Full wwPDB X-ray Structure Validation Report (i)

Dec 1, 2021 – 02:03 PM EST

PDB ID	:	7KNW
Title	:	Crystal structure of SND1 in complex with C-26-A2
Authors	:	Kang, Y.
Deposited on	:	2020-11-06
Resolution	:	2.65 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

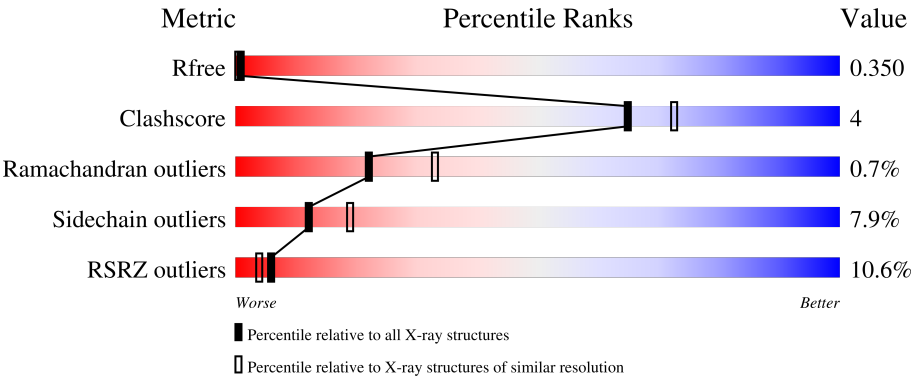
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	9% 78% 12% • 8%
1	B	324	10% 79% 11% • 9%
1	C	324	8% 80% 10% • 9%
1	D	324	11% 77% 12% • 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9991 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	298	Total	C	N	O	S	0	0	0
			2381	1494	445	432	10			
1	B	295	Total	C	N	O	S	0	0	0
			2353	1476	442	425	10			
1	C	296	Total	C	N	O	S	0	0	0
			2361	1483	440	428	10			
1	D	296	Total	C	N	O	S	0	1	0
			2369	1488	443	428	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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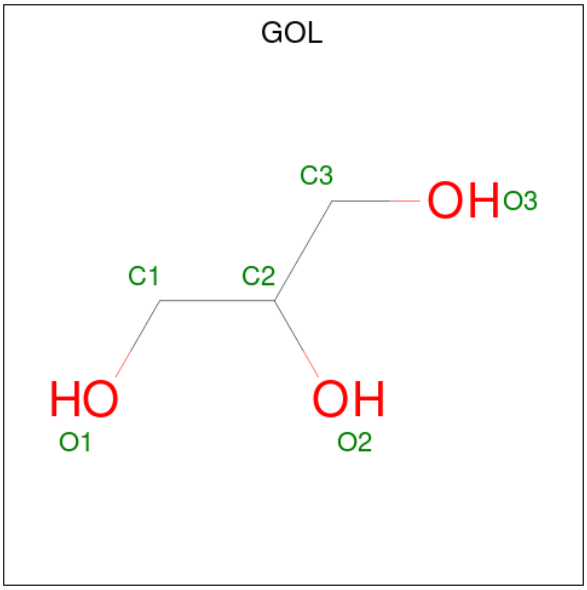
Chain	Residue	Modelled	Actual	Comment	Reference
D	8	GLY	-	expression tag	UNP Q7KZF4
D	9	GLU	-	expression tag	UNP Q7KZF4
D	10	ASN	-	expression tag	UNP Q7KZF4
D	11	LEU	-	expression tag	UNP Q7KZF4
D	12	TYR	-	expression tag	UNP Q7KZF4
D	13	PHE	-	expression tag	UNP Q7KZF4
D	14	GLN	-	expression tag	UNP Q7KZF4
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 GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0

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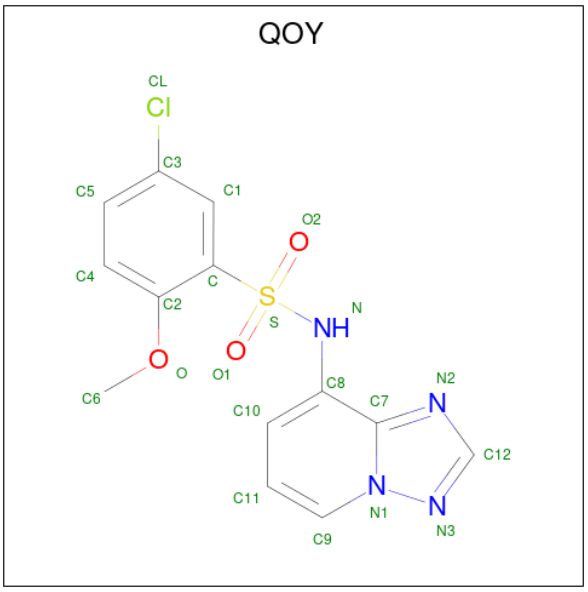
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 6 3 3	0	0

- Molecule 3 is 5-chloro-2-methoxy-N-([1,2,4]triazolo[1,5-a]pyridin-8-yl)benzene-1-sulfonamide (three-letter code: QOY) (formula: $C_{13}H_{11}ClN_4O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Cl N O S 22 13 1 4 3 1	0	0
3	B	1	Total C Cl N O S 22 13 1 4 3 1	0	0
3	C	1	Total C Cl N O S 22 13 1 4 3 1	0	0
3	D	1	Total C Cl N O S 22 13 1 4 3 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	109	Total O 109 109	0	0
4	B	121	Total O 121 121	0	0
4	C	86	Total O 86 86	0	0

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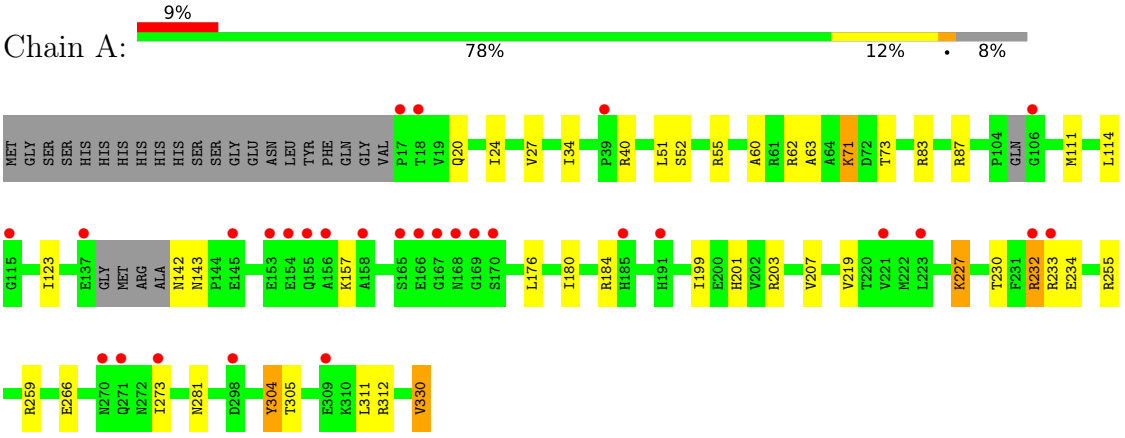
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	105	Total 105	O 105	0	0

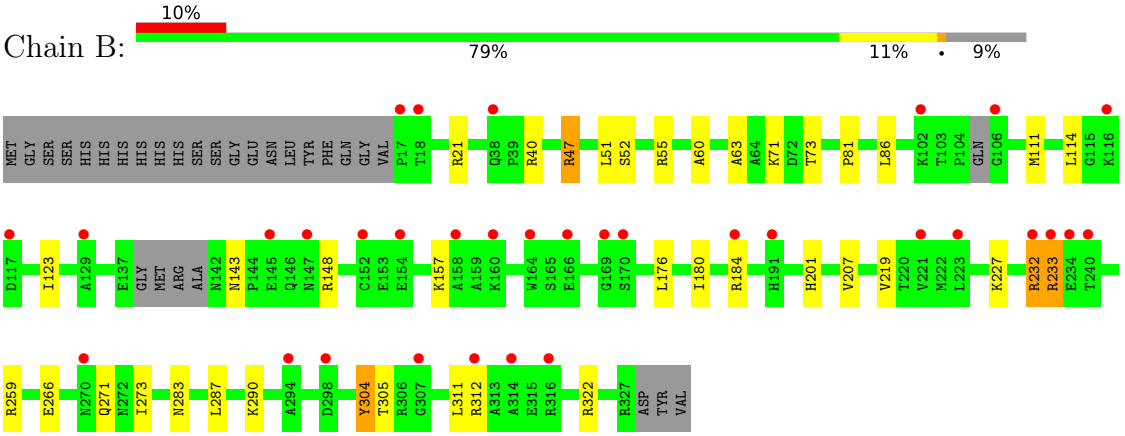
3 Residue-property plots (i)

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.

