



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 10:14 AM EDT

PDB ID : 7YPZ / pdb_00007ypz
Title : Zafirlukast in complex with CRM1-Ran-RanBP1
Authors : Sun, Q.; Lei, Y.
Deposited on : 2022-08-05
Resolution : 2.15 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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

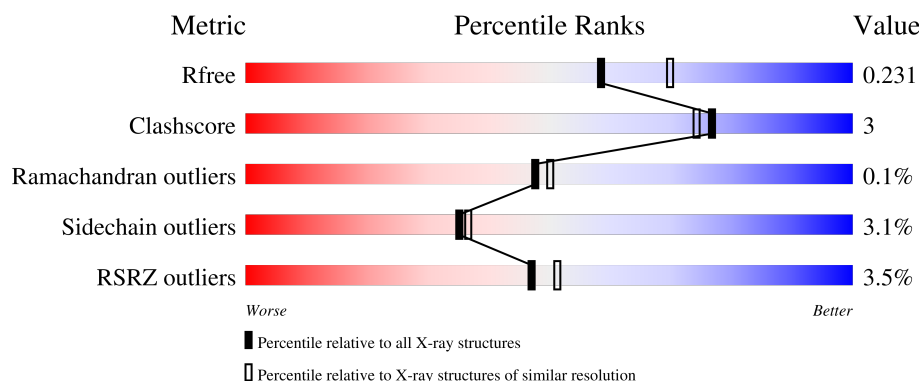
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

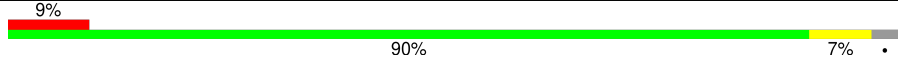
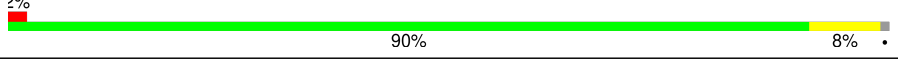
The reported resolution of this entry is 2.15 Å.

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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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 ≥ 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	216	
2	B	140	
3	C	1003	

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 11451 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 GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	1	0
			1680	1083	287	304	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	GLU	GLN	conflict	UNP P62826
A	69	LEU	GLN	engineered mutation	UNP P62826
A	182	ALA	LEU	engineered mutation	UNP P62826

- Molecule 2 is a protein called YRB1 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	123	Total	C	N	O	S	0	0	0
			1007	637	176	189	5			

- Molecule 3 is a protein called CRM1 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	996	Total	C	N	O	S	0	3	0
			8068	5186	1328	1510	44			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP A0A6A5PZI8
C	-1	GLY	-	expression tag	UNP A0A6A5PZI8
C	0	SER	-	expression tag	UNP A0A6A5PZI8
C	27	GLU	SER	engineered mutation	UNP A0A6A5PZI8
C	49	GLU	GLN	engineered mutation	UNP A0A6A5PZI8
C	51	VAL	ALA	engineered mutation	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLN	deletion	UNP A0A6A5PZI8
C	?	-	ARG	deletion	UNP A0A6A5PZI8
C	?	-	LEU	deletion	UNP A0A6A5PZI8
C	?	-	PRO	deletion	UNP A0A6A5PZI8
C	?	-	ALA	deletion	UNP A0A6A5PZI8
C	?	-	THR	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	MET	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	PRO	deletion	UNP A0A6A5PZI8
C	?	-	LEU	deletion	UNP A0A6A5PZI8
C	?	-	ILE	deletion	UNP A0A6A5PZI8
C	?	-	GLN	deletion	UNP A0A6A5PZI8
C	?	-	LEU	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	GLY	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	GLN	deletion	UNP A0A6A5PZI8
C	?	-	ALA	deletion	UNP A0A6A5PZI8
C	?	-	ILE	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	THR	deletion	UNP A0A6A5PZI8
C	?	-	GLY	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	GLY	deletion	UNP A0A6A5PZI8
C	?	-	ALA	deletion	UNP A0A6A5PZI8
C	?	-	LEU	deletion	UNP A0A6A5PZI8
C	?	-	ASN	deletion	UNP A0A6A5PZI8
C	?	-	PRO	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	TYR	deletion	UNP A0A6A5PZI8
C	?	-	MET	deletion	UNP A0A6A5PZI8
C	?	-	LYS	deletion	UNP A0A6A5PZI8
C	?	-	ARG	deletion	UNP A0A6A5PZI8
C	?	-	PHE	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	LEU	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	ASN	deletion	UNP A0A6A5PZI8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ASP	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	GLY	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	ILE	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	ARG	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	PHE	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	LYS	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	ASP	deletion	UNP A0A6A5PZI8
C	?	-	THR	deletion	UNP A0A6A5PZI8
C	537	GLY	ASP	engineered mutation	UNP A0A6A5PZI8
C	539	CYS	THR	engineered mutation	UNP A0A6A5PZI8
C	540	GLU	VAL	engineered mutation	UNP A0A6A5PZI8
C	541	GLN	LYS	engineered mutation	UNP A0A6A5PZI8
C	553	ARG	SER	engineered mutation	UNP A0A6A5PZI8
C	561	GLU	GLN	engineered mutation	UNP A0A6A5PZI8
C	741	THR	ALA	engineered mutation	UNP A0A6A5PZI8
C	1022	CYS	TYR	engineered mutation	UNP A0A6A5PZI8

