



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:10 am BST

PDB ID : 6U3Y
Title : Structure-based discovery of a novel small-molecule inhibitor of methicillin-resistant *S. aureus*
Authors : Liu, J.; Kozhaya, L.; Torres, V.J.; Unutmaz, D.; Lu, M.
Deposited on : 2019-08-22
Resolution : 2.04 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

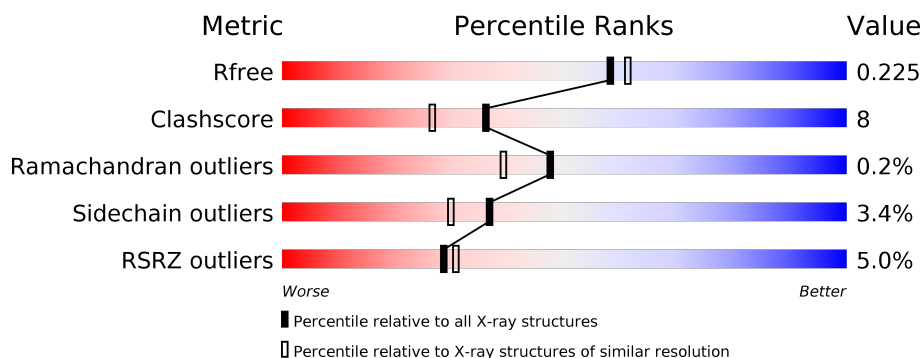
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	301	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• •</div> </div> </div>
2	B	284	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• 5%</div> </div> </div>
2	D	284	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>14%</div> <div>• 10%</div> </div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7154 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.

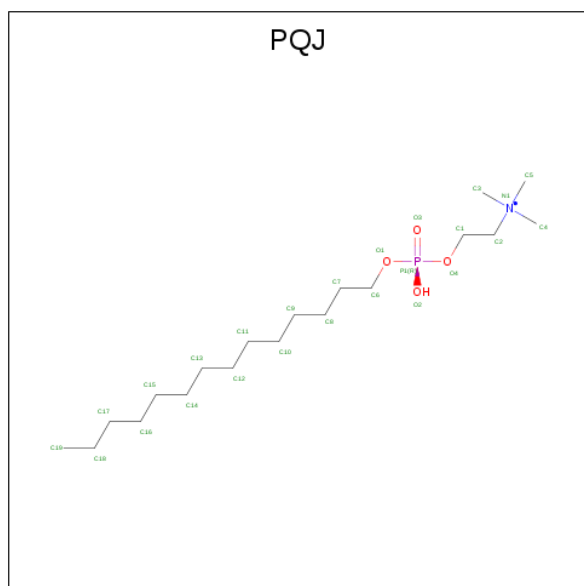
- Molecule 1 is a protein called Panton-Valentine Leucocidin F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2370	1487	409	469	5			

- Molecule 2 is a protein called Gamma-hemolysin subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	270	Total	C	N	O	S	0	0	0
			2195	1385	382	424	4			
2	D	255	Total	C	N	O	S	0	0	0
			2081	1315	363	399	4			

- Molecule 3 is fos-choline-14 (three-letter code: PQJ) (formula: $C_{19}H_{43}NO_4P$).



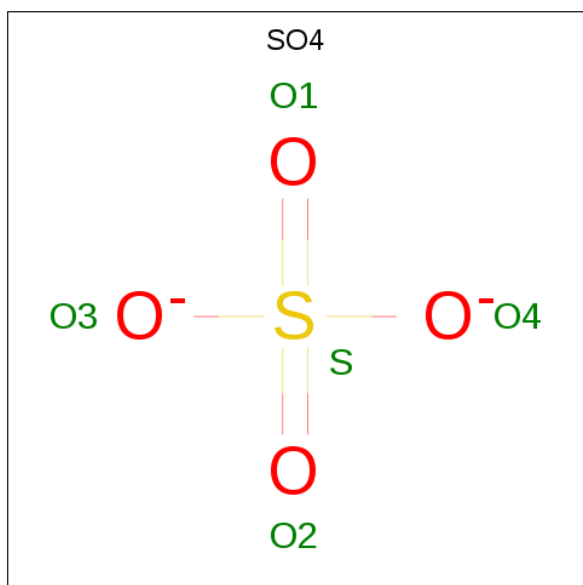
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			19	13	1	4	1		
3	A	1	Total	C	N	O	P	0	0
			16	10	1	4	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



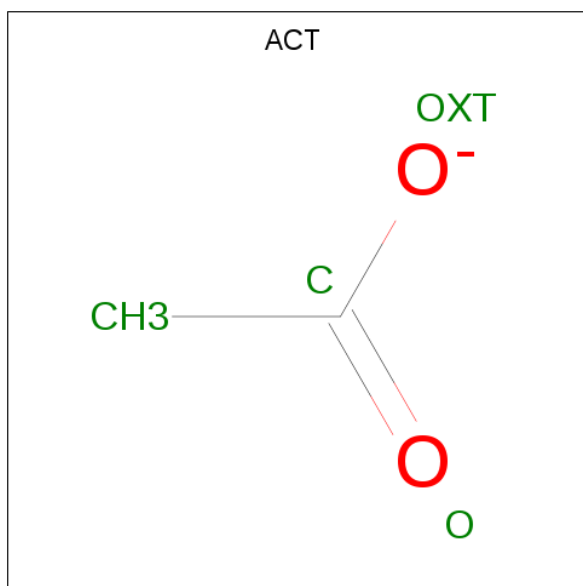
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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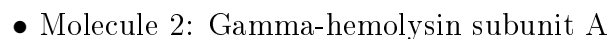
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	144	Total 144	O 144	0	0
6	B	130	Total 130	O 130	0	0
6	D	75	Total 75	O 75	0	0

