



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:51 AM UTC

PDB ID : 4KQV / pdb_00004kqv
Title : Topoisomerase iv atp binding domain of francisella tularensis in complex with a small molecule inhibitor
Authors : Bensen, D.C.; Akers-Rodriguez, S.; Lam, T.; Tari, L.W.
Deposited on : 2013-05-15
Resolution : 2.38 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

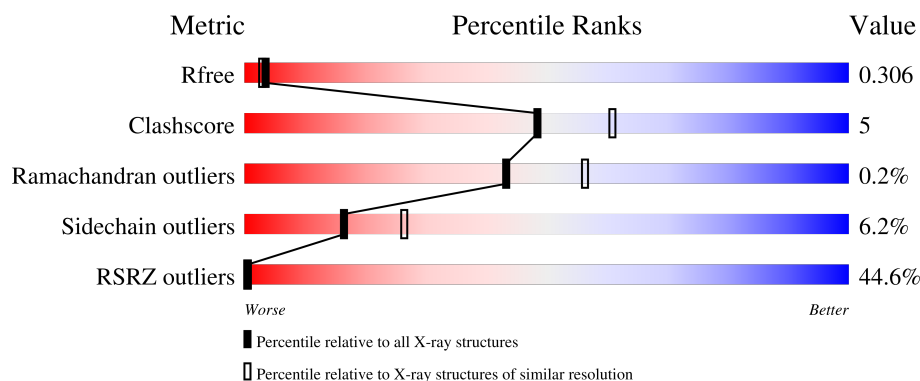
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	390	28% 78% 12% • 9%
1	B	390	35% 42% 8% • 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4586 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 Topoisomerase IV, subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	3	0
			2826	1805	476	537	8			
1	B	196	Total	C	N	O	S	0	1	0
			1559	996	263	294	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	PRO	LEU	variant	UNP Q2A1P5
A	383	LEU	-	expression tag	UNP Q2A1P5
A	384	GLU	-	expression tag	UNP Q2A1P5
A	385	HIS	-	expression tag	UNP Q2A1P5
A	386	HIS	-	expression tag	UNP Q2A1P5
A	387	HIS	-	expression tag	UNP Q2A1P5
A	388	HIS	-	expression tag	UNP Q2A1P5
A	389	HIS	-	expression tag	UNP Q2A1P5
A	390	HIS	-	expression tag	UNP Q2A1P5
B	258	PRO	LEU	variant	UNP Q2A1P5
B	383	LEU	-	expression tag	UNP Q2A1P5
B	384	GLU	-	expression tag	UNP Q2A1P5
B	385	HIS	-	expression tag	UNP Q2A1P5
B	386	HIS	-	expression tag	UNP Q2A1P5
B	387	HIS	-	expression tag	UNP Q2A1P5
B	388	HIS	-	expression tag	UNP Q2A1P5
B	389	HIS	-	expression tag	UNP Q2A1P5
B	390	HIS	-	expression tag	UNP Q2A1P5

- Molecule 2 is IODIDE ION (CCD ID: IOD) (formula: I).

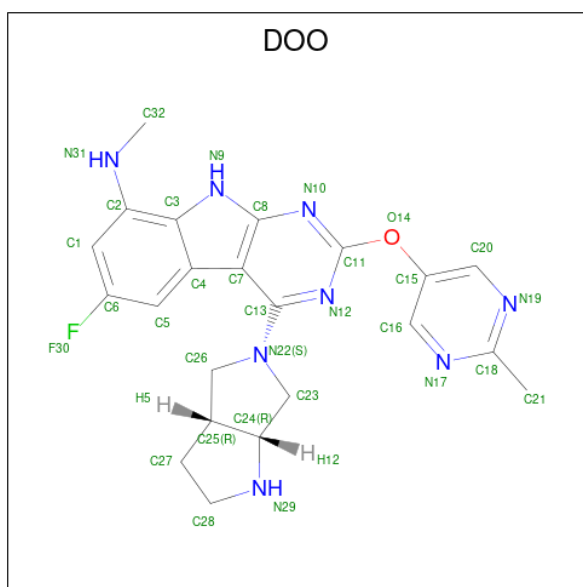
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	I	0	0
			6	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total I 2 2	0	0