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



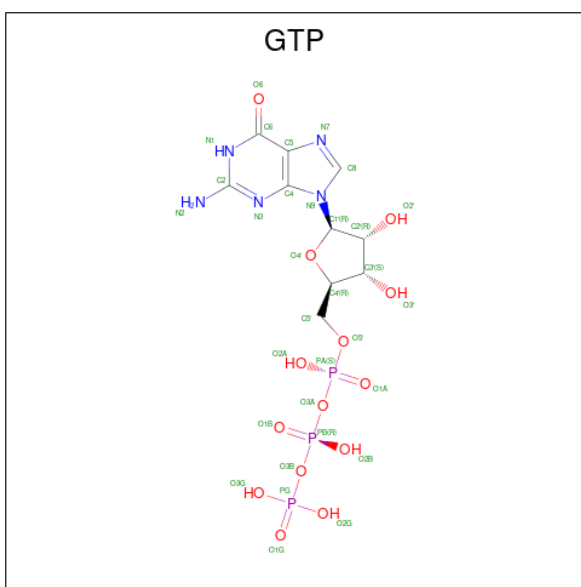
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	
			32	10	5	14	3	

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl		
			1	1	0	0
8	C	3	Total	Cl		
			3	3	0	0

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

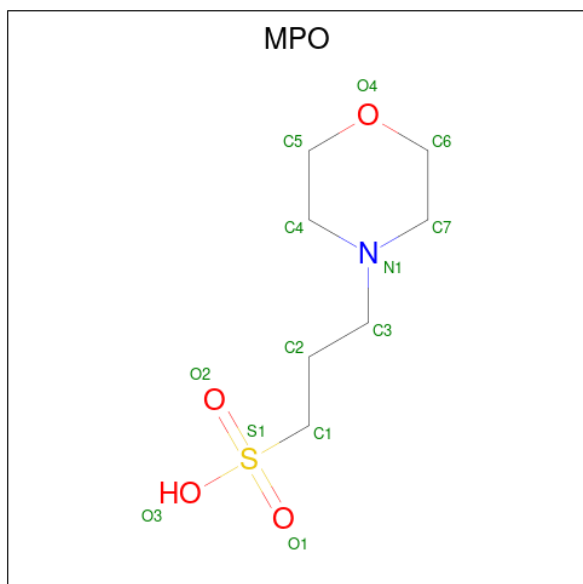
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	Na		
			1	1	0	0

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



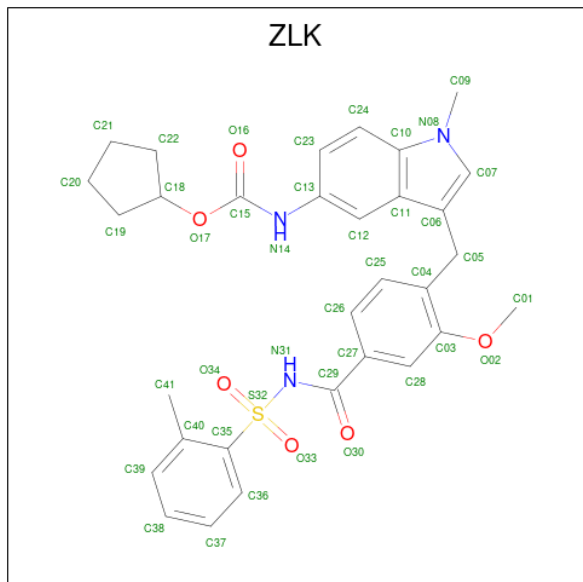
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula: $C_7H_{15}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 12 is zafirlukast (CCD ID: ZLK) (formula: $C_{31}H_{33}N_3O_6S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	N	O	S	0	0
			41	31	3	6	1		

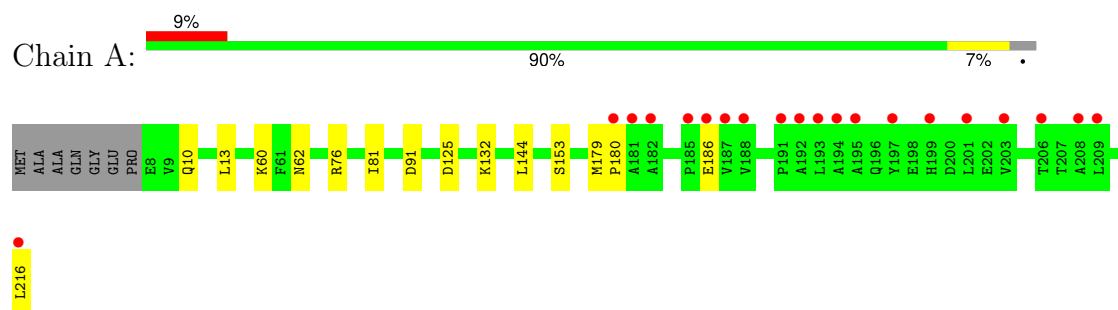
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	110	Total	O	0	0
			110	110		
13	B	27	Total	O	0	0
			27	27		
13	C	399	Total	O	0	0
			399	399		

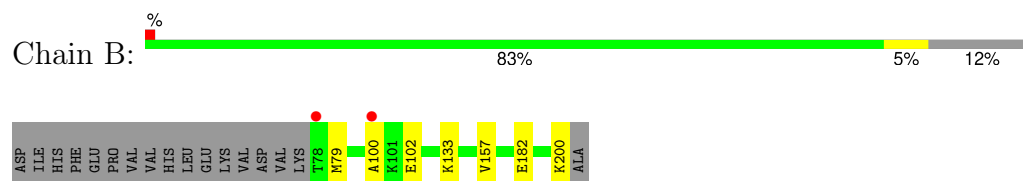
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