- Molecule 1: Panton-Valentine Leucocidin F



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	139.10 Å 139.10 Å 246.77 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.69 – 2.04 38.66 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.69-2.04) 99.9 (38.66-2.04)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.05 Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.182 , 0.225 0.183 , 0.225	Depositor DCC
R_{free} test set	3889 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7154	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: PQJ, SO4, ACT

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	0.82	4/2425 (0.2%)	1.22	15/3272 (0.5%)
2	B	0.78	2/2250 (0.1%)	1.22	13/3044 (0.4%)
2	D	0.59	0/2134	1.01	6/2887 (0.2%)
All	All	0.74	6/6809 (0.1%)	1.16	34/9203 (0.4%)

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
2	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	GLU	CD-OE1	9.72	1.36	1.25
1	A	106	GLU	CD-OE2	7.54	1.33	1.25
2	B	197	GLU	CD-OE2	-7.31	1.17	1.25
1	A	296	GLU	CD-OE2	-6.32	1.18	1.25
1	A	117	SER	CA-CB	-5.76	1.44	1.52
2	B	44	ASP	CG-OD2	5.05	1.36	1.25

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	148	ARG	NE-CZ-NH2	-13.32	113.64	120.30
1	A	218	ARG	CG-CD-NE	-13.00	84.50	111.80
1	A	218	ARG	NE-CZ-NH2	-12.20	114.20	120.30
1	A	218	ARG	NE-CZ-NH1	10.63	125.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	ARG	NE-CZ-NH2	-9.77	115.42	120.30
2	B	148	ARG	CG-CD-NE	-9.64	91.55	111.80
1	A	218	ARG	CD-NE-CZ	9.35	136.68	123.60
1	A	231	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	A	288	LYS	CB-CA-C	-7.10	96.20	110.40
2	B	189	ARG	NE-CZ-NH2	-6.81	116.90	120.30
2	D	241	ARG	NE-CZ-NH1	6.75	123.67	120.30
2	B	148	ARG	NE-CZ-NH1	6.60	123.60	120.30
2	B	148	ARG	CD-NE-CZ	6.52	132.72	123.60
2	D	165	THR	OG1-CB-CG2	-6.52	95.01	110.00
1	A	65	LYS	CB-CA-C	-6.08	98.23	110.40
2	D	207	ASN	CB-CA-C	-6.04	98.33	110.40
1	A	247	ARG	NE-CZ-NH2	-5.94	117.33	120.30
2	B	148	ARG	CB-CG-CD	-5.85	96.38	111.60
1	A	28	ASP	CB-CA-C	5.74	121.89	110.40
2	D	241	ARG	NE-CZ-NH2	-5.73	117.44	120.30
2	B	232	ARG	CB-CA-C	-5.57	99.27	110.40
2	B	232	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	B	159	LYS	CB-CA-C	-5.47	99.45	110.40
2	B	189	ARG	NE-CZ-NH1	5.47	123.04	120.30
2	D	232	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	B	232	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	231	ARG	CB-CG-CD	-5.24	97.99	111.60
1	A	18	LEU	CB-CA-C	5.15	119.99	110.20
1	A	271	ARG	CG-CD-NE	-5.10	101.09	111.80
2	B	255	ARG	CG-CD-NE	5.08	122.48	111.80
1	A	46	TYR	CB-CG-CD1	5.08	124.05	121.00
2	B	263	ARG	NE-CZ-NH2	-5.07	117.76	120.30
2	D	232	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	A	231	ARG	CG-CD-NE	-5.02	101.25	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	255	ARG	Peptide

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	2370	0	2269	45	0
2	B	2195	0	2101	36	0
2	D	2081	0	2002	38	0
3	A	47	0	0	1	0
4	A	30	0	0	0	0
4	B	20	0	0	0	0
4	D	30	0	0	1	0
5	A	12	0	9	0	0
5	B	16	0	12	0	0
5	D	4	0	3	0	0
6	A	144	0	0	5	1
6	B	130	0	0	1	1
6	D	75	0	0	2	0
All	All	7154	0	6396	106	1

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 8.

