



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 08:30 pm BST

PDB ID : 5K7G
Title : IRAK4 in complex with AZ3862
Authors : Ferguson, A.D.
Deposited on : 2016-05-26
Resolution : 2.23 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 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 : 2.11
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) : 2.11

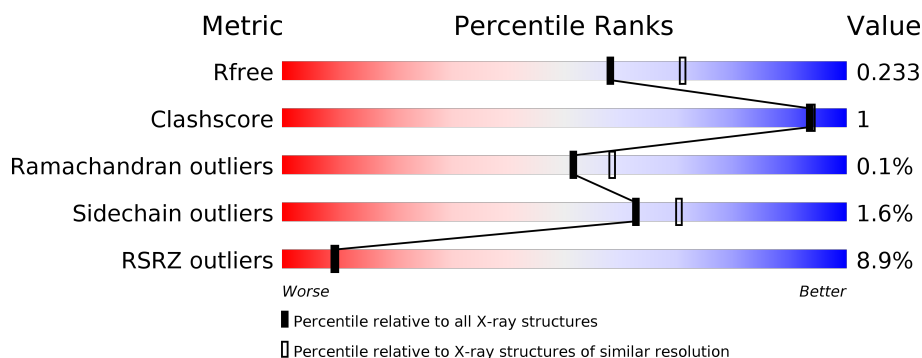
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 $\leq 5\%$. 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	301	<div> <div>7%</div> <div>89%</div> <div>7%</div> </div>
1	B	301	<div> <div>9%</div> <div>88%</div> <div>9%</div> </div>
1	C	301	<div> <div>9%</div> <div>90%</div> <div>5%</div> </div>
1	D	301	<div> <div>8%</div> <div>88%</div> <div>6% 5%</div> </div>

2 Entry composition [i](#)

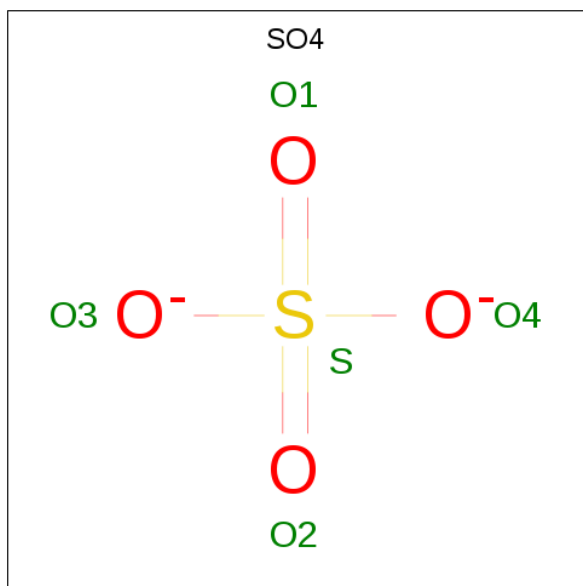
There are 4 unique types of molecules in this entry. The entry contains 9351 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	279	Total	C	N	O	P	S	0	0	0
			2205	1386	373	430	2	14			
1	B	275	Total	C	N	O	P	S	0	0	0
			2170	1370	363	424		13			
1	C	285	Total	C	N	O	P	S	0	0	0
			2253	1414	379	444	2	14			
1	D	285	Total	C	N	O	P	S	0	0	0
			2253	1414	379	444	2	14			

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



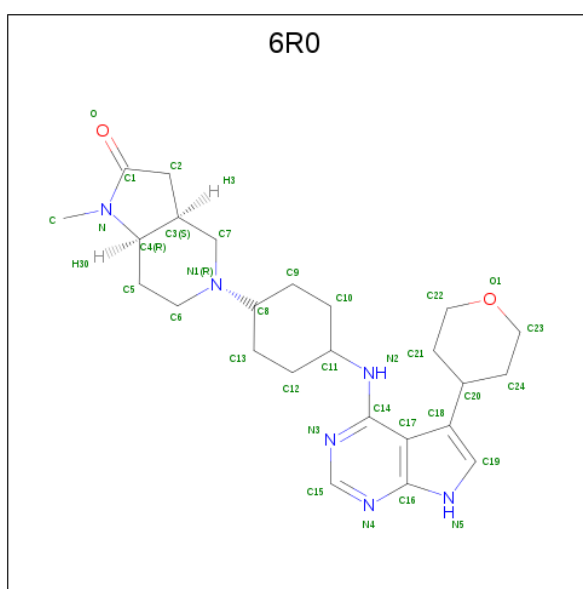
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is (3 {a} {S},7 {a} {R})-1-methyl-5-[4-[[5-(oxan-4-yl)-7 {H}-pyrrolo[2,3-d]pyrimidin-4-yl]amino]cyclohexyl]-3,3 {a},4,6,7,7 {a}-hexahydropyrrolo[3,2-c]pyridin-2-one (three-letter code: 6R0) (formula: C₂₅H₃₆N₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			33	25	6	2		
3	B	1	Total	C	N	O	0	0
			33	25	6	2		
3	C	1	Total	C	N	O	0	0
			33	25	6	2		
3	D	1	Total	C	N	O	0	0
			33	25	6	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total	O	0	0
			71	71		

Continued on next page...

