Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 07:38 AM EDT

PDB ID	:	6O8U
Title	:	Crystal structure of IRAK4 in complex with compound 23
Authors	:	Kiefer, J.R.; Yu, C.; Drobnick, J.; Bryan, M.C.; Lupardus, P.J.
Deposited on	:	2019-03-12
Resolution	:	1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

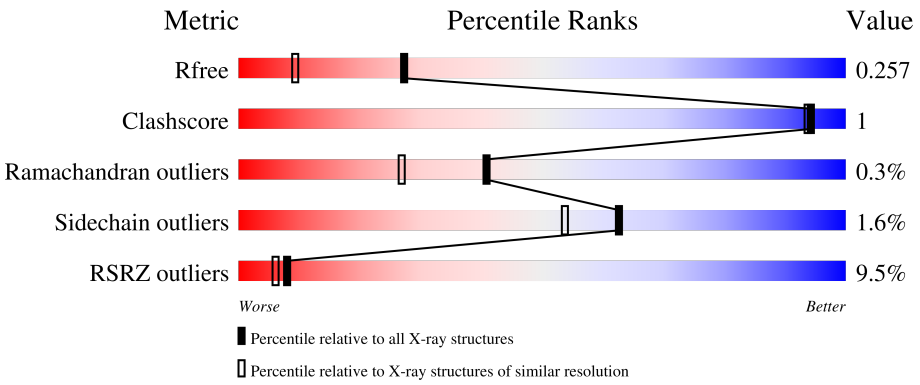
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 >=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 <=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	305	12% 89% • • 7%
1	B	305	10% 88% 6% 6%
1	C	305	7% 90% 6% •
1	D	305	6% 91% • 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9672 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.

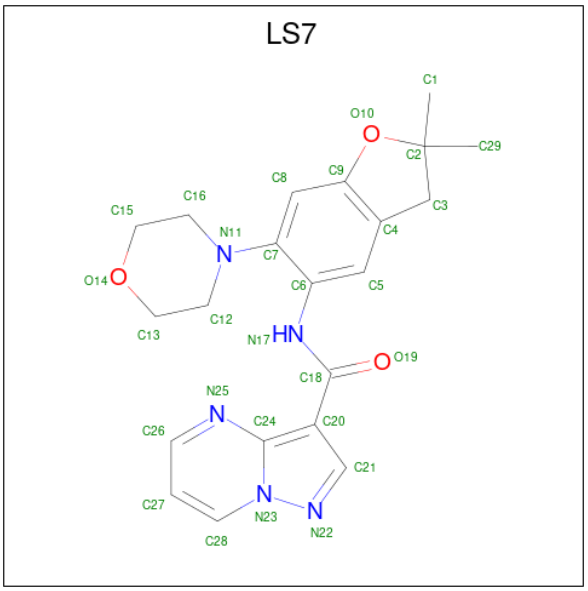
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	283	2234	1404	374	440	2	14	0	5	0
1	B	286	2257	1411	377	453	2	14	0	3	0
1	C	292	2319	1456	391	454	2	16	0	4	0
1	D	290	2257	1418	381	441	2	15	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

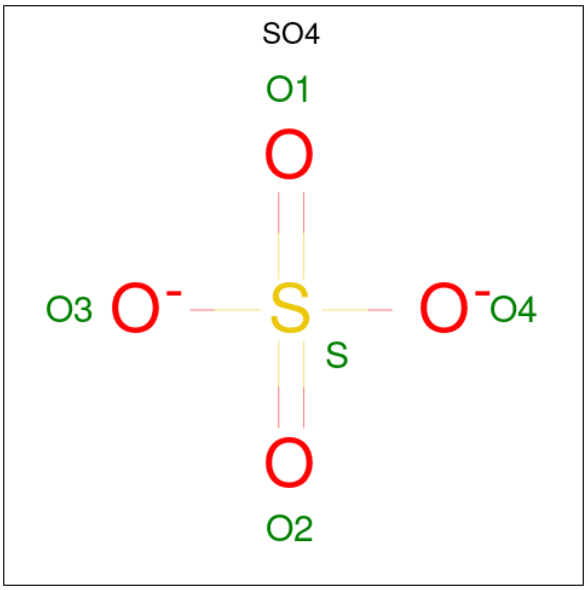
Chain	Residue	Modelled	Actual	Comment	Reference
A	159	SER	-	expression tag	UNP Q9NWZ3
A	461	GLY	-	expression tag	UNP Q9NWZ3
A	462	ASN	-	expression tag	UNP Q9NWZ3
A	463	SER	-	expression tag	UNP Q9NWZ3
B	159	SER	-	expression tag	UNP Q9NWZ3
B	461	GLY	-	expression tag	UNP Q9NWZ3
B	462	ASN	-	expression tag	UNP Q9NWZ3
B	463	SER	-	expression tag	UNP Q9NWZ3
C	159	SER	-	expression tag	UNP Q9NWZ3
C	461	GLY	-	expression tag	UNP Q9NWZ3
C	462	ASN	-	expression tag	UNP Q9NWZ3
C	463	SER	-	expression tag	UNP Q9NWZ3
D	159	SER	-	expression tag	UNP Q9NWZ3
D	461	GLY	-	expression tag	UNP Q9NWZ3
D	462	ASN	-	expression tag	UNP Q9NWZ3
D	463	SER	-	expression tag	UNP Q9NWZ3

- Molecule 2 is N-[2,2-dimethyl-6-(morpholin-4-yl)-2,3-dihydro-1-benzofuran-5-yl]pyrazolo[1,5-a]pyrimidine-3-carboxamide (three-letter code: LS7) (formula: $C_{21}H_{23}N_5O_3$).