All (106) 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)
2:D:93:ASN:ND2	2:D:213:THR:HG22	1.60	1.16
1:A:300:MET:O	1:A:301:SER:HB2	1.52	1.05
2:D:165:THR:HG22	6:D:414:HOH:O	1.58	1.01
2:D:93:ASN:ND2	2:D:213:THR:CG2	2.34	0.90
2:D:272:ASN:HD22	2:D:275:THR:H	1.22	0.86
1:A:175:GLY:HA2	3:A:403:PQJ:C6	2.06	0.85
1:A:285:HIS:HD2	6:A:627:HOH:O	1.60	0.84
2:B:284:ASN:OXT	6:B:401:HOH:O	1.96	0.83
2:D:93:ASN:HD21	2:D:213:THR:HG22	1.47	0.79
2:D:233:ASN:ND2	2:D:262:ASN:H	1.81	0.78
1:A:103:ASN:H	2:B:207:ASN:HD22	1.30	0.77
1:A:111:GLN:HG2	2:B:136:SER:HB2	1.65	0.75
1:A:171:ILE:HB	1:A:192:MET:HE2	1.70	0.73
2:D:93:ASN:HD22	2:D:93:ASN:C	1.92	0.72
2:D:272:ASN:ND2	2:D:275:THR:H	1.87	0.72
1:A:103:ASN:H	2:B:207:ASN:ND2	1.88	0.72
1:A:198:GLN:HE22	1:A:260:HIS:HB3	1.58	0.68
1:A:180:GLY:CA	1:A:192:MET:HE3	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:GLN:HE21	2:B:79:ASN:ND2	1.95	0.65
2:D:53:PHE:HE2	2:D:55:ASN:OD1	1.80	0.65
2:D:70:LYS:HZ1	2:D:186:GLN:HE22	1.45	0.64
1:A:18:LEU:HD21	1:A:39:ASN:HB3	1.80	0.63
1:A:4:ILE:HA	2:B:211:ILE:HD11	1.81	0.63
2:B:95:LEU:HB2	2:B:211:ILE:HG22	1.81	0.62
1:A:107:GLU:HG2	2:B:140:GLN:CG	2.28	0.62
2:B:63:TYR:OH	2:D:238:HIS:HE1	1.82	0.62
1:A:285:HIS:HE1	6:A:630:HOH:O	1.83	0.61
2:D:77:GLN:HE21	2:D:79:ASN:ND2	1.99	0.60
2:D:53:PHE:CE2	2:D:55:ASN:OD1	2.55	0.59
1:A:180:GLY:HA2	1:A:192:MET:CE	2.33	0.58
1:A:174:ASN:HD21	1:A:212:LYS:NZ	2.01	0.58
2:D:94:TYR:C	2:D:95:LEU:HD12	2.24	0.57
2:D:165:THR:CG2	6:D:414:HOH:O	2.32	0.56
2:D:93:ASN:HD21	2:D:213:THR:CG2	2.12	0.56
2:B:184:TYR:OH	2:B:249:SER:HB2	2.06	0.55
1:A:107:GLU:HG2	2:B:140:GLN:HG2	1.87	0.54
1:A:264:ASN:HB3	6:A:607:HOH:O	2.07	0.54
2:D:77:GLN:HE21	2:D:79:ASN:HD21	1.57	0.53
1:A:257:ASN:O	1:A:258:GLN:HB2	2.09	0.53
1:A:180:GLY:N	1:A:192:MET:HE3	2.24	0.53
1:A:213:MET:HB2	1:A:218:ARG:HD3	1.91	0.53
1:A:180:GLY:HA2	1:A:192:MET:HE1	1.92	0.52
2:D:233:ASN:HD22	2:D:262:ASN:H	1.57	0.51
2:D:95:LEU:N	2:D:95:LEU:HD12	2.24	0.51
1:A:117:SER:O	1:A:134:GLY:HA2	2.11	0.50
1:A:241:ILE:HD12	1:A:280:VAL:HG21	1.94	0.50
1:A:18:LEU:CD2	1:A:39:ASN:HB3	2.42	0.50
2:B:244:THR:HB	2:B:246:TYR:CE1	2.46	0.50
2:D:57:LYS:O	2:D:59:THR:HG23	2.12	0.49
2:D:93:ASN:ND2	2:D:93:ASN:C	2.64	0.49
2:B:113:ILE:HG22	2:B:113:ILE:O	2.12	0.49
2:B:242:ARG:NH2	2:D:258:ASN:HB2	2.28	0.49
1:A:210:TYR:O	1:A:218:ARG:HD2	2.13	0.48
1:A:211:HIS:HD2	6:A:502:HOH:O	1.96	0.48
1:A:107:GLU:HG2	2:B:140:GLN:HG3	1.93	0.48
2:B:8:GLY:HA2	2:B:36:VAL:CG1	2.43	0.48
1:A:198:GLN:HE22	1:A:260:HIS:CB	2.23	0.48
2:D:22:SER:HB2	2:D:265:TYR:CE1	2.49	0.47
2:D:16:ARG:NE	2:D:17:THR:H	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:92:ILE:HD11	2:D:215:SER:HB3	1.96	0.47
1:A:56:ALA:HA	1:A:223:PRO:O	2.15	0.47
1:A:18:LEU:C	1:A:18:LEU:HD13	2.35	0.47
2:B:77:GLN:HE21	2:B:79:ASN:HD21	1.62	0.46
2:B:95:LEU:HB2	2:B:211:ILE:CG2	2.46	0.46
2:D:92:ILE:HB	2:D:213:THR:HG23	1.96	0.46
1:A:274:HIS:HE1	1:A:292:THR:OG1	1.99	0.45
2:B:165:THR:HG21	2:B:170:MET:CE	2.45	0.45
1:A:4:ILE:HG12	2:B:34:ASP:OD2	2.17	0.45
2:B:246:TYR:CD1	2:B:246:TYR:N	2.83	0.45
2:B:265:TYR:CE1	2:B:283:HIS:HB2	2.51	0.45
1:A:300:MET:O	1:A:301:SER:CB	2.38	0.45
2:B:41:TYR:CE2	2:B:43:LYS:HB2	2.51	0.44
2:B:242:ARG:HD2	2:B:252:GLU:HB2	1.99	0.44
1:A:174:ASN:HD21	1:A:212:LYS:HZ3	1.66	0.44
1:A:41:ILE:HB	1:A:50:THR:HB	2.00	0.43
2:B:111:TYR:C	2:B:111:TYR:CD1	2.91	0.43
2:D:70:LYS:HZ1	2:D:186:GLN:NE2	2.11	0.43
1:A:179:TYR:C	1:A:192:MET:HE3	2.38	0.43
2:D:133:LYS:HE3	4:D:302:SO4:O4	2.18	0.43
2:B:8:GLY:HA2	2:B:36:VAL:HG11	2.00	0.43
2:D:16:ARG:HE	2:D:17:THR:H	1.67	0.43
2:B:243:THR:HA	2:B:248:ASN:O	2.20	0.42
2:B:266:THR:O	2:B:283:HIS:HA	2.18	0.42
2:D:70:LYS:NZ	2:D:186:GLN:HE22	2.14	0.42
2:B:63:TYR:OH	2:D:238:HIS:CE1	2.67	0.42
2:D:242:ARG:O	2:D:249:SER:HA	2.20	0.42
2:D:70:LYS:NZ	2:D:186:GLN:NE2	2.67	0.42
1:A:169:HIS:CD2	1:A:170:LYS:HG2	2.54	0.42
2:B:223:THR:HA	2:B:271:VAL:O	2.20	0.41
2:D:248:ASN:N	2:D:248:ASN:HD22	2.19	0.41
1:A:264:ASN:CB	6:A:607:HOH:O	2.66	0.41
1:A:58:ASN:HD21	1:A:220:ASN:ND2	2.19	0.41
1:A:4:ILE:HG13	2:B:47:ILE:CG2	2.51	0.41
2:D:33:PHE:CD2	2:D:48:LEU:CD2	3.03	0.41
1:A:94:VAL:HA	1:A:230:SER:O	2.21	0.41
1:A:60:TYR:O	1:A:247:ARG:HD3	2.20	0.41
1:A:18:LEU:HD23	1:A:41:ILE:HG12	2.02	0.41
1:A:64:THR:O	1:A:76:PHE:HB2	2.20	0.41
2:B:227:GLU:HG2	2:B:268:LYS:HG2	2.03	0.41
2:B:57:LYS:O	2:B:59:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:ASN:HD22	2:B:70:LYS:HG2	1.86	0.41
2:D:108:THR:HG23	2:D:134:THR:HG22	2.01	0.41
1:A:8:SER:O	2:B:10:GLY:HA2	2.21	0.40
2:B:231:GLY:HA3	2:B:264:ASN:HA	2.02	0.40
2:D:13:VAL:HG12	2:D:36:VAL:HG22	2.03	0.40
2:D:281:LYS:HD2	2:D:281:LYS:HA	1.93	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:640:HOH:O	6:B:524:HOH:O[13_545]	2.08	0.12

