



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:17 am BST

PDB ID : 5K75  
Title : IRAK4 in complex with Compound 1  
Authors : Ferguson, A.D.  
Deposited on : 2016-05-25  
Resolution : 2.03 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](mailto: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.

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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

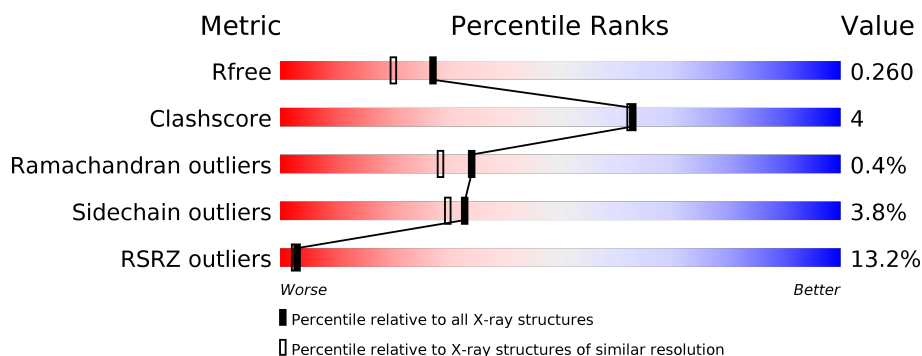
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.03 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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  $\geq 3$ , 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>12%</div> <div> <div></div> <div>82%</div> <div>8%</div> <div>9%</div> </div> </div>
1	B	301	<div> <div>9%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>8%</div> </div> </div>
1	C	301	<div> <div>13%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>6%</div> </div> </div>
1	D	301	<div> <div>15%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>6%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SEP	A	346	-	-	-	X

## 2 Entry composition [i](#)

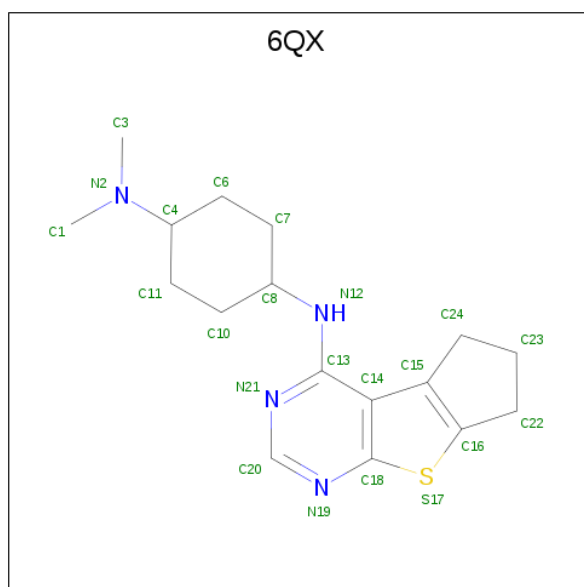
There are 4 unique types of molecules in this entry. The entry contains 9417 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	273	Total	C	N	O	P	S	0	2	0
			2176	1370	367	422	2	15			
1	B	276	Total	C	N	O	P	S	0	2	0
			2207	1388	369	433	2	15			
1	C	284	Total	C	N	O	P	S	0	2	0
			2257	1417	379	445	2	14			
1	D	282	Total	C	N	O	P	S	0	2	0
			2248	1411	377	444	2	14			

- Molecule 2 is {N}1-(7,8-dihydro-6 {H}-cyclopenta[2,3]thieno[2,4- {c}]pyrimidin-1-yl)- {N}4, {N}4-dimethyl-cyclohexane-1,4-diamine (three-letter code: 6QX) (formula: C<sub>17</sub>H<sub>24</sub>N<sub>4</sub>S).



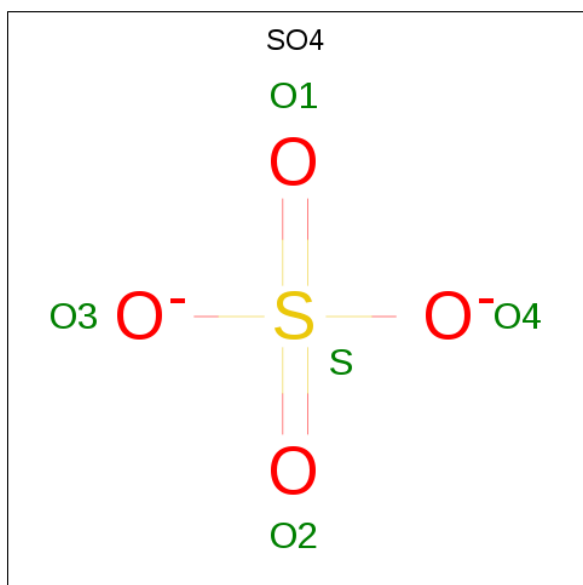
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			22	17	4	1		
2	B	1	Total	C	N	S	0	0
			22	17	4	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	S	0	0
			22	17	4	1		
2	D	1	Total	C	N	S	0	0
			22	17	4	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

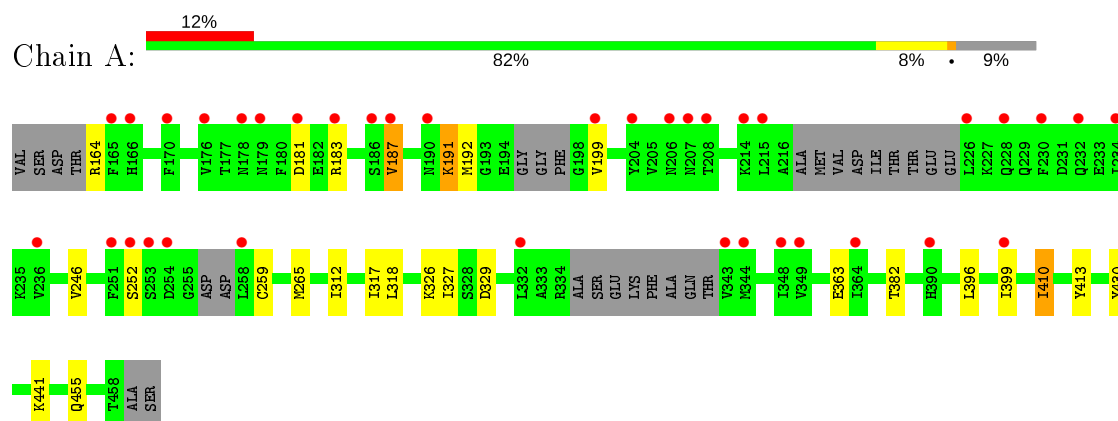
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	90	Total 90	O 90	0	0
4	B	90	Total 90	O 90	0	0
4	C	108	Total 108	O 108	0	0
4	D	118	Total 118	O 118	0	0

