



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 07:53 AM EDT

PDB ID : 6O94
Title : Structure of the IRAK4 kinase domain with compound 17
Authors : Yu, C.; Drobnick, J.; Bryan, M.C.; Kiefer, J.; Lupardus, P.J.
Deposited on : 2019-03-13
Resolution : 1.98 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 : 4.02b-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

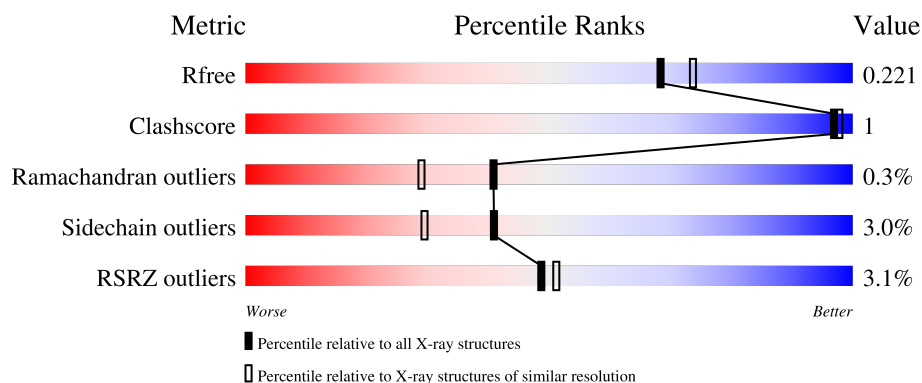
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	320	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; align-items: center;"> </div> </div>
1	B	320	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 2% </div> <div style="display: flex; justify-content: space-between; align-items: center;"> </div> </div>
1	C	320	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 5% </div> <div style="display: flex; justify-content: space-between; align-items: center;"> </div> </div>
1	D	320	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 2% </div> <div style="display: flex; justify-content: space-between; align-items: center;"> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9907 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
1	A	292	Total	C	N	O	P	S	0	0	0
			2306	1443	387	458	3	15			
1	B	293	Total	C	N	O	P	S	0	0	0
			2311	1446	388	459	3	15			
1	C	286	Total	C	N	O	P	S	0	2	0
			2279	1429	381	451	3	15			
1	D	285	Total	C	N	O	P	S	0	0	0
			2256	1412	379	448	3	14			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	144	MET	-	initiating methionine	UNP Q9NWZ3
A	145	HIS	-	expression tag	UNP Q9NWZ3
A	146	HIS	-	expression tag	UNP Q9NWZ3
A	147	HIS	-	expression tag	UNP Q9NWZ3
A	148	HIS	-	expression tag	UNP Q9NWZ3
A	149	HIS	-	expression tag	UNP Q9NWZ3
A	150	HIS	-	expression tag	UNP Q9NWZ3
A	151	GLY	-	expression tag	UNP Q9NWZ3
A	152	GLU	-	expression tag	UNP Q9NWZ3
A	153	ASN	-	expression tag	UNP Q9NWZ3
A	154	LEU	-	expression tag	UNP Q9NWZ3
A	155	TYR	-	expression tag	UNP Q9NWZ3
A	156	PHE	-	expression tag	UNP Q9NWZ3
A	157	GLN	-	expression tag	UNP Q9NWZ3
A	158	GLY	-	expression tag	UNP Q9NWZ3
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	144	MET	-	initiating methionine	UNP Q9NWZ3
B	145	HIS	-	expression tag	UNP Q9NWZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	146	HIS	-	expression tag	UNP Q9NWZ3
B	147	HIS	-	expression tag	UNP Q9NWZ3
B	148	HIS	-	expression tag	UNP Q9NWZ3
B	149	HIS	-	expression tag	UNP Q9NWZ3
B	150	HIS	-	expression tag	UNP Q9NWZ3
B	151	GLY	-	expression tag	UNP Q9NWZ3
B	152	GLU	-	expression tag	UNP Q9NWZ3
B	153	ASN	-	expression tag	UNP Q9NWZ3
B	154	LEU	-	expression tag	UNP Q9NWZ3
B	155	TYR	-	expression tag	UNP Q9NWZ3
B	156	PHE	-	expression tag	UNP Q9NWZ3
B	157	GLN	-	expression tag	UNP Q9NWZ3
B	158	GLY	-	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	144	MET	-	initiating methionine	UNP Q9NWZ3
C	145	HIS	-	expression tag	UNP Q9NWZ3
C	146	HIS	-	expression tag	UNP Q9NWZ3
C	147	HIS	-	expression tag	UNP Q9NWZ3
C	148	HIS	-	expression tag	UNP Q9NWZ3
C	149	HIS	-	expression tag	UNP Q9NWZ3
C	150	HIS	-	expression tag	UNP Q9NWZ3
C	151	GLY	-	expression tag	UNP Q9NWZ3
C	152	GLU	-	expression tag	UNP Q9NWZ3
C	153	ASN	-	expression tag	UNP Q9NWZ3
C	154	LEU	-	expression tag	UNP Q9NWZ3
C	155	TYR	-	expression tag	UNP Q9NWZ3
C	156	PHE	-	expression tag	UNP Q9NWZ3
C	157	GLN	-	expression tag	UNP Q9NWZ3
C	158	GLY	-	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	144	MET	-	initiating methionine	UNP Q9NWZ3
D	145	HIS	-	expression tag	UNP Q9NWZ3
D	146	HIS	-	expression tag	UNP Q9NWZ3
D	147	HIS	-	expression tag	UNP Q9NWZ3
D	148	HIS	-	expression tag	UNP Q9NWZ3
D	149	HIS	-	expression tag	UNP Q9NWZ3