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	287/301 (95%)	280 (98%)	6 (2%)	1 (0%)	41	31
2	B	266/284 (94%)	257 (97%)	8 (3%)	1 (0%)	34	24
2	D	251/284 (88%)	243 (97%)	8 (3%)	0	100	100
All	All	804/869 (92%)	780 (97%)	22 (3%)	2 (0%)	47	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	GLN
2	B	128	SER

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	263/270 (97%)	257 (98%)	6 (2%)	50	44
2	B	244/254 (96%)	239 (98%)	5 (2%)	55	50
2	D	232/254 (91%)	218 (94%)	14 (6%)	19	11
All	All	739/778 (95%)	714 (97%)	25 (3%)	37	30

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	73	SER
1	A	84	ILE
1	A	237	LYS
1	A	300	MET
1	A	301	SER
2	B	128	SER
2	B	148	ARG
2	B	171	SER
2	B	220	SER
2	B	281	LYS
2	D	16	ARG
2	D	17	THR
2	D	39	LYS
2	D	64	LYS
2	D	93	ASN
2	D	109	LEU
2	D	149	GLN
2	D	165	THR
2	D	170	MET
2	D	186	GLN
2	D	204	SER
2	D	207	ASN
2	D	274	LYS
2	D	279	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	87	ASN
1	A	111	GLN
1	A	169	HIS
1	A	174	ASN
1	A	198	GLN
1	A	220	ASN
1	A	260	HIS
1	A	274	HIS
1	A	284	ASN
2	B	62	ASN
2	B	79	ASN
2	B	85	ASN
2	B	203	HIS
2	B	207	ASN
2	D	30	ASN
2	D	42	ASN
2	D	62	ASN
2	D	79	ASN
2	D	93	ASN
2	D	104	ASN
2	D	138	ASN
2	D	186	GLN
2	D	196	ASN
2	D	233	ASN
2	D	238	HIS
2	D	248	ASN
2	D	272	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

