



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:31 PM UTC

PDB ID : 8UW2 / pdb_00008uw2
Title : Structure of AKT1(E17K) with compound 3 (zinc-free)
Authors : Craven, G.B.; Taunton, J.
Deposited on : 2023-11-05
Resolution : 2.20 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

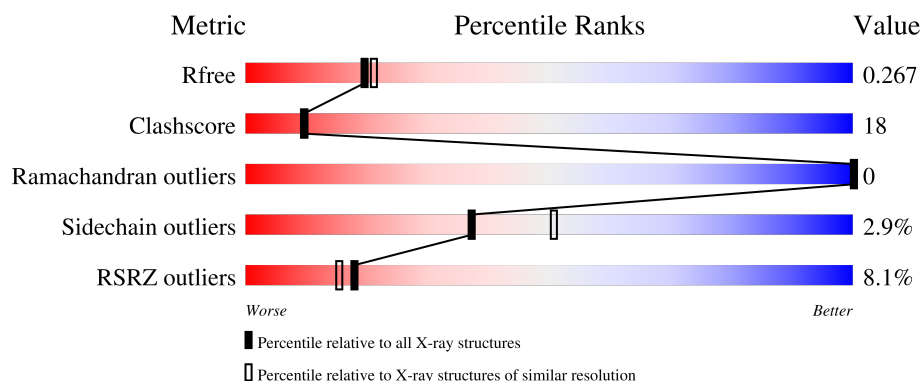
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	438	6% 61% 27% • 11%
2	B	126	11% 51% 40% 10%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4301 atoms, of which 6 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 RAC-alpha serine/threonine-protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	8	0
			3242	2084	547	594	17			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	LYS	GLU	conflict	UNP P31749
A	?	-	PHE	deletion	UNP P31749
A	120	ALA	ARG	conflict	UNP P31749
A	122	ALA	GLY	conflict	UNP P31749
A	123	GLU	SER	conflict	UNP P31749
A	124	HIS	PRO	conflict	UNP P31749
A	125	THR	SER	conflict	UNP P31749
A	?	-	ASN	deletion	UNP P31749
A	?	-	SER	deletion	UNP P31749
A	?	-	GLY	deletion	UNP P31749
A	?	-	ALA	deletion	UNP P31749
A	?	-	GLU	deletion	UNP P31749
A	?	-	GLU	deletion	UNP P31749

- Molecule 2 is a protein called NB41.

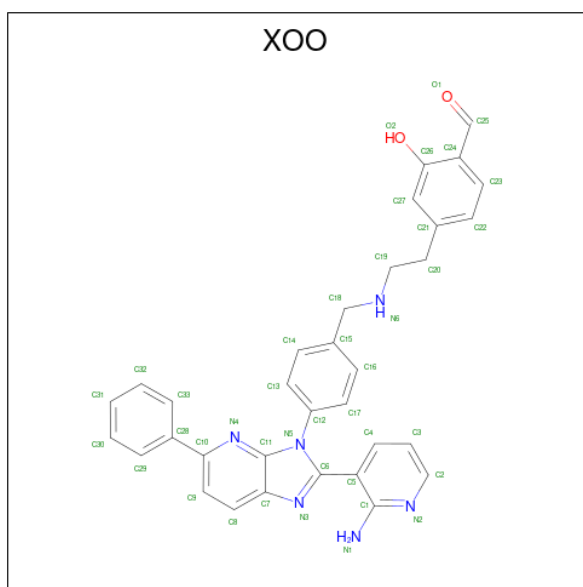
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	114	Total	C	N	O	S	0	0	0
			869	541	160	164	4			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			4	2	2			
3	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is 4-{2-[(4-[(2P)-2-(2-aminopyridin-3-yl)-5-phenyl-3H-imidazo[4,5-b]pyridin-3-yl]phenyl)methyl]amino]ethyl}-2-hydroxybenzaldehyde (CCD ID: XO0) (formula: C₃₃H₂₈N₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			40	33	6	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

