

wwPDB X-ray Structure Validation Summary Report (i)

May 26, 2020 – 12:22 pm BST

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		
Resolution	:	1.98 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references (1)) were used in the production of this report:

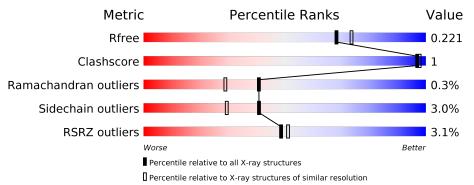
MolProbity		4.02b-467 1.8.5 (274361), CSD as541be (2020)
9		
Xtriage (Phenix)		1.13
EDS	:	2.11
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.98 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
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 on 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	А	320	% 	•	9%
1	В	320	3% 87%	•	8%
1	С	320	5% 82%	7%	11%
1	D	320	^{2%} 85%	••	11%



2 Entry composition (i)

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	Δ	292	Total	С	Ν	Ο	Р	\mathbf{S}	0	0	0
	A	292	2306	1443	387	458	3	15	0	0	
1	В	293	Total	С	Ν	Ο	Р	S	0	0	0
			2311	1446	388	459	3	15			
1	С	286	Total	С	Ν	Ο	Р	S	0	2	0
			2279	1429	381	451	3	15			
1	1 D	295	Total	С	Ν	Ο	Р	S	0	0	0
	285	2256	1412	379	448	3	14	0	U		

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

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
В	144	MET	-	initiating methionine	UNP Q9NWZ3
В	145	HIS	-	expression tag	UNP Q9NWZ3



В В В В В В В В В В В В В В В В В С С С С С С С С С С С С С С С С С С С

Residue	Modelled	Actual	Comment	Reference
146	HIS	-	expression tag	UNP Q9NWZ3
147	HIS	-	expression tag	UNP Q9NWZ3
148	HIS	-	expression tag	UNP Q9NWZ3
149	HIS	-	expression tag	UNP Q9NWZ3
150	HIS	-	expression tag	UNP Q9NWZ3
151	GLY	-	expression tag	UNP Q9NWZ3
152	GLU	-	expression tag	UNP Q9NWZ3
153	ASN	-	expression tag	UNP Q9NWZ3
154	LEU	-	expression tag	UNP Q9NWZ3
155	TYR	-	expression tag	UNP Q9NWZ3
156	PHE	-	expression tag	UNP Q9NWZ3
157	GLN	-	expression tag	UNP Q9NWZ3
158	GLY	-	expression tag	UNP Q9NWZ3
159	SER	-	expression tag	UNP Q9NWZ3
461	GLY	-	expression tag	UNP Q9NWZ3
462	ASN	-	expression tag	UNP Q9NWZ3
463	SER	-	expression tag	UNP Q9NWZ3
144	MET	-	initiating methionine	UNP Q9NWZ3
145	HIS	-	expression tag	UNP Q9NWZ3
146	HIS	-	expression tag	UNP Q9NWZ3
147	HIS	-	expression tag	UNP Q9NWZ3
148	HIS	-	expression tag	UNP Q9NWZ3
149	HIS	-	expression tag	UNP Q9NWZ3
150	HIS	-	expression tag	UNP Q9NWZ3
151	GLY	-	expression tag	UNP Q9NWZ3
152	GLU	-	expression tag	UNP Q9NWZ3
153	ASN	-	expression tag	UNP Q9NWZ3
154	LEU	-	expression tag	UNP Q9NWZ3
155	TYR	-	expression tag	UNP Q9NWZ3
156	PHE	-	expression tag	UNP Q9NWZ3
157	GLN	-	expression tag	UNP Q9NWZ3
158	GLY	-	expression tag	UNP Q9NWZ3
159	SER	-	expression tag	UNP Q9NWZ3
461	GLY	-	expression tag	UNP Q9NWZ3
462	ASN	-	expression tag	UNP Q9NWZ3
100			• •	TIND CONTINUES