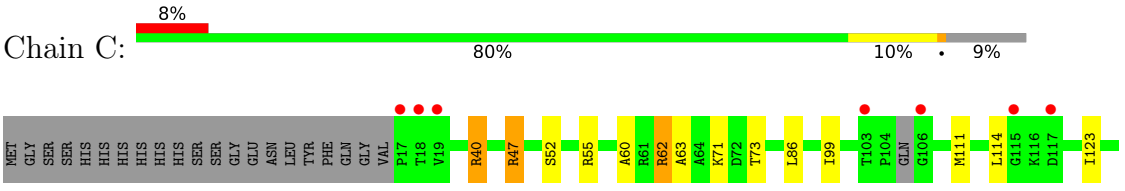
• Molecule 1: Staphylococcal nuclease domain-containing protein 1

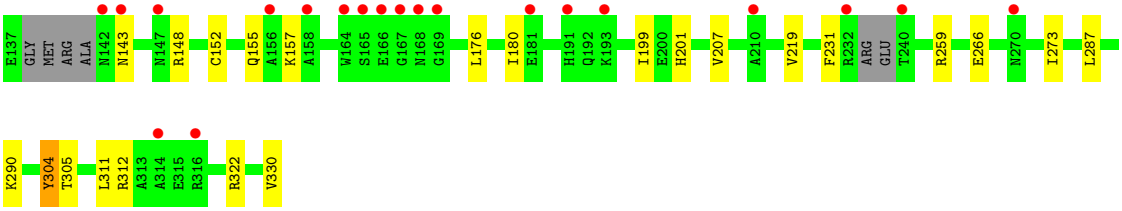


• Molecule 1: Staphylococcal nuclease domain-containing protein 1



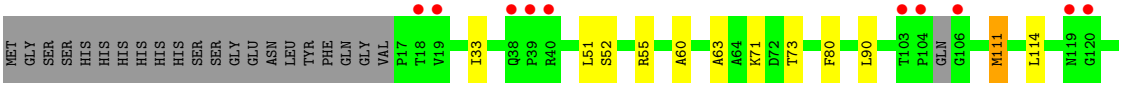
• Molecule 1: Staphylococcal nuclease domain-containing protein 1

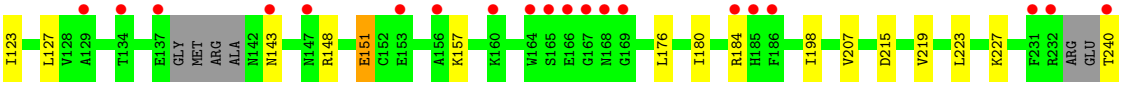


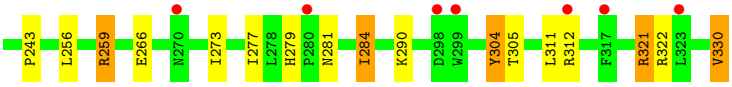


• Molecule 1: Staphylococcal nuclease domain-containing protein 1

Chain D:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	61.24Å 86.15Å 82.43Å 82.71° 72.00° 65.42°	Depositor
Resolution (Å)	30.00 – 2.65 26.12 – 2.65	Depositor EDS
% Data completeness (in resolution range)	91.4 (30.00-2.65) 91.5 (26.12-2.65)	Depositor EDS
R_{merge}	1.00	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 2.64Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.264 , 0.338 0.274 , 0.350	Depositor DCC
R_{free} test set	1995 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	34.4	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 69.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.026 for -h,-h+l,-h+k	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	9991	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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: GOL, QOY

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	0.50	0/2427	0.77	0/3272
1	B	0.50	0/2398	0.77	1/3233 (0.0%)
1	C	0.50	0/2406	0.74	0/3243
1	D	0.49	0/2417	0.79	4/3257 (0.1%)
All	All	0.50	0/9648	0.77	5/13005 (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	D	284	ILE	CG1-CB-CG2	6.35	125.37	111.40
1	D	321	ARG	NE-CZ-NH1	-6.29	117.16	120.30
1	D	111	MET	CA-CB-CG	5.69	122.97	113.30
1	D	321	ARG	NE-CZ-NH2	5.63	123.11	120.30
1	B	47	ARG	CA-CB-CG	5.11	124.64	113.40

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	2381	0	2402	23	0
1	B	2353	0	2380	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2361	0	2382	16	0
1	D	2369	0	2395	28	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	D	6	0	8	0	0
3	A	22	0	0	1	0
3	B	22	0	0	1	0
3	C	22	0	0	1	0
3	D	22	0	0	1	0
4	A	109	0	0	13	0
4	B	121	0	0	3	1
4	C	86	0	0	4	0
4	D	105	0	0	11	1
All	All	9991	0	9583	78	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 4.

