



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:16 AM UTC

PDB ID : 8R4V / pdb_00008r4v
Title : Structure of Salt-inducible kinase 3 in complex with inhibitor
Authors : Kack, H.; Oster, L.
Deposited on : 2023-11-14
Resolution : 1.90 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

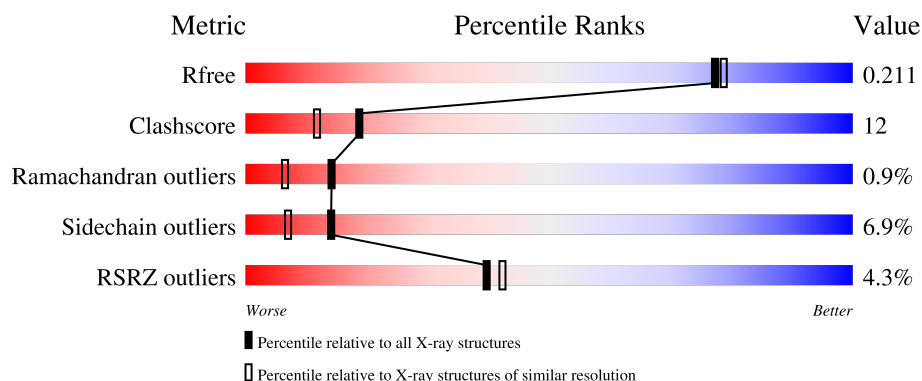
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	328	7% 76% 18% • •
1	B	328	2% 69% 23% • •
1	C	328	3% 76% 19% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7672 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.

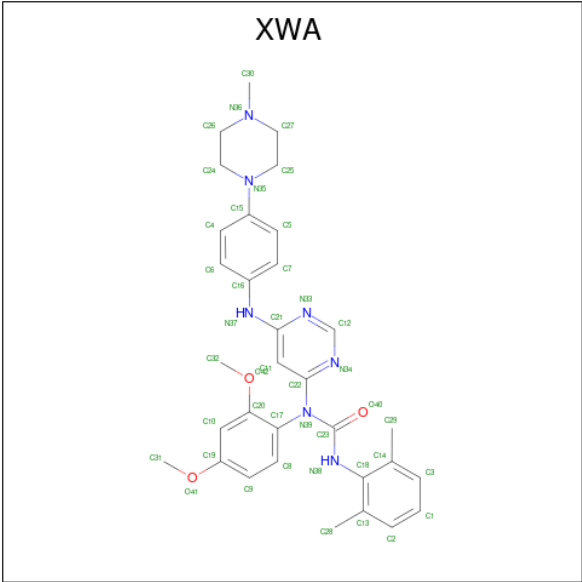
- Molecule 1 is a protein called Serine/threonine-protein kinase SIK3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	P	S	0	0	0
			2462	1571	427	446	1	17			
1	B	316	Total	C	N	O	P	S	0	0	0
			2453	1570	418	447	1	17			
1	C	319	Total	C	N	O	P	S	0	0	0
			2516	1604	435	459	1	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	58	SER	-	expression tag	UNP Q9Y2K2
A	121	SER	CYS	engineered mutation	UNP Q9Y2K2
A	181	SER	CYS	engineered mutation	UNP Q9Y2K2
A	333	SER	CYS	engineered mutation	UNP Q9Y2K2
B	58	SER	-	expression tag	UNP Q9Y2K2
B	121	SER	CYS	engineered mutation	UNP Q9Y2K2
B	181	SER	CYS	engineered mutation	UNP Q9Y2K2
B	333	SER	CYS	engineered mutation	UNP Q9Y2K2
C	58	SER	-	expression tag	UNP Q9Y2K2
C	121	SER	CYS	engineered mutation	UNP Q9Y2K2
C	181	SER	CYS	engineered mutation	UNP Q9Y2K2
C	333	SER	CYS	engineered mutation	UNP Q9Y2K2

- Molecule 2 is 1-(2,4-dimethoxyphenyl)-3-(2,6-dimethylphenyl)-1-[6-[[4-(4-methylpiperazin-1-yl)phenyl]amino]pyrimidin-4-yl]urea (CCD ID: XWA) (formula: C₃₂H₃₇N₇O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			42	32	7	3		
2	B	1	Total	C	N	O	0	0
			42	32	7	3		
2	C	1	Total	C	N	O	0	0
			42	32	7	3		

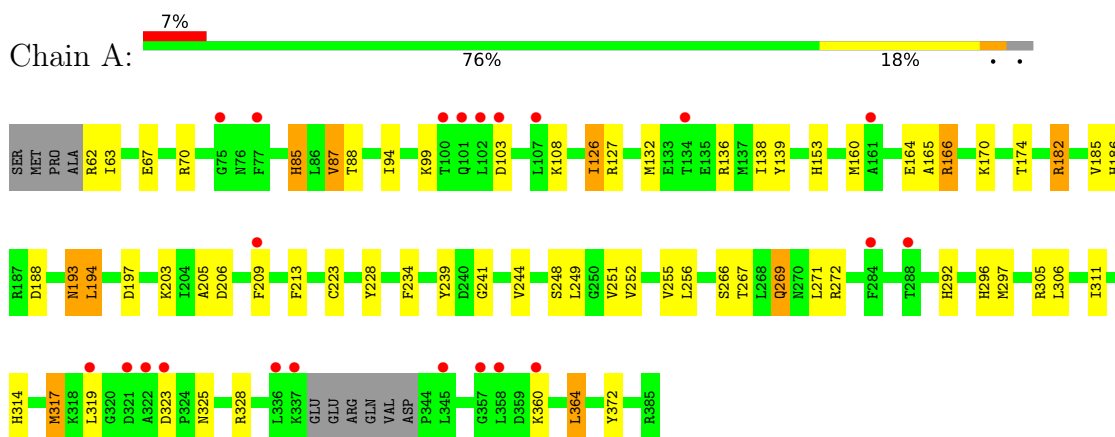
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		
3	B	40	Total	O	0	0
			40	40		
3	C	37	Total	O	0	0
			37	37		

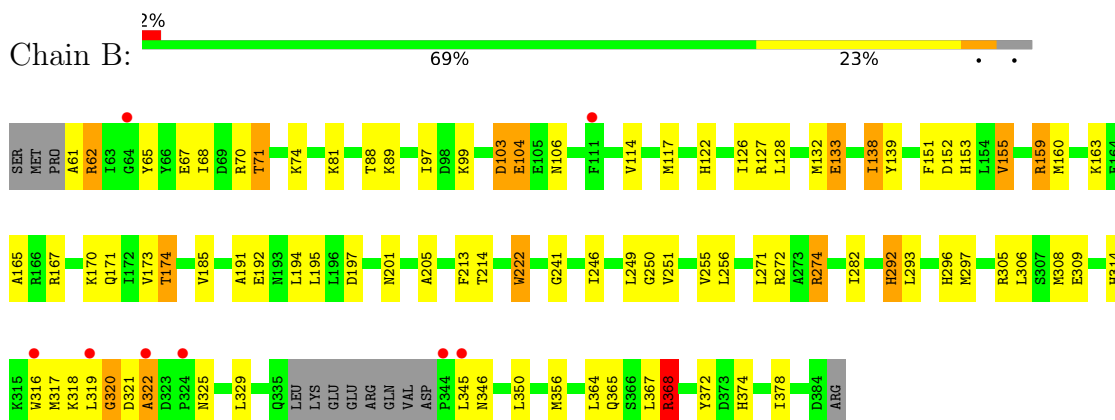
3 Residue-property plots [i](#)

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.