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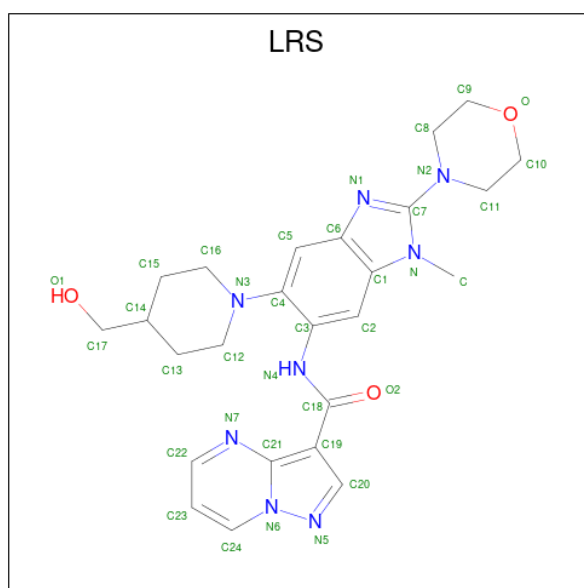
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Chain	Residue	Modelled	Actual	Comment	Reference
D	150	HIS	-	expression tag	UNP Q9NWZ3
D	151	GLY	-	expression tag	UNP Q9NWZ3
D	152	GLU	-	expression tag	UNP Q9NWZ3
D	153	ASN	-	expression tag	UNP Q9NWZ3
D	154	LEU	-	expression tag	UNP Q9NWZ3
D	155	TYR	-	expression tag	UNP Q9NWZ3
D	156	PHE	-	expression tag	UNP Q9NWZ3
D	157	GLN	-	expression tag	UNP Q9NWZ3
D	158	GLY	-	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 CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0

- Molecule 3 is N-{5-[4-(hydroxymethyl)piperidin-1-yl]-1-methyl-2-(morpholin-4-yl)-1H-benzimidazol-6-yl}pyrazolo[1,5-a]pyrimidine-3-carboxamide (three-letter code: LRS) (formula: C₂₅H₃₀N₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			36	25	8	3		
3	B	1	Total	C	N	O	0	0
			36	25	8	3		
3	C	1	Total	C	N	O	0	0
			36	25	8	3		
3	D	1	Total	C	N	O	0	0
			36	25	8	3		

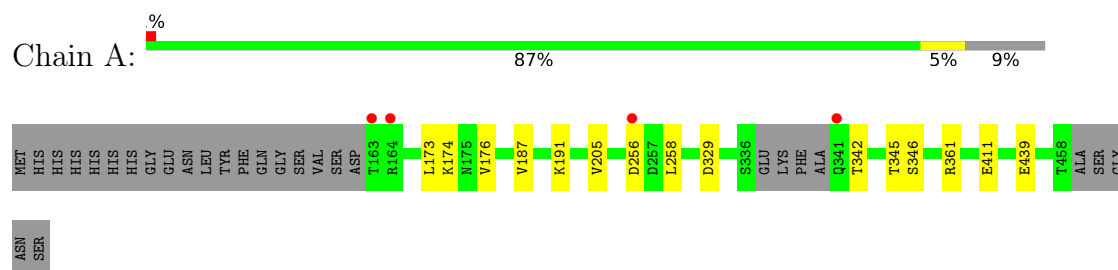
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	194	Total	O	0	0
			194	194		
4	B	147	Total	O	0	0
			147	147		
4	C	116	Total	O	0	0
			116	116		
4	D	152	Total	O	0	0
			152	152		

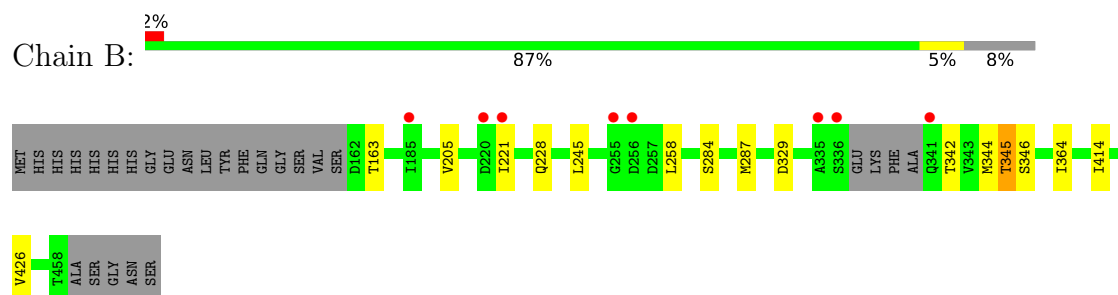
3 Residue-property plots [i](#)

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.

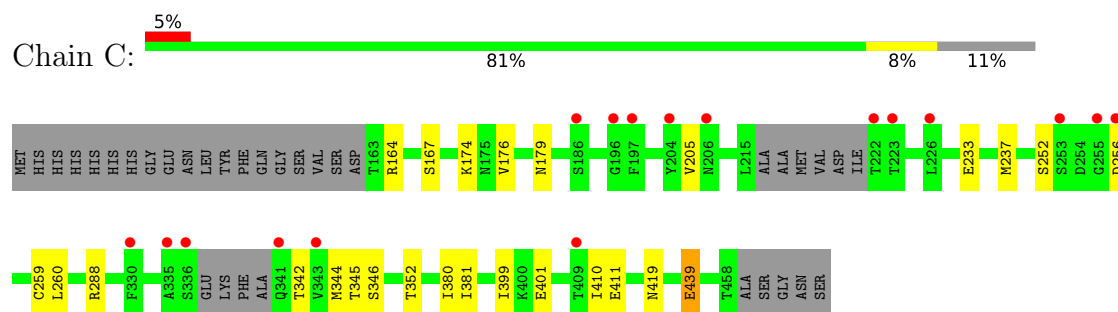
- Molecule 1: Interleukin-1 receptor-associated kinase 4



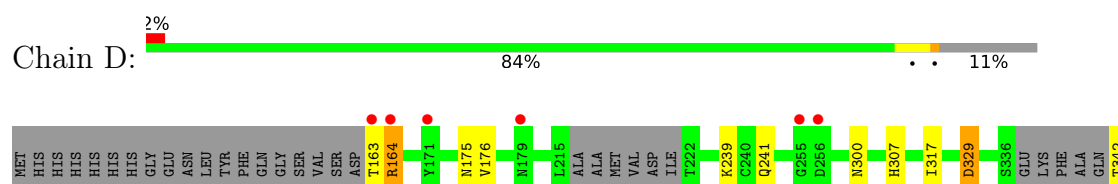
- Molecule 1: Interleukin-1 receptor-associated kinase 4