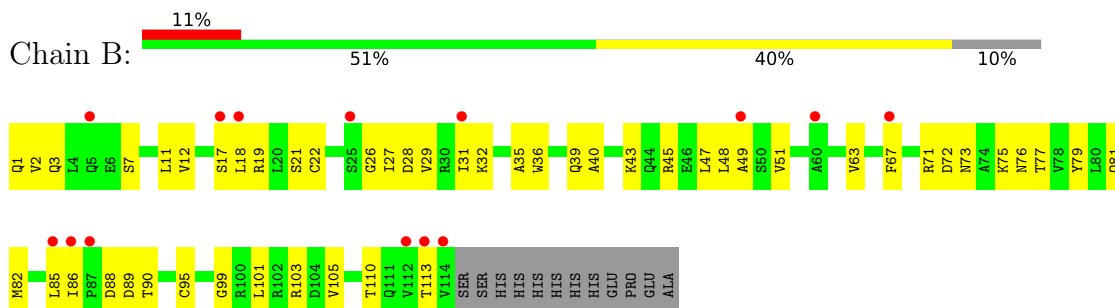


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	92	Total	O	0	0
			92	92		
6	B	14	Total	O	0	0
			14	14		

- Molecule 1: RAC-alpha serine/threonine-protein kinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	76.01Å 87.63Å 197.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.82 – 2.20 43.82 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (43.82-2.20) 99.0 (43.82-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.220 , 0.279 (Not available) , 0.267	Depositor DCC
R_{free} test set	1699 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4301	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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, EDO, XO0

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	0.37	0/3317	0.55	0/4472
2	B	0.31	0/883	0.54	0/1196
All	All	0.36	0/4200	0.55	0/5668

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

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	3242	0	3132	104	0
2	B	869	0	868	45	0
3	A	8	6	12	2	0
4	A	40	0	0	1	0
5	A	25	0	0	1	0
5	B	5	0	0	0	0
6	A	92	0	0	3	0
6	B	14	0	0	0	0
All	All	4295	6	4012	145	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 18.