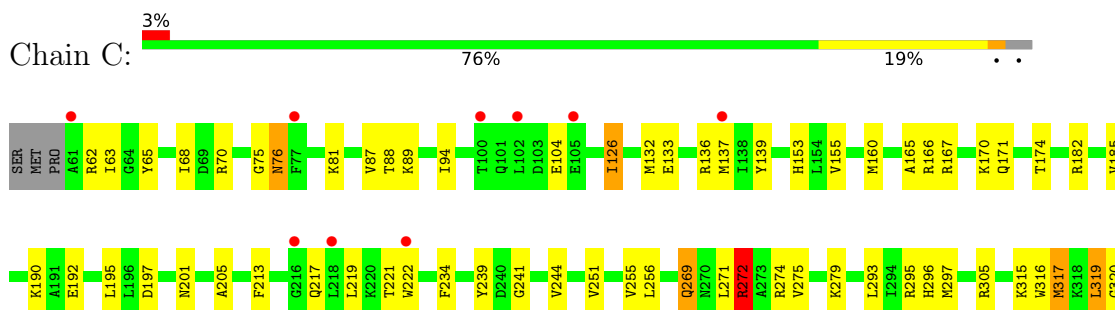
- Molecule 1: Serine/threonine-protein kinase SIK3

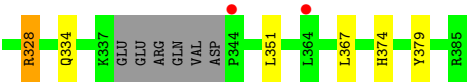


- Molecule 1: Serine/threonine-protein kinase SIK3



- Molecule 1: Serine/threonine-protein kinase SIK3





4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	104.25Å 104.25Å 95.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.64 – 1.90 65.64 – 1.90	Depositor EDS
% Data completeness (in resolution range)	60.4 (65.64-1.90) 61.7 (65.64-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.204 , 0.240 0.180 , 0.211	Depositor DCC
R_{free} test set	2866 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.097 for -h,-k,l 0.027 for h,-h-k,-l 0.011 for -k,-h,-l	Xtriage
Reported twinning fraction	0.509 for H, K, L 0.491 for -h,-k,l	Depositor
Outliers	0 of 56513 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7672	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: XWA, 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	0.55	1/2498 (0.0%)	0.91	0/3378
1	B	0.57	2/2491 (0.1%)	0.96	1/3372 (0.0%)
1	C	0.56	2/2555 (0.1%)	0.95	0/3455
All	All	0.56	5/7544 (0.1%)	0.94	1/10205 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
1	C	0	5
All	All	0	14

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	153	HIS	CE1-NE2	5.46	1.38	1.32
1	A	85	HIS	CE1-NE2	5.25	1.37	1.32
1	C	296	HIS	CE1-NE2	5.22	1.37	1.32
1	B	153	HIS	CE1-NE2	5.04	1.37	1.32
1	B	292	HIS	CE1-NE2	5.02	1.37	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	THR	CB-CA-C	5.69	119.53	110.19

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	ARG	Sidechain
1	A	166	ARG	Sidechain
1	A	182	ARG	Sidechain
1	A	305	ARG	Sidechain
1	A	62	ARG	Sidechain
1	B	159	ARG	Sidechain
1	B	274	ARG	Sidechain
1	B	305	ARG	Sidechain
1	B	368	ARG	Sidechain
1	C	136	ARG	Sidechain
1	C	166	ARG	Sidechain
1	C	182	ARG	Sidechain
1	C	272	ARG	Sidechain
1	C	305	ARG	Sidechain

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	2462	0	2403	56	0
1	B	2453	0	2397	68	0
1	C	2516	0	2468	48	0
2	A	42	0	0	1	0
2	B	42	0	0	3	0
2	C	42	0	0	1	0
3	A	38	0	0	1	0
3	B	40	0	0	3	0
3	C	37	0	0	1	0
All	All	7672	0	7268	176	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 12.