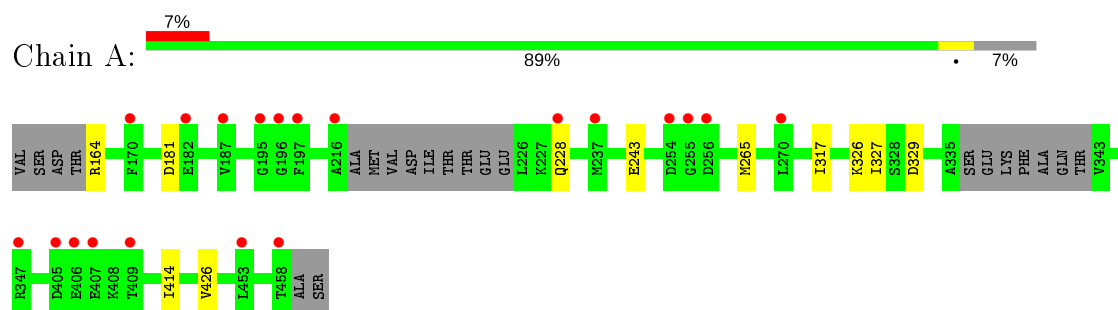
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	70	Total	O	0	0
			70	70		
4	C	88	Total	O	0	0
			88	88		
4	D	84	Total	O	0	0
			84	84		

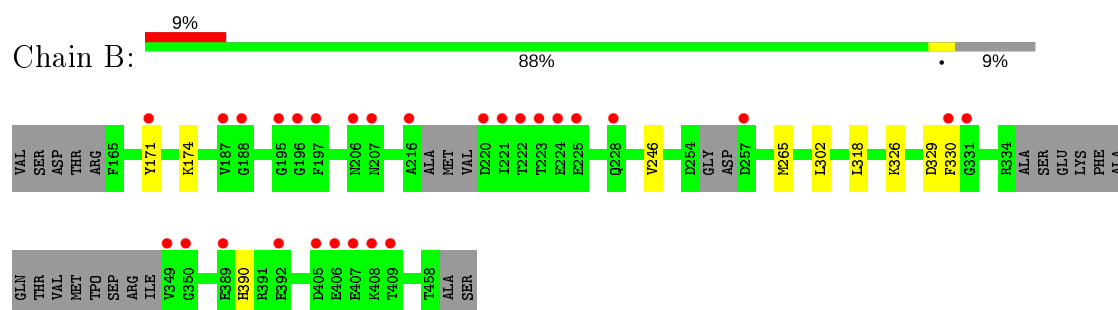
3 Residue-property plots [i](#)

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.

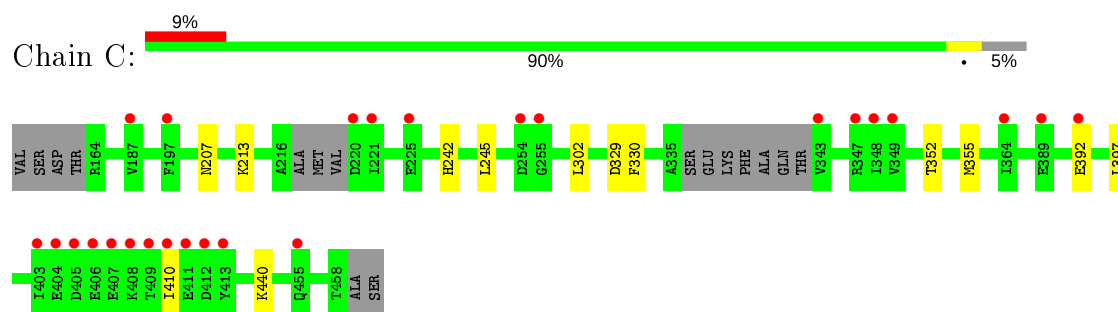
- Molecule 1: Interleukin-1 receptor-associated kinase 4



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

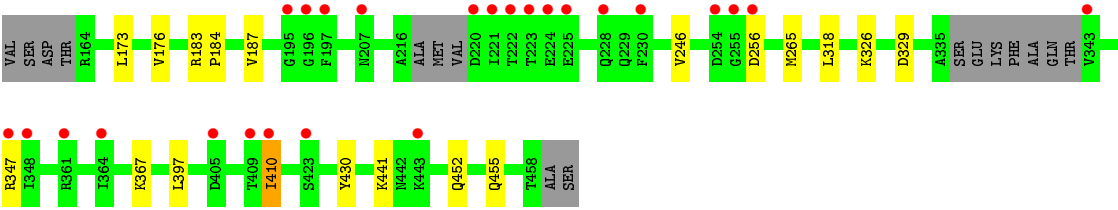


- Molecule 1: Interleukin-1 receptor-associated kinase 4



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





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.21Å 141.00Å 86.84Å 90.00° 126.19° 90.00°	Depositor
Resolution (Å)	45.29 – 2.23 45.29 – 2.23	Depositor EDS
% Data completeness (in resolution range)	95.5 (45.29-2.23) 95.8 (45.29-2.23)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.22Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.7	Depositor
R, R_{free}	0.206 , 0.227 0.214 , 0.233	Depositor DCC
R_{free} test set	3037 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9351	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.2629e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: TPO, 6R0, SO4, 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	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/2220	0.59	0/2989
1	B	0.41	0/2206	0.59	0/2973
1	C	0.40	0/2268	0.60	0/3055
1	D	0.40	0/2268	0.60	0/3055
All	All	0.40	0/8962	0.60	0/12072

