



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:04 AM UTC

PDB ID : 5WAD / pdb_00005wad
Title : ADC-7 in complex with boronic acid transition state inhibitor CR161
Authors : Powers, R.A.; Wallar, B.J.
Deposited on : 2017-06-26
Resolution : 2.09 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

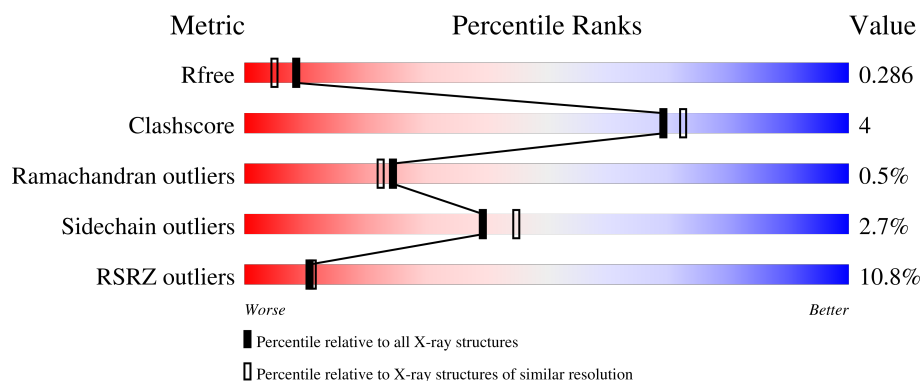
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	361	5% 80% 17% ..
1	B	361	90% 8% ..
1	C	361	12% 88% 9% ..
1	D	361	25% 82% 12% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11263 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.

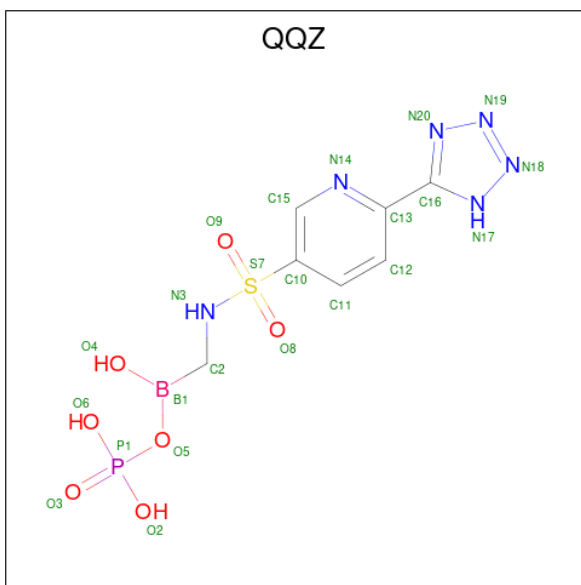
- Molecule 1 is a protein called Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2713	1746	449	509	9			
1	B	357	Total	C	N	O	S	0	1	0
			2805	1802	464	530	9			
1	C	354	Total	C	N	O	S	0	0	0
			2692	1728	450	505	9			
1	D	343	Total	C	N	O	S	0	0	0
			2581	1661	428	483	9			

There are 4 discrepancies between the modelled and reference sequences:

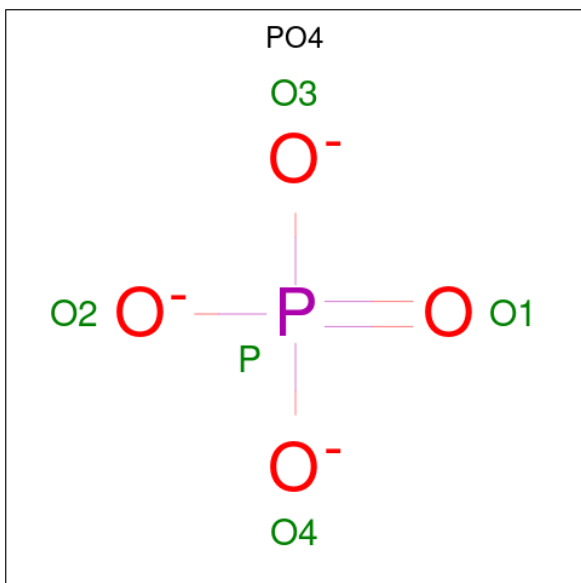
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP Q6DRA1
B	-1	MET	-	expression tag	UNP Q6DRA1
C	-1	MET	-	expression tag	UNP Q6DRA1
D	-1	MET	-	expression tag	UNP Q6DRA1

- Molecule 2 is phosphonoxy-[[[6-(1 {H}-1,2,3,4-tetrazol-5-yl)pyridin-3-yl]sulfonylamino]methyl]borinic acid (CCD ID: QQZ) (formula: C₇H₁₀BN₆O₇PS).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	B	C	N	O	P	S	0	0
			23	1	7	6	7	1	1		
2	B	1	Total	B	C	N	O	P	S	0	0
			23	1	7	6	7	1	1		
2	C	1	Total	B	C	N	O	P	S	0	0
			23	1	7	6	7	1	1		
2	D	1	Total	B	C	N	O	P	S	0	0
			23	1	7	6	7	1	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		

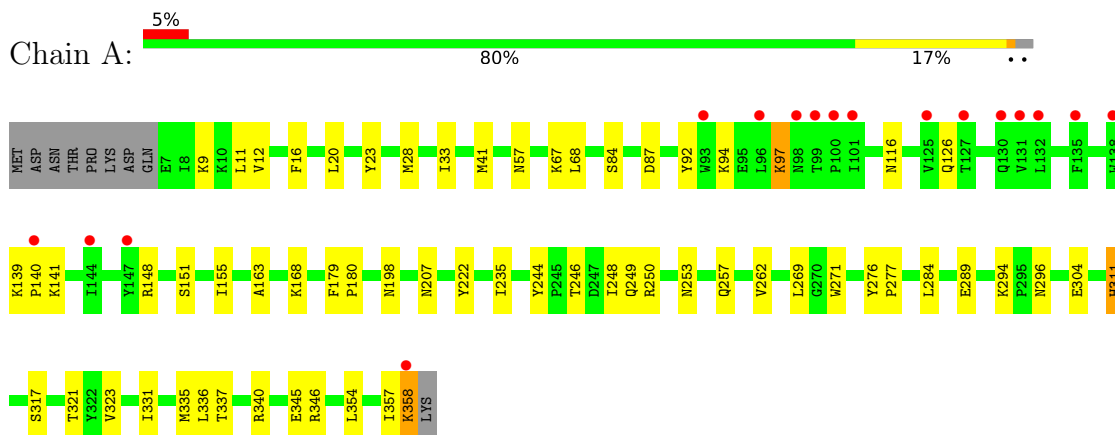
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	83	Total	O	0	0
			83	83		
4	B	170	Total	O	0	3
			173	173		
4	C	67	Total	O	0	1
			68	68		
4	D	50	Total	O	0	1
			51	51		

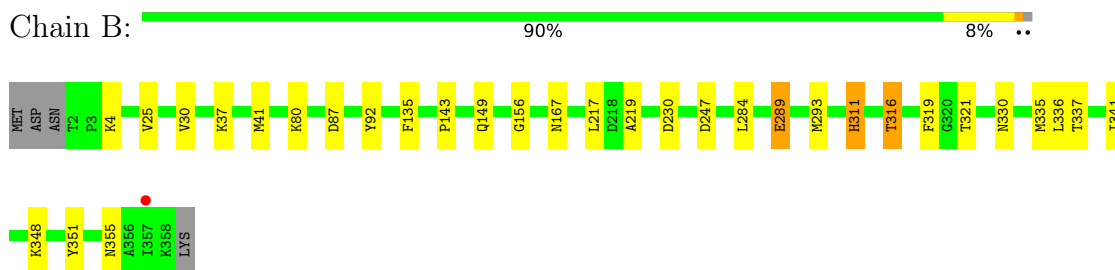
3 Residue-property plots [i](#)

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.