All (176) 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:160:MET:CE	1:C:165:ALA:HA	2.04	0.88
1:A:160:MET:CE	1:A:165:ALA:HA	2.08	0.84
1:B:160:MET:CE	1:B:165:ALA:HA	2.09	0.83
1:C:319:LEU:HD23	1:C:320:GLY:N	1.94	0.81
1:B:314:HIS:HD1	1:B:316:TRP:H	1.31	0.76
1:B:151:PHE:O	1:B:155:VAL:HG12	1.85	0.75
1:B:103:ASP:OD1	1:B:106:ASN:ND2	2.22	0.73
1:A:360:LYS:O	1:A:364:LEU:HD22	1.89	0.73
1:A:193:ASN:C	1:A:193:ASN:HD22	1.97	0.72
1:A:249:LEU:HA	1:A:252:VAL:HG22	1.71	0.72
1:C:171:GLN:HE22	1:C:201:ASN:HD22	1.37	0.72
1:C:170:LYS:HG3	1:C:317:MET:HE2	1.70	0.72
1:C:317:MET:HE3	1:C:317:MET:HA	1.72	0.71
1:C:160:MET:HE3	1:C:165:ALA:HA	1.71	0.71
1:A:160:MET:HE3	1:A:165:ALA:HA	1.75	0.69
1:A:193:ASN:HB3	3:A:509:HOH:O	1.91	0.69
1:C:167:ARG:HH21	1:C:201:ASN:HD21	1.41	0.69
1:C:269:GLN:H	1:C:269:GLN:HE21	1.39	0.69
1:B:99:LYS:NZ	1:B:133:GLU:OE2	2.25	0.69
1:B:122:HIS:HE1	1:B:174:THR:CG2	2.06	0.69
1:C:171:GLN:HE22	1:C:201:ASN:ND2	1.91	0.68
1:B:246:ILE:HG13	1:B:308:MET:HE2	1.75	0.67
1:B:350:LEU:HD21	1:B:364:LEU:HD11	1.75	0.67
1:B:171:GLN:HE22	1:B:201:ASN:HD22	1.43	0.66
1:A:228:TYR:HD1	1:A:251:VAL:HG13	1.61	0.66
1:B:171:GLN:HE22	1:B:201:ASN:ND2	1.95	0.65
1:C:272:ARG:O	1:C:275:VAL:HG22	1.97	0.65
1:C:160:MET:HE1	1:C:165:ALA:HA	1.79	0.64
1:B:122:HIS:HE1	1:B:174:THR:HG22	1.61	0.64
1:B:246:ILE:CG1	1:B:308:MET:HE2	2.26	0.64
1:C:160:MET:HE2	1:C:256:LEU:HB3	1.81	0.63
1:B:356:MET:HE1	1:B:378:ILE:HG21	1.80	0.63
1:C:293:LEU:HG	1:C:297:MET:HE2	1.80	0.63
1:B:160:MET:HE3	1:B:165:ALA:HA	1.80	0.61
1:A:160:MET:HE1	1:A:165:ALA:HA	1.83	0.61
1:A:292:HIS:ND1	1:A:314:HIS:HE1	1.98	0.61
1:C:160:MET:HE3	1:C:165:ALA:CA	2.30	0.61
1:A:228:TYR:CD1	1:A:251:VAL:HG13	2.34	0.61
1:A:160:MET:HE2	1:A:256:LEU:HB3	1.83	0.60
1:B:122:HIS:CE1	1:B:174:THR:CG2	2.84	0.60
1:B:249:LEU:HD12	1:B:308:MET:HE1	1.83	0.60
1:B:160:MET:HE2	1:B:256:LEU:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ASN:HD22	1:A:194:LEU:N	1.99	0.60
1:B:160:MET:HE1	1:B:165:ALA:HA	1.83	0.60
1:A:248:SER:O	1:A:251:VAL:CG1	2.51	0.58
1:A:160:MET:HE3	1:A:165:ALA:CA	2.33	0.58
1:B:152:ASP:HA	1:B:155:VAL:CG1	2.34	0.58
1:A:228:TYR:CD1	1:A:251:VAL:CG1	2.87	0.58
1:C:328:ARG:HH11	1:C:328:ARG:HB3	1.68	0.57
1:B:62:ARG:NH1	1:B:67:GLU:OE1	2.37	0.56
1:A:292:HIS:ND1	1:A:314:HIS:CE1	2.73	0.56
1:B:152:ASP:HA	1:B:155:VAL:HG13	1.87	0.56
1:C:334:GLN:HA	3:C:505:HOH:O	2.04	0.56
1:A:249:LEU:HB3	1:A:297:MET:HE1	1.88	0.56
1:A:249:LEU:HA	1:A:252:VAL:CG2	2.36	0.55
1:C:269:GLN:HE21	1:C:269:GLN:N	2.05	0.55
2:C:401:XWA:N34	2:C:401:XWA:N38	2.52	0.55
2:B:401:XWA:C30	3:B:518:HOH:O	2.55	0.55
1:A:228:TYR:HD1	1:A:251:VAL:CG1	2.19	0.54
1:A:267:THR:HB	1:A:269:GLN:NE2	2.23	0.54
1:A:325:ASN:HD22	1:A:328:ARG:HH21	1.54	0.53
1:A:249:LEU:CA	1:A:252:VAL:HG22	2.37	0.53
1:B:160:MET:HE3	1:B:165:ALA:CA	2.39	0.53
1:B:185:VAL:HG13	1:B:213:PHE:CD1	2.44	0.53
1:A:248:SER:O	1:A:251:VAL:HG12	2.09	0.53
1:B:365:GLN:HA	1:B:368:ARG:HG2	1.91	0.53
1:A:85:HIS:CE1	1:A:87:VAL:HG22	2.45	0.52
1:B:104:GLU:C	1:B:106:ASN:H	2.18	0.51
1:B:325:ASN:O	1:B:329:LEU:HD13	2.10	0.51
1:B:293:LEU:HG	1:B:297:MET:HE2	1.92	0.51
1:A:153:HIS:HE1	1:A:164:GLU:OE2	1.94	0.51
1:B:271:LEU:HD23	1:B:271:LEU:C	2.36	0.51
1:A:185:VAL:HG13	1:A:213:PHE:CD1	2.45	0.51
1:A:209:PHE:CD1	1:A:223:CYS:HB2	2.46	0.51
1:A:234:PHE:CD1	1:A:272:ARG:HG3	2.46	0.51
1:A:271:LEU:C	1:A:271:LEU:HD23	2.36	0.51
2:A:401:XWA:N34	2:A:401:XWA:N38	2.58	0.51
1:C:234:PHE:CD1	1:C:272:ARG:HG3	2.46	0.51
1:A:228:TYR:HA	1:A:251:VAL:HG11	1.94	0.50
1:B:292:HIS:CE1	1:B:296:HIS:CE1	3.00	0.50
1:A:193:ASN:C	1:A:193:ASN:ND2	2.67	0.50
1:C:367:LEU:HD11	1:C:379:TYR:CD2	2.46	0.50
1:A:87:VAL:HG22	1:A:88:THR:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:SER:O	1:A:251:VAL:HG13	2.12	0.49
1:B:68:ILE:HG21	1:B:81:LYS:HD3	1.93	0.49
1:B:114:VAL:HA	1:B:117:MET:HE2	1.95	0.49
1:B:127:ARG:NH2	1:B:372:TYR:OH	2.45	0.49
2:B:401:XWA:N34	2:B:401:XWA:N38	2.59	0.49
1:C:319:LEU:HD23	1:C:320:GLY:H	1.75	0.49
1:A:99:LYS:HD2	1:A:138:ILE:HG13	1.95	0.48
