



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2023 – 04:11 PM JST

PDB ID : 8ILA  
Title : Crystal structure of LmbT from *Streptomyces lincolnensis* NRRL ISP-5355 in complex with substrates  
Authors : Dai, Y.; Qiao, H.; Xia, M.; Fang, P.; Liu, W.  
Deposited on : 2023-03-03  
Resolution : 2.79 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)  
Xtrriage (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

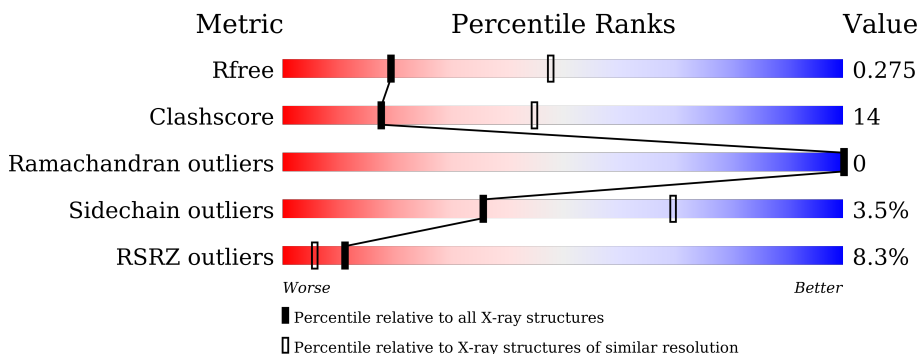
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 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 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	457	
1	B	457	
1	C	457	
1	D	457	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	Q3L	B	502	-	-	-	X

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 13278 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 Glycosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	429	Total 3252	C 2036	N 611	O 598	S 7	0	0	0
1	C	429	Total 3258	C 2039	N 614	O 598	S 7	0	0	0
1	B	429	Total 3225	C 2023	N 599	O 596	S 7	0	0	0
1	D	429	Total 3258	C 2039	N 614	O 598	S 7	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A9Y8T1
A	-19	GLY	-	expression tag	UNP A9Y8T1
A	-18	SER	-	expression tag	UNP A9Y8T1
A	-17	SER	-	expression tag	UNP A9Y8T1
A	-16	HIS	-	expression tag	UNP A9Y8T1
A	-15	HIS	-	expression tag	UNP A9Y8T1
A	-14	HIS	-	expression tag	UNP A9Y8T1
A	-13	HIS	-	expression tag	UNP A9Y8T1
A	-12	HIS	-	expression tag	UNP A9Y8T1
A	-11	HIS	-	expression tag	UNP A9Y8T1
A	-10	SER	-	expression tag	UNP A9Y8T1
A	-9	SER	-	expression tag	UNP A9Y8T1
A	-8	GLY	-	expression tag	UNP A9Y8T1
A	-7	LEU	-	expression tag	UNP A9Y8T1
A	-6	VAL	-	expression tag	UNP A9Y8T1
A	-5	PRO	-	expression tag	UNP A9Y8T1
A	-4	ARG	-	expression tag	UNP A9Y8T1
A	-3	GLY	-	expression tag	UNP A9Y8T1
A	-2	SER	-	expression tag	UNP A9Y8T1
A	-1	HIS	-	expression tag	UNP A9Y8T1
A	0	MET	-	expression tag	UNP A9Y8T1

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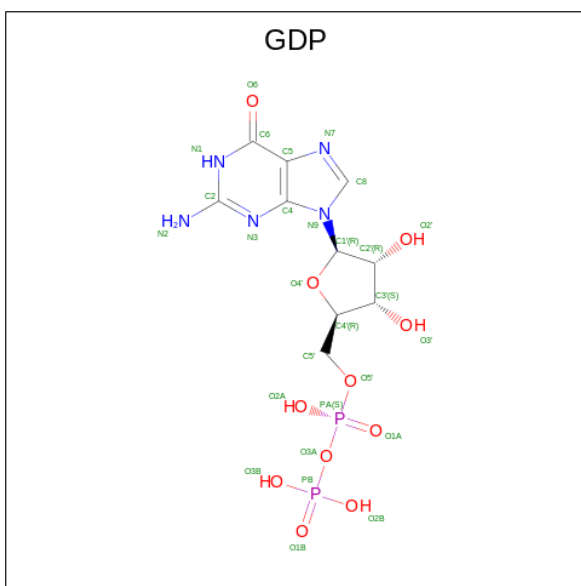
Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	MET	-	initiating methionine	UNP A9Y8T1
C	-19	GLY	-	expression tag	UNP A9Y8T1
C	-18	SER	-	expression tag	UNP A9Y8T1
C	-17	SER	-	expression tag	UNP A9Y8T1
C	-16	HIS	-	expression tag	UNP A9Y8T1
C	-15	HIS	-	expression tag	UNP A9Y8T1
C	-14	HIS	-	expression tag	UNP A9Y8T1
C	-13	HIS	-	expression tag	UNP A9Y8T1
C	-12	HIS	-	expression tag	UNP A9Y8T1
C	-11	HIS	-	expression tag	UNP A9Y8T1
C	-10	SER	-	expression tag	UNP A9Y8T1
C	-9	SER	-	expression tag	UNP A9Y8T1
C	-8	GLY	-	expression tag	UNP A9Y8T1
C	-7	LEU	-	expression tag	UNP A9Y8T1
C	-6	VAL	-	expression tag	UNP A9Y8T1
C	-5	PRO	-	expression tag	UNP A9Y8T1
C	-4	ARG	-	expression tag	UNP A9Y8T1
C	-3	GLY	-	expression tag	UNP A9Y8T1
C	-2	SER	-	expression tag	UNP A9Y8T1
C	-1	HIS	-	expression tag	UNP A9Y8T1
C	0	MET	-	expression tag	UNP A9Y8T1
B	-20	MET	-	initiating methionine	UNP A9Y8T1
B	-19	GLY	-	expression tag	UNP A9Y8T1
B	-18	SER	-	expression tag	UNP A9Y8T1
B	-17	SER	-	expression tag	UNP A9Y8T1
B	-16	HIS	-	expression tag	UNP A9Y8T1
B	-15	HIS	-	expression tag	UNP A9Y8T1
B	-14	HIS	-	expression tag	UNP A9Y8T1
B	-13	HIS	-	expression tag	UNP A9Y8T1
B	-12	HIS	-	expression tag	UNP A9Y8T1
B	-11	HIS	-	expression tag	UNP A9Y8T1
B	-10	SER	-	expression tag	UNP A9Y8T1
B	-9	SER	-	expression tag	UNP A9Y8T1
B	-8	GLY	-	expression tag	UNP A9Y8T1
B	-7	LEU	-	expression tag	UNP A9Y8T1
B	-6	VAL	-	expression tag	UNP A9Y8T1
B	-5	PRO	-	expression tag	UNP A9Y8T1
B	-4	ARG	-	expression tag	UNP A9Y8T1
B	-3	GLY	-	expression tag	UNP A9Y8T1
B	-2	SER	-	expression tag	UNP A9Y8T1
B	-1	HIS	-	expression tag	UNP A9Y8T1
B	0	MET	-	expression tag	UNP A9Y8T1

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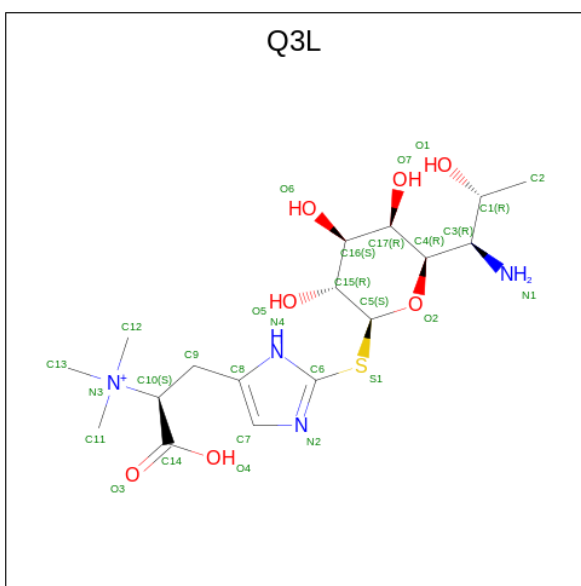
Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	initiating methionine	UNP A9Y8T1
D	-19	GLY	-	expression tag	UNP A9Y8T1
D	-18	SER	-	expression tag	UNP A9Y8T1
D	-17	SER	-	expression tag	UNP A9Y8T1
D	-16	HIS	-	expression tag	UNP A9Y8T1
D	-15	HIS	-	expression tag	UNP A9Y8T1
D	-14	HIS	-	expression tag	UNP A9Y8T1
D	-13	HIS	-	expression tag	UNP A9Y8T1
D	-12	HIS	-	expression tag	UNP A9Y8T1
D	-11	HIS	-	expression tag	UNP A9Y8T1
D	-10	SER	-	expression tag	UNP A9Y8T1
D	-9	SER	-	expression tag	UNP A9Y8T1
D	-8	GLY	-	expression tag	UNP A9Y8T1
D	-7	LEU	-	expression tag	UNP A9Y8T1
D	-6	VAL	-	expression tag	UNP A9Y8T1
D	-5	PRO	-	expression tag	UNP A9Y8T1
D	-4	ARG	-	expression tag	UNP A9Y8T1
D	-3	GLY	-	expression tag	UNP A9Y8T1
D	-2	SER	-	expression tag	UNP A9Y8T1
D	-1	HIS	-	expression tag	UNP A9Y8T1
D	0	MET	-	expression tag	UNP A9Y8T1

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	28	10	5	11	2	0	0
2	C	1	28	10	5	11	2	0	0
2	B	1	28	10	5	11	2	3	0
2	D	1	28	10	5	11	2	1	0

- Molecule 3 is (2 {S})-3-[2-[(2 {S},3 {R}),4 {S},5 {R},6 {R})-6-[(1 {R}),2 {R})-1-azanyl-2-oxidanyl-propyl]-3,4,5-tris(oxidanyl)oxan-2-yl]sulfanyl-1 {H}-imidazol-5-yl]-2-(trimethyl- $l^{\{4\}}$ -azanyl)propanoic acid (three-letter code: Q3L) (formula:  $C_{17}H_{31}N_4O_7S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	29	17	4	7	1	1	0
3	C	1	29	17	4	7	1	0	0
3	B	1	29	17	4	7	1	1	0
3	D	1	29	17	4	7	1	0	0

- Molecule 4 is water.

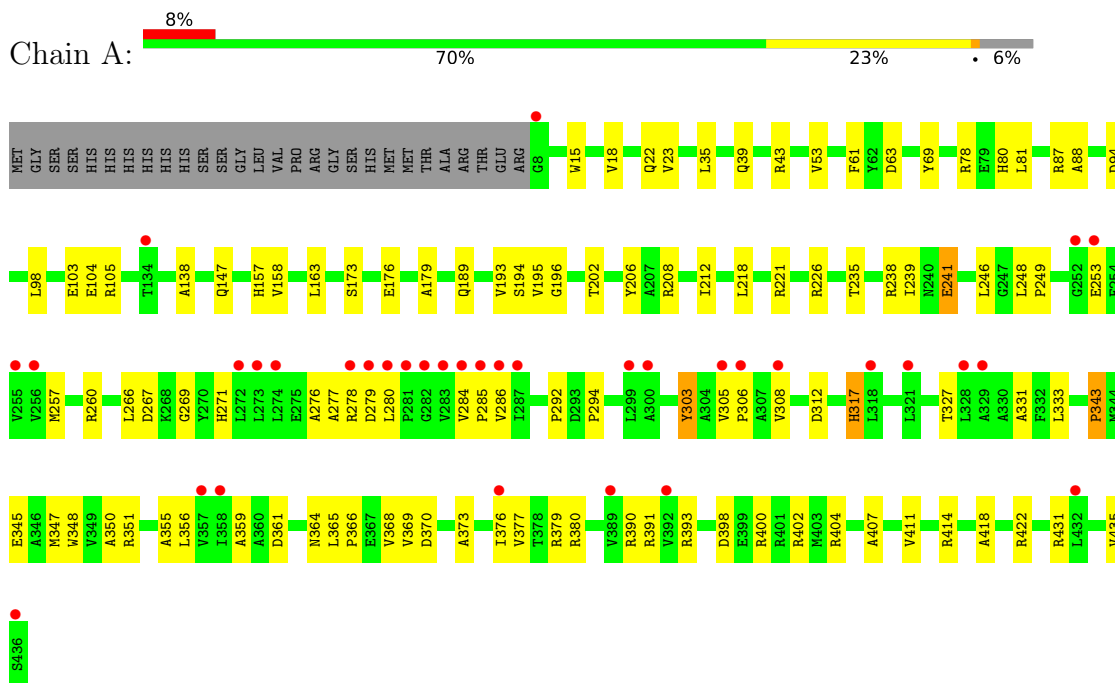
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	19	Total O 19 19	0	0
4	C	18	Total O 18 18	0	0
4	B	7	Total O 7 7	0	0
4	D	13	Total O 13 13	0	0