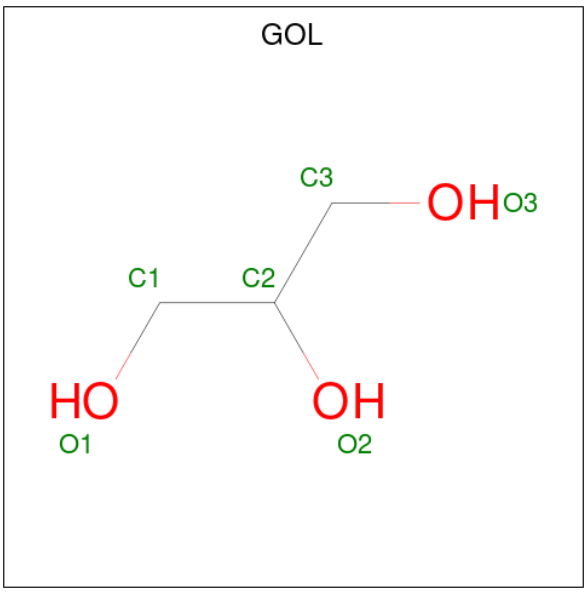
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	29	21	5	3	0	0
			Total	C	N	O		
2	B	1	29	21	5	3	0	0
			Total	C	N	O		
2	C	1	29	21	5	3	0	0
			Total	C	N	O		
2	D	1	29	21	5	3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0
3	B	1	5	4	1	0	0
3	C	1	5	4	1	0	0
3	D	1	5	4	1	0	0
3	D	1	5	4	1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

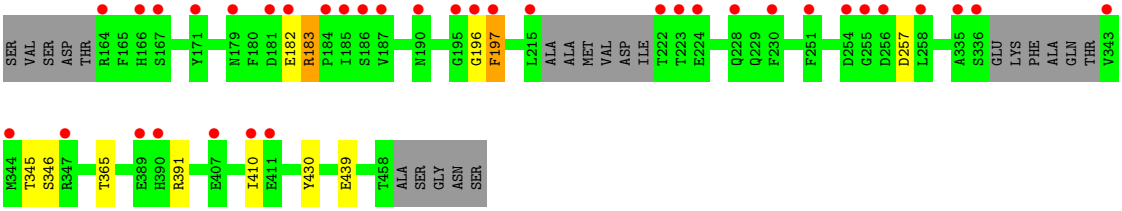
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	113	113	113	0	0
5	B	106	108	108	0	2
5	C	110	112	112	0	2
5	D	125	125	125	0	0

3 Residue-property plots (i)

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

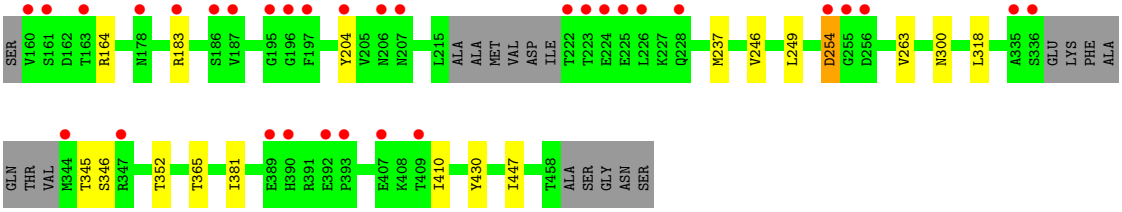
• Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain A:



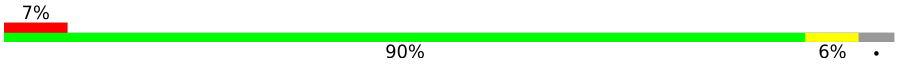
• Molecule 1: Interleukin-1 receptor-associated kinase 4

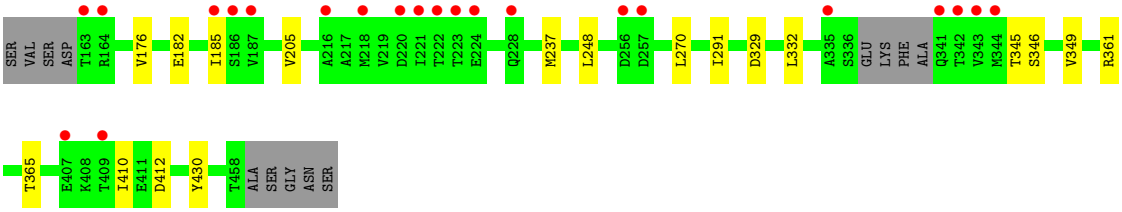
Chain B:



• Molecule 1: Interleukin-1 receptor-associated kinase 4

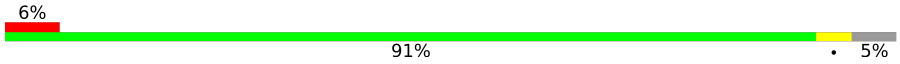
Chain C:

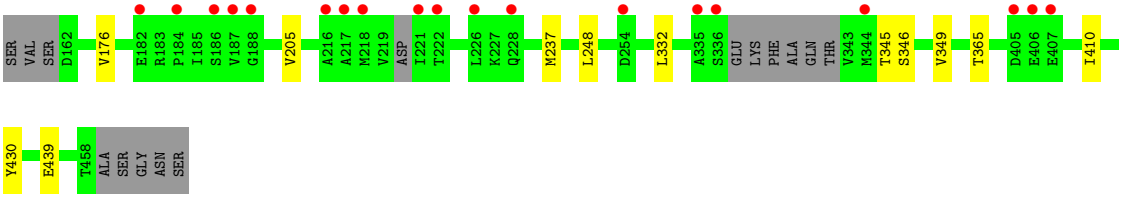




• Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain D:




SER
VAL
SER
D162
V176
E182
R183
P184
I185
S186
V187
G188
V205
A216
A217
M218
V219
ASP
I221
T222
L226
K227
Q228
M237
L248
D254
L332
A335
S336
GLU
LYS
PHE
ALA
GLN
THR
V343
M344
T345
S346
V349
T365
D405
E406
E407
I410

Y430
E439
T458
ALA
SER
GLY
ASN
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.12Å 140.51Å 87.52Å 90.00° 123.97° 90.00°	Depositor
Resolution (Å)	35.00 – 1.80 34.94 – 1.80	Depositor EDS
% Data completeness (in resolution range)	89.1 (35.00-1.80) 89.1 (34.94-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.231 , 0.255 0.234 , 0.257	Depositor DCC
R_{free} test set	5765 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	28.6	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9672	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: LS7, SO4, SEP, GOL, TPO

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	0.36	0/2250	0.54	0/3036
1	B	0.35	0/2273	0.55	0/3070
1	C	0.36	0/2335	0.56	0/3149
1	D	0.36	0/2272	0.57	0/3063
All	All	0.36	0/9130	0.56	0/12318

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	182	GLU	Peptide
1	A	183	ARG	Peptide

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	2234	0	2157	6	0
1	B	2257	0	2165	7	0
1	C	2319	0	2284	8	0
1	D	2257	0	2210	4	0
2	A	29	0	0	0	0
2	B	29	0	0	0	0
2	C	29	0	0	0	0
2	D	29	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
4	A	6	0	8	0	0
5	A	113	0	0	0	0
5	B	108	0	0	0	0
5	C	112	0	0	0	0
5	D	125	0	0	0	0
All	All	9672	0	8824	24	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 1.