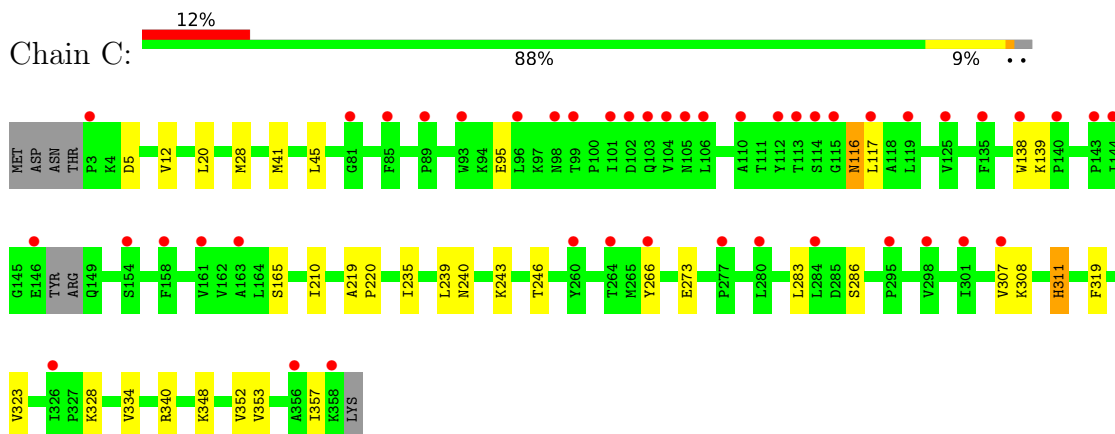
• Molecule 1: Beta-lactamase



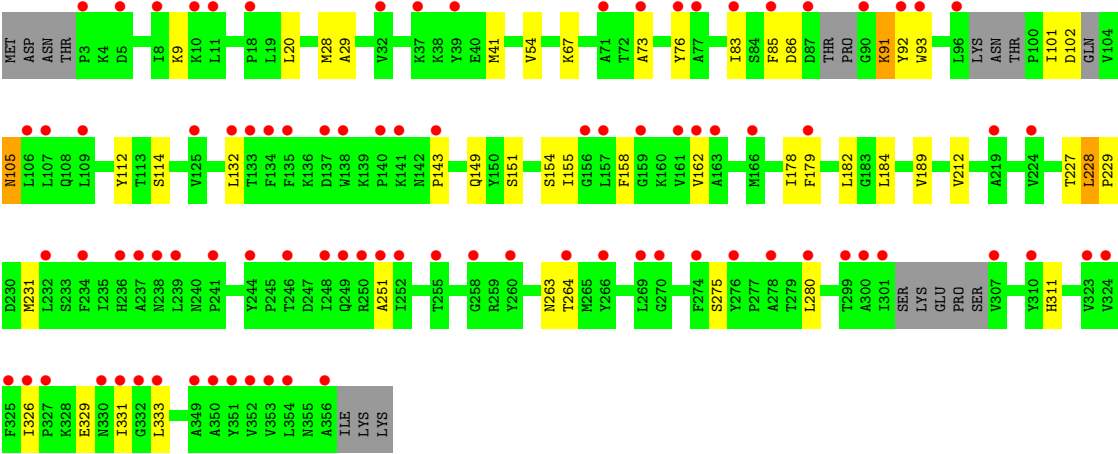
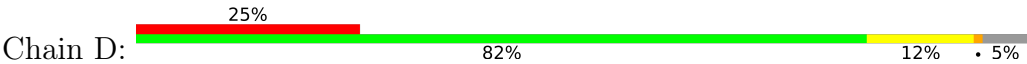
• Molecule 1: Beta-lactamase



• Molecule 1: Beta-lactamase



● Molecule 1: Beta-lactamase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.27Å 81.47Å 105.91Å 90.00° 112.50° 90.00°	Depositor
Resolution (Å)	97.84 – 2.09 97.84 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.3 (97.84-2.09) 99.3 (97.84-2.09)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.214 , 0.286 0.219 , 0.286	Depositor DCC
R_{free} test set	4124 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11263	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.46 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3165e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, QQZ

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	1.11	2/2780 (0.1%)	1.15	10/3790 (0.3%)
1	B	1.14	2/2873 (0.1%)	1.11	9/3908 (0.2%)
1	C	0.99	0/2758	1.09	7/3758 (0.2%)
1	D	1.00	1/2643 (0.0%)	1.09	3/3603 (0.1%)
All	All	1.06	5/11054 (0.0%)	1.11	29/15059 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	219	ALA	C-O	-6.04	1.19	1.24
1	A	289	GLU	C-O	5.96	1.31	1.24
1	D	228	LEU	CA-C	5.96	1.59	1.52
1	B	143	PRO	CA-C	5.12	1.58	1.52
1	A	284	LEU	N-CA	5.11	1.52	1.46

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	SER	N-CA-C	8.02	121.16	107.93
1	C	117	LEU	N-CA-C	7.13	119.88	108.41
1	C	45	LEU	CA-C-N	6.83	129.32	120.44
1	C	45	LEU	C-N-CA	6.83	129.32	120.44
1	A	97	LYS	N-CA-C	6.65	120.99	113.01
1	A	304	GLU	CA-C-N	-6.59	113.17	119.76
1	A	304	GLU	C-N-CA	-6.59	113.17	119.76
1	A	11	LEU	N-CA-C	6.55	118.08	111.07
1	B	230	ASP	N-CA-C	6.08	117.91	111.28
1	B	135	PHE	N-CA-C	6.03	118.82	111.82
1	B	284	LEU	N-CA-C	5.98	117.47	111.07
1	B	341	ILE	CA-C-N	-5.97	113.61	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	341	ILE	C-N-CA	-5.97	113.61	119.76
1	C	319	PHE	CA-C-N	5.90	125.66	121.65
1	C	319	PHE	C-N-CA	5.90	125.66	121.65
1	B	167	ASN	N-CA-C	5.89	119.67	111.90
1	D	189	VAL	N-CA-C	-5.86	106.10	111.67
1	A	139	LYS	CA-C-N	5.68	126.95	119.84
1	A	139	LYS	C-N-CA	5.68	126.95	119.84
1	D	73	ALA	N-CA-C	5.48	117.26	111.28
1	A	116	ASN	N-CA-C	5.45	119.59	109.56
1	B	316	THR	N-CA-C	-5.30	102.32	109.95
1	A	262	VAL	N-CA-C	-5.24	98.44	109.34
1	B	25	VAL	CA-C-N	-5.18	113.21	118.85
1	B	25	VAL	C-N-CA	-5.18	113.21	118.85
1	C	116	ASN	N-CA-C	5.08	120.10	112.94
1	A	253	ASN	N-CA-C	5.04	116.77	111.28
1	C	246	THR	N-CA-C	5.03	117.16	111.02
1	D	151	SER	N-CA-C	5.03	116.78	108.13