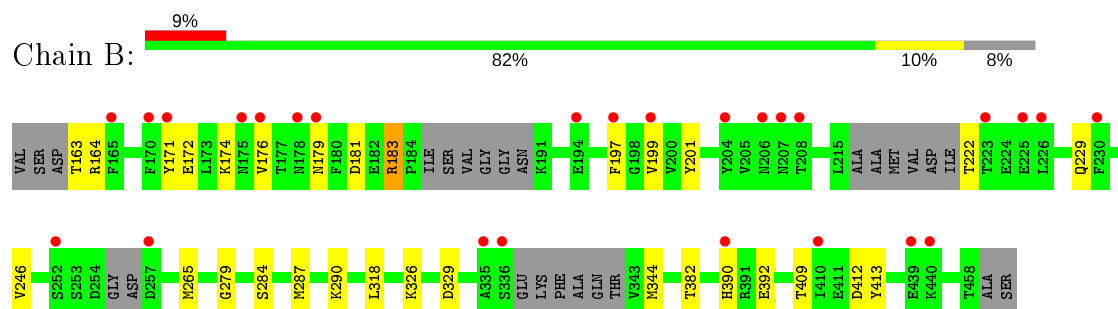
### 3 Residue-property plots [i](#)

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.

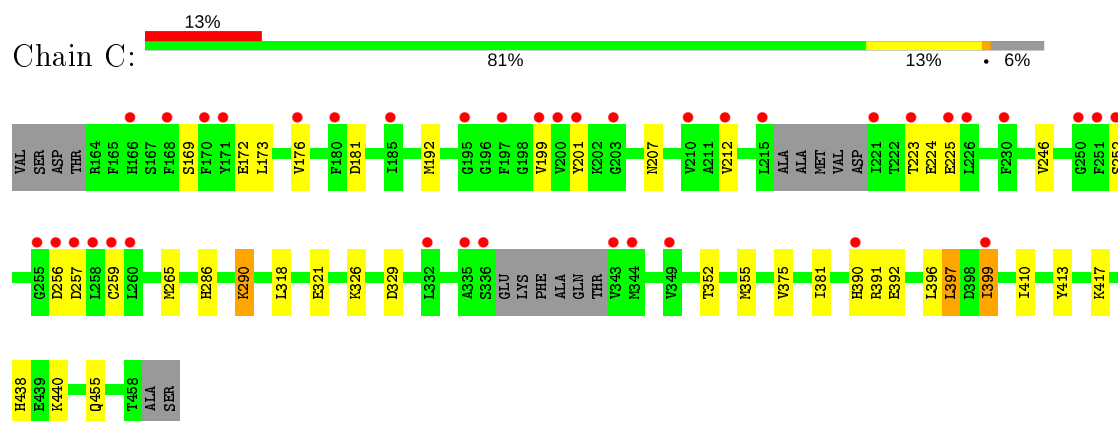
- Molecule 1: Interleukin-1 receptor-associated kinase 4



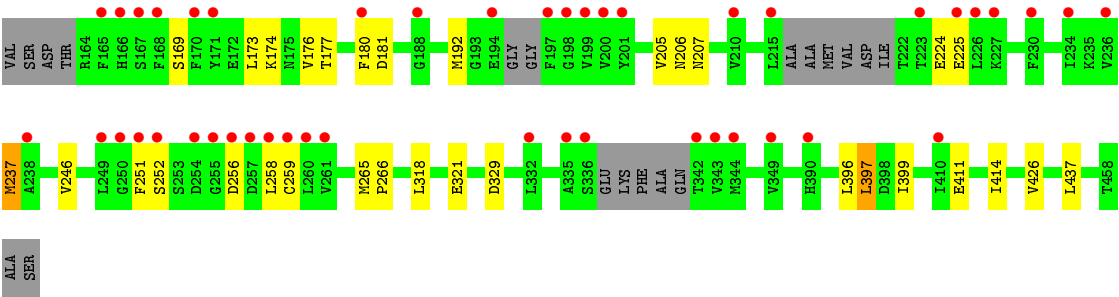
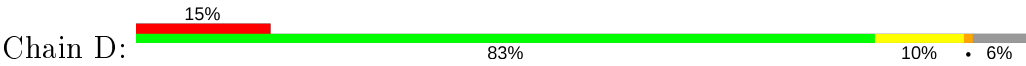
- Molecule 1: Interleukin-1 receptor-associated kinase 4



- 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, $\alpha$ , $\beta$ , $\gamma$	144.87Å 141.62Å 88.06Å 90.00° 125.92° 90.00°	Depositor
Resolution (Å)	45.18 – 2.03 45.17 – 2.03	Depositor EDS
% Data completeness (in resolution range)	97.0 (45.18-2.03) 97.0 (45.17-2.03)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 2.03Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.7	Depositor
R, $R_{free}$	0.239 , 0.253 0.245 , 0.260	Depositor DCC
$R_{free}$ test set	4493 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.4	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.169 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9417	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, 6QX, 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	0.45	0/2194	0.63	0/2950
1	B	0.46	0/2226	0.62	0/2994
1	C	0.50	0/2278	0.66	0/3068
1	D	0.50	0/2268	0.67	0/3054
All	All	0.48	0/8966	0.64	0/12066

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	2176	0	2161	15	0
1	B	2207	0	2178	18	0
1	C	2257	0	2226	31	0
1	D	2248	0	2214	18	0
2	A	22	0	0	0	0
2	B	22	0	0	0	0
2	C	22	0	0	0	0
2	D	22	0	0	0	0
3	B	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	10	0	0	0	0
3	D	10	0	0	0	0
4	A	90	0	0	0	0
4	B	90	0	0	0	0
4	C	108	0	0	2	0
4	D	118	0	0	3	0
All	All	9417	0	8779	77	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 4.

