Full wwPDB X-ray Structure Validation Report ⓘ

Dec 1, 2021 – 02:03 PM EST

PDB ID	:	7KNX
Title	:	Crystal structure of SND1 in complex with C-26-A6
Authors	:	Kang, Y.
Deposited on	:	2020-11-06
Resolution	:	2.70 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:

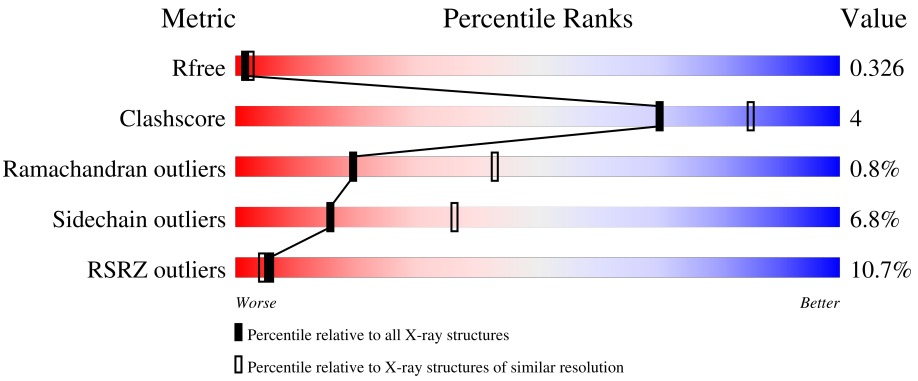
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	324	8% 78% 11% • 10%
1	B	324	9% 79% 11% • 9%
1	C	324	12% 77% 12% • 10%
1	D	324	10% 77% 12% • 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	D	1001	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9995 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 Staphylococcal nuclease domain-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2334	1464	438	422	10			
1	B	295	Total	C	N	O	S	0	0	0
			2353	1478	439	426	10			
1	C	290	Total	C	N	O	S	0	1	0
			2320	1457	434	419	10			
1	D	290	Total	C	N	O	S	0	0	0
			2318	1458	431	419	10			

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	initiating methionine	UNP Q7KZF4
A	-3	GLY	-	expression tag	UNP Q7KZF4
A	-2	SER	-	expression tag	UNP Q7KZF4
A	-1	SER	-	expression tag	UNP Q7KZF4
A	0	HIS	-	expression tag	UNP Q7KZF4
A	1	HIS	-	expression tag	UNP Q7KZF4
A	2	HIS	-	expression tag	UNP Q7KZF4
A	3	HIS	-	expression tag	UNP Q7KZF4
A	4	HIS	-	expression tag	UNP Q7KZF4
A	5	HIS	-	expression tag	UNP Q7KZF4
A	6	SER	-	expression tag	UNP Q7KZF4
A	7	SER	-	expression tag	UNP Q7KZF4
A	8	GLY	-	expression tag	UNP Q7KZF4
A	9	GLU	-	expression tag	UNP Q7KZF4
A	10	ASN	-	expression tag	UNP Q7KZF4
A	11	LEU	-	expression tag	UNP Q7KZF4
A	12	TYR	-	expression tag	UNP Q7KZF4
A	13	PHE	-	expression tag	UNP Q7KZF4
A	14	GLN	-	expression tag	UNP Q7KZF4
A	15	GLY	-	expression tag	UNP Q7KZF4
A	?	-	ALA	deletion	UNP Q7KZF4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP Q7KZF4
A	?	-	THR	deletion	UNP Q7KZF4
A	?	-	GLN	deletion	UNP Q7KZF4
A	?	-	PRO	deletion	UNP Q7KZF4
A	?	-	ASP	deletion	UNP Q7KZF4
A	?	-	GLU	deletion	UNP Q7KZF4
A	?	-	ALA	deletion	UNP Q7KZF4
A	?	-	ASP	deletion	UNP Q7KZF4
A	?	-	GLY	deletion	UNP Q7KZF4
A	?	-	SER	deletion	UNP Q7KZF4
B	-4	MET	-	initiating methionine	UNP Q7KZF4
B	-3	GLY	-	expression tag	UNP Q7KZF4
B	-2	SER	-	expression tag	UNP Q7KZF4
B	-1	SER	-	expression tag	UNP Q7KZF4
B	0	HIS	-	expression tag	UNP Q7KZF4
B	1	HIS	-	expression tag	UNP Q7KZF4
B	2	HIS	-	expression tag	UNP Q7KZF4
B	3	HIS	-	expression tag	UNP Q7KZF4
B	4	HIS	-	expression tag	UNP Q7KZF4
B	5	HIS	-	expression tag	UNP Q7KZF4
B	6	SER	-	expression tag	UNP Q7KZF4
B	7	SER	-	expression tag	UNP Q7KZF4
B	8	GLY	-	expression tag	UNP Q7KZF4
B	9	GLU	-	expression tag	UNP Q7KZF4
B	10	ASN	-	expression tag	UNP Q7KZF4
B	11	LEU	-	expression tag	UNP Q7KZF4
B	12	TYR	-	expression tag	UNP Q7KZF4
B	13	PHE	-	expression tag	UNP Q7KZF4
B	14	GLN	-	expression tag	UNP Q7KZF4
B	15	GLY	-	expression tag	UNP Q7KZF4
B	?	-	ALA	deletion	UNP Q7KZF4
B	?	-	ALA	deletion	UNP Q7KZF4
B	?	-	THR	deletion	UNP Q7KZF4
B	?	-	GLN	deletion	UNP Q7KZF4
B	?	-	PRO	deletion	UNP Q7KZF4
B	?	-	ASP	deletion	UNP Q7KZF4
B	?	-	GLU	deletion	UNP Q7KZF4
B	?	-	ALA	deletion	UNP Q7KZF4
B	?	-	ASP	deletion	UNP Q7KZF4
B	?	-	GLY	deletion	UNP Q7KZF4
B	?	-	SER	deletion	UNP Q7KZF4
C	-4	MET	-	initiating methionine	UNP Q7KZF4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP Q7KZF4
C	-2	SER	-	expression tag	UNP Q7KZF4
C	-1	SER	-	expression tag	UNP Q7KZF4
C	0	HIS	-	expression tag	UNP Q7KZF4
C	1	HIS	-	expression tag	UNP Q7KZF4
C	2	HIS	-	expression tag	UNP Q7KZF4
C	3	HIS	-	expression tag	UNP Q7KZF4
C	4	HIS	-	expression tag	UNP Q7KZF4
C	5	HIS	-	expression tag	UNP Q7KZF4
C	6	SER	-	expression tag	UNP Q7KZF4
C	7	SER	-	expression tag	UNP Q7KZF4
C	8	GLY	-	expression tag	UNP Q7KZF4
C	9	GLU	-	expression tag	UNP Q7KZF4
C	10	ASN	-	expression tag	UNP Q7KZF4
C	11	LEU	-	expression tag	UNP Q7KZF4
C	12	TYR	-	expression tag	UNP Q7KZF4
C	13	PHE	-	expression tag	UNP Q7KZF4
C	14	GLN	-	expression tag	UNP Q7KZF4
C	15	GLY	-	expression tag	UNP Q7KZF4
C	?	-	ALA	deletion	UNP Q7KZF4
C	?	-	ALA	deletion	UNP Q7KZF4
C	?	-	THR	deletion	UNP Q7KZF4
C	?	-	GLN	deletion	UNP Q7KZF4
C	?	-	PRO	deletion	UNP Q7KZF4
C	?	-	ASP	deletion	UNP Q7KZF4
C	?	-	GLU	deletion	UNP Q7KZF4
C	?	-	ALA	deletion	UNP Q7KZF4
C	?	-	ASP	deletion	UNP Q7KZF4
C	?	-	GLY	deletion	UNP Q7KZF4
C	?	-	SER	deletion	UNP Q7KZF4
D	-4	MET	-	initiating methionine	UNP Q7KZF4
D	-3	GLY	-	expression tag	UNP Q7KZF4
D	-2	SER	-	expression tag	UNP Q7KZF4
D	-1	SER	-	expression tag	UNP Q7KZF4
D	0	HIS	-	expression tag	UNP Q7KZF4
D	1	HIS	-	expression tag	UNP Q7KZF4
D	2	HIS	-	expression tag	UNP Q7KZF4
D	3	HIS	-	expression tag	UNP Q7KZF4
D	4	HIS	-	expression tag	UNP Q7KZF4
D	5	HIS	-	expression tag	UNP Q7KZF4
D	6	SER	-	expression tag	UNP Q7KZF4
D	7	SER	-	expression tag	UNP Q7KZF4