- Molecule 3 is 6-fluoro-4-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl]-N-methyl-2-[(2-methylpyrimidin-5-yl)oxy]-9H-pyrimido[4,5-b]indol-8-amine (CCD ID: DOO) (formula: C₂₂H₂₃FN₈O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C F N O 32 22 1 8 1	0	0
3	B	1	Total C F N O 32 22 1 8 1	0	0

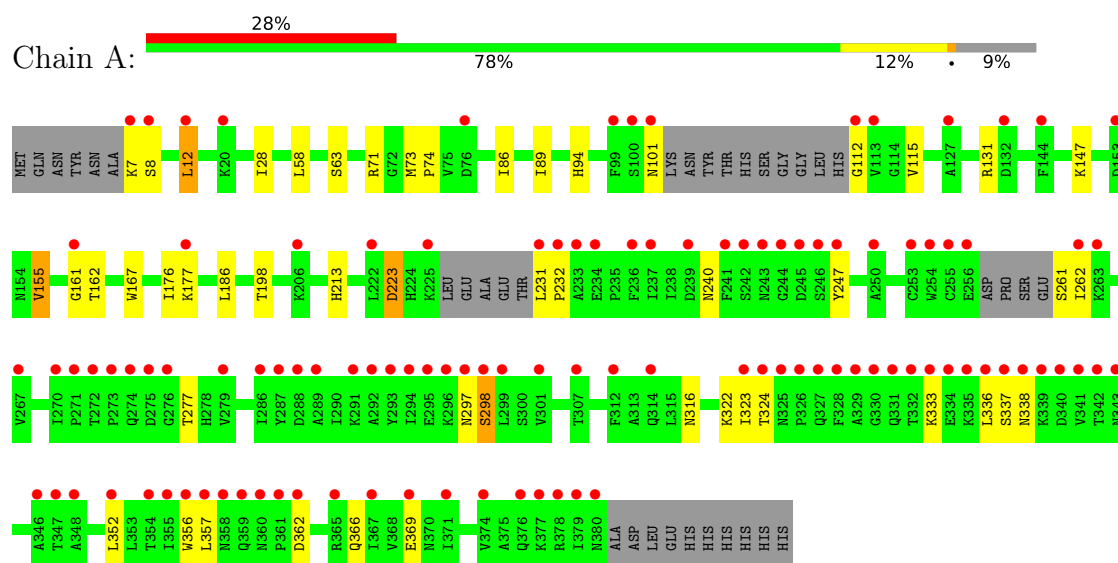
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	107	Total O 107 107	0	0
4	B	22	Total O 22 22	0	0