1:A:94:ILE:HD11	1:A:139:TYR:HD2	1.78	0.48
1:A:186:HIS:HE1	1:A:205:ALA:O	1.96	0.48
1:A:170:LYS:O	1:A:174:THR:HG23	2.14	0.48
1:B:122:HIS:CE1	1:B:174:THR:HG23	2.49	0.48
1:C:75:GLY:O	1:C:76:ASN:C	2.56	0.48
1:C:170:LYS:O	1:C:174:THR:HG23	2.14	0.48
1:C:185:VAL:HG13	1:C:213:PHE:CD1	2.48	0.48
1:C:62:ARG:O	1:C:63:ILE:HD13	2.13	0.47
1:C:219:LEU:HD22	1:C:219:LEU:N	2.29	0.47
1:C:234:PHE:CE2	1:C:275:VAL:HG21	2.50	0.47
1:B:133:GLU:HG3	1:B:138:ILE:CD1	2.44	0.47
1:B:249:LEU:CD1	1:B:308:MET:HE1	2.44	0.47
1:A:249:LEU:C	1:A:252:VAL:HG22	2.39	0.47
1:B:214:THR:N	1:C:295:ARG:HH21	2.13	0.47
1:C:271:LEU:C	1:C:271:LEU:HD23	2.40	0.47
1:C:185:VAL:HG11	1:C:241:GLY:HA3	1.97	0.47
1:A:166:ARG:O	1:A:170:LYS:HG3	2.15	0.47
1:B:97:ILE:HD12	1:B:138:ILE:CG2	2.46	0.46
1:B:126:ILE:HG12	1:B:205:ALA:HA	1.95	0.46
1:C:132:MET:HB2	1:C:139:TYR:HB2	1.96	0.46
1:B:246:ILE:HD13	1:B:306:LEU:O	2.15	0.46
1:B:122:HIS:CE1	1:B:174:THR:HG22	2.46	0.46
1:A:296:HIS:HB3	1:A:306:LEU:HG	1.98	0.46
1:B:65:TYR:CE2	1:B:374:HIS:NE2	2.83	0.46
1:C:167:ARG:NH2	1:C:201:ASN:HD21	2.09	0.46
1:A:132:MET:HB2	1:A:139:TYR:HB2	1.98	0.46
1:A:251:VAL:O	1:A:255:VAL:HG23	2.15	0.46
1:B:117:MET:HE3	1:B:128:LEU:HD22	1.97	0.46
1:B:246:ILE:HG12	1:B:308:MET:HE2	1.98	0.46
1:B:88:THR:O	1:B:89:LYS:HB2	2.15	0.45
1:B:104:GLU:C	1:B:106:ASN:N	2.74	0.45
1:B:185:VAL:HG11	1:B:241:GLY:HA3	1.99	0.45
1:C:68:ILE:HG21	1:C:81:LYS:HD3	1.98	0.45
1:B:132:MET:HB2	1:B:139:TYR:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:LYS:O	1:B:320:GLY:N	2.50	0.45
1:C:315:LYS:O	1:C:319:LEU:HB2	2.16	0.45
1:A:170:LYS:HG2	1:A:317:MET:HE3	1.99	0.45
1:B:368:ARG:NH1	1:B:368:ARG:HB3	2.31	0.45
1:A:267:THR:HB	1:A:269:GLN:HE22	1.81	0.45
1:B:368:ARG:NH1	1:B:368:ARG:CB	2.80	0.45
1:C:269:GLN:H	1:C:269:GLN:NE2	2.12	0.45
1:C:274:ARG:NH2	1:C:279:LYS:O	2.44	0.45
2:B:401:XWA:C6	2:B:401:XWA:C11	2.94	0.44
1:A:323:ASP:OD1	1:A:323:ASP:N	2.50	0.44
1:B:127:ARG:NH1	3:B:501:HOH:O	2.50	0.44
1:C:251:VAL:O	1:C:255:VAL:HG23	2.18	0.44
1:B:321:ASP:O	1:B:322:ALA:HB3	2.18	0.43
1:A:126:ILE:HD13	1:A:126:ILE:HA	1.94	0.43
1:A:197:ASP:OD1	1:A:197:ASP:C	2.61	0.43
1:B:191:ALA:HA	1:B:194:LEU:HD12	2.00	0.43
1:B:195:LEU:HD12	1:B:205:ALA:HB2	1.99	0.43
1:C:195:LEU:HD12	1:C:205:ALA:HB2	1.99	0.43
1:C:317:MET:HA	1:C:317:MET:CE	2.45	0.43
1:A:239:TYR:CD2	1:A:244:VAL:HG21	2.54	0.43
1:B:346:ASN:O	1:B:350:LEU:CD1	2.66	0.43
1:A:85:HIS:CE1	1:A:87:VAL:HG13	2.54	0.43
1:A:292:HIS:CE1	1:A:314:HIS:HE1	2.37	0.43
1:B:133:GLU:HG3	1:B:138:ILE:HD11	2.01	0.43
1:B:250:GLY:HA2	1:B:297:MET:HE3	2.00	0.43
1:B:170:LYS:HA	1:B:173:VAL:HG22	2.00	0.43
1:A:297:MET:HE3	1:A:311:ILE:HD13	2.01	0.42
1:A:185:VAL:HG11	1:A:241:GLY:HA3	2.01	0.42
1:A:249:LEU:O	1:A:252:VAL:HG22	2.18	0.42
1:C:65:TYR:HD2	1:C:87:VAL:HG23	1.84	0.42
1:C:239:TYR:CD2	1:C:244:VAL:HG21	2.54	0.42
1:B:292:HIS:HD2	1:B:314:HIS:NE2	2.17	0.42
1:C:197:ASP:C	1:C:197:ASP:OD1	2.61	0.42
1:C:234:PHE:CD2	1:C:275:VAL:HG21	2.54	0.42
1:B:346:ASN:O	1:B:350:LEU:HD13	2.20	0.42
1:B:197:ASP:OD1	1:B:197:ASP:C	2.62	0.42
1:B:103:ASP:CG	1:B:106:ASN:HD22	2.28	0.41
1:C:88:THR:O	1:C:89:LYS:HB2	2.20	0.41
1:B:222:TRP:CD1	1:B:222:TRP:C	2.97	0.41
1:B:61:ALA:N	3:B:506:HOH:O	2.53	0.41
1:B:97:ILE:HD12	1:B:138:ILE:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:VAL:O	1:B:255:VAL:HG23	2.20	0.41
1:B:68:ILE:HD12	1:B:68:ILE:N	2.36	0.41
1:A:127:ARG:NH2	1:A:372:TYR:OH	2.48	0.41
1:B:296:HIS:HB3	1:B:306:LEU:HG	2.02	0.40
1:A:267:THR:CB	1:A:269:GLN:NE2	2.84	0.40
1:C:126:ILE:HD13	1:C:126:ILE:HA	1.97	0.40
1:C:328:ARG:HB3	1:C:328:ARG:NH1	2.35	0.40
1:C:65:TYR:CE1	1:C:374:HIS:CE1	3.09	0.40
1:C:316:TRP:CZ3	1:C:317:MET:HE1	2.56	0.40
1:A:188:ASP:O	1:A:188:ASP:CG	2.64	0.40
1:C:167:ARG:HG3	1:C:167:ARG:HH11	1.87	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	313/328 (95%)	303 (97%)	9 (3%)	1 (0%)	36	29
1	B	311/328 (95%)	293 (94%)	13 (4%)	5 (2%)	7	2
1	C	314/328 (96%)	304 (97%)	8 (2%)	2 (1%)	21	13
All	All	938/984 (95%)	900 (96%)	30 (3%)	8 (1%)	14	6