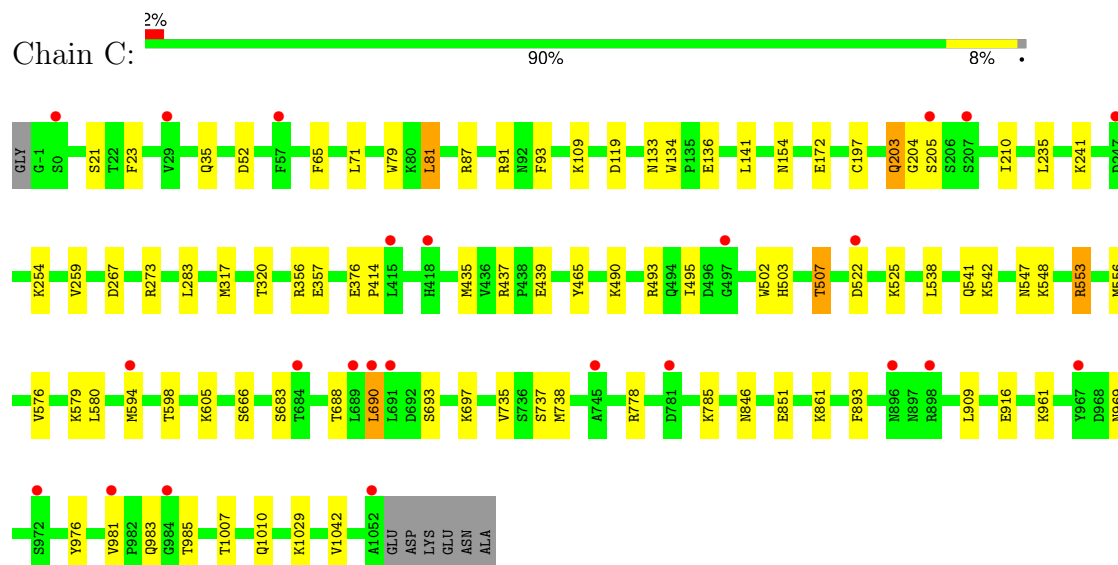
- Molecule 1: GTP-binding nuclear protein Ran



- Molecule 2: YRB1 isoform 1



- Molecule 3: CRM1 isoform 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.78Å 105.78Å 304.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.15 50.01 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.01-2.15) 99.2 (50.01-2.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.183 , 0.216 0.197 , 0.231	Depositor DCC
R_{free} test set	4788 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11451	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: DMS, MG, EDO, MPO, GOL, GTP, ZLK, CL, NA

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	0.59	0/1721	0.98	1/2333 (0.0%)
2	B	0.53	0/1024	0.98	0/1367
3	C	0.55	0/8224	1.05	3/11142 (0.0%)
All	All	0.55	0/10969	1.04	4/14842 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	893	PHE	CB-CA-C	-6.91	98.93	110.68
1	A	91	ASP	CA-CB-CG	5.11	117.71	112.60
3	C	52	ASP	CA-C-N	5.02	126.97	120.44
3	C	52	ASP	C-N-CA	5.02	126.97	120.44

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	1680	0	1677	11	0
2	B	1007	0	1008	3	0
3	C	8068	0	8158	52	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	8	0	12	0	0
5	C	16	0	24	2	0
6	A	16	0	24	4	0
6	C	16	0	24	0	0
7	A	32	0	12	0	0
8	A	1	0	0	0	0
8	C	3	0	0	0	0
9	C	1	0	0	0	0
10	C	12	0	16	1	0
11	C	13	0	14	4	0
12	C	41	0	0	0	0
13	A	110	0	0	1	0
13	B	27	0	0	0	0
13	C	399	0	0	6	0
All	All	11451	0	10969	63	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 3.