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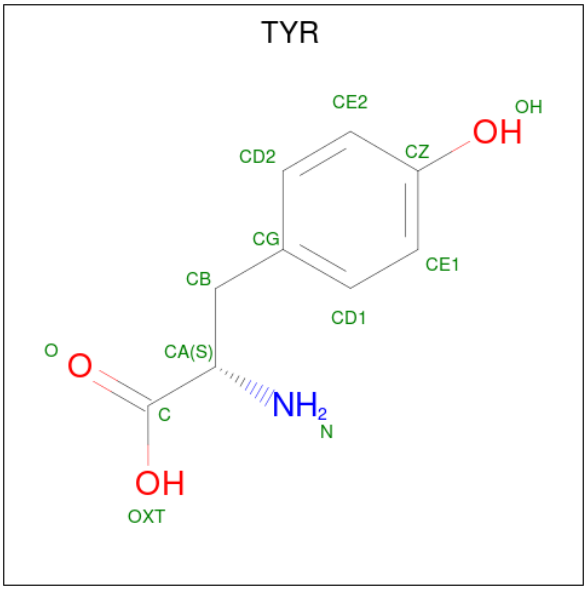
Chain	Residue	Modelled	Actual	Comment	Reference
D	8	GLY	-	expression tag	UNP Q7KZF4
D	9	GLU	-	expression tag	UNP Q7KZF4
D	10	ASN	-	expression tag	UNP Q7KZF4
D	11	LEU	-	expression tag	UNP Q7KZF4
D	12	TYR	-	expression tag	UNP Q7KZF4
D	13	PHE	-	expression tag	UNP Q7KZF4
D	14	GLN	-	expression tag	UNP Q7KZF4
D	15	GLY	-	expression tag	UNP Q7KZF4
D	?	-	ALA	deletion	UNP Q7KZF4
D	?	-	ALA	deletion	UNP Q7KZF4
D	?	-	THR	deletion	UNP Q7KZF4
D	?	-	GLN	deletion	UNP Q7KZF4
D	?	-	PRO	deletion	UNP Q7KZF4
D	?	-	ASP	deletion	UNP Q7KZF4
D	?	-	GLU	deletion	UNP Q7KZF4
D	?	-	ALA	deletion	UNP Q7KZF4
D	?	-	ASP	deletion	UNP Q7KZF4
D	?	-	GLY	deletion	UNP Q7KZF4
D	?	-	SER	deletion	UNP Q7KZF4

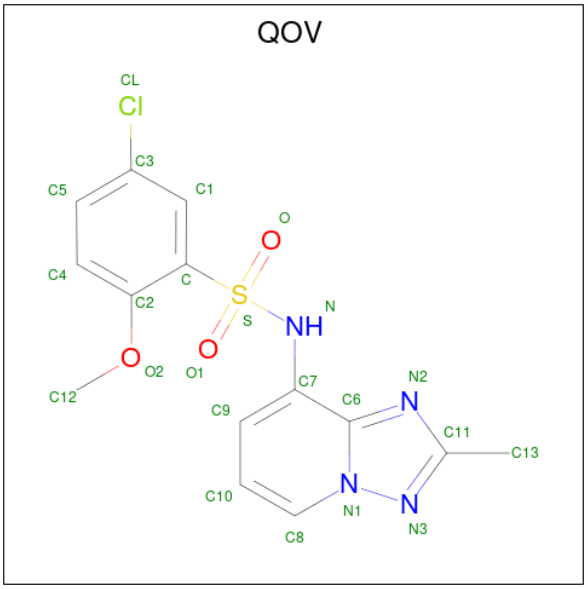
- Molecule 2 is TYROSINE (three-letter code: TYR) (formula: $C_9H_{11}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	12	9	1	2	0	0

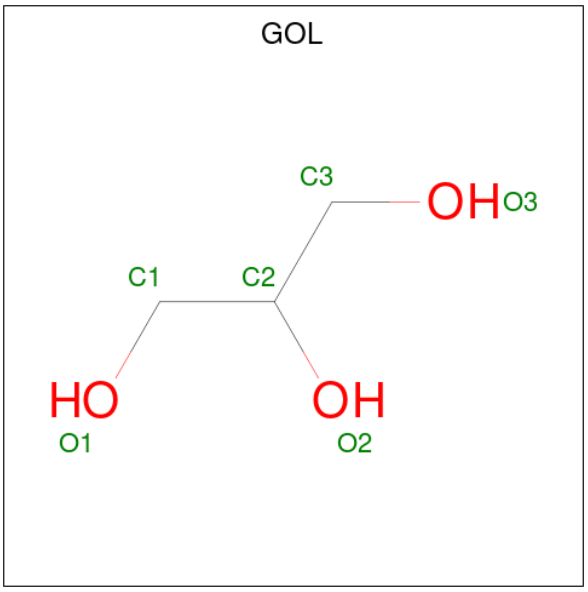
- Molecule 3 is 5-chloro-2-methoxy-N-(2-methyl[1,2,4]triazolo[1,5-a]pyridin-8-yl)benzene-

1-sulfonamide (three-letter code: QOV) (formula: $C_{14}H_{13}ClN_4O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			23	14	1	4	3	1		
3	B	1	Total	C	Cl	N	O	S	0	0
			23	14	1	4	3	1		
3	C	1	Total	C	Cl	N	O	S	0	0
			23	14	1	4	3	1		
3	D	1	Total	C	Cl	N	O	S	0	0
			23	14	1	4	3	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

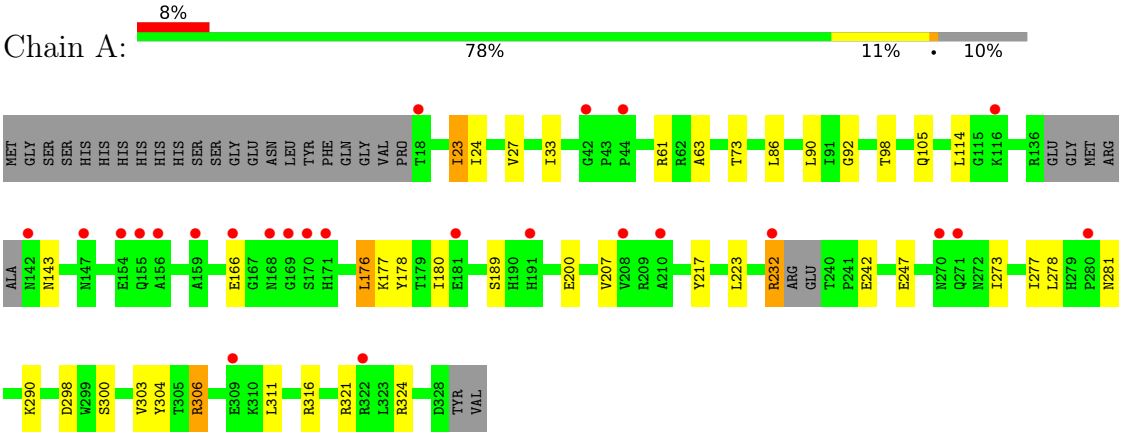
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	134	Total O 134 134	0	0
5	B	151	Total O 151 151	0	0
5	C	132	Total O 132 132	0	0
5	D	143	Total O 143 143	0	0

3 Residue-property plots (i)

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

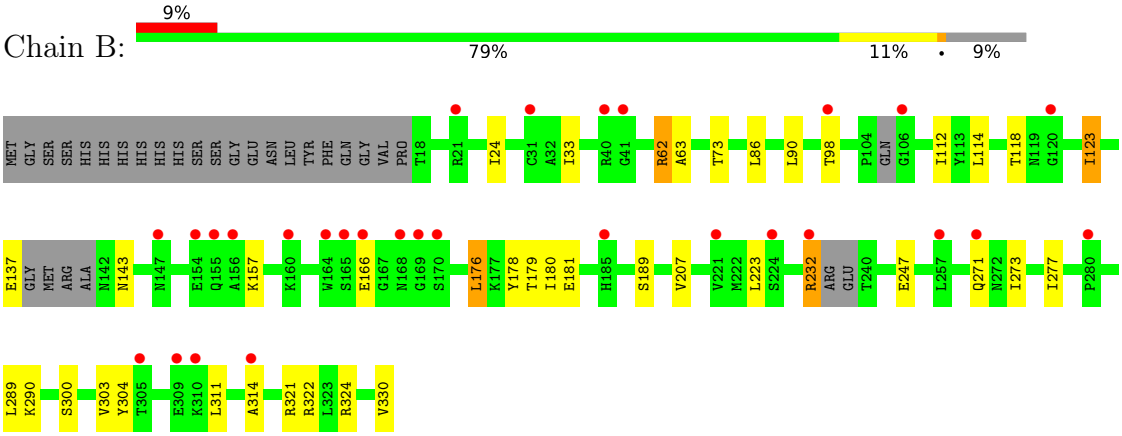
• Molecule 1: Staphylococcal nuclease domain-containing protein 1