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	2205	0	2176	4	0
1	B	2170	0	2141	7	0
1	C	2253	0	2218	4	0
1	D	2253	0	2217	10	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	D	5	0	0	0	0
3	A	33	0	0	0	0
3	B	33	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	33	0	0	0	0
3	D	33	0	0	0	0
4	A	71	0	0	0	0
4	B	70	0	0	0	0
4	C	88	0	0	0	0
4	D	84	0	0	0	0
All	All	9351	0	8752	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:B:265:MET:HE1	1:B:326:LYS:HG3	1.56	0.88
1:B:265:MET:CE	1:B:326:LYS:HG3	2.12	0.80
1:A:265:MET:HE1	1:A:326:LYS:HG3	1.64	0.79
1:C:352:THR:HA	1:C:355:MET:HE3	1.67	0.77
1:B:246:VAL:HG11	1:B:318:LEU:HD12	1.77	0.64
1:D:246:VAL:HG11	1:D:318:LEU:HD12	1.82	0.61
1:B:171:TYR:HA	1:B:174:LYS:HD3	1.90	0.53
1:A:265:MET:CE	1:A:326:LYS:HG3	2.34	0.53
1:D:173:LEU:HA	1:D:176:VAL:HG22	1.91	0.52
1:D:410:ILE:HG12	1:D:430:TYR:CG	2.46	0.51
1:D:265:MET:CE	1:D:326:LYS:HG3	2.43	0.49
1:B:265:MET:HE2	1:B:326:LYS:HG3	1.95	0.48
1:D:183:ARG:HB3	1:D:187:VAL:CG2	2.45	0.47
1:D:452:GLN:O	1:D:455:GLN:HG2	2.16	0.46
1:D:410:ILE:HG12	1:D:430:TYR:CD2	2.50	0.46
1:D:265:MET:HE1	1:D:326:LYS:HG3	1.97	0.46
1:A:317:ILE:HG12	1:A:327:ILE:HD13	2.00	0.43
1:C:242:HIS:HB3	1:C:245:LEU:HG	2.01	0.42
1:D:184:PRO:HD2	1:D:187:VAL:HG22	2.02	0.42
1:D:367:LYS:HD2	1:D:441:LYS:O	2.21	0.41
1:A:414:ILE:HG12	1:A:426:VAL:HG11	2.03	0.40
1:B:302:LEU:HD11	1:B:330:PHE:HE1	1.86	0.40
1:C:302:LEU:HD11	1:C:330:PHE:HE1	1.87	0.40
1:B:390:HIS:HB3	1:C:392:GLU:O	2.21	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	271/301 (90%)	265 (98%)	5 (2%)	1 (0%)	34	35
1	B	267/301 (89%)	260 (97%)	7 (3%)	0	100	100
1	C	277/301 (92%)	272 (98%)	5 (2%)	0	100	100
1	D	277/301 (92%)	271 (98%)	6 (2%)	0	100	100
All	All	1092/1204 (91%)	1068 (98%)	23 (2%)	1 (0%)	51	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	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	241/260 (93%)	237 (98%)	4 (2%)	60	68
1	B	241/260 (93%)	240 (100%)	1 (0%)	91	93
1	C	247/260 (95%)	241 (98%)	6 (2%)	49	55
1	D	247/260 (95%)	242 (98%)	5 (2%)	55	62
All	All	976/1040 (94%)	960 (98%)	16 (2%)	62	70

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	ARG
1	A	228	GLN
1	A	243	GLU
1	A	329	ASP
1	B	329	ASP
1	C	207	ASN
1	C	213	LYS
1	C	329	ASP
1	C	397	LEU
1	C	410	ILE
1	C	440	LYS
1	D	256	ASP
1	D	329	ASP
1	D	347	ARG
1	D	397	LEU
1	D	410	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	394	GLN
1	A	438	HIS
1	B	179	ASN
1	B	293	GLN
1	C	394	GLN
1	C	438	HIS
1	D	166	HIS
1	D	438	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	345	1	8,10,11	1.02	0	10,14,16	1.13	1 (10%)
1	TPO	D	345	1	8,10,11	1.08	0	10,14,16	1.11	1 (10%)
1	SEP	D	346	1	8,9,10	0.85	0	8,12,14	1.91	3 (37%)
1	SEP	C	346	1	8,9,10	0.76	0	8,12,14	3.25	3 (37%)
1	SEP	A	346	1	8,9,10	0.90	0	8,12,14	1.10	1 (12%)
1	TPO	C	345	1	8,10,11	0.84	0	10,14,16	1.87	2 (20%)

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	345	1	-	6/9/11/13	-
1	TPO	D	345	1	-	4/9/11/13	-
1	SEP	D	346	1	-	0/5/8/10	-
1	SEP	C	346	1	-	0/5/8/10	-
1	SEP	A	346	1	-	0/5/8/10	-
1	TPO	C	345	1	-	7/9/11/13	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	346	SEP	OG-CB-CA	8.10	116.03	108.14
1	C	345	TPO	CG2-CB-CA	4.64	122.31	113.16
1	D	346	SEP	OG-P-O1P	3.13	115.24	106.47
1	D	346	SEP	OG-CB-CA	2.90	110.97	108.14
1	C	346	SEP	P-OG-CB	-2.70	110.86	118.30
1	C	346	SEP	O3P-P-OG	2.63	113.74	106.73
1	D	346	SEP	P-OG-CB	-2.62	111.07	118.30
1	A	346	SEP	O2P-P-OG	2.34	112.96	106.73
1	C	345	TPO	O3P-P-OG1	2.21	115.92	105.99
1	A	345	TPO	O3P-P-OG1	2.19	115.80	105.99
1	D	345	TPO	O3P-P-OG1	2.13	115.54	105.99

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	CA-CB-OG1-P
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	CA-CB-OG1-P
1	D	345	TPO	CB-OG1-P-O1P
1	C	345	TPO	N-CA-CB-CG2
1	C	345	TPO	N-CA-CB-OG1
1	C	345	TPO	C-CA-CB-CG2
1	C	345	TPO	O-C-CA-CB
1	C	345	TPO	CB-OG1-P-O2P
1	A	345	TPO	CB-OG1-P-O1P
1	C	345	TPO	CB-OG1-P-O1P
1	C	345	TPO	CA-CB-OG1-P
1	A	345	TPO	CB-OG1-P-O2P
1	A	345	TPO	CB-OG1-P-O3P
1	A	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