27 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	ACT	D	307	-	1,3,3	3.82	1 (100%)	0,3,3	0.00	-
4	SO4	D	304	-	4,4,4	0.39	0	6,6,6	0.17	0
3	PQJ	A	403	-	15,15,24	0.79	1 (6%)	19,20,29	1.01	0
5	ACT	B	308	-	1,3,3	4.64	1 (100%)	0,3,3	0.00	-
5	ACT	B	307	-	1,3,3	3.67	1 (100%)	0,3,3	0.00	-
3	PQJ	A	402	-	18,18,24	0.60	0	22,23,29	0.90	1 (4%)
5	ACT	B	305	-	1,3,3	3.23	1 (100%)	0,3,3	0.00	-
4	SO4	A	406	-	4,4,4	0.40	0	6,6,6	0.11	0
4	SO4	D	302	-	4,4,4	0.38	0	6,6,6	0.17	0
5	ACT	A	410	-	1,3,3	3.94	1 (100%)	0,3,3	0.00	-
4	SO4	A	405	-	4,4,4	0.37	0	6,6,6	0.18	0
3	PQJ	A	401	-	11,11,24	0.63	0	15,16,29	0.86	0
4	SO4	B	304	-	4,4,4	0.38	0	6,6,6	0.10	0
4	SO4	A	404	-	4,4,4	0.46	0	6,6,6	0.18	0
4	SO4	D	303	-	4,4,4	0.49	0	6,6,6	0.14	0
5	ACT	A	412	-	1,3,3	3.15	1 (100%)	0,3,3	0.00	-
4	SO4	A	407	-	4,4,4	0.40	0	6,6,6	0.09	0
5	ACT	B	306	-	1,3,3	4.13	1 (100%)	0,3,3	0.00	-
4	SO4	A	409	-	4,4,4	0.27	0	6,6,6	0.17	0
4	SO4	B	302	-	4,4,4	0.31	0	6,6,6	0.17	0
4	SO4	D	306	-	4,4,4	0.38	0	6,6,6	0.20	0
4	SO4	D	301	-	4,4,4	0.39	0	6,6,6	0.09	0
4	SO4	A	408	-	4,4,4	0.34	0	6,6,6	0.09	0
4	SO4	B	301	-	4,4,4	0.49	0	6,6,6	0.22	0
4	SO4	D	305	-	4,4,4	0.38	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	B	303	-	4,4,4	0.31	0	6,6,6	0.16	0
5	ACT	A	411	-	1,3,3	3.65	1 (100%)	0,3,3	0.00	-

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	PQJ	A	402	-	-	4/18/18/24	-
3	PQJ	A	403	-	-	5/15/15/24	-
3	PQJ	A	401	-	-	3/11/11/24	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	308	ACT	CH3-C	4.64	1.54	1.48
5	B	306	ACT	CH3-C	4.13	1.54	1.48
5	A	410	ACT	CH3-C	3.94	1.53	1.48
5	D	307	ACT	CH3-C	3.82	1.53	1.48
5	B	307	ACT	CH3-C	3.67	1.53	1.48
5	A	411	ACT	CH3-C	3.65	1.53	1.48
5	B	305	ACT	CH3-C	3.23	1.52	1.48
5	A	412	ACT	CH3-C	3.15	1.52	1.48
3	A	403	PQJ	P1-O1	2.17	1.68	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	PQJ	C8-C7-C6	-2.35	103.08	113.49

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	PQJ	C6-O1-P1-O2
3	A	403	PQJ	C6-O1-P1-O4
3	A	402	PQJ	C6-O1-P1-O2
3	A	402	PQJ	C6-O1-P1-O3
3	A	402	PQJ	C6-O1-P1-O4

