



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:25 AM UTC

PDB ID : 5K75 / pdb_00005k75
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

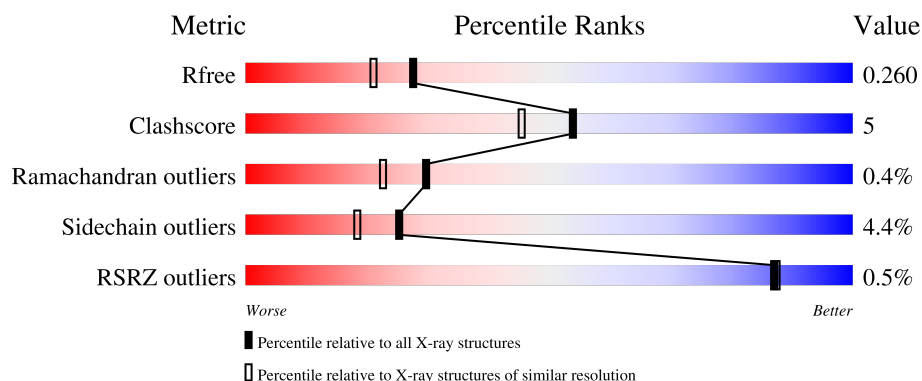
1 Overall quality at a glance

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}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	301	79% 10% • 9%
1	B	301	79% 11% • 8%
1	C	301	75% 17% • 6%
1	D	301	79% 14% • 6%

2 Entry composition [i](#)

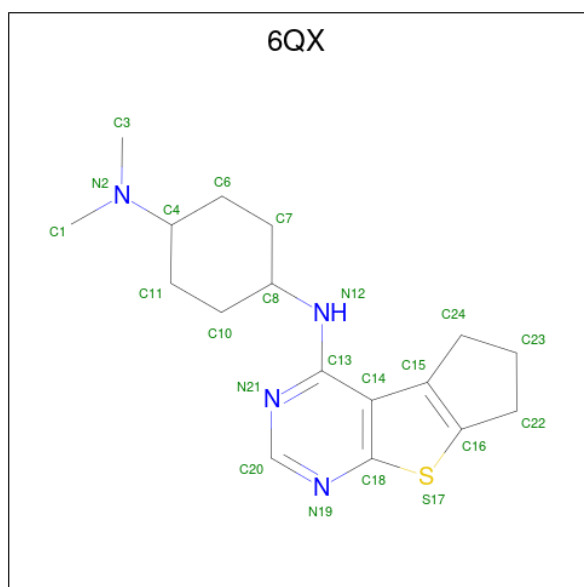
There are 4 unique types of molecules in this entry. The entry contains 9417 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 6QX) (formula: C₁₇H₂₄N₄S).



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		

Continued on next page...

Continued from previous page...

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 (CCD ID: SO4) (formula: O₄S).



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		

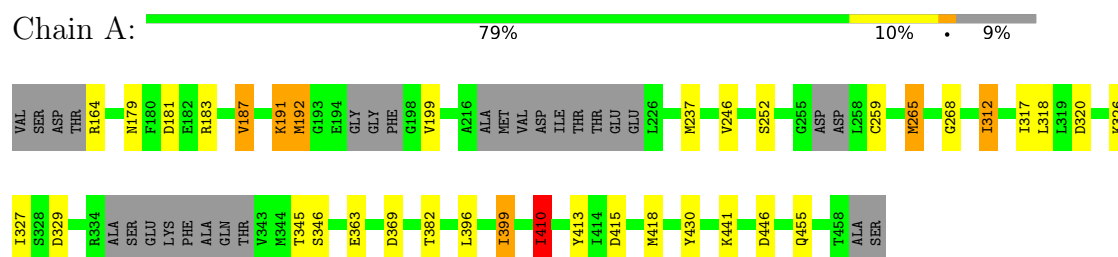
- Molecule 4 is water.

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

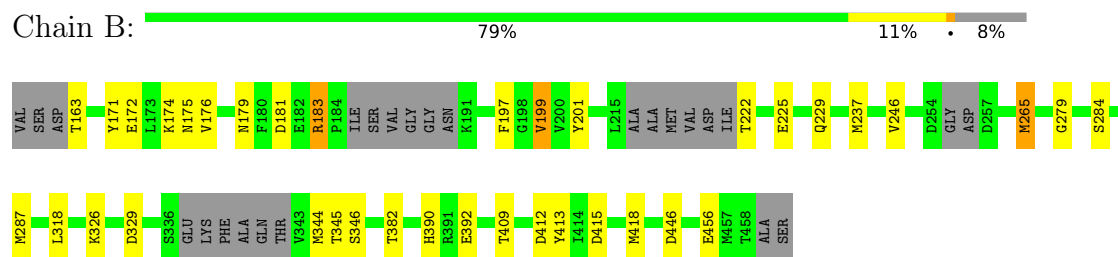
3 Residue-property plots [i](#)