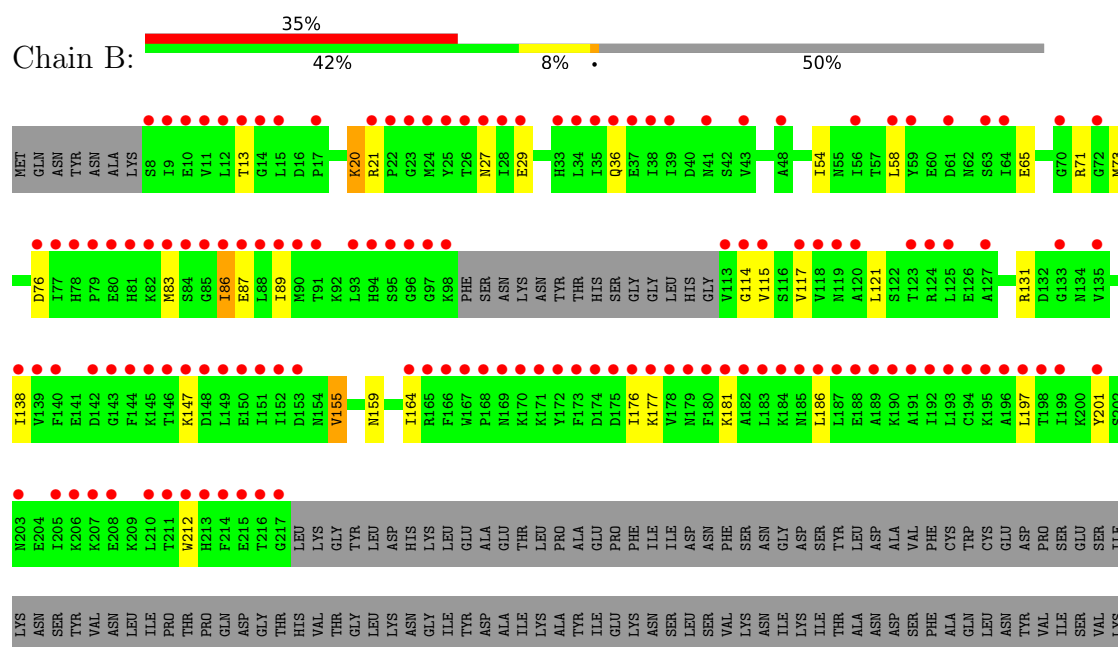
3 Residue-property plots

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: Topoisomerase IV, subunit B



• Molecule 1: Topoisomerase IV, subunit B



LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS	ILE	THR	THR	ASN	GLN	GLY	ALA	PHE	GLN	PRO	THR	THR	ASP	LYS	LYS	ASN	VAL	THR	THR	ASP	LYS	LYS	GLN	GLY	ALA	PHE	GLN	PRO	THR	THR	ASN	ILE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.20Å 163.16Å 72.28Å 90.00° 91.81° 90.00°	Depositor
Resolution (Å)	66.06 – 2.38 66.06 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.1 (66.06-2.38) 98.1 (66.06-2.38)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.255 , 0.299 0.262 , 0.306	Depositor DCC
R_{free} test set	2010 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.067 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4586	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.69	0/2885	0.85	1/3896 (0.0%)
1	B	0.66	0/1588	0.82	0/2138
All	All	0.68	0/4473	0.84	1/6034 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	GLY	N-CA-C	6.15	118.27	110.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2826	0	2865	28	0
1	B	1559	0	1595	17	0
2	A	6	0	0	0	0
2	B	2	0	0	1	0
3	A	32	0	23	7	0
3	B	32	0	23	3	0
4	A	107	0	0	1	0
4	B	22	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4586	0	4506	49	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 5.