Chain A:



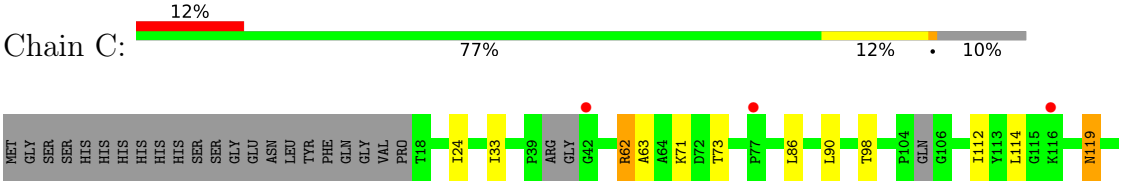
• Molecule 1: Staphylococcal nuclease domain-containing protein 1

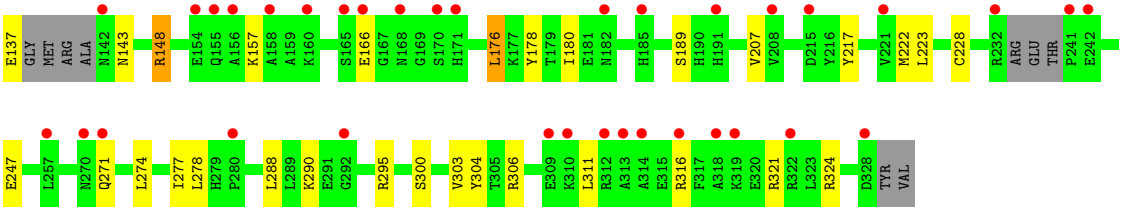
Chain B:



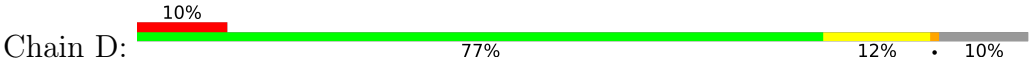
• Molecule 1: Staphylococcal nuclease domain-containing protein 1

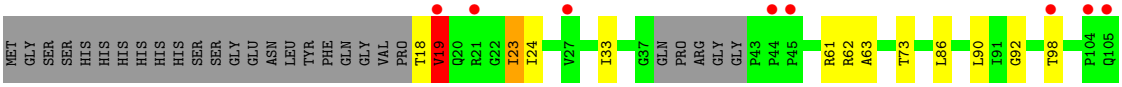
Chain C:

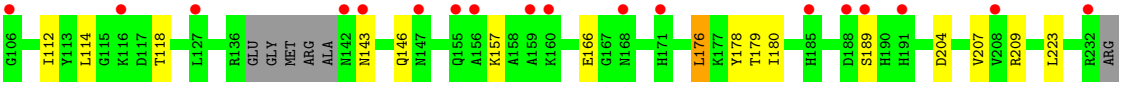


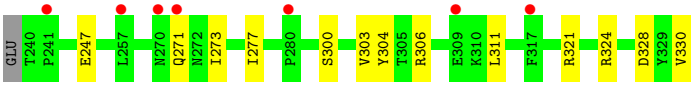


• Molecule 1: Staphylococcal nuclease domain-containing protein 1









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	61.13Å 81.88Å 81.88Å 83.77° 70.89° 70.91°	Depositor
Resolution (Å)	30.00 – 2.70 27.82 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.4 (30.00-2.70) 96.5 (27.82-2.70)	Depositor EDS
R_{merge}	1.00	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.260 , 0.329 0.267 , 0.326	Depositor DCC
R_{free} test set	1849 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	32.9	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 57.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.020 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	9995	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: QOV, GOL

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	0.54	0/2378	0.79	3/3207 (0.1%)
1	B	0.53	0/2397	0.76	0/3232
1	C	0.53	0/2365	0.77	0/3185
1	D	0.53	0/2361	0.78	2/3183 (0.1%)
All	All	0.53	0/9501	0.78	5/12807 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	61	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	D	19	VAL	CB-CA-C	-6.01	99.98	111.40
1	A	232	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	A	61	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	D	61	ARG	NE-CZ-NH1	-5.42	117.59	120.30

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	2334	0	2359	20	0
1	B	2353	0	2374	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2320	0	2346	18	0
1	D	2318	0	2343	16	0
2	A	12	0	8	0	0
3	A	23	0	0	0	0
3	B	23	0	0	0	0
3	C	23	0	0	0	0
3	D	23	0	0	0	0
4	D	6	0	8	0	0
5	A	134	0	0	4	0
5	B	151	0	0	2	0
5	C	132	0	0	4	0
5	D	143	0	0	2	0
All	All	9995	0	9438	68	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 (68) 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:27:VAL:HG22	1:A:33:ILE:HD12	1.49	0.94
1:C:228:CYS:SG	5:C:2108:HOH:O	2.16	0.88
1:C:222:MET:HG3	1:C:274:LEU:HD23	1.71	0.72
1:A:232:ARG:NH1	1:A:242:GLU:OE1	2.23	0.72
1:C:180:ILE:HD13	1:C:217:TYR:CD1	2.27	0.68
1:C:71:LYS:O	5:C:2101:HOH:O	2.14	0.65
1:C:278:LEU:HD23	1:C:306:ARG:NH2	2.11	0.64
1:C:33:ILE:HD11	1:C:112:ILE:HG12	1.82	0.62
1:B:33:ILE:HD11	1:B:112:ILE:HG12	1.83	0.60
1:D:33:ILE:HD11	1:D:112:ILE:HG12	1.82	0.60
1:A:281:ASN:O	1:B:232:ARG:NH1	2.34	0.60
1:A:23:ILE:HD11	1:A:92:GLY:HA2	1.83	0.59
1:C:288:LEU:HD22	5:C:2108:HOH:O	2.01	0.59
1:D:23:ILE:HD11	1:D:92:GLY:HA2	1.83	0.59
1:C:223:LEU:HD21	1:C:277:ILE:HD12	1.86	0.56
1:A:180:ILE:CD1	1:A:273:ILE:HD11	2.36	0.56
1:B:223:LEU:HD21	1:B:277:ILE:HD12	1.87	0.56
1:B:314:ALA:HB3	5:B:2200:HOH:O	2.04	0.56
1:D:223:LEU:HD21	1:D:277:ILE:HD12	1.87	0.55
1:D:180:ILE:CD1	1:D:273:ILE:HD11	2.36	0.55
1:B:180:ILE:CD1	1:B:273:ILE:HD11	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LEU:HD21	1:A:277:ILE:HD12	1.88	0.54
1:A:27:VAL:HG22	1:A:33:ILE:CD1	2.32	0.53
1:B:112:ILE:HB	1:B:123:ILE:HD12	1.91	0.53
1:D:18:THR:O	1:D:19:VAL:HG22	2.09	0.52
1:A:278:LEU:HD23	5:A:501:HOH:O	2.11	0.50
1:C:176:LEU:HD13	1:C:178:TYR:CZ	2.47	0.49
1:A:306:ARG:NH2	5:A:501:HOH:O	2.45	0.49
1:D:209:ARG:O	5:D:1101:HOH:O	2.20	0.48
1:D:204:ASP:HB2	5:D:1132:HOH:O	2.13	0.48
1:A:277:ILE:O	5:A:501:HOH:O	2.20	0.48
1:B:300:SER:O	1:B:303:VAL:HG22	2.14	0.47
1:A:180:ILE:HD11	1:A:273:ILE:HD11	1.96	0.47
1:B:176:LEU:HD13	1:B:178:TYR:CZ	2.49	0.47
1:D:300:SER:O	1:D:303:VAL:HG22	2.13	0.47
1:C:300:SER:O	1:C:303:VAL:HG22	2.15	0.46
1:D:176:LEU:HD13	1:D:178:TYR:CZ	2.50	0.46
1:B:289:LEU:HD12	5:B:2200:HOH:O	2.14	0.46
1:A:24:ILE:HD12	1:A:33:ILE:HG21	1.97	0.46
1:C:148[A]:ARG:HD3	1:C:148[A]:ARG:HA	1.74	0.45
1:A:300:SER:O	1:A:303:VAL:HG22	2.15	0.45
1:B:180:ILE:HD11	1:B:273:ILE:HD11	1.97	0.45
1:B:247:GLU:OE1	1:B:247:GLU:N	2.50	0.44
1:D:180:ILE:HD11	1:D:273:ILE:HD11	1.99	0.44
1:A:176:LEU:HD13	1:A:178:TYR:CZ	2.52	0.44
1:C:247:GLU:OE1	1:C:247:GLU:N	2.49	0.44
1:D:247:GLU:OE1	1:D:247:GLU:N	2.50	0.44
1:A:247:GLU:OE1	1:A:247:GLU:N	2.50	0.44
1:A:200:GLU:N	5:A:502:HOH:O	2.50	0.43
1:D:179:THR:HB	1:D:271:GLN:HE21	1.83	0.43
1:B:179:THR:HB	1:B:271:GLN:HE21	1.83	0.43
1:D:86:LEU:HB3	1:D:90:LEU:HD12	2.00	0.42
1:C:86:LEU:HB3	1:C:90:LEU:HD12	2.01	0.42
1:A:304:TYR:CZ	1:A:311:LEU:HD21	2.55	0.42
1:B:304:TYR:CZ	1:B:311:LEU:HD21	2.55	0.42
1:B:247:GLU:HG2	1:D:328:ASP:HB3	2.02	0.41
1:D:304:TYR:CZ	1:D:311:LEU:HD21	2.55	0.41
1:B:86:LEU:HB3	1:B:90:LEU:HD12	2.02	0.41
1:C:119:ASN:O	1:C:119:ASN:ND2	2.51	0.41
1:C:304:TYR:CZ	1:C:311:LEU:HD21	2.55	0.41
1:A:86:LEU:HB3	1:A:90:LEU:HD12	2.01	0.41
1:C:24:ILE:HG13	1:C:90:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:ILE:HG13	1:D:90:LEU:HB3	2.03	0.41
1:A:24:ILE:HG13	1:A:90:LEU:HB3	2.03	0.41
1:A:177:LYS:HD2	1:A:217:TYR:CE1	2.56	0.40
1:B:24:ILE:HG13	1:B:90:LEU:HB3	2.04	0.40
1:B:62:ARG:HB3	1:C:62:ARG:HB3	2.04	0.40
1:C:295:ARG:NH1	5:C:2110:HOH:O	2.53	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	287/324 (89%)	276 (96%)	9 (3%)	2 (1%)	22	46
1	B	287/324 (89%)	275 (96%)	10 (4%)	2 (1%)	22	46
1	C	281/324 (87%)	273 (97%)	6 (2%)	2 (1%)	22	46
1	D	282/324 (87%)	271 (96%)	8 (3%)	3 (1%)	14	34
All	All	1137/1296 (88%)	1095 (96%)	33 (3%)	9 (1%)	19	43