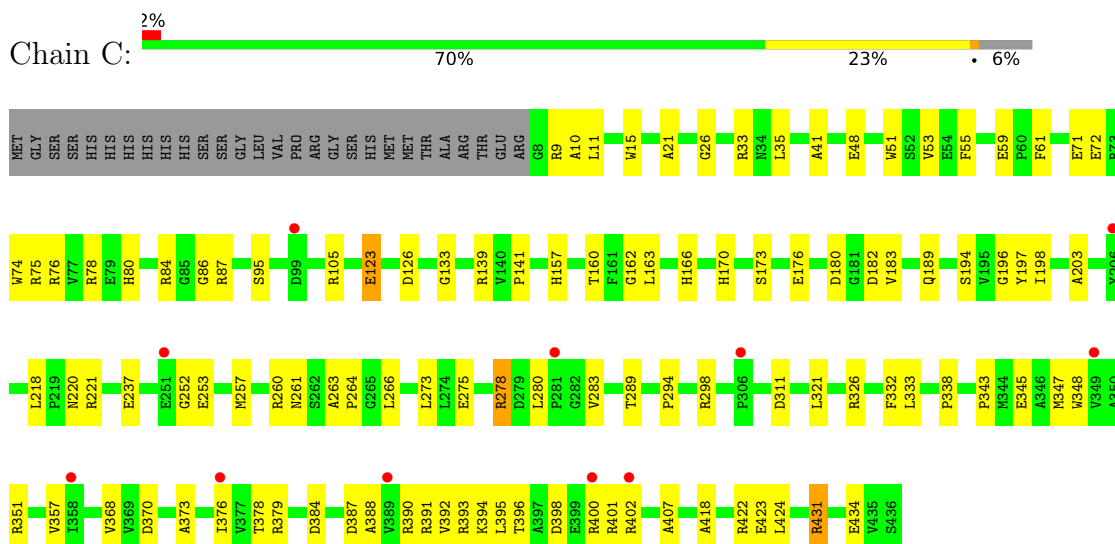
### 3 Residue-property plots

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.

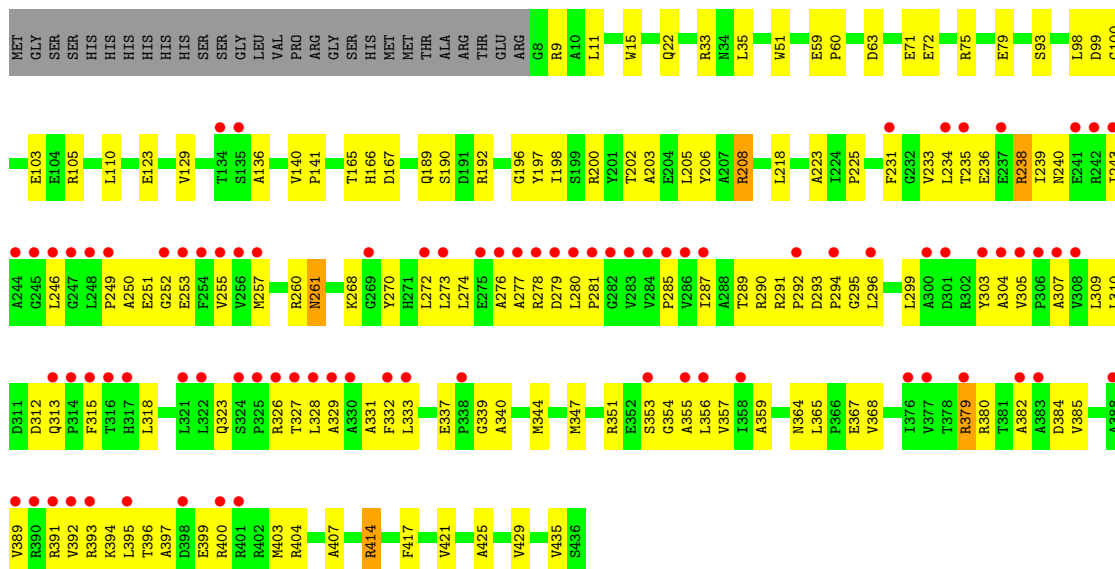
- Molecule 1: Glycosyltransferase



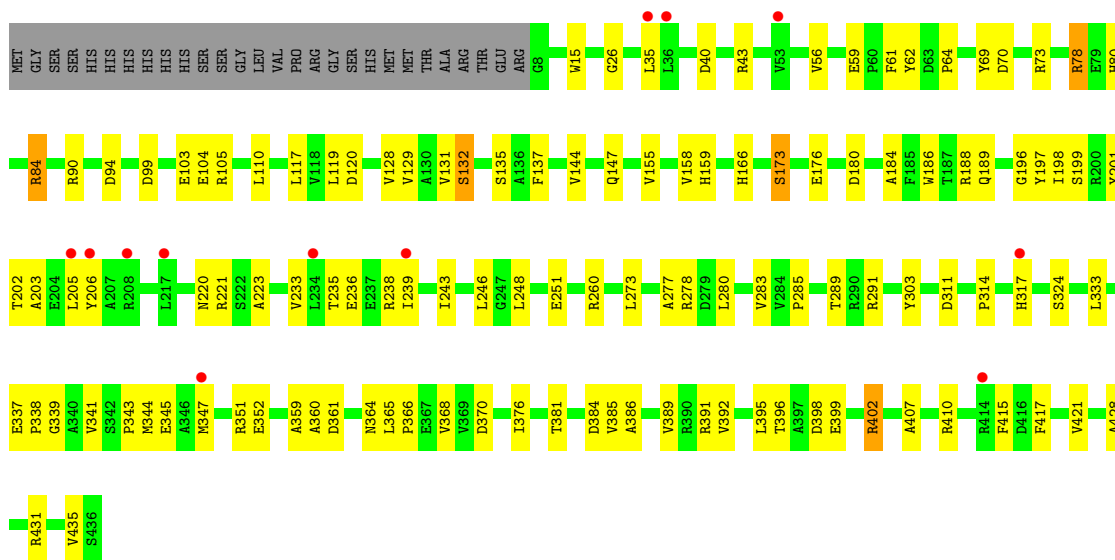
- Molecule 1: Glycosyltransferase



• Molecule 1: Glycosyltransferase



• Molecule 1: Glycosyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.38Å 137.74Å 146.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.87 – 2.79 68.87 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.3 (68.87-2.79) 99.3 (68.87-2.79)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 2.77Å)	Xtrriage
Refinement program	PHENIX 1.13	Depositor
R, $R_{free}$	0.238 , 0.279 0.231 , 0.275	Depositor DCC
$R_{free}$ test set	3095 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.5	Xtrriage
Anisotropy	0.424	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13278	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: GDP, Q3L

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	0.54	0/3320	0.73	1/4519 (0.0%)
1	B	0.52	2/3293 (0.1%)	0.72	0/4487
1	C	0.52	0/3326	0.73	0/4526
1	D	0.47	0/3326	0.68	0/4526
All	All	0.51	2/13265 (0.0%)	0.71	1/18058 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	261	ASN	C-N	-5.42	1.21	1.34
1	B	379	ARG	C-N	5.41	1.46	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	ASP	C-N-CA	-5.20	108.70	121.70

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	3252	0	3207	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3225	0	3160	124	0
1	C	3258	0	3218	78	0
1	D	3258	0	3218	94	0
2	A	28	0	12	2	0
2	B	28	0	12	0	0
2	C	28	0	12	2	0
2	D	28	0	12	2	0
3	A	29	0	0	1	0
3	B	29	0	0	0	0
3	C	29	0	0	1	0
3	D	29	0	0	0	0
4	A	19	0	0	1	0
4	B	7	0	0	0	0
4	C	18	0	0	0	0
4	D	13	0	0	0	0
All	All	13278	0	12851	358	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 14.

