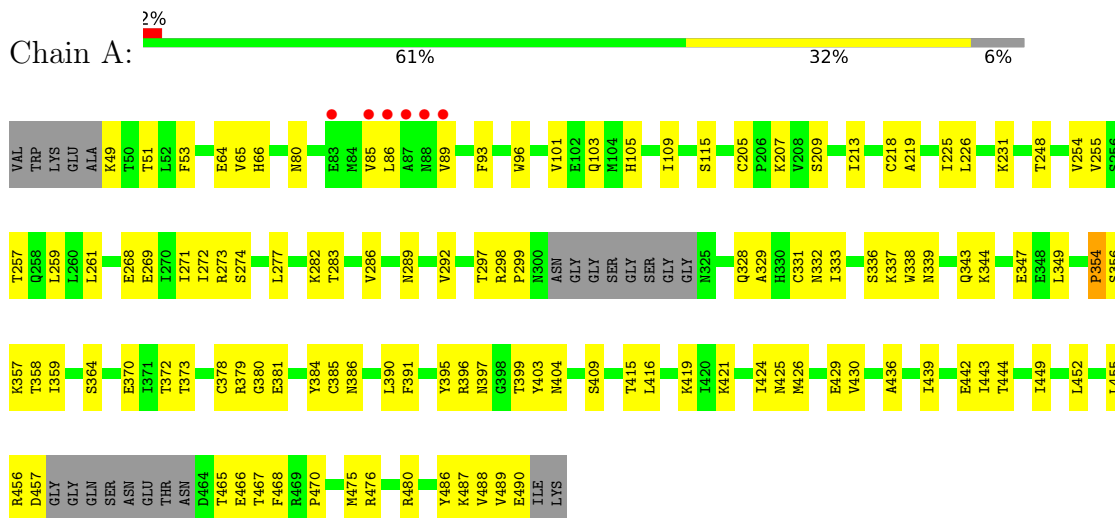
### 3 Residue-property plots

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: Glycoprotein 120

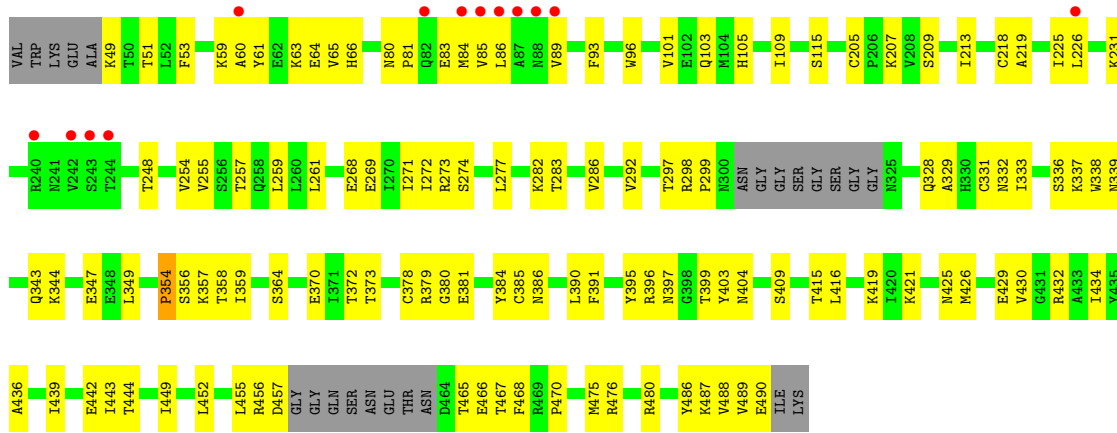


- Molecule 1: Glycoprotein 120

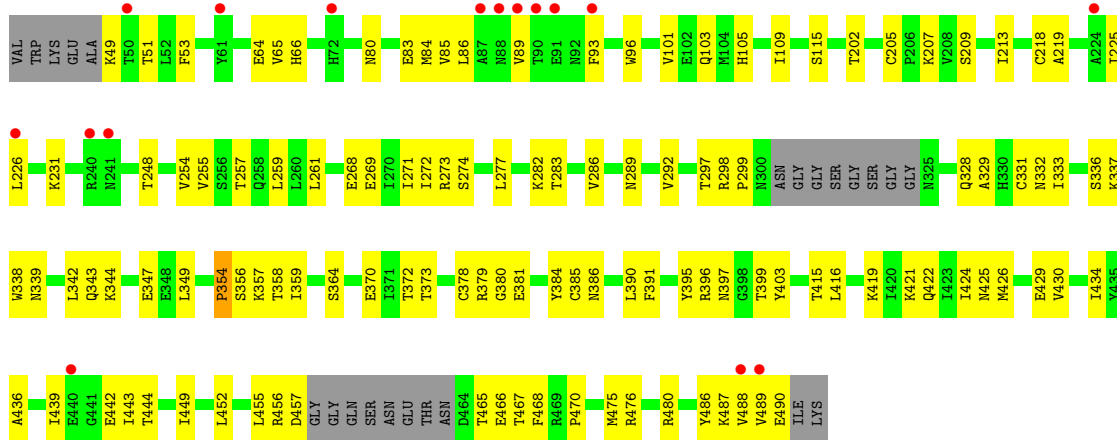


- Molecule 1: Glycoprotein 120





● Molecule 1: Glycoprotein 120



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.34Å 121.83Å 195.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.93 – 3.07 48.93 – 3.07	Depositor EDS
% Data completeness (in resolution range)	73.4 (48.93-3.07) 73.4 (48.93-3.07)	Depositor EDS
$R_{merge}$	0.28	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 3.07Å)	Xtrriage
Refinement program	PHENIX 1.20rc3_4406, PHENIX 1.20rc3_4406	Depositor
R, $R_{free}$	0.229 , 0.268 0.230 , 0.269	Depositor DCC
$R_{free}$ test set	1997 reflections (8.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.9	Xtrriage
Anisotropy	0.049	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11229	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.04% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IMD, NAG, I6Q

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	0.30	0/2682	0.51	0/3640
1	B	0.30	0/2682	0.51	0/3640
1	C	0.30	0/2682	0.51	0/3640
1	D	0.30	0/2682	0.52	0/3640
All	All	0.30	0/10728	0.51	0/14560

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2627	0	2539	101	0
1	B	2627	0	2539	97	2
1	C	2627	0	2539	111	0
1	D	2627	0	2539	108	2
2	A	35	0	0	1	0
2	B	35	0	0	1	0
2	C	35	0	0	1	0
2	D	35	0	0	1	0
3	A	126	0	117	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	126	0	117	7	0
3	C	126	0	117	17	0
3	D	126	0	117	11	0
4	A	5	5	5	0	0
5	A	15	0	0	0	0
5	B	15	0	0	0	0
5	C	19	0	0	0	0
5	D	18	0	0	0	0
All	All	11224	5	10629	421	2

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 19.