All (24) 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:A:196[B]:GLY:O	1:A:197[B]:PHE:CD2	1.74	1.40
1:A:196[B]:GLY:O	1:A:197[B]:PHE:CG	2.06	1.08
1:C:205[B]:VAL:O	1:C:205[B]:VAL:HG23	1.93	0.68
1:B:237:MET:HE1	1:B:246:VAL:HG23	1.78	0.66
1:D:176:VAL:HG21	1:D:205:VAL:HG22	1.81	0.61
1:D:237:MET:HE2	1:D:248:LEU:HB2	1.87	0.57
1:C:205[B]:VAL:O	1:C:205[B]:VAL:CG2	2.52	0.57
1:B:410:ILE:HD13	1:B:430:TYR:CD1	2.48	0.49
1:C:332:LEU:HD22	1:C:349:VAL:HG21	1.93	0.48
1:B:249:LEU:HD21	1:B:263:VAL:HG22	1.97	0.47
1:B:246:VAL:HG11	1:B:318:LEU:HD12	1.98	0.45
1:D:332:LEU:HD22	1:D:349:VAL:HG21	1.99	0.45
1:C:237:MET:HE2	1:C:248:LEU:HB2	1.99	0.45
1:C:410:ILE:HD13	1:C:430:TYR:CD1	2.53	0.43
1:A:410:ILE:HD13	1:A:430:TYR:CD1	2.53	0.43
1:A:196[B]:GLY:O	1:A:197[B]:PHE:CB	2.60	0.42
1:D:410:ILE:HD13	1:D:430:TYR:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196[B]:GLY:C	1:A:197[B]:PHE:CG	2.90	0.41
1:B:300:ASN:HA	1:B:447:ILE:HG21	2.02	0.41
1:B:352:THR:CG2	1:C:361:ARG:HA	2.51	0.41
1:A:196[B]:GLY:O	1:A:197[B]:PHE:CE2	2.57	0.41
1:C:176:VAL:HG21	1:C:205[B]:VAL:HG12	2.03	0.40
1:C:270:LEU:HD13	1:C:291:ILE:HG21	2.02	0.40
1:B:381:ILE:HG21	1:B:410:ILE:HD11	2.02	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	280/305 (92%)	264 (94%)	13 (5%)	3 (1%)	14 4
1	B	281/305 (92%)	273 (97%)	7 (2%)	1 (0%)	34 21
1	C	290/305 (95%)	284 (98%)	6 (2%)	0	100 100
1	D	282/305 (92%)	279 (99%)	3 (1%)	0	100 100
All	All	1133/1220 (93%)	1100 (97%)	29 (3%)	4 (0%)	41 21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	ARG
1	A	197[A]	PHE
1	A	197[B]	PHE
1	B	254	ASP

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	239/263 (91%)	234 (98%)	5 (2%)	53	42
1	B	245/263 (93%)	240 (98%)	5 (2%)	55	44
1	C	253/263 (96%)	248 (98%)	5 (2%)	55	44
1	D	243/263 (92%)	241 (99%)	2 (1%)	81	78
All	All	980/1052 (93%)	963 (98%)	17 (2%)	62	51

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	ASP
1	A	365	THR
1	A	391	ARG
1	A	439[A]	GLU
1	A	439[B]	GLU
1	B	164	ARG
1	B	183	ARG
1	B	204	TYR
1	B	254	ASP
1	B	365	THR
1	C	182	GLU
1	C	185	ILE
1	C	329	ASP
1	C	365	THR
1	C	412	ASP
1	D	365	THR
1	D	439	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	241	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)

8 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	SEP	B	346	1	8,9,10	0.63	0	8,12,14	1.48	1 (12%)
1	TPO	A	345	1	8,10,11	0.90	0	10,14,16	1.04	1 (10%)
1	TPO	D	345	1	8,10,11	0.90	0	10,14,16	1.13	1 (10%)
1	SEP	C	346	1	8,9,10	0.61	0	8,12,14	1.35	1 (12%)
1	SEP	D	346	1	8,9,10	0.63	0	8,12,14	1.39	1 (12%)
1	TPO	C	345	1	8,10,11	0.93	0	10,14,16	1.07	1 (10%)
1	SEP	A	346	1	8,9,10	0.62	0	8,12,14	1.35	1 (12%)
1	TPO	B	345	1	8,10,11	0.83	0	10,14,16	1.32	1 (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
1	SEP	B	346	1	-	1/5/8/10	-
1	TPO	A	345	1	-	3/9/11/13	-
1	TPO	D	345	1	-	2/9/11/13	-
1	SEP	C	346	1	-	0/5/8/10	-
1	SEP	D	346	1	-	3/5/8/10	-
1	TPO	C	345	1	-	3/9/11/13	-
1	SEP	A	346	1	-	0/5/8/10	-
1	TPO	B	345	1	-	2/9/11/13	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	345	TPO	P-OG1-CB	-3.57	112.42	123.21
1	B	346	SEP	OG-CB-CA	3.00	111.07	108.14
1	D	346	SEP	OG-CB-CA	2.72	110.79	108.14
1	C	345	TPO	P-OG1-CB	-2.57	115.45	123.21
1	A	345	TPO	P-OG1-CB	-2.56	115.47	123.21
1	C	346	SEP	OG-CB-CA	2.51	110.59	108.14
1	D	345	TPO	P-OG1-CB	-2.47	115.75	123.21
1	A	346	SEP	OG-CB-CA	2.35	110.43	108.14