All (49) 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:B:73[B]:MET:SD	3:B:403:DOO:H4	2.07	0.93
1:A:73[A]:MET:SD	3:A:403:DOO:H4	2.20	0.82
1:B:86:ILE:HD12	1:B:138:ILE:HG21	1.70	0.73
1:A:261:SER:HB2	1:A:316:ASN:HD21	1.55	0.72
1:B:73[B]:MET:SD	3:B:403:DOO:C26	2.78	0.70
3:A:403:DOO:H2	3:A:403:DOO:C23	2.25	0.67
1:B:155:VAL:HG13	1:B:159:ASN:HB3	1.80	0.64
1:A:73[B]:MET:HE3	1:A:86:ILE:HD13	1.81	0.62
1:B:86:ILE:O	1:B:89:ILE:HG22	2.03	0.58
1:A:262:ILE:H	1:A:316:ASN:HD22	1.51	0.57
1:A:247:TYR:HB2	1:A:322:LYS:HB2	1.88	0.56
1:A:240:ASN:HD21	1:A:247:TYR:HD1	1.53	0.55
3:A:403:DOO:H2	3:A:403:DOO:H13	1.89	0.54
3:A:403:DOO:H2	3:A:403:DOO:H14	1.87	0.54
1:A:240:ASN:ND2	1:A:247:TYR:HD1	2.05	0.53
1:A:115:VAL:HG11	3:A:403:DOO:F30	2.00	0.52
1:B:20:LYS:HG3	1:B:21:ARG:HG3	1.92	0.51
1:B:83:MET:HG2	1:B:87:GLU:HB3	1.92	0.51
1:A:297:ASN:O	1:A:298:SER:HB3	2.11	0.50
1:B:54:ILE:HG13	1:B:197:LEU:HD11	1.94	0.49
3:A:403:DOO:H14	3:A:403:DOO:C5	2.42	0.49
1:A:112:GLY:HA3	1:A:333:LYS:NZ	2.28	0.49
1:A:73[A]:MET:SD	3:A:403:DOO:C26	2.99	0.49
1:A:198:THR:HG23	1:A:213:HIS:HB2	1.94	0.48
1:B:36:GLN:HG3	1:B:186:LEU:HD21	1.96	0.47
1:A:223:ASP:OD1	1:A:223:ASP:N	2.45	0.47
1:A:362:ASP:O	1:A:366:GLN:HG3	2.15	0.47
1:B:164:ILE:HD12	3:B:403:DOO:C1	2.45	0.47
1:B:186:LEU:HD22	2:B:401:IOD:I	2.85	0.46
1:B:71:ARG:O	1:B:131:ARG:HG3	2.15	0.46
1:A:323:ILE:HD11	1:A:336:LEU:HD11	1.98	0.46
1:A:12:LEU:HD11	1:A:94:HIS:CE1	2.50	0.45
1:A:112:GLY:HA3	1:A:333:LYS:HZ1	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73[B]:MET:HE2	1:B:86:ILE:HA	1.99	0.45
1:B:201:TYR:HB2	1:B:212:TRP:HZ3	1.80	0.45
1:A:232:PRO:HG3	1:A:356:TRP:CH2	2.52	0.45
1:A:262:ILE:H	1:A:316:ASN:ND2	2.14	0.44
1:B:27:ASN:OD1	1:B:29:GLU:HG2	2.17	0.44
1:B:65:GLU:HA	1:B:164:ILE:O	2.17	0.43
1:A:73[A]:MET:SD	1:A:74:PRO:HD2	2.59	0.43
1:A:63:SER:HB3	1:A:167:TRP:CD1	2.54	0.42
1:B:114:GLY:O	1:B:117:VAL:HB	2.18	0.42
1:A:155:VAL:HG22	4:A:569:HOH:O	2.18	0.42
1:A:71:ARG:O	1:A:131:ARG:HG2	2.20	0.42
1:A:297:ASN:O	1:A:298:SER:CB	2.68	0.42
1:A:337:SER:O	1:A:338:ASN:C	2.63	0.42
1:A:262:ILE:N	1:A:316:ASN:HD22	2.17	0.41
1:A:73[B]:MET:HE2	1:A:162:THR:HG21	2.02	0.41
1:A:231:LEU:HA	1:A:232:PRO:C	2.46	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	350/390 (90%)	335 (96%)	14 (4%)	1 (0%)	36	48
1	B	193/390 (50%)	183 (95%)	10 (5%)	0	100	100
All	All	543/780 (70%)	518 (95%)	24 (4%)	1 (0%)	43	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	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	317/344 (92%)	299 (94%)	18 (6%)	18	30
1	B	174/344 (51%)	162 (93%)	12 (7%)	14	22
All	All	491/688 (71%)	461 (94%)	30 (6%)	16	27