All (358) 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:310:LEU:CG	1:B:313:GLN:HG3	1.56	1.33
1:B:310:LEU:HG	1:B:313:GLN:CG	1.68	1.23
1:B:234:LEU:HD22	1:B:238:ARG:HH21	1.16	1.08
1:D:198:ILE:H	1:D:202:THR:HG21	1.23	1.02
1:B:251:GLU:OE1	1:B:251:GLU:N	1.93	1.00
1:B:310:LEU:CD2	1:B:313:GLN:HG3	1.99	0.92
1:B:253:GLU:N	1:B:253:GLU:OE1	2.06	0.88
1:B:382:ALA:HA	1:B:385:VAL:HG12	1.57	0.86
1:B:382:ALA:O	1:B:385:VAL:HG12	1.76	0.86
1:D:198:ILE:HD12	1:D:339:GLY:HA3	1.58	0.86
1:A:103:GLU:OE1	1:B:103:GLU:HG3	1.75	0.85
1:B:310:LEU:HG	1:B:313:GLN:HG3	0.85	0.85
1:D:273:LEU:HD12	1:D:273:LEU:O	1.76	0.84
1:C:275:GLU:O	1:C:278:ARG:HG3	1.78	0.83
1:A:257:MET:CE	1:A:333:LEU:HD12	2.14	0.78
1:B:234:LEU:HD22	1:B:238:ARG:NH2	1.98	0.77
1:A:173:SER:HB3	1:A:176:GLU:HG3	1.65	0.77
1:B:233:VAL:HG23	1:B:323:GLN:OE1	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:PRO:O	1:A:347:MET:HG3	1.85	0.76
1:C:347:MET:HG2	1:C:407:ALA:HB1	1.67	0.76
1:B:293:ASP:H	1:B:309:LEU:HD11	1.49	0.76
1:C:376:ILE:HG13	1:C:392:VAL:HG22	1.66	0.76
1:B:354:GLY:N	1:B:404:ARG:HH12	1.84	0.75
1:B:110:LEU:HD23	1:B:136:ALA:HB1	1.70	0.74
1:A:278:ARG:HB2	1:A:303:TYR:HD2	1.52	0.74
1:B:260:ARG:HG3	1:B:261:ASN:H	1.53	0.74
1:B:240:ASN:HA	1:B:243:ILE:HB	1.70	0.73
1:B:261:ASN:OD1	1:B:261:ASN:O	2.06	0.73
1:B:425:ALA:O	1:B:429:VAL:HG23	1.89	0.73
1:D:199:SER:O	1:D:202:THR:HG22	1.88	0.73
1:B:396:THR:HB	1:B:399:GLU:HB2	1.70	0.73
1:B:246:LEU:HD21	1:B:310:LEU:HD11	1.69	0.73
1:D:236:GLU:HA	1:D:239:ILE:HD13	1.70	0.73
1:B:382:ALA:CA	1:B:385:VAL:HG12	2.20	0.72
1:B:293:ASP:HB3	1:B:296:LEU:HD23	1.71	0.72
1:D:197:TYR:HB2	1:D:202:THR:HG23	1.70	0.71
1:D:343:PRO:HB2	1:D:368:VAL:HG11	1.71	0.71
1:C:400:ARG:HH21	1:C:401:ARG:HE	1.39	0.70
1:D:398:ASP:CB	1:D:402:ARG:HH22	2.04	0.69
1:D:398:ASP:CB	1:D:402:ARG:NH2	2.54	0.69
1:B:260:ARG:HB3	1:B:268:LYS:HE3	1.75	0.69
1:A:418:ALA:O	1:A:422:ARG:HD2	1.92	0.69
1:A:15:TRP:CD2	1:A:35:LEU:HD21	2.27	0.69
1:A:94:ASP:OD2	1:C:139:ARG:NH2	2.25	0.69
1:C:105:ARG:HH12	1:D:103:GLU:CD	1.95	0.69
1:D:376:ILE:HG13	1:D:392:VAL:HG22	1.75	0.69
1:B:382:ALA:O	1:B:385:VAL:CG1	2.42	0.68
1:C:392:VAL:O	1:C:395:LEU:HD13	1.92	0.68
1:A:202:THR:HG23	1:A:206:TYR:CE2	2.28	0.68
1:B:234:LEU:CD2	1:B:238:ARG:HH21	2.03	0.67
1:B:382:ALA:C	1:B:385:VAL:HG12	2.15	0.67
1:D:280:LEU:HB3	1:D:283:VAL:HG21	1.75	0.67
1:C:21:ALA:HB3	1:C:59:GLU:OE1	1.94	0.66
1:D:128:VAL:HB	1:D:155:VAL:HG22	1.77	0.66
1:B:367:GLU:OE2	1:B:414:ARG:NH1	2.29	0.66
1:D:15:TRP:CH2	1:D:35:LEU:HD11	2.31	0.66
1:D:94:ASP:HB3	1:D:105:ARG:HG2	1.77	0.66
1:D:173:SER:HB3	1:D:176:GLU:HG3	1.78	0.66
1:A:257:MET:HE1	1:A:333:LEU:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:MET:HE3	1:A:333:LEU:HD12	1.78	0.65
1:C:391:ARG:O	1:C:395:LEU:CD1	2.45	0.65
1:D:35:LEU:HD22	1:D:417:PHE:HZ	1.61	0.65
1:C:105:ARG:NH1	1:D:103:GLU:OE1	2.30	0.64
1:B:276:ALA:CB	1:B:385:VAL:HG13	2.27	0.64
1:B:250:ALA:HB1	1:B:326:ARG:HH22	1.62	0.64
1:B:261:ASN:OD1	1:B:261:ASN:C	2.35	0.64
1:C:278:ARG:HB3	1:C:278:ARG:CZ	2.28	0.64
1:B:231:PHE:O	1:B:351:ARG:NH2	2.32	0.63
1:B:280:LEU:HD12	1:B:281:PRO:HD2	1.78	0.63
1:C:257:MET:HE2	1:C:273:LEU:CD2	2.29	0.63
1:B:323:GLN:HG2	1:B:353:SER:O	1.98	0.63
1:D:396:THR:OG1	1:D:399:GLU:HG3	1.99	0.63
1:D:132:SER:HB2	1:D:159:HIS:ND1	2.14	0.63
1:C:257:MET:HE2	1:C:273:LEU:HD22	1.81	0.62
1:B:223:ALA:HA	1:B:344:MET:HE1	1.79	0.62
1:A:94:ASP:HB3	1:A:105:ARG:HG2	1.81	0.62
1:A:257:MET:HE3	1:A:333:LEU:CD1	2.30	0.62
1:A:278:ARG:HB2	1:A:303:TYR:CD2	2.34	0.62
1:B:382:ALA:HA	1:B:385:VAL:CG1	2.27	0.62
1:B:396:THR:O	1:B:400:ARG:HG3	2.00	0.61
1:B:379:ARG:NH2	1:B:384:ASP:OD1	2.34	0.61
1:A:269:GLY:HA3	1:A:333:LEU:HB2	1.81	0.61
1:A:356:LEU:HD11	1:A:400:ARG:HG2	1.82	0.61
1:D:431:ARG:HH11	1:D:431:ARG:HG3	1.65	0.61
1:A:286:VAL:HG13	1:A:308:VAL:HB	1.82	0.61
1:A:138:ALA:HB3	1:A:179:ALA:HB1	1.82	0.61
1:C:15:TRP:CD2	1:C:35:LEU:HD21	2.35	0.61
1:C:392:VAL:C	1:C:395:LEU:HD13	2.21	0.61
1:B:289:THR:HG21	1:B:291:ARG:O	2.01	0.61
1:A:347:MET:HE3	1:A:407:ALA:HB1	1.82	0.60
1:A:195:VAL:HG21	1:A:212:ILE:HD13	1.83	0.60
1:D:239:ILE:HD12	1:D:239:ILE:H	1.66	0.60
1:B:234:LEU:HD13	1:B:238:ARG:HE	1.67	0.60
1:D:385:VAL:O	1:D:389:VAL:HG23	2.01	0.60
1:A:253:GLU:CD	1:A:393:ARG:HH21	2.04	0.59
1:D:243:ILE:HG23	1:D:248:LEU:HD12	1.83	0.59
1:A:359:ALA:HB1	1:A:365:LEU:HB3	1.85	0.59
1:C:74:TRP:CZ2	1:C:78:ARG:HD2	2.37	0.59
1:A:246:LEU:HB2	1:A:248:LEU:HD11	1.84	0.59
1:B:257:MET:SD	1:B:273:LEU:HD22	2.43	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:LEU:HB2	1:B:400:ARG:HG2	1.85	0.59
1:B:273:LEU:O	1:B:274:LEU:C	2.41	0.58
1:D:198:ILE:N	1:D:202:THR:HG21	2.06	0.58
1:C:370:ASP:OD1	1:C:370:ASP:O	2.21	0.58
1:D:198:ILE:HA	1:D:221:ARG:HA	1.85	0.58
1:A:257:MET:HG2	1:A:331:ALA:O	2.02	0.58
1:A:347:MET:HB3	1:A:407:ALA:HB1	1.85	0.58
1:B:328:LEU:HD12	1:B:393:ARG:HA	1.86	0.58
1:D:280:LEU:HB3	1:D:283:VAL:CG2	2.33	0.58
1:C:418:ALA:O	1:C:422:ARG:HD2	2.04	0.58
1:B:72:GLU:OE1	1:B:72:GLU:HA	2.04	0.57
1:B:277:ALA:CB	1:B:285:PRO:HG3	2.34	0.57
1:A:364:ASN:O	1:A:368:VAL:HG23	2.05	0.57
1:D:347:MET:HB3	1:D:407:ALA:HB1	1.87	0.57
1:B:356:LEU:HD13	1:B:403:MET:SD	2.44	0.56
1:A:39:GLN:OE1	1:A:80:HIS:NE2	2.37	0.56
1:B:9:ARG:HB2	1:B:51:TRP:CZ3	2.40	0.56
1:D:260:ARG:NH1	2:D:501:GDP:O1B	2.39	0.56
1:A:15:TRP:CE2	1:A:35:LEU:HD21	2.40	0.56
1:A:226:ARG:HD3	1:A:411:VAL:HG12	1.87	0.56
1:C:173:SER:OG	1:C:176:GLU:HG3	2.05	0.56
1:B:289:THR:HG23	1:B:290:ARG:N	2.21	0.56
1:D:345:GLU:OE2	2:D:501:GDP:O3'	2.21	0.56
1:B:257:MET:HE3	1:B:333:LEU:HG	1.89	0.55
1:D:391:ARG:O	1:D:395:LEU:HG	2.06	0.55
1:C:105:ARG:HD3	1:D:104:GLU:OE2	2.06	0.55
1:D:15:TRP:CZ2	1:D:35:LEU:HD11	2.42	0.55
1:A:431:ARG:O	1:A:435:VAL:HG22	2.06	0.55
1:D:64:PRO:HA	1:D:69:TYR:CD2	2.41	0.55
1:A:189:GLN:HB2	1:D:166:HIS:ND1	2.22	0.54
1:C:189:GLN:HB2	1:B:166:HIS:HD1	1.71	0.54
1:B:347:MET:HG2	1:B:407:ALA:HB1	1.90	0.54
1:A:15:TRP:CZ2	1:A:35:LEU:HD11	2.42	0.54
1:D:198:ILE:HG22	1:D:220:ASN:O	2.08	0.54
1:A:361:ASP:HA	1:A:366:PRO:HG3	1.88	0.54
1:B:295:GLY:O	1:B:299:LEU:HD13	2.08	0.54
1:C:343:PRO:HB2	1:C:368:VAL:HG11	1.89	0.54
1:C:9:ARG:HB3	1:C:51:TRP:CZ3	2.43	0.53
1:C:289:THR:O	1:C:311:ASP:HA	2.07	0.53
1:B:257:MET:CE	1:B:333:LEU:HG	2.38	0.53
1:D:110:LEU:HG	1:D:137:PHE:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:MET:CE	1:A:407:ALA:HB1	2.38	0.53
1:C:263:ALA:HB1	1:C:264:PRO:HD2	1.90	0.53
1:A:18:VAL:HG22	4:A:609:HOH:O	2.08	0.53
1:A:277:ALA:HB3	1:A:305:VAL:HG11	1.89	0.53
1:B:272:LEU:HD13	1:B:380:ARG:O	2.09	0.52
1:A:257:MET:CE	1:A:333:LEU:CD1	2.84	0.52
1:D:289:THR:HG23	1:D:291:ARG:O	2.08	0.52
1:B:225:PRO:HD2	1:B:231:PHE:HE2	1.74	0.52
1:D:273:LEU:HD12	1:D:273:LEU:C	2.23	0.52
1:A:348:TRP:O	1:A:351:ARG:HG3	2.10	0.52
1:D:417:PHE:CZ	1:D:421:VAL:HG11	2.45	0.52
1:C:166:HIS:HD1	1:B:189:GLN:HB2	1.74	0.52
1:A:63:ASP:HB3	1:A:98:LEU:HD23	1.92	0.52
1:C:11:LEU:HB2	1:C:51:TRP:CE3	2.44	0.52
1:A:235:THR:O	1:A:239:ILE:HG13	2.10	0.52
1:B:310:LEU:CD2	1:B:313:GLN:CG	2.82	0.52
1:C:198:ILE:HD11	1:C:338:PRO:HB2	1.91	0.52
1:C:388:ALA:O	1:C:392:VAL:HG23	2.10	0.52
1:C:26:GLY:HA3	1:C:260:ARG:HD3	1.91	0.51
1:B:15:TRP:CH2	1:B:35:LEU:HD11	2.45	0.51
1:B:260:ARG:NH1	1:B:289:THR:OG1	2.43	0.51
1:B:289:THR:CG2	1:B:291:ARG:O	2.58	0.51
1:A:78:ARG:NH1	1:C:123:GLU:OE2	2.37	0.51
1:D:364:ASN:O	1:D:368:VAL:HG23	2.11	0.51
1:C:166:HIS:ND1	1:B:189:GLN:HB2	2.26	0.51
1:D:396:THR:HG23	1:D:399:GLU:OE1	2.11	0.50
1:D:15:TRP:CZ2	1:D:35:LEU:CD1	2.95	0.50
1:D:314:PRO:HG2	1:D:317:HIS:ND1	2.26	0.50
1:B:332:PHE:C	1:B:333:LEU:HD23	2.32	0.50
1:D:351:ARG:HG2	1:D:351:ARG:HH11	1.76	0.50
1:C:141:PRO:HA	1:C:157:HIS:CE1	2.47	0.50
1:C:261:ASN:ND2	1:C:289:THR:OG1	2.45	0.50
1:B:202:THR:HG23	1:B:206:TYR:CE2	2.47	0.50
1:D:70:ASP:OD1	1:D:73:ARG:N	2.45	0.50
1:C:87:ARG:HG3	1:C:87:ARG:HH11	1.76	0.50
1:C:252:GLY:O	1:C:326:ARG:NH1	2.45	0.50
1:B:292:PRO:O	1:B:294:PRO:HD3	2.12	0.50
1:B:260:ARG:NH1	1:B:261:ASN:N	2.60	0.50
1:B:304:ALA:O	1:B:305:VAL:CG1	2.60	0.50
1:A:147:GLN:OE1	1:C:95:SER:O	2.31	0.49
1:B:277:ALA:C	1:B:279:ASP:N	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:GLU:HG3	1:C:76:ARG:NH1	2.26	0.49