All (77) 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:C:286:HIS:NE2	1:C:290:LYS:NZ	1.89	1.20
1:B:265:MET:HE1	1:B:326:LYS:HG3	1.34	1.09
1:C:265:MET:HE1	1:C:326:LYS:HG3	1.35	1.08
1:C:265:MET:CE	1:C:326:LYS:HG3	1.82	1.08
1:C:375:VAL:HG22	1:C:397:LEU:HD11	1.48	0.92
1:C:212:VAL:HG13	4:C:618:HOH:O	1.72	0.88
1:C:375:VAL:HG22	1:C:397:LEU:CD1	2.05	0.86
1:B:265:MET:CE	1:B:326:LYS:HG3	2.07	0.85
1:B:390:HIS:O	1:C:390:HIS:O	1.97	0.82
1:D:177:THR:HG23	1:D:180:PHE:H	1.44	0.80
1:A:265:MET:HE1	1:A:326:LYS:HG3	1.64	0.79
1:A:363:GLU:OE1	1:A:441:LYS:NZ	2.15	0.79
1:C:286:HIS:CE1	1:C:290:LYS:HZ2	2.01	0.76
1:D:173:LEU:O	1:D:177:THR:HG22	1.87	0.75
1:C:265:MET:HE2	1:C:326:LYS:HG3	1.64	0.74
1:C:352:THR:HA	1:C:355:MET:HE3	1.70	0.73
1:A:246:VAL:HG11	1:A:318:LEU:HD12	1.75	0.69
1:A:191:LYS:HD2	1:A:199:VAL:CG1	2.24	0.68
1:B:390:HIS:HB3	1:C:392:GLU:H	1.60	0.67
1:C:259:CYS:HB3	4:C:618:HOH:O	1.95	0.66
1:C:169:SER:HB3	1:C:172:GLU:HG3	1.77	0.66
1:D:237:MET:HA	1:D:237:MET:CE	2.27	0.64
1:C:381:ILE:HG21	1:C:410:ILE:HD11	1.79	0.64
1:D:266:PRO:HG2	1:D:321:GLU:HG3	1.78	0.64
1:C:375:VAL:CG2	1:C:397:LEU:HD11	2.25	0.64
1:A:265:MET:CE	1:A:326:LYS:HG3	2.28	0.62
1:B:197:PHE:HE2	1:B:229:GLN:NE2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:THR:HG21	1:D:180:PHE:CD1	2.37	0.60
1:A:396:LEU:HD12	1:A:399:ILE:HD13	1.83	0.59
1:B:246:VAL:HG11	1:B:318:LEU:HD12	1.83	0.59
1:C:246:VAL:HG11	1:C:318:LEU:HD12	1.84	0.59
1:C:265:MET:HE1	1:C:326:LYS:CG	2.22	0.58
1:B:390:HIS:O	1:C:391:ARG:HA	2.02	0.58
1:D:246:VAL:HG11	1:D:318:LEU:HD12	1.86	0.58
1:B:409:THR:HG22	1:B:412:ASP:OD1	2.03	0.58
1:B:284:SER:H	1:B:287[A]:MET:HE3	1.67	0.57
1:D:177:THR:HB	4:D:680:HOH:O	2.04	0.57
1:C:286:HIS:CD2	1:C:290:LYS:NZ	2.73	0.56
1:A:191:LYS:HD2	1:A:199:VAL:HG13	1.88	0.54
1:D:173:LEU:HA	1:D:176:VAL:HG22	1.89	0.54
1:D:237:MET:HE2	1:D:237:MET:HA	1.90	0.53
1:C:173:LEU:HA	1:C:176:VAL:HG22	1.92	0.52
1:A:399:ILE:HG12	1:A:413:TYR:CE1	2.45	0.51
1:C:172:GLU:O	1:C:176:VAL:HG13	2.10	0.50
1:D:251:PHE:HD2	4:D:646:HOH:O	1.93	0.50
1:B:171:TYR:HA	1:B:174:LYS:HD3	1.93	0.49
1:C:396:LEU:O	1:C:399:ILE:HB	2.13	0.48
1:B:172:GLU:O	1:B:176:VAL:HG13	2.13	0.48
1:D:176:VAL:HG11	1:D:205:VAL:HG22	1.95	0.48
1:B:181:ASP:OD1	1:B:183:ARG:HB2	2.12	0.48
1:A:191:LYS:HE2	1:A:191:LYS:HB3	1.53	0.47
1:B:392:GLU:H	1:C:390:HIS:HB3	1.79	0.47
1:B:197:PHE:CE2	1:B:229:GLN:NE2	2.81	0.47
1:D:396:LEU:O	1:D:399:ILE:HG12	2.15	0.46
1:C:207:ASN:HD22	1:C:207:ASN:N	2.13	0.46
1:C:252:SER:HB3	1:C:259:CYS:HB2	1.96	0.46
1:C:399:ILE:HG12	1:C:413:TYR:CZ	2.52	0.45
1:A:317:ILE:HG12	1:A:327:ILE:HD13	1.98	0.45
1:B:199:VAL:HG13	1:B:201:TYR:CE1	2.53	0.44
1:A:382:THR:HG22	1:A:413:TYR:HB3	2.00	0.43
1:D:252:SER:HB3	1:D:259:CYS:HB2	1.99	0.43
1:D:414:ILE:HG12	1:D:426:VAL:HG11	2.00	0.43
1:A:183:ARG:HB3	1:A:187:VAL:CG1	2.49	0.43
1:A:191:LYS:HD2	1:A:199:VAL:HG11	1.99	0.43
1:C:169:SER:CB	1:C:172:GLU:HG3	2.48	0.43
1:C:199:VAL:HG13	1:C:201:TYR:CE1	2.54	0.42
1:B:382:THR:HG22	1:B:413:TYR:HB3	2.02	0.42
1:D:397:LEU:HD11	1:D:437:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:SER:HB3	1:A:259:CYS:HB2	2.00	0.42
1:C:438:HIS:HE1	1:C:440:LYS:HD2	1.85	0.42
1:A:410:ILE:HG12	1:A:430:TYR:CD2	2.54	0.42
1:D:397:LEU:HA	1:D:397:LEU:HD12	1.86	0.41
1:D:265:MET:HE3	4:D:657:HOH:O	2.20	0.41
1:B:287[B]:MET:HE1	1:B:290:LYS:HD2	2.03	0.40
1:D:206:ASN:O	1:D:207:ASN:HB2	2.21	0.40
1:B:279:GLY:HA2	1:C:417:LYS:O	2.22	0.40
1:C:397:LEU:HD12	1:C:397:LEU:HA	1.92	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	263/301 (87%)	257 (98%)	5 (2%)	1 (0%)	34	28
1	B	266/301 (88%)	254 (96%)	12 (4%)	0	100	100
1	C	278/301 (92%)	268 (96%)	9 (3%)	1 (0%)	34	28
1	D	274/301 (91%)	265 (97%)	7 (3%)	2 (1%)	22	15
All	All	1081/1204 (90%)	1044 (97%)	33 (3%)	4 (0%)	34	28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	258	LEU
1	C	181	ASP
1	A	181	ASP
1	D	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	240/260 (92%)	232 (97%)	8 (3%)	38	36
1	B	244/260 (94%)	237 (97%)	7 (3%)	42	41
1	C	249/260 (96%)	237 (95%)	12 (5%)	25	21
1	D	249/260 (96%)	239 (96%)	10 (4%)	31	28
All	All	982/1040 (94%)	945 (96%)	37 (4%)	33	30