All (63) 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:C:556[B]:MET:HE3	3:C:556[B]:MET:HA	1.45	0.98
3:C:503:HIS:O	3:C:507:THR:HG23	1.66	0.95
3:C:556[A]:MET:HE3	3:C:594[A]:MET:CG	2.17	0.74
3:C:356:ARG:HA	10:C:1106:GOL:H12	1.72	0.71
3:C:197[A]:CYS:SG	13:C:1226:HOH:O	2.49	0.69
3:C:735:VAL:HA	3:C:738:MET:HE3	1.73	0.69
3:C:556[A]:MET:HE3	3:C:594[A]:MET:HG3	1.75	0.69
1:A:179:MET:HE3	2:B:133:LYS:HG2	1.74	0.68
3:C:317:MET:SD	11:C:1112:MPO:H21	2.34	0.68
3:C:542:LYS:O	3:C:548:LYS:HE2	1.95	0.67
3:C:846:ASN:HB2	5:C:1107:DMS:H21	1.78	0.64
3:C:320:THR:HB	11:C:1112:MPO:H61	1.80	0.64
1:A:10:GLN:OE1	1:A:62[B]:ASN:ND2	2.25	0.62
3:C:556[B]:MET:HE3	3:C:556[B]:MET:CA	2.24	0.62
3:C:556[B]:MET:HA	3:C:556[B]:MET:CE	2.23	0.59
3:C:502:TRP:HE1	3:C:547:ASN:HD22	1.48	0.59
3:C:556[A]:MET:HE3	3:C:594[A]:MET:HG2	1.85	0.58
3:C:683:SER:OG	3:C:690:LEU:HD23	2.04	0.58
3:C:1029:LYS:NZ	13:C:1205:HOH:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:503:HIS:O	3:C:507:THR:CG2	2.50	0.55
3:C:435:MET:HE1	3:C:465:TYR:CD1	2.41	0.55
3:C:553:ARG:HD3	3:C:594[A]:MET:HG2	1.88	0.55
3:C:435:MET:HE1	3:C:465:TYR:CE1	2.41	0.55
6:A:309:EDO:H21	3:C:357:GLU:HB2	1.89	0.53
3:C:556[B]:MET:HE1	3:C:576:VAL:HG13	1.91	0.53
3:C:553:ARG:HB2	3:C:553:ARG:HH21	1.74	0.53
3:C:693:SER:O	3:C:697:LYS:HG3	2.09	0.52
1:A:125:ASP:HA	6:A:305:EDO:H12	1.93	0.51
3:C:273:ARG:NH1	13:C:1202:HOH:O	2.33	0.50
3:C:141:LEU:C	3:C:141:LEU:HD23	2.36	0.49
3:C:204:GLY:HA2	3:C:210:ILE:HD11	1.95	0.49
3:C:119:ASP:OD2	3:C:154:ASN:ND2	2.44	0.48
3:C:79:TRP:NE1	3:C:87:ARG:HD2	2.29	0.48
1:A:144:LEU:O	6:A:309:EDO:H22	2.13	0.48
1:A:180:PRO:HB3	2:B:79:MET:HG3	1.96	0.47
3:C:81:LEU:HD13	3:C:1042:VAL:HG11	1.96	0.47
3:C:235:LEU:HD21	3:C:259:VAL:HG11	1.97	0.47
3:C:556[B]:MET:HE2	3:C:598:THR:HG21	1.96	0.46
2:B:100:ALA:O	2:B:102:GLU:N	2.47	0.46
3:C:502:TRP:HE1	3:C:547:ASN:ND2	2.11	0.46
3:C:1007:THR:H	3:C:1010:GLN:HE21	1.64	0.45
3:C:241:LYS:NZ	13:C:1216:HOH:O	2.48	0.45
3:C:495:ILE:HG23	3:C:541:GLN:HE22	1.82	0.45
11:C:1112:MPO:H42	13:C:1563:HOH:O	2.17	0.44
3:C:203:GLN:HE21	3:C:203:GLN:CA	2.31	0.44
1:A:81:ILE:HD11	3:C:65:PHE:CD1	2.54	0.43
1:A:10:GLN:HA	1:A:60:LYS:O	2.19	0.43
3:C:254:LYS:NZ	13:C:1228:HOH:O	2.52	0.42
1:A:153:SER:OG	6:A:305:EDO:H11	2.19	0.42
3:C:437:ARG:HD3	3:C:439:GLU:HB2	2.01	0.42
3:C:556[B]:MET:HE2	3:C:580:LEU:HD21	2.02	0.42
1:A:76:ARG:HD2	13:A:415:HOH:O	2.18	0.42
3:C:93:PHE:CD1	5:C:1111:DMS:H11	2.55	0.42
3:C:376:GLU:HA	3:C:414:PRO:HD3	1.91	0.41
3:C:556[A]:MET:CE	3:C:594[A]:MET:CG	2.93	0.41
1:A:81:ILE:HD11	3:C:65:PHE:CG	2.54	0.41
1:A:13:LEU:C	1:A:13:LEU:HD23	2.45	0.41
3:C:23:PHE:CE1	3:C:35:GLN:HG2	2.56	0.41
3:C:317:MET:SD	11:C:1112:MPO:C2	3.05	0.41
3:C:91:ARG:HG3	3:C:134:TRP:CZ3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:916:GLU:OE1	3:C:961:LYS:NZ	2.41	0.40
3:C:356:ARG:HA	3:C:356:ARG:HD3	2.00	0.40
3:C:976:TYR:OH	3:C:985:THR:O	2.38	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	208/216 (96%)	204 (98%)	4 (2%)	0	100	100
2	B	121/140 (86%)	112 (93%)	9 (7%)	0	100	100
3	C	997/1003 (99%)	980 (98%)	16 (2%)	1 (0%)	48	50
All	All	1326/1359 (98%)	1296 (98%)	29 (2%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	205	SER

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	181/184 (98%)	178 (98%)	3 (2%)	53	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	105/121 (87%)	102 (97%)	3 (3%)	37	39
3	C	913/915 (100%)	882 (97%)	31 (3%)	32	33
All	All	1199/1220 (98%)	1162 (97%)	37 (3%)	35	37

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	LYS
1	A	186	GLU
1	A	216	LEU
2	B	157	VAL
2	B	182	GLU
2	B	200	LYS
3	C	21	SER
3	C	71	LEU
3	C	81	LEU
3	C	109	LYS
3	C	133	ASN
3	C	136	GLU
3	C	172	GLU
3	C	203	GLN
3	C	267	ASP
3	C	283	LEU
3	C	490	LYS
3	C	493	ARG
3	C	507	THR
3	C	522	ASP
3	C	525	LYS
3	C	538	LEU
3	C	553	ARG
3	C	579	LYS
3	C	605	LYS
3	C	666	SER
3	C	688	THR
3	C	690	LEU
3	C	737	SER
3	C	778	ARG
3	C	785	LYS
3	C	851	GLU
3	C	861	LYS
3	C	909	LEU