All (145) 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:A:164:VAL:HG23	1:A:295:LEU:HD11	1.45	0.94
2:B:28:ASP:HB3	2:B:31:ILE:HG12	1.55	0.88
1:A:403:MET:HE2	1:A:413:TRP:CD2	2.15	0.81
1:A:65:THR:HG23	1:A:72:THR:OG1	1.82	0.80
1:A:164:VAL:HG22	1:A:179:LYS:HG3	1.63	0.78
1:A:387:ASP:OD1	1:A:389:LYS:HE2	1.86	0.76
1:A:237[A]:PHE:CE1	1:A:241:ARG:HD3	2.20	0.76
2:B:7:SER:HA	2:B:110:THR:HG21	1.70	0.73
1:A:403:MET:HE2	1:A:413:TRP:CG	2.24	0.73
1:A:264:LEU:HD22	1:A:270:VAL:HG22	1.69	0.73
2:B:28:ASP:HB3	2:B:31:ILE:CG1	2.19	0.71
1:A:237[A]:PHE:CZ	1:A:241:ARG:HD3	2.26	0.71
1:A:5:ALA:H	1:A:31:ASN:HD21	1.39	0.70
1:A:403:MET:HB3	1:A:413:TRP:CE2	2.26	0.70
1:A:6:ILE:HD13	1:A:28:LEU:HD12	1.74	0.70
2:B:99:GLY:O	2:B:103:ARG:HG3	1.93	0.69
1:A:186:ILE:HD13	1:A:223:LEU:HD23	1.76	0.68
1:A:353:ASP:OD2	1:A:356:LYS:HG3	1.93	0.68
1:A:5:ALA:H	1:A:31:ASN:ND2	1.91	0.68
1:A:17:LYS:NZ	4:A:502:XOO:O2	2.28	0.67
2:B:67:PHE:CD1	2:B:82:MET:HA	2.30	0.67
1:A:119:ASP:HB3	2:B:32:LYS:HG2	1.76	0.67
2:B:2:VAL:HG13	2:B:27:ILE:HD11	1.76	0.66
2:B:2:VAL:HG13	2:B:27:ILE:CD1	2.24	0.66
1:A:163:LYS:HE2	5:A:507:SO4:O2	1.96	0.65
1:A:161:PHE:HD1	1:A:185:VAL:HG11	1.61	0.65
2:B:85:LEU:HD23	2:B:89:ASP:OD2	1.98	0.64
1:A:264:LEU:HD22	1:A:270:VAL:CG2	2.27	0.64
1:A:210:LEU:O	1:A:289:LYS:HE3	1.99	0.62
1:A:164:VAL:HG23	1:A:295:LEU:CD1	2.24	0.62
1:A:416:VAL:HG22	1:A:421:LEU:HD12	1.82	0.62
1:A:247:GLU:HG3	6:A:678:HOH:O	1.99	0.62
1:A:38:TYR:CD1	1:A:42:PRO:HG3	2.35	0.61
1:A:28:LEU:HD23	1:A:38:TYR:CE1	2.36	0.61
1:A:72:THR:HG22	1:A:89:HIS:HB2	1.84	0.60
2:B:19:ARG:HG3	2:B:81:GLN:OE1	2.02	0.60
1:A:239:LEU:HD23	1:A:277:LEU:CD2	2.33	0.59
1:A:28:LEU:HD23	1:A:38:TYR:HE1	1.66	0.59
1:A:152[B]:TYR:HD1	1:A:165:ILE:HD12	1.68	0.59
1:A:12:LEU:HD21	1:A:99:TRP:NE1	2.18	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ASP:HB3	2:B:32:LYS:CG	2.34	0.58
1:A:152[A]:TYR:O	1:A:153[A]:LEU:HD23	2.02	0.58
1:A:127:MET:O	2:B:101:LEU:HD21	2.04	0.57
2:B:1:GLN:HG3	2:B:3:GLN:HG2	1.86	0.57
2:B:67:PHE:CZ	2:B:82:MET:HG2	2.40	0.57
1:A:343:MET:HE1	1:A:407:PHE:CZ	2.40	0.57
2:B:12:VAL:HG11	2:B:18:LEU:HG	1.86	0.57
1:A:151[B]:GLU:OE1	1:A:168:LYS:HE2	2.05	0.57
1:A:228:GLU:OE2	1:A:289:LYS:HE2	2.04	0.57
1:A:428:GLN:O	1:A:429:VAL:HG13	2.05	0.57
2:B:2:VAL:HG22	2:B:26:GLY:HA3	1.87	0.57
1:A:76:ARG:NE	1:A:85:GLU:OE2	2.37	0.56
1:A:153[A]:LEU:HD11	1:A:168:LYS:HB2	1.87	0.56
2:B:11:LEU:HD23	2:B:12:VAL:N	2.20	0.56
1:A:81:THR:OG1	1:A:179:LYS:NZ	2.37	0.55
2:B:17:SER:HA	2:B:82:MET:O	2.05	0.55
1:A:64:LYS:NZ	1:A:97:GLU:OE2	2.38	0.55
2:B:67:PHE:HA	2:B:81:GLN:O	2.07	0.54
1:A:147:MET:HG3	1:A:152[B]:TYR:OH	2.08	0.54
1:A:399:ALA:O	1:A:403:MET:HG3	2.07	0.54
1:A:5:ALA:N	1:A:31:ASN:HD21	2.06	0.54
1:A:313:PRO:HD2	1:A:314:GLU:OE1	2.08	0.53
1:A:238:HIS:O	1:A:242:GLU:HG3	2.09	0.53
1:A:366:ILE:HD13	1:A:368:PHE:CZ	2.43	0.52
1:A:152[B]:TYR:CD1	1:A:165:ILE:HD12	2.45	0.52
2:B:2:VAL:CG1	2:B:27:ILE:HD11	2.40	0.52
2:B:51:VAL:O	2:B:51:VAL:HG13	2.09	0.52
2:B:63:VAL:CG1	2:B:67:PHE:HB2	2.39	0.52
1:A:359:GLU:OE1	1:A:363:MET:HG3	2.09	0.52
1:A:366:ILE:HD12	1:A:384:LEU:HD12	1.91	0.52
2:B:22:CYS:O	2:B:77:THR:HG23	2.10	0.52
2:B:40:ALA:HB3	2:B:43:LYS:HG3	1.91	0.51
2:B:7:SER:CA	2:B:110:THR:HG21	2.40	0.51
1:A:148:ASN:O	1:A:170:LYS:HE2	2.10	0.51
1:A:76:ARG:NH2	1:A:85:GLU:OE2	2.44	0.51
1:A:182:LYS:O	1:A:185:VAL:HG22	2.10	0.51