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	2713	0	2623	28	0
1	B	2805	0	2762	10	0
1	C	2692	0	2566	14	0
1	D	2581	0	2409	23	0
2	A	23	0	0	0	0
2	B	23	0	0	0	0
2	C	23	0	0	0	0
2	D	23	0	0	0	0
3	B	5	0	0	0	0
4	A	83	0	0	0	0
4	B	173	0	0	0	0
4	C	68	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	51	0	0	1	0
All	All	11263	0	10360	75	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 (75) 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:235:ILE:HD11	1:A:323:VAL:CG1	2.14	0.78
1:A:235:ILE:HD11	1:A:323:VAL:HG13	1.69	0.74
1:A:20:LEU:HD11	1:A:28:MET:HE2	1.73	0.70
1:D:112:TYR:HB3	1:D:149:GLN:O	1.93	0.69
1:B:87:ASP:OD2	1:B:92:TYR:OH	2.07	0.69
1:A:12:VAL:HG21	1:A:41:MET:HE3	1.77	0.66
1:D:178:ILE:HG22	1:D:182:LEU:HD12	1.80	0.64
1:C:20:LEU:HD11	1:C:28:MET:HE2	1.79	0.64
1:D:20:LEU:HD11	1:D:28:MET:HE2	1.79	0.63
1:D:83:ILE:HA	1:D:92:TYR:OH	1.99	0.62
1:D:54:VAL:O	4:D:501:HOH:O	2.16	0.62
1:A:23:TYR:OH	1:A:345:GLU:OE2	2.16	0.62
1:B:321:THR:HG23	1:B:336:LEU:HD23	1.83	0.61
1:A:357:ILE:HG22	1:A:357:ILE:O	2.04	0.57
1:C:12:VAL:HG21	1:C:41:MET:HE3	1.88	0.56
1:D:85:PHE:O	1:D:105:ASN:ND2	2.39	0.56
1:B:80:LYS:NZ	1:B:247:ASP:OD2	2.39	0.55
1:D:333:LEU:C	1:D:333:LEU:HD23	2.32	0.55
1:A:294:LYS:O	1:A:296:ASN:ND2	2.40	0.55
1:C:307:VAL:HG11	1:C:328:LYS:HD3	1.88	0.54
1:B:289:GLU:OE2	1:B:293:MET:HG3	2.07	0.54
1:C:116:ASN:ND2	1:C:139:LYS:O	2.40	0.54
1:D:86:ASP:HA	1:D:105:ASN:HD22	1.72	0.54
1:C:235:ILE:HG22	1:C:239:LEU:HD12	1.90	0.52
1:D:263:ASN:OD1	1:D:264:THR:N	2.40	0.52
1:A:357:ILE:O	1:A:358:LYS:HG2	2.08	0.52
1:D:158:PHE:O	1:D:162:VAL:HG23	2.09	0.52
1:C:283:LEU:O	1:C:286:SER:OG	2.23	0.51
1:A:235:ILE:HD11	1:A:323:VAL:HG11	1.91	0.51
1:A:331:ILE:HD12	1:A:354:LEU:HD22	1.92	0.51
1:C:348:LYS:O	1:C:352:VAL:HG23	2.10	0.51
1:A:321:THR:HG23	1:A:336:LEU:HD23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:VAL:HG12	1:C:334:VAL:HG22	1.93	0.49
1:D:263:ASN:CG	1:D:264:THR:H	2.21	0.49
1:B:30:VAL:O	1:B:41:MET:HE3	2.14	0.47
1:B:335:MET:HE3	1:B:337:THR:HG23	1.97	0.47
1:C:353:VAL:O	1:C:357:ILE:HG13	2.15	0.47
1:A:67:LYS:HE3	1:A:155:ILE:HG21	1.95	0.47
1:A:87:ASP:OD2	1:A:92:TYR:OH	2.22	0.47
1:A:357:ILE:C	1:A:358:LYS:HD3	2.40	0.46
1:D:93:TRP:CZ2	1:D:132:LEU:HD13	2.50	0.46
1:D:329:GLU:HB2	1:D:331:ILE:HG22	1.97	0.46
1:D:179:PHE:CD1	1:D:184:LEU:HD12	2.50	0.46
1:C:116:ASN:HB3	1:C:138:TRP:NE1	2.31	0.46
1:A:148:ARG:N	1:A:296:ASN:O	2.46	0.45
1:A:179:PHE:HB2	1:A:180:PRO:HD3	1.99	0.45
1:C:240:ASN:HD22	1:C:243:LYS:HE3	1.81	0.45
1:A:94:LYS:O	1:A:97:LYS:CB	2.65	0.45
1:A:57:ASN:O	1:A:198:ASN:HB3	2.17	0.44
1:A:68:LEU:HD13	1:A:271:TRP:CZ2	2.52	0.44
1:A:16:PHE:HB3	1:A:28:MET:HE1	2.00	0.44
1:A:311:HIS:CD2	1:A:311:HIS:C	2.95	0.44
1:D:227:THR:HB	1:D:229:PRO:HD2	2.00	0.44
1:D:29:ALA:HB1	1:D:228:LEU:HD22	2.00	0.43
1:D:101:ILE:O	1:D:102:ASP:HB2	2.18	0.43
1:A:276:TYR:CD1	1:A:277:PRO:HA	2.54	0.42
1:B:156:GLY:C	1:B:217:LEU:HD13	2.44	0.42
1:D:91:LYS:HD2	1:D:92:TYR:CE2	2.54	0.42
1:A:317:SER:HA	1:A:340:ARG:HD2	2.01	0.42
1:A:246:THR:O	1:A:250:ARG:HG2	2.20	0.42
1:A:244:TYR:HB3	1:A:248:ILE:CG2	2.50	0.41
1:C:266:TYR:HB2	1:C:273:GLU:HB3	2.02	0.41
1:C:311:HIS:CD2	1:C:311:HIS:C	2.98	0.41
1:B:311:HIS:CD2	1:B:311:HIS:C	2.98	0.41
1:D:212:VAL:O	1:D:212:VAL:HG13	2.20	0.41
1:B:316:THR:OG1	1:B:319:PHE:HB2	2.21	0.41
1:D:179:PHE:HD1	1:D:184:LEU:HD12	1.84	0.41
1:A:163:ALA:HB1	1:A:168:LYS:O	2.21	0.41
1:A:335:MET:HE3	1:A:337:THR:HG23	2.03	0.41
1:B:351:TYR:O	1:B:355:ASN:ND2	2.50	0.41
1:D:67:LYS:HG2	1:D:155:ILE:HG21	2.03	0.41
1:A:335:MET:HE1	1:A:346:ARG:HG2	2.02	0.40
1:D:9:LYS:HD2	1:D:41:MET:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:ALA:HB3	1:C:220:PRO:HD3	2.03	0.40
1:D:76:TYR:HA	1:D:251:ALA:HB2	2.03	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	350/361 (97%)	331 (95%)	16 (5%)	3 (1%)	14	10
1	B	356/361 (99%)	347 (98%)	9 (2%)	0	100	100
1	C	350/361 (97%)	333 (95%)	16 (5%)	1 (0%)	36	36
1	D	333/361 (92%)	315 (95%)	15 (4%)	3 (1%)	14	10
All	All	1389/1444 (96%)	1326 (96%)	56 (4%)	7 (0%)	24	22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	PRO
1	C	95	GLU
1	D	143	PRO
1	D	114	SER
1	A	207	ASN
1	A	222	TYR
1	D	154	SER