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



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



T345	T346	V376	T447	T448	T458	ALA	SER	GLY	ASN	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.54Å 140.11Å 87.82Å 90.00° 123.36° 90.00°	Depositor
Resolution (Å)	28.99 – 1.98 90.36 – 1.98	Depositor EDS
% Data completeness (in resolution range)	96.9 (28.99-1.98) 96.8 (90.36-1.98)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 1.98Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.183 , 0.215 0.189 , 0.221	Depositor DCC
R_{free} test set	4776 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9907	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.71% 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: SEP, TPO, CA, LRS

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	0.51	0/2310	0.64	0/3112
1	B	0.51	0/2315	0.63	0/3119
1	C	0.49	0/2289	0.62	0/3081
1	D	0.51	0/2260	0.62	0/3044
All	All	0.50	0/9174	0.63	0/12356

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2306	0	2267	5	0
1	B	2311	0	2269	3	0
1	C	2279	0	2242	7	0
1	D	2256	0	2218	4	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	36	0	0	0	0
3	B	36	0	0	0	0
3	C	36	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	36	0	0	0	0
4	A	194	0	0	1	0
4	B	147	0	0	0	0
4	C	116	0	0	0	0
4	D	152	0	0	0	0
All	All	9907	0	8996	17	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 (17) 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:284:SER:H	1:B:287:MET:HE3	1.25	0.97
1:A:176:VAL:HG11	1:A:205:VAL:HG22	1.81	0.63
1:A:173:LEU:HA	1:A:176:VAL:HG22	1.85	0.59
1:C:252:SER:HB3	1:C:259:CYS:HB2	1.88	0.56
1:A:439:GLU:HB2	1:C:439:GLU:HG2	1.89	0.54
1:D:239:LYS:HD3	1:D:307:HIS:HE1	1.79	0.48
1:A:191:LYS:HE2	4:A:717:HOH:O	2.14	0.46
1:B:345:TPO:HB	1:B:364:ILE:HD11	1.97	0.46
1:C:176:VAL:HG11	1:C:205:VAL:HG22	1.97	0.46
1:A:361:ARG:HA	1:C:352:THR:CG2	2.47	0.45
1:C:233:GLU:HG2	1:C:260:LEU:HD13	2.00	0.43
1:B:414:ILE:HD13	1:B:426:VAL:HG11	2.02	0.42
1:D:163:THR:HG22	1:D:164:ARG:H	1.85	0.41
1:D:300:ASN:HA	1:D:447:ILE:HG21	2.02	0.41
1:C:288:ARG:HB3	1:C:380:ILE:HG23	2.03	0.41
1:C:381:ILE:HG21	1:C:410:ILE:HD11	2.03	0.41
1:D:317:ILE:HD12	1:D:376:VAL:HG11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	285/320 (89%)	280 (98%)	4 (1%)	1 (0%)	34	22
1	B	286/320 (89%)	279 (98%)	7 (2%)	0	100	100
1	C	279/320 (87%)	272 (98%)	6 (2%)	1 (0%)	34	22
1	D	277/320 (87%)	267 (96%)	9 (3%)	1 (0%)	34	22
All	All	1127/1280 (88%)	1098 (97%)	26 (2%)	3 (0%)	41	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	256	ASP
1	A	329	ASP
1	D	329	ASP

5.3.2 Protein sidechains ⓘ

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	252/275 (92%)	247 (98%)	5 (2%)	55	48
1	B	252/275 (92%)	244 (97%)	8 (3%)	39	28
1	C	250/275 (91%)	239 (96%)	11 (4%)	28	16
1	D	247/275 (90%)	241 (98%)	6 (2%)	49	41
All	All	1001/1100 (91%)	971 (97%)	30 (3%)	41	29

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	LYS
1	A	187	VAL
1	A	256	ASP
1	A	258	LEU
1	A	411	GLU

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Mol	Chain	Res	Type
1	B	163	THR
1	B	205	VAL
1	B	221	ILE
1	B	228	GLN
1	B	245	LEU
1	B	258	LEU
1	B	329	ASP
1	B	344	MET
1	C	164	ARG
1	C	167	SER
1	C	174	LYS
1	C	179	ASN
1	C	237	MET
1	C	344	MET
1	C	399	ILE
1	C	401	GLU
1	C	411	GLU
1	C	419	ASN
1	C	439	GLU
1	D	164	ARG
1	D	175	ASN
1	D	176	VAL
1	D	241	GLN
1	D	329	ASP
1	D	448	LYS

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

Mol	Chain	Res	Type
1	A	207	ASN
1	A	293	GLN
1	A	316	ASN
1	B	228	GLN
1	C	293	GLN
1	C	419	ASN
1	D	166	HIS
1	D	286	HIS
1	D	293	GLN
1	D	307	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

12 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	TPO	A	342	1	8,10,11	1.07	1 (12%)	10,14,16	1.62	3 (30%)
1	SEP	C	346	1	8,9,10	0.86	0	8,12,14	2.24	2 (25%)
1	SEP	B	346	1	8,9,10	1.06	1 (12%)	8,12,14	1.57	1 (12%)
1	TPO	B	345	1	8,10,11	1.44	2 (25%)	10,14,16	1.34	1 (10%)
1	TPO	D	345	1	8,10,11	1.46	2 (25%)	10,14,16	1.03	0
1	TPO	D	342	1	8,10,11	1.05	0	10,14,16	1.40	2 (20%)
1	SEP	D	346	1	8,9,10	1.04	0	8,12,14	1.81	1 (12%)
1	TPO	C	345	1	8,10,11	1.22	1 (12%)	10,14,16	1.26	1 (10%)
1	TPO	A	345	1	8,10,11	1.07	1 (12%)	10,14,16	1.41	1 (10%)
1	TPO	C	342	1	8,10,11	1.31	1 (12%)	10,14,16	1.12	0
1	TPO	B	342	1	8,10,11	1.05	1 (12%)	10,14,16	1.47	1 (10%)
1	SEP	A	346	1	8,9,10	0.85	0	8,12,14	2.32	3 (37%)