All (78) 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:D:284:ILE:HG23	3:D:1002:QOY:CL	1.99	1.00
1:A:199:ILE:HG22	4:A:1102:HOH:O	1.62	0.99
1:A:201:HIS:N	4:A:1102:HOH:O	2.00	0.92
1:A:83:ARG:O	4:A:1101:HOH:O	1.93	0.86
1:C:199:ILE:HG22	4:C:2106:HOH:O	1.80	0.82
1:A:87:ARG:N	4:A:1101:HOH:O	2.14	0.79
1:D:277:ILE:HD12	1:D:284:ILE:HD11	1.67	0.76
1:D:127:LEU:HA	4:D:1144:HOH:O	1.85	0.76
1:A:51:LEU:HD21	1:A:123:ILE:HD11	1.70	0.74
1:D:51:LEU:HD21	1:D:123:ILE:HD11	1.71	0.72
1:A:34:ILE:O	4:A:1103:HOH:O	2.07	0.71
1:D:223:LEU:HD11	1:D:284:ILE:HD12	1.74	0.67
1:B:51:LEU:HD23	4:B:1116:HOH:O	1.94	0.66
1:A:27:VAL:HG11	4:A:1101:HOH:O	1.97	0.65
1:A:20:GLN:NE2	4:A:1104:HOH:O	2.32	0.63
1:B:283:ASN:ND2	4:B:1102:HOH:O	2.33	0.62
1:D:198:ILE:CD1	4:D:1158:HOH:O	2.53	0.55
1:D:304:TYR:CZ	1:D:311:LEU:HD21	2.42	0.55
1:C:304:TYR:CZ	1:C:311:LEU:HD21	2.42	0.55
1:A:304:TYR:CZ	1:A:311:LEU:HD21	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:TYR:CZ	1:B:311:LEU:HD21	2.42	0.54
1:D:279:HIS:HD1	1:D:281:ASN:H	1.54	0.54
1:D:198:ILE:HD12	4:D:1158:HOH:O	2.07	0.53
1:D:33:ILE:CD1	4:D:1198:HOH:O	2.56	0.53
1:C:152:CYS:HA	1:C:155:GLN:HE21	1.73	0.53
1:D:240:THR:HG23	4:D:1180:HOH:O	2.09	0.52
1:B:287:LEU:HD12	3:B:1002:QOY:CL	2.48	0.51
1:A:203:ARG:HG2	4:A:1132:HOH:O	2.11	0.50
1:D:223:LEU:CD1	1:D:284:ILE:HD12	2.43	0.49
1:B:232:ARG:HB2	1:B:233:ARG:NE	2.27	0.49
1:D:90:LEU:CD1	4:D:1198:HOH:O	2.60	0.49
1:D:80:PHE:HZ	4:D:1158:HOH:O	1.96	0.49
1:A:281:ASN:HD21	1:D:240:THR:HG22	1.77	0.48
1:D:180:ILE:CD1	1:D:273:ILE:HD11	2.43	0.48
1:C:201:HIS:N	4:C:2106:HOH:O	2.47	0.48
1:A:180:ILE:CD1	1:A:273:ILE:HD11	2.44	0.48
1:A:230:THR:HG23	1:A:232:ARG:HD3	1.95	0.48
1:B:86:LEU:HD22	1:B:123:ILE:CG2	2.44	0.48
1:B:180:ILE:CD1	1:B:273:ILE:HD11	2.44	0.48
1:C:180:ILE:CD1	1:C:273:ILE:HD11	2.44	0.48
1:B:60:ALA:CB	1:B:176:LEU:HD12	2.44	0.47
1:B:81:PRO:O	4:B:1101:HOH:O	2.20	0.47
1:B:232:ARG:C	1:B:233:ARG:HG2	2.35	0.47
1:C:219:VAL:HG21	1:C:273:ILE:HD12	1.97	0.47
1:A:219:VAL:HG21	1:A:273:ILE:HD12	1.95	0.47
1:C:86:LEU:HD22	1:C:123:ILE:CG2	2.45	0.47
1:A:60:ALA:CB	1:A:176:LEU:HD12	2.45	0.47
1:D:259[A]:ARG:CD	1:D:279:HIS:NE2	2.78	0.47
1:D:60:ALA:CB	1:D:176:LEU:HD12	2.44	0.47
1:C:60:ALA:CB	1:C:176:LEU:HD12	2.44	0.47
1:A:330:VAL:HG22	4:A:1118:HOH:O	2.15	0.46
1:C:231:PHE:HD1	4:C:2175:HOH:O	1.96	0.46
1:D:219:VAL:HG21	1:D:273:ILE:HD12	1.98	0.46
1:C:152:CYS:HA	1:C:155:GLN:NE2	2.30	0.46
1:B:219:VAL:HG21	1:B:273:ILE:HD12	1.96	0.46
1:D:330:VAL:HG22	4:D:1184:HOH:O	2.16	0.46
1:B:86:LEU:HD22	1:B:123:ILE:HG23	1.98	0.46
1:C:40:ARG:HD2	1:D:322:ARG:CZ	2.46	0.46
1:C:287:LEU:HD12	3:C:2001:QOY:CL	2.51	0.46
1:A:266:GLU:HG2	1:A:305:THR:HG23	1.99	0.45
1:B:266:GLU:HG2	1:B:305:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:GLU:HG2	1:C:305:THR:HG23	1.99	0.45
1:D:243:PRO:HB3	4:D:1182:HOH:O	2.16	0.44
1:D:223:LEU:HD11	1:D:284:ILE:CD1	2.43	0.44
1:D:256:LEU:HD11	1:D:284:ILE:HG12	1.99	0.44
1:D:266:GLU:HG2	1:D:305:THR:HG23	2.00	0.44
1:A:24:ILE:HG23	4:A:1103:HOH:O	2.17	0.44
1:A:27:VAL:HG21	4:A:1101:HOH:O	2.18	0.44
1:C:86:LEU:HD22	1:C:123:ILE:HG23	2.00	0.43
1:D:33:ILE:HD12	4:D:1198:HOH:O	2.17	0.43
1:C:62:ARG:HG3	4:C:2103:HOH:O	2.19	0.43
1:D:127:LEU:HD23	4:D:1144:HOH:O	2.19	0.43
1:D:151:GLU:OE2	1:D:151:GLU:HA	2.19	0.42
1:A:255:ARG:HB3	3:A:1002:QOY:C4	2.50	0.42
1:A:83:ARG:NH1	4:A:1107:HOH:O	2.45	0.41
1:A:71:LYS:HE2	1:B:201:HIS:CE1	2.56	0.41
1:A:227:LYS:NZ	4:A:1115:HOH:O	2.53	0.41
1:C:47:ARG:HH22	1:C:99:ILE:HD11	1.85	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)
4:B:1215:HOH:O	4:D:1189:HOH:O[1_545]	2.09	0.11

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	292/324 (90%)	280 (96%)	10 (3%)	2 (1%)	22	33
1	B	289/324 (89%)	277 (96%)	10 (4%)	2 (1%)	22	33
1	C	288/324 (89%)	277 (96%)	9 (3%)	2 (1%)	22	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	289/324 (89%)	279 (96%)	8 (3%)	2 (1%)	22 33
All	All	1158/1296 (89%)	1113 (96%)	37 (3%)	8 (1%)	22 33

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ALA
1	B	63	ALA
1	C	63	ALA
1	D	63	ALA
1	A	304	TYR
1	B	304	TYR
1	C	304	TYR
1	D	304	TYR

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	253/274 (92%)	233 (92%)	20 (8%)	12 19
1	B	250/274 (91%)	228 (91%)	22 (9%)	10 14
1	C	251/274 (92%)	233 (93%)	18 (7%)	14 22
1	D	252/274 (92%)	232 (92%)	20 (8%)	12 19
All	All	1006/1096 (92%)	926 (92%)	80 (8%)	12 18

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	52	SER
1	A	55	ARG
1	A	62	ARG
1	A	71	LYS
1	A	73	THR

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Mol	Chain	Res	Type
1	A	111	MET
1	A	114	LEU
1	A	142	ASN
1	A	143	ASN
1	A	157	LYS
1	A	184	ARG
1	A	207	VAL
1	A	227	LYS
1	A	232	ARG
1	A	233	ARG
1	A	234	GLU
1	A	259	ARG
1	A	312	ARG
1	A	330	VAL
1	B	21	ARG
1	B	40	ARG
1	B	47	ARG
1	B	52	SER
1	B	55	ARG
1	B	71	LYS
1	B	73	THR
1	B	111	MET
1	B	114	LEU
1	B	143	ASN
1	B	148	ARG
1	B	157	LYS
1	B	184	ARG
1	B	207	VAL
1	B	227	LYS
1	B	232	ARG
1	B	233	ARG
1	B	259	ARG
1	B	271	GLN
1	B	290	LYS
1	B	312	ARG
1	B	322	ARG
1	C	40	ARG
1	C	47	ARG
1	C	52	SER
1	C	55	ARG
1	C	62	ARG
1	C	71	LYS

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Mol	Chain	Res	Type
1	C	73	THR
1	C	111	MET
1	C	114	LEU
1	C	143	ASN
1	C	148	ARG
1	C	157	LYS
1	C	207	VAL
1	C	259	ARG
1	C	290	LYS
1	C	312	ARG
1	C	322	ARG
1	C	330	VAL
1	D	52	SER
1	D	55	ARG
1	D	71	LYS
1	D	73	THR
1	D	111	MET
1	D	114	LEU
1	D	143	ASN
1	D	148	ARG
1	D	151	GLU
1	D	157	LYS
1	D	184	ARG
1	D	207	VAL
1	D	215	ASP
1	D	227	LYS
1	D	259[A]	ARG
1	D	259[B]	ARG
1	D	290	LYS
1	D	312	ARG
1	D	321	ARG
1	D	330	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	119	ASN
1	A	142	ASN
1	A	143	ASN
1	A	146	GLN
1	A	147	ASN

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Mol	Chain	Res	Type
1	A	171	HIS
1	A	269	HIS
1	A	270	ASN
1	A	271	GLN
1	B	119	ASN
1	B	143	ASN
1	B	146	GLN
1	B	147	ASN
1	B	269	HIS
1	B	270	ASN
1	C	119	ASN
1	C	143	ASN
1	C	146	GLN
1	C	147	ASN
1	C	155	GLN
1	C	269	HIS
1	C	270	ASN
1	D	147	ASN
1	D	270	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 monosaccharides in this entry.