Continued Chain | I

463

144

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SER

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HIS

HIS

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UNP Q9NWZ3



expression tag

initiating methionine

expression tag

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expression tag

expression tag

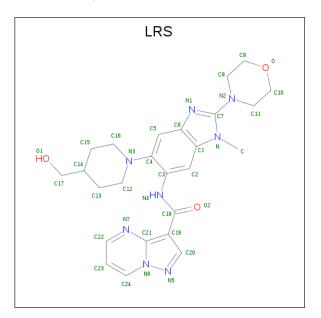
expression tag

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	В	1	Total Ca 1 1	0	0
2	А	1	Total Ca 1 1	0	0

• Molecule 3 is N-{5-[4-(hydroxymethyl)piperidin-1-yl]-1-methyl-2-(morpholin-4-yl)-1H-ben zimidazol-6-yl}pyrazolo[1,5-a]pyrimidine-3-carboxamide (three-letter code: LRS) (formula: $C_{25}H_{30}N_8O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total C N O 36 25 8 3	0	0
3	В	1	Total C N O 36 25 8 3	0	0
3	С	1	Total C N O 36 25 8 3	0	0
3	D	1	$\begin{array}{cccccc} {\rm Total} & {\rm C} & {\rm N} & {\rm O} \\ {\rm 36} & {\rm 25} & {\rm 8} & {\rm 3} \end{array}$	0	0

• Molecule 4 is water.

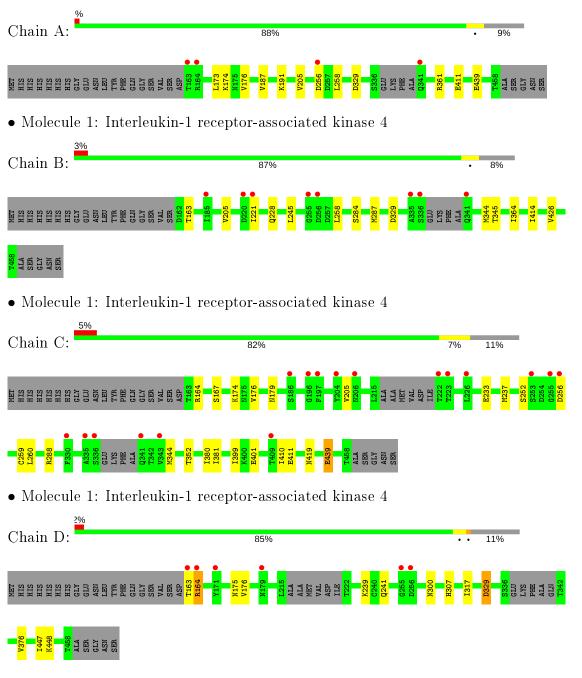
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	194	Total O 194 194	0	0
4	В	147	Total O 147 147	0	0
4	С	116	Total O 116 116	0	0
4	D	152	Total O 152 152	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	141.54Å 140.11 Å 87.82 Å	Depositor
a, b, c, α , β , γ	90.00° 123.36° 90.00°	Depositor
Resolution (Å)	28.99 - 1.98	Depositor
Resolution (A)	90.36 - 1.98	EDS
% Data completeness	96.9 (28.99-1.98)	Depositor
(in resolution range)	96.8 (90.36 - 1.98)	EDS
R _{merge}	0.05	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.30 (at 1.98 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
D D.	0.183 , 0.215	Depositor
R, R_{free}	0.189 , 0.221	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.

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.



¹Intensities estimated from amplitudes.

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: TPO, CA, LRS, SEP

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		
	Cham	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.51	0/2310	0.64	0/3112	
1	В	0.51	0/2315	0.63	0/3119	
1	С	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	А	2306	0	2267	5	0
1	В	2311	0	2269	3	0
1	С	2279	0	2242	7	0
1	D	2256	0	2218	4	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
3	А	36	0	0	0	0
3	В	36	0	0	0	0
3	С	36	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	36	0	0	0	0
4	А	194	0	0	1	0
4	В	147	0	0	0	0
4	С	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.