9 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	SO4	B	501	-	4,4,4	0.17	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	6R0	A	503	-	37,38,38	0.90	2 (5%)	43,55,55	0.86	1 (2%)
3	6R0	B	503	-	37,38,38	1.02	2 (5%)	43,55,55	1.45	5 (11%)
3	6R0	D	502	-	37,38,38	0.98	2 (5%)	43,55,55	1.65	6 (13%)
2	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.05	0
3	6R0	C	501	-	37,38,38	1.09	2 (5%)	43,55,55	1.53	5 (11%)
2	SO4	A	502	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	D	501	-	4,4,4	0.12	0	6,6,6	0.05	0
2	SO4	B	502	-	4,4,4	0.15	0	6,6,6	0.05	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
3	6R0	A	503	-	-	6/10/55/55	0/6/6/6
3	6R0	B	503	-	-	4/10/55/55	0/6/6/6
3	6R0	C	501	-	-	7/10/55/55	0/6/6/6
3	6R0	D	502	-	-	3/10/55/55	0/6/6/6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	6R0	C18-C17	4.83	1.46	1.40
3	D	502	6R0	C18-C17	4.35	1.45	1.40
3	B	503	6R0	C18-C17	4.04	1.45	1.40
3	A	503	6R0	C18-C17	3.69	1.44	1.40
3	B	503	6R0	C4-N	3.44	1.51	1.46
3	C	501	6R0	C4-N	3.30	1.50	1.46
3	A	503	6R0	C4-N	2.73	1.50	1.46
3	D	502	6R0	C4-N	2.70	1.50	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	6R0	C14-N2-C11	7.02	137.50	124.16
3	C	501	6R0	C14-N2-C11	6.80	137.09	124.16
3	B	503	6R0	C14-N2-C11	6.53	136.57	124.16
3	D	502	6R0	C6-C5-C4	5.36	118.33	109.91
3	C	501	6R0	C13-C8-N1	4.24	123.53	112.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	6R0	C13-C8-N1	4.03	122.98	112.52
3	D	502	6R0	C9-C8-N1	3.49	121.58	112.52
3	A	503	6R0	C6-C5-C4	2.80	114.30	109.91
3	C	501	6R0	C12-C11-N2	2.78	114.94	110.60
3	D	502	6R0	C10-C11-N2	2.72	114.83	110.60
3	C	501	6R0	C10-C11-N2	2.67	114.75	110.60
3	B	503	6R0	C12-C11-N2	2.41	114.36	110.60
3	D	502	6R0	C12-C11-N2	2.30	114.17	110.60
3	C	501	6R0	C9-C8-N1	2.27	118.42	112.52
3	B	503	6R0	C10-C11-N2	2.22	114.06	110.60
3	D	502	6R0	C13-C8-N1	2.17	118.14	112.52
3	B	503	6R0	C9-C8-N1	2.10	117.97	112.52

There are no chirality outliers.

All (20) torsion outliers are listed below:

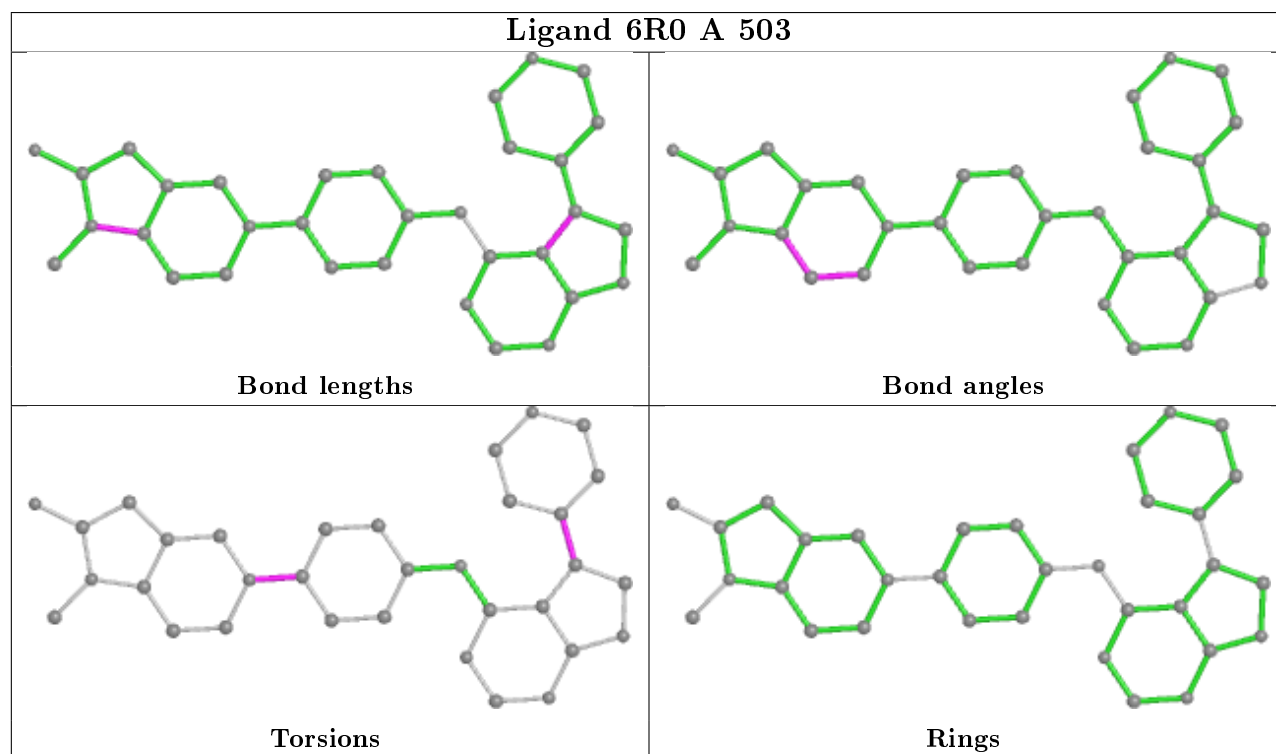
Mol	Chain	Res	Type	Atoms
3	A	503	6R0	C9-C8-N1-C7
3	B	503	6R0	C9-C8-N1-C7
3	B	503	6R0	C9-C8-N1-C6
3	B	503	6R0	C10-C11-N2-C14
3	D	502	6R0	C10-C11-N2-C14
3	C	501	6R0	C9-C8-N1-C7
3	C	501	6R0	C9-C8-N1-C6
3	C	501	6R0	C10-C11-N2-C14
3	A	503	6R0	C9-C8-N1-C6
3	A	503	6R0	C13-C8-N1-C7
3	C	501	6R0	C13-C8-N1-C6
3	B	503	6R0	C13-C8-N1-C6
3	A	503	6R0	C13-C8-N1-C6
3	D	502	6R0	C13-C8-N1-C7
3	D	502	6R0	C13-C8-N1-C6
3	C	501	6R0	C13-C8-N1-C7
3	A	503	6R0	C19-C18-C20-C21
3	A	503	6R0	C19-C18-C20-C24
3	C	501	6R0	C19-C18-C20-C21
3	C	501	6R0	C19-C18-C20-C24