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

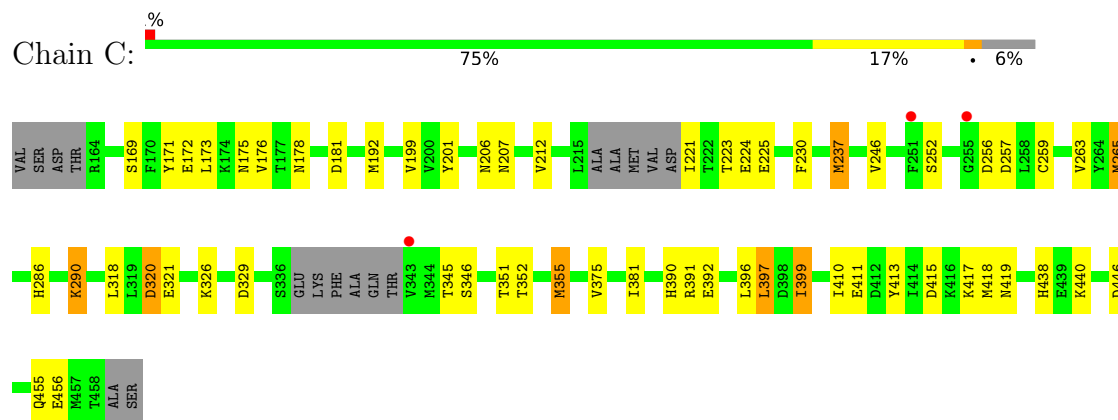
- Molecule 1: Interleukin-1 receptor-associated kinase 4



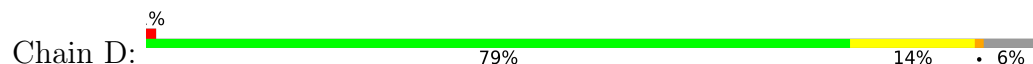
- Molecule 1: Interleukin-1 receptor-associated kinase 4

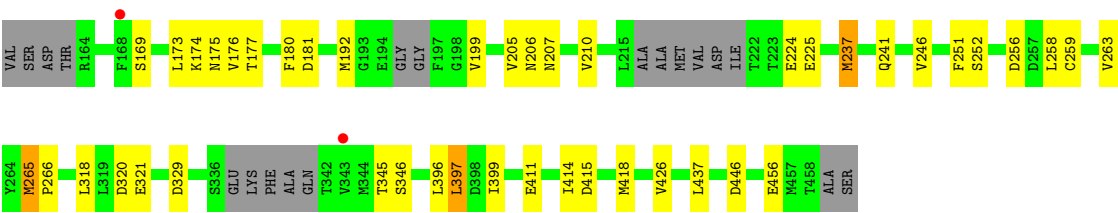


- Molecule 1: Interleukin-1 receptor-associated kinase 4



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





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.87Å 141.62Å 88.06Å 90.00° 125.92° 90.00°	Depositor
Resolution (Å)	45.18 – 2.03 45.18 – 2.03	Depositor EDS
% Data completeness (in resolution range)	97.0 (45.18-2.03) 97.0 (45.18-2.03)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.169 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9417	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, SEP, 6QX, TPO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.79	1/2194 (0.0%)	1.30	7/2950 (0.2%)
1	B	0.80	1/2226 (0.0%)	1.26	4/2994 (0.1%)
1	C	0.87	3/2278 (0.1%)	1.32	13/3068 (0.4%)
1	D	0.84	1/2268 (0.0%)	1.34	7/3054 (0.2%)
All	All	0.83	6/8966 (0.1%)	1.31	31/12066 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	265	MET	SD-CE	-9.56	1.55	1.79
1	A	265	MET	SD-CE	-8.27	1.58	1.79
1	B	265	MET	SD-CE	-7.50	1.60	1.79
1	D	265	MET	SD-CE	-5.44	1.66	1.79
1	C	355	MET	SD-CE	-5.21	1.66	1.79
1	C	175	ASN	CA-CB	-5.19	1.44	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	ILE	N-CA-CB	7.57	118.78	110.53
1	B	175	ASN	CA-CB-CG	7.44	120.04	112.60
1	D	175	ASN	CA-CB-CG	-6.88	105.72	112.60
1	C	263	VAL	N-CA-C	-6.77	100.83	109.30
1	D	263	VAL	N-CA-C	-6.33	100.49	108.84
1	C	411	GLU	CB-CG-CD	6.02	122.83	112.60
1	C	320	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	446	ASP	CA-CB-CG	5.77	118.37	112.60
1	D	446	ASP	CA-CB-CG	5.61	118.21	112.60
1	B	446	ASP	CA-CB-CG	5.51	118.11	112.60
1	D	320	ASP	CA-CB-CG	5.41	118.01	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	ASN	CA-CB-CG	5.41	118.01	112.60
1	A	179	ASN	CA-CB-CG	5.40	118.00	112.60
1	C	419	ASN	CA-CB-CG	5.36	117.95	112.60
1	D	456	GLU	CA-C-N	5.36	127.45	120.28
1	D	456	GLU	C-N-CA	5.36	127.45	120.28
1	D	210	VAL	CB-CA-C	-5.29	103.94	111.19
1	A	320	ASP	CA-CB-CG	5.27	117.87	112.60
1	C	456	GLU	CA-C-N	5.19	127.24	120.28
1	C	456	GLU	C-N-CA	5.19	127.24	120.28
1	A	369	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	446	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	178	ASN	CA-C-N	5.11	129.44	122.34
1	C	178	ASN	C-N-CA	5.11	129.44	122.34
1	B	456	GLU	CA-C-N	5.11	127.12	120.28
1	B	456	GLU	C-N-CA	5.11	127.12	120.28
1	C	230	PHE	CA-CB-CG	5.05	118.85	113.80
1	A	410	ILE	CA-C-N	5.04	127.04	120.28
1	A	410	ILE	C-N-CA	5.04	127.04	120.28
1	C	351	THR	CA-C-N	5.02	128.35	120.82
1	C	351	THR	C-N-CA	5.02	128.35	120.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	18	0
1	B	2207	0	2178	19	0
1	C	2257	0	2226	36	0
1	D	2248	0	2214	19	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