The worst 5 of 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

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	Perce	ntiles
1	А	285/320~(89%)	280~(98%)	4 (1%)	1 (0%)	34	22
1	В	286/320~(89%)	279~(98%)	7(2%)	0	100	100
1	С	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	С	256	ASP
1	А	329	ASP
1	D	329	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	А	252/275~(92%)	247 (98%)	5(2%)	55	48	
1	В	252/275~(92%)	244 (97%)	8 (3%)	39	28	
1	С	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	

 $5~{\rm of}~30$ residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	С	164	ARG
1	С	179	ASN
1	D	241	GLN
1	С	174	LYS
1	С	237	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	С	293	GLN
1	С	419	ASN
1	D	286	HIS
1	В	228	GLN
1	D	166	HIS



5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	B	Bond lengths			ond ang	les
WIOI	туре	Cham	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	С	342	1	8,10,11	1.31	1(12%)	10, 14, 16	1.12	0
1	TPO	С	345	1	8,10,11	1.22	1 (12%)	10, 14, 16	1.26	1 (10%)
1	TPO	А	345	1	8,10,11	1.07	1 (12%)	10, 14, 16	1.41	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	SEP	С	346	1	8,9,10	0.86	0	8,12,14	2.24	2 (25%)
1	SEP	В	346	1	8,9,10	1.06	1 (12%)	8,12,14	1.57	1 (12%)
1	SEP	А	346	1	8,9,10	0.85	0	8,12,14	2.32	3 (37%)
1	TPO	А	342	1	8,10,11	1.07	1 (12%)	10, 14, 16	1.62	3 (30%)
1	TPO	В	342	1	8,10,11	1.05	1 (12%)	10, 14, 16	1.47	1 (10%)
1	TPO	В	345	1	8,10,11	1.44	2 (25%)	10, 14, 16	1.34	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	TPO	С	342	1	-	1/9/11/13	-
1	TPO	С	345	1	-	5/9/11/13	-
1	TPO	А	345	1	-	2/9/11/13	-
1	TPO	D	345	1	-	3/9/11/13	-



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	SEP	С	346	1	-	1/5/8/10	-
1	SEP	В	346	1	-	1/5/8/10	-
1	SEP	А	346	1	-	3/5/8/10	-
1	TPO	А	342	1	-	1/9/11/13	-
1	TPO	В	342	1	-	1/9/11/13	-
1	TPO	В	345	1	-	2/9/11/13	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms		$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	В	345	TPO	P-OG1	-2.75	1.54	1.59
1	С	342	TPO	P-OG1	-2.71	1.54	1.59
1	D	345	TPO	CB-CA	2.47	1.59	1.53
1	В	346	SEP	P-OG	-2.23	1.53	1.60
1	А	345	TPO	CB-CA	2.16	1.58	1.53

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	С	346	SEP	OG-CB-CA	5.38	113.38	108.14
1	А	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	А	346	SEP	O3P-P-OG	3.88	117.06	106.73
1	А	342	TPO	P-OG1-CB	-3.57	112.44	123.21

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	С	342	TPO	O-C-CA-CB
1	С	345	TPO	N-CA-CB-OG1
1	С	345	TPO	CB-OG1-P-O1P
1	А	345	TPO	N-CA-CB-OG1
1	D	345	TPO	N-CA-CB-OG1

There are no ring outliers.

1 monomer is involved in 1 short contact:



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

5.5 Carbohydrates (i)

There are no carbohydrates 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	Tune	Chain	in Res Link		Bond lengths			Bond angles		
	Type	Cham	ILES		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	LRS	А	502	-	$33,\!41,\!41$	0.71	1(3%)	$38,\!59,\!59$	0.90	<mark>1 (2%)</mark>
3	LRS	С	501	-	33,41,41	0.75	1(3%)	$38,\!59,\!59$	0.92	<mark>1 (2%)</mark>
3	LRS	В	502	-	$33,\!41,\!41$	0.72	1(3%)	$38,\!59,\!59$	1.31	<mark>3 (7%)</mark>
3	LRS	D	501	-	$33,\!41,\!41$	0.78	1(3%)	$38,\!59,\!59$	1.17	<mark>3 (7%)</mark>