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Mol	Chain	Res	Type
3	C	969	ASN
3	C	981	VAL
3	C	983	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
3	C	30	GLN
3	C	35	GLN
3	C	203	GLN
3	C	233	ASN
3	C	274	GLN
3	C	345	GLN
3	C	426	GLN
3	C	494	GLN
3	C	541	GLN
3	C	547	ASN
3	C	928	HIS
3	C	1010	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 6 are monoatomic - leaving 19 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	A	302	-	3,3,3	0.25	0	3,3,3	0.06	0
6	EDO	C	1114	-	3,3,3	0.12	0	2,2,2	0.03	0
5	DMS	C	1110	-	3,3,3	0.29	0	3,3,3	0.15	0
6	EDO	C	1115	-	3,3,3	0.11	0	2,2,2	0.24	0
5	DMS	C	1107	-	3,3,3	0.32	0	3,3,3	0.19	0
6	EDO	A	304	-	3,3,3	0.27	0	2,2,2	0.31	0
6	EDO	A	309	-	3,3,3	0.26	0	2,2,2	0.35	0
10	GOL	C	1109	-	5,5,5	0.15	0	5,5,5	0.49	0
5	DMS	C	1111	9	3,3,3	0.22	0	3,3,3	0.08	0
10	GOL	C	1106	-	5,5,5	0.14	0	5,5,5	0.43	0
6	EDO	C	1113	-	3,3,3	0.12	0	2,2,2	0.19	0
6	EDO	C	1105	-	3,3,3	0.31	0	2,2,2	0.63	0
11	MPO	C	1112	-	13,13,13	1.22	1 (7%)	17,17,17	1.19	2 (11%)
6	EDO	A	305	-	3,3,3	0.03	0	2,2,2	0.10	0
5	DMS	A	303	-	3,3,3	0.23	0	3,3,3	0.11	0
6	EDO	A	306	-	3,3,3	0.07	0	2,2,2	0.13	0
12	ZLK	C	1116	-	45,45,45	3.07	22 (48%)	64,65,65	3.42	23 (35%)
7	GTP	A	307	4	33,34,34	1.15	4 (12%)	50,54,54	0.56	0
5	DMS	C	1108	-	3,3,3	0.25	0	3,3,3	0.08	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
10	GOL	C	1106	-	-	4/4/4/4	-
11	MPO	C	1112	-	-	5/7/15/15	0/1/1/1
6	EDO	C	1113	-	-	1/1/1/1	-
6	EDO	A	305	-	-	1/1/1/1	-
6	EDO	C	1105	-	-	1/1/1/1	-
6	EDO	A	304	-	-	1/1/1/1	-
6	EDO	C	1114	-	-	1/1/1/1	-
6	EDO	A	306	-	-	0/1/1/1	-
12	ZLK	C	1116	-	-	6/29/36/36	0/5/5/5
6	EDO	A	309	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	C	1109	-	-	0/4/4/4	-
6	EDO	C	1115	-	-	1/1/1/1	-
7	GTP	A	307	4	-	3/22/38/38	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	1116	ZLK	C35-S32	6.88	1.87	1.77
12	C	1116	ZLK	O17-C15	6.58	1.46	1.35
12	C	1116	ZLK	C05-C04	6.45	1.60	1.51
12	C	1116	ZLK	O33-S32	6.21	1.50	1.43
12	C	1116	ZLK	C15-N14	5.47	1.47	1.36
12	C	1116	ZLK	C29-N31	4.83	1.44	1.39
12	C	1116	ZLK	C40-C35	4.32	1.45	1.40
12	C	1116	ZLK	C41-C40	4.17	1.58	1.51
11	C	1112	MPO	O2-S1	4.01	1.56	1.45
12	C	1116	ZLK	S32-N31	3.90	1.73	1.64
12	C	1116	ZLK	O02-C03	3.83	1.43	1.37
12	C	1116	ZLK	C13-N14	3.49	1.48	1.41
12	C	1116	ZLK	C36-C35	3.49	1.43	1.39
12	C	1116	ZLK	C20-C19	-3.46	1.37	1.51
12	C	1116	ZLK	C24-C10	3.46	1.45	1.39
12	C	1116	ZLK	C11-C10	-3.27	1.36	1.41
12	C	1116	ZLK	C19-C18	3.21	1.68	1.52
7	A	307	GTP	PG-O3G	-3.05	1.43	1.54
12	C	1116	ZLK	C28-C03	3.02	1.44	1.38
12	C	1116	ZLK	O34-S32	3.01	1.47	1.43
12	C	1116	ZLK	C22-C18	-2.67	1.38	1.52
7	A	307	GTP	PG-O2G	-2.64	1.45	1.54
12	C	1116	ZLK	C05-C06	2.60	1.57	1.50
7	A	307	GTP	PG-O1G	-2.48	1.42	1.50
12	C	1116	ZLK	C27-C29	2.41	1.55	1.50
12	C	1116	ZLK	C21-C22	2.39	1.61	1.51
7	A	307	GTP	PB-O2B	-2.29	1.44	1.55

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	1116	ZLK	O34-S32-O33	-17.21	98.62	119.52
12	C	1116	ZLK	O17-C15-N14	10.98	122.47	108.97
12	C	1116	ZLK	C36-C35-C40	-6.19	115.56	121.17
12	C	1116	ZLK	C05-C04-C03	5.02	125.68	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	1116	ZLK	O34-S32-C35	4.77	115.56	107.68
12	C	1116	ZLK	C29-N31-S32	4.46	129.22	123.38
12	C	1116	ZLK	C13-N14-C15	-4.29	119.60	126.39
12	C	1116	ZLK	C39-C40-C35	4.28	120.78	116.27
12	C	1116	ZLK	O33-S32-C35	4.08	114.41	107.68
12	C	1116	ZLK	C18-O17-C15	4.06	122.32	116.52
12	C	1116	ZLK	C24-C10-C11	-3.96	117.53	121.95
12	C	1116	ZLK	O17-C15-O16	-3.82	118.94	124.55
12	C	1116	ZLK	O02-C03-C04	3.66	121.41	115.96
12	C	1116	ZLK	O16-C15-N14	-3.55	118.59	126.12
12	C	1116	ZLK	C05-C04-C25	-3.32	114.64	120.06
12	C	1116	ZLK	C40-C35-S32	3.08	124.74	122.02
12	C	1116	ZLK	C24-C10-N08	2.94	133.92	129.91
12	C	1116	ZLK	C41-C40-C39	-2.89	114.70	120.28
12	C	1116	ZLK	C28-C03-C04	-2.39	118.02	120.49
11	C	1112	MPO	C6-C7-N1	2.32	113.65	110.12
12	C	1116	ZLK	C23-C13-C12	-2.27	116.91	119.66
11	C	1112	MPO	O3-S1-O1	2.15	116.78	111.40
12	C	1116	ZLK	C05-C06-C07	2.12	130.77	127.04
12	C	1116	ZLK	C37-C36-C35	2.12	122.56	118.76
12	C	1116	ZLK	O02-C03-C28	-2.04	120.56	124.08