1:D:119:LEU:HD21	1:D:144:VAL:HG13	1.94	0.49
1:D:398:ASP:CA	1:D:402:ARG:NH2	2.76	0.49
1:A:350:ALA:O	1:A:404:ARG:HD2	2.13	0.49
1:B:235:THR:O	1:B:239:ILE:HG13	2.12	0.49
1:D:40:ASP:OD1	1:D:84:ARG:NH1	2.46	0.49
1:B:59:GLU:HG2	1:B:60:PRO:HD2	1.94	0.49
1:B:123:GLU:OE2	1:D:78:ARG:NH1	2.46	0.49
1:D:159:HIS:O	1:D:196:GLY:N	2.22	0.49
1:B:287:ILE:HD11	1:B:307:ALA:HB1	1.95	0.49
1:D:197:TYR:HB2	1:D:202:THR:CG2	2.38	0.49
1:C:257:MET:CE	1:C:273:LEU:HB2	2.44	0.48
1:B:323:GLN:O	1:B:353:SER:OG	2.28	0.48
1:C:221:ARG:NH1	1:C:423:GLU:OE1	2.46	0.48
1:D:201:TYR:CZ	1:D:205:LEU:HD22	2.48	0.48
1:B:260:ARG:HH11	1:B:261:ASN:N	2.12	0.48
1:D:26:GLY:HA3	1:D:260:ARG:HD2	1.96	0.48
1:D:206:TYR:N	1:D:206:TYR:CD1	2.81	0.48
1:D:280:LEU:HD11	1:D:386:ALA:HA	1.95	0.48
1:C:345:GLU:OE2	2:C:501:GDP:O3'	2.31	0.48
1:C:392:VAL:HA	1:C:395:LEU:CD1	2.44	0.48
1:C:345:GLU:CD	2:C:501:GDP:HO3'	2.17	0.47
1:D:381:THR:OG1	1:D:384:ASP:OD1	2.28	0.47
1:A:400:ARG:NH2	1:A:404:ARG:NH2	2.63	0.47
1:C:10:ALA:H	1:C:126:ASP:HB2	1.79	0.47
1:D:56:VAL:HG11	1:D:117:LEU:HD11	1.96	0.47
1:C:197:TYR:CD2	1:C:203:ALA:HB2	2.49	0.47
1:B:276:ALA:O	1:B:280:LEU:N	2.40	0.47
1:B:140:VAL:HB	1:B:141:PRO:HD3	1.95	0.47
1:A:365:LEU:O	1:A:369:VAL:HG22	2.14	0.47
1:B:385:VAL:O	1:B:389:VAL:HG23	2.14	0.47
1:C:332:PHE:O	1:C:333:LEU:HD23	2.15	0.47
1:C:392:VAL:HA	1:C:395:LEU:HD13	1.97	0.47
1:B:197:TYR:CD2	1:B:203:ALA:HB2	2.49	0.47
1:B:304:ALA:O	1:B:305:VAL:HG12	2.14	0.47
1:B:347:MET:HG3	1:B:357:VAL:HG21	1.97	0.47
1:A:104:GLU:OE1	1:B:105:ARG:HD3	2.15	0.47
1:C:48:GLU:OE1	1:C:48:GLU:HA	2.14	0.47
1:C:263:ALA:O	1:C:264:PRO:C	2.52	0.47
1:B:198:ILE:HD12	1:B:339:GLY:HA3	1.97	0.47
1:C:71:GLU:O	1:C:75:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:GLY:HA2	1:C:218:LEU:O	2.14	0.47
1:B:435:VAL:HG23	1:B:435:VAL:O	2.14	0.47
1:C:15:TRP:CE3	1:C:35:LEU:HD21	2.50	0.46
1:A:196:GLY:HA2	1:A:218:LEU:O	2.15	0.46
1:A:361:ASP:OD1	1:A:379:ARG:NH1	2.43	0.46
1:C:294:PRO:O	1:C:298:ARG:HG3	2.15	0.46
1:B:196:GLY:HA2	1:B:218:LEU:O	2.14	0.46
1:C:139:ARG:HD2	1:C:182:ASP:CG	2.36	0.46
1:B:71:GLU:O	1:B:75:ARG:HG3	2.15	0.46
1:B:315:PHE:HA	1:B:318:LEU:HG	1.98	0.46
1:A:260:ARG:NE	2:A:501:GDP:O2B	2.41	0.46
1:C:257:MET:CE	1:C:273:LEU:CB	2.93	0.46
1:D:199:SER:H	1:D:202:THR:HG22	1.80	0.46
1:C:347:MET:HG3	1:C:357:VAL:HG21	1.98	0.46
1:C:55:PHE:O	1:C:86:GLY:HA3	2.16	0.46
1:C:392:VAL:CA	1:C:395:LEU:HD13	2.45	0.46
1:B:252:GLY:HA2	1:B:326:ARG:HH21	1.81	0.46
1:D:80:HIS:O	1:D:84:ARG:HD2	2.16	0.46
1:C:257:MET:HE1	1:C:273:LEU:HB2	1.97	0.46
1:C:400:ARG:HH21	1:C:401:ARG:NE	2.11	0.46
1:B:276:ALA:HB2	1:B:385:VAL:HG13	1.98	0.46
1:C:162:GLY:O	1:C:163:LEU:HD22	2.16	0.46
1:B:417:PHE:O	1:B:421:VAL:HG22	2.16	0.46
1:C:390:ARG:O	1:C:394:LYS:HG2	2.16	0.45
1:B:268:LYS:HB2	1:B:270:TYR:CE2	2.51	0.45
1:A:226:ARG:HB3	1:A:348:TRP:CE2	2.52	0.45
1:C:280:LEU:HB3	1:C:283:VAL:HB	1.97	0.45
1:A:22:GLN:O	1:A:69:TYR:HA	2.16	0.45
1:D:431:ARG:O	1:D:435:VAL:HG22	2.17	0.45
1:A:241:GLU:C	1:A:241:GLU:OE1	2.55	0.45
1:A:246:LEU:HB2	1:A:248:LEU:CD1	2.46	0.45
1:B:99:ASP:OD1	1:B:100:GLY:N	2.50	0.45
1:B:260:ARG:CG	1:B:261:ASN:H	2.28	0.45
1:B:249:PRO:HB2	1:B:251:GLU:OE2	2.17	0.45
1:B:257:MET:HG3	1:B:331:ALA:O	2.17	0.45
1:D:202:THR:HG23	1:D:203:ALA:N	2.32	0.45
1:D:278:ARG:HD2	1:D:303:TYR:CG	2.52	0.45
1:C:431:ARG:HA	1:C:434:GLU:HG2	1.98	0.45
1:B:397:ALA:HA	1:B:400:ARG:NH2	2.32	0.44
1:D:235:THR:O	1:D:238:ARG:N	2.44	0.44
1:A:347:MET:HE3	1:A:407:ALA:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:GLY:HA2	1:C:160:THR:O	2.17	0.44
1:D:277:ALA:HA	1:D:280:LEU:HB2	1.99	0.44
1:B:327:THR:HG22	1:B:355:ALA:HB2	1.99	0.44
1:A:376:ILE:CG2	1:A:391:ARG:HH21	2.31	0.44
1:A:221:ARG:NH2	1:A:414:ARG:O	2.49	0.44
1:A:43:ARG:HA	1:A:53:VAL:HG12	2.00	0.44
1:A:249:PRO:HG2	1:A:284:VAL:HG11	1.99	0.44
1:A:359:ALA:O	1:A:377:VAL:HA	2.17	0.44
1:A:157:HIS:HB2	1:A:193:VAL:HG22	1.99	0.44
1:A:266:LEU:HD13	3:A:502:Q3L:O4	2.18	0.44
1:A:285:PRO:HD2	1:A:306:PRO:O	2.18	0.44
1:D:94:ASP:O	1:D:105:ARG:NE	2.50	0.44
1:D:381:THR:O	1:D:385:VAL:HG23	2.18	0.44
1:C:257:MET:HE1	1:C:273:LEU:CB	2.48	0.43
1:A:246:LEU:HD21	1:A:317:HIS:CD2	2.53	0.43
1:C:253:GLU:OE1	1:C:393:ARG:NH1	2.51	0.43
1:B:140:VAL:N	1:B:141:PRO:CD	2.80	0.43
1:D:370:ASP:HB2	1:D:410:ARG:HD2	2.00	0.43
1:A:267:ASP:OD2	1:A:380:ARG:NH2	2.50	0.43
1:B:364:ASN:O	1:B:368:VAL:HG23	2.19	0.43
1:B:255:VAL:CG2	1:B:328:LEU:HD21	2.49	0.43
1:B:236:GLU:HA	1:B:239:ILE:HG13	1.99	0.43
1:B:246:LEU:HD12	1:B:246:LEU:HA	1.86	0.43
1:D:59:GLU:O	1:D:90:ARG:HA	2.18	0.43
1:C:80:HIS:O	1:C:84:ARG:HD2	2.19	0.43
1:C:220:ASN:OD1	1:C:424:LEU:HD22	2.19	0.43
1:D:64:PRO:HA	1:D:69:TYR:CE2	2.54	0.43
1:B:15:TRP:CZ2	1:B:35:LEU:HD11	2.54	0.43
1:D:360:ALA:O	1:D:365:LEU:HB2	2.18	0.43
1:C:11:LEU:O	1:C:53:VAL:HA	2.19	0.43
1:C:370:ASP:HB3	1:C:373:ALA:HB3	2.01	0.43
1:B:277:ALA:O	1:B:278:ARG:C	2.57	0.43
1:B:200:ARG:HH11	1:B:200:ARG:HB3	1.84	0.43
1:B:337:GLU:HB3	1:B:340:ALA:HB2	2.01	0.43
1:D:131:VAL:HG22	1:D:158:VAL:HB	1.99	0.43
1:B:93:SER:O	1:D:147:GLN:OE1	2.37	0.42
1:B:255:VAL:HG22	1:B:328:LEU:HD21	2.00	0.42
1:A:345:GLU:OE2	2:A:501:GDP:O3'	2.37	0.42
1:C:348:TRP:O	1:C:351:ARG:HG3	2.20	0.42
1:B:11:LEU:HD11	1:B:129:VAL:HG23	2.01	0.42
1:D:99:ASP:N	1:D:99:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:LEU:HG	1:D:285:PRO:HB3	2.02	0.42
1:D:147:GLN:O	1:D:147:GLN:HG2	2.19	0.42
1:D:243:ILE:HA	1:D:246:LEU:HD11	2.02	0.42
1:A:81:LEU:HD12	1:A:88:ALA:HB2	2.02	0.42
1:C:41:ALA:HB1	1:C:422:ARG:HH22	1.84	0.42
1:A:195:VAL:HG21	1:A:212:ILE:CD1	2.48	0.42
1:A:158:VAL:HA	1:A:194:SER:O	2.20	0.42
1:C:387:ASP:O	1:C:391:ARG:HG3	2.20	0.42
1:B:359:ALA:HB1	1:B:365:LEU:HB3	2.01	0.42
1:A:279:ASP:OD1	1:A:390:ARG:NH1	2.45	0.42
1:B:225:PRO:HD2	1:B:231:PHE:CE2	2.54	0.42
1:D:239:ILE:HD12	1:D:239:ILE:N	2.33	0.41
1:B:296:LEU:HD13	1:B:296:LEU:HA	1.92	0.41
1:D:347:MET:HE1	1:D:368:VAL:O	2.20	0.41
1:B:167:ASP:OD1	1:B:167:ASP:N	2.46	0.41
1:A:327:THR:CG2	1:A:355:ALA:HB2	2.51	0.41
1:B:22:GLN:NE2	1:B:60:PRO:O	2.53	0.41
1:D:184:ALA:O	1:D:188:ARG:HG3	2.20	0.41
1:B:299:LEU:O	1:B:303:TYR:CD2	2.74	0.41
1:D:337:GLU:HA	1:D:338:PRO:HD3	1.84	0.41
1:B:347:MET:CG	1:B:407:ALA:HB1	2.50	0.41
1:D:251:GLU:OE1	1:D:251:GLU:HA	2.21	0.41
1:A:276:ALA:O	1:A:280:LEU:HD22	2.21	0.41
1:C:266:LEU:HD13	3:C:502:Q3L:O4	2.20	0.41
1:C:180:ASP:HA	1:C:183:VAL:HG12	2.03	0.41
1:B:260:ARG:HA	1:B:260:ARG:HD2	1.86	0.41
1:B:276:ALA:HB2	1:B:385:VAL:CG1	2.51	0.41
1:D:233:VAL:HG21	1:D:352:GLU:HG2	2.01	0.41
1:D:243:ILE:HG23	1:D:248:LEU:CD1	2.50	0.41
1:D:431:ARG:HG3	1:D:431:ARG:NH1	2.33	0.41
1:A:370:ASP:HB3	1:A:373:ALA:HB3	2.02	0.41
1:C:398:ASP:O	1:C:402:ARG:HG2	2.21	0.41
1:B:404:ARG:HE	1:B:404:ARG:HB2	1.72	0.41
1:D:135:SER:OG	1:D:180:ASP:OD2	2.38	0.41
1:D:186:TRP:HA	1:D:189:GLN:HB3	2.03	0.41
1:D:223:ALA:HB1	1:D:415:PHE:O	2.20	0.41
1:D:361:ASP:HA	1:D:366:PRO:HG3	2.03	0.41
1:B:63:ASP:HB3	1:B:98:LEU:HD23	2.02	0.40
1:B:205:LEU:CD1	1:B:208:ARG:NH2	2.84	0.40
1:D:129:VAL:HG21	1:D:428:ALA:HB1	2.03	0.40
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ASP:N	1:B:309:LEU:HD11	2.26	0.40
1:B:304:ALA:C	1:B:305:VAL:HG13	2.42	0.40
1:D:341:VAL:O	1:D:344:MET:HB2	2.21	0.40
1:D:235:THR:O	1:D:239:ILE:HD12	2.22	0.40
1:A:292:PRO:O	1:A:294:PRO:HD3	2.22	0.40
1:C:321:LEU:HD23	1:C:321:LEU:HA	1.78	0.40
1:B:329:ALA:HB2	1:B:392:VAL:HG11	2.04	0.40
1:D:333:LEU:HA	1:D:360:ALA:HB2	2.04	0.40
1:A:398:ASP:O	1:A:402:ARG:NH1	2.54	0.40
1:A:418:ALA:O	1:A:422:ARG:CD	2.65	0.40
1:B:304:ALA:C	1:B:305:VAL:CG1	2.90	0.40
1:D:359:ALA:HB1	1:D:365:LEU:HB3	2.03	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	427/457 (93%)	404 (95%)	23 (5%)	0	100	100
1	B	427/457 (93%)	395 (92%)	32 (8%)	0	100	100
1	C	427/457 (93%)	412 (96%)	15 (4%)	0	100	100
1	D	427/457 (93%)	413 (97%)	14 (3%)	0	100	100
All	All	1708/1828 (93%)	1624 (95%)	84 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	315/341 (92%)	305 (97%)	10 (3%)	39	73
1	B	310/341 (91%)	299 (96%)	11 (4%)	36	70
1	C	316/341 (93%)	304 (96%)	12 (4%)	33	67
1	D	316/341 (93%)	305 (96%)	11 (4%)	36	70
All	All	1257/1364 (92%)	1213 (96%)	44 (4%)	36	70