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	А	502	-	-	4/12/36/36	0/6/6/6
3	LRS	С	501	-	-	4/12/36/36	0/6/6/6
3	LRS	В	502	-	-	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



			10			0	
Mol	Chain	\mathbf{Res}	Type	Atoms		Observed(Å)	Ideal(Å) $ $
3	С	501	LRS	C7-N1	-2.23	1.31	1.35
3	А	502	LRS	C7-N1	-2.20	1.31	1.35
3	В	502	LRS	C7-N1	-2.13	1.31	1.35

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	В	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	В	502	LRS	C8-N2-C7	-3.93	113.60	122.03
3	С	501	LRS	C3-C2-C1	-3.53	118.27	121.32
3	В	502	LRS	C3-C2-C1	-3.52	118.28	121.32

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

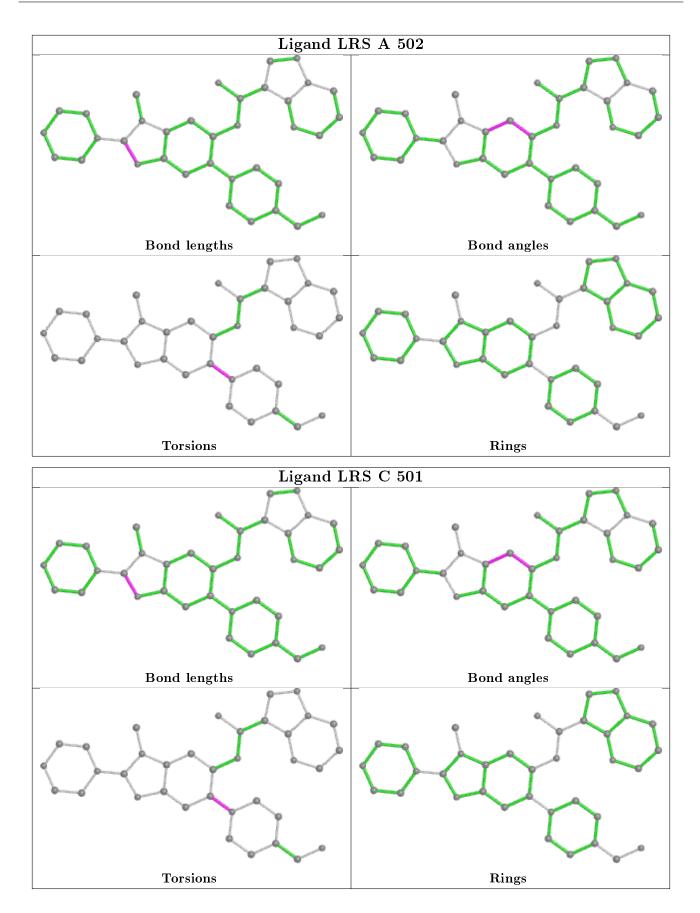
Mol	Chain	Res	Type	Atoms
3	D	501	LRS	C5-C4-N3-C16
3	С	501	LRS	C5-C4-N3-C16
3	В	502	LRS	C5-C4-N3-C16
3	А	502	LRS	C5-C4-N3-C16
3	D	501	LRS	C5-C4-N3-C12

There are no ring outliers.

No monomer is involved in short contacts.