1:A:249:ARG:HD2	3:A:503:EDO:H21	1.93	0.51
1:A:163:LYS:HD3	6:A:617:HOH:O	2.10	0.51
1:A:32:ASP:OD1	1:A:34:THR:HG23	2.12	0.50
1:A:248[B]:ASP:OD1	6:A:601:HOH:O	2.20	0.50
1:A:127:MET:HA	2:B:47:LEU:HD22	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLU:N	1:A:149:GLU:OE1	2.45	0.49
2:B:72:ASP:OD2	2:B:75:LYS:HD3	2.11	0.49
1:A:428:GLN:N	1:A:437:TYR:OH	2.44	0.49
1:A:236:PHE:CD2	1:A:278[A]:GLU:HG3	2.48	0.49
2:B:22:CYS:C	2:B:77:THR:HG23	2.38	0.49
1:A:11:TRP:O	1:A:12:LEU:HD23	2.13	0.48
1:A:12:LEU:HD21	1:A:99:TRP:CE2	2.48	0.48
1:A:214:LYS:HA	1:A:214:LYS:HE2	1.96	0.48
1:A:239:LEU:HD23	1:A:277:LEU:HD21	1.95	0.48
2:B:103:ARG:HB2	2:B:105:VAL:HG23	1.95	0.47
1:A:214:LYS:HE2	1:A:214:LYS:CA	2.45	0.47
1:A:57:VAL:O	1:A:60:CYS:HB3	2.15	0.47
2:B:7:SER:HA	2:B:110:THR:CG2	2.42	0.47
1:A:20:LYS:O	1:A:21:THR:CB	2.63	0.47
1:A:271:VAL:CG1	1:A:328:ARG:HA	2.46	0.46
1:A:362:LEU:O	1:A:386:LYS:HD3	2.16	0.46
2:B:35:ALA:HA	2:B:49:ALA:O	2.14	0.46
2:B:71:ARG:HD3	2:B:73:ASN:OD1	2.16	0.46
1:A:27:PHE:CZ	1:A:88:PHE:HE1	2.34	0.45
1:A:69:ARG:O	1:A:72:THR:HG23	2.16	0.45
1:A:67:ARG:HA	1:A:68:PRO:C	2.41	0.45
1:A:212:ALA:H	1:A:228:GLU:CG	2.29	0.45
1:A:5:ALA:HB3	1:A:31:ASN:ND2	2.32	0.45
1:A:249:ARG:CD	3:A:503:EDO:H21	2.47	0.45
1:A:237[A]:PHE:CZ	1:A:241:ARG:CD	2.99	0.45
2:B:39:GLN:HB2	2:B:45:ARG:HG3	1.99	0.45
2:B:36:TRP:O	2:B:48:LEU:HB2	2.17	0.44
1:A:38:TYR:CG	1:A:42:PRO:HG3	2.52	0.44
1:A:118:MET:HE2	1:A:118:MET:HB3	1.89	0.44
1:A:213:LEU:CD1	1:A:227[A]:MET:HG3	2.49	0.43
2:B:90:THR:HG23	2:B:113:THR:HG22	2.00	0.43
2:B:63:VAL:HG11	2:B:67:PHE:CD2	2.54	0.43
1:A:239:LEU:HD23	1:A:277:LEU:HD22	2.00	0.43
1:A:16:GLY:N	1:A:21:THR:O	2.44	0.43
1:A:213:LEU:HD12	1:A:227[A]:MET:HG3	2.00	0.42
1:A:61:GLN:HG2	1:A:76:ARG:HB3	2.02	0.42
1:A:156:LEU:HA	1:A:156:LEU:HD23	1.67	0.42
1:A:366:ILE:CD1	1:A:384:LEU:HD12	2.50	0.42
1:A:271:VAL:HG11	1:A:327:GLY:O	2.20	0.42
1:A:346:ARG:NH2	1:A:369:PRO:HG3	2.35	0.41
2:B:63:VAL:CG1	2:B:67:PHE:CD2	3.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:SER:HB2	2:B:79:TYR:CE1	2.56	0.41
2:B:63:VAL:HG13	2:B:67:PHE:CG	2.55	0.41
2:B:67:PHE:CE1	2:B:82:MET:HG2	2.56	0.41
1:A:411:ILE:HD13	1:A:411:ILE:HA	1.93	0.41
1:A:415:HIS:HB3	1:A:420:LYS:HB2	2.02	0.41
1:A:162:GLY:HA3	1:A:180:ILE:O	2.21	0.41
1:A:262:ASP:HB2	1:A:399:ALA:CB	2.51	0.41
2:B:75:LYS:O	2:B:76:ASN:C	2.63	0.41
1:A:227[B]:MET:HE2	1:A:227[B]:MET:HB3	1.92	0.41
2:B:29:VAL:HG22	2:B:76:ASN:OD1	2.20	0.41
2:B:63:VAL:CG1	2:B:63:VAL:O	2.69	0.41
1:A:9:GLU:HG3	1:A:26:TYR:OH	2.20	0.41
1:A:65:THR:HG23	1:A:72:THR:HG1	1.83	0.41
1:A:97:GLU:OE1	1:A:97:GLU:HA	2.21	0.41
1:A:275:LEU:HD23	1:A:335:LEU:N	2.36	0.41
1:A:434:ASP:C	1:A:436:ARG:H	2.28	0.41
1:A:62:LEU:C	1:A:63:MET:HG3	2.46	0.41
2:B:2:VAL:HG22	2:B:26:GLY:CA	2.50	0.41
2:B:86:ILE:HG22	2:B:88:ASP:H	1.85	0.40
1:A:326:TYR:HB2	1:A:330:VAL:CG1	2.52	0.40
1:A:201:VAL:HG21	1:A:214:LYS:O	2.21	0.40
1:A:62:LEU:HD12	1:A:104:GLN:OE1	2.22	0.40
1:A:114:GLU:O	1:A:118:MET:HG3	2.21	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	222/438 (51%)	215 (97%)	7 (3%)	0	100	100
2	B	112/126 (89%)	104 (93%)	8 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	334/564 (59%)	319 (96%)	15 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	338/387 (87%)	327 (97%)	11 (3%)	33	45
2	B	91/104 (88%)	90 (99%)	1 (1%)	65	79
All	All	429/491 (87%)	417 (97%)	12 (3%)	37	52