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	61	PHE
1	A	87	ARG
1	A	208	ARG
1	A	238	ARG
1	A	241	GLU
1	A	271	HIS
1	A	303	TYR
1	A	317	HIS
1	A	343	PRO
1	C	33	ARG
1	C	61	PHE
1	C	123	GLU
1	C	170	HIS
1	C	194	SER
1	C	237	GLU
1	C	278	ARG
1	C	378	THR
1	C	379	ARG
1	C	384	ASP
1	C	396	THR
1	C	431	ARG
1	B	33	ARG
1	B	79	GLU
1	B	165	THR
1	B	190	SER
1	B	192	ARG
1	B	208	ARG

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Mol	Chain	Res	Type
1	B	238	ARG
1	B	312	ASP
1	B	391	ARG
1	B	394	LYS
1	B	414	ARG
1	D	43	ARG
1	D	61	PHE
1	D	62	TYR
1	D	78	ARG
1	D	84	ARG
1	D	120	ASP
1	D	132	SER
1	D	173	SER
1	D	311	ASP
1	D	324	SER
1	D	402	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	HIS
1	C	45	HIS
1	C	157	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 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	GDP	D	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.32	4 (13%)
3	Q3L	C	502	-	23,30,30	2.44	8 (34%)	28,45,45	1.36	3 (10%)
2	GDP	B	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.33	4 (13%)
2	GDP	A	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.27	4 (13%)
2	GDP	C	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.32	4 (13%)
3	Q3L	D	502	-	23,30,30	2.43	8 (34%)	28,45,45	1.41	3 (10%)
3	Q3L	B	502	-	23,30,30	2.45	8 (34%)	28,45,45	1.43	3 (10%)
3	Q3L	A	502	-	23,30,30	2.47	8 (34%)	28,45,45	1.37	3 (10%)

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	GDP	D	501	-	-	4/12/32/32	0/3/3/3
3	Q3L	C	502	-	-	7/24/46/46	0/2/2/2
2	GDP	B	501	-	-	4/12/32/32	0/3/3/3
2	GDP	A	501	-	-	5/12/32/32	0/3/3/3
2	GDP	C	501	-	-	4/12/32/32	0/3/3/3
3	Q3L	D	502	-	-	12/24/46/46	0/2/2/2
3	Q3L	B	502	-	-	8/24/46/46	0/2/2/2
3	Q3L	A	502	-	-	9/24/46/46	0/2/2/2

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	Q3L	C4-C3	-6.66	1.44	1.52
3	A	502	Q3L	C4-C3	-6.64	1.44	1.52
3	C	502	Q3L	C4-C3	-6.51	1.44	1.52
3	D	502	Q3L	C4-C3	-6.46	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	Q3L	O2-C4	5.98	1.53	1.44
3	C	502	Q3L	O2-C4	5.94	1.53	1.44
3	D	502	Q3L	O2-C4	5.91	1.53	1.44
3	B	502	Q3L	O2-C4	5.86	1.53	1.44
3	C	502	Q3L	O2-C5	3.66	1.48	1.42
3	D	502	Q3L	O2-C5	3.64	1.48	1.42
3	B	502	Q3L	O2-C5	3.63	1.48	1.42
3	A	502	Q3L	O2-C5	3.60	1.48	1.42
3	D	502	Q3L	C15-C16	-2.67	1.45	1.52
3	A	502	Q3L	C15-C16	-2.67	1.45	1.52
3	C	502	Q3L	C15-C16	-2.65	1.45	1.52
3	B	502	Q3L	C15-C16	-2.64	1.45	1.52
3	B	502	Q3L	O5-C15	2.57	1.49	1.43
3	C	502	Q3L	O5-C15	2.56	1.49	1.43
3	A	502	Q3L	O6-C16	2.54	1.49	1.43
3	A	502	Q3L	O5-C15	2.53	1.48	1.43
3	D	502	Q3L	O5-C15	2.52	1.48	1.43
3	B	502	Q3L	O6-C16	2.52	1.48	1.43
3	C	502	Q3L	O6-C16	2.52	1.48	1.43
3	D	502	Q3L	O6-C16	2.49	1.48	1.43
3	B	502	Q3L	C7-N2	-2.38	1.32	1.36
2	A	501	GDP	C6-N1	-2.31	1.34	1.37
2	D	501	GDP	C6-N1	-2.28	1.34	1.37
2	C	501	GDP	C6-N1	-2.26	1.34	1.37
2	B	501	GDP	C6-N1	-2.26	1.34	1.37
3	A	502	Q3L	C7-N2	-2.24	1.32	1.36
3	D	502	Q3L	C7-N2	-2.20	1.33	1.36
3	C	502	Q3L	C7-N2	-2.15	1.33	1.36
3	B	502	Q3L	O1-C1	2.10	1.48	1.43
3	C	502	Q3L	O1-C1	2.07	1.48	1.43
3	D	502	Q3L	O1-C1	2.06	1.48	1.43
3	A	502	Q3L	O1-C1	2.03	1.48	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	Q3L	C11-N3-C12	3.96	118.92	108.10
3	D	502	Q3L	C11-N3-C12	3.95	118.89	108.10
3	C	502	Q3L	C11-N3-C12	3.91	118.77	108.10
3	A	502	Q3L	C11-N3-C12	3.82	118.54	108.10
2	D	501	GDP	PA-O3A-PB	-3.56	120.62	132.83
2	B	501	GDP	C3'-C2'-C1'	3.45	106.17	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	GDP	PA-O3A-PB	-3.43	121.07	132.83
3	B	502	Q3L	O4-C14-C10	3.41	119.97	111.87
2	C	501	GDP	PA-O3A-PB	-3.30	121.49	132.83
2	A	501	GDP	PA-O3A-PB	-3.26	121.64	132.83
3	C	502	Q3L	O4-C14-C10	3.15	119.35	111.87
3	D	502	Q3L	O4-C14-C10	3.13	119.31	111.87
2	C	501	GDP	C3'-C2'-C1'	3.13	105.69	100.98
3	A	502	Q3L	O4-C14-C10	3.12	119.28	111.87
2	D	501	GDP	C3'-C2'-C1'	2.98	105.47	100.98
2	A	501	GDP	C3'-C2'-C1'	2.87	105.30	100.98
3	A	502	Q3L	O2-C5-C15	2.43	113.37	110.31
3	B	502	Q3L	O2-C5-C15	2.43	113.36	110.31
3	D	502	Q3L	O2-C5-C15	2.42	113.36	110.31
2	D	501	GDP	C8-N7-C5	2.42	107.59	102.99
3	C	502	Q3L	O2-C5-C15	2.35	113.26	110.31
2	A	501	GDP	C8-N7-C5	2.32	107.42	102.99
2	C	501	GDP	C8-N7-C5	2.32	107.41	102.99
2	B	501	GDP	C8-N7-C5	2.32	107.41	102.99
2	B	501	GDP	C5-C6-N1	2.27	117.96	113.95
2	C	501	GDP	C5-C6-N1	2.22	117.87	113.95
2	A	501	GDP	C5-C6-N1	2.20	117.83	113.95
2	D	501	GDP	C5-C6-N1	2.16	117.76	113.95

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GDP	C5'-O5'-PA-O3A
2	A	501	GDP	C5'-O5'-PA-O1A
2	A	501	GDP	C5'-O5'-PA-O2A
2	C	501	GDP	C5'-O5'-PA-O3A
2	C	501	GDP	C5'-O5'-PA-O1A
2	C	501	GDP	C5'-O5'-PA-O2A
2	B	501	GDP	C5'-O5'-PA-O3A
2	B	501	GDP	C5'-O5'-PA-O1A
2	B	501	GDP	C5'-O5'-PA-O2A
2	D	501	GDP	C5'-O5'-PA-O3A
2	D	501	GDP	C5'-O5'-PA-O2A
3	A	502	Q3L	O1-C1-C3-C4
3	A	502	Q3L	C2-C1-C3-N1
3	A	502	Q3L	N4-C8-C9-C10
3	C	502	Q3L	O1-C1-C3-C4

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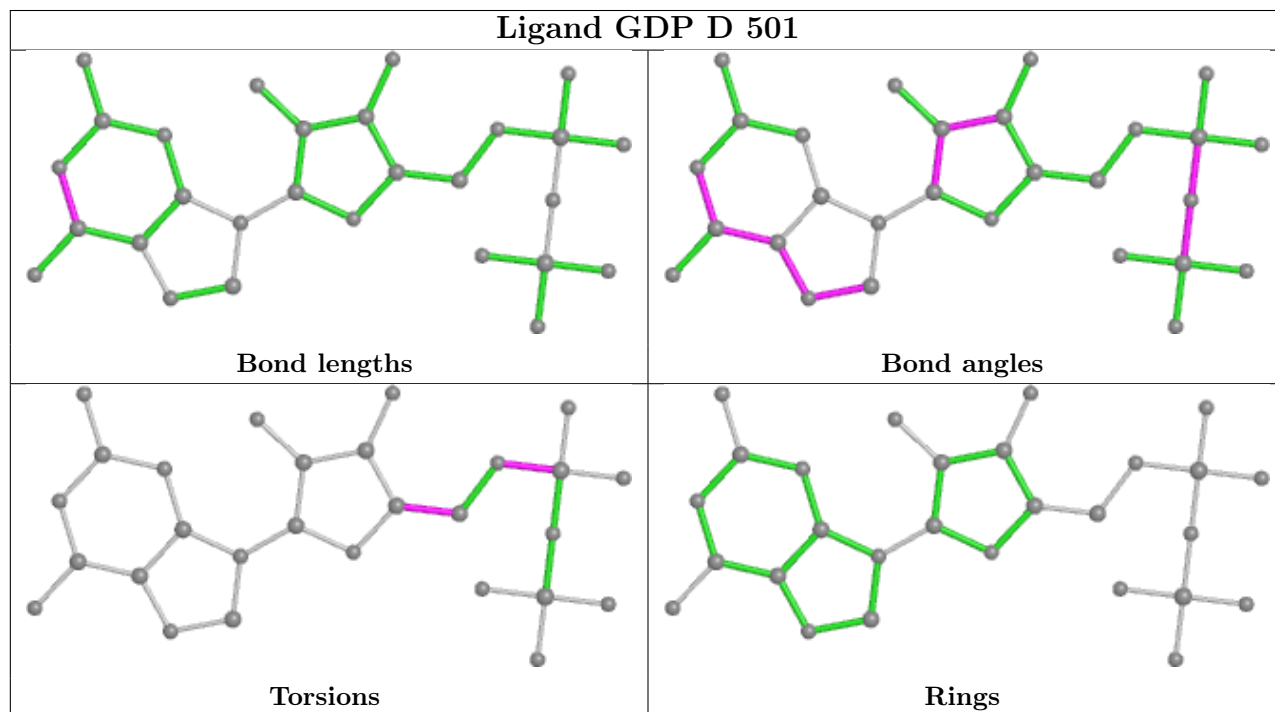
Mol	Chain	Res	Type	Atoms
3	C	502	Q3L	C14-C10-C9-C8
3	B	502	Q3L	O1-C1-C3-C4
3	B	502	Q3L	C2-C1-C3-N1
3	D	502	Q3L	N1-C3-C4-O2
3	D	502	Q3L	O1-C1-C3-C4
3	D	502	Q3L	C2-C1-C3-N1
3	D	502	Q3L	O1-C1-C3-N1
3	D	502	Q3L	C14-C10-C9-C8
3	A	502	Q3L	O2-C5-S1-C6
3	C	502	Q3L	O2-C5-S1-C6
3	B	502	Q3L	O2-C5-S1-C6
3	D	502	Q3L	O2-C5-S1-C6
3	A	502	Q3L	C15-C5-S1-C6
3	C	502	Q3L	C15-C5-S1-C6
3	B	502	Q3L	C15-C5-S1-C6
3	D	502	Q3L	C15-C5-S1-C6
3	D	502	Q3L	C1-C3-C4-O2
3	B	502	Q3L	N3-C10-C14-O4
2	A	501	GDP	O4'-C4'-C5'-O5'
2	A	501	GDP	PB-O3A-PA-O1A
3	A	502	Q3L	O1-C1-C3-N1
3	A	502	Q3L	C14-C10-C9-C8
3	B	502	Q3L	O1-C1-C3-N1
2	D	501	GDP	C5'-O5'-PA-O1A
3	D	502	Q3L	N4-C8-C9-C10
2	D	501	GDP	O4'-C4'-C5'-O5'
2	B	501	GDP	O4'-C4'-C5'-O5'
3	A	502	Q3L	N3-C10-C14-O4
3	C	502	Q3L	N3-C10-C14-O4
3	D	502	Q3L	N3-C10-C14-O4
2	C	501	GDP	O4'-C4'-C5'-O5'
3	A	502	Q3L	C2-C1-C3-C4
3	C	502	Q3L	C2-C1-C3-C4
3	B	502	Q3L	C2-C1-C3-C4
3	D	502	Q3L	C2-C1-C3-C4
3	C	502	Q3L	O1-C1-C3-N1
3	D	502	Q3L	C9-C10-N3-C12
3	B	502	Q3L	C7-C8-C9-C10