5.6 Ligand geometry

7 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	$\#\|Z\| > 2$
3	QOY	C	2001	-	19,24,24	1.20	1 (5%)	25,35,35	3.01	5 (20%)
3	QOY	B	1002	-	19,24,24	1.05	0	25,35,35	2.73	6 (24%)
3	QOY	A	1002	-	19,24,24	0.90	0	25,35,35	3.28	9 (36%)
3	QOY	D	1002	-	19,24,24	1.08	1 (5%)	25,35,35	3.89	7 (28%)
2	GOL	B	1001	-	5,5,5	0.33	0	5,5,5	0.57	0
2	GOL	A	1001	-	5,5,5	0.35	0	5,5,5	0.76	0
2	GOL	D	1001	-	5,5,5	0.23	0	5,5,5	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	QOY	C	2001	-	-	8/13/13/13	0/3/3/3
3	QOY	B	1002	-	-	7/13/13/13	0/3/3/3
3	QOY	A	1002	-	-	9/13/13/13	0/3/3/3
3	QOY	D	1002	-	-	9/13/13/13	0/3/3/3
2	GOL	B	1001	-	-	2/4/4/4	-
2	GOL	A	1001	-	-	0/4/4/4	-
2	GOL	D	1001	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1002	QOY	C-S	-2.23	1.74	1.77
3	C	2001	QOY	C-S	-2.19	1.74	1.77

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1002	QOY	C-S-N	13.08	122.56	107.27
3	C	2001	QOY	C-S-N	11.54	120.75	107.27
3	A	1002	QOY	O1-S-O2	-9.73	107.59	119.55
3	A	1002	QOY	C-S-N	9.36	118.20	107.27
3	B	1002	QOY	O1-S-O2	-8.84	108.68	119.55
3	D	1002	QOY	O1-S-O2	-8.36	109.27	119.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1002	QOY	C6-O-C2	7.83	129.34	117.53
3	B	1002	QOY	C-S-N	7.53	116.07	107.27
3	C	2001	QOY	O1-S-O2	-7.09	110.83	119.55
3	D	1002	QOY	O-C2-C	6.24	121.34	116.50
3	A	1002	QOY	C6-O-C2	4.94	124.98	117.53
3	B	1002	QOY	O-C2-C	4.15	119.72	116.50
3	C	2001	QOY	C6-O-C2	4.03	123.62	117.53
3	B	1002	QOY	C6-O-C2	3.11	122.23	117.53
3	A	1002	QOY	C10-C8-C7	-2.85	114.73	119.68
3	A	1002	QOY	O-C2-C	2.79	118.67	116.50
3	A	1002	QOY	C7-C8-N	2.75	119.40	115.50
3	C	2001	QOY	C10-C8-C7	-2.65	115.08	119.68
3	A	1002	QOY	C1-C3-CL	2.61	122.41	119.15
3	B	1002	QOY	C3-C1-C	2.59	121.64	119.36
3	D	1002	QOY	O-C2-C4	-2.56	119.98	124.37
3	A	1002	QOY	O1-S-C	-2.54	103.48	107.66
3	D	1002	QOY	O2-S-C	-2.30	103.88	107.66
3	C	2001	QOY	C7-C8-N	2.20	118.62	115.50
3	D	1002	QOY	C10-C8-C7	-2.14	115.96	119.68
3	A	1002	QOY	C1-C-S	2.12	122.24	118.51
3	B	1002	QOY	C10-C8-C7	-2.02	116.18	119.68

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1001	GOL	C1-C2-C3-O3
3	A	1002	QOY	C2-C-S-O2
3	A	1002	QOY	C2-C-S-N
3	B	1002	QOY	C2-C-S-O2
3	B	1002	QOY	C2-C-S-N
3	C	2001	QOY	C2-C-S-O2
3	C	2001	QOY	C2-C-S-N
3	D	1002	QOY	C2-C-S-O2
3	D	1002	QOY	C2-C-S-N
3	B	1002	QOY	C-C2-O-C6
3	B	1002	QOY	C1-C-S-O2
3	C	2001	QOY	C1-C-S-O2
3	A	1002	QOY	C1-C-S-N
3	B	1002	QOY	C1-C-S-N
3	C	2001	QOY	C1-C-S-N
3	D	1002	QOY	C-C2-O-C6

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Mol	Chain	Res	Type	Atoms
3	B	1002	QOY	C2-C-S-O1
3	D	1002	QOY	C1-C-S-N
3	D	1002	QOY	C8-N-S-O1
3	A	1002	QOY	C1-C-S-O2
2	B	1001	GOL	C1-C2-C3-O3
2	D	1001	GOL	O1-C1-C2-C3
3	D	1002	QOY	C1-C-S-O2
2	B	1001	GOL	O2-C2-C3-O3
2	D	1001	GOL	O2-C2-C3-O3
3	A	1002	QOY	C2-C-S-O1
3	C	2001	QOY	C2-C-S-O1
3	B	1002	QOY	C4-C2-O-C6
3	D	1002	QOY	C4-C2-O-C6
2	D	1001	GOL	O1-C1-C2-O2
3	C	2001	QOY	C8-N-S-O1
3	D	1002	QOY	C2-C-S-O1
3	A	1002	QOY	C10-C8-N-S
3	A	1002	QOY	C-C2-O-C6
3	C	2001	QOY	C-C2-O-C6
3	A	1002	QOY	C4-C2-O-C6
3	D	1002	QOY	C8-N-S-O2
3	A	1002	QOY	C8-N-S-O1
3	C	2001	QOY	C4-C2-O-C6

There are no ring outliers.

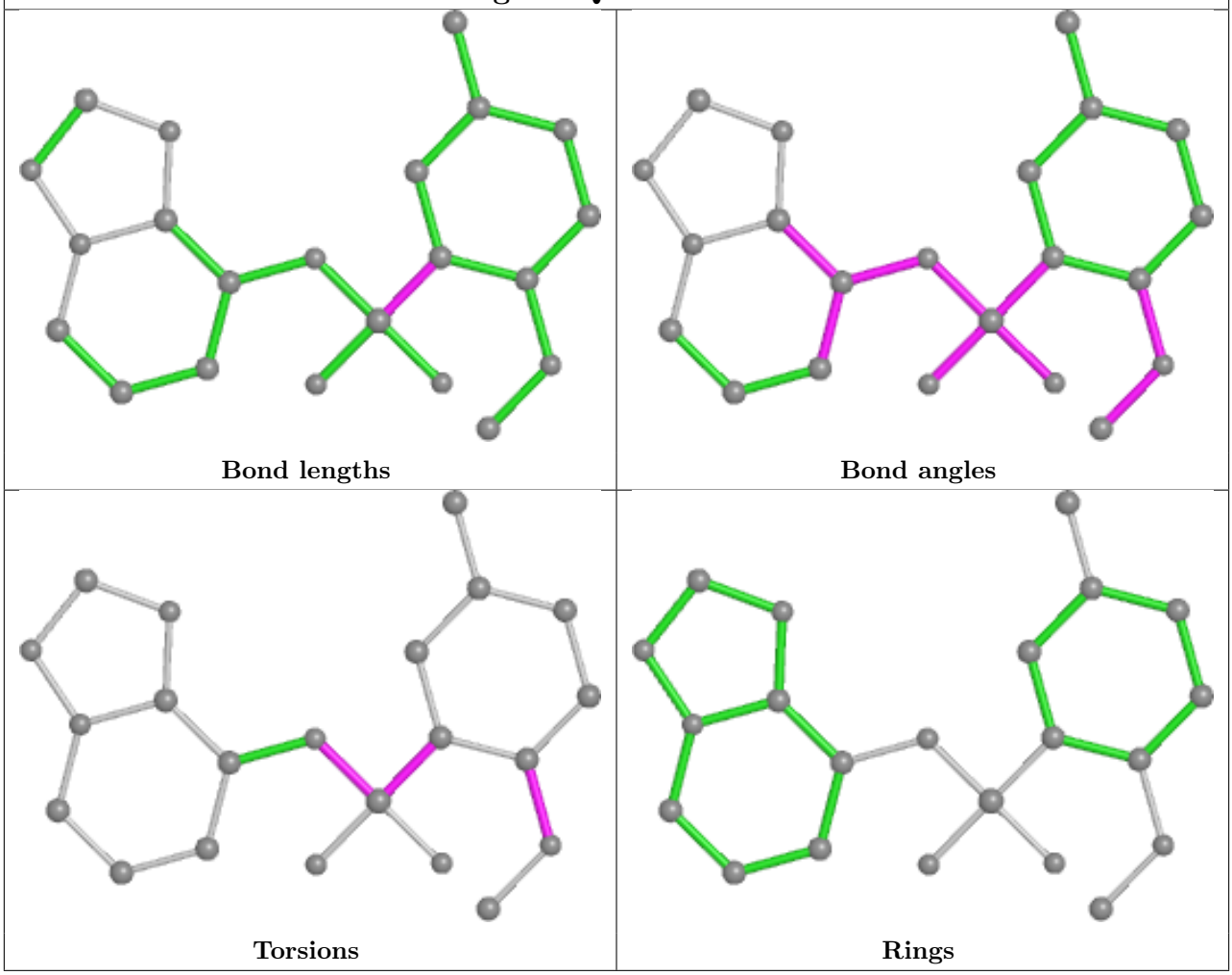
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2001	QOY	1	0
3	B	1002	QOY	1	0
3	A	1002	QOY	1	0
3	D	1002	QOY	1	0