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	19	ILE
1	A	28	LEU
1	A	69	ARG
1	A	145	VAL
1	A	149	GLU
1	A	244	VAL
1	A	270	VAL
1	A	271	VAL
1	A	312	THR
1	A	366	ILE
2	B	95	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	354	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
5	SO4	A	507	-	4,4,4	0.26	0	6,6,6	0.14	0
3	EDO	A	501	-	3,3,3	0.50	0	2,2,2	0.27	0
3	EDO	A	503	-	3,3,3	0.60	0	2,2,2	0.29	0
5	SO4	A	505	-	4,4,4	0.28	0	6,6,6	0.10	0
4	XOO	A	502	1	45,45,46	0.62	1 (2%)	58,63,64	0.80	1 (1%)
5	SO4	A	508	-	4,4,4	0.34	0	6,6,6	0.12	0
5	SO4	B	201	-	4,4,4	0.27	0	6,6,6	0.24	0
5	SO4	A	506	-	4,4,4	0.29	0	6,6,6	0.19	0
5	SO4	A	504	-	4,4,4	0.19	0	6,6,6	0.15	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	EDO	A	501	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	503	-	-	1/1/1/1	-
4	XOO	A	502	1	-	2/19/19/21	0/6/6/6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	XOO	C25-C24	-2.65	1.46	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	XOO	C12-N5-C11	-2.25	122.25	125.11