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	1106	GOL	O1-C1-C2-C3
10	C	1106	GOL	C1-C2-C3-O3
12	C	1116	ZLK	C19-C18-O17-C15
12	C	1116	ZLK	C40-C35-S32-O33
11	C	1112	MPO	C2-C1-S1-O3
12	C	1116	ZLK	C29-N31-S32-C35
10	C	1106	GOL	O1-C1-C2-O2
12	C	1116	ZLK	C36-C35-S32-O33
11	C	1112	MPO	C2-C3-N1-C4
12	C	1116	ZLK	C40-C35-S32-N31
11	C	1112	MPO	C2-C3-N1-C7
12	C	1116	ZLK	C36-C35-S32-N31
6	C	1113	EDO	O1-C1-C2-O2
11	C	1112	MPO	C2-C1-S1-O1
11	C	1112	MPO	C2-C1-S1-O2
10	C	1106	GOL	O2-C2-C3-O3

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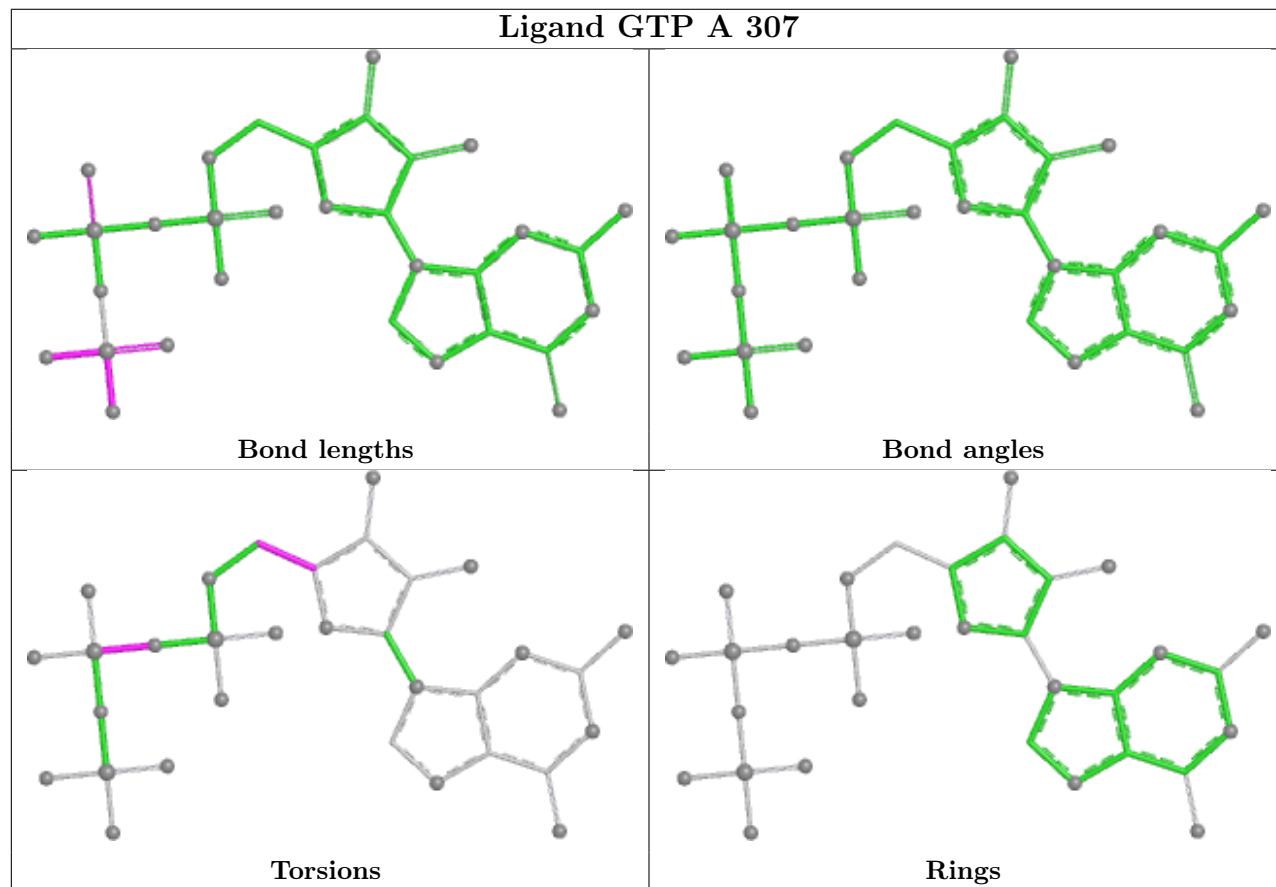
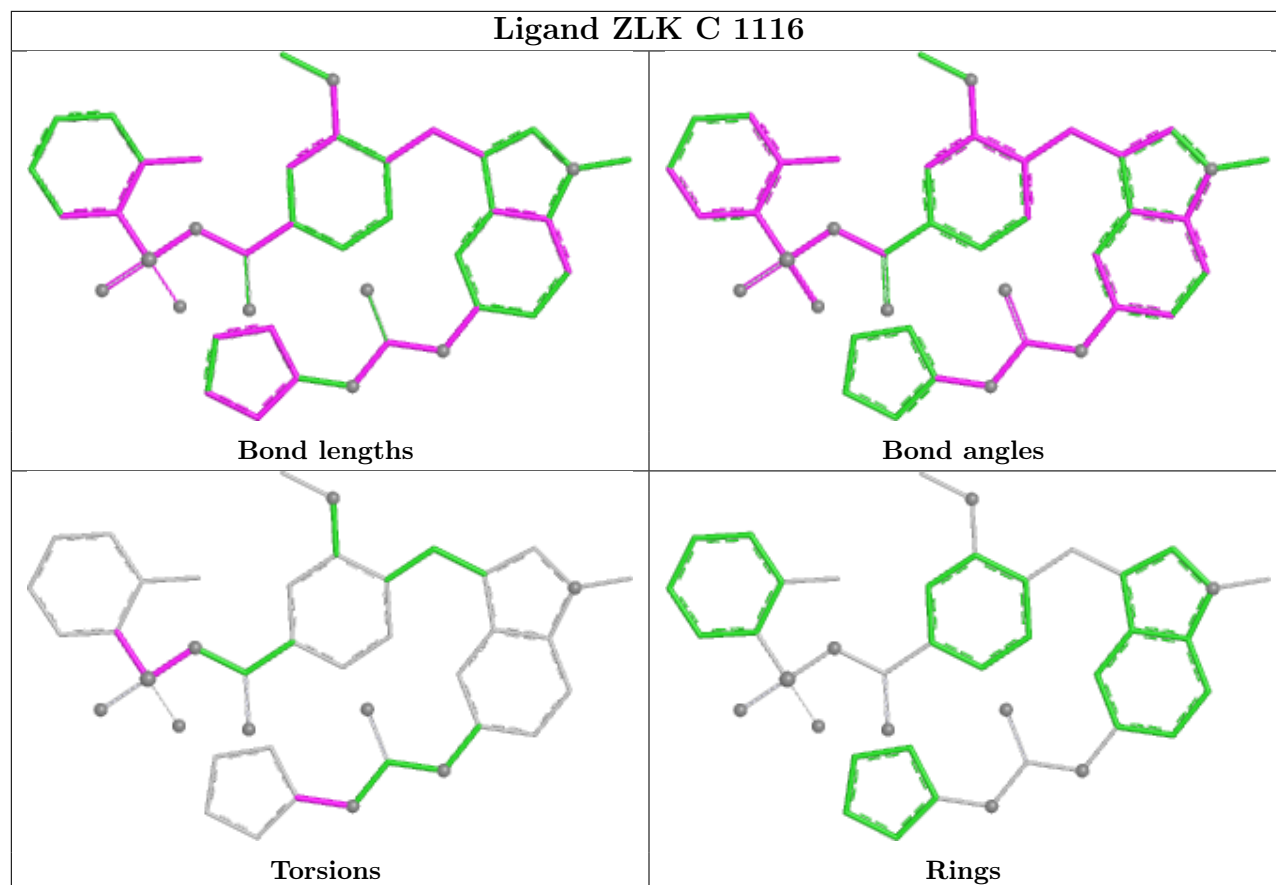
Mol	Chain	Res	Type	Atoms
6	C	1115	EDO	O1-C1-C2-O2
7	A	307	GTP	PA-O3A-PB-O2B
6	A	304	EDO	O1-C1-C2-O2
7	A	307	GTP	O4'-C4'-C5'-O5'
6	A	305	EDO	O1-C1-C2-O2
6	C	1105	EDO	O1-C1-C2-O2
6	C	1114	EDO	O1-C1-C2-O2
7	A	307	GTP	PA-O3A-PB-O1B