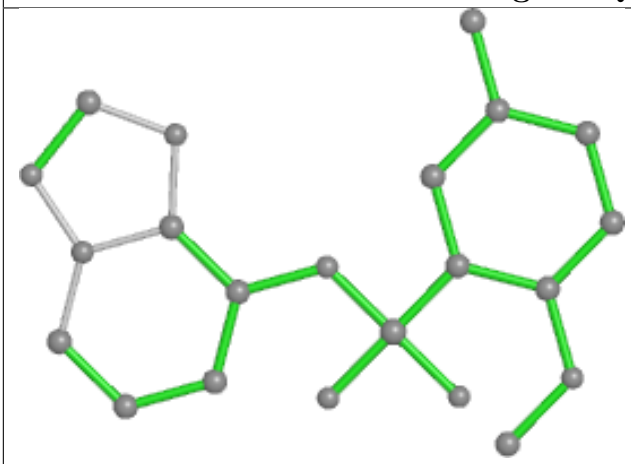
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

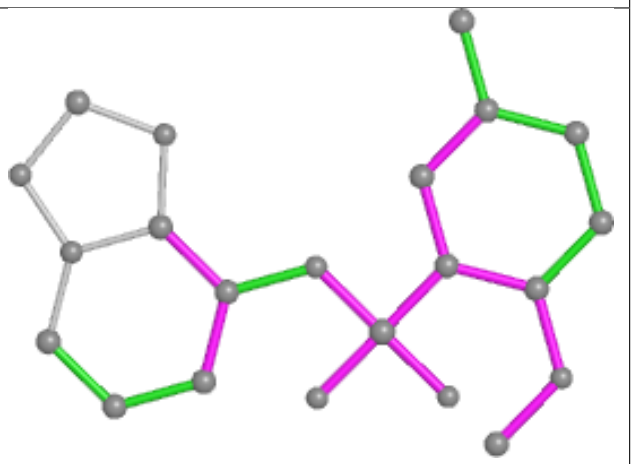
Ligand QOY C 2001



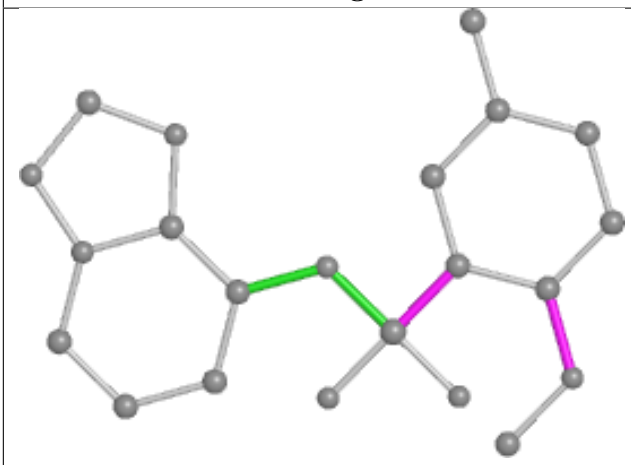
Ligand QOY B 1002



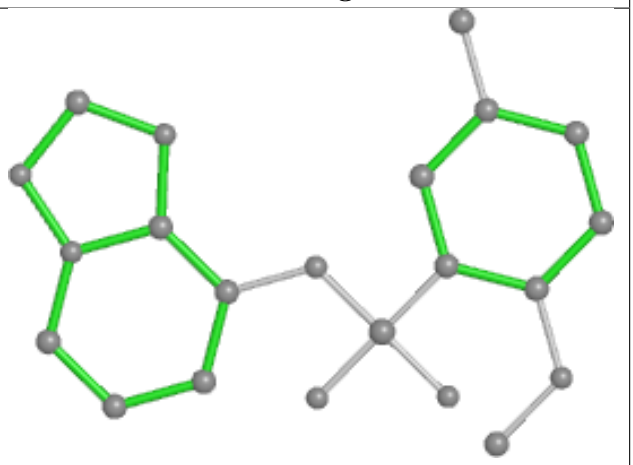
Bond lengths



Bond angles

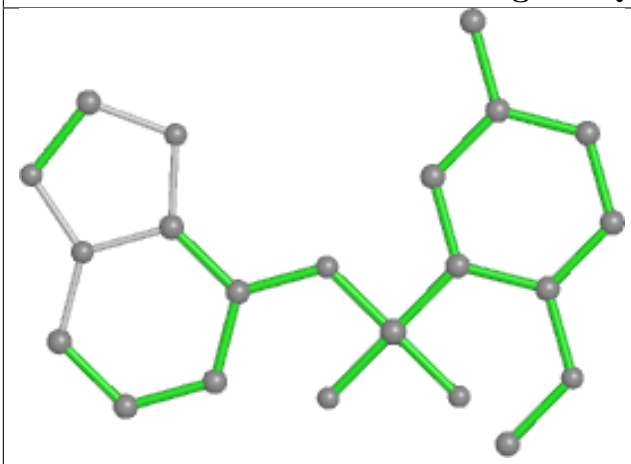


Torsions

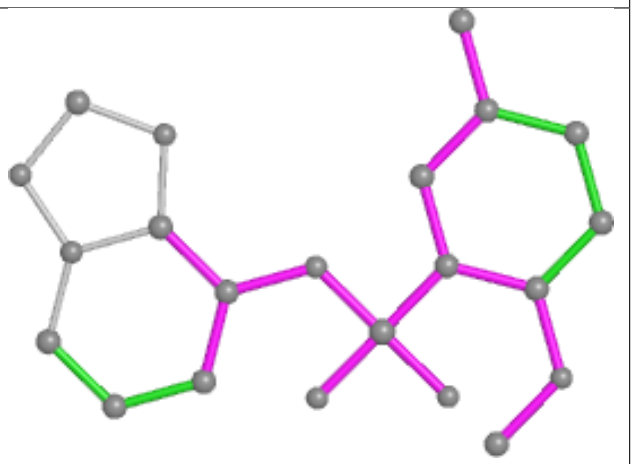


Rings

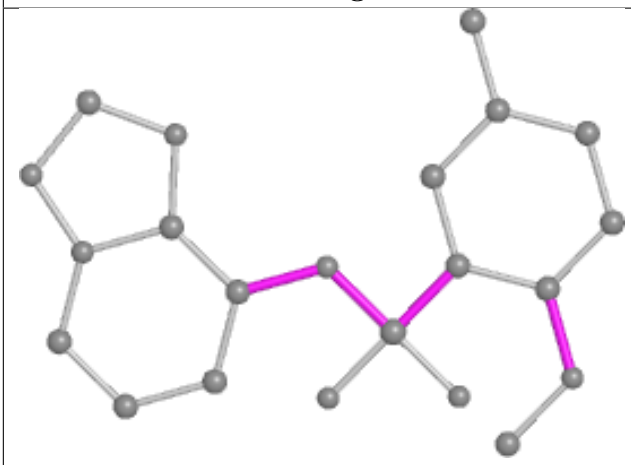
Ligand QOY A 1002



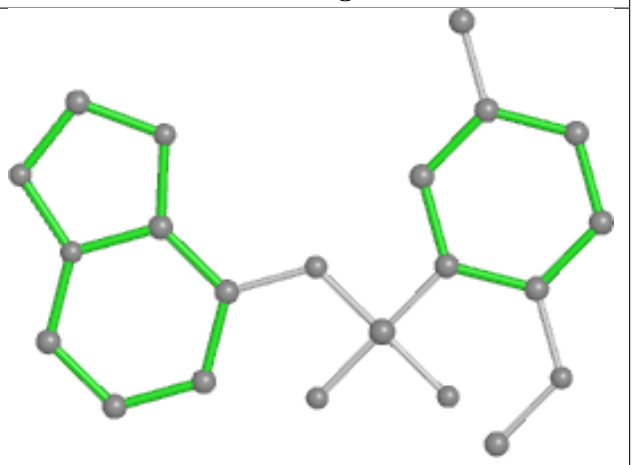
Bond lengths



Bond angles

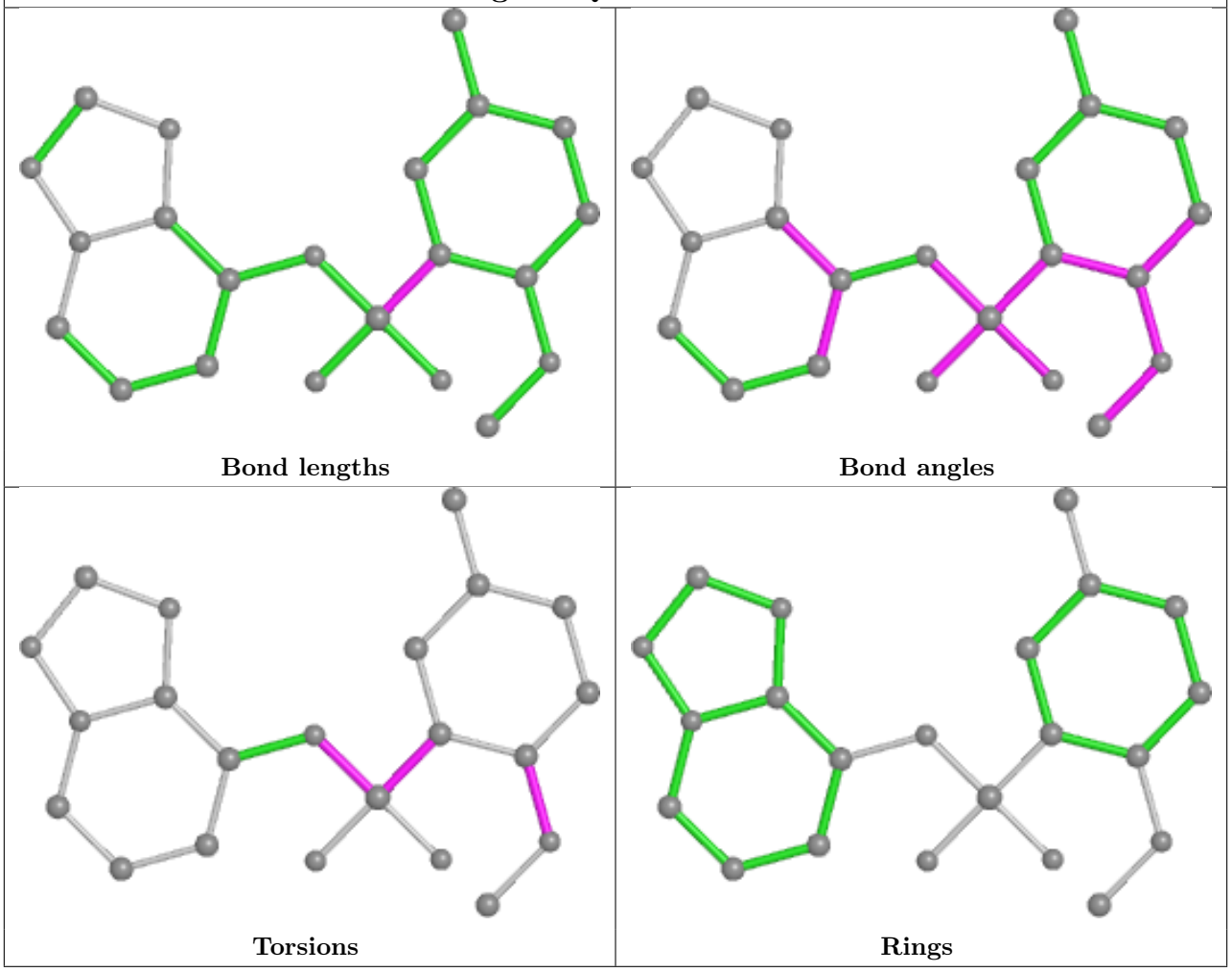


Torsions



Rings

Ligand QOY D 1002



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	298/324 (91%)	0.52	29 (9%) 7 6	18, 46, 85, 125	0
1	B	295/324 (91%)	0.65	33 (11%) 5 3	23, 49, 89, 121	0
1	C	296/324 (91%)	0.43	27 (9%) 9 7	18, 47, 81, 110	0
1	D	296/324 (91%)	0.74	37 (12%) 3 2	24, 52, 94, 110	0
All	All	1185/1296 (91%)	0.59	126 (10%) 6 4	18, 48, 87, 125	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	ALA	6.3
1	A	165	SER	5.2
1	B	234	GLU	5.0
1	D	167	GLY	4.9
1	B	17	PRO	4.8
1	B	18	THR	4.7
1	D	39	PRO	4.7
1	C	18	THR	4.6
1	B	106	GLY	4.6
1	D	168	ASN	4.5
1	B	158	ALA	4.5
1	A	166	GLU	4.4
1	D	19	VAL	4.4
1	B	166	GLU	4.2
1	A	233	ARG	4.2
1	C	147	ASN	4.2
1	A	168	ASN	4.1
1	B	160	LYS	4.0
1	C	166	GLU	4.0
1	D	166	GLU	4.0
1	B	233	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	116	LYS	4.0
1	D	165	SER	3.8
1	B	184	ARG	3.8
1	C	103	THR	3.7
1	B	147	ASN	3.7
1	C	106	GLY	3.6
1	A	17	PRO	3.6
1	A	298	ASP	3.5
1	B	232	ARG	3.5
1	A	309	GLU	3.5
1	C	17	PRO	3.4
1	B	223	LEU	3.4
1	B	298	ASP	3.4
1	D	317	PHE	3.4
1	A	232	ARG	3.3
1	B	221	VAL	3.3
1	A	169	GLY	3.3