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	19	VAL
1	B	63	ALA
1	C	63	ALA
1	D	63	ALA
1	A	63	ALA
1	A	324	ARG
1	B	324	ARG
1	C	324	ARG
1	D	324	ARG

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	248/274 (90%)	233 (94%)	15 (6%)	19	42
1	B	250/274 (91%)	231 (92%)	19 (8%)	13	30
1	C	247/274 (90%)	229 (93%)	18 (7%)	14	33
1	D	247/274 (90%)	231 (94%)	16 (6%)	17	38
All	All	992/1096 (90%)	924 (93%)	68 (7%)	16	35

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ILE
1	A	73	THR
1	A	98	THR
1	A	105	GLN
1	A	114	LEU
1	A	143	ASN
1	A	166	GLU
1	A	176	LEU
1	A	189	SER
1	A	207	VAL
1	A	290	LYS
1	A	298	ASP
1	A	306	ARG
1	A	316	ARG
1	A	321	ARG
1	B	62	ARG
1	B	73	THR
1	B	98	THR
1	B	114	LEU
1	B	118	THR
1	B	123	ILE
1	B	137	GLU
1	B	143	ASN
1	B	157	LYS

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Mol	Chain	Res	Type
1	B	166	GLU
1	B	176	LEU
1	B	181	GLU
1	B	189	SER
1	B	207	VAL
1	B	232	ARG
1	B	290	LYS
1	B	321	ARG
1	B	322	ARG
1	B	330	VAL
1	C	62	ARG
1	C	73	THR
1	C	98	THR
1	C	114	LEU
1	C	119	ASN
1	C	137	GLU
1	C	143	ASN
1	C	148[A]	ARG
1	C	148[B]	ARG
1	C	157	LYS
1	C	166	GLU
1	C	176	LEU
1	C	189	SER
1	C	207	VAL
1	C	271	GLN
1	C	290	LYS
1	C	316	ARG
1	C	321	ARG
1	D	23	ILE
1	D	62	ARG
1	D	73	THR
1	D	98	THR
1	D	114	LEU
1	D	118	THR
1	D	143	ASN
1	D	146	GLN
1	D	157	LYS
1	D	166	GLU
1	D	176	LEU
1	D	189	SER
1	D	207	VAL
1	D	306	ARG

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Mol	Chain	Res	Type
1	D	321	ARG
1	D	330	VAL

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

Mol	Chain	Res	Type
1	A	20	GLN
1	A	58	ASN
1	A	105	GLN
1	A	143	ASN
1	A	155	GLN
1	A	182	ASN
1	A	270	ASN
1	B	20	GLN
1	B	58	ASN
1	B	119	ASN
1	B	143	ASN
1	B	155	GLN
1	B	182	ASN
1	B	270	ASN
1	B	271	GLN
1	C	20	GLN
1	C	58	ASN
1	C	119	ASN
1	C	143	ASN
1	C	155	GLN
1	C	182	ASN
1	D	20	GLN
1	D	58	ASN
1	D	143	ASN
1	D	155	GLN
1	D	182	ASN
1	D	270	ASN
1	D	271	GLN

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
4	GOL	D	1001	-	5,5,5	0.42	0	5,5,5	0.32	0
3	QOV	A	402	-	21,25,25	0.81	0	28,37,37	2.83	11 (39%)
3	QOV	B	2001	-	21,25,25	0.92	1 (4%)	28,37,37	3.16	11 (39%)
3	QOV	D	1002	-	21,25,25	1.02	0	28,37,37	2.82	6 (21%)
2	TYR	A	401	-	11,12,13	0.59	0	12,15,17	0.28	0
3	QOV	C	2001	-	21,25,25	0.86	0	28,37,37	3.19	8 (28%)

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
4	GOL	D	1001	-	-	2/4/4/4	-
3	QOV	A	402	-	-	4/13/13/13	0/3/3/3
3	QOV	B	2001	-	-	6/13/13/13	0/3/3/3
3	QOV	D	1002	-	-	4/13/13/13	0/3/3/3
2	TYR	A	401	-	-	1/5/6/8	0/1/1/1
3	QOV	C	2001	-	-	6/13/13/13	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	QOV	C-S	-2.44	1.74	1.77

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2001	QOV	O1-S-O	-10.25	106.95	119.55
3	B	2001	QOV	O1-S-O	-10.03	107.22	119.55
3	C	2001	QOV	C12-O2-C2	9.78	132.30	117.53
3	D	1002	QOV	O1-S-O	-9.24	108.19	119.55
3	B	2001	QOV	C12-O2-C2	9.20	131.42	117.53
3	D	1002	QOV	C12-O2-C2	8.79	130.80	117.53
3	A	402	QOV	O1-S-O	-8.32	109.32	119.55
3	A	402	QOV	C12-O2-C2	7.75	129.22	117.53
3	B	2001	QOV	C-S-N	5.74	113.98	107.27
3	C	2001	QOV	O2-C2-C	5.33	120.64	116.50
3	D	1002	QOV	C-S-N	4.20	112.18	107.27
3	A	402	QOV	C-S-N	4.07	112.02	107.27
3	A	402	QOV	C1-C3-CL	3.61	123.66	119.15
3	A	402	QOV	O-S-C	3.51	113.43	107.66
3	B	2001	QOV	C6-C7-N	3.26	120.12	115.50
3	D	1002	QOV	C6-C7-N	3.05	119.83	115.50
3	B	2001	QOV	C13-C11-N3	3.00	127.77	123.85
3	C	2001	QOV	C6-C7-N	2.86	119.56	115.50
3	C	2001	QOV	C-S-N	2.75	110.49	107.27
3	A	402	QOV	C6-C7-N	2.71	119.34	115.50
3	C	2001	QOV	C3-C1-C	2.66	121.71	119.36
3	A	402	QOV	O2-C2-C	2.62	118.53	116.50
3	D	1002	QOV	O1-S-C	2.57	111.89	107.66
3	B	2001	QOV	C5-C3-C1	-2.47	118.25	121.53
3	D	1002	QOV	C7-N-S	2.46	131.41	124.20
3	B	2001	QOV	C7-N-S	2.35	131.08	124.20
3	C	2001	QOV	C5-C3-C1	-2.33	118.44	121.53
3	A	402	QOV	C1-C-S	2.29	122.54	118.51
3	B	2001	QOV	O2-C2-C	2.24	118.24	116.50
3	A	402	QOV	C2-C-S	-2.20	117.80	120.62
3	B	2001	QOV	C9-C7-C6	-2.19	115.89	119.68
3	A	402	QOV	C9-C7-C6	-2.13	115.99	119.68
3	B	2001	QOV	O-S-C	2.06	111.05	107.66
3	A	402	QOV	C13-C11-N3	2.04	126.51	123.85
3	C	2001	QOV	C9-C7-C6	-2.02	116.17	119.68
3	B	2001	QOV	C5-C3-CL	2.01	122.49	119.35

There are no chirality outliers.