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

Mol	Chain	Res	Type
1	A	164	ARG
1	A	187	VAL
1	A	191	LYS
1	A	192	MET
1	A	312	ILE
1	A	329	ASP
1	A	410	ILE
1	A	455	GLN
1	B	163	THR
1	B	164	ARG
1	B	179	ASN
1	B	183	ARG
1	B	222	THR
1	B	329	ASP
1	B	344	MET
1	C	192	MET
1	C	223	THR
1	C	224	GLU
1	C	225	GLU
1	C	256	ASP
1	C	257	ASP
1	C	290	LYS
1	C	321	GLU
1	C	329	ASP

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Mol	Chain	Res	Type
1	C	397	LEU
1	C	399	ILE
1	C	455	GLN
1	D	169	SER
1	D	174	LYS
1	D	192	MET
1	D	224	GLU
1	D	225	GLU
1	D	237	MET
1	D	256	ASP
1	D	329	ASP
1	D	397	LEU
1	D	411	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	ASN
1	B	206	ASN
1	B	293	GLN
1	C	206	ASN
1	C	207	ASN
1	C	229	GLN
1	D	286	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	A	346	1	8,9,10	0.61	0	8,12,14	2.29	3 (37%)
1	SEP	C	346	1	8,9,10	0.75	0	8,12,14	3.09	2 (25%)
1	SEP	B	346	1	8,9,10	0.75	0	8,12,14	2.72	3 (37%)
1	TPO	B	345	1	8,10,11	1.08	1 (12%)	10,14,16	1.22	1 (10%)
1	TPO	D	345	1	8,10,11	1.09	0	10,14,16	1.15	1 (10%)
1	TPO	A	345	1	8,10,11	1.03	0	10,14,16	1.15	0
1	TPO	C	345	1	8,10,11	0.73	0	10,14,16	1.92	2 (20%)
1	SEP	D	346	1	8,9,10	0.80	0	8,12,14	1.87	4 (50%)

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	A	346	1	-	3/5/8/10	-
1	SEP	C	346	1	-	0/5/8/10	-
1	SEP	B	346	1	-	1/5/8/10	-
1	TPO	B	345	1	-	3/9/11/13	-
1	TPO	D	345	1	-	4/9/11/13	-
1	TPO	A	345	1	-	5/9/11/13	-
1	TPO	C	345	1	-	5/9/11/13	-
1	SEP	D	346	1	-	0/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	345	TPO	CB-CA	2.07	1.58	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	346	SEP	OG-CB-CA	7.69	115.63	108.14
1	B	346	SEP	OG-CB-CA	6.71	114.68	108.14
1	A	346	SEP	O2P-P-OG	4.47	118.63	106.73
1	C	345	TPO	CG2-CB-CA	4.45	121.95	113.16
1	D	346	SEP	OG-CB-CA	3.23	111.29	108.14
1	A	346	SEP	OG-CB-CA	3.18	111.24	108.14
1	D	346	SEP	OG-P-O1P	2.70	114.04	106.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	346	SEP	P-OG-CB	-2.62	111.07	118.30
1	A	346	SEP	P-OG-CB	-2.56	111.23	118.30
1	C	345	TPO	O3P-P-OG1	2.47	117.05	105.99
1	B	346	SEP	O3P-P-OG	2.39	113.08	106.73
1	D	346	SEP	P-OG-CB	-2.27	112.05	118.30
1	B	345	TPO	O3P-P-OG1	2.26	116.14	105.99
1	D	345	TPO	O3P-P-OG1	2.16	115.65	105.99
1	B	346	SEP	OG-P-O1P	2.02	112.13	106.47
1	D	346	SEP	O3P-P-OG	2.02	112.10	106.73

There are no chirality outliers.