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	TPO	A	342	1	-	1/9/11/13	-
1	SEP	C	346	1	-	1/5/8/10	-
1	SEP	B	346	1	-	1/5/8/10	-
1	TPO	B	345	1	-	2/9/11/13	-
1	TPO	D	345	1	-	3/9/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	D	342	1	-	1/9/11/13	-
1	SEP	D	346	1	-	1/5/8/10	-
1	TPO	C	345	1	-	5/9/11/13	-
1	TPO	A	345	1	-	2/9/11/13	-
1	TPO	C	342	1	-	1/9/11/13	-
1	TPO	B	342	1	-	1/9/11/13	-
1	SEP	A	346	1	-	3/5/8/10	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	345	TPO	P-OG1	-2.75	1.54	1.59
1	C	342	TPO	P-OG1	-2.71	1.54	1.59
1	D	345	TPO	CB-CA	2.47	1.59	1.53
1	B	346	SEP	P-OG	-2.23	1.53	1.60
1	A	345	TPO	CB-CA	2.16	1.58	1.53
1	B	345	TPO	CG2-CB	2.10	1.56	1.51
1	A	342	TPO	P-OG1	-2.08	1.55	1.59
1	B	342	TPO	P-OG1	-2.05	1.55	1.59
1	D	345	TPO	P-OG1	-2.01	1.55	1.59
1	C	345	TPO	P-OG1	-2.00	1.55	1.59

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	346	SEP	OG-CB-CA	5.38	113.38	108.14
1	A	346	SEP	OG-CB-CA	4.64	112.66	108.14
1	D	346	SEP	OG-CB-CA	4.26	112.29	108.14
1	A	346	SEP	O3P-P-OG	3.88	117.06	106.73
1	A	342	TPO	P-OG1-CB	-3.57	112.44	123.21
1	B	346	SEP	OG-P-O1P	3.26	115.62	106.47
1	D	342	TPO	P-OG1-CB	-3.18	113.61	123.21
1	B	342	TPO	P-OG1-CB	-2.92	114.40	123.21
1	C	346	SEP	OG-P-O1P	2.79	114.31	106.47
1	B	345	TPO	O2P-P-OG1	2.64	117.80	105.99
1	A	345	TPO	O3P-P-OG1	2.42	116.84	105.99
1	A	346	SEP	P-OG-CB	-2.24	112.14	118.30
1	C	345	TPO	O2P-P-OG1	2.21	115.89	105.99
1	A	342	TPO	CG2-CB-CA	2.13	117.37	113.16
1	D	342	TPO	O3P-P-OG1	2.02	115.05	105.99
1	A	342	TPO	O3P-P-OG1	2.01	114.98	105.99

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	346	SEP	CB-OG-P-O1P
1	A	346	SEP	CB-OG-P-O2P
1	A	346	SEP	CB-OG-P-O3P
1	B	342	TPO	CB-OG1-P-O3P
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
1	C	342	TPO	O-C-CA-CB
1	C	345	TPO	N-CA-CB-OG1
1	C	345	TPO	CB-OG1-P-O1P
1	C	346	SEP	N-CA-CB-OG
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	O-C-CA-CB
1	D	346	SEP	N-CA-CB-OG
1	B	346	SEP	CB-OG-P-O2P
1	C	345	TPO	CA-CB-OG1-P
1	D	345	TPO	CB-OG1-P-O1P
1	C	345	TPO	CB-OG1-P-O2P
1	A	342	TPO	O-C-CA-CB
1	A	345	TPO	O-C-CA-CB
1	C	345	TPO	O-C-CA-CB
1	D	342	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	345	TPO	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
3	LRS	A	502	-	33,41,41	0.71	1 (3%)	38,59,59	0.90	1 (2%)
3	LRS	B	502	-	33,41,41	0.72	1 (3%)	38,59,59	1.31	3 (7%)
3	LRS	C	501	-	33,41,41	0.75	1 (3%)	38,59,59	0.92	1 (2%)
3	LRS	D	501	-	33,41,41	0.78	1 (3%)	38,59,59	1.17	3 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LRS	A	502	-	-	4/12/36/36	0/6/6/6
3	LRS	B	502	-	-	4/12/36/36	0/6/6/6
3	LRS	C	501	-	-	4/12/36/36	0/6/6/6
3	LRS	D	501	-	-	4/12/36/36	0/6/6/6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	LRS	C7-N1	-2.51	1.30	1.35
3	C	501	LRS	C7-N1	-2.23	1.31	1.35
3	A	502	LRS	C7-N1	-2.20	1.31	1.35
3	B	502	LRS	C7-N1	-2.13	1.31	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	LRS	C11-N2-C7	-4.80	111.76	122.03
3	D	501	LRS	C8-N2-C7	-4.12	113.21	122.03
3	B	502	LRS	C8-N2-C7	-3.93	113.60	122.03
3	C	501	LRS	C3-C2-C1	-3.53	118.27	121.32
3	B	502	LRS	C3-C2-C1	-3.52	118.28	121.32
3	D	501	LRS	C3-C2-C1	-3.47	118.33	121.32
3	A	502	LRS	C3-C2-C1	-3.43	118.35	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	LRS	C11-N2-C7	-2.76	116.12	122.03

There are no chirality outliers.