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

Mol	Chain	Res	Type
1	A	7	LYS
1	A	8	SER
1	A	12	LEU
1	A	28	ILE
1	A	58	LEU
1	A	89	ILE
1	A	101	ASN
1	A	147	LYS
1	A	155	VAL
1	A	176	ILE
1	A	177	LYS
1	A	186	LEU
1	A	223	ASP
1	A	277	THR
1	A	324	THR
1	A	352	LEU
1	A	357	LEU
1	A	369	GLU
1	B	13	THR
1	B	20	LYS
1	B	58	LEU
1	B	76	ASP
1	B	86	ILE
1	B	115	VAL
1	B	121	LEU
1	B	147	LYS
1	B	155	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	176	ILE
1	B	177	LYS
1	B	181	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	81	HIS
1	A	134	ASN
1	A	137	HIS
1	A	154	ASN
1	A	224	HIS
1	A	240	ASN
1	A	243	ASN
1	A	264	ASN
1	A	314	GLN
1	A	316	ASN
1	A	325	ASN
1	A	343	ASN
1	A	358	ASN
1	A	370	ASN
1	B	36	GLN
1	B	119	ASN
1	B	134	ASN
1	B	137	HIS
1	B	154	ASN
1	B	185	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

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	DOO	A	403	-	37,37,37	1.71	5 (13%)	45,55,55	2.92	19 (42%)
3	DOO	B	403	-	37,37,37	2.01	5 (13%)	45,55,55	3.11	19 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DOO	A	403	-	-	0/10/28/28	0/6/6/6
3	DOO	B	403	-	-	3/10/28/28	0/6/6/6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	DOO	C3-C2	7.70	1.48	1.40
3	A	403	DOO	C3-C2	5.49	1.46	1.40
3	B	403	DOO	C4-C3	5.38	1.48	1.41
3	A	403	DOO	C4-C3	4.84	1.47	1.41
3	B	403	DOO	C7-C13	4.57	1.50	1.42
3	A	403	DOO	C7-C13	3.61	1.48	1.42
3	A	403	DOO	C7-C8	3.32	1.48	1.43
3	B	403	DOO	C7-C8	2.81	1.47	1.43
3	A	403	DOO	C13-N12	2.37	1.37	1.34
3	B	403	DOO	C13-N12	2.04	1.36	1.34

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	DOO	C7-C8-N10	-12.64	118.68	126.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	DOO	C7-C8-N10	-11.04	119.70	126.75
3	B	403	DOO	C3-N9-C8	7.24	113.13	108.85
3	A	403	DOO	C7-C13-N12	-6.63	114.29	122.39
3	A	403	DOO	C3-N9-C8	6.57	112.73	108.85
3	B	403	DOO	C7-C13-N12	-5.71	115.41	122.39
3	B	403	DOO	N9-C8-N10	5.19	132.86	124.66
3	A	403	DOO	N9-C8-N10	4.95	132.48	124.66
3	B	403	DOO	C16-C15-C20	4.65	119.61	116.59
3	A	403	DOO	C13-C7-C8	4.10	118.97	115.61
3	A	403	DOO	C16-C15-C20	4.10	119.25	116.59
3	B	403	DOO	C7-C13-N22	3.42	128.44	120.29
3	B	403	DOO	C2-C3-N9	3.38	133.73	128.92
3	B	403	DOO	C13-C7-C8	3.25	118.27	115.61
3	A	403	DOO	C15-C20-N19	-3.17	118.76	122.67
3	A	403	DOO	C20-N19-C18	3.10	121.16	116.07
3	B	403	DOO	N17-C18-N19	-3.09	120.45	125.46
3	B	403	DOO	C15-C16-N17	-3.03	118.93	122.67
3	B	403	DOO	N10-C11-N12	-2.99	122.21	127.65
3	B	403	DOO	C20-N19-C18	2.98	120.97	116.07
3	A	403	DOO	N17-C18-N19	-2.94	120.69	125.46
3	B	403	DOO	C16-N17-C18	2.87	120.78	116.07
3	B	403	DOO	C21-C18-N17	2.85	120.24	117.20
3	A	403	DOO	C2-C3-N9	2.77	132.87	128.92
3	B	403	DOO	C15-C20-N19	-2.76	119.26	122.67
3	A	403	DOO	C7-C13-N22	2.76	126.87	120.29
3	A	403	DOO	C21-C18-N19	2.60	119.97	117.20
3	B	403	DOO	C4-C7-C8	-2.58	104.71	106.05
3	A	403	DOO	C16-N17-C18	2.57	120.29	116.07
3	A	403	DOO	C26-C25-C24	2.52	108.32	103.97
3	B	403	DOO	C2-C1-C6	2.51	121.93	117.62
3	A	403	DOO	C15-C16-N17	-2.29	119.84	122.67
3	A	403	DOO	N10-C11-N12	-2.19	123.67	127.65
3	A	403	DOO	C27-C25-C24	2.15	107.52	103.94
3	B	403	DOO	C27-C25-C24	2.12	107.47	103.94
3	A	403	DOO	C4-C3-C2	-2.10	118.89	121.55
3	B	403	DOO	C4-C3-C2	-2.07	118.93	121.55
3	A	403	DOO	C21-C18-N17	2.00	119.33	117.20