Continued on next page...

Continued from previous page...

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	87	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 5.

All (87) 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:C:265:MET:CE	1:C:326:LYS:HG3	1.82	1.08
1:C:265:MET:HE2	1:C:326:LYS:HG3	1.41	0.99
1:B:265:MET:HE1	1:B:326:LYS:HG3	1.44	0.99
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:A:265:MET:HE1	1:A:326:LYS:HG3	1.58	0.86
1:C:375:VAL:HG22	1:C:397:LEU:CD1	2.05	0.86
1:C:265:MET:HE1	1:C:326:LYS:HG3	1.58	0.85
1:B:265:MET:CE	1:B:326:LYS:HG3	2.07	0.85
1:B:284:SER:H	1:B:287[A]:MET:HE3	1.41	0.82
1:B:390:HIS:O	1:C:390:HIS:O	1.97	0.82
1:D:237:MET:HA	1:D:237:MET:HE2	1.63	0.80
1:D:177:THR:HG23	1:D:180:PHE:H	1.44	0.80
1:A:363:GLU:OE1	1:A:441:LYS:NZ	2.15	0.79
1:C:286:HIS:CE1	1:C:290:LYS:HZ2	2.02	0.76
1:D:173:LEU:O	1:D:177:THR:HG22	1.87	0.75
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:C:237:MET:HE2	1:C:237:MET:HA	1.78	0.65
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:THR:HA	1:C:355:MET:HE3	1.80	0.63
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
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: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:C:286:HIS:CD2	1:C:290:LYS:HZ2	2.13	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:C:173:LEU:HA	1:C:176:VAL:HG22	1.92	0.52
1:B:237:MET:HE1	1:B:246:VAL:HG23	1.92	0.52
1:C:265:MET:HE2	1:C:326:LYS:CG	2.29	0.51
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:D:265:MET:HE3	4:D:657:HOH:O	2.10	0.50
1:B:171:TYR:HA	1:B:174:LYS:HD3	1.93	0.49
1:A:192:MET:HE1	1:A:268:GLY:HA2	1.95	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:HB3	1:A:191:LYS:HE2	1.53	0.47
1:A:237:MET:HE1	1:A:246:VAL:HG23	1.97	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:C:265:MET:HE1	1:C:320:ASP:HB3	1.98	0.44
1:B:199:VAL:HG13	1:B:201:TYR:CE1	2.53	0.44
1:D:415:ASP:HB3	1:D:418:MET:HE2	2.00	0.43
1:A:382:THR:HG22	1:A:413:TYR:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:415:ASP:HB3	1:A:418:MET:HE2	2.00	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
1:C:415:ASP:HB3	1:C:418:MET:HE2	2.00	0.42
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:HD12	1:D:397:LEU:HA	1.86	0.41
1:B:415:ASP:HB3	1:B:418:MET:HE2	2.01	0.41
1:C:171:TYR:CD1	1:C:171:TYR:C	2.99	0.41
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

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	263/301 (87%)	257 (98%)	5 (2%)	1 (0%)	30	22
1	B	266/301 (88%)	254 (96%)	12 (4%)	0	100	100
1	C	278/301 (92%)	268 (96%)	9 (3%)	1 (0%)	30	22
1	D	274/301 (91%)	265 (97%)	7 (3%)	2 (1%)	18	10
All	All	1081/1204 (90%)	1044 (97%)	33 (3%)	4 (0%)	30	22

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%)	231 (96%)	9 (4%)	29	23
1	B	244/260 (94%)	236 (97%)	8 (3%)	33	29
1	C	249/260 (96%)	235 (94%)	14 (6%)	19	12
1	D	249/260 (96%)	237 (95%)	12 (5%)	23	15
All	All	982/1040 (94%)	939 (96%)	43 (4%)	25	18