1	D	147	ASN	3.3
1	D	270	ASN	3.3
1	D	106	GLY	3.2
1	B	240	THR	3.2
1	C	191	HIS	3.2
1	D	298	ASP	3.2
1	C	232	ARG	3.1
1	C	117	ASP	3.1
1	B	169	GLY	3.0
1	A	271	GLN	3.0
1	B	117	ASP	3.0
1	A	106	GLY	3.0
1	D	312	ARG	3.0
1	A	167	GLY	3.0
1	C	168	ASN	2.9
1	D	232	ARG	2.9
1	D	153	GLU	2.9
1	D	186	PHE	2.9
1	C	181	GLU	2.8
1	D	120	GLY	2.8
1	A	221	VAL	2.8
1	D	18	THR	2.8
1	C	142	ASN	2.8
1	B	316	ARG	2.8
1	B	191	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	145	GLU	2.7
1	D	185	HIS	2.7
1	A	155	GLN	2.7
1	B	170	SER	2.7
1	A	115	GLY	2.7
1	D	156	ALA	2.7
1	A	223	LEU	2.6
1	A	158	ALA	2.6
1	B	270	ASN	2.6
1	D	160	LYS	2.6
1	C	316	ARG	2.6
1	C	156	ALA	2.6
1	B	38	GLN	2.6
1	D	184	ARG	2.6
1	C	169	GLY	2.5
1	D	164	TRP	2.5
1	B	102	LYS	2.5
1	B	129	ALA	2.4
1	C	165	SER	2.4
1	D	169	GLY	2.4
1	A	145	GLU	2.4
1	D	143	ASN	2.4
1	D	38	GLN	2.3
1	C	115	GLY	2.3
1	A	18	THR	2.3
1	B	154	GLU	2.3
1	A	170	SER	2.3
1	C	193	LYS	2.3
1	A	191	HIS	2.3
1	A	137	GLU	2.3
1	A	270	ASN	2.3
1	B	152	CYS	2.3
1	A	273	ILE	2.3
1	D	299	TRP	2.2
1	B	294	ALA	2.2
1	C	314	ALA	2.2
1	C	143	ASN	2.2
1	D	40	ARG	2.2
1	C	210	ALA	2.2
1	B	314	ALA	2.2
1	D	119	ASN	2.2
1	A	153	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	103	THR	2.2
1	D	240	THR	2.2
1	A	185	HIS	2.1
1	D	323	LEU	2.1
1	B	312	ARG	2.1
1	C	158	ALA	2.1
1	A	154	GLU	2.1
1	D	129	ALA	2.1
1	C	270	ASN	2.1
1	D	137	GLU	2.1
1	D	134	THR	2.1
1	A	39	PRO	2.1
1	C	240	THR	2.1
1	C	19	VAL	2.0
1	D	104	PRO	2.0
1	B	307	GLY	2.0
1	C	164	TRP	2.0
1	D	280	PRO	2.0
1	C	167	GLY	2.0
1	D	231	PHE	2.0
1	B	164	TRP	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	GOL	B	1001	6/6	0.89	0.33	43,54,57,62	0
3	QOY	D	1002	22/22	0.89	0.20	35,44,52,56	0