All (421) 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)
3:D:505:NAG:HN2	3:C:510:NAG:H61	1.20	1.00
1:D:61:TYR:OH	1:C:60:ALA:HB1	1.66	0.94
3:A:506:NAG:O3	1:C:409:SER:OG	1.85	0.94
3:A:504:NAG:H83	3:A:504:NAG:H3	1.58	0.86
3:D:504:NAG:H83	3:D:504:NAG:H3	1.58	0.85
3:B:504:NAG:H83	3:B:504:NAG:H3	1.58	0.85
1:D:59:LYS:HE2	1:C:61:TYR:HA	1.56	0.84
3:C:504:NAG:H3	3:C:504:NAG:H83	1.58	0.84
1:C:343:GLN:HG3	1:C:403:TYR:HB3	1.61	0.83
1:A:343:GLN:HG3	1:A:403:TYR:HB3	1.61	0.82
1:A:357:LYS:HB3	1:A:465:THR:HA	1.62	0.82
1:C:357:LYS:HB3	1:C:465:THR:HA	1.62	0.82
3:A:506:NAG:HO3	1:C:409:SER:HG	1.17	0.81
1:D:343:GLN:HG3	1:D:403:TYR:HB3	1.61	0.81
1:B:343:GLN:HG3	1:B:403:TYR:HB3	1.61	0.81
1:D:357:LYS:HB3	1:D:465:THR:HA	1.62	0.80
1:A:409:SER:HG	3:C:506:NAG:HO3	1.26	0.79
1:B:357:LYS:HB3	1:B:465:THR:HA	1.62	0.79
1:D:442:GLU:HG2	1:C:81:PRO:HD3	1.64	0.78
1:B:259:LEU:HD22	1:B:449:ILE:HD13	1.66	0.78
1:D:259:LEU:HD22	1:D:449:ILE:HD13	1.66	0.77
1:A:259:LEU:HD22	1:A:449:ILE:HD13	1.66	0.77
1:C:259:LEU:HD22	1:C:449:ILE:HD13	1.66	0.76
1:D:57:ASP:OD2	1:C:63:LYS:HE2	1.86	0.75
1:A:409:SER:OG	3:C:506:NAG:O3	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:ASP:OD2	1:C:59:LYS:HE3	1.88	0.73
1:C:344:LYS:HD3	3:C:504:NAG:H5	1.71	0.72
1:A:344:LYS:HD3	3:A:504:NAG:H5	1.71	0.72
1:B:344:LYS:HD3	3:B:504:NAG:H5	1.71	0.71
3:D:505:NAG:N2	3:C:510:NAG:H61	2.01	0.71
1:B:343:GLN:HG3	1:B:403:TYR:CB	2.21	0.71
1:C:343:GLN:HG3	1:C:403:TYR:CB	2.21	0.70
1:A:49:LYS:HG2	1:A:488:VAL:HG13	1.73	0.70
1:A:343:GLN:HG3	1:A:403:TYR:CB	2.21	0.70
1:D:49:LYS:HG2	1:D:488:VAL:HG13	1.73	0.70
1:B:49:LYS:HG2	1:B:488:VAL:HG13	1.73	0.70
1:D:344:LYS:HD3	3:D:504:NAG:H5	1.72	0.70
1:C:49:LYS:HG2	1:C:488:VAL:HG13	1.73	0.70
1:D:343:GLN:HG3	1:D:403:TYR:CB	2.21	0.69
1:A:370:GLU:HG3	1:A:384:TYR:CE2	2.27	0.69
1:C:370:GLU:HG3	1:C:384:TYR:CE2	2.27	0.69
1:B:370:GLU:HG3	1:B:384:TYR:CE2	2.28	0.69
1:A:65:VAL:HB	1:A:115:SER:HB3	1.75	0.69
1:A:404:ASN:HD22	3:C:508:NAG:H62	1.57	0.69
1:C:456:ARG:HG2	1:C:457:ASP:H	1.58	0.69
1:D:370:GLU:HG3	1:D:384:TYR:CE2	2.27	0.69
1:B:65:VAL:HB	1:B:115:SER:HB3	1.75	0.68
1:D:65:VAL:HB	1:D:115:SER:HB3	1.75	0.68
1:B:331:CYS:HB2	1:B:416:LEU:HD12	1.76	0.68
1:A:456:ARG:HG2	1:A:457:ASP:H	1.58	0.68
1:C:65:VAL:HB	1:C:115:SER:HB3	1.75	0.68
1:D:456:ARG:HG2	1:D:457:ASP:H	1.58	0.67
1:A:331:CYS:HB2	1:A:416:LEU:HD12	1.76	0.67
1:D:331:CYS:HB2	1:D:416:LEU:HD12	1.76	0.67
1:C:51:THR:HA	1:C:103:GLN:HE22	1.59	0.67
1:A:51:THR:HA	1:A:103:GLN:HE22	1.59	0.67
1:D:51:THR:HA	1:D:103:GLN:HE22	1.59	0.67
1:B:456:ARG:HG2	1:B:457:ASP:H	1.58	0.66
1:C:331:CYS:HB2	1:C:416:LEU:HD12	1.76	0.66
1:A:370:GLU:CD	1:A:425:ASN:HB2	2.16	0.66
1:D:370:GLU:CD	1:D:425:ASN:HB2	2.17	0.66
1:A:336:SER:O	1:A:339:ASN:HB2	1.96	0.66
1:B:51:THR:HA	1:B:103:GLN:HE22	1.59	0.66
1:C:336:SER:O	1:C:339:ASN:HB2	1.96	0.65
1:B:336:SER:O	1:B:339:ASN:HB2	1.96	0.65
1:D:61:TYR:OH	1:C:60:ALA:CB	2.42	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:SER:O	1:D:339:ASN:HB2	1.96	0.65
1:B:269:GLU:O	1:B:271:ILE:HD12	1.97	0.65
1:A:219:ALA:HB2	1:A:225:ILE:HG13	1.79	0.65
1:C:370:GLU:CD	1:C:425:ASN:HB2	2.17	0.65
1:A:269:GLU:O	1:A:271:ILE:HD12	1.97	0.65
1:B:370:GLU:CD	1:B:425:ASN:HB2	2.17	0.65
1:D:213:ILE:HG22	1:C:61:TYR:CE2	2.32	0.64
1:D:269:GLU:O	1:D:271:ILE:HD12	1.97	0.64
1:D:442:GLU:CG	1:C:81:PRO:HD3	2.27	0.64
1:B:89:VAL:HG13	1:B:89:VAL:O	1.98	0.64
1:C:269:GLU:O	1:C:271:ILE:HD12	1.97	0.64
1:A:89:VAL:O	1:A:89:VAL:HG13	1.98	0.64
1:C:89:VAL:HG13	1:C:89:VAL:O	1.98	0.64
1:D:373:THR:HB	1:D:385:CYS:O	1.97	0.64
1:B:373:THR:HB	1:B:385:CYS:O	1.98	0.64
1:B:219:ALA:HB2	1:B:225:ILE:HG13	1.79	0.64
1:A:51:THR:HA	1:A:103:GLN:NE2	2.14	0.63
1:D:51:THR:HA	1:D:103:GLN:NE2	2.14	0.63
1:D:89:VAL:HG13	1:D:89:VAL:O	1.98	0.63
1:D:457:ASP:OD2	1:D:467:THR:HG23	1.98	0.63
1:C:373:THR:HB	1:C:385:CYS:O	1.98	0.63
1:C:51:THR:HA	1:C:103:GLN:NE2	2.14	0.63
1:D:442:GLU:HG3	1:D:442:GLU:O	1.98	0.63
1:A:331:CYS:O	1:A:415:THR:HA	1.99	0.63
1:A:373:THR:HB	1:A:385:CYS:O	1.98	0.63
1:B:457:ASP:OD2	1:B:467:THR:HG23	1.99	0.63
1:B:51:THR:HA	1:B:103:GLN:NE2	2.13	0.63
1:C:219:ALA:HB2	1:C:225:ILE:HG13	1.79	0.62
1:D:219:ALA:HB2	1:D:225:ILE:HG13	1.79	0.62
1:C:248:THR:HG22	1:C:486:TYR:CD1	2.34	0.62
1:C:457:ASP:OD2	1:C:467:THR:HG23	1.99	0.62
1:D:248:THR:HG22	1:D:486:TYR:CD1	2.34	0.62
1:A:457:ASP:OD2	1:A:467:THR:HG23	1.98	0.62
1:C:442:GLU:O	1:C:442:GLU:HG3	1.98	0.62
1:B:248:THR:HG22	1:B:486:TYR:CD1	2.35	0.62
1:D:358:THR:O	1:D:465:THR:HB	2.00	0.62
1:A:248:THR:HG22	1:A:486:TYR:CD1	2.34	0.62
1:A:358:THR:O	1:A:465:THR:HB	1.99	0.62
1:D:274:SER:HB3	1:D:277:LEU:HD13	1.82	0.62
1:A:404:ASN:ND2	3:C:508:NAG:H62	2.14	0.62
1:A:274:SER:HB3	1:A:277:LEU:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:CYS:O	1:D:415:THR:HA	1.99	0.61
1:A:442:GLU:HG3	1:A:442:GLU:O	1.98	0.61
1:C:358:THR:O	1:C:465:THR:HB	2.00	0.61
1:D:57:ASP:O	1:C:61:TYR:HB2	2.01	0.61
1:C:274:SER:HB3	1:C:277:LEU:HD13	1.82	0.61
1:B:331:CYS:O	1:B:415:THR:HA	1.99	0.61
1:B:358:THR:O	1:B:465:THR:HB	1.99	0.61
1:B:442:GLU:O	1:B:442:GLU:HG3	1.98	0.61
1:C:331:CYS:O	1:C:415:THR:HA	1.99	0.61
1:B:274:SER:HB3	1:B:277:LEU:HD13	1.82	0.61
1:C:332:ASN:OD1	1:C:415:THR:HG22	2.01	0.60
1:C:426:MET:HE2	1:C:429:GLU:HG2	1.83	0.60
1:B:343:GLN:O	1:B:347:GLU:HG3	2.02	0.60
1:A:332:ASN:OD1	1:A:415:THR:HG22	2.01	0.60
1:D:66:HIS:HB3	1:D:213:ILE:HG12	1.84	0.60
1:C:298:ARG:HG2	1:C:328:GLN:O	2.02	0.60
1:B:66:HIS:HB3	1:B:213:ILE:HG12	1.84	0.60
1:A:298:ARG:HG2	1:A:328:GLN:O	2.02	0.60
1:B:298:ARG:HG2	1:B:328:GLN:O	2.02	0.60
1:C:66:HIS:HB3	1:C:213:ILE:HG12	1.84	0.60
1:B:332:ASN:OD1	1:B:415:THR:HG22	2.01	0.60
1:D:332:ASN:OD1	1:D:415:THR:HG22	2.01	0.60
1:D:343:GLN:O	1:D:347:GLU:HG3	2.01	0.60
1:D:298:ARG:HG2	1:D:328:GLN:O	2.02	0.59
1:B:426:MET:HE2	1:B:429:GLU:HG2	1.83	0.59
1:A:343:GLN:O	1:A:347:GLU:HG3	2.01	0.59
1:A:426:MET:HE2	1:A:429:GLU:HG2	1.83	0.59
1:D:426:MET:HE2	1:D:429:GLU:HG2	1.85	0.59
1:C:343:GLN:O	1:C:347:GLU:HG3	2.01	0.59
1:A:66:HIS:HB3	1:A:213:ILE:HG12	1.84	0.58
1:D:255:VAL:HG13	1:D:475:MET:CE	2.33	0.58
1:D:442:GLU:HG2	1:C:80:ASN:HA	1.84	0.58
1:B:255:VAL:HG13	1:B:475:MET:CE	2.33	0.58
1:A:255:VAL:HG13	1:A:475:MET:CE	2.33	0.58
1:D:255:VAL:HG13	1:D:475:MET:HE2	1.86	0.58
1:C:255:VAL:HG13	1:C:475:MET:CE	2.33	0.58
1:A:207:LYS:HE2	1:A:436:ALA:HB3	1.86	0.58
1:B:456:ARG:HG2	1:B:457:ASP:N	2.20	0.57
1:C:456:ARG:HG2	1:C:457:ASP:N	2.20	0.57
3:C:504:NAG:H3	3:C:504:NAG:C8	2.33	0.57
1:B:207:LYS:HE2	1:B:436:ALA:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:LYS:HE2	1:D:436:ALA:HB3	1.86	0.57
1:D:59:LYS:HE2	1:C:60:ALA:O	2.05	0.57
1:D:59:LYS:CE	1:C:61:TYR:HA	2.33	0.57
3:A:504:NAG:H3	3:A:504:NAG:C8	2.33	0.57
3:B:504:NAG:H3	3:B:504:NAG:C8	2.33	0.57
3:D:504:NAG:H3	3:D:504:NAG:C8	2.33	0.56
1:D:456:ARG:HG2	1:D:457:ASP:N	2.20	0.56
1:A:456:ARG:HG2	1:A:457:ASP:N	2.20	0.56
1:C:207:LYS:HE2	1:C:436:ALA:HB3	1.86	0.56
1:D:397:ASN:O	1:D:399:THR:HG23	2.06	0.56
1:B:397:ASN:O	1:B:399:THR:HG23	2.06	0.56
1:A:397:ASN:O	1:A:399:THR:HG23	2.06	0.56
1:C:257:THR:O	1:C:259:LEU:N	2.39	0.56
1:C:397:ASN:O	1:C:399:THR:HG23	2.06	0.55
1:A:426:MET:CE	1:A:429:GLU:HG2	2.36	0.55
1:B:426:MET:CE	1:B:429:GLU:HG2	2.36	0.55
1:B:257:THR:O	1:B:259:LEU:N	2.39	0.55
1:D:391:PHE:CE2	1:D:470:PRO:HB3	2.42	0.55
1:B:391:PHE:CE2	1:B:470:PRO:HB3	2.42	0.55
1:C:426:MET:CE	1:C:429:GLU:HG2	2.36	0.55
1:C:434:ILE:HD11	1:B:434:ILE:CD1	2.36	0.55
1:A:344:LYS:NZ	3:A:504:NAG:O4	2.33	0.54
1:A:370:GLU:HG3	1:A:384:TYR:HE2	1.71	0.54
1:C:391:PHE:CE2	1:C:470:PRO:HB3	2.42	0.54
1:A:391:PHE:CE2	1:A:470:PRO:HB3	2.42	0.54
3:D:505:NAG:H82	3:C:510:NAG:H5	1.89	0.53
1:D:426:MET:CE	1:D:429:GLU:HG2	2.36	0.53
1:D:379:ARG:NH1	1:D:444:THR:H	2.06	0.53
1:A:379:ARG:NH1	1:A:444:THR:H	2.07	0.53
1:B:379:ARG:NH1	1:B:444:THR:H	2.07	0.53
1:A:257:THR:O	1:A:259:LEU:N	2.39	0.53
1:C:370:GLU:HG3	1:C:384:TYR:HE2	1.71	0.53
1:D:257:THR:O	1:D:259:LEU:N	2.39	0.53
1:B:370:GLU:HG3	1:B:384:TYR:HE2	1.71	0.53
1:C:379:ARG:NH1	1:C:444:THR:H	2.07	0.53
1:D:344:LYS:NZ	3:D:504:NAG:O4	2.33	0.53
1:D:370:GLU:HG3	1:D:384:TYR:HE2	1.71	0.52
1:B:370:GLU:OE1	1:B:425:ASN:HB2	2.09	0.52
1:C:370:GLU:OE1	1:C:425:ASN:HB2	2.09	0.52
1:C:255:VAL:HG13	1:C:475:MET:HE3	1.92	0.52
1:D:386:ASN:O	1:D:416:LEU:HD22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:GLU:OE1	1:D:425:ASN:HB2	2.09	0.51
1:A:370:GLU:OE1	1:A:425:ASN:HB2	2.09	0.51
1:A:105:HIS:O	1:A:109:ILE:HG13	2.11	0.51
1:A:386:ASN:O	1:A:416:LEU:HD22	2.11	0.51
1:A:404:ASN:HD22	3:C:508:NAG:C6	2.22	0.51
1:B:105:HIS:O	1:B:109:ILE:HG13	2.11	0.51
1:D:105:HIS:O	1:D:109:ILE:HG13	2.11	0.51
1:C:85:VAL:HG12	1:C:86:LEU:N	2.26	0.51
1:C:386:ASN:O	1:C:416:LEU:HD22	2.11	0.51
1:D:80:ASN:OD1	1:D:80:ASN:O	2.29	0.50
1:C:80:ASN:OD1	1:C:80:ASN:O	2.29	0.50
1:B:80:ASN:OD1	1:B:80:ASN:O	2.30	0.50
1:D:85:VAL:HG12	1:D:86:LEU:N	2.26	0.50
1:D:297:THR:O	1:D:329:ALA:HB1	2.12	0.50
1:A:80:ASN:OD1	1:A:80:ASN:O	2.29	0.50
1:B:85:VAL:HG12	1:B:86:LEU:N	2.26	0.50
1:D:64:GLU:OE1	1:D:66:HIS:HB2	2.12	0.50
1:C:64:GLU:OE1	1:C:66:HIS:HB2	2.12	0.50
1:B:386:ASN:O	1:B:416:LEU:HD22	2.11	0.50
1:A:85:VAL:HG12	1:A:86:LEU:N	2.26	0.50
1:C:65:VAL:CB	1:C:115:SER:HB3	2.41	0.50
1:A:96:TRP:CZ2	1:A:274:SER:HA	2.47	0.50
1:A:297:THR:O	1:A:329:ALA:HB1	2.12	0.50