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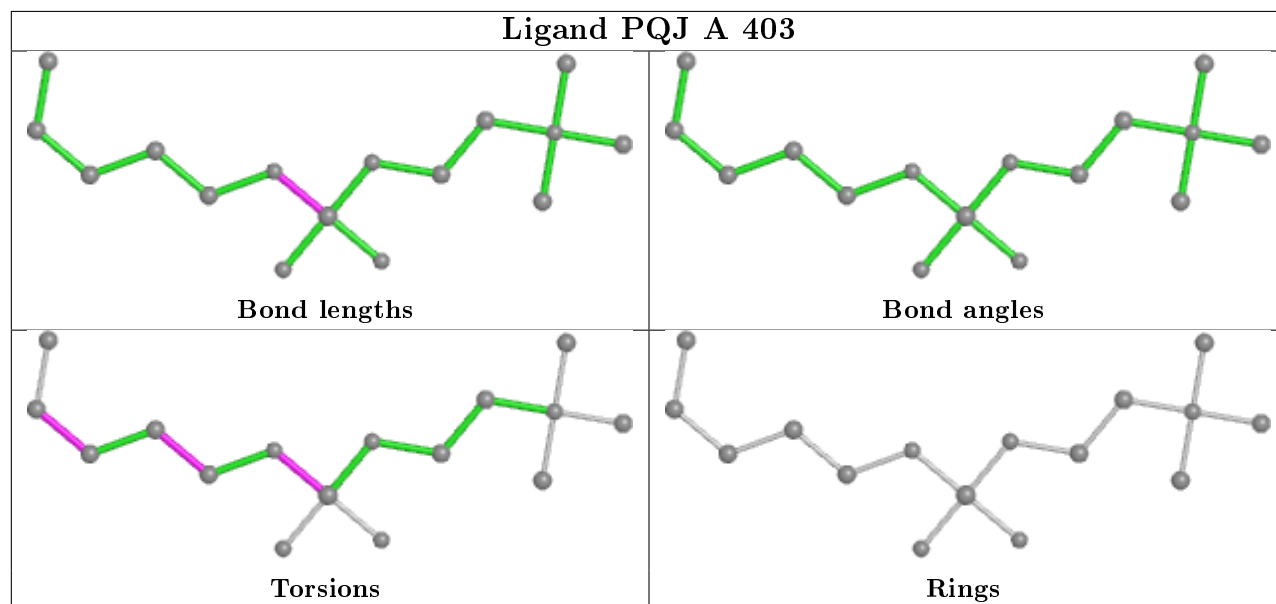
Mol	Chain	Res	Type	Atoms
3	A	401	PQJ	C6-O1-P1-O2
3	A	401	PQJ	C6-O1-P1-O3
3	A	403	PQJ	O1-C6-C7-C8
3	A	402	PQJ	O4-C1-C2-N1
3	A	403	PQJ	C7-C8-C9-C10
3	A	401	PQJ	C6-O1-P1-O4
3	A	403	PQJ	C6-O1-P1-O3

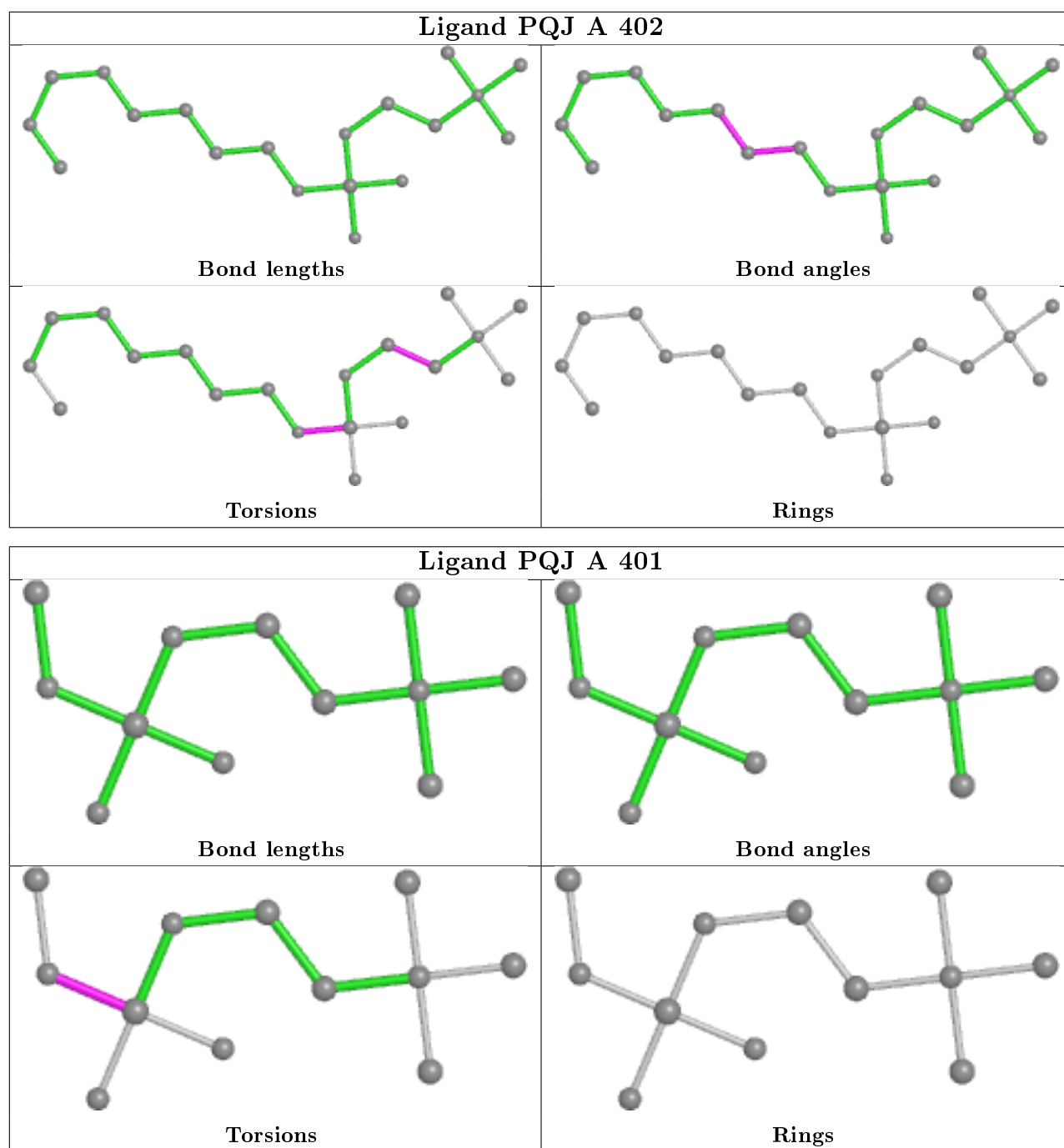
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	PQJ	1	0
4	D	302	SO4	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	291/301 (96%)	-0.18	19 (6%)	18 20	25, 36, 76, 112	0
2	B	270/284 (95%)	-0.21	9 (3%)	46 50	25, 34, 67, 104	0
2	D	255/284 (89%)	-0.05	13 (5%)	28 30	29, 49, 76, 93	0
All	All	816/869 (93%)	-0.15	41 (5%)	28 31	25, 38, 75, 112	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	113	ILE	6.5
1	A	13	ASP	5.8
2	B	114	GLY	5.5
1	A	118	TYR	5.4
1	A	12	VAL	5.4
2	D	111	TYR	4.9
2	D	40	LYS	4.4
2	B	127	GLY	4.2
1	A	120	GLY	4.2
1	A	119	GLY	4.2
2	D	12	GLU	4.1
1	A	7	VAL	4.0
2	B	126	ASN	4.0
1	A	121	ASP	3.9
2	D	223	THR	3.7
2	B	167	LEU	3.6
2	D	41	TYR	3.5
1	A	133	ASN	3.4
1	A	132	GLY	3.4
2	D	11	ALA	3.3
2	D	39	LYS	3.2
1	A	8	SER	3.1
2	D	36	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	5	THR	3.0
1	A	134	GLY	2.9
1	A	301	SER	2.8
2	B	246	TYR	2.8
2	D	10	GLY	2.7
2	D	273	TRP	2.7
1	A	6	PRO	2.6
1	A	11	LYS	2.6
2	B	245	HIS	2.4
2	B	247	GLY	2.4
2	D	110	GLY	2.3
1	A	14	ASP	2.3
1	A	9	GLU	2.3
1	A	234	ASN	2.2
2	D	277	GLU	2.2
2	D	35	PHE	2.1
1	A	10	LYS	2.1
2	B	282	GLY	2.1