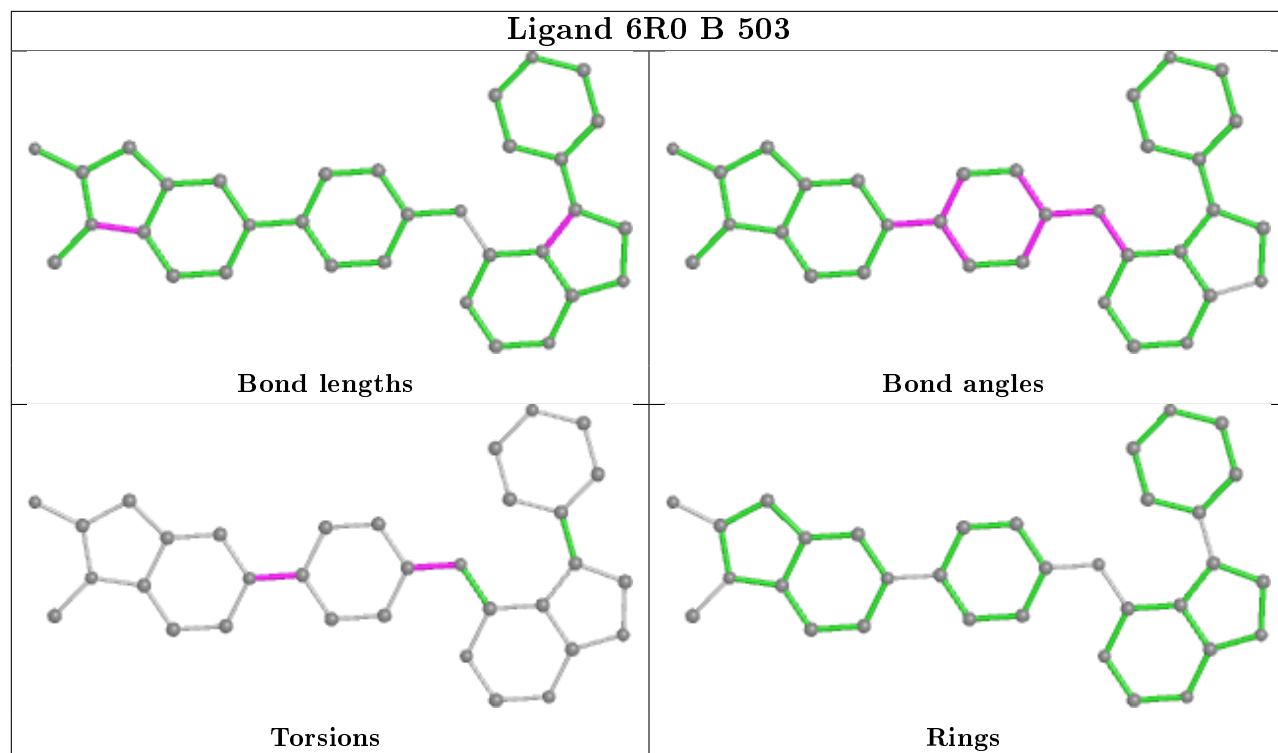
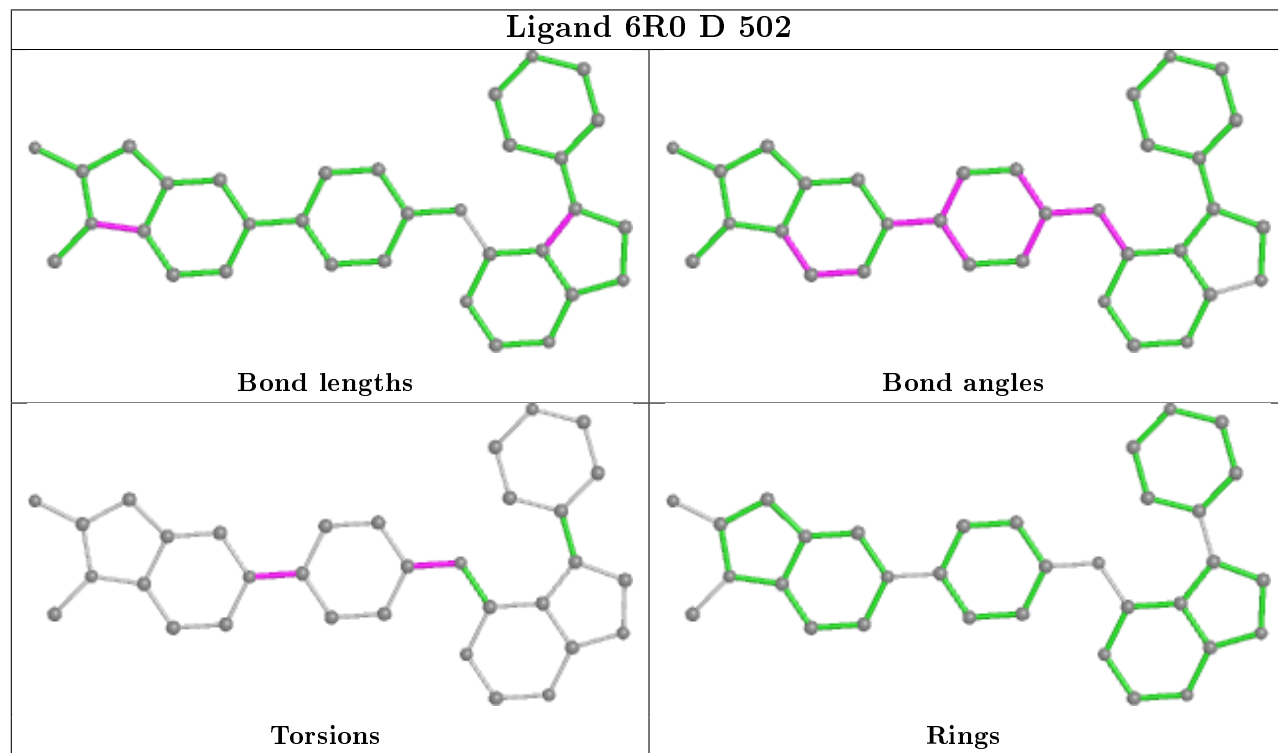
There are no ring outliers.