5.3.2 Protein sidechains [i](#)

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	286/319 (90%)	276 (96%)	10 (4%)	32	35
1	B	305/319 (96%)	298 (98%)	7 (2%)	44	51
1	C	277/319 (87%)	271 (98%)	6 (2%)	45	53
1	D	257/319 (81%)	250 (97%)	7 (3%)	39	45
All	All	1125/1276 (88%)	1095 (97%)	30 (3%)	39	45

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	33	ILE
1	A	84	SER
1	A	126	GLN
1	A	141	LYS
1	A	249	GLN
1	A	257	GLN
1	A	269	LEU
1	A	311	HIS
1	A	358	LYS
1	B	4	LYS
1	B	37	LYS
1	B	149	GLN
1	B	289	GLU
1	B	311	HIS
1	B	330	ASN
1	B	348	LYS
1	C	5	ASP
1	C	165	SER
1	C	210	ILE
1	C	308	LYS
1	C	311	HIS
1	C	340	ARG
1	D	91	LYS
1	D	105	ASN
1	D	231	MET
1	D	275	SER
1	D	280	LEU
1	D	311	HIS
1	D	326	ILE

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	15	ASN
1	A	35	ASN
1	A	36	ASN
1	A	126	GLN
1	A	205	GLN
1	A	236	HIS
1	A	296	ASN
1	A	343	ASN
1	B	149	GLN
1	B	186	HIS
1	C	35	ASN
1	C	172	GLN
1	C	240	ASN
1	D	287	ASN
1	D	343	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	QQZ	D	401	1	22,24,24	2.95	5 (22%)	28,35,35	3.25	11 (39%)
2	QQZ	B	401	1	22,24,24	2.96	6 (27%)	28,35,35	4.11	11 (39%)
3	PO4	B	402	-	4,4,4	0.74	0	6,6,6	0.96	0
2	QQZ	A	401	1	22,24,24	3.40	7 (31%)	28,35,35	2.91	15 (53%)
2	QQZ	C	401	1	22,24,24	3.25	6 (27%)	28,35,35	3.19	12 (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
2	QQZ	A	401	1	-	3/13/21/21	0/2/2/2
2	QQZ	B	401	1	-	7/13/21/21	0/2/2/2
2	QQZ	C	401	1	-	3/13/21/21	0/2/2/2
2	QQZ	D	401	1	-	5/13/21/21	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	QQZ	C10-S7	-10.66	1.60	1.76
2	D	401	QQZ	C10-S7	-9.64	1.61	1.76
2	C	401	QQZ	C10-S7	-9.28	1.62	1.76
2	C	401	QQZ	P1-O5	8.37	1.64	1.56
2	B	401	QQZ	C10-S7	-7.83	1.64	1.76
2	A	401	QQZ	P1-O5	7.68	1.63	1.56
2	B	401	QQZ	N18-N19	6.15	1.42	1.30
2	B	401	QQZ	P1-O5	5.87	1.61	1.56
2	B	401	QQZ	N17-N18	5.84	1.42	1.35
2	D	401	QQZ	N18-N19	5.69	1.41	1.30
2	C	401	QQZ	N18-N19	5.39	1.40	1.30
2	A	401	QQZ	N18-N19	4.96	1.39	1.30
2	A	401	QQZ	N17-N18	4.89	1.41	1.35
2	C	401	QQZ	N17-N18	4.87	1.41	1.35
2	D	401	QQZ	N17-N18	4.86	1.41	1.35
2	D	401	QQZ	P1-O5	4.27	1.60	1.56
2	A	401	QQZ	N20-N19	3.05	1.40	1.36
2	D	401	QQZ	C2-N3	-2.98	1.43	1.47
2	A	401	QQZ	B1-C2	2.90	1.62	1.57
2	C	401	QQZ	C15-C10	2.55	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	QQZ	C2-N3	-2.42	1.44	1.47
2	B	401	QQZ	C2-N3	-2.40	1.44	1.47
2	B	401	QQZ	C16-N20	-2.24	1.28	1.32
2	C	401	QQZ	C2-N3	-2.24	1.44	1.47