All (21) torsion outliers are listed below:

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

11 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	6QX	C	503	-	20,25,25	1.13	2 (10%)	24,36,36	1.53	4 (16%)
3	SO4	B	501	-	4,4,4	0.12	0	6,6,6	0.11	0
3	SO4	B	503	-	4,4,4	0.12	0	6,6,6	0.06	0
3	SO4	C	501	-	4,4,4	0.17	0	6,6,6	0.11	0
3	SO4	D	501	-	4,4,4	0.14	0	6,6,6	0.14	0
2	6QX	B	504	-	20,25,25	1.10	2 (10%)	24,36,36	1.62	4 (16%)
3	SO4	C	502	-	4,4,4	0.13	0	6,6,6	0.07	0
2	6QX	D	503	-	20,25,25	1.20	1 (5%)	24,36,36	1.65	7 (29%)
3	SO4	B	502	-	4,4,4	0.18	0	6,6,6	0.04	0
3	SO4	D	502	-	4,4,4	0.15	0	6,6,6	0.09	0
2	6QX	A	501	-	20,25,25	1.12	2 (10%)	24,36,36	1.43	2 (8%)

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	6QX	B	504	-	-	2/8/24/24	0/4/4/4
2	6QX	C	503	-	-	0/8/24/24	0/4/4/4
2	6QX	D	503	-	-	1/8/24/24	0/4/4/4
2	6QX	A	501	-	-	0/8/24/24	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	503	6QX	C13-C14	-3.27	1.40	1.44
2	C	503	6QX	C13-C14	-2.54	1.41	1.44
2	A	501	6QX	C13-C14	-2.31	1.41	1.44
2	B	504	6QX	C15-C14	2.31	1.46	1.40
2	B	504	6QX	C14-C18	-2.27	1.38	1.42
2	C	503	6QX	C15-C14	2.27	1.46	1.40
2	A	501	6QX	C15-C14	2.07	1.46	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	6QX	C22-C16-C15	5.03	114.71	111.09
2	B	504	6QX	C22-C16-C15	4.76	114.52	111.09
2	C	503	6QX	C22-C16-C15	4.33	114.20	111.09
2	D	503	6QX	C22-C16-C15	4.19	114.10	111.09
2	B	504	6QX	C6-C7-C8	-3.97	107.09	111.48
2	C	503	6QX	C23-C22-C16	-2.84	101.86	103.93
2	D	503	6QX	C14-C13-N21	-2.72	119.11	121.35
2	D	503	6QX	C20-N21-C13	2.61	118.82	116.59
2	D	503	6QX	C23-C22-C16	-2.49	102.11	103.93
2	C	503	6QX	C20-N21-C13	2.45	118.69	116.59
2	B	504	6QX	C1-N2-C4	2.35	116.44	112.39
2	D	503	6QX	C1-N2-C4	2.35	116.43	112.39
2	D	503	6QX	C6-C7-C8	-2.34	108.90	111.48
2	B	504	6QX	C23-C22-C16	-2.32	102.24	103.93
2	D	503	6QX	C10-C8-N12	2.10	113.86	110.60
2	A	501	6QX	C20-N21-C13	2.05	118.35	116.59
2	C	503	6QX	C24-C15-C16	-2.05	108.54	110.96

There are no chirality outliers.

All (3) torsion outliers are listed below:

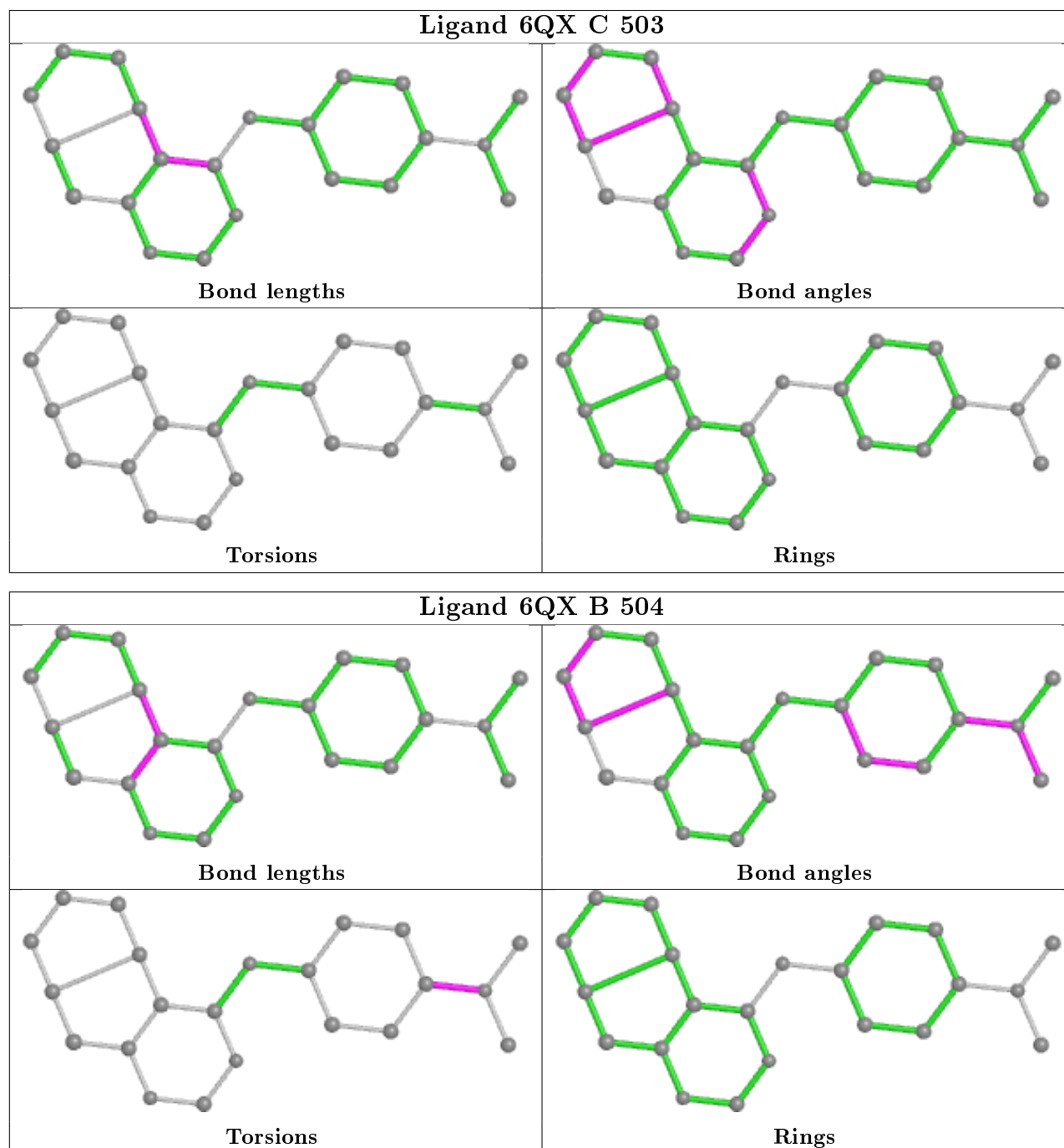
Mol	Chain	Res	Type	Atoms
2	B	504	6QX	C11-C4-N2-C3
2	B	504	6QX	C6-C4-N2-C3
2	D	503	6QX	C11-C4-N2-C3