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1107	DMS	1	0
6	A	309	EDO	2	0
5	C	1111	DMS	1	0
10	C	1106	GOL	1	0
11	C	1112	MPO	4	0
6	A	305	EDO	2	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, 95th 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 ²)	Q < 0.9
1	A	209/216 (96%)	0.53	20 (9%)	13 15	25, 49, 129, 156	1 (0%)
2	B	123/140 (87%)	0.52	2 (1%)	70 74	52, 64, 96, 109	0
3	C	996/1003 (99%)	0.36	24 (2%)	59 63	25, 54, 84, 116	3 (0%)
All	All	1328/1359 (97%)	0.40	46 (3%)	47 51	25, 55, 91, 156	4 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	192	ALA	5.1
1	A	191	PRO	5.1
1	A	195	ALA	4.7
1	A	193	LEU	4.5
3	C	0	SER	4.2
3	C	691	LEU	4.0
1	A	203	VAL	3.8
1	A	187	VAL	3.6
2	B	100	ALA	3.4
1	A	188	VAL	3.3
1	A	216	LEU	3.3
3	C	1052	ALA	3.2
1	A	197	TYR	3.1
3	C	522	ASP	3.0
3	C	689	LEU	2.9
3	C	896	ASN	2.9
1	A	201	LEU	2.7
1	A	194	ALA	2.7
3	C	745	ALA	2.6
1	A	185	PRO	2.6
1	A	209	LEU	2.6
3	C	898	ARG	2.6
1	A	182	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	418	HIS	2.5
3	C	497	GLY	2.5
3	C	972	SER	2.4
1	A	208	ALA	2.4
3	C	984	GLY	2.3
2	B	78	THR	2.3
3	C	684	THR	2.3
3	C	247	ASP	2.2
1	A	186	GLU	2.2
3	C	415	LEU	2.2
3	C	594[A]	MET	2.2
3	C	29	VAL	2.2
3	C	981	VAL	2.1
1	A	199	HIS	2.1
3	C	967	TYR	2.1
3	C	57	PHE	2.1
1	A	181	ALA	2.1
3	C	690	LEU	2.1
1	A	206	THR	2.1
3	C	205	SER	2.1
3	C	207	SER	2.1
3	C	781	ASP	2.0
1	A	180	PRO	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 oligosaccharides 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, 95th 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.