There are no chirality outliers.

All (3) torsion outliers are listed below:

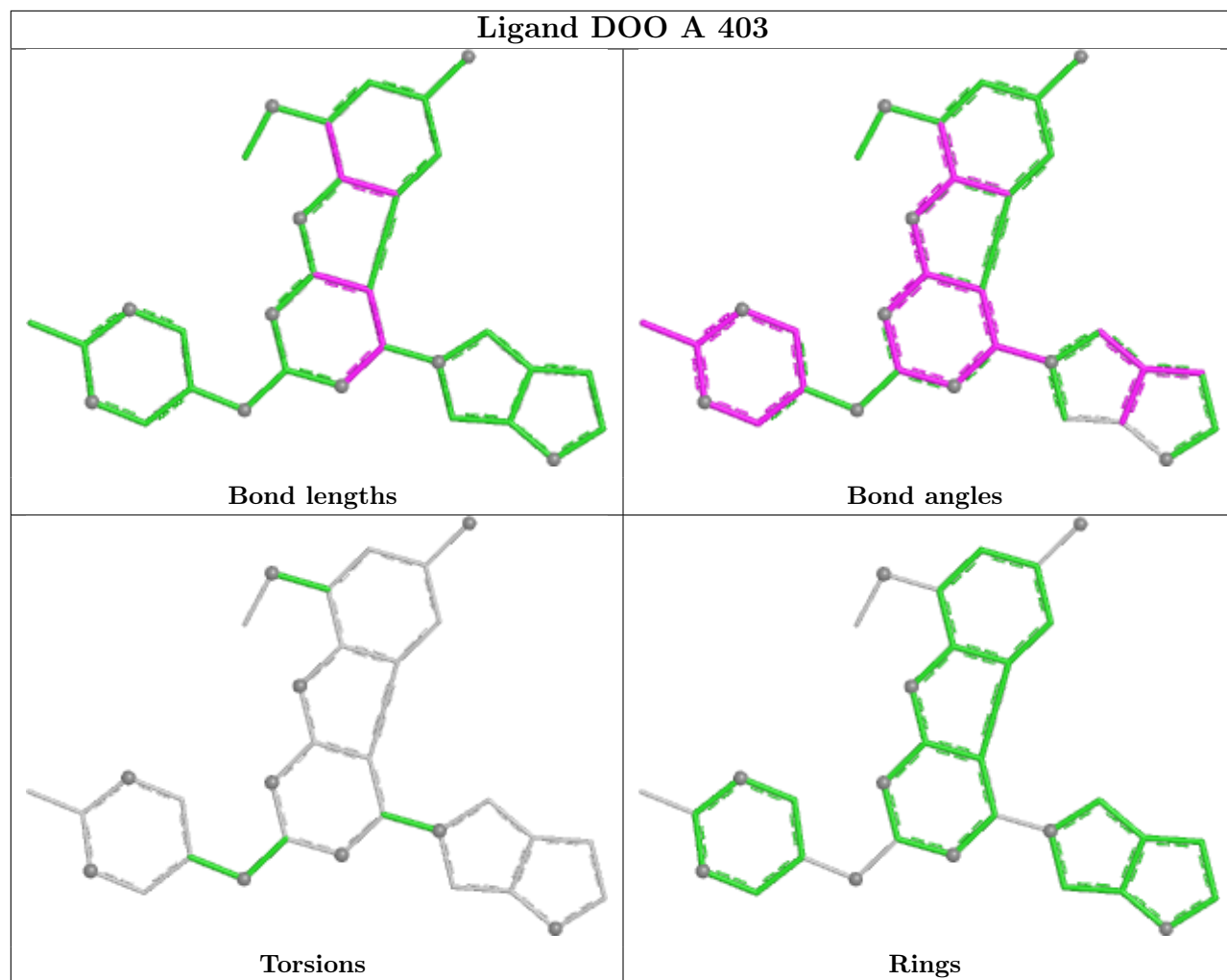
Mol	Chain	Res	Type	Atoms
3	B	403	DOO	N12-C13-N22-C26
3	B	403	DOO	C7-C13-N22-C26
3	B	403	DOO	N12-C13-N22-C23