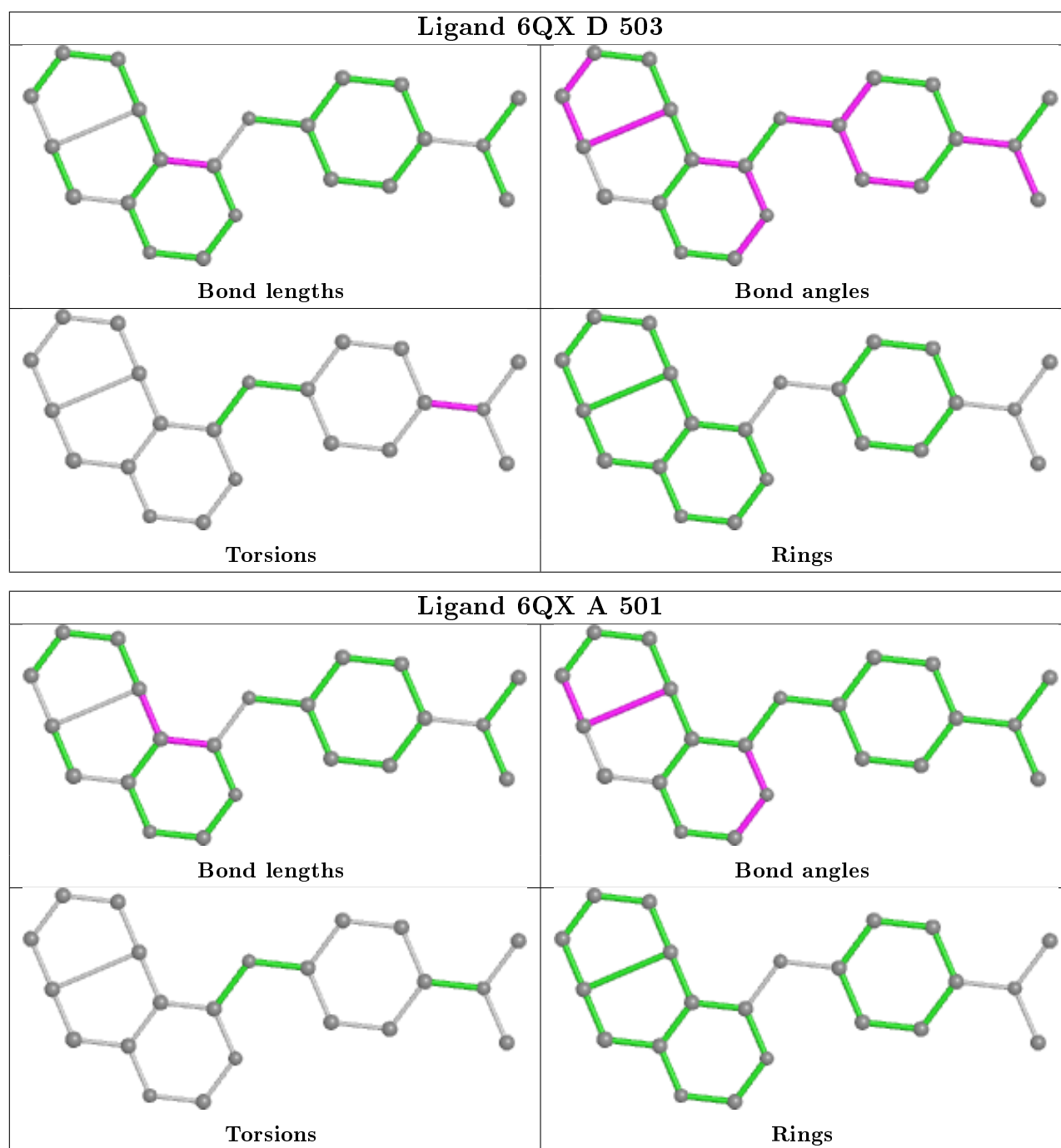
There are no ring outliers.

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.