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	O-C-CA-CB
1	B	345	TPO	N-CA-CB-OG1
1	C	345	TPO	N-CA-CB-OG1
1	C	345	TPO	O-C-CA-CB
1	D	345	TPO	N-CA-CB-OG1
1	D	346	SEP	CB-OG-P-O3P
1	D	346	SEP	CB-OG-P-O1P
1	D	346	SEP	CB-OG-P-O2P
1	B	346	SEP	N-CA-CB-OG
1	A	345	TPO	CB-OG1-P-O2P
1	C	345	TPO	CB-OG1-P-O2P
1	B	345	TPO	O-C-CA-CB
1	D	345	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 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	LS7	B	501	-	28,33,33	1.18	1 (3%)	38,49,49	2.43	7 (18%)
4	GOL	A	503	-	5,5,5	0.31	0	5,5,5	0.14	0
3	SO4	B	502	-	4,4,4	0.32	0	6,6,6	0.05	0
2	LS7	C	501	-	28,33,33	1.19	1 (3%)	38,49,49	2.33	7 (18%)
3	SO4	D	503	-	4,4,4	0.33	0	6,6,6	0.06	0
2	LS7	D	501	-	28,33,33	1.18	1 (3%)	38,49,49	2.39	7 (18%)
3	SO4	D	502	-	4,4,4	0.32	0	6,6,6	0.05	0
2	LS7	A	501	-	28,33,33	1.20	1 (3%)	38,49,49	2.33	6 (15%)
3	SO4	C	502	-	4,4,4	0.32	0	6,6,6	0.05	0
3	SO4	A	502	-	4,4,4	0.32	0	6,6,6	0.06	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
2	LS7	B	501	-	-	4/10/30/30	0/5/5/5
2	LS7	C	501	-	-	4/10/30/30	0/5/5/5
2	LS7	D	501	-	-	4/10/30/30	0/5/5/5
4	GOL	A	503	-	-	2/4/4/4	-
2	LS7	A	501	-	-	4/10/30/30	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	LS7	O10-C2	-4.75	1.44	1.48
2	C	501	LS7	O10-C2	-4.71	1.44	1.48
2	B	501	LS7	O10-C2	-4.66	1.44	1.48
2	D	501	LS7	O10-C2	-4.62	1.44	1.48

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	LS7	C21-N22-N23	8.99	110.24	103.70
2	D	501	LS7	C21-N22-N23	8.77	110.08	103.70
2	A	501	LS7	C21-N22-N23	8.53	109.91	103.70
2	C	501	LS7	C21-N22-N23	8.34	109.77	103.70
2	B	501	LS7	C2-O10-C9	6.24	111.46	107.27
2	D	501	LS7	C2-O10-C9	6.18	111.42	107.27
2	A	501	LS7	C2-O10-C9	6.05	111.33	107.27
2	C	501	LS7	C2-O10-C9	5.71	111.10	107.27
2	C	501	LS7	O10-C2-C1	4.90	110.64	106.54
2	B	501	LS7	O10-C2-C1	4.89	110.64	106.54
2	A	501	LS7	O10-C2-C1	4.68	110.47	106.54
2	D	501	LS7	O10-C2-C29	4.58	110.38	106.54
2	D	501	LS7	O10-C2-C1	4.41	110.24	106.54
2	B	501	LS7	O10-C2-C29	4.01	109.90	106.54
2	A	501	LS7	O10-C2-C29	3.87	109.78	106.54
2	C	501	LS7	O10-C2-C29	3.83	109.75	106.54
2	B	501	LS7	C8-C9-C4	-3.63	118.86	123.18
2	D	501	LS7	C8-C9-C4	-3.56	118.95	123.18
2	C	501	LS7	C8-C9-C4	-3.56	118.95	123.18
2	A	501	LS7	C8-C9-C4	-3.50	119.02	123.18
2	D	501	LS7	C26-N25-C24	2.82	120.27	116.77
2	B	501	LS7	C26-N25-C24	2.76	120.19	116.77
2	C	501	LS7	C26-N25-C24	2.72	120.15	116.77
2	A	501	LS7	C26-N25-C24	2.70	120.12	116.77
2	C	501	LS7	C20-C18-N17	2.22	118.11	114.79
2	B	501	LS7	C20-C18-N17	2.15	118.00	114.79
2	D	501	LS7	C16-N11-C12	2.08	116.10	111.52

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	LS7	C8-C7-N11-C16
2	D	501	LS7	C8-C7-N11-C16
2	C	501	LS7	C8-C7-N11-C12
2	D	501	LS7	C8-C7-N11-C12
2	A	501	LS7	C8-C7-N11-C12
2	A	501	LS7	C8-C7-N11-C16
2	B	501	LS7	C8-C7-N11-C16
2	B	501	LS7	C8-C7-N11-C12
4	A	503	GOL	C1-C2-C3-O3
2	D	501	LS7	C6-C7-N11-C12
2	C	501	LS7	C6-C7-N11-C12

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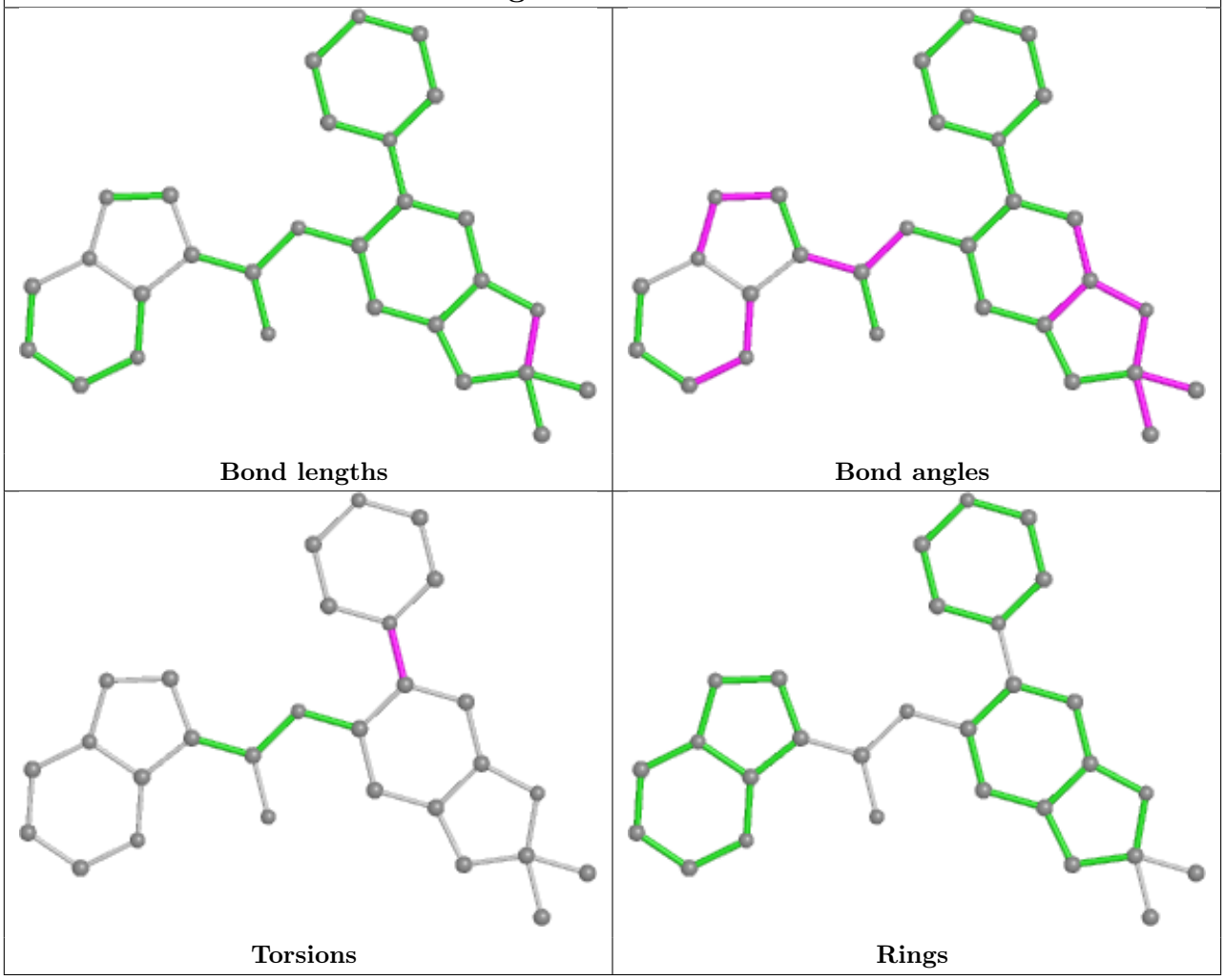
Mol	Chain	Res	Type	Atoms
2	A	501	LS7	C6-C7-N11-C12
2	B	501	LS7	C6-C7-N11-C16
2	C	501	LS7	C6-C7-N11-C16
4	A	503	GOL	O1-C1-C2-C3
2	D	501	LS7	C6-C7-N11-C16
2	A	501	LS7	C6-C7-N11-C16
2	B	501	LS7	C6-C7-N11-C12