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ASP
1	B	319	LEU
1	C	76	ASN
1	B	104	GLU
1	B	345	LEU
1	C	319	LEU

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Mol	Chain	Res	Type
1	B	322	ALA
1	B	320	GLY

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	252/288 (88%)	236 (94%)	16 (6%)	16	8
1	B	253/288 (88%)	232 (92%)	21 (8%)	10	4
1	C	263/288 (91%)	247 (94%)	16 (6%)	17	9
All	All	768/864 (89%)	715 (93%)	53 (7%)	14	7

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ILE
1	A	67	GLU
1	A	70	ARG
1	A	87	VAL
1	A	103	ASP
1	A	108	LYS
1	A	126	ILE
1	A	182	ARG
1	A	193	ASN
1	A	194	LEU
1	A	203	LYS
1	A	266	SER
1	A	269	GLN
1	A	317	MET
1	A	319	LEU
1	A	364	LEU
1	B	62	ARG
1	B	70	ARG
1	B	71	THR
1	B	74	LYS

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Mol	Chain	Res	Type
1	B	103	ASP
1	B	133	GLU
1	B	138	ILE
1	B	155	VAL
1	B	159	ARG
1	B	163	LYS
1	B	167	ARG
1	B	174	THR
1	B	192	GLU
1	B	222	TRP
1	B	272	ARG
1	B	274	ARG
1	B	282	ILE
1	B	309	GLU
1	B	317	MET
1	B	367	LEU
1	B	368	ARG
1	C	70	ARG
1	C	94	ILE
1	C	104	GLU
1	C	126	ILE
1	C	133	GLU
1	C	137	MET
1	C	155	VAL
1	C	190	LYS
1	C	192	GLU
1	C	217	GLN
1	C	222	TRP
1	C	269	GLN
1	C	272	ARG
1	C	317	MET
1	C	328	ARG
1	C	351	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	153	HIS
1	A	157	HIS
1	A	186	HIS
1	A	193	ASN

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Mol	Chain	Res	Type
1	A	269	GLN
1	A	296	HIS
1	A	314	HIS
1	A	325	ASN
1	A	334	GLN
1	B	106	ASN
1	B	115	GLN
1	B	183	ASN
1	B	201	ASN
1	B	292	HIS
1	B	362	GLN
1	C	106	ASN
1	C	115	GLN
1	C	201	ASN
1	C	269	GLN
1	C	303	ASN
1	C	334	GLN
1	C	362	GLN
1	C	374	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	TPO	C	221	1	8,10,11	0.64	0	10,14,16	1.08	1 (10%)
1	TPO	B	221	1	8,10,11	0.83	0	10,14,16	1.05	0
1	TPO	A	221	1	8,10,11	0.59	0	10,14,16	0.99	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
1	TPO	C	221	1	-	0/9/11/13	-
1	TPO	B	221	1	-	0/9/11/13	-
1	TPO	A	221	1	-	0/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	221	TPO	O-C-CA	-2.10	119.37	124.77

There are no chirality outliers.

There are no torsion outliers.

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](#)

3 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	XWA	A	401	-	46,46,46	0.90	2 (4%)	61,64,64	1.73	13 (21%)
2	XWA	C	401	-	46,46,46	0.86	1 (2%)	61,64,64	2.03	14 (22%)
2	XWA	B	401	-	46,46,46	0.95	2 (4%)	61,64,64	2.03	13 (21%)

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	XWA	A	401	-	-	6/28/38/38	0/5/5/5
2	XWA	C	401	-	-	3/28/38/38	0/5/5/5
2	XWA	B	401	-	-	6/28/38/38	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	XWA	C17-N39	-4.21	1.40	1.44
2	A	401	XWA	C17-N39	-3.20	1.41	1.44
2	C	401	XWA	O42-C20	2.89	1.41	1.37
2	A	401	XWA	O42-C20	2.30	1.40	1.37
2	B	401	XWA	O42-C20	2.28	1.40	1.37

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	XWA	C32-O42-C20	-9.33	103.82	117.51
2	B	401	XWA	C32-O42-C20	-9.01	104.29	117.51
2	A	401	XWA	C31-O41-C19	-5.92	104.80	117.50
2	B	401	XWA	N34-C22-N39	5.35	121.51	115.55
2	A	401	XWA	C32-O42-C20	-5.29	109.75	117.51
2	C	401	XWA	C31-O41-C19	-4.88	107.04	117.50
2	B	401	XWA	C21-C11-C22	4.70	120.40	116.64
2	C	401	XWA	N34-C22-N39	4.43	120.48	115.55
2	C	401	XWA	C24-N35-C15	-3.96	107.32	118.11
2	B	401	XWA	C25-N35-C15	-3.48	108.63	118.11
2	A	401	XWA	N34-C22-N39	3.18	119.09	115.55
2	A	401	XWA	C30-N36-C26	-3.07	104.79	110.63
2	B	401	XWA	C16-N37-C21	-3.03	120.96	128.75
2	C	401	XWA	O42-C20-C17	2.87	119.61	116.04
2	B	401	XWA	C28-C13-C18	2.87	124.92	121.42
2	A	401	XWA	C24-N35-C15	-2.86	110.32	118.11
2	A	401	XWA	C8-C17-C20	2.80	122.77	118.62
2	C	401	XWA	C24-C26-N36	-2.71	106.50	110.86
2	C	401	XWA	C8-C17-C20	2.64	122.53	118.62
2	A	401	XWA	C5-C7-C16	-2.62	117.29	120.30
2	B	401	XWA	C28-C13-C2	-2.58	115.30	120.28
2	A	401	XWA	C18-N38-C23	-2.50	117.55	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	XWA	N38-C23-N39	2.50	117.58	114.80
2	C	401	XWA	C25-N35-C15	-2.46	111.41	118.11
2	B	401	XWA	C26-C24-N35	-2.40	105.74	110.78
2	B	401	XWA	C31-O41-C19	-2.39	112.37	117.50
2	B	401	XWA	C30-N36-C26	-2.38	106.09	110.63
2	B	401	XWA	C24-N35-C15	-2.29	111.86	118.11
2	C	401	XWA	C11-C22-N39	-2.27	117.98	121.23
2	C	401	XWA	C2-C13-C18	2.27	120.91	117.76
2	C	401	XWA	C13-C18-N38	2.25	122.34	118.99
2	B	401	XWA	C29-C14-C3	-2.22	116.00	120.28
2	B	401	XWA	C30-N36-C27	-2.21	106.42	110.63
2	A	401	XWA	N34-C12-N33	-2.18	125.29	128.58
2	C	401	XWA	C5-C15-N35	-2.12	118.45	121.39
2	A	401	XWA	C4-C15-N35	-2.07	118.52	121.39
2	A	401	XWA	C9-C19-C10	2.05	123.27	120.50
2	C	401	XWA	C18-N38-C23	-2.03	118.48	122.43
2	C	401	XWA	C21-C11-C22	2.01	118.25	116.64
2	A	401	XWA	C7-C5-C15	2.01	122.84	120.30

There are no chirality outliers.