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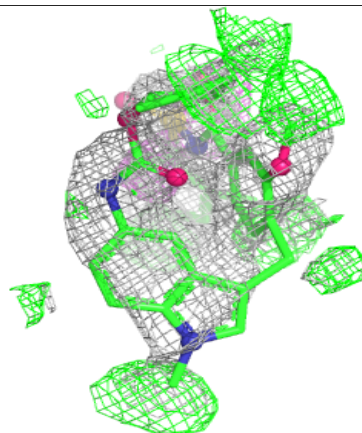
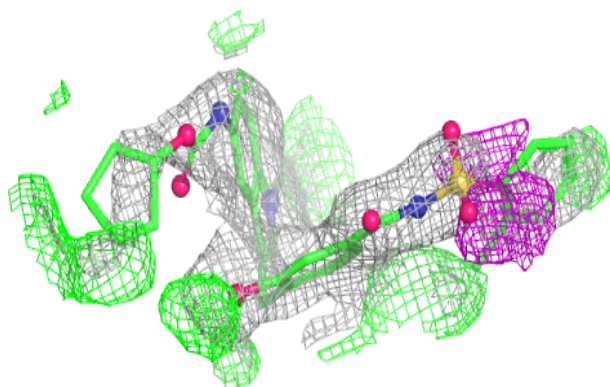
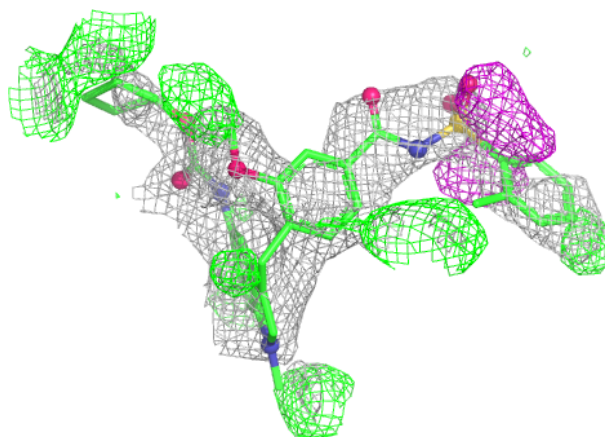
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	C	1108	4/4	0.60	0.23	99,99,100,100	0
5	DMS	A	302	4/4	0.63	0.32	99,104,105,106	0
12	ZLK	C	1116	41/41	0.67	0.27	104,126,135,143	0
5	DMS	A	303	4/4	0.68	0.28	97,99,102,105	0
9	NA	C	1104	1/1	0.75	0.12	99,99,99,99	0
5	DMS	C	1110	4/4	0.75	0.29	95,97,100,109	0
6	EDO	C	1115	4/4	0.78	0.25	86,88,89,89	0
5	DMS	C	1107	4/4	0.78	0.22	95,97,98,99	0
6	EDO	A	305	4/4	0.78	0.20	70,71,74,76	0
5	DMS	C	1111	4/4	0.84	0.27	121,122,123,123	0
6	EDO	A	304	4/4	0.84	0.21	68,69,69,71	0
10	GOL	C	1109	6/6	0.88	0.15	77,78,80,80	0
6	EDO	A	309	4/4	0.89	0.17	57,62,64,64	0
11	MPO	C	1112	13/13	0.89	0.15	56,60,63,63	0
10	GOL	C	1106	6/6	0.89	0.13	67,76,78,78	0
6	EDO	C	1105	4/4	0.90	0.13	55,57,58,62	0
8	CL	A	308	1/1	0.90	0.15	87,87,87,87	0
8	CL	C	1103	1/1	0.90	0.15	82,82,82,82	0
6	EDO	C	1114	4/4	0.90	0.12	80,81,81,82	0
6	EDO	C	1113	4/4	0.91	0.12	70,71,73,75	0
6	EDO	A	306	4/4	0.91	0.10	78,79,79,85	0
7	GTP	A	307	32/32	0.95	0.09	20,20,20,20	0
8	CL	C	1102	1/1	0.95	0.10	92,92,92,92	0
8	CL	C	1101	1/1	0.96	0.11	79,79,79,79	0
4	MG	A	301	1/1	0.99	0.04	40,40,40,40	0

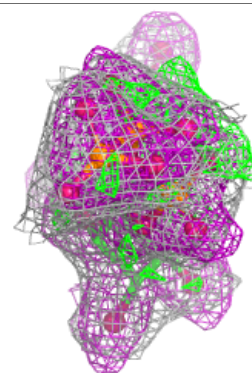
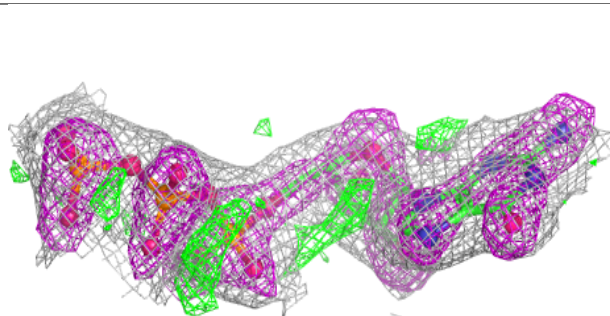
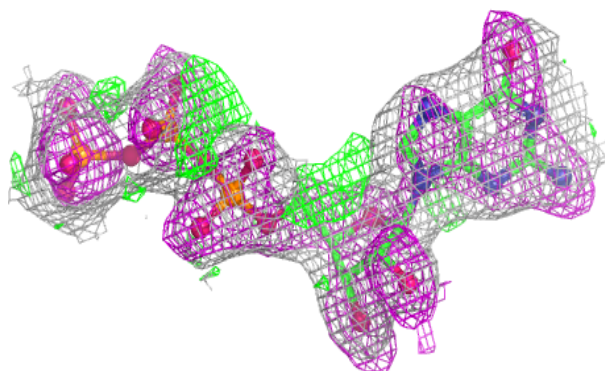
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZLK C 1116:

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

**Electron density around GTP A 307:**

$2mF_o-DF_c$ (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.