All (43) 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	399	ILE
1	A	410	ILE
1	A	455	GLN
1	B	163	THR
1	B	179	ASN
1	B	183	ARG
1	B	199	VAL
1	B	222	THR
1	B	225	GLU
1	B	329	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	344	MET
1	C	192	MET
1	C	221	ILE
1	C	223	THR
1	C	224	GLU
1	C	225	GLU
1	C	237	MET
1	C	256	ASP
1	C	257	ASP
1	C	290	LYS
1	C	321	GLU
1	C	329	ASP
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	199	VAL
1	D	224	GLU
1	D	225	GLU
1	D	237	MET
1	D	241	GLN
1	D	256	ASP
1	D	329	ASP
1	D	397	LEU
1	D	411	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	190	ASN
1	A	293	GLN
1	A	452	GLN
1	B	206	ASN
1	B	293	GLN
1	B	452	GLN
1	C	166	HIS
1	C	175	ASN
1	C	206	ASN
1	C	207	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	419	ASN
1	C	451	GLN
1	C	452	GLN
1	D	451	GLN

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	B	346	1	8,9,10	0.78	0	7,12,14	2.87	3 (42%)
1	TPO	C	345	1	8,10,11	0.76	0	10,14,16	2.02	2 (20%)
1	TPO	A	345	1	8,10,11	1.09	0	10,14,16	1.27	2 (20%)
1	SEP	C	346	1	8,9,10	0.78	0	7,12,14	3.17	1 (14%)
1	TPO	B	345	1	8,10,11	1.13	1 (12%)	10,14,16	1.35	1 (10%)
1	TPO	D	345	1	8,10,11	1.17	1 (12%)	10,14,16	1.25	1 (10%)
1	SEP	A	346	1	8,9,10	0.64	0	7,12,14	2.29	2 (28%)
1	SEP	D	346	1	8,9,10	0.83	0	7,12,14	1.85	3 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	B	346	1	-	2/6/8/10	-
1	TPO	C	345	1	-	5/9/11/13	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	345	1	-	4/9/11/13	-
1	SEP	C	346	1	-	0/6/8/10	-
1	TPO	B	345	1	-	3/9/11/13	-
1	TPO	D	345	1	-	4/9/11/13	-
1	SEP	A	346	1	-	3/6/8/10	-
1	SEP	D	346	1	-	0/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	345	TPO	CB-CA	2.20	1.58	1.53
1	D	345	TPO	P-OG1	-2.06	1.55	1.59

All (15) 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	4.59	118.63	106.67
1	C	345	TPO	CG2-CB-CA	4.46	121.95	113.26
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	C	345	TPO	O3P-P-OG1	2.87	117.05	105.85
1	D	346	SEP	OG-P-O1P	2.81	114.04	106.44
1	B	345	TPO	O3P-P-OG1	2.64	116.14	105.85
1	D	345	TPO	O3P-P-OG1	2.52	115.65	105.85
1	B	346	SEP	O3P-P-OG	2.46	113.08	106.67
1	A	345	TPO	P-OG1-CB	-2.14	117.50	123.33
1	B	346	SEP	OG-P-O1P	2.10	112.13	106.44
1	D	346	SEP	O3P-P-OG	2.08	112.10	106.67
1	A	345	TPO	O2P-P-OG1	2.06	113.88	105.85

There are no chirality outliers.

All (21) 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	A	346	SEP	CB-OG-P-O3P
1	B	345	TPO	N-CA-CB-OG1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	B	345	TPO	O-C-CA-CB
1	B	346	SEP	N-CA-CB-OG
1	B	346	SEP	C-CA-CB-OG
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	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	CA-CB-OG1-P
1	B	345	TPO	CB-OG1-P-O1P
1	A	346	SEP	CB-OG-P-O1P
1	A	345	TPO	CB-OG1-P-O1P
1	D	345	TPO	CB-OG1-P-O1P
1	A	346	SEP	CB-OG-P-O2P
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 oligosaccharides 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	$\# Z > 2$
3	SO4	C	501	-	4,4,4	0.20	0	6,6,6	0.13	0
3	SO4	D	501	-	4,4,4	0.24	0	6,6,6	0.17	0
3	SO4	D	502	-	4,4,4	0.25	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	6QX	A	501	-	24,25,25	0.88	0	28,36,36	1.06	2 (7%)
2	6QX	C	503	-	24,25,25	0.84	0	28,36,36	1.03	2 (7%)
3	SO4	B	502	-	4,4,4	0.28	0	6,6,6	0.07	0
2	6QX	D	503	-	24,25,25	0.97	1 (4%)	28,36,36	1.18	4 (14%)
3	SO4	B	503	-	4,4,4	0.23	0	6,6,6	0.10	0
2	6QX	B	504	-	24,25,25	0.87	0	28,36,36	1.25	4 (14%)
3	SO4	B	501	-	4,4,4	0.23	0	6,6,6	0.13	0
3	SO4	C	502	-	4,4,4	0.24	0	6,6,6	0.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	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	A	501	-	-	0/8/24/24	0/4/4/4
2	6QX	D	503	-	-	1/8/24/24	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	503	6QX	C13-N12	3.00	1.39	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	504	6QX	C6-C7-C8	-4.02	107.09	111.49
2	A	501	6QX	C14-C15-C16	-2.87	110.34	111.64
2	B	504	6QX	C14-C15-C16	-2.50	110.52	111.64
2	D	503	6QX	C14-C15-C16	-2.48	110.52	111.64
2	A	501	6QX	C15-C16-S17	2.45	114.87	113.53
2	C	503	6QX	C15-C16-S17	2.45	114.87	113.53
2	D	503	6QX	C6-C7-C8	-2.37	108.90	111.49
2	B	504	6QX	C1-N2-C4	2.35	116.44	112.39
2	D	503	6QX	C15-C16-S17	2.35	114.82	113.53
2	D	503	6QX	C1-N2-C4	2.35	116.43	112.39
2	B	504	6QX	C15-C16-S17	2.30	114.79	113.53
2	C	503	6QX	C14-C15-C16	-2.25	110.63	111.64

There are no chirality outliers.