There are no ring outliers.

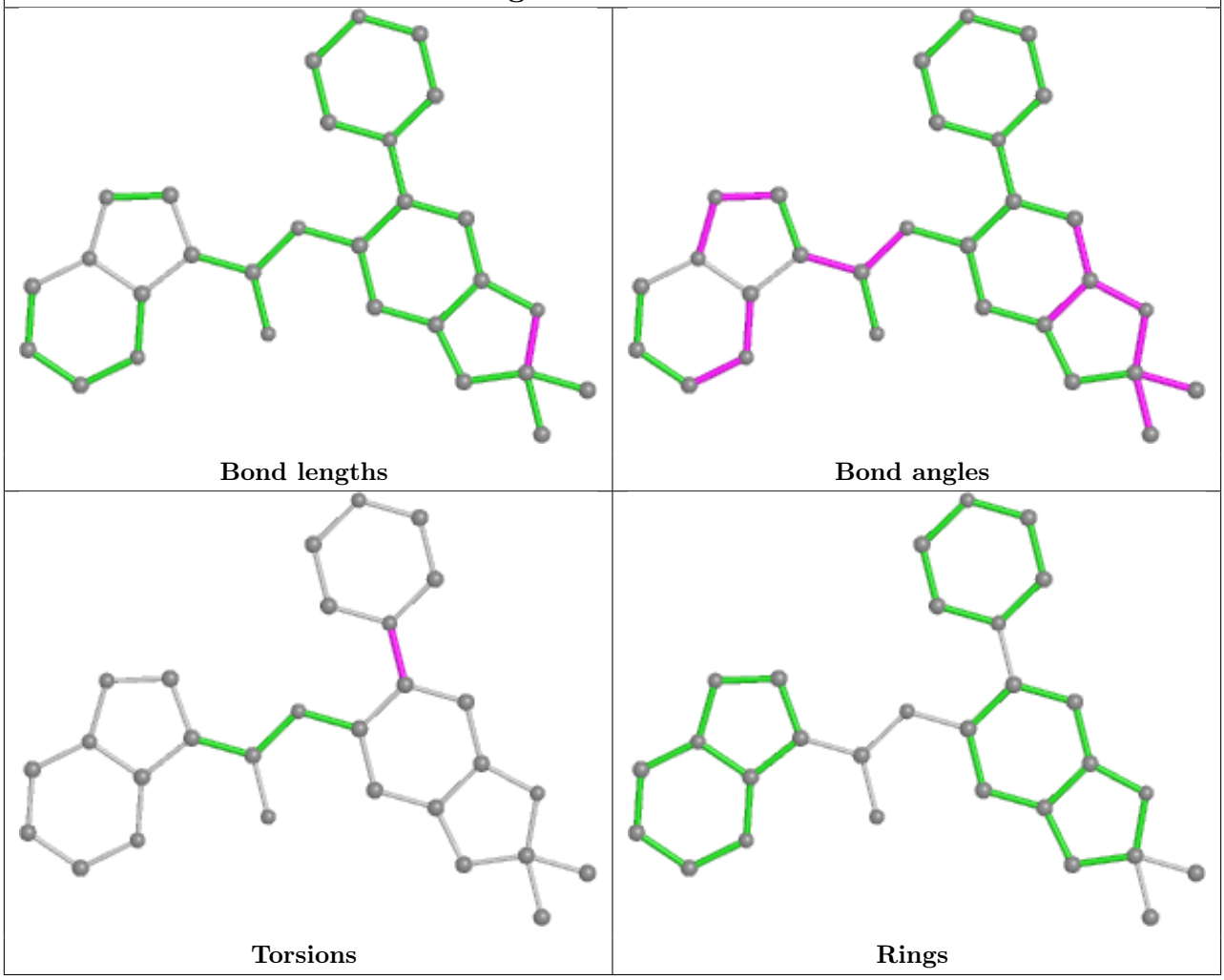
No monomer is involved in short contacts.

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 then 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.