1:C:105:HIS:O	1:C:109:ILE:HG13	2.11	0.50
1:B:344:LYS:NZ	3:B:504:NAG:O4	2.33	0.50
1:B:64:GLU:OE1	1:B:66:HIS:HB2	2.12	0.49
1:C:96:TRP:CZ2	1:C:274:SER:HA	2.47	0.49
1:A:65:VAL:CB	1:A:115:SER:HB3	2.41	0.49
3:A:508:NAG:H62	1:C:404:ASN:ND2	2.27	0.49
1:B:96:TRP:CZ2	1:B:274:SER:HA	2.47	0.49
1:B:292:VAL:HG22	1:B:337:LYS:HG3	1.95	0.49
1:D:64:GLU:HA	1:D:209:SER:OG	2.13	0.49
1:B:297:THR:O	1:B:329:ALA:HB1	2.12	0.49
1:D:96:TRP:CZ2	1:D:274:SER:HA	2.47	0.49
1:C:64:GLU:HA	1:C:209:SER:OG	2.13	0.49
1:C:297:THR:O	1:C:329:ALA:HB1	2.12	0.49
1:A:64:GLU:OE1	1:A:66:HIS:HB2	2.12	0.49
3:D:510:NAG:C6	3:C:503:NAG:H61	2.43	0.49
1:A:364:SER:OG	1:A:372:THR:HA	2.12	0.49
1:B:65:VAL:CB	1:B:115:SER:HB3	2.41	0.49
1:A:255:VAL:HG13	1:A:475:MET:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:SER:HB2	1:A:470:PRO:HG2	1.95	0.49
1:C:292:VAL:HG22	1:C:337:LYS:HG3	1.95	0.49
1:B:364:SER:OG	1:B:372:THR:HA	2.12	0.49
3:B:504:NAG:C1	3:B:504:NAG:H82	2.43	0.49
1:D:364:SER:OG	1:D:372:THR:HA	2.13	0.49
1:C:364:SER:OG	1:C:372:THR:HA	2.12	0.49
3:C:504:NAG:H82	3:C:504:NAG:C1	2.43	0.48
3:D:504:NAG:C1	3:D:504:NAG:H82	2.43	0.48
1:C:344:LYS:NZ	3:C:504:NAG:O4	2.33	0.48
1:B:64:GLU:HA	1:B:209:SER:OG	2.13	0.48
1:D:65:VAL:CB	1:D:115:SER:HB3	2.41	0.48
3:A:504:NAG:H82	3:A:504:NAG:C1	2.43	0.48
1:D:292:VAL:HG22	1:D:337:LYS:HG3	1.95	0.48
1:D:364:SER:HB2	1:D:470:PRO:HG2	1.95	0.48
1:A:64:GLU:HA	1:A:209:SER:OG	2.13	0.48
1:A:292:VAL:HG22	1:A:337:LYS:HG3	1.95	0.48
1:B:65:VAL:HB	1:B:115:SER:CB	2.43	0.48
1:B:105:HIS:ND1	1:B:476:ARG:HG2	2.29	0.48
1:B:364:SER:HB2	1:B:470:PRO:HG2	1.95	0.48
1:A:65:VAL:HB	1:A:115:SER:CB	2.43	0.48
1:A:105:HIS:ND1	1:A:476:ARG:HG2	2.29	0.48
1:D:419:LYS:HD3	1:D:421:LYS:HG3	1.96	0.47
1:A:419:LYS:HD3	1:A:421:LYS:HG3	1.96	0.47
1:D:456:ARG:HD2	1:D:466:GLU:OE1	2.14	0.47
1:A:354:PRO:HG2	1:A:356:SER:H	1.80	0.47
1:C:364:SER:HB2	1:C:470:PRO:HG2	1.95	0.47
1:B:96:TRP:HA	1:B:480:ARG:HD3	1.96	0.47
1:B:282:LYS:HA	1:B:282:LYS:HD3	1.66	0.47
1:B:354:PRO:HG2	1:B:356:SER:H	1.80	0.47
1:C:419:LYS:HD3	1:C:421:LYS:HG3	1.96	0.47
1:B:419:LYS:HD3	1:B:421:LYS:HG3	1.96	0.47
1:A:456:ARG:HD2	1:A:466:GLU:OE1	2.14	0.47
1:C:105:HIS:ND1	1:C:476:ARG:HG2	2.29	0.47
1:C:354:PRO:HG2	1:C:356:SER:H	1.80	0.47
1:B:456:ARG:HD2	1:B:466:GLU:OE1	2.14	0.47
1:D:96:TRP:HA	1:D:480:ARG:HD3	1.96	0.47
1:D:105:HIS:ND1	1:D:476:ARG:HG2	2.29	0.47
1:A:96:TRP:HA	1:A:480:ARG:HD3	1.96	0.47
1:A:286:VAL:HG11	1:A:452:LEU:HD12	1.97	0.47
1:C:432:ARG:NH2	1:B:422:GLN:HB2	2.30	0.47
1:D:354:PRO:HG2	1:D:356:SER:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ILE:HD13	1:A:286:VAL:HG22	1.97	0.47
1:C:96:TRP:HA	1:C:480:ARG:HD3	1.96	0.47
1:C:456:ARG:HD2	1:C:466:GLU:OE1	2.14	0.47
1:D:442:GLU:CD	1:C:81:PRO:HD3	2.35	0.47
1:D:286:VAL:HG11	1:D:452:LEU:HD12	1.97	0.47
1:C:286:VAL:HG11	1:C:452:LEU:HD12	1.96	0.47
1:C:378:CYS:C	1:C:380:GLY:H	2.19	0.47
1:B:255:VAL:HG13	1:B:475:MET:HE3	1.95	0.47
1:A:338:TRP:CZ2	1:A:390:LEU:HG	2.50	0.46
1:A:378:CYS:C	1:A:380:GLY:H	2.19	0.46
1:C:272:ILE:HD13	1:C:286:VAL:HG22	1.97	0.46
1:C:338:TRP:CZ2	1:C:390:LEU:HG	2.50	0.46
1:B:286:VAL:HG11	1:B:452:LEU:HD12	1.96	0.46
1:B:378:CYS:C	1:B:380:GLY:H	2.19	0.46
1:A:277:LEU:HD12	1:A:277:LEU:HA	1.72	0.46
1:C:65:VAL:HB	1:C:115:SER:CB	2.43	0.46
1:D:272:ILE:HD13	1:D:286:VAL:HG22	1.97	0.46
1:A:101:VAL:HG21	1:A:480:ARG:HG3	1.98	0.46
1:C:283:THR:HA	1:C:455:LEU:CD2	2.46	0.46
1:A:283:THR:HA	1:A:455:LEU:CD2	2.46	0.46
1:D:378:CYS:C	1:D:380:GLY:H	2.19	0.46
1:B:272:ILE:HD13	1:B:286:VAL:HG22	1.97	0.46
1:B:338:TRP:CZ2	1:B:390:LEU:HG	2.50	0.46
1:D:338:TRP:CZ2	1:D:390:LEU:HG	2.50	0.46
1:B:358:THR:HG21	1:B:396:ARG:HG3	1.98	0.46
1:A:359:ILE:HB	1:A:395:TYR:HB3	1.98	0.46
3:C:504:NAG:H83	3:C:504:NAG:C3	2.39	0.46
1:B:283:THR:HA	1:B:455:LEU:CD2	2.46	0.46
1:C:358:THR:HG21	1:C:396:ARG:HG3	1.98	0.46
1:D:358:THR:HG21	1:D:396:ARG:HG3	1.98	0.46
1:D:283:THR:HA	1:D:455:LEU:CD2	2.46	0.45
1:C:282:LYS:HA	1:C:282:LYS:HD3	1.66	0.45
1:D:403:TYR:O	3:D:506:NAG:H81	2.16	0.45
1:A:358:THR:HG21	1:A:396:ARG:HG3	1.98	0.45
1:B:101:VAL:HG21	1:B:480:ARG:HG3	1.98	0.45
1:D:65:VAL:HB	1:D:115:SER:CB	2.43	0.45
1:A:283:THR:HA	1:A:455:LEU:HD21	1.99	0.45
1:A:403:TYR:O	3:A:506:NAG:H81	2.16	0.45
1:A:489:VAL:O	1:A:490:GLU:HB3	2.17	0.45
1:B:277:LEU:HD12	1:B:277:LEU:HA	1.72	0.45
3:D:505:NAG:HN2	3:C:510:NAG:C6	2.09	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:ILE:HB	1:B:395:TYR:HB3	1.98	0.45
1:B:489:VAL:O	1:B:490:GLU:HB3	2.17	0.45
1:D:101:VAL:HG21	1:D:480:ARG:HG3	1.98	0.45
1:D:359:ILE:HB	1:D:395:TYR:HB3	1.98	0.45
1:D:283:THR:HA	1:D:455:LEU:HD21	1.99	0.45
1:C:101:VAL:HG21	1:C:480:ARG:HG3	1.98	0.45
3:B:504:NAG:H83	3:B:504:NAG:C3	2.39	0.45
1:C:489:VAL:O	1:C:490:GLU:HB3	2.17	0.45
1:D:489:VAL:O	1:D:490:GLU:HB3	2.17	0.44
1:B:298:ARG:O	1:B:442:GLU:HA	2.17	0.44
1:C:359:ILE:HB	1:C:395:TYR:HB3	1.98	0.44
1:C:403:TYR:O	3:C:506:NAG:H81	2.16	0.44
3:A:508:NAG:H5	1:C:404:ASN:HD22	1.83	0.44
1:C:259:LEU:HD23	1:C:452:LEU:HD23	1.99	0.44
1:D:93:PHE:CE2	1:D:487:LYS:HB3	2.53	0.44
1:C:283:THR:HA	1:C:455:LEU:HD21	1.99	0.44
1:B:403:TYR:O	3:B:506:NAG:H81	2.16	0.44
1:C:93:PHE:CE2	1:C:487:LYS:HB3	2.53	0.44
1:C:298:ARG:O	1:C:442:GLU:HA	2.17	0.44
1:D:259:LEU:HD23	1:D:452:LEU:HD23	1.99	0.44
1:D:298:ARG:O	1:D:442:GLU:HA	2.17	0.44
1:D:381:GLU:HG3	1:D:443:ILE:HD13	2.00	0.44
1:B:381:GLU:HG3	1:B:443:ILE:HD13	2.00	0.44
1:D:349:LEU:HD13	1:D:468:PHE:CZ	2.53	0.43
1:A:298:ARG:O	1:A:442:GLU:HA	2.17	0.43
1:D:342:LEU:HD23	1:D:342:LEU:HA	1.80	0.43
1:C:381:GLU:HG3	1:C:443:ILE:HD13	2.00	0.43
1:A:381:GLU:HG3	1:A:443:ILE:HD13	2.00	0.43
1:B:349:LEU:HD13	1:B:468:PHE:CZ	2.53	0.43
1:B:93:PHE:CE2	1:B:487:LYS:HB3	2.53	0.43
1:B:213:ILE:O	1:B:213:ILE:HG13	2.19	0.43
1:D:86:LEU:HB2	1:D:89:VAL:HG11	2.01	0.43
1:A:93:PHE:CE2	1:A:487:LYS:HB3	2.53	0.43
1:B:259:LEU:HD23	1:B:452:LEU:HD23	1.99	0.43
1:B:283:THR:HA	1:B:455:LEU:HD21	1.99	0.43
1:A:259:LEU:HD23	1:A:452:LEU:HD23	1.99	0.43
1:C:86:LEU:HB2	1:C:89:VAL:CG1	2.49	0.43
1:B:86:LEU:HB2	1:B:89:VAL:HG11	2.01	0.43
1:A:86:LEU:HB2	1:A:89:VAL:CG1	2.49	0.43
1:A:86:LEU:HB2	1:A:89:VAL:HG11	2.01	0.43
1:A:349:LEU:HD13	1:A:468:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:ILE:O	1:C:213:ILE:HG13	2.19	0.43
1:C:333:ILE:HD11	1:C:416:LEU:HD11	2.01	0.43
1:C:349:LEU:HD13	1:C:468:PHE:CZ	2.53	0.42
1:A:213:ILE:O	1:A:213:ILE:HG13	2.19	0.42
1:B:254:VAL:HG11	1:B:261:LEU:HB2	2.01	0.42
1:B:333:ILE:HD11	1:B:416:LEU:HD11	2.01	0.42
1:D:213:ILE:O	1:D:213:ILE:HG13	2.19	0.42
1:B:349:LEU:HD23	1:B:349:LEU:HA	1.85	0.42
1:D:254:VAL:HG11	1:D:261:LEU:HB2	2.01	0.42
1:D:333:ILE:HD11	1:D:416:LEU:HD11	2.01	0.42
1:D:282:LYS:HD3	1:D:282:LYS:HA	1.66	0.42
1:B:86:LEU:HB2	1:B:89:VAL:CG1	2.49	0.42
1:A:231:LYS:HB2	1:A:268:GLU:HG3	2.02	0.42
1:D:231:LYS:HB2	1:D:268:GLU:HG3	2.02	0.42
1:A:254:VAL:HG11	1:A:261:LEU:HB2	2.01	0.42
1:C:254:VAL:HG11	1:C:261:LEU:HB2	2.01	0.42
1:B:231:LYS:HB2	1:B:268:GLU:HG3	2.02	0.42
1:B:53:PHE:CZ	1:B:218:CYS:HB2	2.55	0.42
1:D:337:LYS:HD2	1:D:337:LYS:HA	1.72	0.42
1:A:226:LEU:O	1:A:486:TYR:HA	2.20	0.42
1:C:271:ILE:HD12	1:C:271:ILE:N	2.35	0.42
1:C:378:CYS:C	1:C:380:GLY:N	2.73	0.42
1:B:271:ILE:HD12	1:B:271:ILE:N	2.35	0.42
1:D:53:PHE:CZ	1:D:218:CYS:HB2	2.55	0.41
1:A:349:LEU:HD23	1:A:349:LEU:HA	1.85	0.41
1:C:86:LEU:HB2	1:C:89:VAL:HG11	2.01	0.41
1:B:226:LEU:O	1:B:486:TYR:HA	2.20	0.41
1:B:269:GLU:O	1:B:271:ILE:CD1	2.67	0.41
1:C:269:GLU:O	1:C:271:ILE:CD1	2.67	0.41
1:A:333:ILE:HD11	1:A:416:LEU:HD11	2.01	0.41
1:B:271:ILE:HG21	1:B:273:ARG:NH1	2.36	0.41
1:D:86:LEU:HB2	1:D:89:VAL:CG1	2.49	0.41
1:D:378:CYS:C	1:D:380:GLY:N	2.73	0.41
1:A:282:LYS:HA	1:A:282:LYS:HD3	1.66	0.41
1:C:83:GLU:HG3	1:C:84:MET:N	2.35	0.41
1:C:226:LEU:O	1:C:486:TYR:HA	2.20	0.41
1:C:271:ILE:HG21	1:C:273:ARG:NH1	2.36	0.41
1:C:277:LEU:HA	1:C:277:LEU:HD12	1.72	0.41
1:B:378:CYS:C	1:B:380:GLY:N	2.73	0.41
1:D:277:LEU:HD12	1:D:277:LEU:HA	1.72	0.41
3:A:504:NAG:H83	3:A:504:NAG:C3	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:ILE:HD12	1:D:271:ILE:N	2.35	0.41
1:A:378:CYS:C	1:A:380:GLY:N	2.73	0.41
1:B:269:GLU:HA	1:B:289:ASN:HD22	1.86	0.41
1:D:271:ILE:HG21	1:D:273:ARG:NH1	2.36	0.41
1:A:269:GLU:O	1:A:271:ILE:CD1	2.67	0.41
1:D:59:LYS:HE2	1:C:61:TYR:CA	2.39	0.41
1:D:226:LEU:O	1:D:486:TYR:HA	2.20	0.41
1:A:269:GLU:HA	1:A:289:ASN:HD22	1.86	0.41
1:A:430:VAL:HG22	2:A:501:I6Q:N24	2.36	0.41
1:C:53:PHE:CZ	1:C:218:CYS:HB2	2.55	0.41
1:D:269:GLU:HA	1:D:289:ASN:HD22	1.86	0.41
1:D:430:VAL:HG22	2:D:501:I6Q:N24	2.36	0.41
1:A:53:PHE:CZ	1:A:218:CYS:HB2	2.55	0.41
1:A:86:LEU:CD1	1:A:89:VAL:HG11	2.51	0.41
1:A:255:VAL:HG13	1:A:475:MET:HE2	2.03	0.41
1:C:430:VAL:HG22	2:C:501:I6Q:N24	2.36	0.41
1:B:83:GLU:HG3	1:B:84:MET:N	2.35	0.41
1:A:271:ILE:HG21	1:A:273:ARG:NH1	2.36	0.40
1:C:231:LYS:HB2	1:C:268:GLU:HG3	2.02	0.40
1:B:424:ILE:HD13	1:B:424:ILE:N	2.36	0.40
1:B:430:VAL:HG22	2:B:501:I6Q:N24	2.36	0.40
1:D:86:LEU:CD1	1:D:89:VAL:HG11	2.51	0.40
1:A:337:LYS:HA	1:A:337:LYS:HD2	1.71	0.40
1:A:424:ILE:N	1:A:424:ILE:HD13	2.36	0.40
1:B:342:LEU:HD23	1:B:342:LEU:HA	1.80	0.40
1:D:378:CYS:O	1:D:380:GLY:N	2.55	0.40
1:A:226:LEU:HD12	1:A:489:VAL:HG11	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:SER:OG	1:B:356:SER:OG[3_454]	2.00	0.20
1:D:202:THR:OG1	1:B:202:THR:OG1[4_555]	2.11	0.09