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	QQZ	O9-S7-O8	-10.58	106.67	119.52
2	B	401	QQZ	C13-C16-N17	8.02	137.22	124.02
2	B	401	QQZ	N20-N19-N18	-7.99	100.97	110.50
2	C	401	QQZ	O9-S7-O8	-7.63	110.25	119.52
2	C	401	QQZ	C13-C16-N17	7.60	136.53	124.02
2	B	401	QQZ	C16-N20-N19	7.53	114.11	106.10
2	D	401	QQZ	C13-C16-N17	7.43	136.25	124.02
2	D	401	QQZ	O9-S7-O8	-7.32	110.64	119.52
2	B	401	QQZ	O8-S7-N3	7.26	118.33	107.03
2	D	401	QQZ	C10-S7-N3	6.19	116.08	107.54
2	B	401	QQZ	O4-B1-C2	-6.14	106.49	120.88
2	A	401	QQZ	O9-S7-O8	-5.88	112.38	119.52
2	A	401	QQZ	N20-N19-N18	-5.79	103.59	110.50
2	B	401	QQZ	C16-C13-N14	5.68	122.60	115.96
2	D	401	QQZ	N20-N19-N18	-5.33	104.14	110.50
2	C	401	QQZ	N20-N19-N18	-5.32	104.16	110.50
2	C	401	QQZ	O4-B1-C2	-5.06	109.04	120.88
2	D	401	QQZ	C16-C13-N14	5.05	121.85	115.96
2	D	401	QQZ	C16-N20-N19	5.01	111.42	106.10
2	A	401	QQZ	C13-C16-N17	4.84	131.98	124.02
2	D	401	QQZ	O4-B1-C2	-4.74	109.78	120.88
2	A	401	QQZ	O4-B1-C2	-4.49	110.38	120.88
2	C	401	QQZ	C16-N20-N19	4.45	110.83	106.10
2	A	401	QQZ	O8-S7-N3	4.32	113.75	107.03
2	C	401	QQZ	O9-S7-C10	-4.01	102.92	107.98
2	A	401	QQZ	C16-N20-N19	3.95	110.30	106.10
2	A	401	QQZ	O9-S7-C10	3.74	112.70	107.98
2	C	401	QQZ	C16-C13-N14	3.72	120.31	115.96
2	B	401	QQZ	C12-C13-C16	-3.55	116.72	121.18
2	A	401	QQZ	C15-N14-C13	3.44	122.85	117.46
2	A	401	QQZ	C10-C15-N14	-3.28	119.19	123.19
2	D	401	QQZ	C15-N14-C13	3.26	122.56	117.46
2	C	401	QQZ	O8-S7-N3	3.16	111.95	107.03
2	C	401	QQZ	O6-P1-O5	-3.12	99.79	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	QQZ	O2-P1-O5	-3.09	99.91	109.50
2	D	401	QQZ	C10-C15-N14	-2.75	119.84	123.19
2	A	401	QQZ	C2-N3-S7	2.63	124.84	119.57
2	D	401	QQZ	C12-C13-N14	-2.44	119.45	122.74
2	C	401	QQZ	O9-S7-N3	2.42	110.80	107.03
2	A	401	QQZ	N17-N18-N19	2.38	110.07	106.68
2	B	401	QQZ	C16-N17-N18	-2.27	105.02	108.56
2	C	401	QQZ	N17-C16-N20	2.24	110.97	108.26
2	C	401	QQZ	C10-S7-N3	2.20	110.59	107.54
2	B	401	QQZ	C15-N14-C13	2.12	120.78	117.46
2	B	401	QQZ	C10-C15-N14	-2.11	120.61	123.19
2	D	401	QQZ	O9-S7-C10	-2.10	105.33	107.98
2	A	401	QQZ	O6-P1-O2	2.09	115.63	107.80
2	A	401	QQZ	C16-N17-N18	-2.07	105.33	108.56
2	A	401	QQZ	N17-C16-N20	2.02	110.71	108.26

There are no chirality outliers.

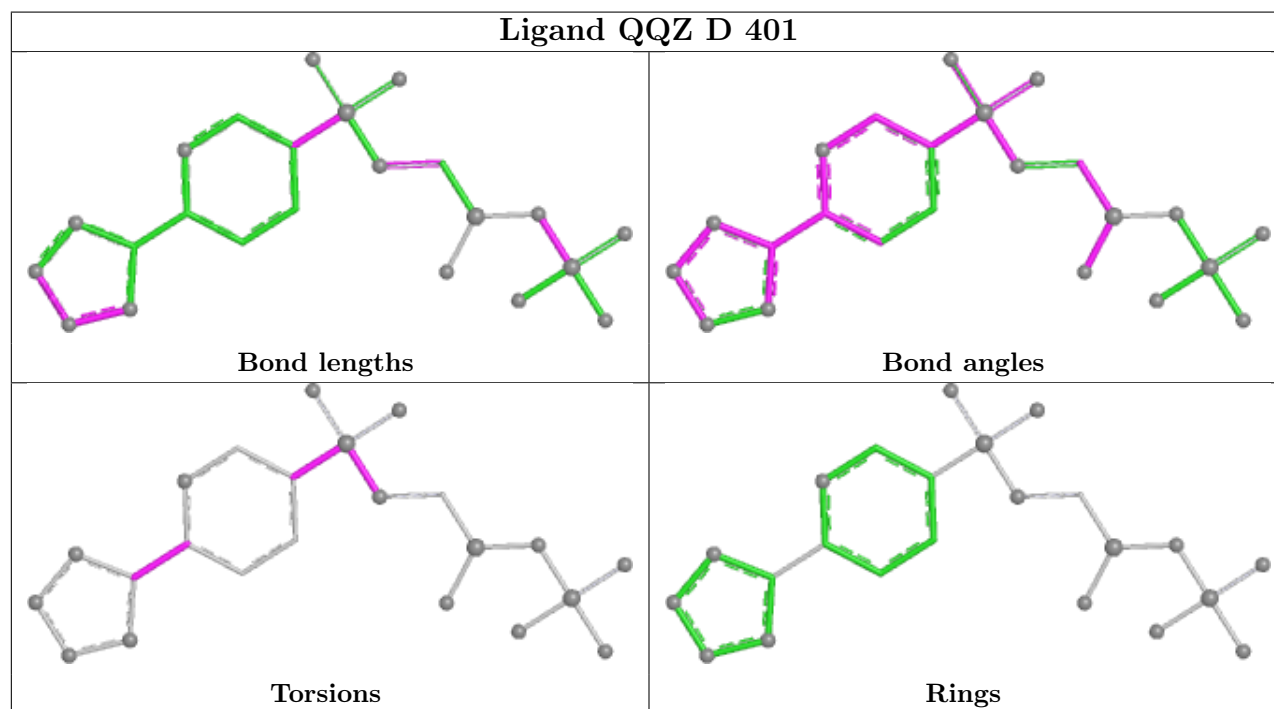
All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	QQZ	C2-N3-S7-O9
2	A	401	QQZ	C2-N3-S7-O8
2	A	401	QQZ	C2-N3-S7-C10
2	D	401	QQZ	C2-N3-S7-O9
2	B	401	QQZ	C2-N3-S7-O9
2	B	401	QQZ	C12-C13-C16-N17
2	B	401	QQZ	N14-C13-C16-N17
2	C	401	QQZ	N14-C13-C16-N17
2	D	401	QQZ	N14-C13-C16-N17
2	B	401	QQZ	C2-N3-S7-C10
2	B	401	QQZ	C2-N3-S7-O8
2	D	401	QQZ	C2-N3-S7-C10
2	C	401	QQZ	C2-N3-S7-O9
2	D	401	QQZ	C2-N3-S7-O8
2	B	401	QQZ	C12-C13-C16-N20
2	B	401	QQZ	N14-C13-C16-N20
2	D	401	QQZ	C11-C10-S7-O9
2	C	401	QQZ	C2-N3-S7-C10