All (16) torsion outliers are listed below:

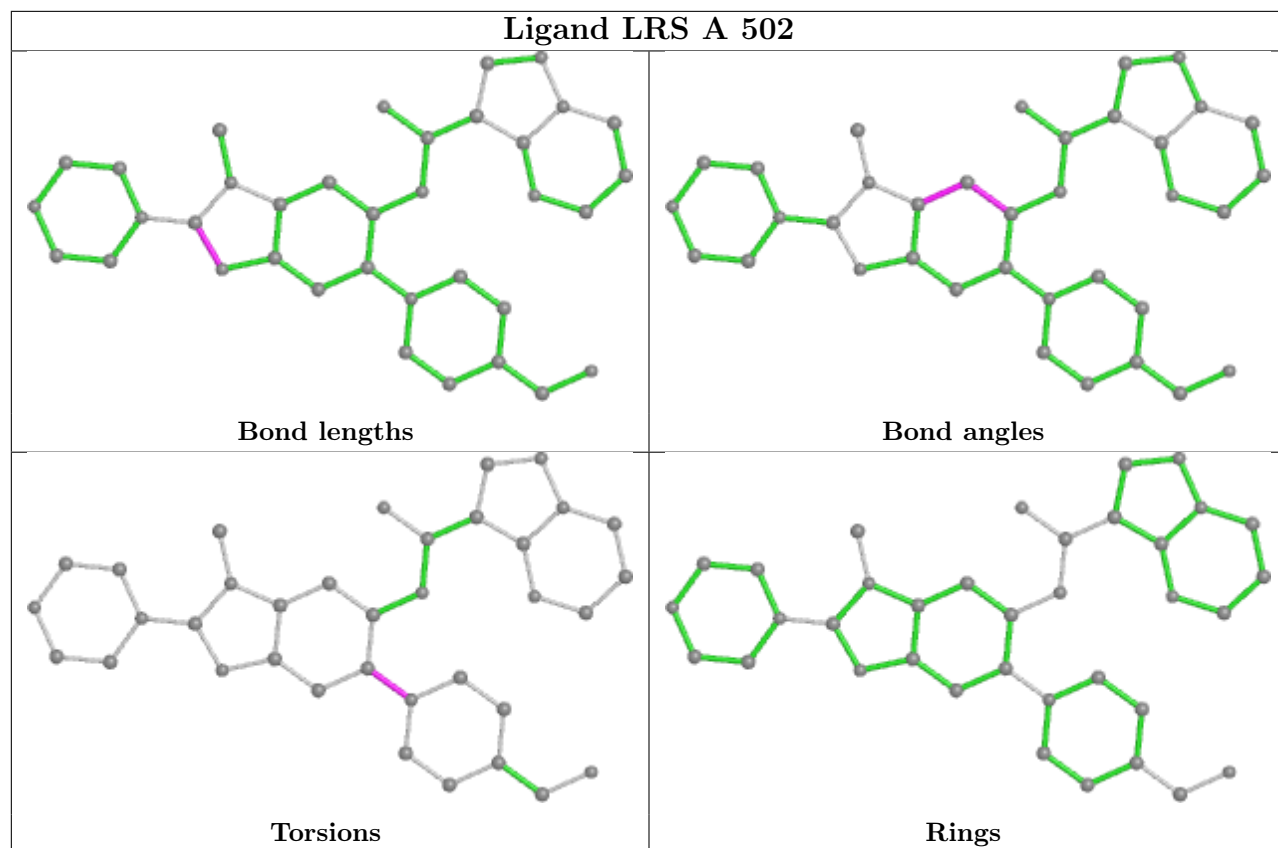
Mol	Chain	Res	Type	Atoms
3	C	501	LRS	C5-C4-N3-C16
3	D	501	LRS	C5-C4-N3-C16
3	B	502	LRS	C5-C4-N3-C16
3	A	502	LRS	C5-C4-N3-C16
3	D	501	LRS	C5-C4-N3-C12
3	B	502	LRS	C5-C4-N3-C12
3	C	501	LRS	C5-C4-N3-C12
3	A	502	LRS	C5-C4-N3-C12
3	A	502	LRS	C3-C4-N3-C12
3	A	502	LRS	C3-C4-N3-C16
3	B	502	LRS	C3-C4-N3-C12
3	C	501	LRS	C3-C4-N3-C12
3	C	501	LRS	C3-C4-N3-C16
3	D	501	LRS	C3-C4-N3-C12
3	B	502	LRS	C3-C4-N3-C16
3	D	501	LRS	C3-C4-N3-C16

There are no ring outliers.

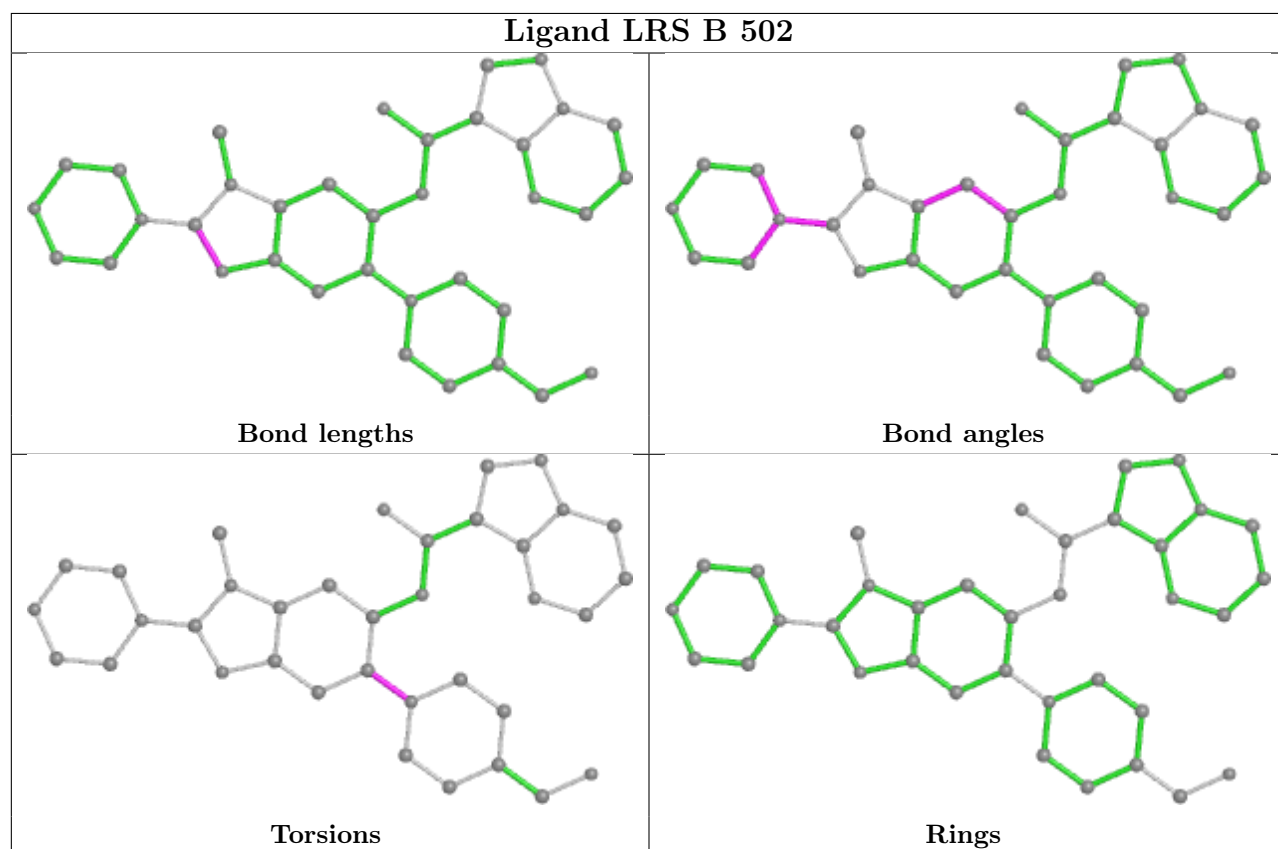
No monomer is involved in short contacts.