## 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	329/358 (92%)	306 (93%)	20 (6%)	3 (1%)	17	49
1	B	329/358 (92%)	306 (93%)	20 (6%)	3 (1%)	17	49
1	C	329/358 (92%)	306 (93%)	20 (6%)	3 (1%)	17	49
1	D	329/358 (92%)	306 (93%)	20 (6%)	3 (1%)	17	49
All	All	1316/1432 (92%)	1224 (93%)	80 (6%)	12 (1%)	17	49

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	354	PRO
1	A	354	PRO
1	C	354	PRO
1	B	354	PRO
1	D	439	ILE
1	A	439	ILE
1	C	439	ILE
1	B	439	ILE
1	D	299	PRO
1	A	299	PRO
1	C	299	PRO
1	B	299	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	297/312 (95%)	296 (100%)	1 (0%)	92	96
1	B	297/312 (95%)	296 (100%)	1 (0%)	92	96
1	C	297/312 (95%)	296 (100%)	1 (0%)	92	96
1	D	297/312 (95%)	296 (100%)	1 (0%)	92	96
All	All	1188/1248 (95%)	1184 (100%)	4 (0%)	92	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	205	CYS
1	A	205	CYS
1	C	205	CYS
1	B	205	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	103	GLN
1	A	103	GLN
1	A	404	ASN
1	C	103	GLN
1	C	404	ASN
1	B	103	GLN