All (15) torsion outliers are listed below:

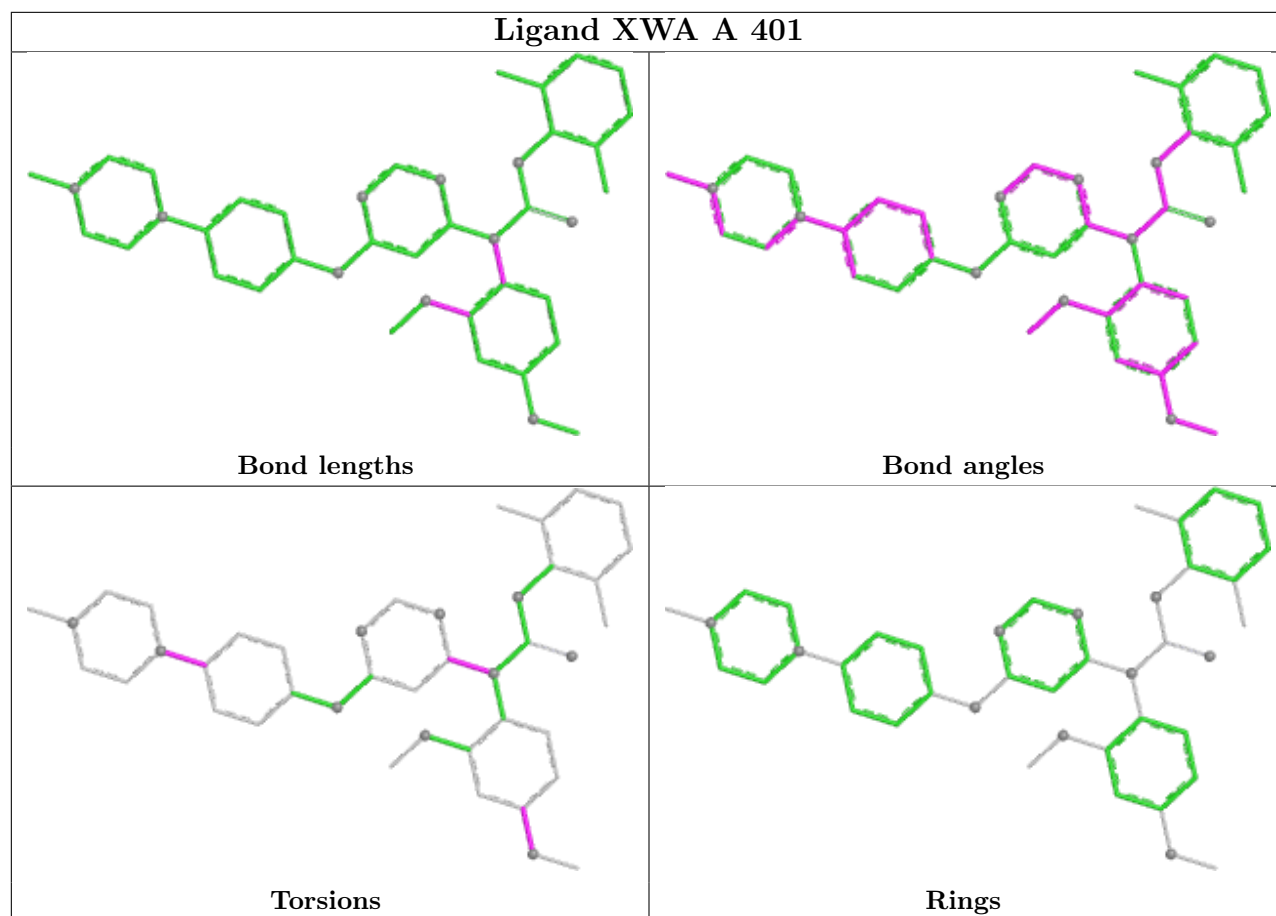
Mol	Chain	Res	Type	Atoms
2	A	401	XWA	C10-C19-O41-C31
2	A	401	XWA	C9-C19-O41-C31
2	B	401	XWA	C9-C19-O41-C31
2	B	401	XWA	C10-C19-O41-C31
2	B	401	XWA	N34-C22-N39-C23
2	B	401	XWA	C11-C22-N39-C23
2	A	401	XWA	N34-C22-N39-C23
2	A	401	XWA	C11-C22-N39-C23
2	B	401	XWA	C5-C15-N35-C24
2	C	401	XWA	N34-C22-N39-C23
2	C	401	XWA	C11-C22-N39-C23
2	B	401	XWA	C4-C15-N35-C24
2	A	401	XWA	C5-C15-N35-C25
2	A	401	XWA	C4-C15-N35-C25
2	C	401	XWA	C5-C15-N35-C25

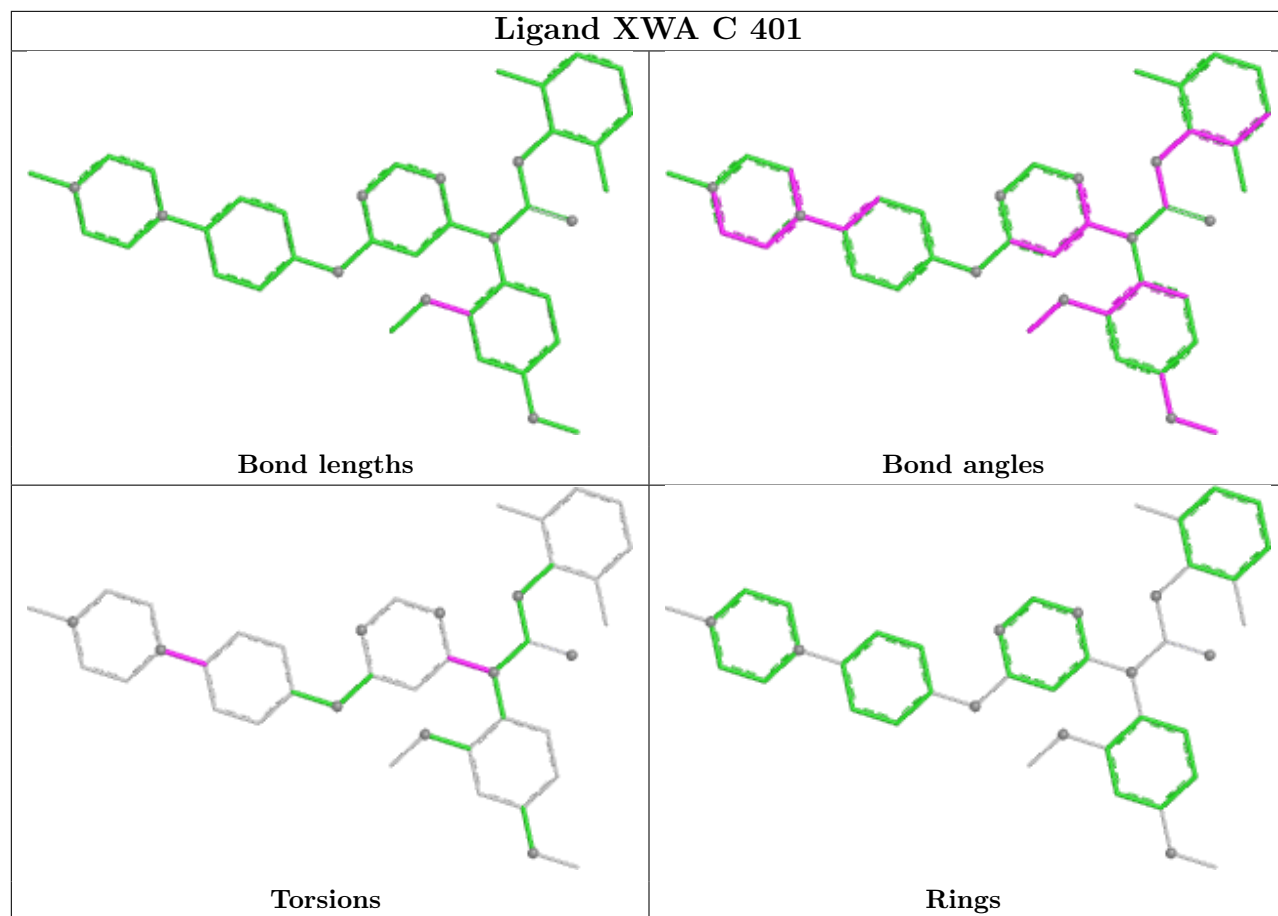
There are no ring outliers.