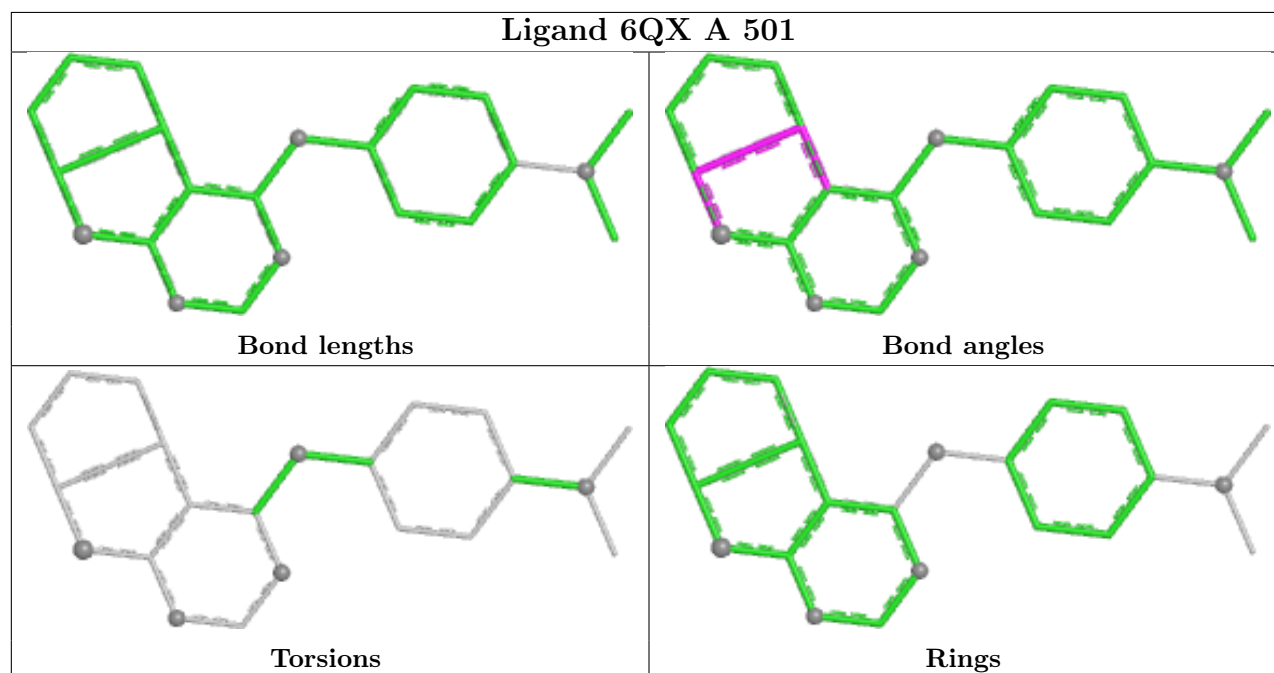
All (3) torsion outliers are listed below:

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

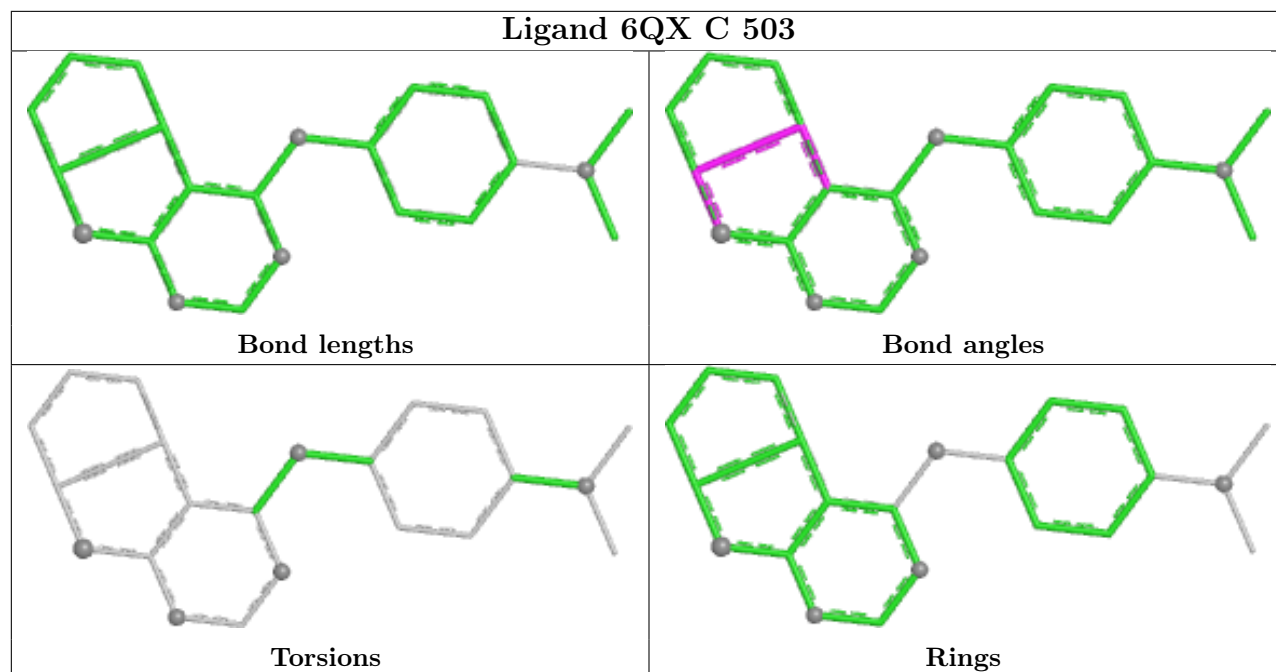
There are no ring outliers.