All (23) torsion outliers are listed below:

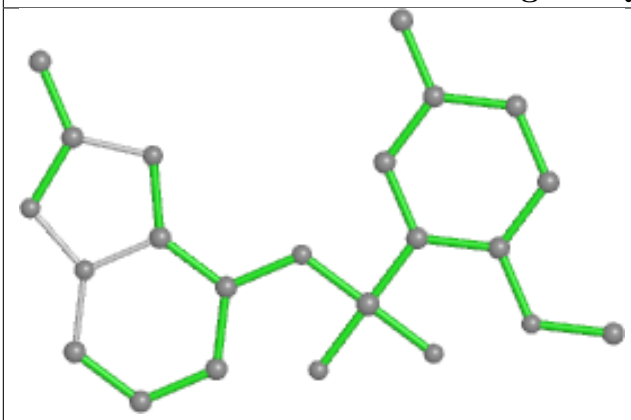
Mol	Chain	Res	Type	Atoms
2	A	401	TYR	O-C-CA-CB
3	A	402	QOV	C2-C-S-O
3	A	402	QOV	C2-C-S-N
3	B	2001	QOV	C2-C-S-N
3	C	2001	QOV	C-C2-O2-C12
3	C	2001	QOV	C2-C-S-N
3	D	1002	QOV	C2-C-S-N
4	D	1001	GOL	O1-C1-C2-C3
3	C	2001	QOV	C4-C2-O2-C12
3	A	402	QOV	C1-C-S-N
3	B	2001	QOV	C1-C-S-N
3	C	2001	QOV	C1-C-S-N
3	D	1002	QOV	C1-C-S-N
4	D	1001	GOL	O1-C1-C2-O2
3	A	402	QOV	C1-C-S-O
3	B	2001	QOV	C-C2-O2-C12
3	B	2001	QOV	C4-C2-O2-C12
3	C	2001	QOV	C1-C-S-O
3	C	2001	QOV	C2-C-S-O
3	D	1002	QOV	C7-N-S-O1
3	D	1002	QOV	C1-C-S-O
3	B	2001	QOV	C1-C-S-O
3	B	2001	QOV	C2-C-S-O

There are no ring outliers.

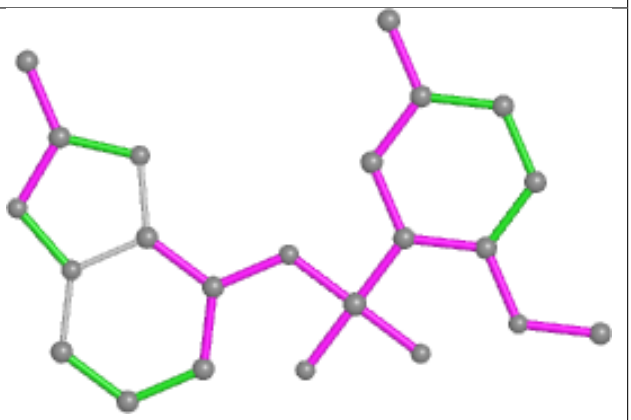
No monomer is involved in short contacts.

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 then 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.