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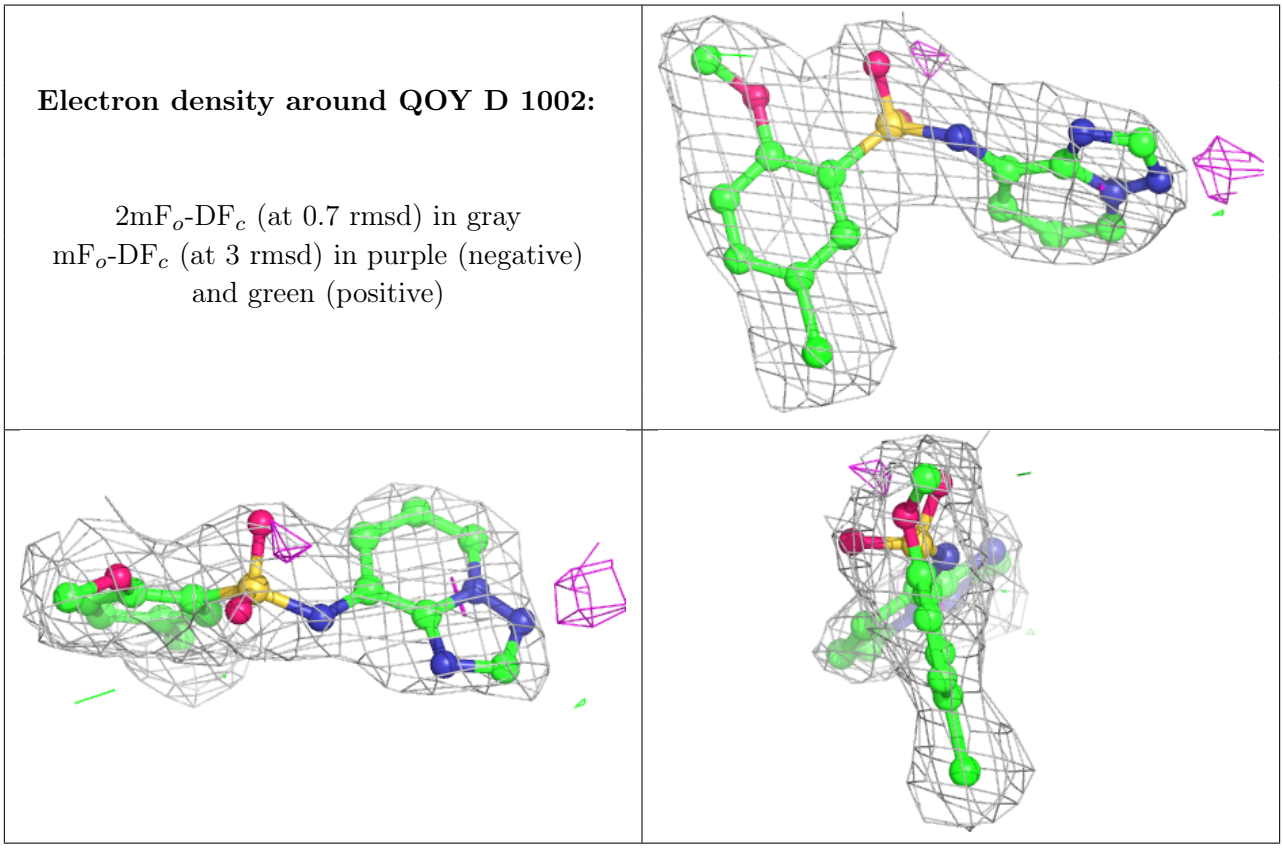
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	A	1001	6/6	0.90	0.27	29,41,42,45	0
3	QOY	B	1002	22/22	0.93	0.15	38,44,46,51	0
2	GOL	D	1001	6/6	0.93	0.25	28,45,48,50	0
3	QOY	C	2001	22/22	0.94	0.15	27,35,44,49	0
3	QOY	A	1002	22/22	0.96	0.13	22,28,37,39	0

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.