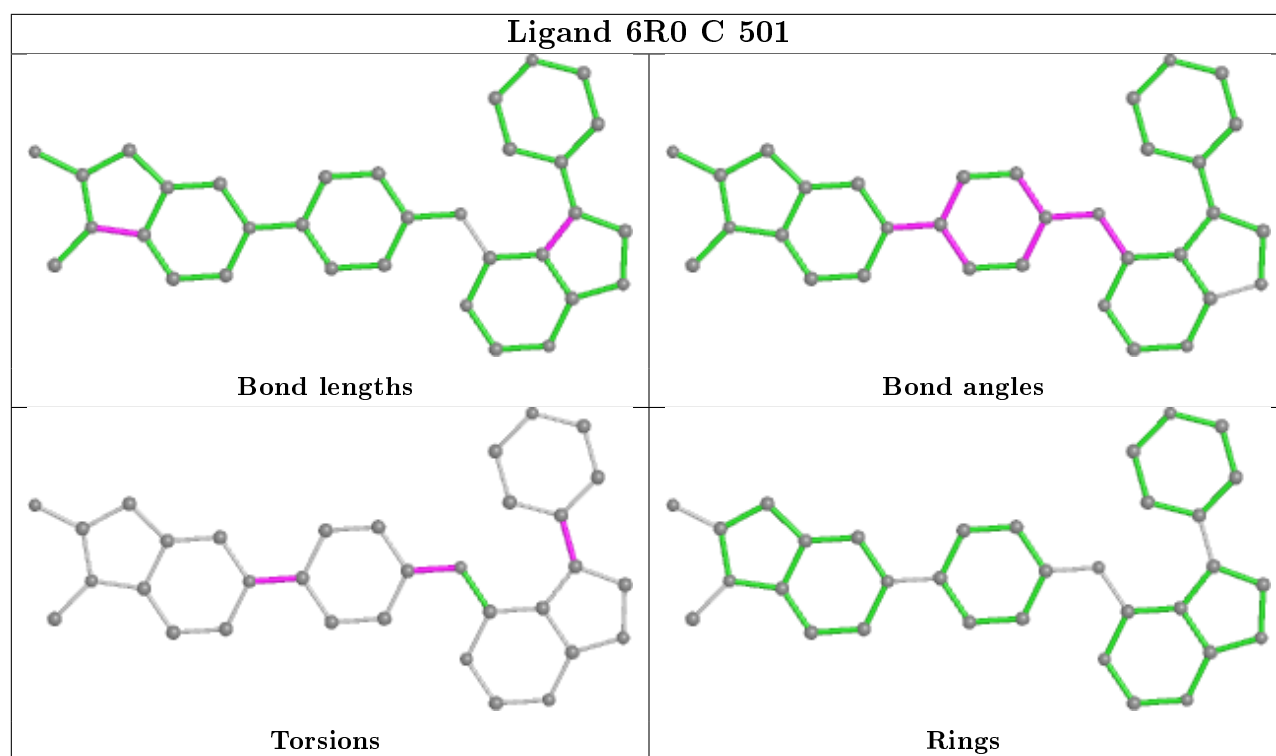
No monomer is involved in short contacts.