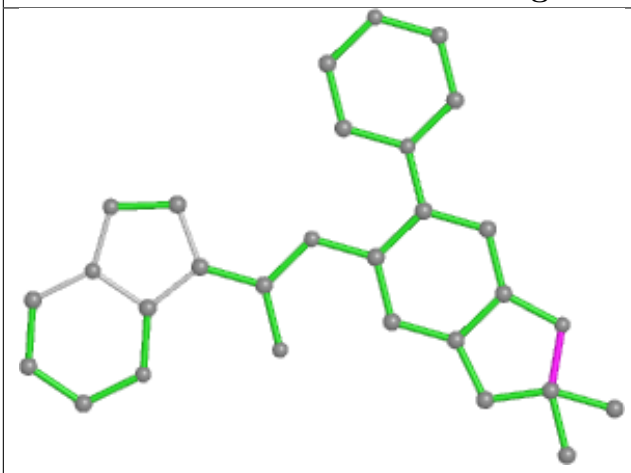
Ligand LS7 B 501



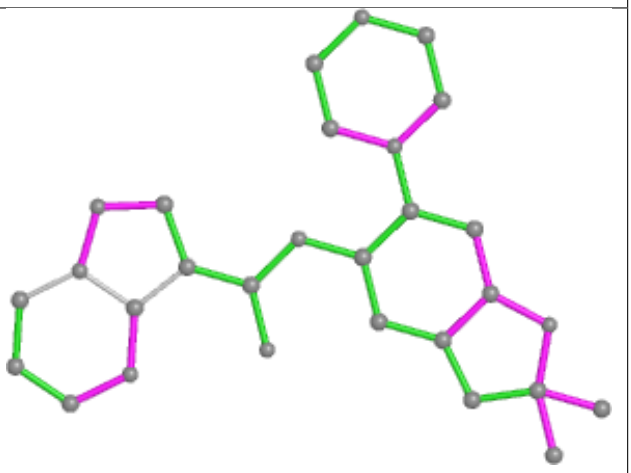
Ligand LS7 C 501



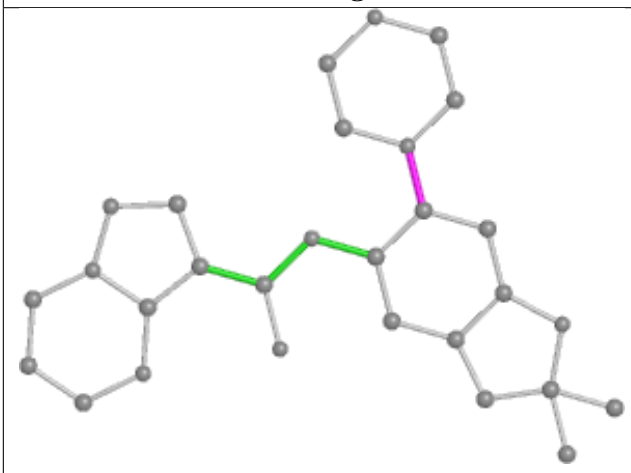
Ligand LS7 D 501



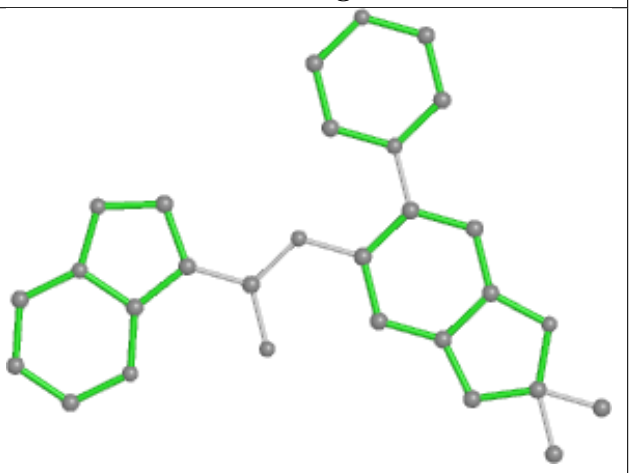
Bond lengths



Bond angles

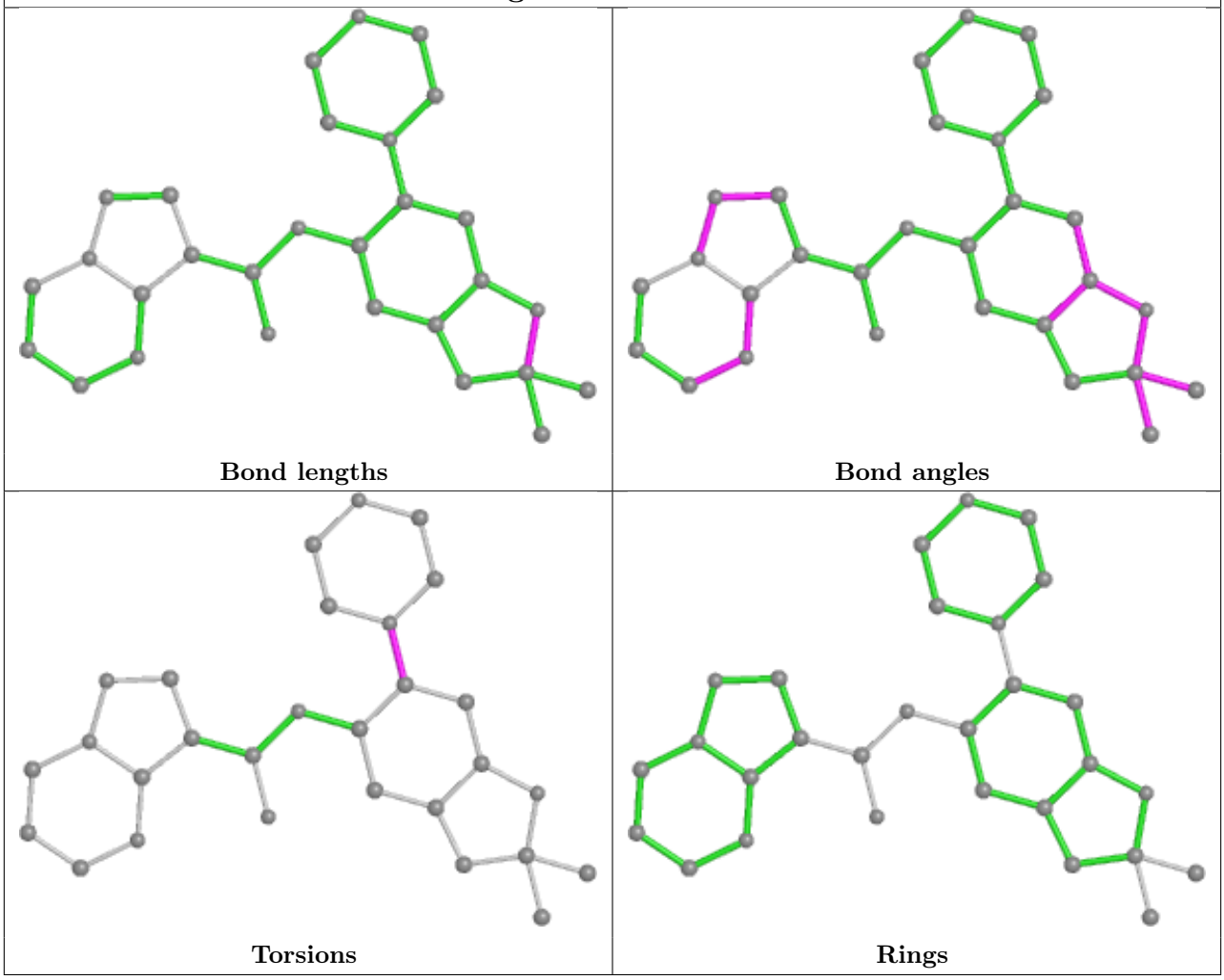


Torsions



Rings

Ligand LS7 A 501



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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	281/305 (92%)	0.63	36 (12%)	3	2	23, 40, 74, 95	0
1	B	284/305 (93%)	0.67	32 (11%)	5	3	22, 41, 68, 103	0
1	C	290/305 (95%)	0.40	22 (7%)	13	10	22, 38, 63, 74	0
1	D	288/305 (94%)	0.37	19 (6%)	18	14	23, 37, 62, 76	0
All	All	1143/1220 (93%)	0.52	109 (9%)	8	6	22, 39, 67, 103	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	226	LEU	11.0
1	B	196	GLY	7.4
1	B	223	THR	7.3
1	A	255	GLY	7.2
1	B	255	GLY	6.9
1	A	196[A]	GLY	6.8
1	A	197[A]	PHE	6.1
1	B	336	SER	5.5
1	B	160	VAL	5.5
1	C	164	ARG	5.4
1	A	195[A]	GLY	5.4
1	B	224	GLU	5.1
1	D	217	ALA	4.9
1	C	341	GLN	4.9
1	A	335	ALA	4.9
1	C	163	THR	4.8
1	D	335	ALA	4.7
1	B	344	MET	4.6
1	B	204	TYR	4.6
1	B	187	VAL	4.5
1	C	220	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	256	ASP	4.3
1	B	256	ASP	4.2
1	B	197	PHE	4.2
1	A	347	ARG	4.1
1	A	336	SER	4.1
1	B	161	SER	4.1
1	C	223	THR	4.1
1	B	228	GLN	4.0
1	B	335	ALA	4.0
1	D	336	SER	4.0
1	A	224	GLU	3.8
1	A	171	TYR	3.7
1	A	167	SER	3.6
1	B	222	THR	3.6
1	C	221	ILE	3.6
1	B	195	GLY	3.6
1	A	228	GLN	3.5
1	B	225	GLU	3.4
1	B	207	ASN	3.4
1	C	407	GLU	3.4
1	A	164	ARG	3.3
1	A	223	THR	3.3
1	A	256	ASP	3.3
1	C	222	THR	3.3
1	D	222	THR	3.3
1	B	347	ARG	3.2
1	D	186	SER	3.2
1	C	218[A]	MET	3.2
1	D	406	GLU	3.2
1	A	343	VAL	3.1
1	C	185	ILE	3.1
1	D	407	GLU	3.1
1	B	407	GLU	3.1