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 carbohydrates 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	PQJ	A	403	16/25	0.81	0.18	54,60,70,71	0
5	ACT	B	308	4/4	0.83	0.27	52,65,65,67	0
5	ACT	D	307	4/4	0.85	0.10	69,72,73,73	0
5	ACT	B	306	4/4	0.89	0.10	48,62,65,66	0
4	SO4	A	408	5/5	0.89	0.10	80,87,95,96	0

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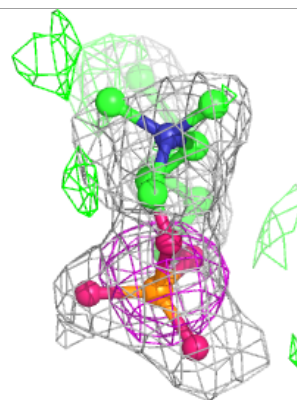
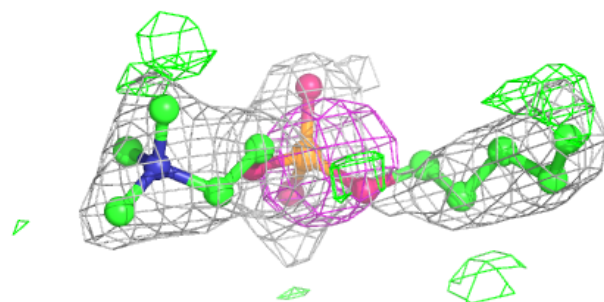
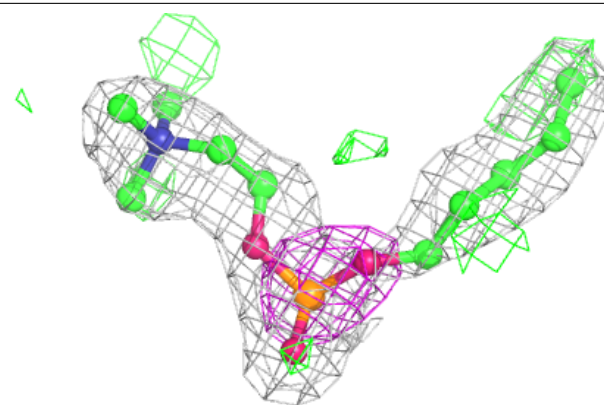
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	405	5/5	0.90	0.11	77,79,87,91	0
4	SO4	A	409	5/5	0.92	0.12	72,77,88,91	0
4	SO4	D	306	5/5	0.93	0.09	57,59,72,76	0
5	ACT	B	307	4/4	0.94	0.28	50,52,62,64	0
5	ACT	B	305	4/4	0.94	0.11	50,55,58,62	0
4	SO4	D	302	5/5	0.94	0.13	71,78,81,82	0
4	SO4	D	304	5/5	0.94	0.10	71,75,85,92	0
4	SO4	B	304	5/5	0.95	0.18	78,80,88,89	0
4	SO4	B	302	5/5	0.95	0.16	64,66,74,75	0
5	ACT	A	410	4/4	0.96	0.12	49,51,53,69	0
4	SO4	A	406	5/5	0.96	0.08	76,79,80,81	0
3	PQJ	A	402	19/25	0.96	0.16	52,57,82,86	0
5	ACT	A	412	4/4	0.96	0.10	54,56,59,63	0
4	SO4	A	407	5/5	0.96	0.14	78,78,87,92	0
4	SO4	D	305	5/5	0.96	0.11	65,68,78,84	0
4	SO4	D	303	5/5	0.97	0.09	68,71,72,80	0
4	SO4	D	301	5/5	0.98	0.09	72,79,81,89	0
4	SO4	A	404	5/5	0.98	0.06	52,57,61,64	0
3	PQJ	A	401	12/25	0.98	0.10	44,55,63,70	0
4	SO4	B	303	5/5	0.98	0.06	47,52,57,58	0
5	ACT	A	411	4/4	0.98	0.13	49,54,60,63	0
4	SO4	B	301	5/5	0.99	0.08	51,52,55,60	0