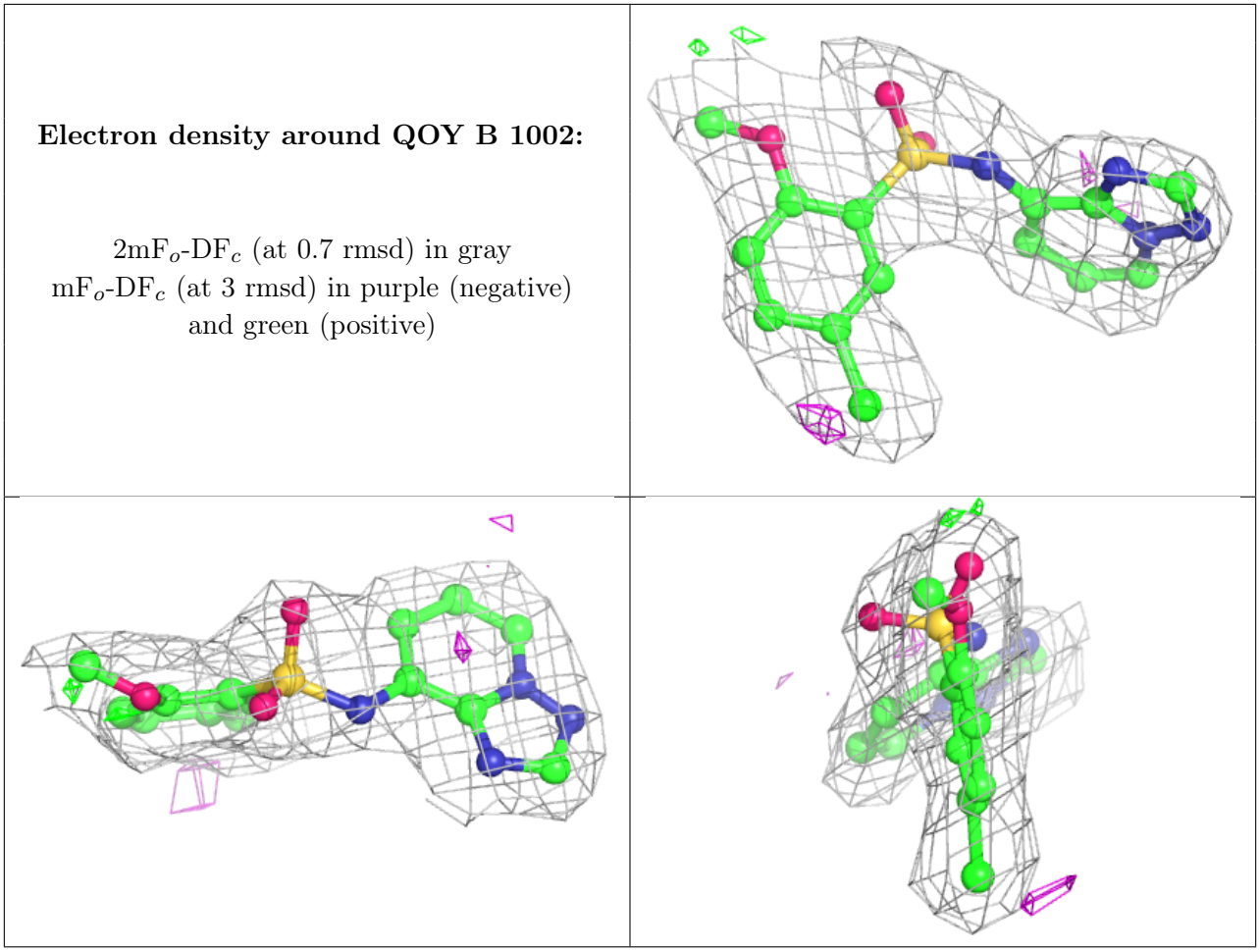
Electron density around QOY D 1002:

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



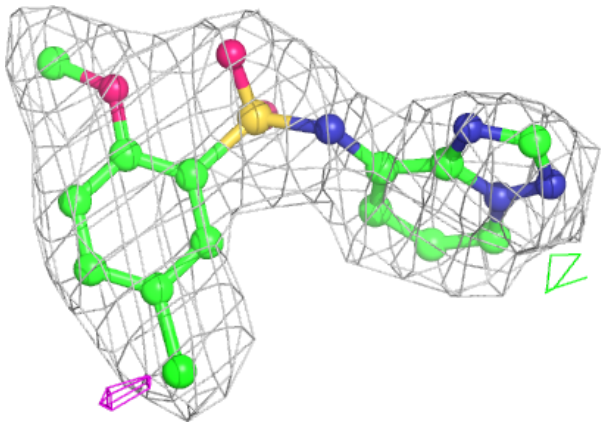
Electron density around QOY B 1002:

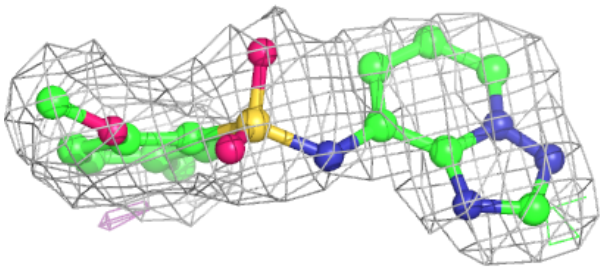
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

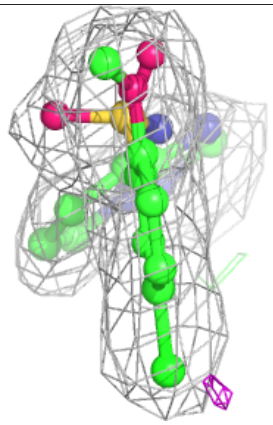


Electron density around QOY C 2001:

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

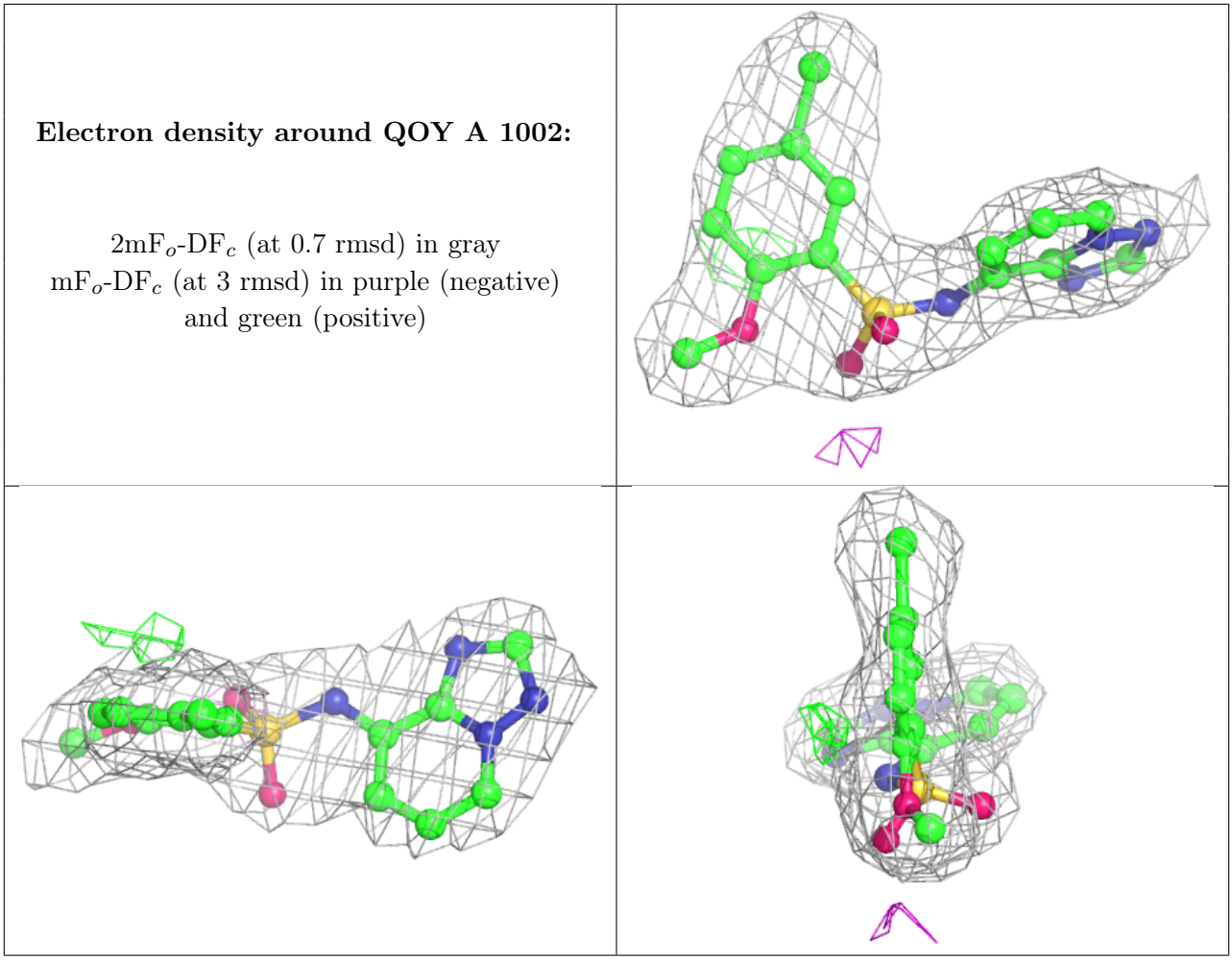






Electron density around QOY A 1002:

$2mF_o$-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.