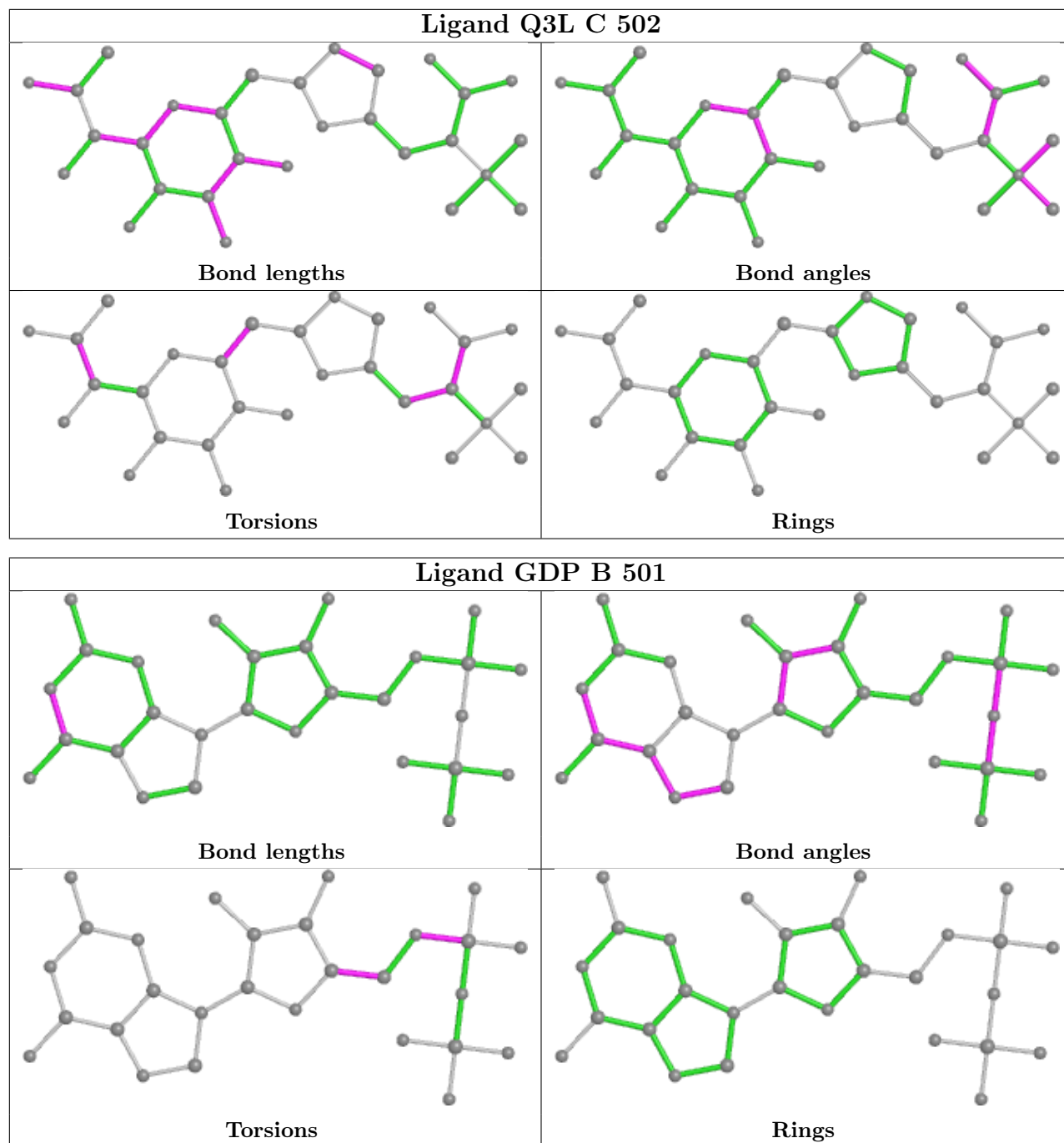
There are no ring outliers.

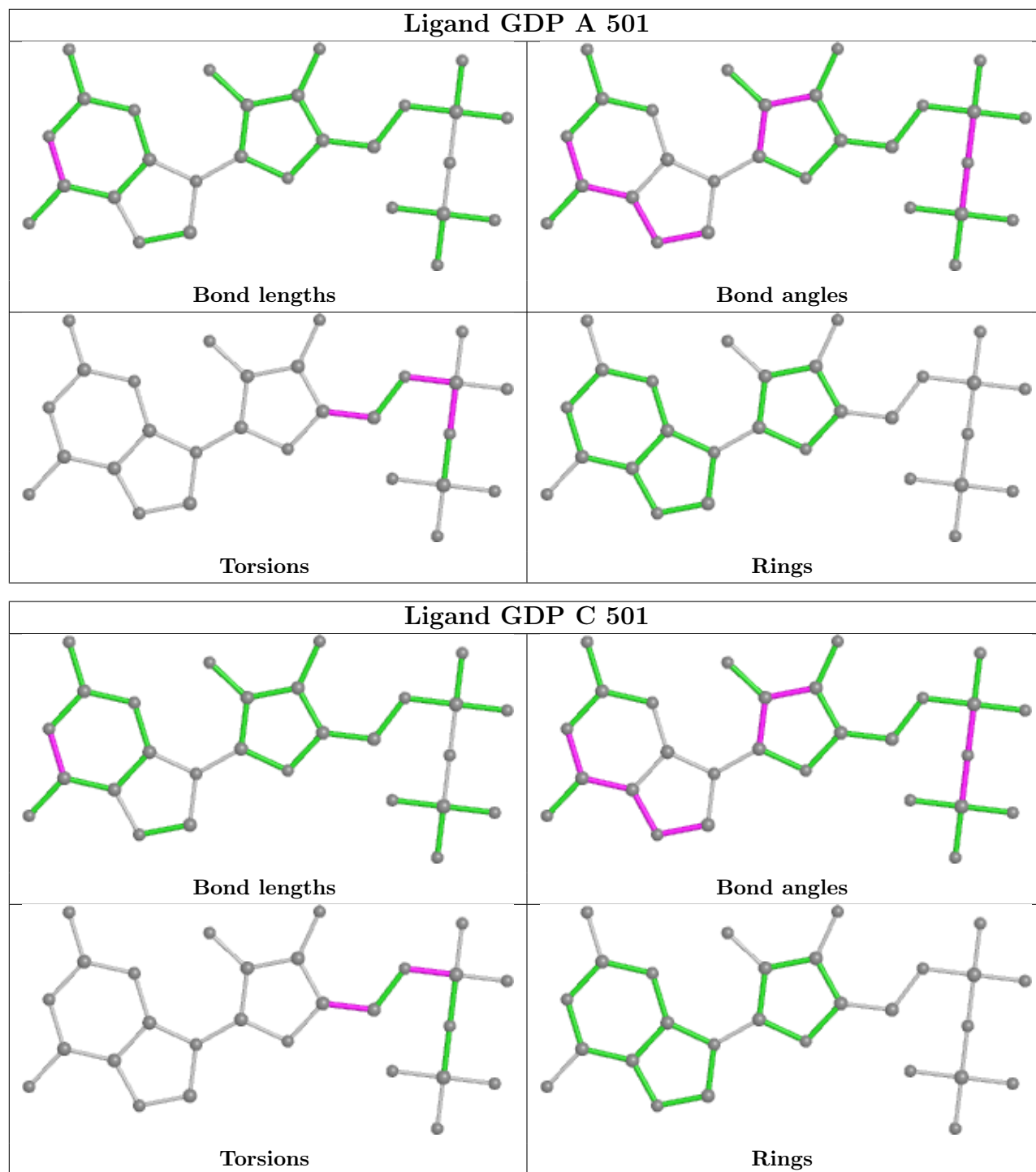
5 monomers are involved in 8 short contacts:

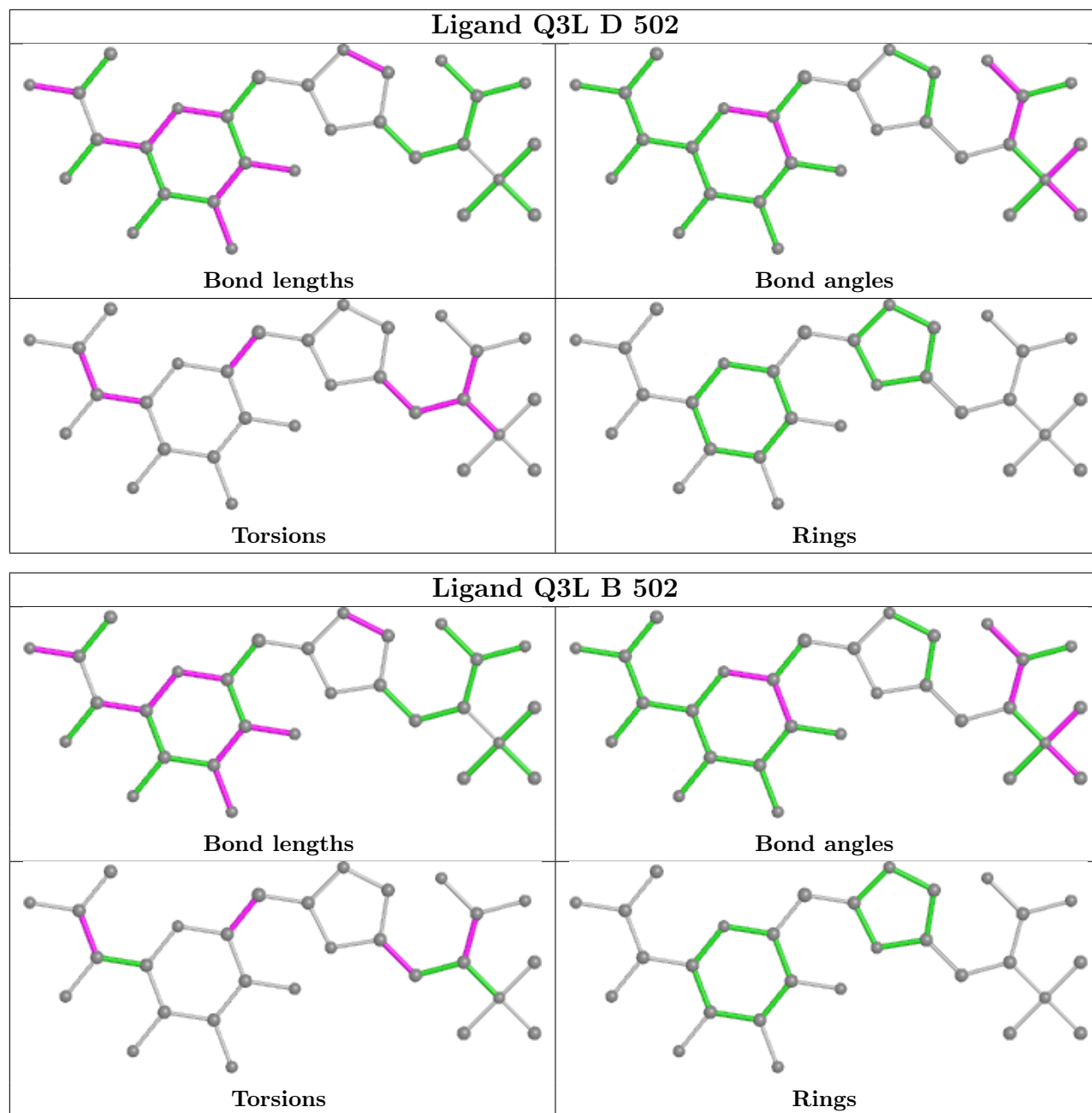
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	GDP	2	0
3	C	502	Q3L	1	0
2	A	501	GDP	2	0
2	C	501	GDP	2	0
3	A	502	Q3L	1	0

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.