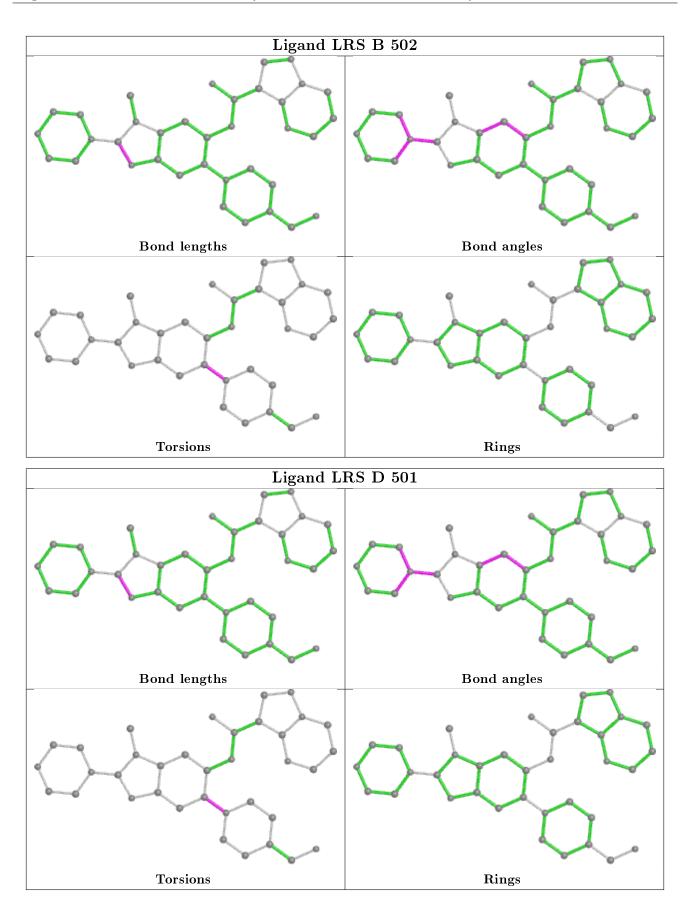
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.













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, 95^{th} 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	А	289/320~(90%)	-0.09	4 (1%) 75 77	18,30,54,84	0
1	В	290/320~(90%)	0.07	8 (2%) 53 55	20,35,63,87	0
1	С	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

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	С	343	VAL	9.1
1	С	341	GLN	9.0
1	D	255	GLY	6.5
1	С	226	LEU	6.0
1	С	223	THR	5.6

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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	$Q{<}0.9$
1	TPO	С	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	В	342	11/12	0.81	0.14	$69,\!70,\!71,\!71$	3
1	SEP	С	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	А	342	11/12	0.87	0.12	$58,\!59,\!62,\!63$	3
1	TPO	С	345	11/12	0.90	0.13	$74,\!76,\!77,\!77$	0



Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	RSR	${f B} ext{-factors}({ m \AA}^2)$	$Q{<}0.9$
1	SEP	В	346	10/11	0.90	0.09	$57,\!60,\!62,\!63$	3
1	SEP	А	346	10/11	0.91	0.11	$44,\!48,\!51,\!53$	3
1	TPO	D	345	11/12	0.97	0.09	$52,\!54,\!57,\!58$	0
1	TPO	А	345	11/12	0.97	0.08	43,44,48,49	0
1	TPO	В	345	11/12	0.97	0.10	$54,\!56,\!58,\!59$	0

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6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