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	271/301 (90%)	0.80	37 (13%) 3 2	35, 65, 117, 143	0
1	B	274/301 (91%)	0.51	26 (9%) 8 8	34, 60, 106, 126	0
1	C	282/301 (93%)	0.77	38 (13%) 3 2	32, 59, 100, 128	0
1	D	280/301 (93%)	0.86	45 (16%) 1 1	31, 57, 99, 128	0
All	All	1107/1204 (91%)	0.73	146 (13%) 3 2	31, 60, 107, 143	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	256	ASP	11.2
1	D	335	ALA	9.4
1	A	230	PHE	7.9
1	A	207	ASN	7.9
1	C	343	VAL	7.9
1	D	343	VAL	7.6
1	A	258	LEU	7.2
1	D	255	GLY	6.9
1	D	168	PHE	6.7
1	D	230	PHE	6.7
1	C	255	GLY	6.7
1	D	225	GLU	6.2
1	C	225	GLU	6.2
1	C	335	ALA	6.1
1	B	206	ASN	5.8
1	B	207	ASN	5.8
1	A	204	TYR	5.7
1	D	251	PHE	5.6
1	C	257	ASP	5.5
1	C	256	ASP	5.4
1	A	348	ILE	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	349	VAL	5.3
1	C	252	SER	5.1
1	B	225	GLU	5.1
1	D	227	LYS	5.1
1	A	226	LEU	5.1
1	A	254	ASP	5.0
1	A	253	SER	5.0
1	D	258	LEU	5.0
1	D	336	SER	4.9
1	C	258	LEU	4.9
1	D	259	CYS	4.8
1	D	171	TYR	4.8
1	C	259	CYS	4.8
1	A	179	ASN	4.8
1	C	251	PHE	4.8
1	D	194	GLU	4.5
1	C	250	GLY	4.5
1	D	252	SER	4.5
1	A	178	ASN	4.4
1	D	250	GLY	4.4
1	A	186	SER	4.3
1	C	171	TYR	4.0
1	C	168	PHE	4.0
1	A	332	LEU	3.9
1	A	187	VAL	3.9
1	D	223	THR	3.8
1	C	203	GLY	3.8
1	B	178	ASN	3.7
1	C	230	PHE	3.7
1	B	223	THR	3.7
1	A	343	VAL	3.6
1	D	349	VAL	3.6
1	C	180	PHE	3.6
1	B	204	TYR	3.6
1	A	176	VAL	3.5
1	C	201	TYR	3.5
1	C	332	LEU	3.5
1	C	195	GLY	3.4
1	D	344	MET	3.4
1	C	226	LEU	3.4
1	A	170	PHE	3.4
1	B	335	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	166	HIS	3.3
1	C	176	VAL	3.3
1	B	171	TYR	3.3
1	B	226	LEU	3.3
1	A	252	SER	3.3
1	B	165	PHE	3.3
1	D	249	LEU	3.2
1	B	257	ASP	3.2
1	D	226	LEU	3.2
1	B	197	PHE	3.1
1	C	221	ILE	3.1
1	D	166	HIS	3.1
1	D	170	PHE	3.1
1	A	199	VAL	3.1
1	B	199	VAL	3.1
1	D	198	GLY	3.0
1	D	234	ILE	3.0
1	D	254	ASP	3.0
1	C	212	VAL	2.9
1	D	390	HIS	2.9
1	B	410	ILE	2.9
1	B	175	ASN	2.9
1	A	183	ARG	2.9
1	B	170	PHE	2.9
1	D	201	TYR	2.9
1	C	170	PHE	2.8
1	C	390	HIS	2.8
1	C	344	MET	2.8
1	A	181	ASP	2.8
1	C	349	VAL	2.8
1	D	410	ILE	2.8
1	C	215	LEU	2.8
1	B	230	PHE	2.7
1	B	179	ASN	2.7
1	C	197	PHE	2.6
1	D	180	PHE	2.6
1	D	197	PHE	2.6
1	A	190	ASN	2.6
1	A	390	HIS	2.6
1	D	260	LEU	2.6
1	D	215	LEU	2.6
1	D	261	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	176	VAL	2.6
1	C	199	VAL	2.6
1	A	251	PHE	2.6
1	A	165	PHE	2.5
1	C	336	SER	2.5
1	A	214	LYS	2.5
1	B	194	GLU	2.5
1	A	236	VAL	2.4
1	C	210	VAL	2.4
1	A	208	THR	2.4
1	C	200	VAL	2.4
1	C	166	HIS	2.4
1	B	252	SER	2.4
1	D	332	LEU	2.4
1	D	199	VAL	2.4
1	A	206	ASN	2.4
1	D	188	GLY	2.4
1	B	439	GLU	2.3
1	C	185	ILE	2.3
1	A	215	LEU	2.3
1	B	390	HIS	2.3
1	A	399	ILE	2.3
1	D	257	ASP	2.2
1	C	399	ILE	2.2
1	B	440	LYS	2.2
1	D	200	VAL	2.2
1	A	228	GLN	2.2
1	A	234	ILE	2.2
1	A	344	MET	2.2
1	C	223	THR	2.2
1	A	364	ILE	2.1
1	D	236	VAL	2.1
1	D	165	PHE	2.1
1	D	167	SER	2.1
1	B	208	THR	2.1
1	A	232	GLN	2.1
1	C	260	LEU	2.1
1	D	210	VAL	2.0
1	D	342	THR	2.0
1	B	336	SER	2.0
1	D	238	ALA	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	SEP	A	346	10/11	0.05	0.43	129,137,146,146	0
1	SEP	C	346	10/11	0.54	0.23	108,114,124,126	0
1	SEP	D	346	10/11	0.57	0.24	113,118,124,125	0
1	SEP	B	346	10/11	0.73	0.21	101,106,114,114	0
1	TPO	A	345	11/12	0.77	0.24	124,130,133,136	0
1	TPO	B	345	11/12	0.83	0.19	96,101,105,108	0
1	TPO	C	345	11/12	0.84	0.17	106,110,113,114	0
1	TPO	D	345	11/12	0.84	0.25	108,111,117,117	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, 95<sup>th</sup> 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.

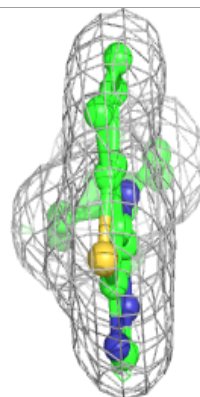
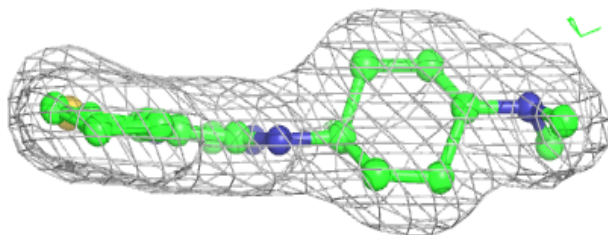
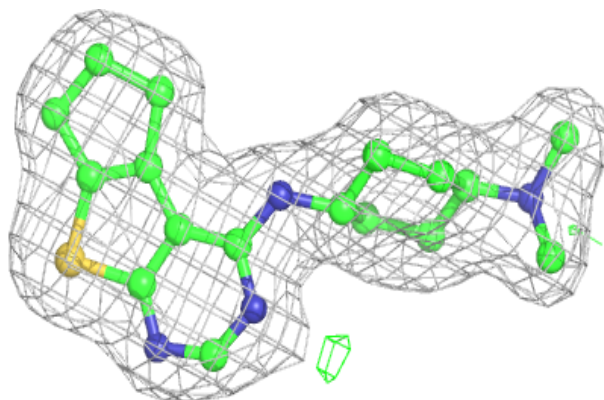
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	B	502	5/5	0.76	0.17	149,150,150,150	0
3	SO4	D	502	5/5	0.76	0.17	160,160,160,161	0
3	SO4	C	502	5/5	0.78	0.24	157,157,158,158	0
3	SO4	C	501	5/5	0.88	0.15	129,130,130,130	0
3	SO4	B	503	5/5	0.90	0.10	125,125,125,126	0
3	SO4	D	501	5/5	0.91	0.19	108,108,108,110	0
3	SO4	B	501	5/5	0.95	0.12	106,106,107,107	0
2	6QX	D	503	22/22	0.96	0.12	30,33,35,37	0
2	6QX	C	503	22/22	0.97	0.11	31,33,35,37	0
2	6QX	B	504	22/22	0.97	0.11	34,37,39,40	0
2	6QX	A	501	22/22	0.97	0.10	35,38,39,42	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.