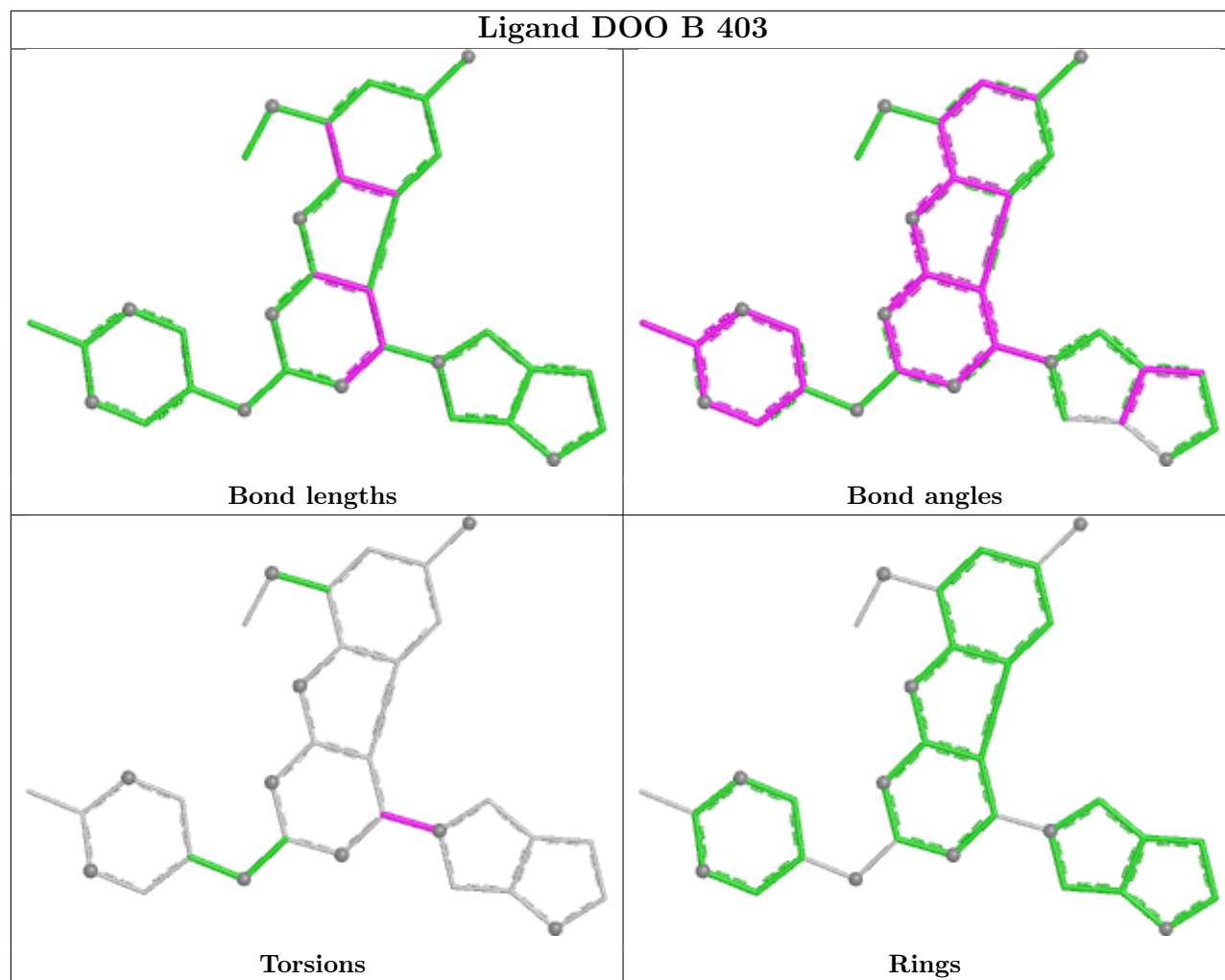
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	DOO	7	0
3	B	403	DOO	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	355/390 (91%)	1.63	110 (30%) 1 1	22, 50, 87, 117	3 (0%)
1	B	196/390 (50%)	2.76	136 (69%) 0 0	30, 64, 90, 108	1 (0%)
All	All	551/780 (70%)	2.03	246 (44%) 0 0	22, 57, 88, 117	4 (0%)