There are no chirality outliers.

All (3) torsion outliers are listed below:

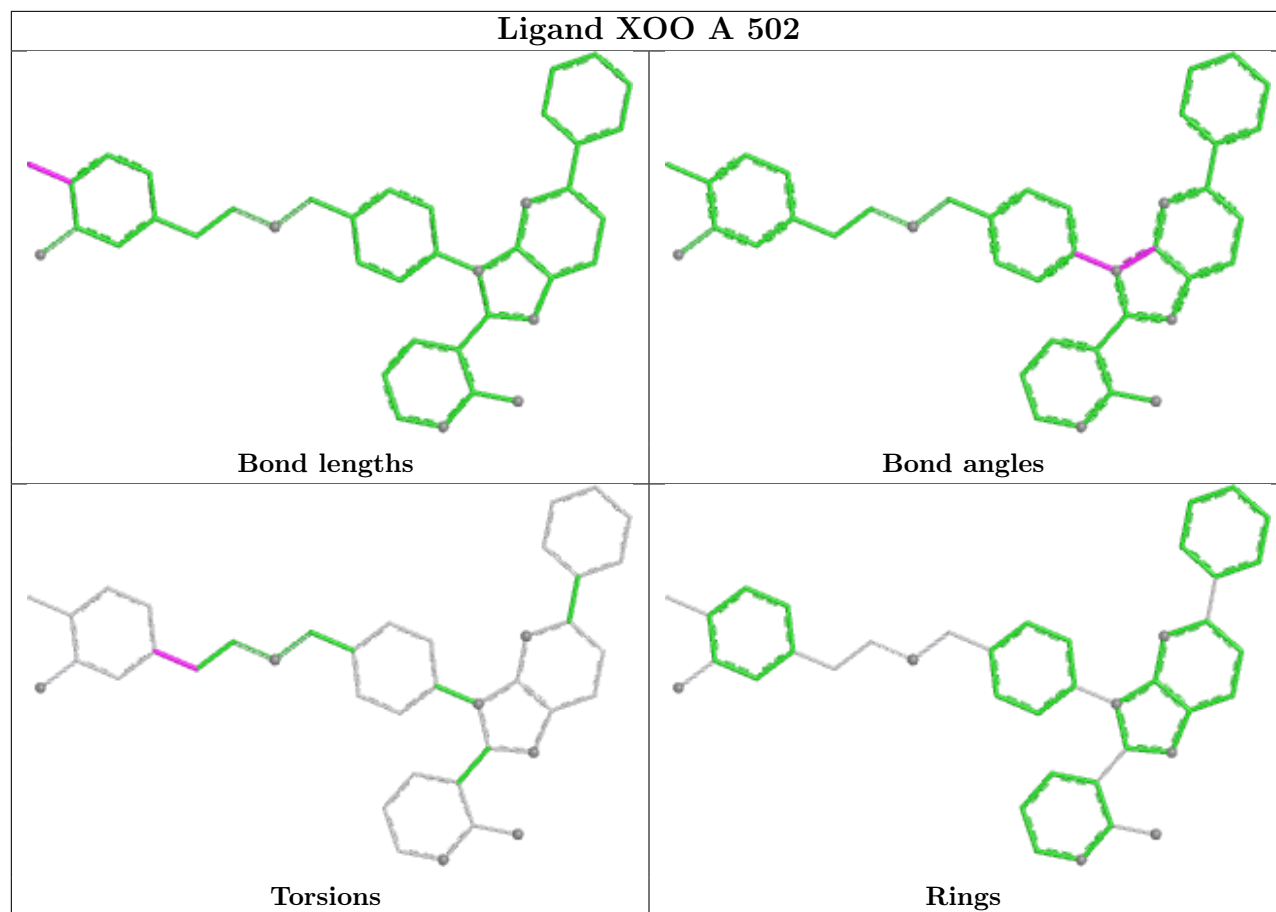
Mol	Chain	Res	Type	Atoms
4	A	502	XOO	C19-C20-C21-C22
4	A	502	XOO	C19-C20-C21-C27
3	A	503	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	507	SO4	1	0
3	A	503	EDO	2	0
4	A	502	XOO	1	0