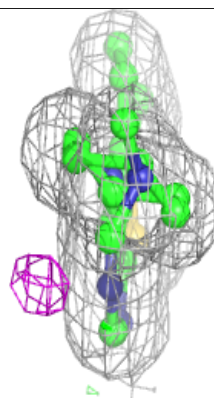
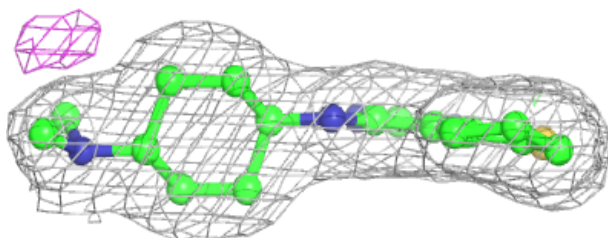
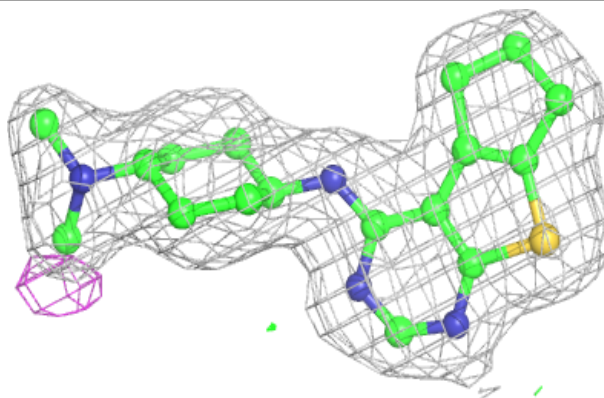
**Electron density around 6QX D 503:**

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



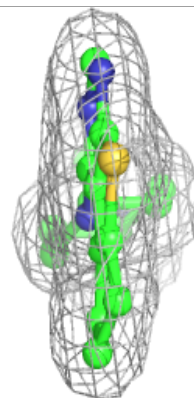
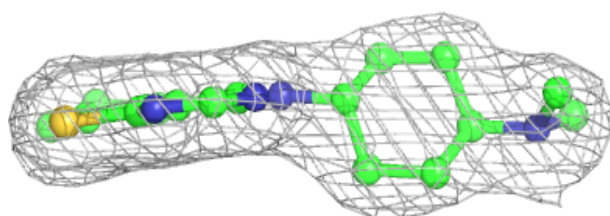
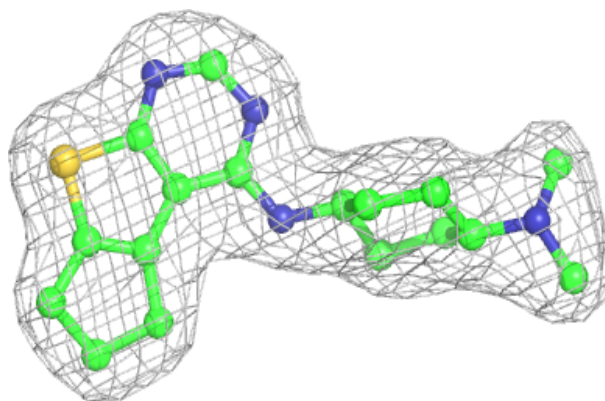
**Electron density around 6QX C 503:**

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

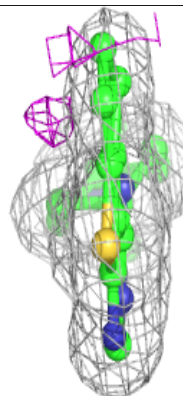
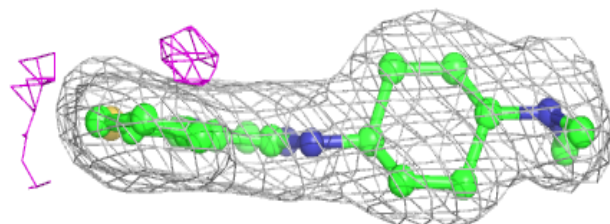
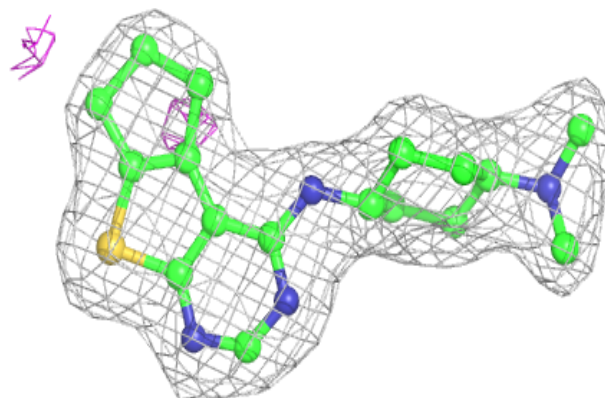


**Electron density around 6QX B 504:**

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

**Electron density around 6QX 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.