No monomer is involved in short contacts.

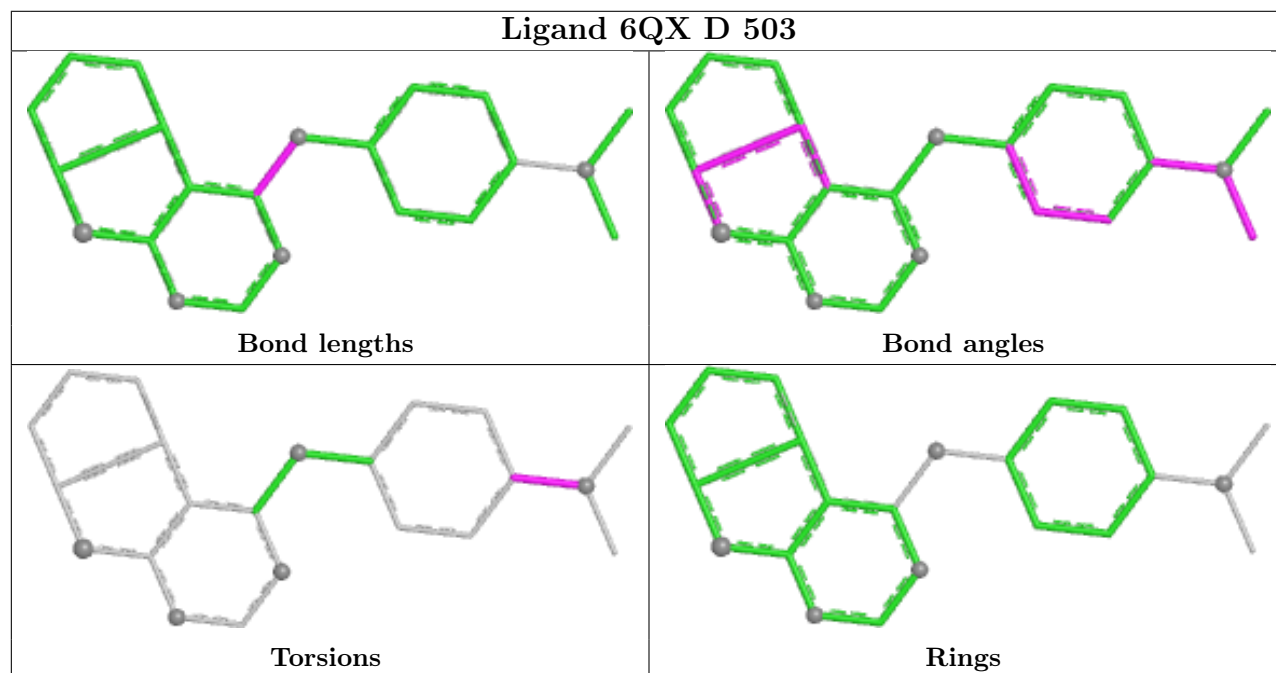
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