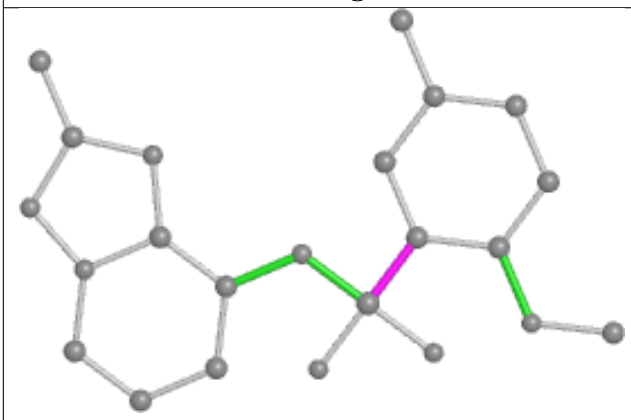
Ligand QOV A 402



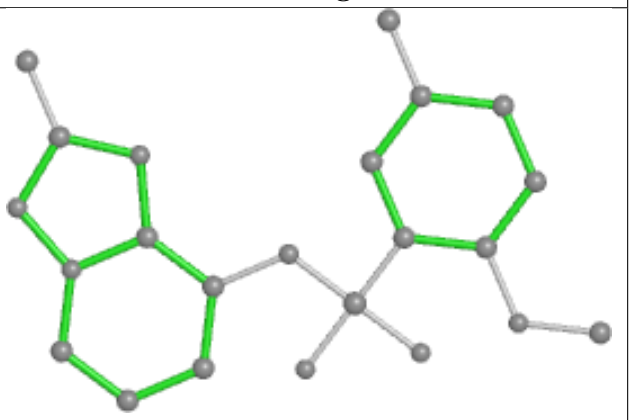
Bond lengths



Bond angles

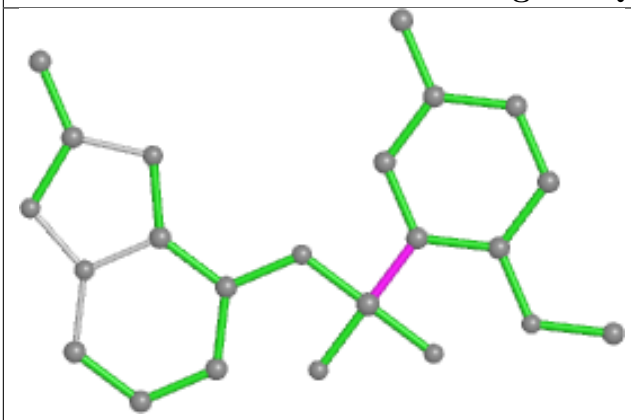


Torsions

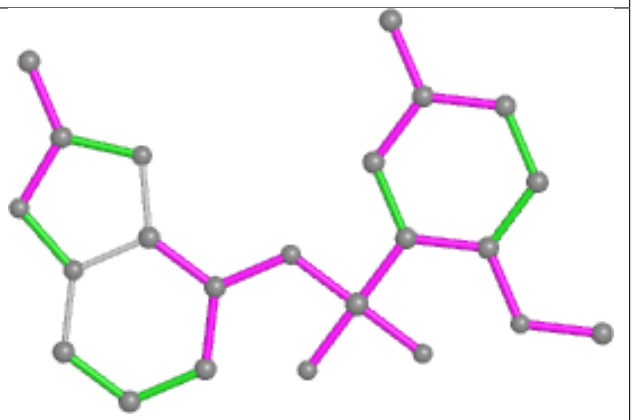


Rings

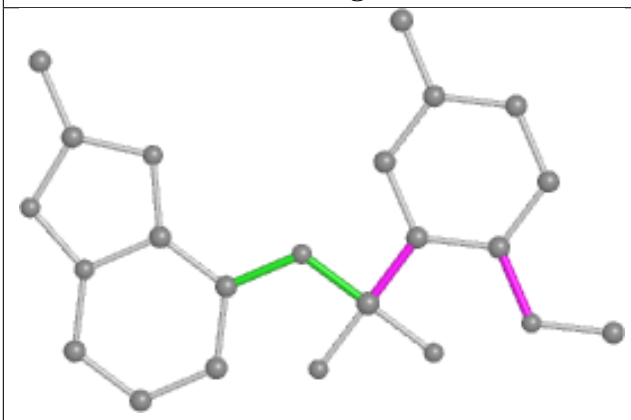
Ligand QOV B 2001



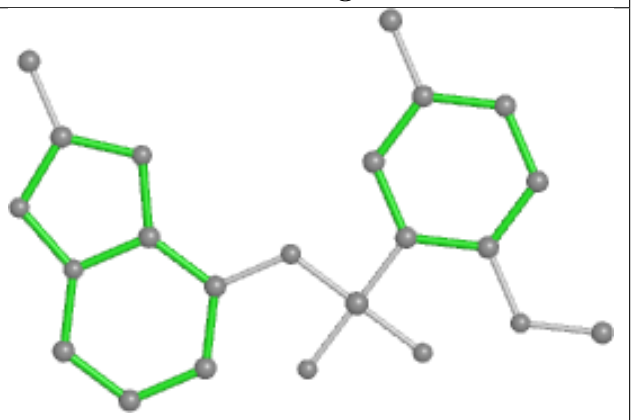
Bond lengths



Bond angles

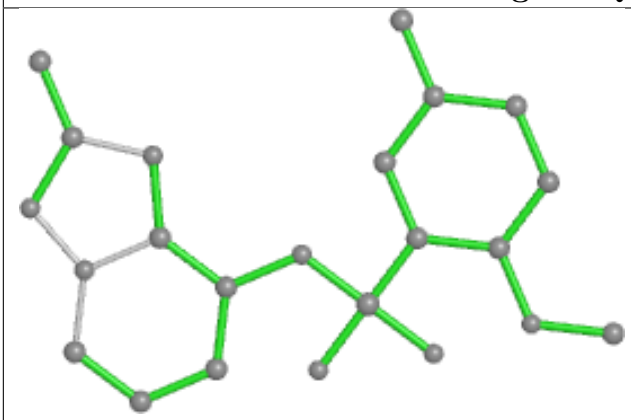


Torsions

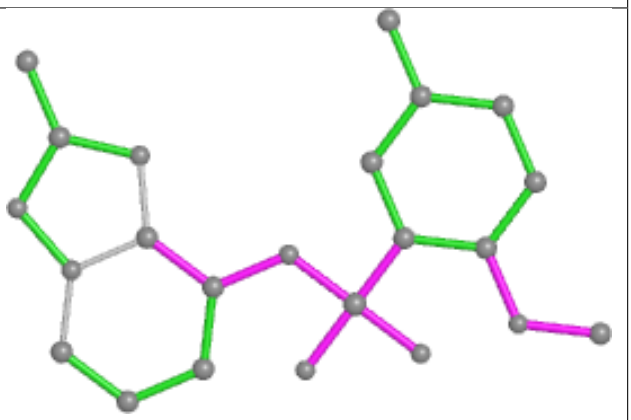


Rings

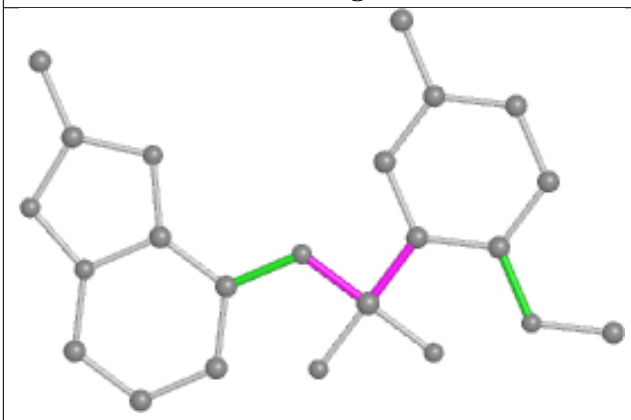
Ligand QOV D 1002



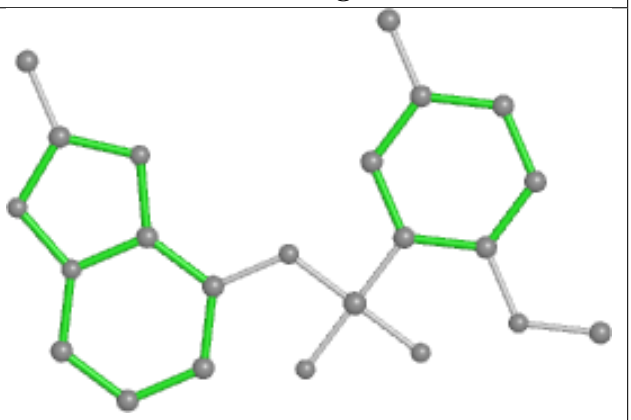
Bond lengths



Bond angles

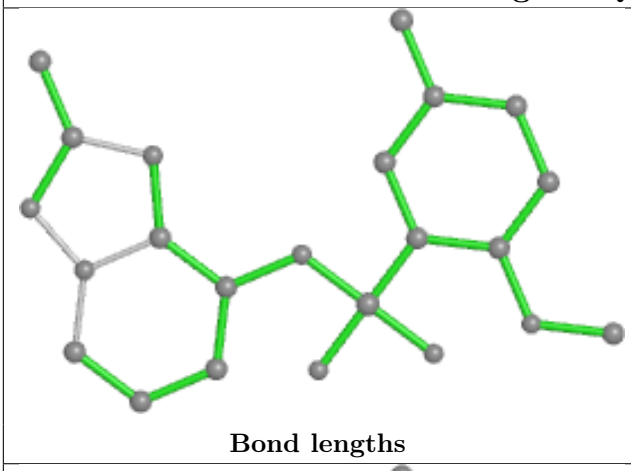


Torsions

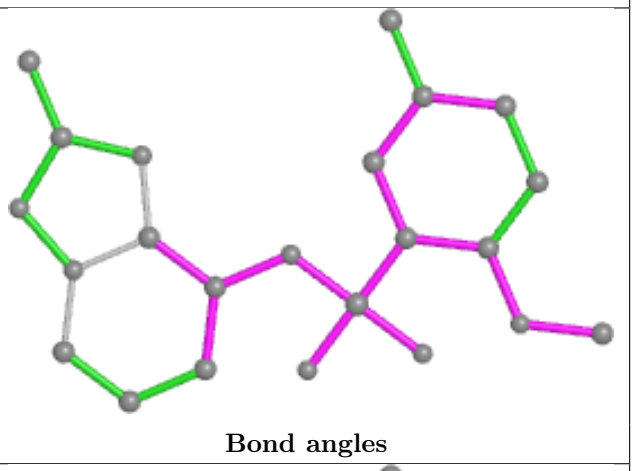


Rings

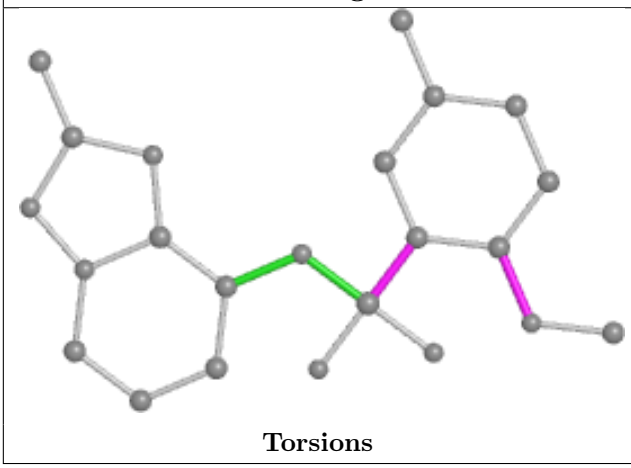
Ligand QOV C 2001



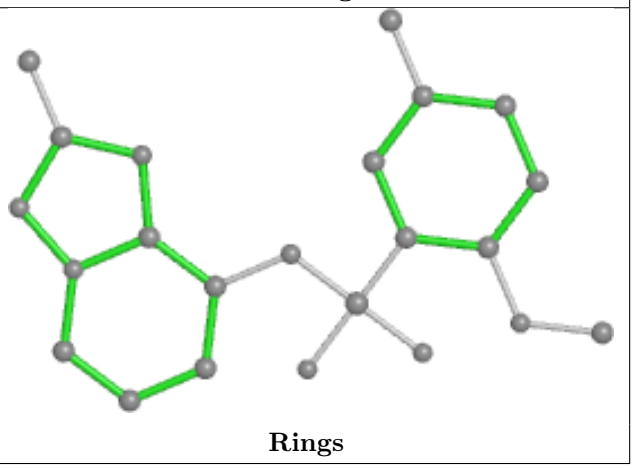
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	293/324 (90%)	0.59	25 (8%) 10 9	25, 51, 85, 104	0
1	B	295/324 (91%)	0.71	29 (9%) 7 5	29, 52, 85, 98	0
1	C	290/324 (89%)	0.81	38 (13%) 3 2	27, 54, 86, 100	0
1	D	290/324 (89%)	0.86	33 (11%) 5 4	31, 57, 89, 101	0
All	All	1168/1296 (90%)	0.74	125 (10%) 6 4	25, 54, 87, 104	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	155	GLN	7.3
1	C	314	ALA	6.6
1	B	166	GLU	6.0
1	A	42	GLY	5.0
1	B	155	GLN	4.9
1	C	142	ASN	4.7
1	C	242	GLU	4.6
1	B	156	ALA	4.5
1	A	155	GLN	4.3
1	C	42	GLY	4.3
1	C	168	ASN	4.2
1	C	313	ALA	4.2
1	B	98	THR	4.2
1	C	322	ARG	3.9
1	C	156	ALA	3.7
1	D	168	ASN	3.7
1	B	185	HIS	3.7
1	D	271	GLN	3.6
1	C	232	ARG	3.6
1	D	160	LYS	3.5
1	D	21	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	166	GLU	3.5
1	D	185	HIS	3.5
1	A	232	ARG	3.5
1	D	241	PRO	3.4
1	B	232	ARG	3.4
1	D	280	PRO	3.4
1	D	143	ASN	3.4
1	A	156	ALA	3.3
1	A	147	ASN	3.3
1	A	171	HIS	3.3
1	B	40	ARG	3.3
1	C	221	VAL	3.3
1	A	168	ASN	3.2
1	D	191	HIS	3.2
1	A	170	SER	3.2
1	D	98	THR	3.2
1	B	147	ASN	3.1
1	D	105	GLN	3.1
1	D	127	LEU	3.1
1	B	169	GLY	3.1
1	A	271	GLN	3.1
1	B	154	GLU	3.0
1	C	116	LYS	3.0
1	C	166	GLU	3.0
1	A	142	ASN	3.0
1	D	147	ASN	2.9
1	D	232	ARG	2.9
1	D	156	ALA	2.9
1	C	165	SER	2.9
1	C	280	PRO	2.8
1	D	44	PRO	2.8
1	A	116	LYS	2.8
1	B	165	SER	2.8
1	D	19	VAL	2.7
1	A	270	ASN	2.7
1	C	270	ASN	2.7