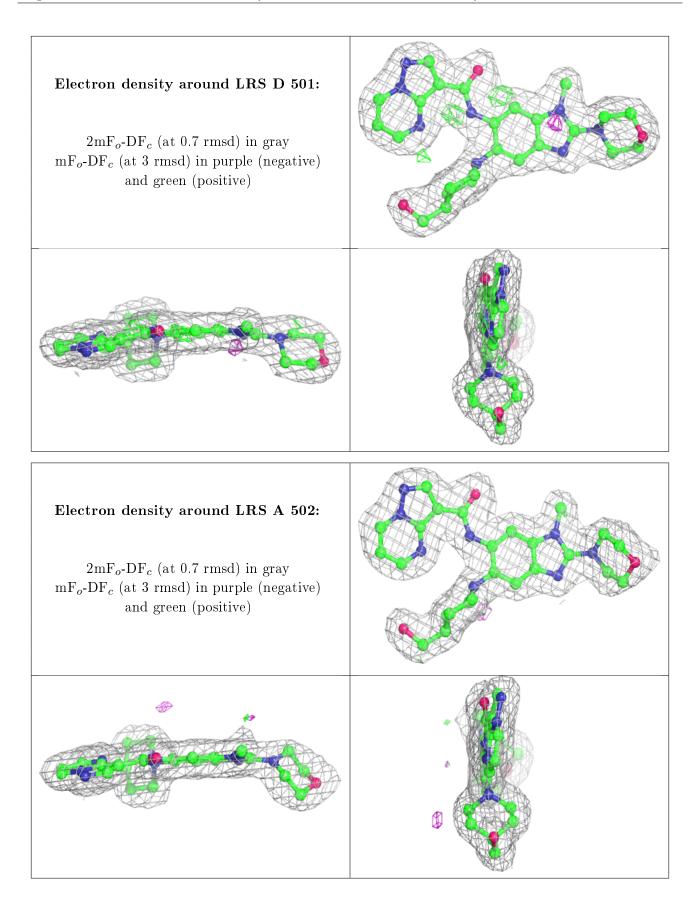
6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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.

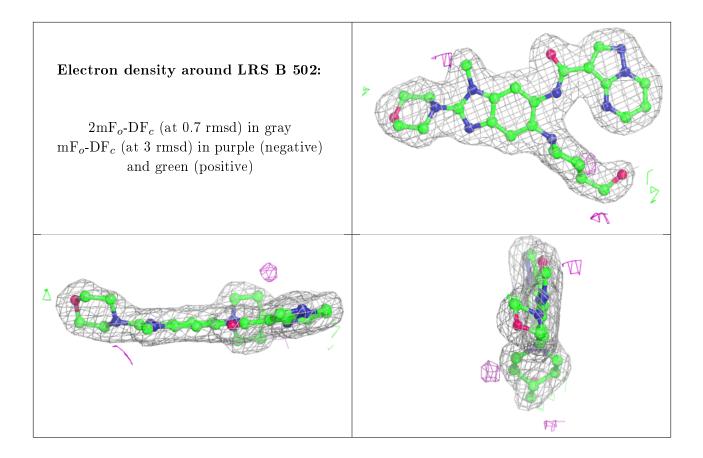
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	$Q{<}0.9$
2	CA	А	501	1/1	0.94	0.19	$63,\!63,\!63,\!63$	0
3	LRS	D	501	36/36	0.96	0.10	$17,\!24,\!30,\!37$	0
2	CA	В	501	1/1	0.97	0.22	$54,\!54,\!54,\!54$	0
3	LRS	А	502	36/36	0.97	0.10	$16,\!19,\!33,\!34$	0
3	LRS	В	502	36/36	0.97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

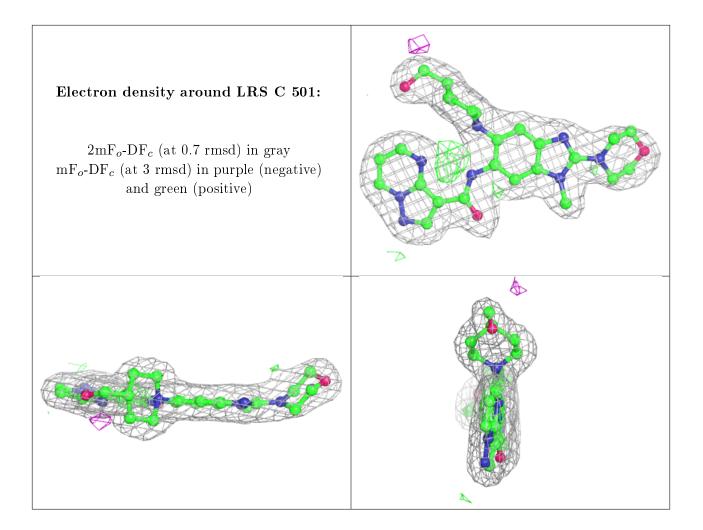












6.5 Other polymers (i)

There are no such residues in this entry.