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, 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	392/438 (89%)	0.55	27 (6%) 23 20	15, 45, 74, 93	8 (2%)
2	B	114/126 (90%)	1.11	14 (12%) 8 6	43, 60, 73, 85	0
All	All	506/564 (89%)	0.68	41 (8%) 18 15	15, 49, 74, 93	8 (1%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	310	CYS	4.3
1	A	309	PHE	4.2
1	A	201	VAL	4.1
1	A	296	CYS	4.0
2	B	114	VAL	3.9
1	A	202	LEU	3.8
1	A	125	THR	3.7
2	B	67	PHE	3.5
1	A	152[A]	TYR	3.5
1	A	186	ILE	3.2
1	A	200	ARG	3.1
1	A	437	TYR	3.0
1	A	429	VAL	3.0
1	A	205	SER	2.9
1	A	187	VAL	2.9
1	A	145	VAL	2.8
1	A	68	PRO	2.7
1	A	203	GLN	2.7
1	A	124	HIS	2.6
1	A	110	LEU	2.6
1	A	128	GLU	2.6
1	A	432	GLU	2.6
2	B	86	ILE	2.5
1	A	20	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	159	GLY	2.4
2	B	112	VAL	2.4
1	A	299	GLY	2.4
1	A	185	VAL	2.4
2	B	49	ALA	2.3
2	B	25	SER	2.3
2	B	87	PRO	2.3
1	A	237[A]	PHE	2.3
2	B	113	THR	2.3
1	A	295	LEU	2.2
1	A	433	THR	2.2
2	B	17	SER	2.1
2	B	60	ALA	2.1
2	B	5	GLN	2.0
2	B	85	LEU	2.0
2	B	18	LEU	2.0
2	B	31	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