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 6R0 B 503**Ligand 6R0 D 502**



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	277/301 (92%)	0.66	20 (7%) 15 14	27, 45, 74, 94	0
1	B	275/301 (91%)	0.67	28 (10%) 6 6	25, 42, 71, 96	0
1	C	283/301 (94%)	0.70	26 (9%) 9 8	24, 41, 78, 103	0
1	D	283/301 (94%)	0.64	25 (8%) 10 9	25, 43, 81, 103	0
All	All	1118/1204 (92%)	0.67	99 (8%) 9 9	24, 43, 78, 103	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	331	GLY	6.7
1	D	221	ILE	6.2
1	D	405	ASP	5.7
1	A	187	VAL	5.5
1	D	220	ASP	5.3
1	A	407	GLU	5.2
1	C	403	ILE	5.1
1	B	220	ASP	4.7
1	A	256	ASP	4.7
1	B	221	ILE	4.7
1	C	220	ASP	4.7
1	D	256	ASP	4.6
1	A	405	ASP	4.4
1	B	349	VAL	4.3
1	C	407	GLU	4.2
1	C	408	LYS	4.2
1	C	405	ASP	4.1
1	B	196	GLY	4.1
1	C	413	TYR	4.0
1	D	255	GLY	4.0
1	C	364	ILE	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	225	GLU	3.8
1	A	254	ASP	3.8
1	B	195	GLY	3.7
1	A	195	GLY	3.7
1	B	187	VAL	3.6
1	B	222	THR	3.5
1	D	347	ARG	3.5
1	B	408	LYS	3.4
1	B	224	GLU	3.3
1	A	196	GLY	3.2
1	A	409	THR	3.2
1	A	255	GLY	3.2
1	C	221	ILE	3.2
1	D	228	GLN	3.1
1	B	406	GLU	3.1
1	B	228	GLN	3.1
1	B	216	ALA	3.1
1	C	343	VAL	3.0
1	A	347	ARG	3.0
1	D	225	GLU	3.0
1	B	171	TYR	3.0
1	B	407	GLU	2.9
1	D	197	PHE	2.9
1	C	410	ILE	2.9
1	A	170	PHE	2.9
1	A	197	PHE	2.9
1	B	197	PHE	2.8
1	A	216	ALA	2.8
1	C	404	GLU	2.8
1	B	188	GLY	2.8
1	D	410	ILE	2.7
1	B	405	ASP	2.7
1	C	348	ILE	2.7
1	C	406	GLU	2.7
1	C	455	GLN	2.6
1	C	197	PHE	2.6
1	C	412	ASP	2.6
1	D	222	THR	2.6
1	A	458	THR	2.6
1	B	225	GLU	2.6
1	D	409	THR	2.5
1	A	237	MET	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	255	GLY	2.5
1	B	206	ASN	2.5
1	C	392	GLU	2.5
1	A	228	GLN	2.5
1	B	223	THR	2.5
1	D	254	ASP	2.5
1	D	343	VAL	2.5
1	B	392	GLU	2.4
1	B	409	THR	2.4
1	D	361	ARG	2.4
1	B	350	GLY	2.4
1	C	347	ARG	2.4
1	B	257	ASP	2.3
1	D	224	GLU	2.3
1	A	453	LEU	2.3
1	D	196	GLY	2.3
1	D	443	LYS	2.2
1	D	207	ASN	2.2
1	A	406	GLU	2.2
1	C	411	GLU	2.2
1	D	364	ILE	2.2
1	A	270	LEU	2.2
1	B	389	GLU	2.2
1	C	389	GLU	2.2
1	D	230	PHE	2.1
1	C	409	THR	2.1
1	C	187	VAL	2.1
1	C	254	ASP	2.1
1	B	207	ASN	2.1
1	D	423	SER	2.1
1	C	349	VAL	2.1
1	A	182	GLU	2.1
1	D	223	THR	2.1
1	B	330	PHE	2.1
1	D	195	GLY	2.1
1	D	348	ILE	2.0

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

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(\AA^2)	Q<0.9
1	SEP	A	346	10/11	0.68	0.36	78,83,88,89	0
1	SEP	D	346	10/11	0.75	0.39	93,98,103,104	0
1	SEP	C	346	10/11	0.76	0.37	90,94,101,102	0
1	TPO	C	345	11/12	0.85	0.33	85,88,92,93	0
1	TPO	D	345	11/12	0.87	0.26	87,91,96,96	0
1	TPO	A	345	11/12	0.88	0.19	71,74,80,80	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

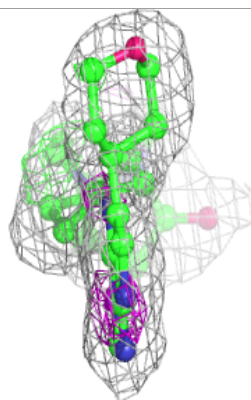
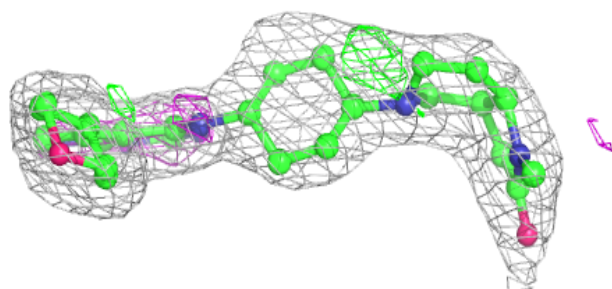
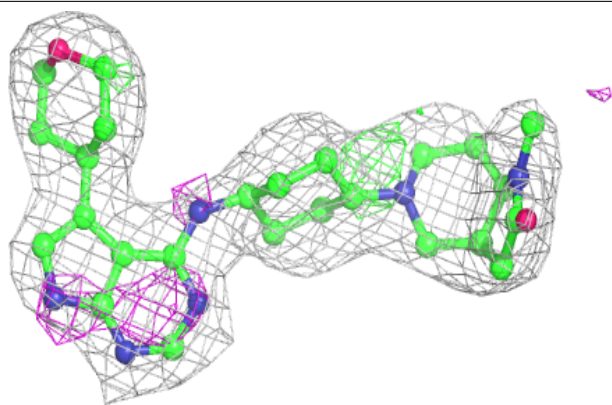
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	B	502	5/5	0.40	0.30	147,147,148,148	0
2	SO4	A	502	5/5	0.51	0.24	132,133,133,133	0
2	SO4	D	501	5/5	0.74	0.38	111,111,112,112	0
2	SO4	A	501	5/5	0.75	0.26	134,134,134,134	0
2	SO4	B	501	5/5	0.87	0.31	83,84,84,85	0
3	6R0	D	502	33/33	0.90	0.17	27,31,43,48	0
3	6R0	C	501	33/33	0.92	0.17	24,29,39,44	0
3	6R0	A	503	33/33	0.93	0.16	29,34,40,43	0
3	6R0	B	503	33/33	0.93	0.15	27,32,40,44	0