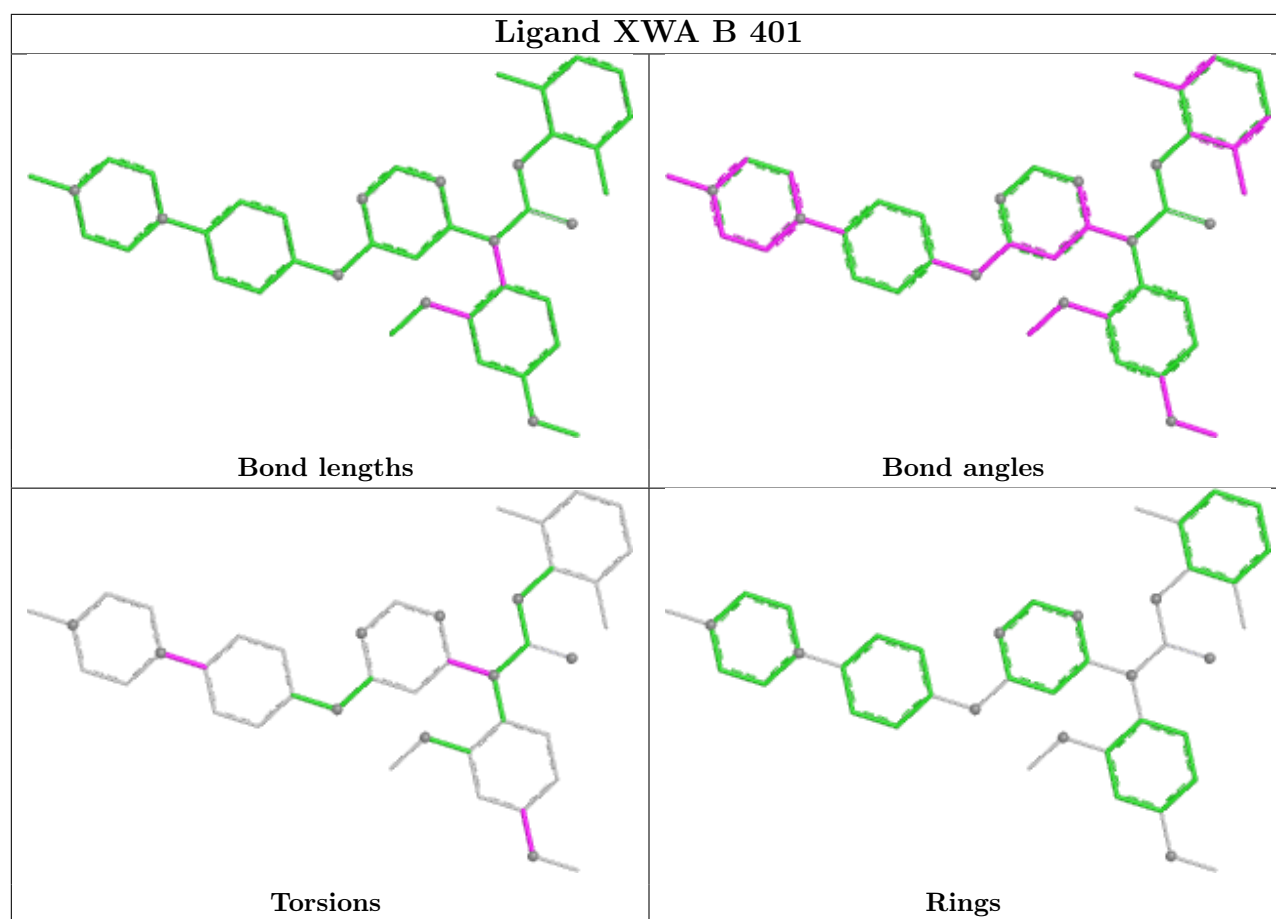
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	XWA	1	0
2	C	401	XWA	1	0
2	B	401	XWA	3	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	317/328 (96%)	0.61	22 (6%) 23 24	23, 45, 78, 108	0
1	B	315/328 (96%)	0.29	8 (2%) 58 62	20, 36, 63, 88	0
1	C	318/328 (96%)	0.26	11 (3%) 47 50	18, 35, 64, 83	0
All	All	950/984 (96%)	0.39	41 (4%) 40 42	18, 39, 69, 108	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	LEU	4.1
1	B	322	ALA	4.0
1	A	358	LEU	3.7
1	C	77	PHE	3.6
1	A	336	LEU	3.3
1	B	324	PRO	3.1
1	A	321	ASP	3.1
1	C	61	ALA	3.1
1	C	364	LEU	3.0
1	A	288	THR	3.0
1	B	344	PRO	2.9
1	C	102	LEU	2.9
1	A	102	LEU	2.8
1	A	100	THR	2.8
1	A	357	GLY	2.7
1	A	103	ASP	2.7
1	A	284	PHE	2.7
1	C	222	TRP	2.6
1	A	337	LYS	2.6
1	B	316	TRP	2.6
1	A	77	PHE	2.6
1	C	137	MET	2.6
1	C	344	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	107	LEU	2.5
1	C	216	GLY	2.4
1	A	101	GLN	2.4
1	C	100	THR	2.4
1	A	322	ALA	2.4
1	A	75	GLY	2.4
1	A	345	LEU	2.3
1	A	209	PHE	2.2
1	B	111	PHE	2.2
1	A	323	ASP	2.2
1	B	64	GLY	2.2
1	B	319	LEU	2.2
1	C	218	LEU	2.2
1	A	134	THR	2.1
1	C	105	GLU	2.1
1	A	360	LYS	2.1
1	A	161	ALA	2.1
1	B	345	LEU	2.0

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($\text{\AA}^2$)	Q<0.9
1	TPO	C	221	11/12	0.93	0.11	47,55,63,64	0
1	TPO	A	221	11/12	0.94	0.09	52,57,60,61	0
1	TPO	B	221	11/12	0.95	0.07	39,42,44,46	0