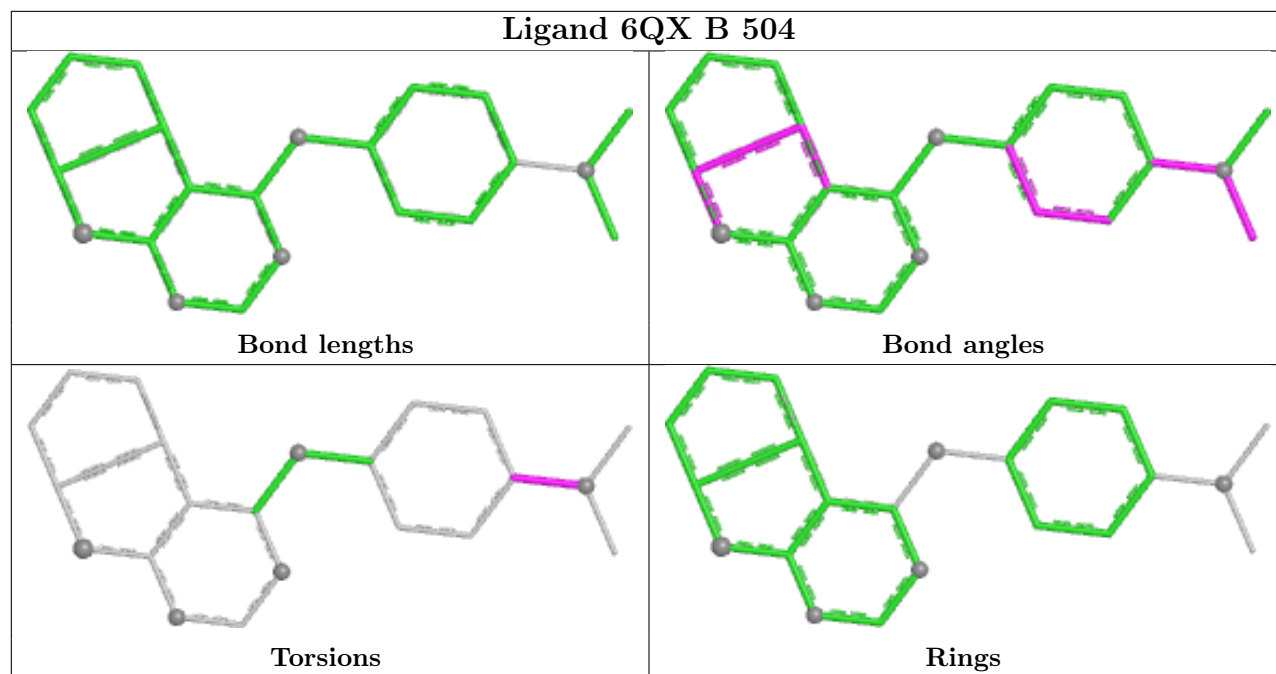


Ligand 6QX C 503



Ligand 6QX D 503





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	271/301 (90%)	-0.67	0 100 100	25, 65, 117, 143	2 (0%)
1	B	274/301 (91%)	-0.81	0 100 100	23, 60, 106, 126	2 (0%)
1	C	282/301 (93%)	-0.70	3 (1%) 78 78	25, 59, 100, 128	2 (0%)
1	D	280/301 (93%)	-0.68	2 (0%) 84 84	26, 57, 99, 128	2 (0%)
All	All	1107/1204 (91%)	-0.72	5 (0%) 87 87	23, 60, 107, 143	8 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	343	VAL	2.6
1	D	343	VAL	2.5
1	C	251	PHE	2.4
1	D	168	PHE	2.1
1	C	255	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	A	346	10/11	0.91	0.06	129,137,146,146	0
1	SEP	C	346	10/11	0.92	0.06	108,114,124,126	0
1	SEP	B	346	10/11	0.94	0.05	101,106,114,114	0
1	TPO	D	345	11/12	0.94	0.08	108,111,117,117	0
1	SEP	D	346	10/11	0.94	0.06	113,118,124,125	0
1	TPO	C	345	11/12	0.96	0.07	106,110,113,114	0
1	TPO	A	345	11/12	0.96	0.07	124,130,133,136	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	TPO	B	345	11/12	0.98	0.05	96,101,105,108	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

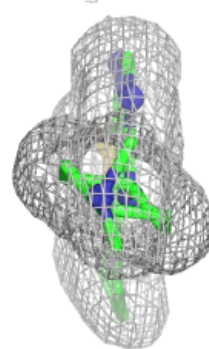
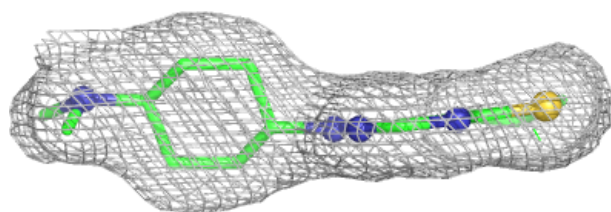
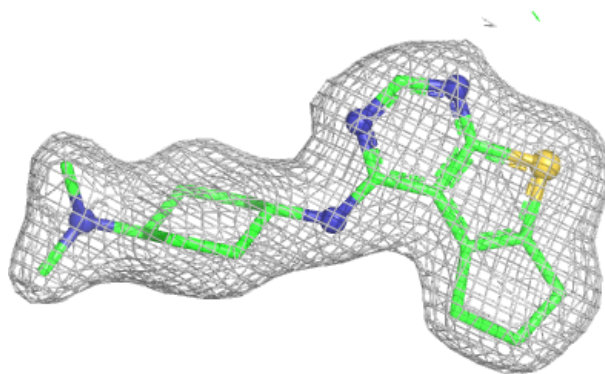
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	C	502	5/5	0.93	0.06	157,157,158,158	0
3	SO4	B	502	5/5	0.96	0.07	149,150,150,150	0
3	SO4	D	502	5/5	0.96	0.04	160,160,160,161	0
3	SO4	D	501	5/5	0.97	0.07	108,108,108,110	0
3	SO4	B	503	5/5	0.97	0.05	125,125,125,126	0
3	SO4	C	501	5/5	0.98	0.08	129,130,130,130	0
3	SO4	B	501	5/5	0.98	0.05	106,106,107,107	0
2	6QX	C	503	22/22	0.99	0.04	31,33,35,37	0
2	6QX	D	503	22/22	0.99	0.04	30,33,35,37	0
2	6QX	A	501	22/22	0.99	0.04	35,38,39,42	0
2	6QX	B	504	22/22	1.00	0.03	34,37,39,40	0