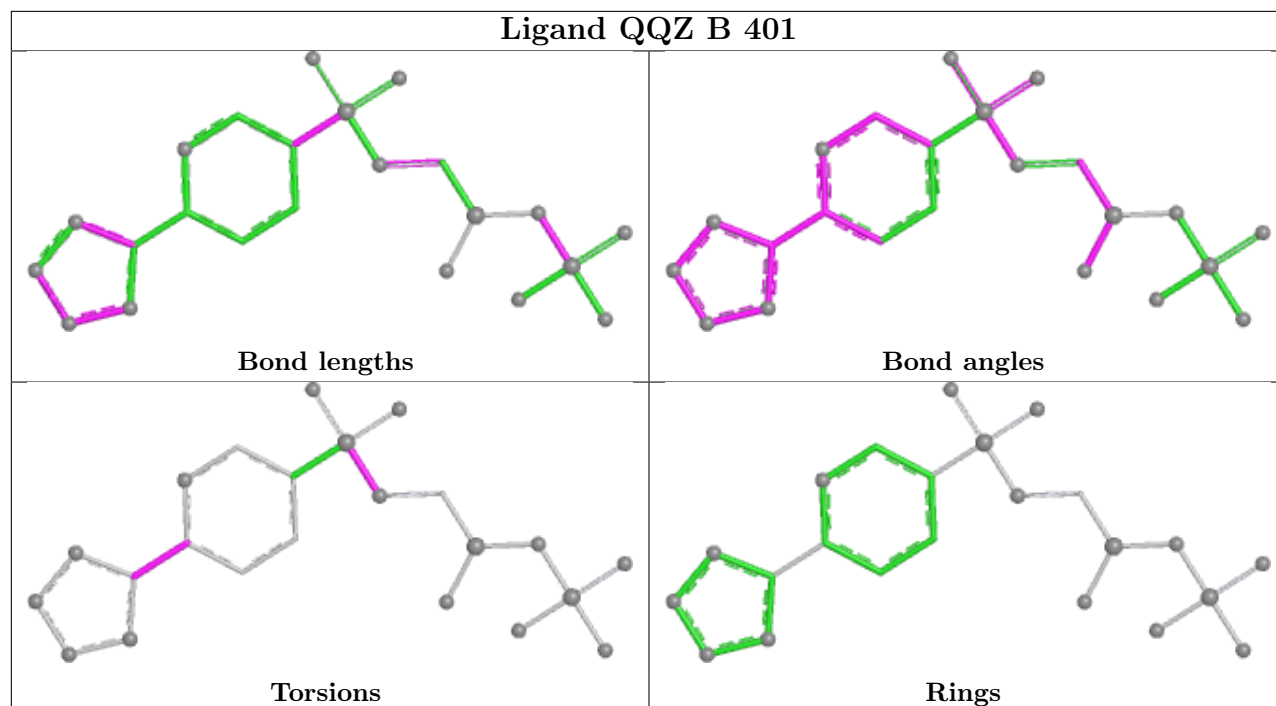
There are no ring outliers.

No monomer is involved in short contacts.

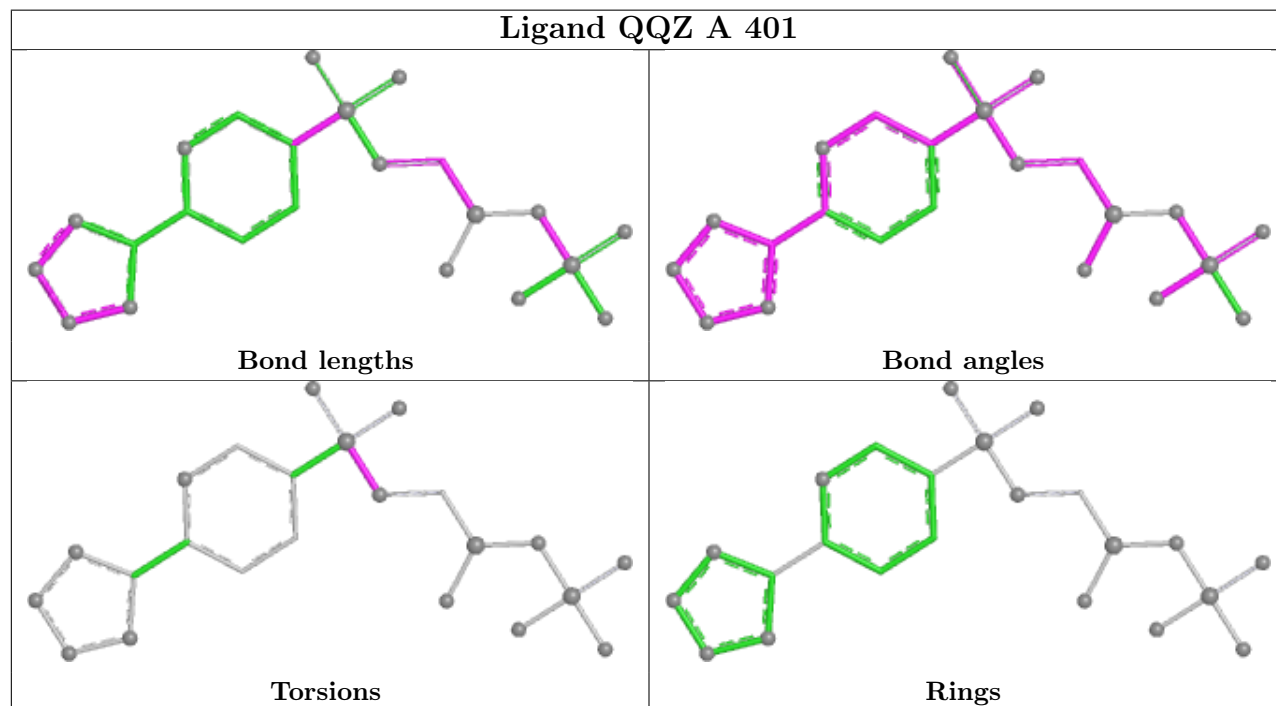
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