### 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

41 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
3	NAG	C	502	1	14,14,15	0.26	0	17,19,21	0.39	0
3	NAG	A	503	1	14,14,15	0.16	0	17,19,21	0.70	1 (5%)
3	NAG	A	506	1	14,14,15	0.60	1 (7%)	17,19,21	0.49	0
3	NAG	D	509	1	14,14,15	0.51	0	17,19,21	0.42	0
3	NAG	D	510	1	14,14,15	0.52	0	17,19,21	0.71	1 (5%)
3	NAG	B	510	1	14,14,15	0.52	0	17,19,21	0.71	1 (5%)
3	NAG	A	505	1	14,14,15	0.33	0	17,19,21	0.53	0
3	NAG	C	505	1	14,14,15	0.33	0	17,19,21	0.53	0
3	NAG	A	504	1	14,14,15	0.25	0	17,19,21	0.64	0
3	NAG	C	510	1	14,14,15	0.52	0	17,19,21	0.71	1 (5%)
3	NAG	A	508	1	14,14,15	0.48	0	17,19,21	0.59	0
3	NAG	D	507	1	14,14,15	0.35	0	17,19,21	0.62	0
3	NAG	B	504	1	14,14,15	0.25	0	17,19,21	0.64	0
3	NAG	A	507	1	14,14,15	0.35	0	17,19,21	0.62	0
3	NAG	B	506	1	14,14,15	0.60	1 (7%)	17,19,21	0.49	0
3	NAG	B	502	1	14,14,15	0.26	0	17,19,21	0.39	0
2	I6Q	B	501	-	38,38,38	5.15	20 (52%)	45,54,54	1.70	7 (15%)
3	NAG	C	503	1	14,14,15	0.17	0	17,19,21	0.70	1 (5%)
2	I6Q	A	501	-	38,38,38	5.15	20 (52%)	45,54,54	1.70	7 (15%)
3	NAG	D	504	1	14,14,15	0.25	0	17,19,21	0.64	0
3	NAG	B	503	1	14,14,15	0.16	0	17,19,21	0.70	1 (5%)
4	IMD	A	511	-	3,5,5	0.49	0	4,5,5	0.63	0
3	NAG	C	508	1	14,14,15	0.48	0	17,19,21	0.59	0
3	NAG	A	509	1	14,14,15	0.51	0	17,19,21	0.42	0
3	NAG	D	503	1	14,14,15	0.16	0	17,19,21	0.70	1 (5%)
2	I6Q	C	501	-	38,38,38	5.15	20 (52%)	45,54,54	1.70	7 (15%)
3	NAG	D	502	1	14,14,15	0.26	0	17,19,21	0.39	0
2	I6Q	D	501	-	38,38,38	5.15	20 (52%)	45,54,54	1.70	7 (15%)
3	NAG	B	507	1	14,14,15	0.35	0	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	D	506	1	14,14,15	0.60	1 (7%)	17,19,21	0.49	0
3	NAG	A	510	1	14,14,15	0.52	0	17,19,21	0.71	1 (5%)
3	NAG	B	505	1	14,14,15	0.33	0	17,19,21	0.53	0
3	NAG	C	507	1	14,14,15	0.35	0	17,19,21	0.62	0
3	NAG	D	508	1	14,14,15	0.48	0	17,19,21	0.59	0
3	NAG	C	509	1	14,14,15	0.51	0	17,19,21	0.42	0
3	NAG	D	505	1	14,14,15	0.33	0	17,19,21	0.53	0
3	NAG	B	509	1	14,14,15	0.51	0	17,19,21	0.42	0
3	NAG	C	504	1	14,14,15	0.25	0	17,19,21	0.64	0
3	NAG	B	508	1	14,14,15	0.48	0	17,19,21	0.59	0
3	NAG	A	502	1	14,14,15	0.26	0	17,19,21	0.39	0
3	NAG	C	506	1	14,14,15	0.60	1 (7%)	17,19,21	0.49	0

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
3	NAG	C	502	1	-	0/6/23/26	0/1/1/1
3	NAG	A	503	1	-	0/6/23/26	0/1/1/1
3	NAG	A	506	1	-	2/6/23/26	0/1/1/1
3	NAG	D	509	1	-	1/6/23/26	0/1/1/1
3	NAG	D	510	1	-	2/6/23/26	0/1/1/1
3	NAG	B	510	1	-	2/6/23/26	0/1/1/1
3	NAG	A	505	1	-	2/6/23/26	0/1/1/1
3	NAG	C	505	1	-	2/6/23/26	0/1/1/1
3	NAG	A	504	1	-	5/6/23/26	0/1/1/1
3	NAG	C	510	1	-	2/6/23/26	0/1/1/1
3	NAG	A	508	1	-	2/6/23/26	0/1/1/1
3	NAG	D	507	1	-	2/6/23/26	0/1/1/1
3	NAG	B	504	1	-	5/6/23/26	0/1/1/1
3	NAG	A	507	1	-	2/6/23/26	0/1/1/1
3	NAG	B	506	1	-	2/6/23/26	0/1/1/1
3	NAG	B	502	1	-	0/6/23/26	0/1/1/1
2	I6Q	B	501	-	-	0/21/42/42	0/4/4/4
3	NAG	C	503	1	-	0/6/23/26	0/1/1/1
2	I6Q	A	501	-	-	0/21/42/42	0/4/4/4
3	NAG	D	504	1	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	503	1	-	0/6/23/26	0/1/1/1
4	IMD	A	511	-	-	-	0/1/1/1
3	NAG	C	508	1	-	2/6/23/26	0/1/1/1
3	NAG	A	509	1	-	1/6/23/26	0/1/1/1
3	NAG	D	503	1	-	0/6/23/26	0/1/1/1
2	I6Q	C	501	-	-	0/21/42/42	0/4/4/4
3	NAG	D	502	1	-	0/6/23/26	0/1/1/1
2	I6Q	D	501	-	-	0/21/42/42	0/4/4/4
3	NAG	B	507	1	-	2/6/23/26	0/1/1/1
3	NAG	D	506	1	-	2/6/23/26	0/1/1/1
3	NAG	A	510	1	-	2/6/23/26	0/1/1/1
3	NAG	B	505	1	-	2/6/23/26	0/1/1/1
3	NAG	C	507	1	-	2/6/23/26	0/1/1/1
3	NAG	D	508	1	-	2/6/23/26	0/1/1/1
3	NAG	C	509	1	-	1/6/23/26	0/1/1/1
3	NAG	D	505	1	-	2/6/23/26	0/1/1/1
3	NAG	B	509	1	-	1/6/23/26	0/1/1/1
3	NAG	C	504	1	-	5/6/23/26	0/1/1/1
3	NAG	B	508	1	-	2/6/23/26	0/1/1/1
3	NAG	A	502	1	-	0/6/23/26	0/1/1/1
3	NAG	C	506	1	-	2/6/23/26	0/1/1/1

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	I6Q	C27-N28	-19.97	1.09	1.47
2	C	501	I6Q	C27-N28	-19.97	1.09	1.47
2	B	501	I6Q	C27-N28	-19.97	1.09	1.47
2	A	501	I6Q	C27-N28	-19.97	1.09	1.47
2	A	501	I6Q	C33-C31	-12.96	1.27	1.52
2	B	501	I6Q	C33-C31	-12.95	1.27	1.52
2	D	501	I6Q	C33-C31	-12.95	1.27	1.52
2	C	501	I6Q	C33-C31	-12.95	1.27	1.52
2	D	501	I6Q	C30-C29	-12.01	1.29	1.52
2	C	501	I6Q	C30-C29	-12.01	1.29	1.52
2	A	501	I6Q	C30-C29	-12.01	1.29	1.52
2	B	501	I6Q	C30-C29	-12.01	1.29	1.52
2	C	501	I6Q	C02-N14	7.70	1.49	1.34
2	D	501	I6Q	C02-N14	7.69	1.49	1.34
2	B	501	I6Q	C02-N14	7.69	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	I6Q	C02-N14	7.69	1.49	1.34
2	C	501	I6Q	C22-N21	6.98	1.47	1.33
2	D	501	I6Q	C22-N21	6.98	1.47	1.33
2	A	501	I6Q	C22-N21	6.98	1.47	1.33
2	B	501	I6Q	C22-N21	6.98	1.47	1.33
2	B	501	I6Q	C03-N04	5.81	1.48	1.35
2	D	501	I6Q	C03-N04	5.81	1.48	1.35
2	C	501	I6Q	C03-N04	5.81	1.48	1.35
2	A	501	I6Q	C03-N04	5.80	1.48	1.35
2	A	501	I6Q	C16-C15	4.99	1.56	1.51
2	C	501	I6Q	C16-C15	4.99	1.56	1.51
2	B	501	I6Q	C16-C15	4.98	1.56	1.51
2	D	501	I6Q	C16-C15	4.98	1.56	1.51
2	D	501	I6Q	C33-N28	3.96	1.52	1.47
2	B	501	I6Q	C33-N28	3.96	1.52	1.47
2	A	501	I6Q	C33-N28	3.95	1.52	1.47
2	C	501	I6Q	C33-N28	3.95	1.52	1.47
2	C	501	I6Q	C22-N23	3.73	1.47	1.32
2	A	501	I6Q	C22-N23	3.73	1.47	1.32
2	B	501	I6Q	C22-N23	3.73	1.47	1.32
2	D	501	I6Q	C22-N23	3.73	1.47	1.32
2	D	501	I6Q	C05-N04	3.66	1.49	1.41
2	A	501	I6Q	C05-N04	3.66	1.49	1.41
2	C	501	I6Q	C05-N04	3.66	1.49	1.41
2	B	501	I6Q	C05-N04	3.66	1.49	1.41
2	D	501	I6Q	C35-C16	3.36	1.44	1.39
2	B	501	I6Q	C35-C16	3.36	1.44	1.39
2	C	501	I6Q	C35-C16	3.36	1.44	1.39
2	A	501	I6Q	C35-C16	3.35	1.44	1.39
2	C	501	I6Q	C31-N32	3.05	1.56	1.46
2	B	501	I6Q	C31-N32	3.05	1.56	1.46
2	A	501	I6Q	C31-N32	3.05	1.56	1.46
2	D	501	I6Q	C31-N32	3.05	1.56	1.46
2	D	501	I6Q	O01-C02	-2.63	1.18	1.23
2	B	501	I6Q	O01-C02	-2.63	1.18	1.23
2	A	501	I6Q	O01-C02	-2.63	1.18	1.23
2	C	501	I6Q	O01-C02	-2.63	1.18	1.23
2	A	501	I6Q	O13-C03	-2.53	1.18	1.23
2	C	501	I6Q	O13-C03	-2.52	1.18	1.23
2	B	501	I6Q	O13-C03	-2.52	1.18	1.23
2	D	501	I6Q	O13-C03	-2.52	1.18	1.23
2	D	501	I6Q	C30-C31	2.43	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	I6Q	C30-C31	2.43	1.57	1.53
2	A	501	I6Q	C30-C31	2.43	1.57	1.53
2	B	501	I6Q	C30-C31	2.42	1.57	1.53
2	D	501	I6Q	C15-N14	-2.31	1.42	1.46
2	B	501	I6Q	C15-N14	-2.31	1.42	1.46
2	C	501	I6Q	C15-N14	-2.30	1.42	1.46
2	A	501	I6Q	C15-N14	-2.30	1.42	1.46
2	B	501	I6Q	C25-C26	2.27	1.43	1.39
2	C	501	I6Q	C25-C26	2.27	1.43	1.39
2	D	501	I6Q	C25-C26	2.27	1.43	1.39
2	A	501	I6Q	C25-C26	2.27	1.43	1.39
2	D	501	I6Q	C18-C17	2.25	1.54	1.50
2	B	501	I6Q	C18-C17	2.25	1.54	1.50
2	C	501	I6Q	C18-C17	2.25	1.54	1.50
2	A	501	I6Q	C18-C17	2.25	1.54	1.50
2	C	501	I6Q	C08-CL09	2.21	1.78	1.73
2	A	501	I6Q	C08-CL09	2.21	1.78	1.73
2	B	501	I6Q	C08-CL09	2.21	1.78	1.73
2	D	501	I6Q	C08-CL09	2.20	1.78	1.73
3	D	506	NAG	O5-C1	-2.14	1.40	1.43
3	B	506	NAG	O5-C1	-2.14	1.40	1.43
3	C	506	NAG	O5-C1	-2.14	1.40	1.43
3	A	506	NAG	O5-C1	-2.14	1.40	1.43
2	C	501	I6Q	C19-C15	-2.04	1.51	1.54
2	D	501	I6Q	C19-C15	-2.04	1.51	1.54
2	A	501	I6Q	C19-C15	-2.04	1.51	1.54
2	B	501	I6Q	C19-C15	-2.04	1.51	1.54