1	C	187	VAL	3.1
1	A	179	ASN	3.1
1	B	409	THR	3.0
1	B	206	ASN	3.0
1	B	390	HIS	3.0
1	B	178	ASN	2.8
1	D	228	GLN	2.8
1	A	390	HIS	2.8
1	D	188	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	216	ALA	2.8
1	B	186	SER	2.8
1	B	392	GLU	2.8
1	A	251	PHE	2.7
1	B	163	THR	2.7
1	A	187	VAL	2.7
1	D	226	LEU	2.7
1	A	186	SER	2.7
1	A	254	ASP	2.6
1	C	228	GLN	2.6
1	A	222	THR	2.6
1	A	184	PRO	2.6
1	A	215	LEU	2.5
1	A	166	HIS	2.5
1	A	181	ASP	2.5
1	A	389	GLU	2.5
1	D	187	VAL	2.5
1	A	185	ILE	2.5
1	C	335	ALA	2.4
1	C	342	THR	2.4
1	C	409	THR	2.4
1	D	182	GLU	2.4
1	D	221	ILE	2.4
1	B	389	GLU	2.4
1	C	224	GLU	2.4
1	B	254	ASP	2.3
1	B	393	PRO	2.3
1	D	405	ASP	2.3
1	C	216	ALA	2.3
1	C	186	SER	2.3
1	A	182	GLU	2.3
1	A	344	MET	2.3
1	C	344	MET	2.3
1	A	407	GLU	2.3
1	C	257	ASP	2.3
1	C	343	VAL	2.2
1	D	254	ASP	2.2
1	D	218	MET	2.2
1	A	258	LEU	2.2
1	B	183	ARG	2.2
1	A	410	ILE	2.2
1	A	230	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	411	GLU	2.1
1	D	184	PRO	2.1
1	D	344	MET	2.1
1	A	190	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SEP	D	346	10/11	0.70	0.30	72,77,84,86	3
1	SEP	C	346	10/11	0.76	0.26	67,73,80,81	3
1	SEP	B	346	10/11	0.84	0.25	79,84,88,90	4
1	SEP	A	346	10/11	0.86	0.24	74,79,84,87	4
1	TPO	C	345	11/12	0.86	0.17	61,66,67,70	0
1	TPO	B	345	11/12	0.91	0.23	74,78,79,79	0
1	TPO	D	345	11/12	0.92	0.18	67,71,72,74	0
1	TPO	A	345	11/12	0.92	0.16	65,69,71,73	0

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, 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	503	6/6	0.65	0.33	49,51,51,52	0
3	SO4	D	502	5/5	0.87	0.32	98,99,99,99	0
3	SO4	C	502	5/5	0.87	0.31	96,96,97,97	0
3	SO4	A	502	5/5	0.88	0.16	81,81,82,82	0
2	LS7	A	501	29/29	0.93	0.09	35,38,40,40	0
2	LS7	B	501	29/29	0.94	0.08	29,31,32,33	0