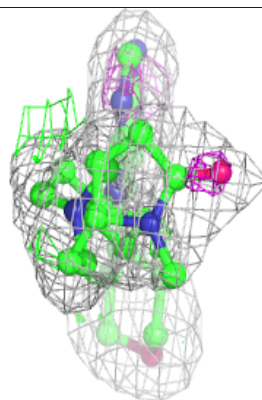
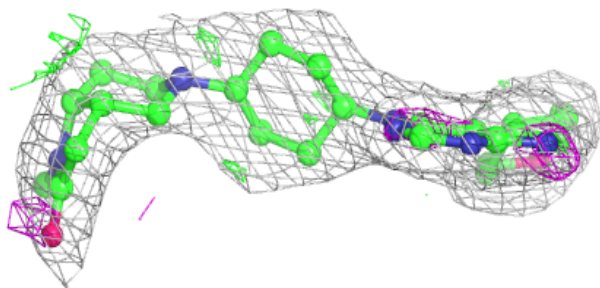
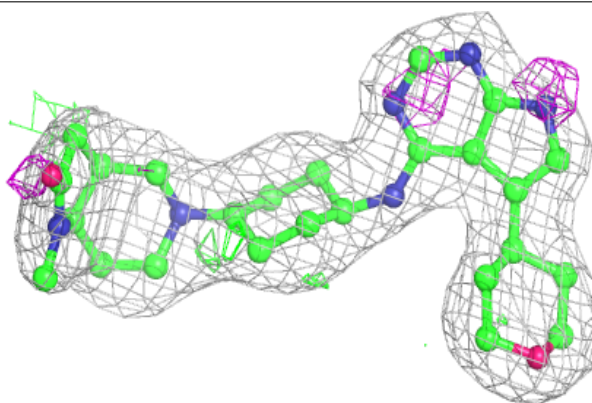
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6R0 D 502:

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

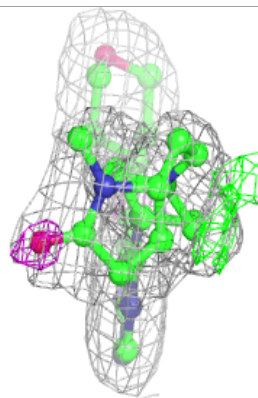
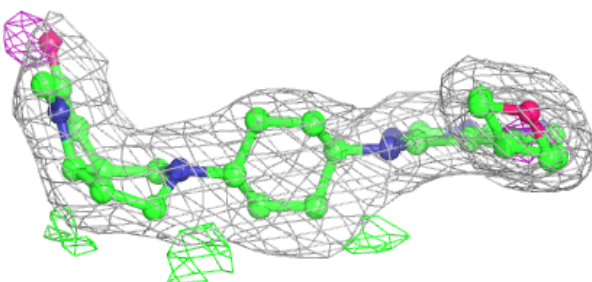
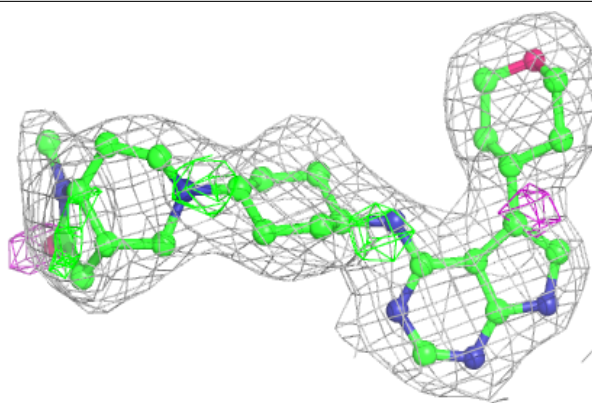
**Electron density around 6R0 C 501:**

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

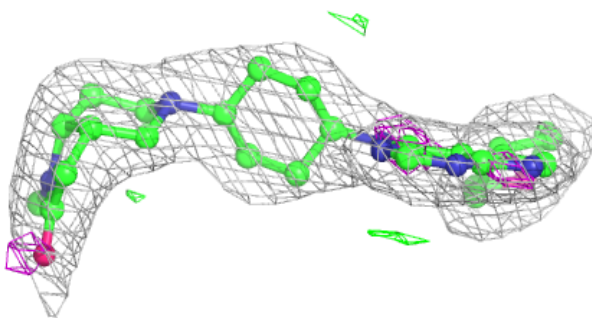
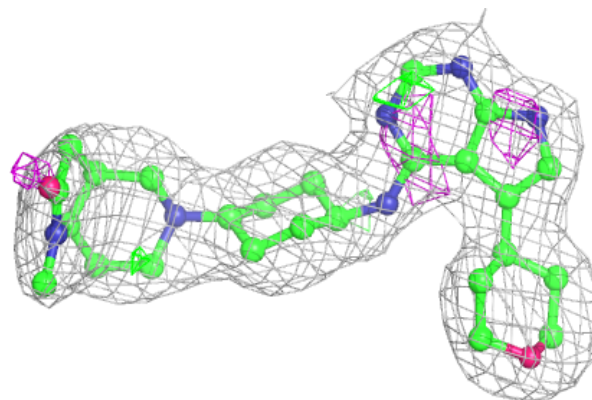


Electron density around 6R0 A 503:

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

**Electron density around 6R0 B 503:**

$2mF_o-DF_c$ (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.