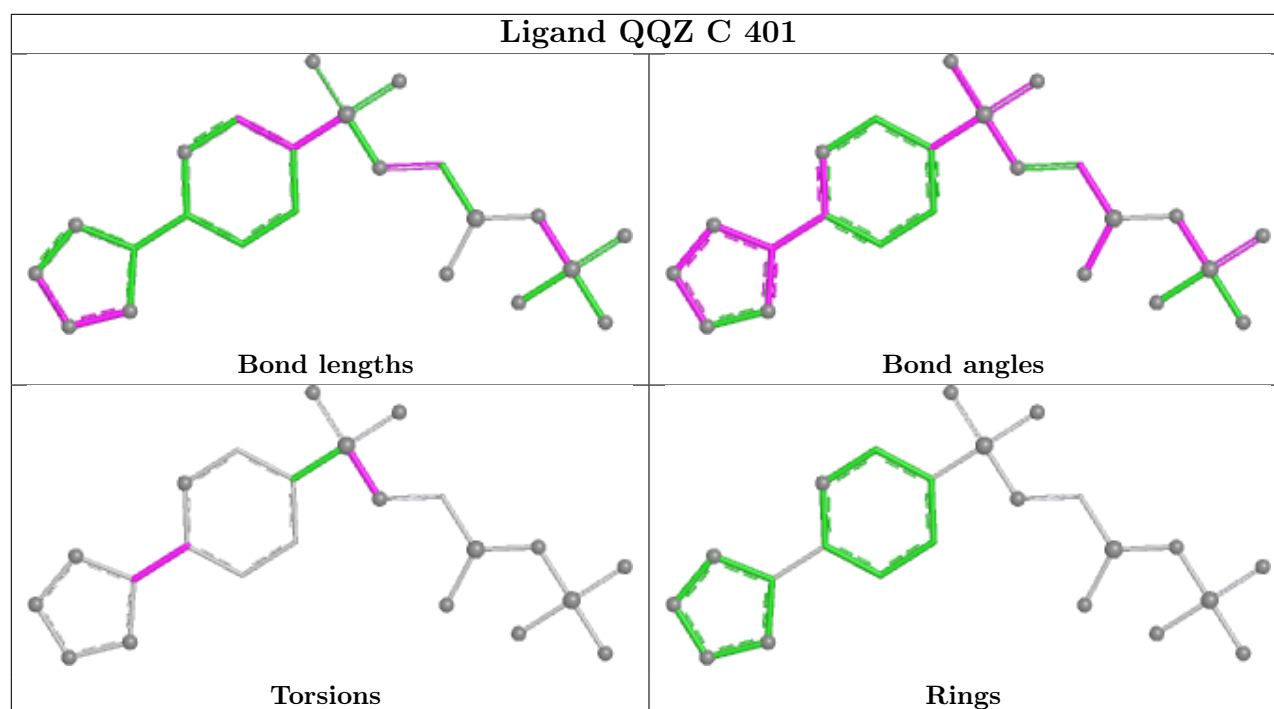


Ligand QQZ B 401



Ligand QQZ A 401





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	352/361 (97%)	0.42	17 (4%) 35 38	18, 34, 54, 70	0
1	B	357/361 (98%)	-0.23	1 (0%) 90 91	10, 25, 41, 53	1 (0%)
1	C	354/361 (98%)	0.90	45 (12%) 8 8	18, 46, 67, 79	0
1	D	343/361 (95%)	1.33	89 (25%) 1 1	21, 50, 69, 80	0
All	All	1406/1444 (97%)	0.60	152 (10%) 11 11	10, 37, 65, 80	1 (0%)

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	73	ALA	6.5
1	C	104	VAL	4.3
1	D	238	ASN	4.3
1	D	109	LEU	4.2
1	A	127	THR	4.1
1	D	331	ILE	4.1
1	D	356	ALA	4.1
1	D	234	PHE	4.0
1	D	5	ASP	4.0
1	D	11	LEU	4.0
1	C	144	ILE	3.9
1	D	3	PRO	3.9
1	D	32	VAL	3.8
1	D	307	VAL	3.7
1	D	251	ALA	3.7
1	D	255	THR	3.7
1	D	250	ARG	3.5
1	D	96	LEU	3.5
1	D	352	VAL	3.5
1	D	241	PRO	3.4
1	C	106	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	298	VAL	3.4
1	D	71	ALA	3.4
1	D	269	LEU	3.4
1	D	301	ILE	3.3
1	A	138	TRP	3.2
1	D	332	GLY	3.2
1	D	132	LEU	3.2
1	D	138	TRP	3.2
1	D	83	ILE	3.2
1	D	324	VAL	3.1
1	D	137	ASP	3.1
1	D	274	PHE	3.1
1	D	140	PRO	3.1
1	D	330	ASN	3.1
1	D	161	VAL	3.1
1	C	101	ILE	3.1
1	D	354	LEU	3.0
1	D	87	ASP	3.0
1	D	77	ALA	3.0
1	D	333	LEU	3.0
1	D	163	ALA	3.0
1	D	300	ALA	3.0
1	D	107	LEU	3.0
1	D	248	ILE	3.0
1	D	133	THR	3.0
1	C	280	LEU	2.9
1	C	3	PRO	2.9
1	C	163	ALA	2.9
1	C	96	LEU	2.9
1	A	130	GLN	2.9
1	C	135	PHE	2.9
1	D	39	TYR	2.9
1	D	244	TYR	2.9
1	D	310	TYR	2.9
1	C	93	TRP	2.9
1	D	106	LEU	2.9
1	D	162	VAL	2.9
1	D	353	VAL	2.9
1	D	159	GLY	2.9
1	C	266	TYR	2.8
1	D	93	TRP	2.8
1	D	326	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	103	GLN	2.8
1	C	98	ASN	2.8
1	D	276	TYR	2.8
1	D	135	PHE	2.7
1	C	112	TYR	2.7
1	D	179	PHE	2.7
1	D	325	PHE	2.7
1	C	264	THR	2.7
1	D	239	LEU	2.7
1	C	143	PRO	2.6
1	D	90	GLY	2.6
1	C	119	LEU	2.6
1	D	280	LEU	2.6
1	A	144	ILE	2.6
1	C	85	PHE	2.5
1	C	154	SER	2.5
1	D	266	TYR	2.5
1	C	260	TYR	2.4
1	C	115	GLY	2.4
1	D	278	ALA	2.4
1	D	252	ILE	2.4
1	C	113	THR	2.4
1	C	140	PRO	2.4
1	C	356	ALA	2.4
1	C	105	ASN	2.4
1	D	258	GLY	2.4
1	C	146	GLU	2.3
1	C	284	LEU	2.3
1	A	358	LYS	2.3
1	D	323	VAL	2.3
1	C	277	PRO	2.3
1	D	246	THR	2.3
1	D	157	LEU	2.3
1	D	270	GLY	2.3
1	A	101	ILE	2.3
1	C	307	VAL	2.3
1	D	125	VAL	2.3
1	C	110	ALA	2.3
1	D	237	ALA	2.3
1	C	81	GLY	2.3
1	D	10	LYS	2.3
1	C	158	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	326	ILE	2.2
1	D	8	ILE	2.2
1	A	99	THR	2.2
1	C	99	THR	2.2
1	C	117	LEU	2.2
1	C	138	TRP	2.2
1	C	301	ILE	2.2
1	D	299	THR	2.2
1	A	131	VAL	2.2
1	C	89	PRO	2.2
1	C	125	VAL	2.2
1	C	102	ASP	2.2
1	A	147	TYR	2.2
1	D	76	TYR	2.2
1	D	92	TYR	2.2
1	D	351	TYR	2.2
1	A	98	ASN	2.2
1	A	140	PRO	2.2
1	D	327	PRO	2.2
1	D	224	VAL	2.2
1	D	232	LEU	2.2
1	D	141	LYS	2.2
1	C	295	PRO	2.1
1	D	143	PRO	2.1
1	A	135	PHE	2.1
1	D	85	PHE	2.1
1	A	125	VAL	2.1
1	D	219	ALA	2.1
1	C	114	SER	2.1
1	C	358	LYS	2.1
1	A	93	TRP	2.1
1	D	156	GLY	2.1
1	D	349	ALA	2.1
1	D	350	ALA	2.1
1	D	260	TYR	2.1
1	D	18	PRO	2.1
1	D	249	GLN	2.1
1	D	264	THR	2.1
1	D	37	LYS	2.1
1	A	96	LEU	2.1
1	D	166	MET	2.1
1	A	100	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	357	ILE	2.1
1	C	161	VAL	2.1
1	D	236	HIS	2.0
1	D	134	PHE	2.0
1	A	132	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