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 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.

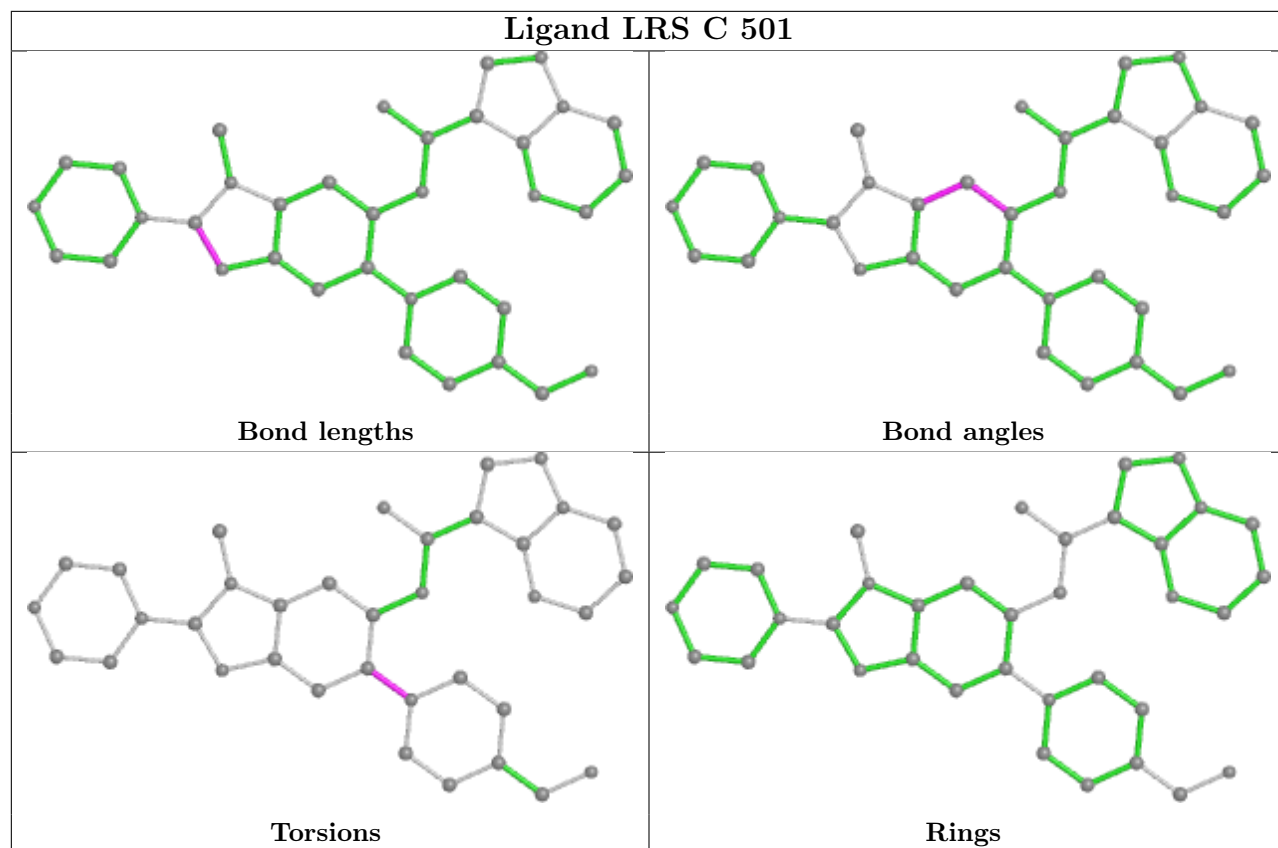
Ligand LRS A 502



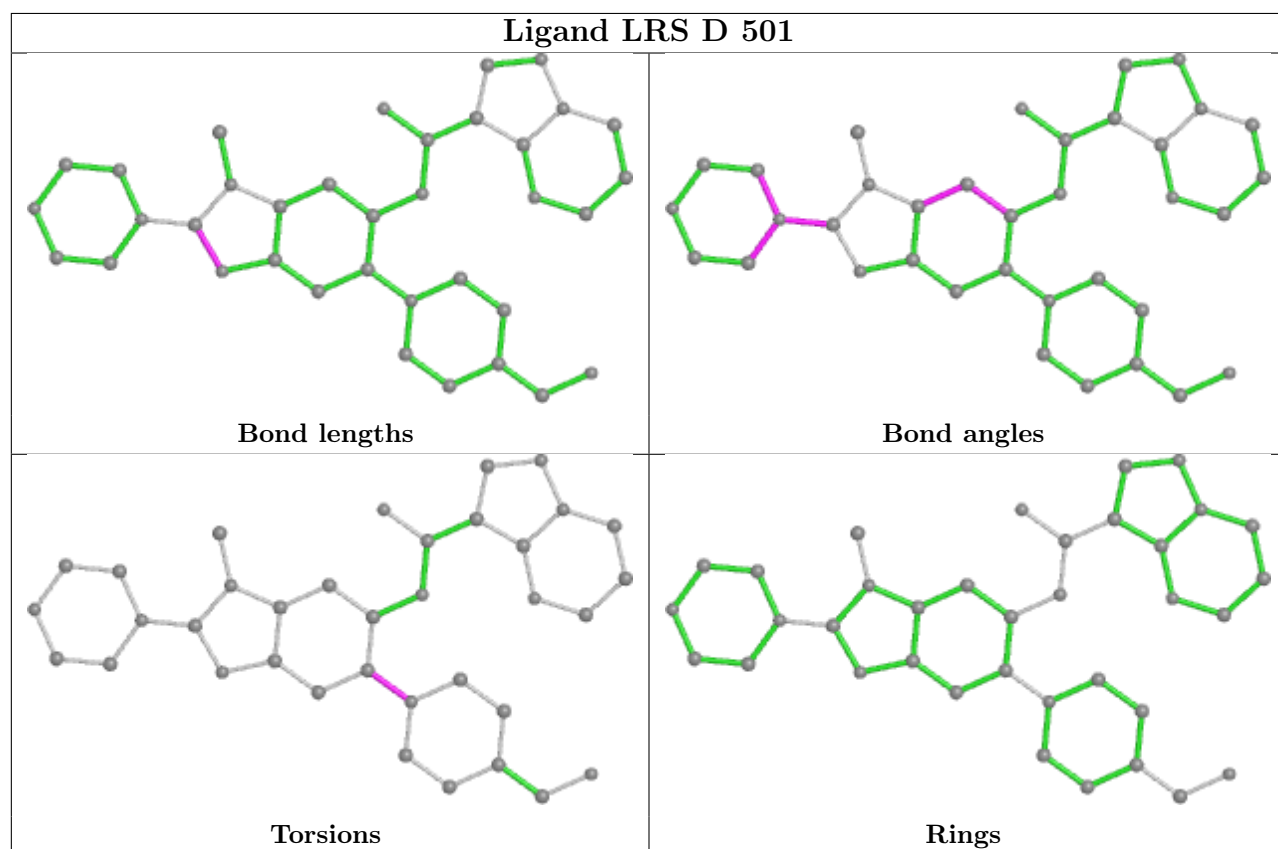
Ligand LRS B 502



Ligand LRS C 501



Ligand LRS D 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

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	289/320 (90%)	-0.09	4 (1%) 75 77	18, 30, 54, 84	0
1	B	290/320 (90%)	0.07	8 (2%) 53 55	20, 35, 63, 87	0
1	C	283/320 (88%)	0.30	17 (6%) 21 23	21, 37, 70, 107	0
1	D	282/320 (88%)	0.01	6 (2%) 63 65	21, 35, 65, 82	0
All	All	1144/1280 (89%)	0.07	35 (3%) 49 51	18, 34, 65, 107	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	343	VAL	9.1
1	C	341	GLN	9.0
1	D	255	GLY	6.5
1	C	226	LEU	6.0
1	C	223	THR	5.6
1	C	335	ALA	5.2
1	B	336	SER	5.2
1	A	341	GLN	5.0
1	D	164	ARG	4.8
1	C	256	ASP	4.7
1	A	164	ARG	4.5
1	C	336	SER	3.9
1	B	335	ALA	3.4
1	D	163	THR	3.3
1	C	253	SER	3.2
1	C	197	PHE	3.0