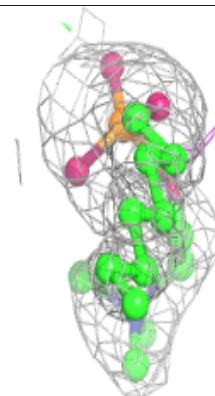
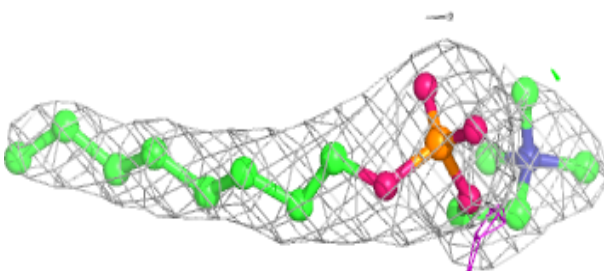
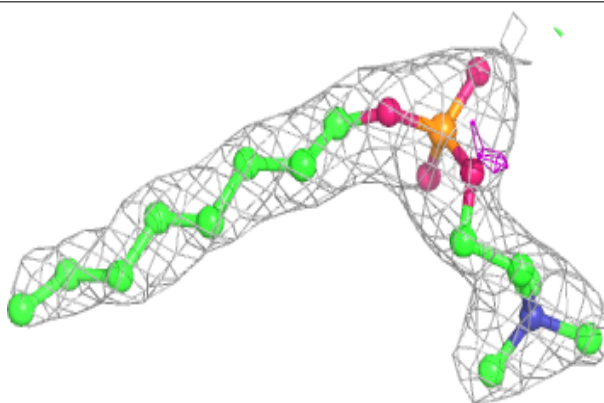
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PQJ A 403:

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

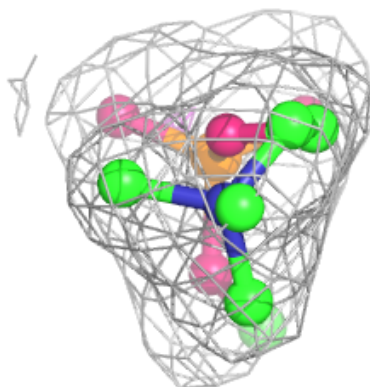
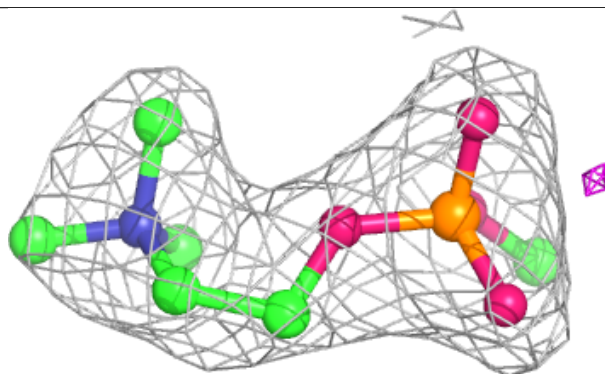
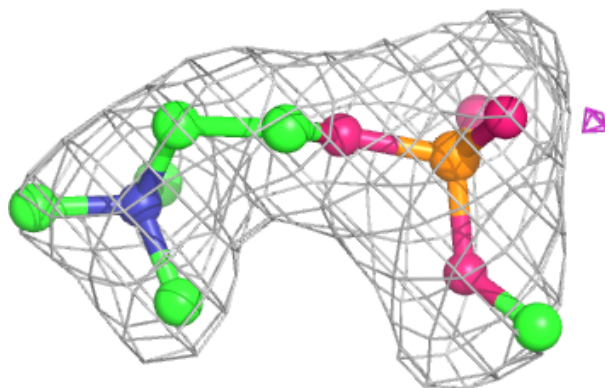
**Electron density around PQJ A 402:**

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



Electron density around PQJ 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.