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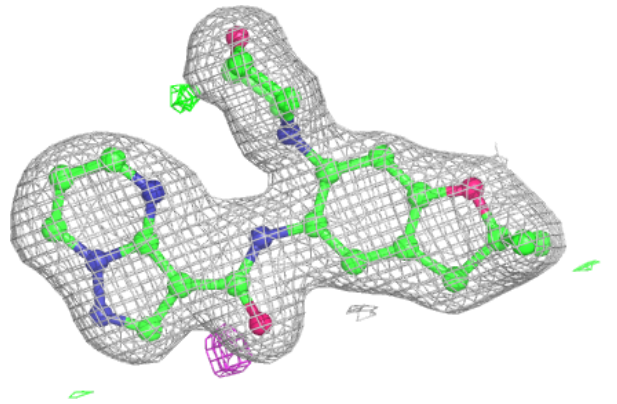
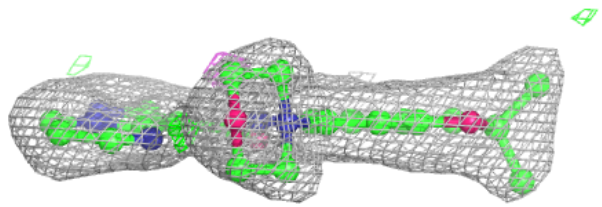
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	D	503	5/5	0.94	0.14	72,72,72,73	0
2	LS7	C	501	29/29	0.94	0.10	32,34,36,36	0
2	LS7	D	501	29/29	0.95	0.08	30,32,33,33	0
3	SO4	B	502	5/5	0.95	0.12	60,61,62,62	0

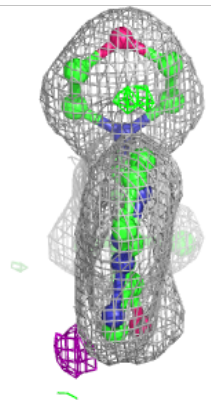
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LS7 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)

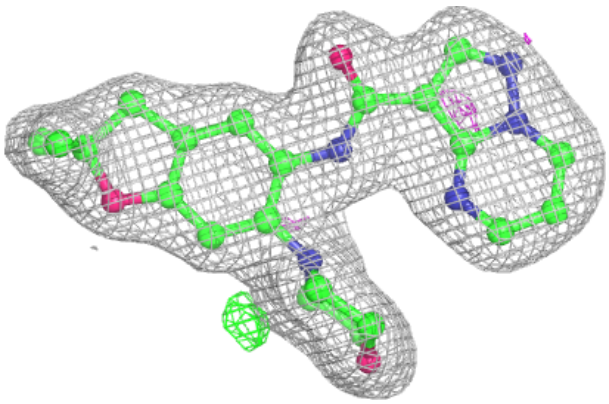


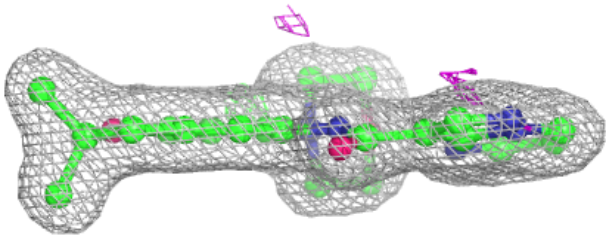


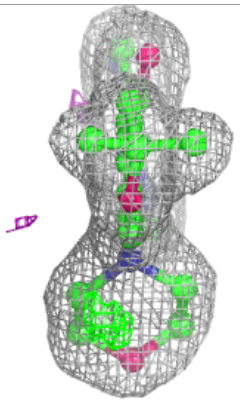


Electron density around LS7 B 501:

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

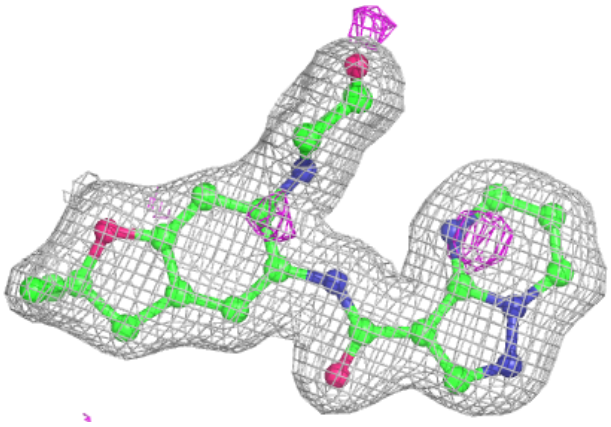


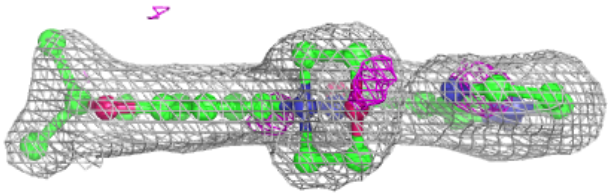


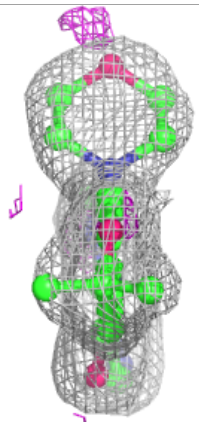


Electron density around LS7 C 501:

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

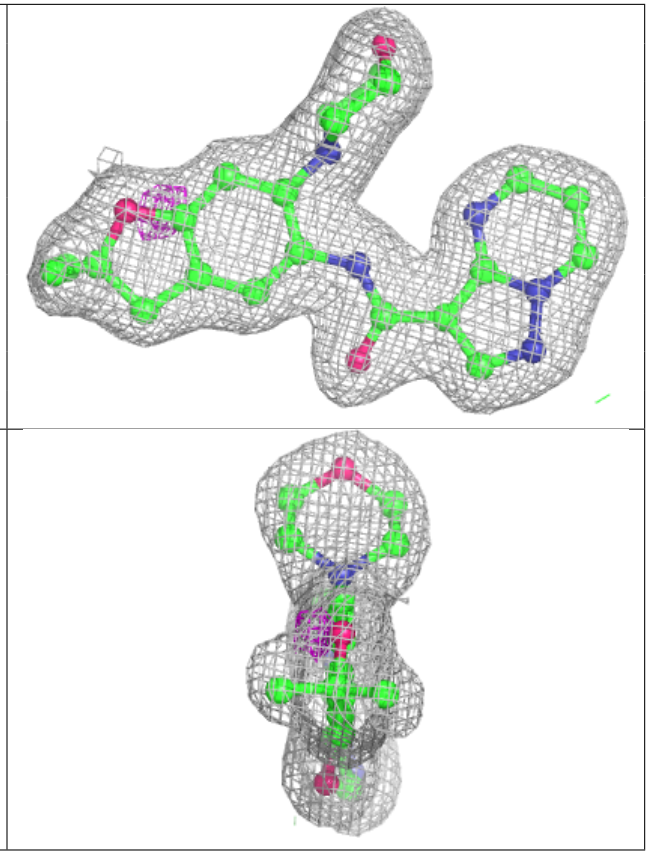






Electron density around LS7 D 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.