1	C	330	PHE	2.8
1	C	186	SER	2.7
1	B	220	ASP	2.7
1	A	163	THR	2.7
1	D	179	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	256	ASP	2.6
1	C	255	GLY	2.6
1	B	221	ILE	2.5
1	D	171	TYR	2.5
1	C	222	THR	2.4
1	C	409	THR	2.4
1	A	256	ASP	2.4
1	B	185	ILE	2.4
1	B	256	ASP	2.3
1	C	204[A]	TYR	2.3
1	C	206	ASN	2.2
1	B	341	GLN	2.2
1	C	196	GLY	2.1
1	B	255	GLY	2.1

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	TPO	C	342	11/12	0.73	0.24	88,88,91,91	3
1	SEP	D	346	10/11	0.80	0.14	56,61,64,64	3
1	TPO	B	342	11/12	0.81	0.14	69,70,71,71	3
1	SEP	C	346	10/11	0.85	0.13	72,74,75,75	3
1	TPO	D	342	11/12	0.86	0.15	61,63,64,64	4
1	TPO	A	342	11/12	0.87	0.12	58,59,62,63	3
1	TPO	C	345	11/12	0.90	0.13	74,76,77,77	0
1	SEP	B	346	10/11	0.90	0.09	57,60,62,63	3
1	SEP	A	346	10/11	0.91	0.11	44,48,51,53	3
1	TPO	A	345	11/12	0.97	0.08	43,44,48,49	0
1	TPO	D	345	11/12	0.97	0.09	52,54,57,58	0
1	TPO	B	345	11/12	0.97	0.10	54,56,58,59	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