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	I6Q	C05-N04-C03	-5.23	118.46	127.53
2	D	501	I6Q	C05-N04-C03	-5.22	118.46	127.53
2	A	501	I6Q	C05-N04-C03	-5.22	118.46	127.53
2	B	501	I6Q	C05-N04-C03	-5.22	118.46	127.53
2	A	501	I6Q	C15-N14-C02	-4.38	115.26	122.32
2	C	501	I6Q	C15-N14-C02	-4.38	115.26	122.32
2	B	501	I6Q	C15-N14-C02	-4.38	115.27	122.32
2	D	501	I6Q	C15-N14-C02	-4.38	115.27	122.32
2	A	501	I6Q	C02-C03-N04	4.32	119.13	112.31
2	D	501	I6Q	C02-C03-N04	4.32	119.13	112.31
2	C	501	I6Q	C02-C03-N04	4.31	119.13	112.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	I6Q	C02-C03-N04	4.31	119.13	112.31
2	C	501	I6Q	C27-N28-C29	-2.82	109.06	113.18
2	B	501	I6Q	C27-N28-C29	-2.82	109.07	113.18
2	A	501	I6Q	C27-N28-C29	-2.82	109.07	113.18
2	D	501	I6Q	C27-N28-C29	-2.82	109.07	113.18
2	D	501	I6Q	C03-C02-N14	2.56	119.86	113.73
2	A	501	I6Q	C03-C02-N14	2.56	119.86	113.73
2	B	501	I6Q	C03-C02-N14	2.56	119.86	113.73
2	C	501	I6Q	C03-C02-N14	2.56	119.86	113.73
3	B	503	NAG	C1-O5-C5	2.37	115.40	112.19
3	C	503	NAG	C1-O5-C5	2.36	115.40	112.19
3	A	503	NAG	C1-O5-C5	2.36	115.39	112.19
3	D	503	NAG	C1-O5-C5	2.36	115.39	112.19
3	B	510	NAG	C1-O5-C5	2.34	115.37	112.19
3	D	510	NAG	C1-O5-C5	2.34	115.37	112.19
3	C	510	NAG	C1-O5-C5	2.34	115.36	112.19
3	A	510	NAG	C1-O5-C5	2.34	115.36	112.19
2	C	501	I6Q	C07-C08-C10	2.10	120.62	118.94
2	A	501	I6Q	C07-C08-C10	2.09	120.62	118.94
2	D	501	I6Q	C07-C08-C10	2.09	120.61	118.94
2	B	501	I6Q	C07-C08-C10	2.09	120.61	118.94
2	A	501	I6Q	C17-C18-C19	2.07	106.99	104.06
2	C	501	I6Q	C17-C18-C19	2.07	106.99	104.06
2	B	501	I6Q	C17-C18-C19	2.07	106.99	104.06
2	D	501	I6Q	C17-C18-C19	2.07	106.99	104.06

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	506	NAG	C4-C5-C6-O6
3	A	506	NAG	C4-C5-C6-O6
3	C	506	NAG	C4-C5-C6-O6
3	B	506	NAG	C4-C5-C6-O6
3	D	507	NAG	O5-C5-C6-O6
3	A	507	NAG	O5-C5-C6-O6
3	C	507	NAG	O5-C5-C6-O6
3	B	507	NAG	O5-C5-C6-O6
3	D	506	NAG	O5-C5-C6-O6
3	A	506	NAG	O5-C5-C6-O6
3	C	506	NAG	O5-C5-C6-O6
3	B	506	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	D	507	NAG	C4-C5-C6-O6
3	A	507	NAG	C4-C5-C6-O6
3	C	507	NAG	C4-C5-C6-O6
3	B	507	NAG	C4-C5-C6-O6
3	D	504	NAG	C8-C7-N2-C2
3	D	504	NAG	O7-C7-N2-C2
3	A	504	NAG	C8-C7-N2-C2
3	A	504	NAG	O7-C7-N2-C2
3	C	504	NAG	C8-C7-N2-C2
3	C	504	NAG	O7-C7-N2-C2
3	B	504	NAG	C8-C7-N2-C2
3	B	504	NAG	O7-C7-N2-C2
3	D	505	NAG	O5-C5-C6-O6
3	A	505	NAG	O5-C5-C6-O6
3	C	505	NAG	O5-C5-C6-O6
3	B	505	NAG	O5-C5-C6-O6
3	D	510	NAG	O5-C5-C6-O6
3	A	510	NAG	O5-C5-C6-O6
3	C	510	NAG	O5-C5-C6-O6
3	B	510	NAG	O5-C5-C6-O6
3	D	505	NAG	C4-C5-C6-O6
3	A	505	NAG	C4-C5-C6-O6
3	C	505	NAG	C4-C5-C6-O6
3	B	505	NAG	C4-C5-C6-O6
3	D	504	NAG	C4-C5-C6-O6
3	A	504	NAG	C4-C5-C6-O6
3	C	504	NAG	C4-C5-C6-O6
3	B	504	NAG	C4-C5-C6-O6
3	D	504	NAG	C3-C2-N2-C7
3	D	510	NAG	C3-C2-N2-C7
3	A	504	NAG	C3-C2-N2-C7
3	A	510	NAG	C3-C2-N2-C7
3	C	504	NAG	C3-C2-N2-C7
3	C	510	NAG	C3-C2-N2-C7
3	B	504	NAG	C3-C2-N2-C7
3	B	510	NAG	C3-C2-N2-C7
3	D	509	NAG	O5-C5-C6-O6
3	A	509	NAG	O5-C5-C6-O6
3	C	509	NAG	O5-C5-C6-O6
3	B	509	NAG	O5-C5-C6-O6
3	A	504	NAG	O5-C5-C6-O6
3	D	504	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	504	NAG	O5-C5-C6-O6
3	B	504	NAG	O5-C5-C6-O6
3	D	508	NAG	C4-C5-C6-O6
3	A	508	NAG	C4-C5-C6-O6
3	C	508	NAG	C4-C5-C6-O6
3	B	508	NAG	C4-C5-C6-O6
3	D	508	NAG	O5-C5-C6-O6
3	A	508	NAG	O5-C5-C6-O6
3	C	508	NAG	O5-C5-C6-O6
3	B	508	NAG	O5-C5-C6-O6

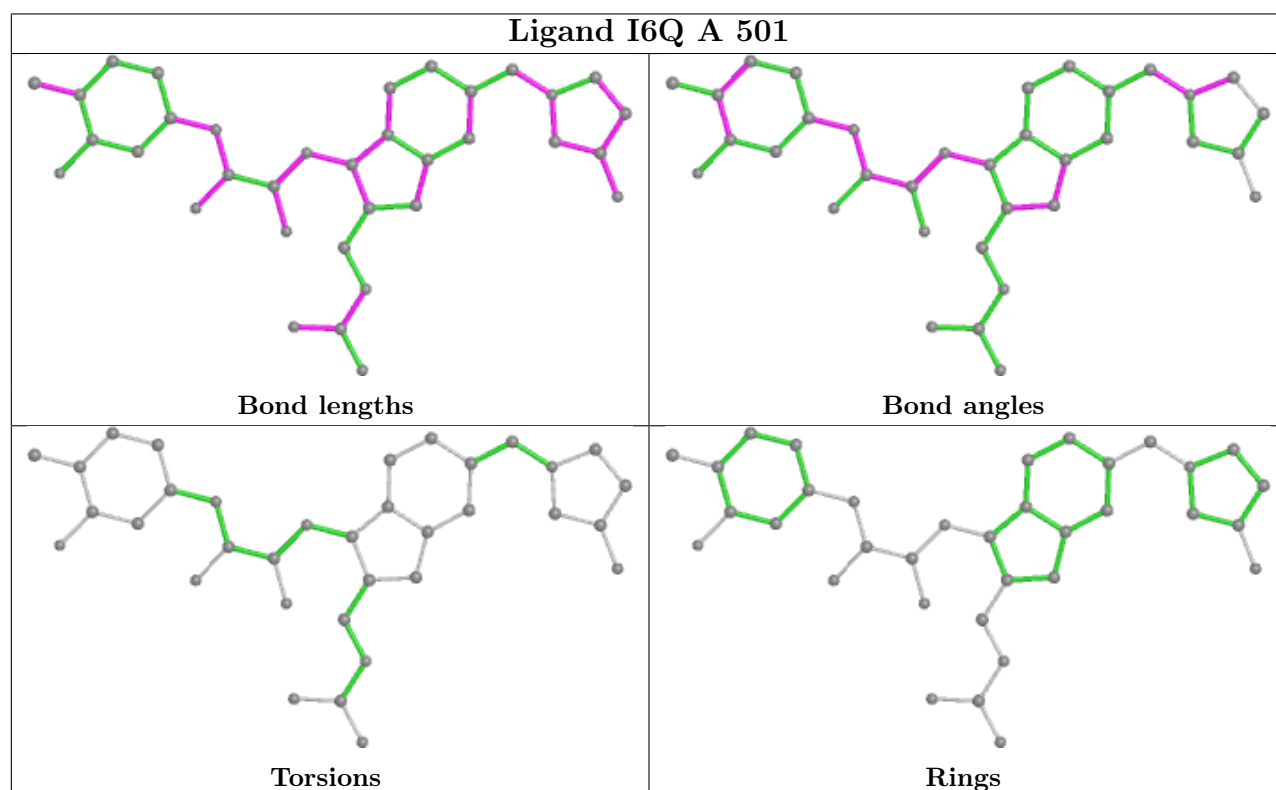
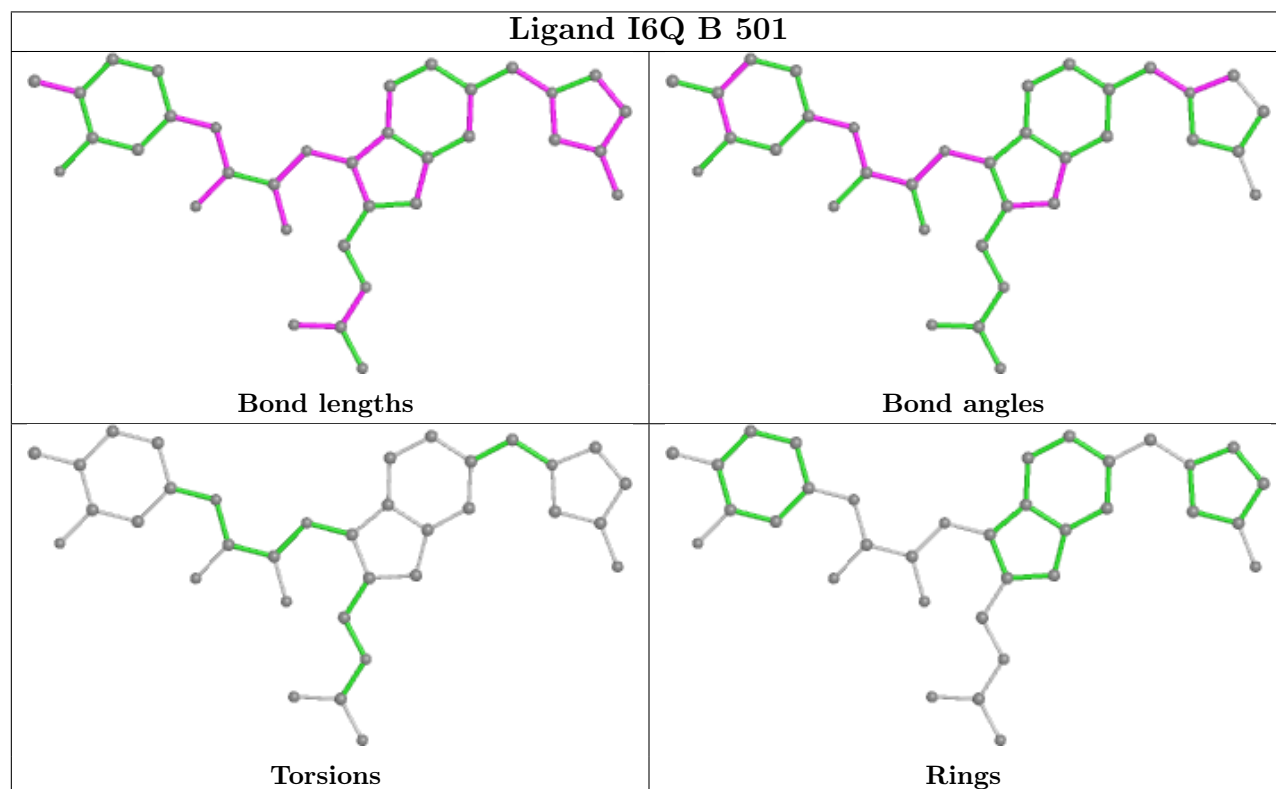
There are no ring outliers.