1	B	309	GLU	2.7
1	C	182	ASN	2.7
1	D	188	ASP	2.7
1	B	41	GLY	2.7
1	D	270	ASN	2.7
1	D	257	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	271	GLN	2.6
1	B	221	VAL	2.6
1	C	215	ASP	2.6
1	B	164	TRP	2.6
1	A	280	PRO	2.5
1	C	155	GLN	2.5
1	B	31	CYS	2.5
1	C	312	ARG	2.5
1	C	191	HIS	2.5
1	D	142	ASN	2.5
1	B	106	GLY	2.5
1	B	21	ARG	2.5
1	A	309	GLU	2.5
1	C	158	ALA	2.5
1	D	309	GLU	2.5
1	D	171	HIS	2.4
1	B	170	SER	2.4
1	D	208	VAL	2.4
1	B	168	ASN	2.4
1	B	280	PRO	2.4
1	A	210	ALA	2.4
1	C	170	SER	2.4
1	D	45	PRO	2.4
1	C	316	ARG	2.4
1	D	116	LYS	2.4
1	C	185	HIS	2.4
1	C	160	LYS	2.4
1	C	154	GLU	2.3
1	B	314	ALA	2.3
1	D	317	PHE	2.3
1	A	169	GLY	2.3
1	A	159	ALA	2.2
1	B	257	LEU	2.2
1	A	154	GLU	2.2
1	A	181	GLU	2.2
1	C	310	LYS	2.2
1	A	191	HIS	2.1
1	A	322	ARG	2.1
1	D	159	ALA	2.1
1	C	257	LEU	2.1
1	B	120	GLY	2.1
1	C	319	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	77	PRO	2.1
1	B	271	GLN	2.1
1	B	224	SER	2.1
1	C	328	ASP	2.1
1	D	104	PRO	2.1
1	B	160	LYS	2.1
1	B	310	LYS	2.1
1	D	27	VAL	2.1
1	C	318	ALA	2.1
1	C	309	GLU	2.1
1	D	106	GLY	2.1
1	A	44	PRO	2.0
1	C	241	PRO	2.0
1	A	18	THR	2.0
1	B	305	THR	2.0
1	A	208	VAL	2.0
1	D	189	SER	2.0
1	C	171	HIS	2.0
1	C	208	VAL	2.0
1	C	292	GLY	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 monosaccharides 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, 95^{th} 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
2	TYR	A	401	12/13	0.61	0.31	61,75,81,83	0
4	GOL	D	1001	6/6	0.78	0.69	83,86,90,91	0
3	QOV	D	1002	23/23	0.85	0.23	49,57,62,64	0

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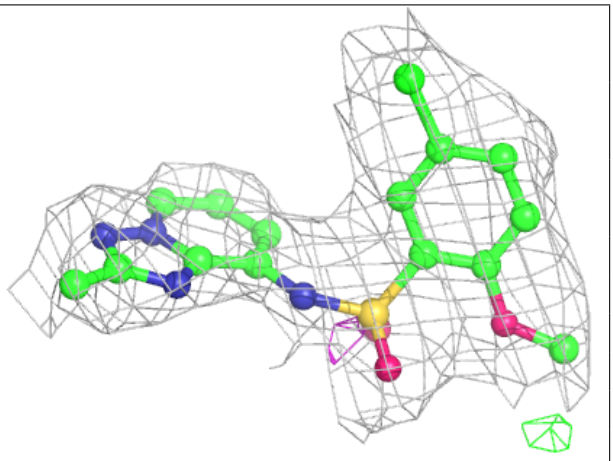
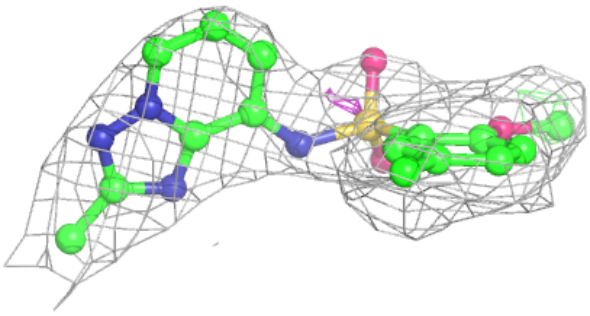
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	QOV	C	2001	23/23	0.94	0.14	41,44,47,47	0
3	QOV	B	2001	23/23	0.95	0.14	42,46,50,50	0
3	QOV	A	402	23/23	0.95	0.14	37,39,41,41	0

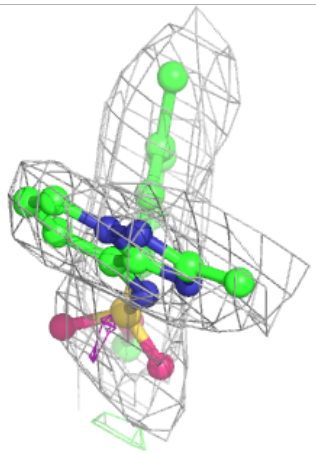
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QOV D 1002:

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

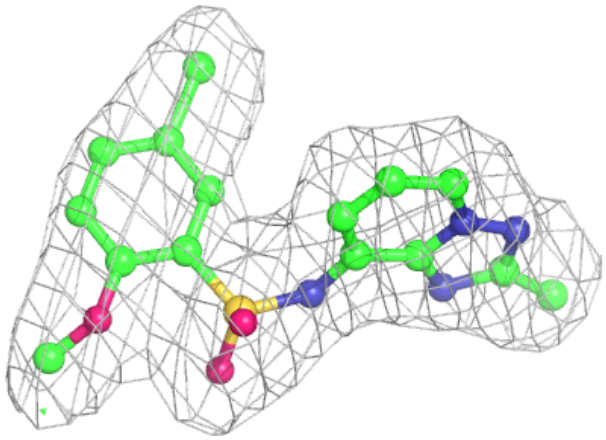


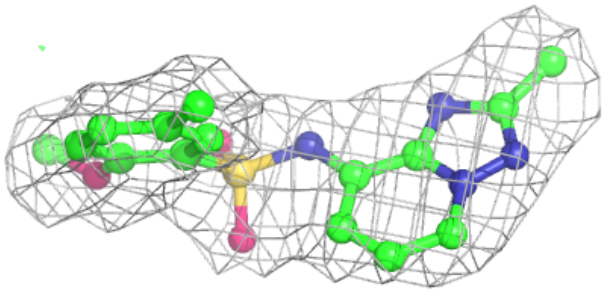


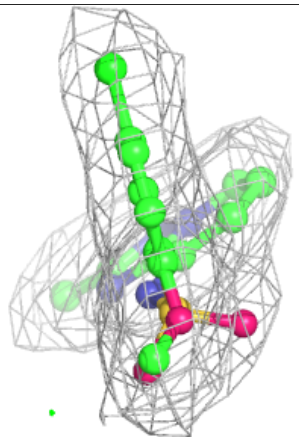


Electron density around QOV C 2001:

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

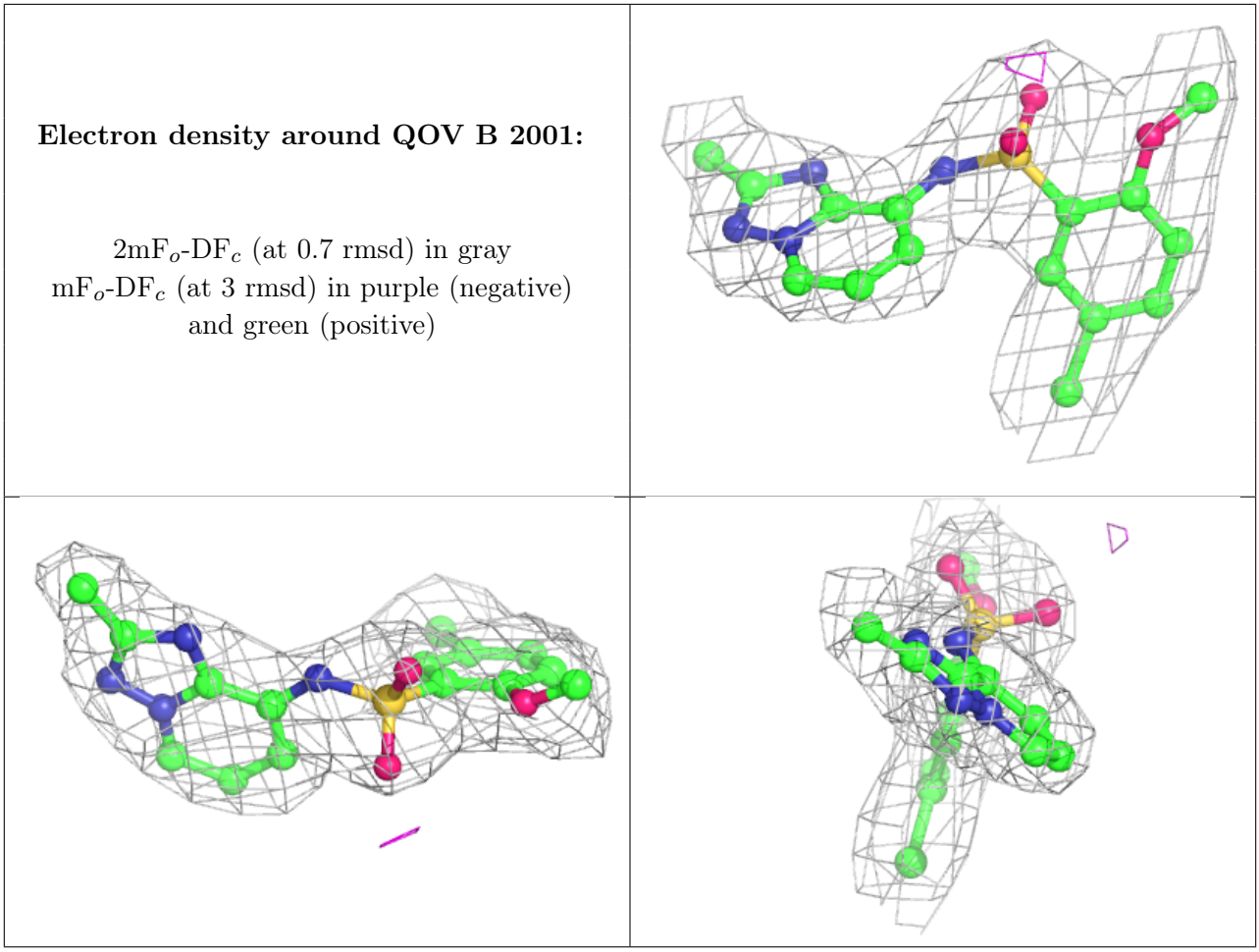






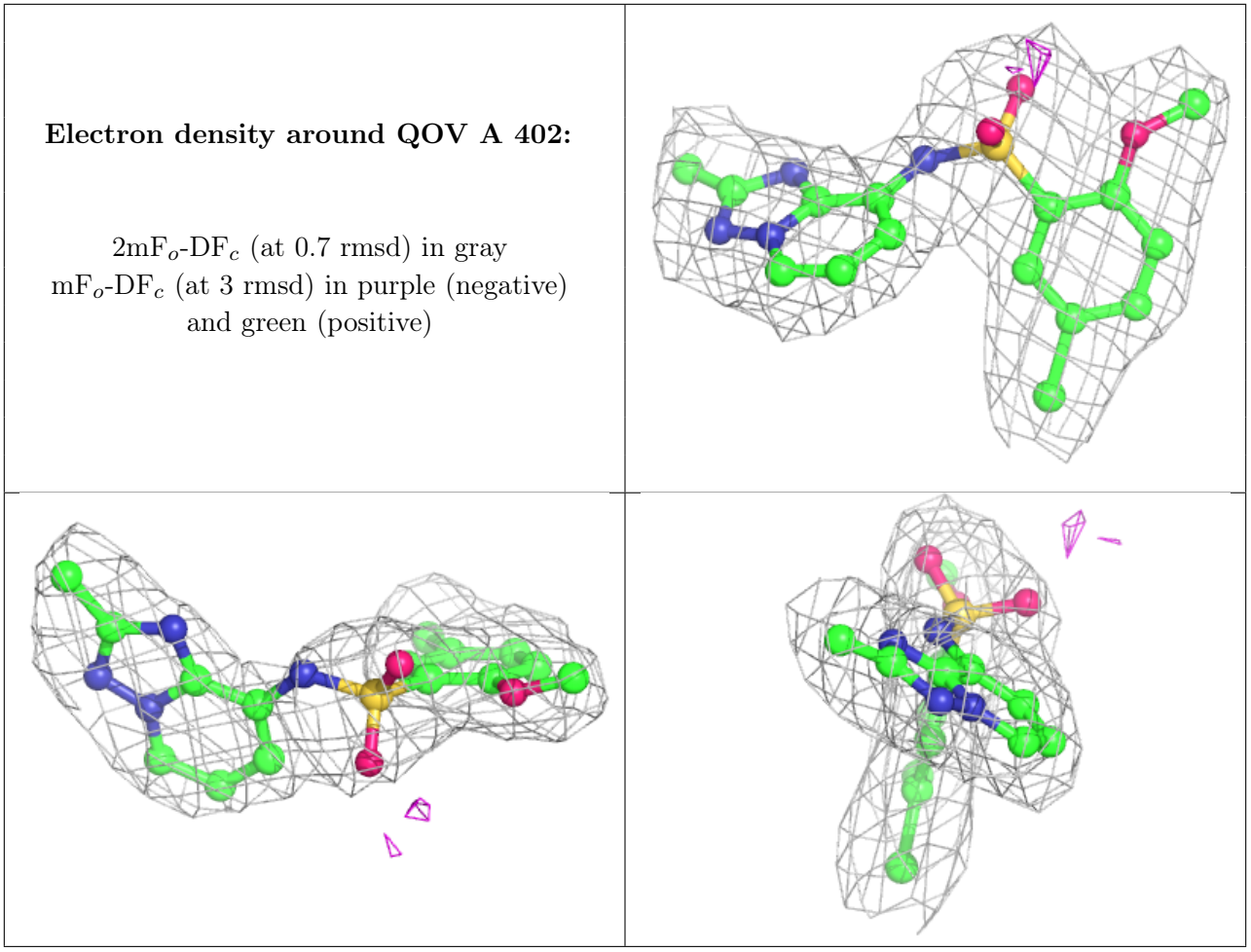
Electron density around QOV B 2001:

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



Electron density around QOV 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)



6.5 Other polymers

There are no such residues in this entry.