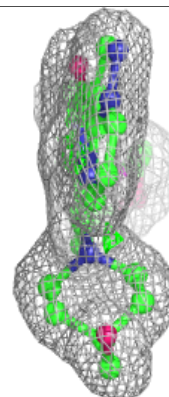
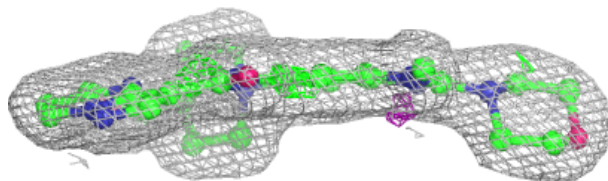
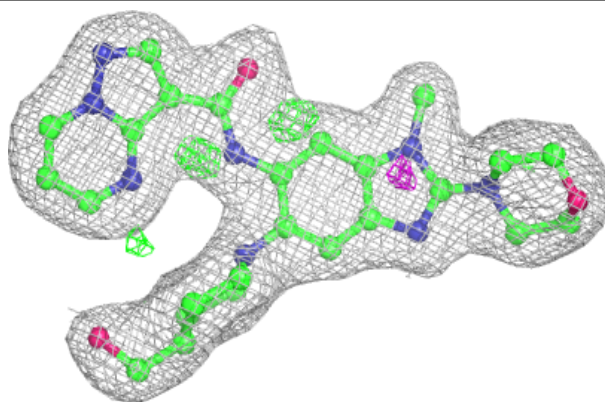
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	501	1/1	0.94	0.19	63,63,63,63	0
3	LRS	D	501	36/36	0.96	0.10	17,24,30,37	0
3	LRS	A	502	36/36	0.97	0.10	16,19,33,34	0
3	LRS	B	502	36/36	0.97	0.10	21,25,41,42	0
3	LRS	C	501	36/36	0.97	0.12	17,24,43,44	0
2	CA	B	501	1/1	0.97	0.22	54,54,54,54	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.

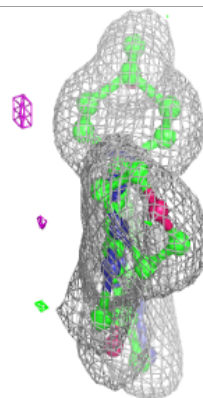
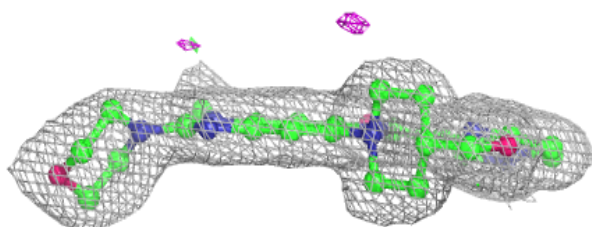
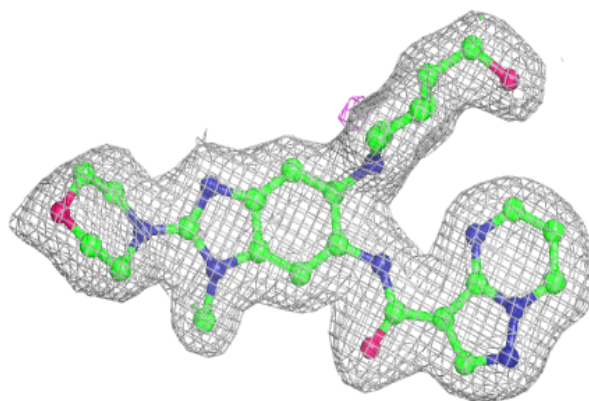
Electron density around LRS D 501:

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

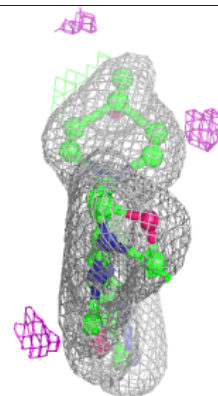
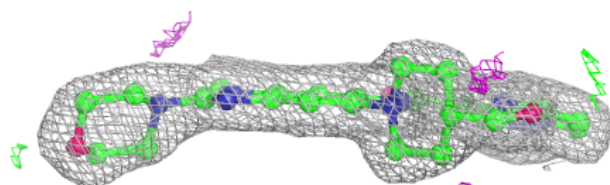
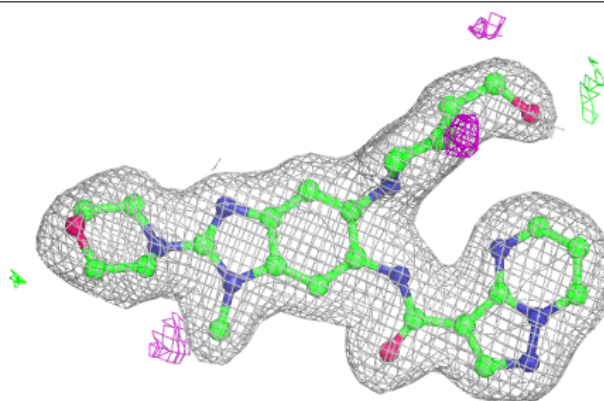


Electron density around LRS A 502:

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

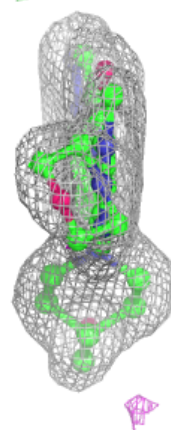
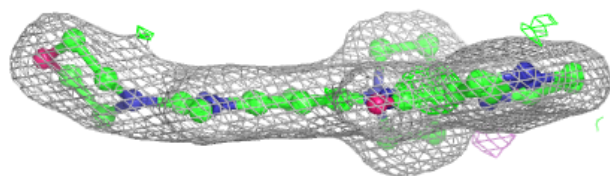
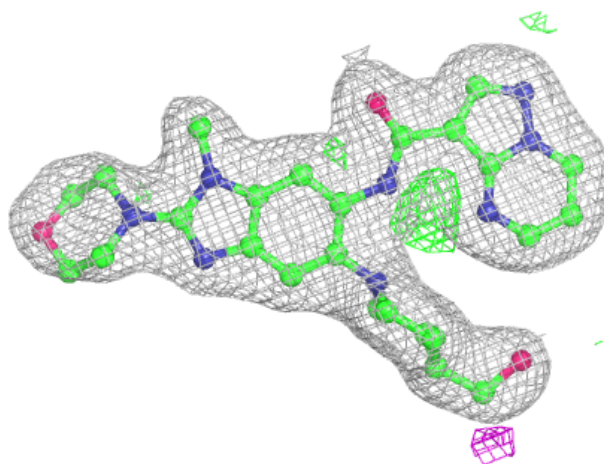
**Electron density around LRS B 502:**

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



Electron density around LRS 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.