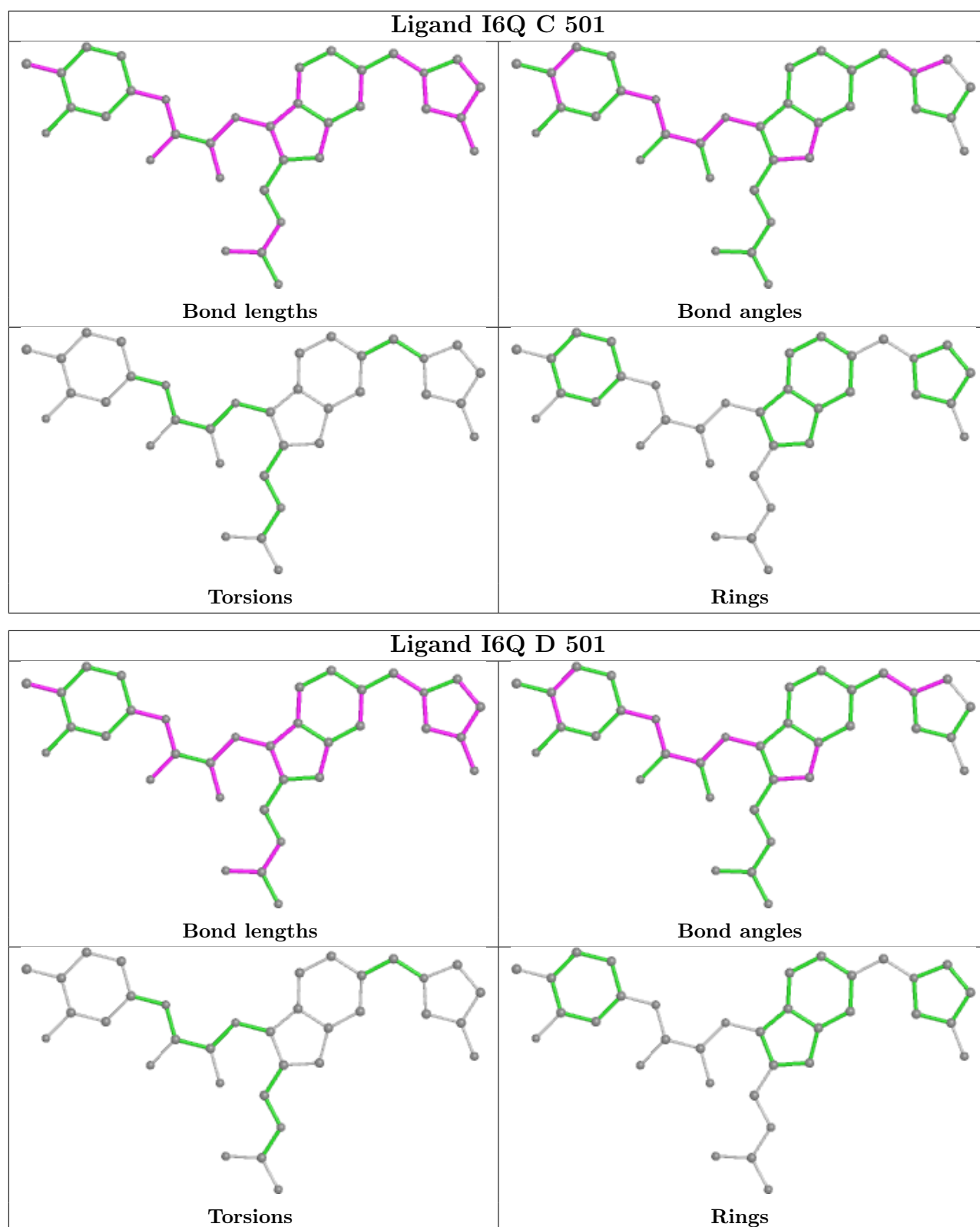
18 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	506	NAG	3	0
3	D	510	NAG	1	0
3	A	504	NAG	6	0
3	C	510	NAG	4	0
3	A	508	NAG	2	0
3	B	504	NAG	6	0
3	B	506	NAG	1	0
2	B	501	I6Q	1	0
3	C	503	NAG	1	0
2	A	501	I6Q	1	0
3	D	504	NAG	5	0
3	C	508	NAG	3	0
2	C	501	I6Q	1	0
2	D	501	I6Q	1	0
3	D	506	NAG	1	0
3	D	505	NAG	4	0
3	C	504	NAG	6	0
3	C	506	NAG	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 [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	335/358 (93%)	-0.04	6 (1%) 68 46	28, 59, 88, 118	0
1	B	335/358 (93%)	0.14	16 (4%) 30 14	34, 68, 104, 124	0
1	C	335/358 (93%)	0.01	13 (3%) 39 19	27, 56, 89, 126	0
1	D	335/358 (93%)	0.06	16 (4%) 30 14	37, 66, 99, 116	0
All	All	1340/1432 (93%)	0.04	51 (3%) 40 20	27, 62, 97, 126	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	91	GLU	8.1
1	D	87	ALA	5.4
1	C	87	ALA	4.6
1	B	87	ALA	4.4
1	D	89	VAL	4.1
1	C	86	LEU	3.9
1	A	87	ALA	3.8
1	D	243	SER	3.8
1	B	88	ASN	3.7
1	C	88	ASN	3.4
1	D	242	VAL	3.4
1	B	50	THR	3.3
1	C	244	THR	3.2
1	A	85	VAL	3.2
1	C	89	VAL	3.1
1	D	488	VAL	3.1
1	C	242	VAL	3.0
1	B	90	THR	3.0
1	C	60	ALA	2.9
1	B	226	LEU	2.9
1	A	83	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	86	LEU	2.8
1	B	89	VAL	2.8
1	B	224	ALA	2.8
1	A	86	LEU	2.7
1	D	88	ASN	2.6
1	D	91	GLU	2.6
1	A	88	ASN	2.6
1	C	243	SER	2.6
1	D	92	ASN	2.6
1	D	240	ARG	2.5
1	B	488	VAL	2.5
1	C	85	VAL	2.5
1	D	238	PRO	2.5
1	B	93	PHE	2.4
1	D	90	THR	2.4
1	C	84	MET	2.3
1	C	82	GLN	2.3
1	A	89	VAL	2.2
1	C	226	LEU	2.2
1	B	72	HIS	2.2
1	B	61	TYR	2.2
1	D	93	PHE	2.2
1	B	241	ASN	2.1
1	D	241	ASN	2.1
1	D	226	LEU	2.1
1	D	124	GLY	2.1
1	B	240	ARG	2.1
1	B	440	GLU	2.1
1	B	489	VAL	2.0
1	C	240	ARG	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.