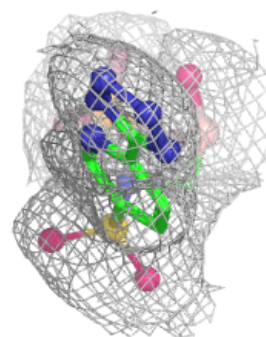
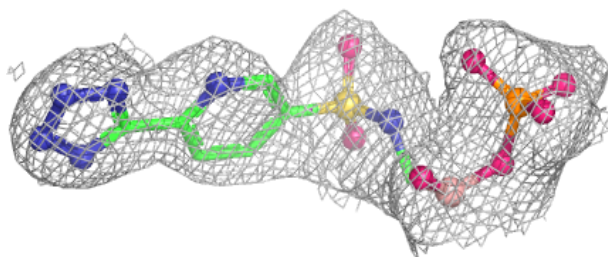
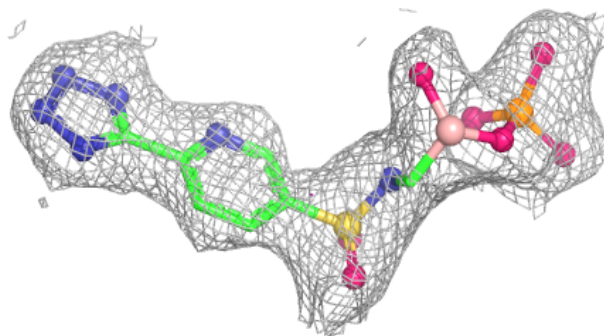
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PO4	B	402	5/5	0.79	0.11	57,61,67,75	0
2	QQZ	C	401	23/23	0.93	0.09	38,47,54,55	0
2	QQZ	D	401	23/23	0.94	0.09	29,45,50,52	0
2	QQZ	A	401	23/23	0.94	0.08	27,38,45,47	0
2	QQZ	B	401	23/23	0.96	0.07	18,31,33,37	0

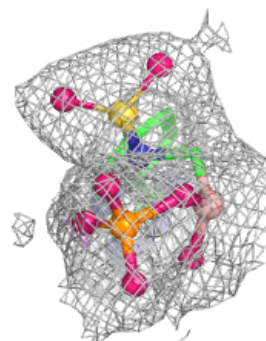
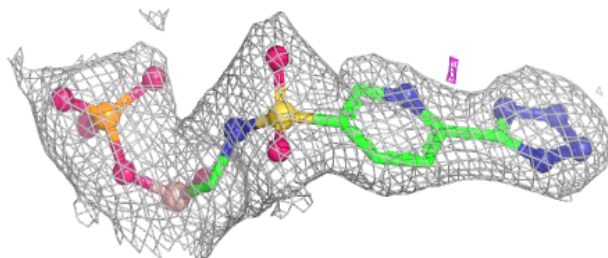
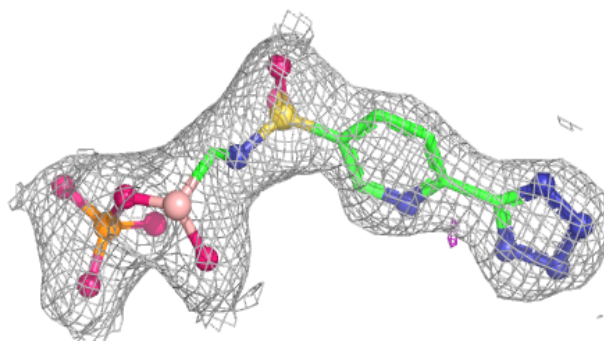
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QQZ 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)

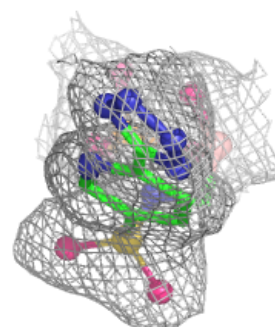
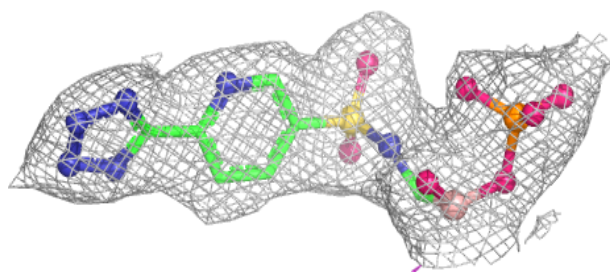
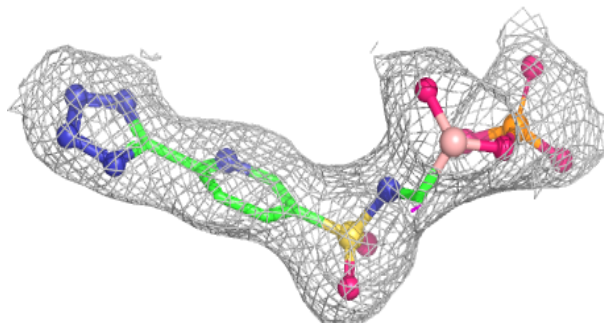
**Electron density around QQZ D 401:**

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

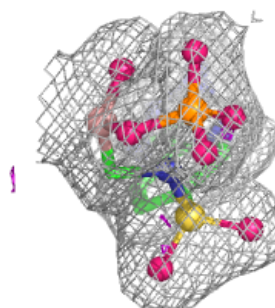
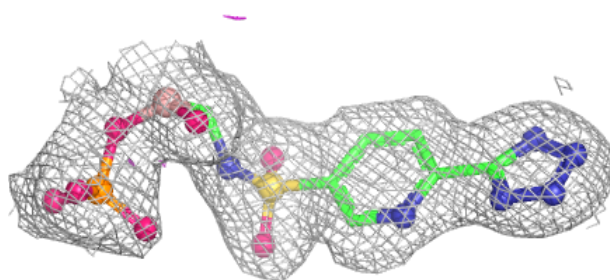
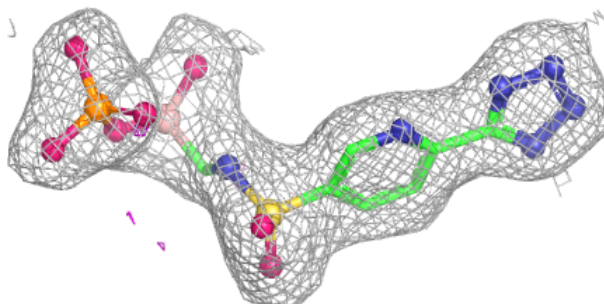


Electron density around QQZ A 401:

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

**Electron density around QQZ 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.