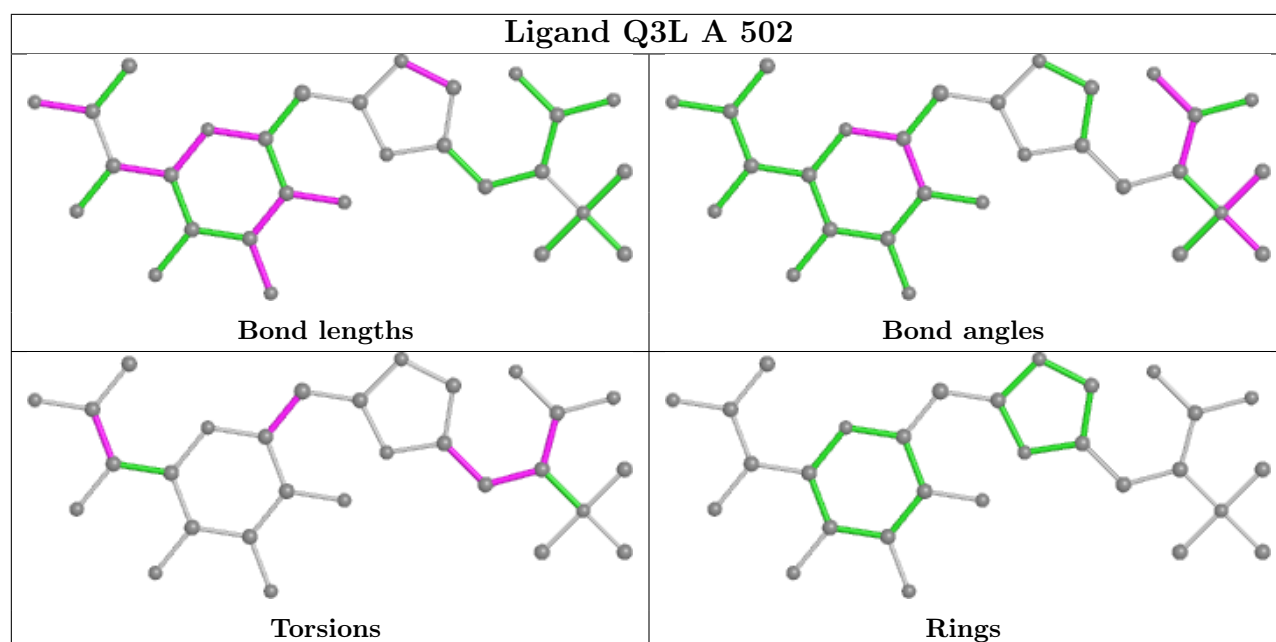












## 5.7 Other polymers [i](#)

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	429/457 (93%)	0.72	35 (8%) <b>11</b> <b>6</b>	50, 68, 103, 127	0
1	B	429/457 (93%)	1.27	84 (19%) <b>1</b> <b>0</b>	55, 79, 143, 177	0
1	C	429/457 (93%)	0.51	11 (2%) 56 46	50, 62, 82, 108	0
1	D	429/457 (93%)	0.59	12 (2%) 53 43	56, 69, 87, 114	0
All	All	1716/1828 (93%)	0.77	142 (8%) <b>11</b> <b>6</b>	50, 69, 120, 177	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	254	PHE	13.0
1	B	256	VAL	7.7
1	B	245	GLY	7.4
1	B	246	LEU	7.4
1	B	281	PRO	7.0
1	B	392	VAL	6.4
1	B	304	ALA	6.4
1	B	234	LEU	6.3
1	B	244	ALA	6.2
1	B	329	ALA	6.0
1	B	327	THR	5.7
1	B	285	PRO	5.7
1	B	326	ARG	5.6
1	B	237	GLU	5.6
1	B	393	ARG	5.4
1	B	315	PHE	5.3
1	B	277	ALA	5.3
1	B	255	VAL	5.2
1	B	389	VAL	5.0
1	B	242	ARG	5.0
1	A	328	LEU	4.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	305	VAL	4.9
1	B	280	LEU	4.8
1	B	287	ILE	4.7
1	B	272	LEU	4.7
1	A	285	PRO	4.7
1	B	276	ALA	4.6
1	A	329	ALA	4.6
1	B	284	VAL	4.5
1	B	286	VAL	4.5
1	B	306	PRO	4.5
1	B	314	PRO	4.5
1	B	307	ALA	4.4
1	B	395	LEU	4.4
1	B	253	GLU	4.3
1	D	206	TYR	4.2
1	B	358	ILE	4.0
1	B	294	PRO	3.9
1	B	379	ARG	3.8
1	B	301	ASP	3.7
1	A	436	SER	3.6
1	B	273	LEU	3.6
1	B	283	VAL	3.5
1	B	333	LEU	3.5
1	B	248	LEU	3.4
1	A	256	VAL	3.4
1	A	280	LEU	3.4
1	B	231	PHE	3.4
1	B	247	GLY	3.3
1	B	398	ASP	3.3
1	B	401	ARG	3.3
1	B	324	SER	3.3
1	B	257	MET	3.2
1	B	278	ARG	3.2
1	A	376	ILE	3.2
1	B	390	ARG	3.2
1	D	35	LEU	3.2
1	A	282	GLY	3.2
1	B	252	GLY	3.2
1	B	292	PRO	3.1
1	B	279	ASP	3.1
1	B	308	VAL	3.1
1	B	400	ARG	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	278	ARG	3.0
1	B	376	ILE	3.0
1	B	316	THR	3.0
1	A	274	LEU	2.9
1	D	234	LEU	2.9
1	B	383	ALA	2.9
1	A	272	LEU	2.9
1	B	322	LEU	2.8
1	A	253	GLU	2.8
1	A	284	VAL	2.8
1	A	286	VAL	2.8
1	A	321	LEU	2.8
1	B	356	LEU	2.8
1	A	357	VAL	2.8
1	B	388	ALA	2.7
1	C	306	PRO	2.7
1	A	392	VAL	2.7
1	B	235	THR	2.7
1	A	8	GLY	2.7
1	A	358	ILE	2.6
1	B	353	SER	2.6
1	B	303	TYR	2.6
1	B	249	PRO	2.6
1	B	355	ALA	2.5
1	A	283	VAL	2.5
1	B	332	PHE	2.5
1	D	205	LEU	2.5
1	B	134	THR	2.5
1	B	321	LEU	2.5
1	B	135	SER	2.5
1	B	275	GLU	2.5
1	C	402	ARG	2.5
1	B	241	GLU	2.4
1	A	305	VAL	2.4
1	C	206	TYR	2.4
1	A	279	ASP	2.4
1	D	36	LEU	2.4
1	B	317	HIS	2.4
1	A	308	VAL	2.4
1	A	300	ALA	2.3
1	C	389	VAL	2.3
1	A	134	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	53	VAL	2.3
1	B	313	GLN	2.3
1	A	255	VAL	2.3
1	A	318	LEU	2.3
1	B	377	VAL	2.3
1	B	300	ALA	2.2
1	D	208	ARG	2.2
1	D	414	ARG	2.2
1	B	243	ILE	2.2
1	C	281	PRO	2.2
1	D	317	HIS	2.2
1	B	282	GLY	2.2
1	B	382	ALA	2.2
1	B	269	GLY	2.2
1	A	287	ILE	2.2
1	C	349	VAL	2.2
1	C	400	ARG	2.2
1	C	99	ASP	2.2
1	A	281	PRO	2.2
1	A	252	GLY	2.2
1	B	328	LEU	2.1
1	A	306	PRO	2.1
1	B	391	ARG	2.1
1	A	432	LEU	2.1
1	C	358	ILE	2.1
1	B	338	PRO	2.1
1	D	347	MET	2.1
1	A	273	LEU	2.1
1	C	376	ILE	2.1
1	A	299	LEU	2.1
1	D	217	LEU	2.1
1	D	239	ILE	2.0
1	B	325	PRO	2.0
1	B	296	LEU	2.0
1	C	251	GLU	2.0
1	B	330	ALA	2.0
1	A	389	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains

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

### 6.3 Carbohydrates

There are no monosaccharides in this entry.

### 6.4 Ligands

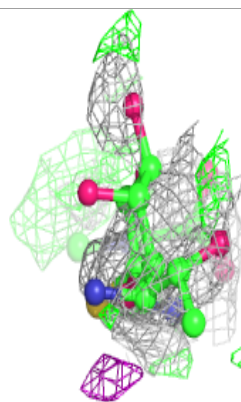
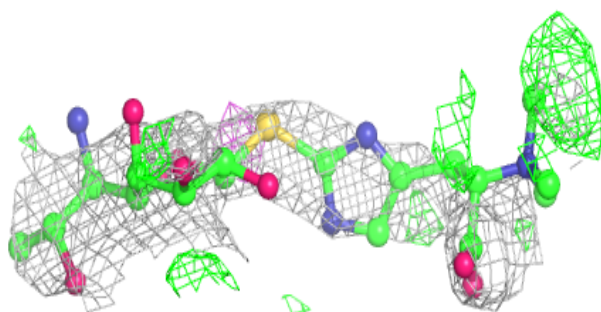
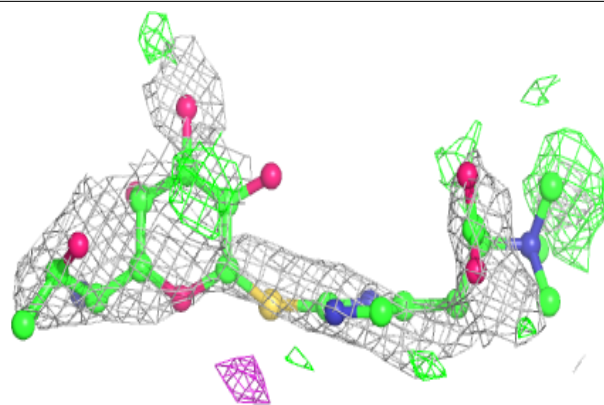
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	Q3L	B	502	29/29	0.66	0.44	97,103,106,107	14
2	GDP	B	501	28/28	0.72	0.34	85,96,119,126	12
3	Q3L	A	502	29/29	0.81	0.35	65,68,72,75	16
3	Q3L	C	502	29/29	0.84	0.34	56,58,60,63	17
3	Q3L	D	502	29/29	0.87	0.30	58,59,60,61	17
2	GDP	D	501	28/28	0.92	0.23	59,60,63,64	12
2	GDP	A	501	28/28	0.95	0.19	61,63,65,67	14
2	GDP	C	501	28/28	0.95	0.24	55,56,58,60	14