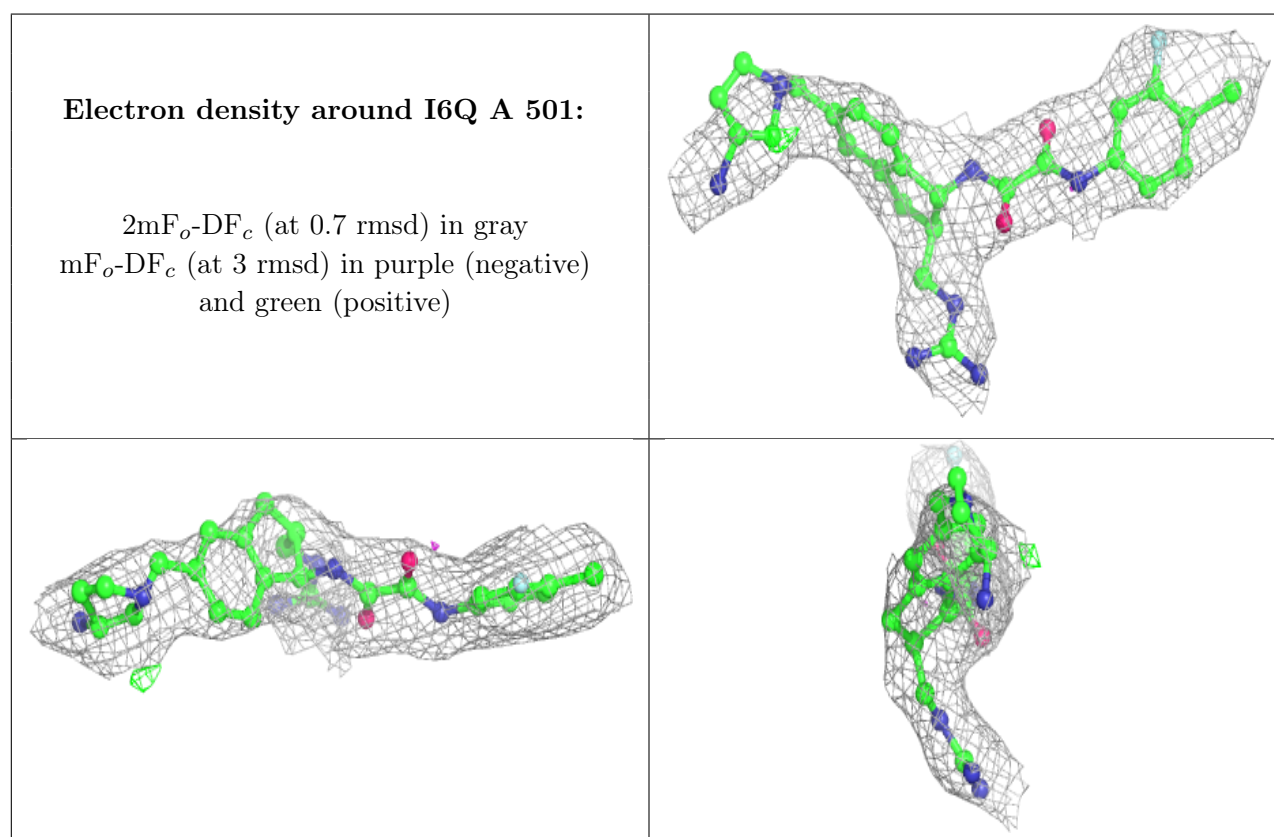
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	D	506	14/15	0.34	0.55	95,134,139,140	0
3	NAG	D	505	14/15	0.59	0.71	110,124,130,135	0
3	NAG	A	510	14/15	0.59	0.47	80,110,115,122	0
3	NAG	B	506	14/15	0.61	0.48	109,126,139,144	0
3	NAG	B	510	14/15	0.61	0.48	75,113,128,137	0
3	NAG	C	510	14/15	0.62	0.54	66,112,124,124	0
3	NAG	A	505	14/15	0.65	0.42	87,102,114,123	0
3	NAG	B	505	14/15	0.66	0.68	104,123,131,139	0
3	NAG	D	510	14/15	0.70	0.42	73,109,123,126	0
3	NAG	A	509	14/15	0.74	0.34	88,101,108,111	0
3	NAG	D	509	14/15	0.75	0.27	65,76,87,100	0
3	NAG	D	504	14/15	0.79	0.27	67,82,94,100	0
3	NAG	C	505	14/15	0.81	0.39	85,109,121,122	0
3	NAG	C	509	14/15	0.82	0.31	64,85,97,101	0
3	NAG	D	507	14/15	0.83	0.22	70,75,83,89	0
3	NAG	B	504	14/15	0.84	0.24	71,86,93,97	0
3	NAG	A	506	14/15	0.85	0.23	78,100,113,118	0
3	NAG	C	506	14/15	0.85	0.24	83,99,113,118	0
3	NAG	B	507	14/15	0.86	0.21	55,64,73,82	0
3	NAG	A	502	14/15	0.88	0.29	63,75,81,83	0
3	NAG	B	509	14/15	0.88	0.23	63,78,86,86	0
3	NAG	D	508	14/15	0.88	0.26	69,78,90,90	0
3	NAG	C	502	14/15	0.89	0.23	64,74,82,82	0
3	NAG	D	502	14/15	0.90	0.29	66,75,81,84	0
3	NAG	A	508	14/15	0.90	0.22	39,53,70,73	0
2	I6Q	A	501	35/35	0.90	0.25	36,54,79,88	0
3	NAG	A	507	14/15	0.91	0.20	49,55,64,67	0
2	I6Q	B	501	35/35	0.91	0.21	35,49,88,95	0
3	NAG	A	503	14/15	0.91	0.29	41,49,59,62	0
3	NAG	B	502	14/15	0.92	0.25	73,81,91,96	0
3	NAG	B	503	14/15	0.92	0.25	53,71,82,86	0
2	I6Q	C	501	35/35	0.92	0.21	26,39,69,96	0
3	NAG	D	503	14/15	0.92	0.28	53,59,68,84	0
3	NAG	C	507	14/15	0.92	0.17	58,61,81,82	0
3	NAG	C	508	14/15	0.92	0.18	42,53,61,67	0
3	NAG	C	503	14/15	0.92	0.30	38,53,76,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	C	504	14/15	0.92	0.15	62,76,88,108	0
4	IMD	A	511	5/5	0.92	0.22	49,64,81,89	0
3	NAG	A	504	14/15	0.93	0.18	49,65,76,83	0
2	I6Q	D	501	35/35	0.93	0.20	28,50,99,100	0
3	NAG	B	508	14/15	0.93	0.29	67,76,90,92	0

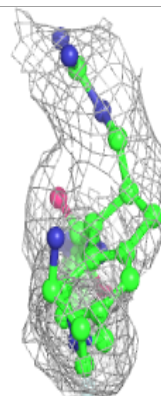
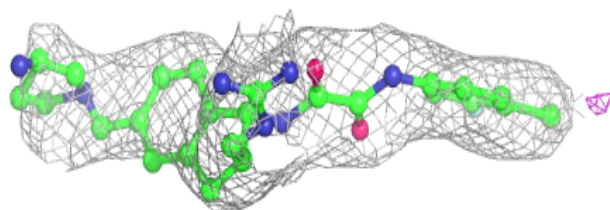
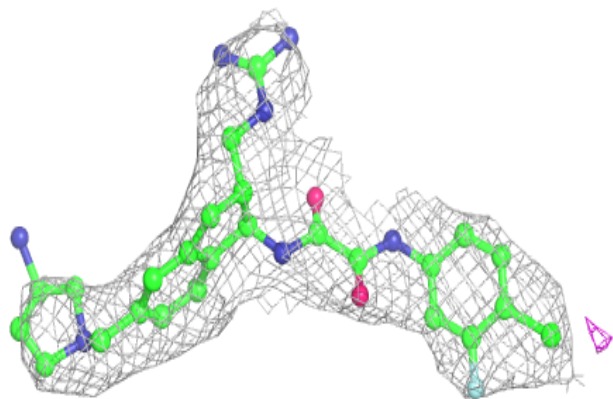
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



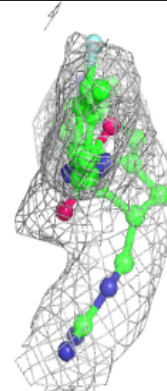
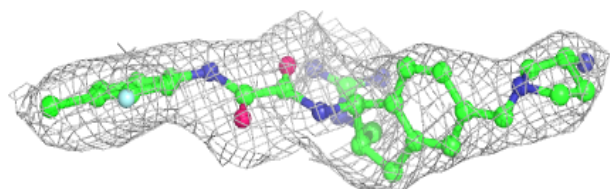
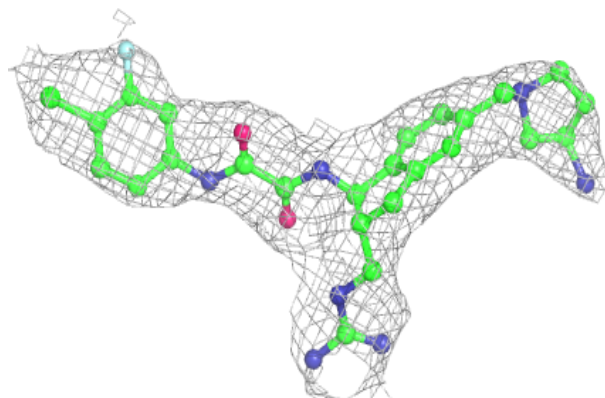


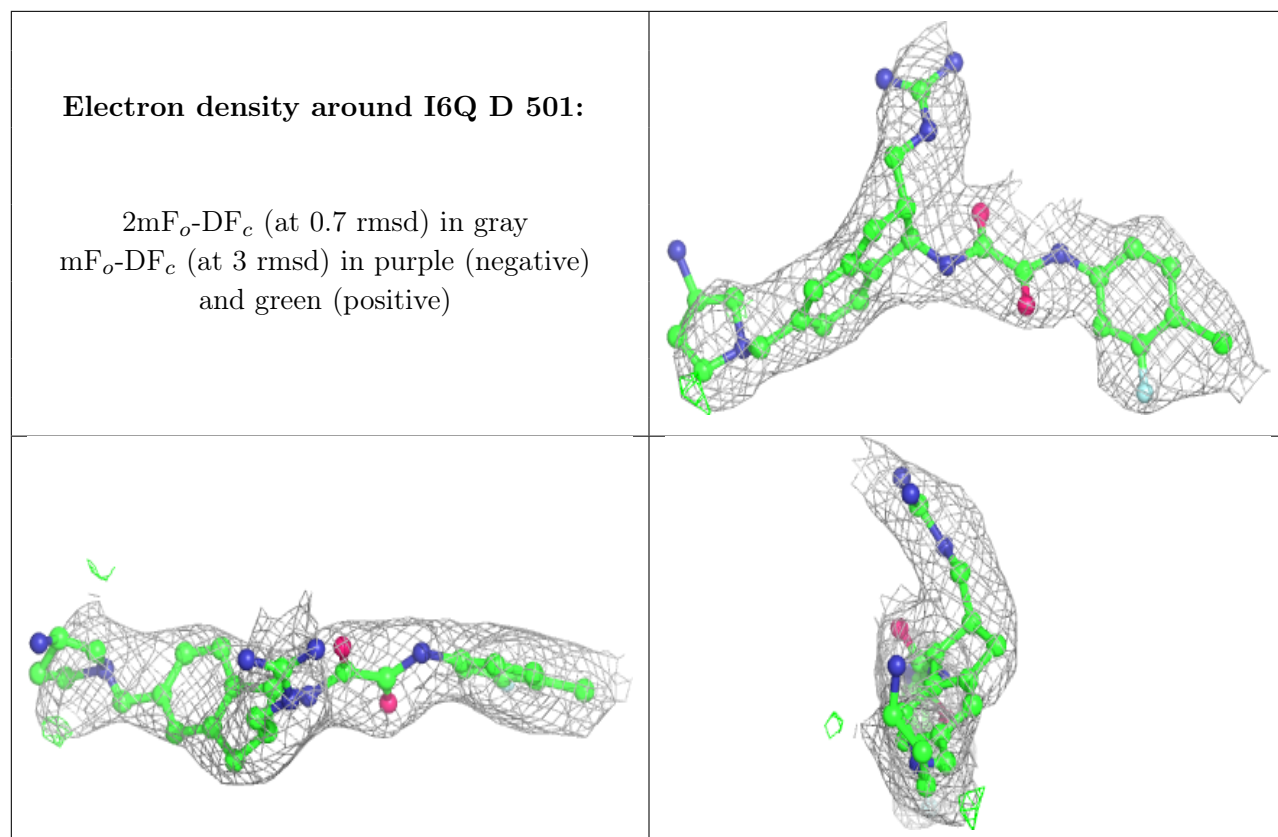
**Electron density around I6Q B 501:**

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

**Electron density around I6Q C 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.