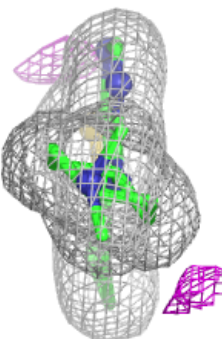
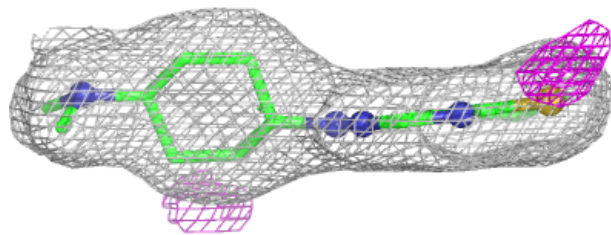
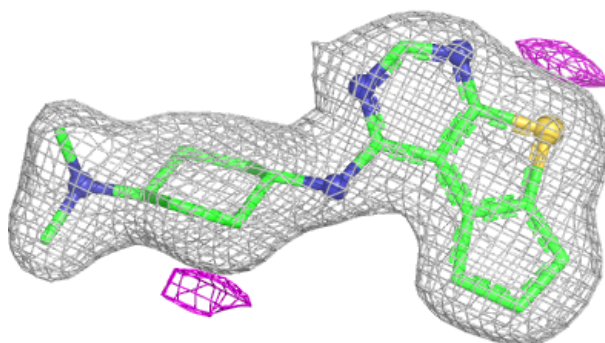
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6QX 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)

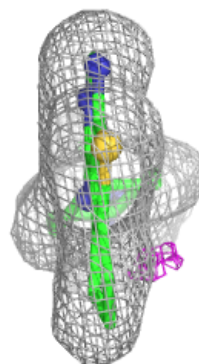
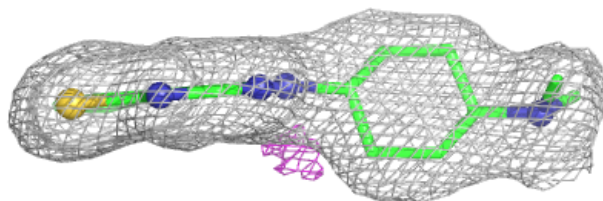
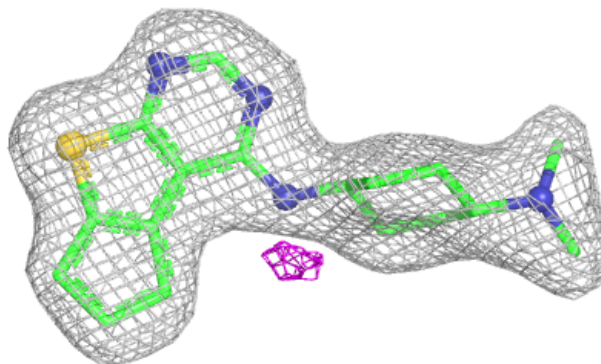
**Electron density around 6QX D 503:**

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

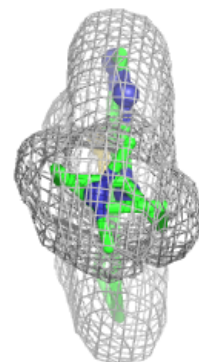
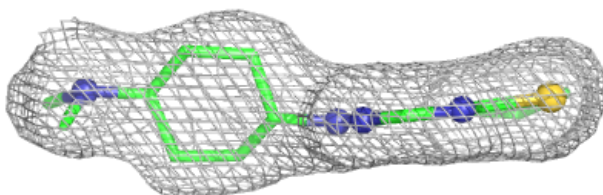
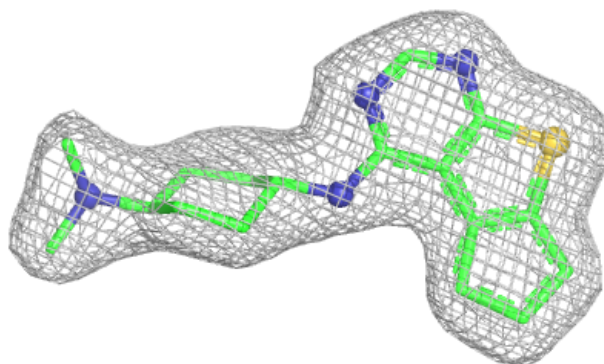


Electron density around 6QX A 501:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.