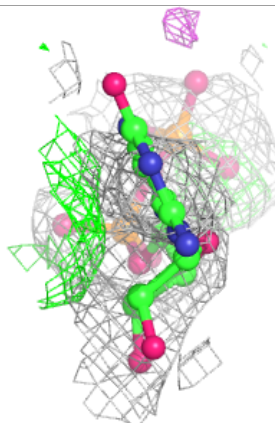
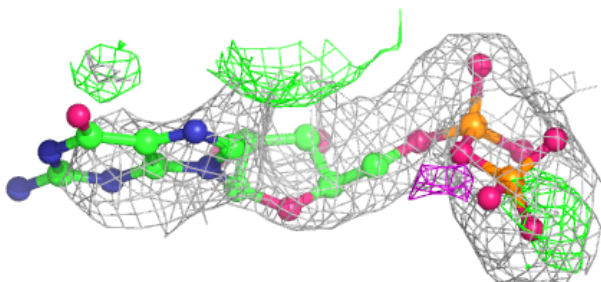
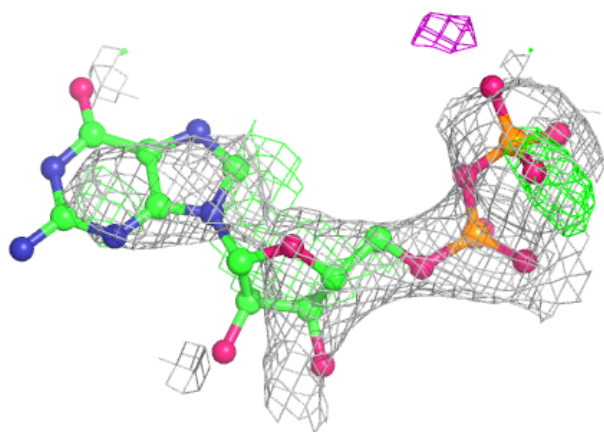
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around Q3L B 502:**

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

**Electron density around GDP B 501:**

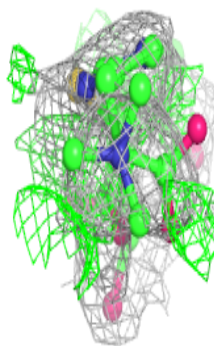
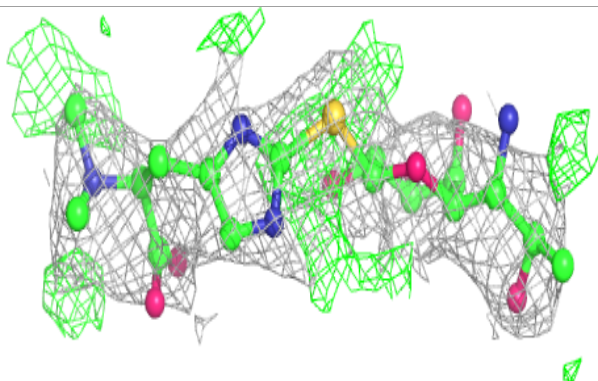
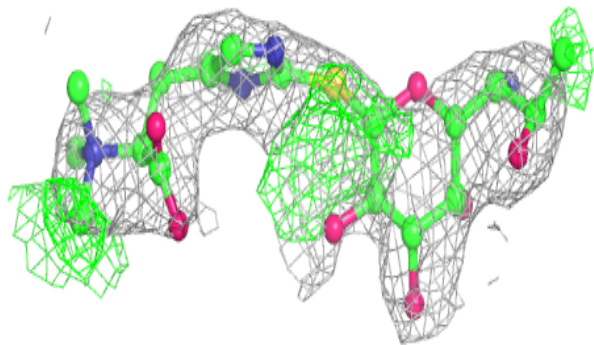
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



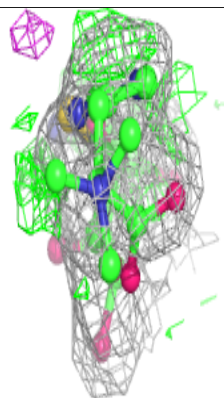
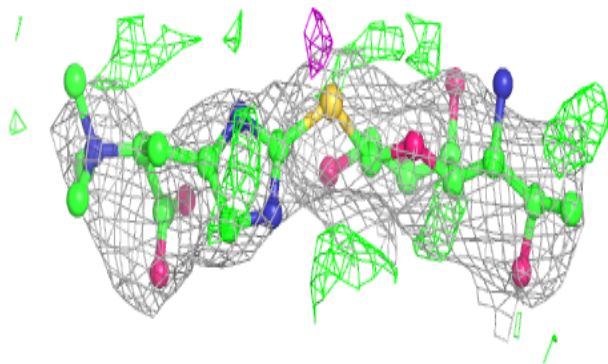
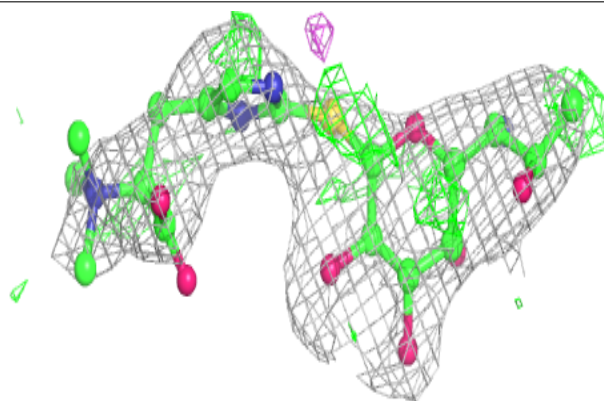


**Electron density around Q3L A 502:**

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

**Electron density around Q3L C 502:**

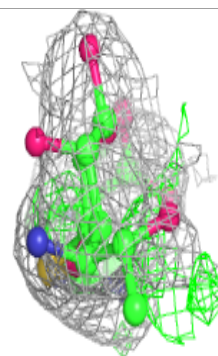
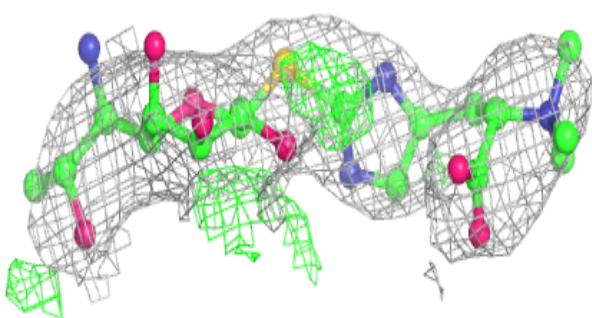
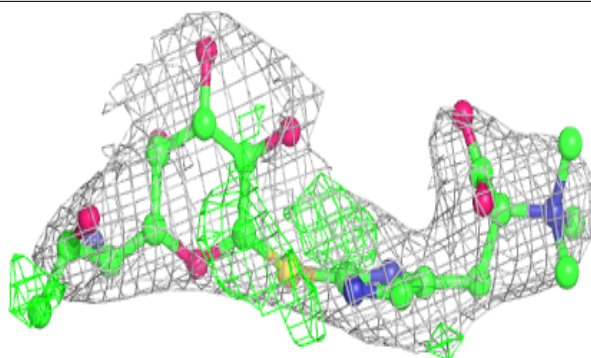
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



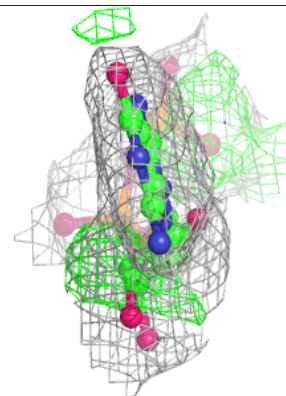
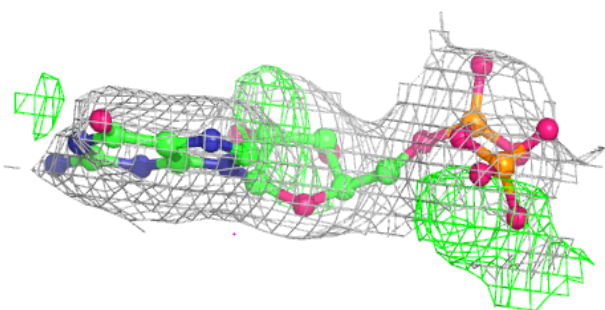
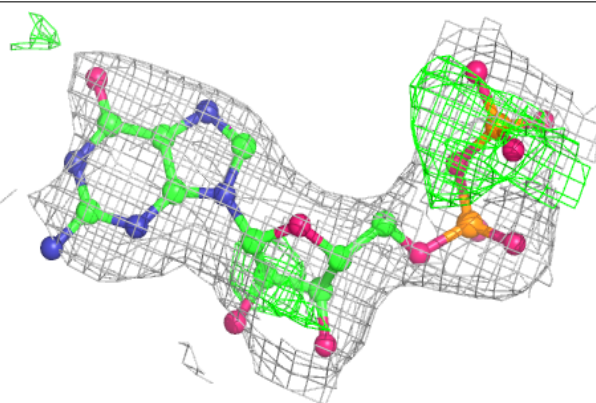


**Electron density around Q3L D 502:**

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

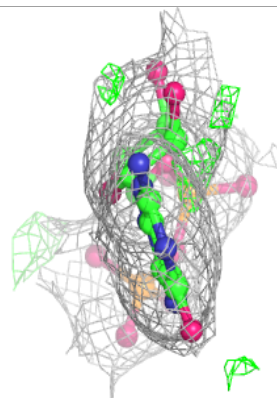
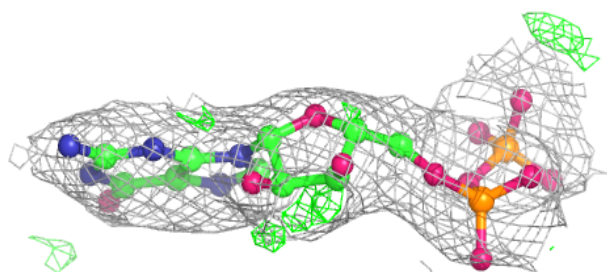
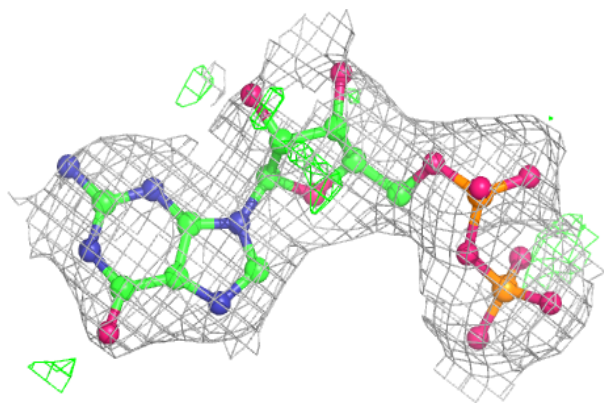
**Electron density around GDP D 501:**

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

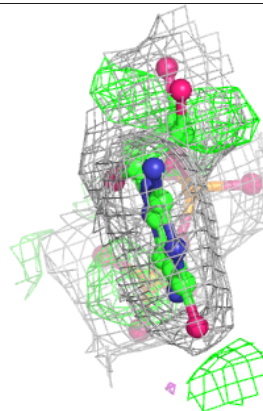
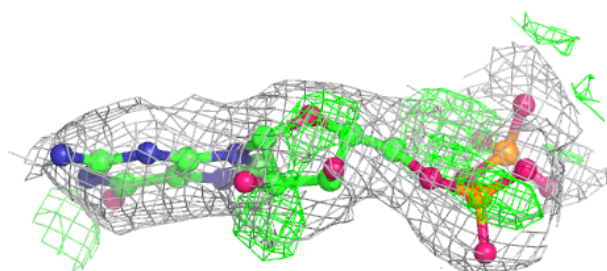
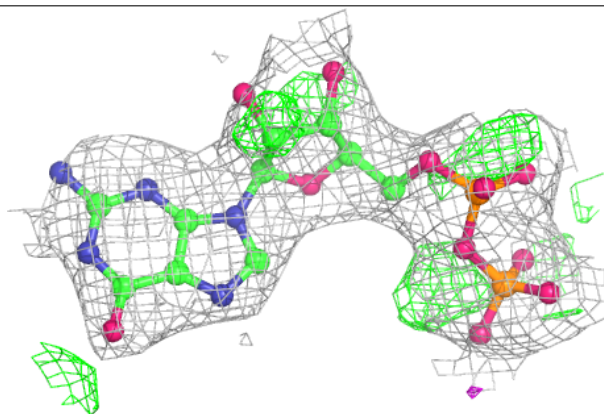


**Electron density around GDP A 501:**

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

**Electron density around GDP 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.