6.3 Carbohydrates [i](#)

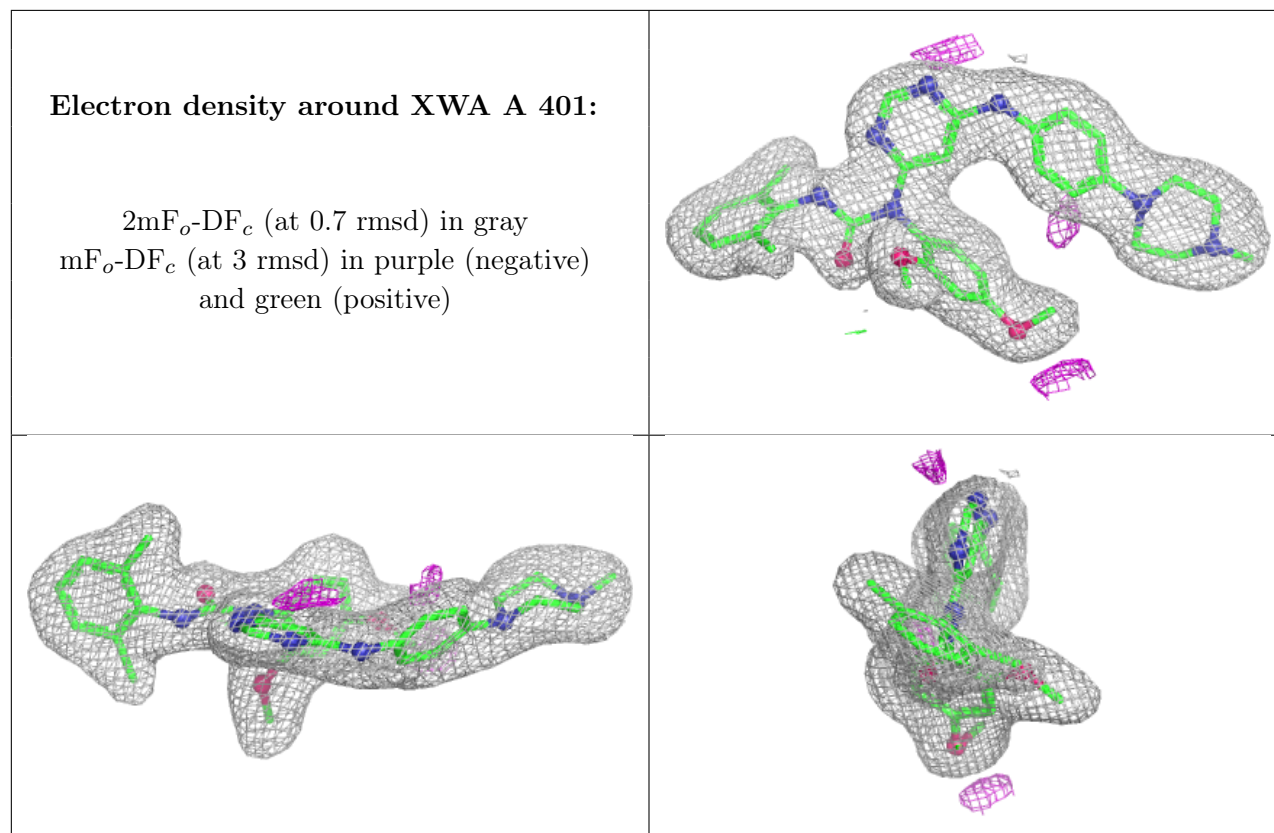
There are no oligosaccharides in this entry.

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.

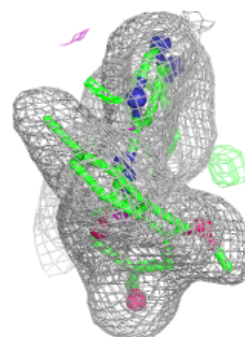
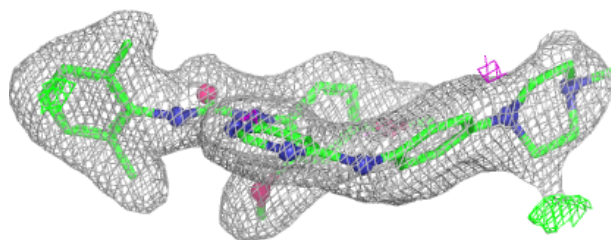
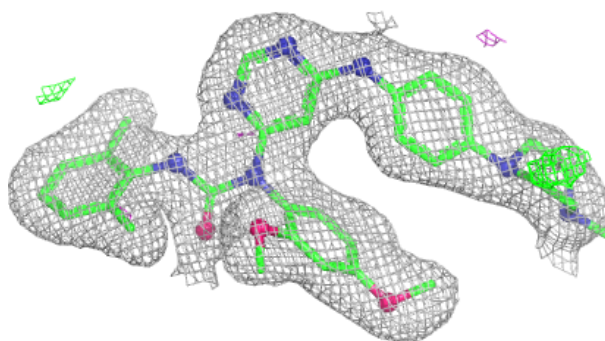
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	XWA	A	401	42/42	0.95	0.06	18,28,35,40	0
2	XWA	B	401	42/42	0.96	0.06	18,22,44,52	0
2	XWA	C	401	42/42	0.96	0.06	15,25,31,35	0

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.

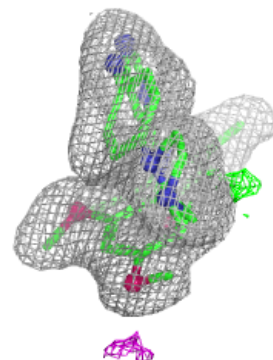
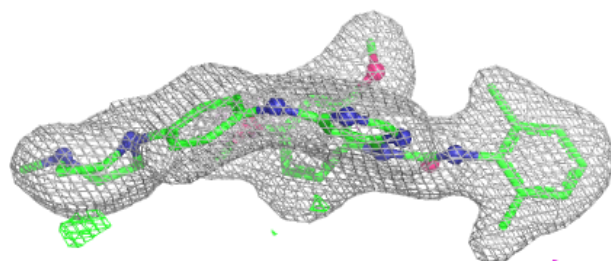
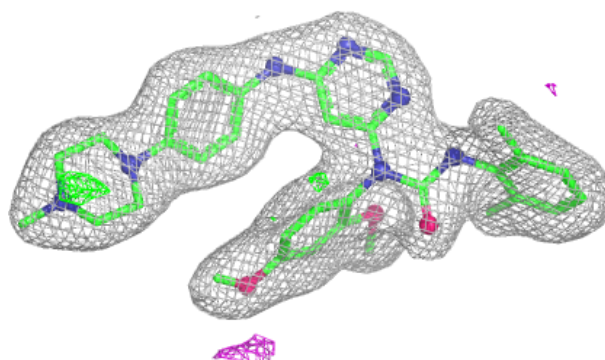


Electron density around XWA B 401:

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

**Electron density around XWA C 401:**

$2mF_o-DF_c$ (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.