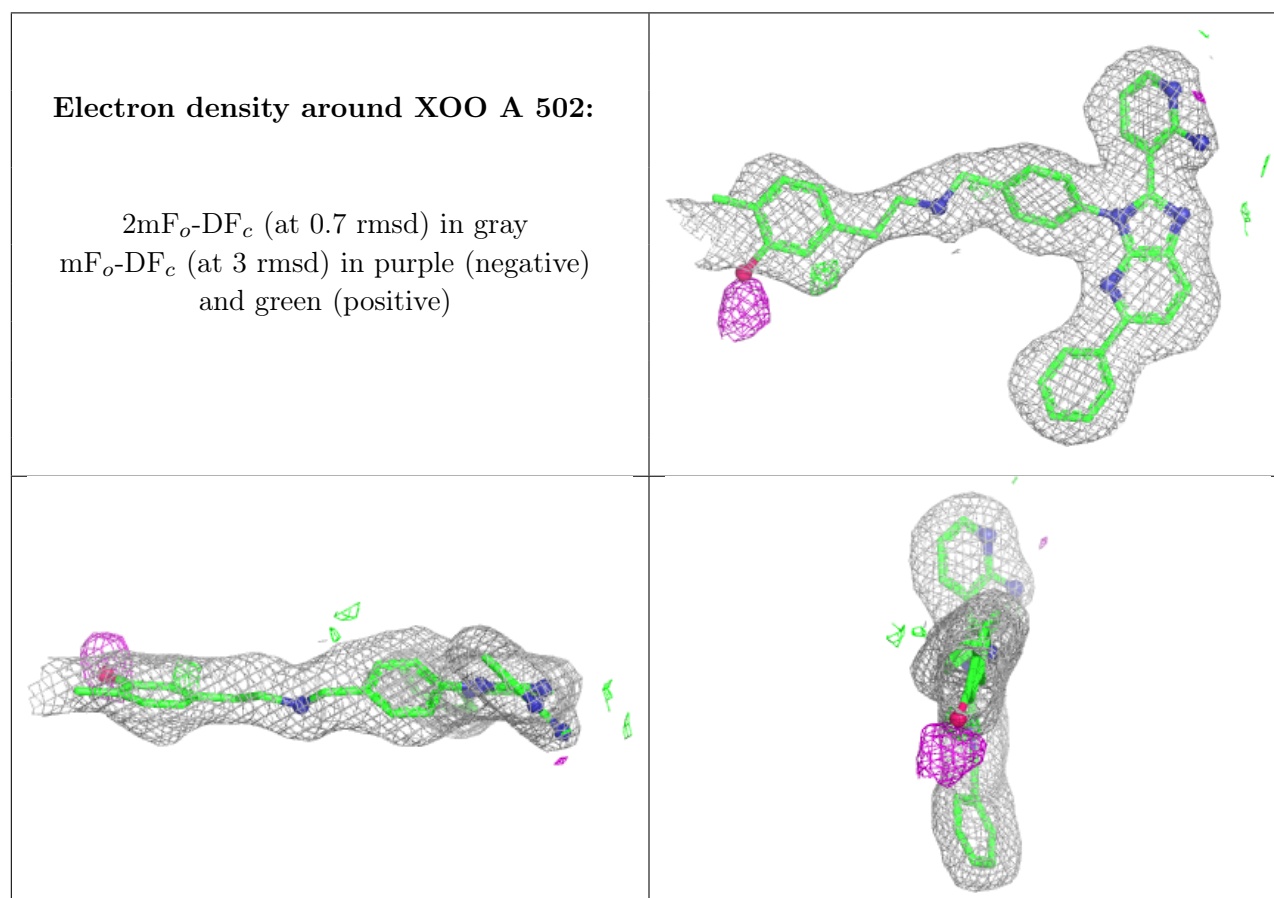
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	A	507	5/5	0.47	0.13	93,106,109,122	0
5	SO4	A	505	5/5	0.75	0.14	66,66,86,97	0
5	SO4	A	506	5/5	0.79	0.12	57,70,79,84	0
3	EDO	A	503	4/4	0.80	0.13	49,59,64,67	0
5	SO4	A	508	5/5	0.82	0.14	50,65,75,77	0
5	SO4	B	201	5/5	0.83	0.12	75,76,87,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	501	4/4	0.90	0.14	48,49,53,57	0
4	XOO	A	502	40/41	0.92	0.10	22,35,65,73	0
5	SO4	A	504	5/5	0.93	0.07	64,66,72,72	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.