All (246) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	214	PHE	7.6
1	A	333	LYS	7.4
1	B	196	ALA	7.3
1	B	113	VAL	6.8
1	B	12	LEU	6.4
1	A	329	ALA	6.3
1	B	98	LYS	6.3
1	A	332	THR	6.3
1	B	213	HIS	5.8
1	B	193	LEU	5.7
1	B	9	ILE	5.5
1	A	339	LYS	5.5
1	A	245	ASP	5.5
1	A	361	PRO	5.4
1	B	192	ILE	5.4
1	B	28	ILE	5.3
1	A	299	LEU	5.3
1	A	330	GLY	5.2
1	B	13	THR	5.2
1	B	15	LEU	5.2
1	B	194	CYS	5.2
1	A	359	GLN	5.1
1	A	328	PHE	4.9
1	A	256	GLU	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	144	PHE	4.8
1	A	331	GLN	4.8
1	A	326	PRO	4.7
1	B	89	ILE	4.7
1	A	231	LEU	4.7
1	A	335	LYS	4.7
1	B	125	LEU	4.7
1	B	167	TRP	4.6
1	B	21	ARG	4.6
1	B	191	ALA	4.5
1	B	139	VAL	4.5
1	A	273	PRO	4.5
1	B	118	VAL	4.5
1	A	327	GLN	4.3
1	B	217	GLY	4.3
1	B	33	HIS	4.2
1	B	207	LYS	4.2
1	B	8	SER	4.2
1	B	59	TYR	4.2
1	A	101	ASN	4.2
1	B	24	MET	4.2
1	A	379	ILE	4.1
1	B	64	ILE	4.1
1	B	27	ASN	4.1
1	B	195	LYS	4.1
1	B	79	PRO	4.1
1	B	182	ALA	4.1
1	B	185	ASN	4.0
1	A	343	ASN	4.0
1	B	176	ILE	4.0
1	A	292	ALA	4.0
1	A	272	THR	4.0
1	B	86	ILE	4.0
1	A	337	SER	3.9
1	B	88	LEU	3.9
1	A	244	GLY	3.9
1	B	77	ILE	3.9
1	A	342	THR	3.8
1	B	123	THR	3.8
1	A	298	SER	3.8
1	A	357	LEU	3.8
1	A	360	ASN	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	215	GLU	3.7
1	A	7	LYS	3.7
1	A	222	LEU	3.7
1	B	83	MET	3.7
1	A	293	TYR	3.6
1	B	70	GLY	3.6
1	B	85	GLY	3.6
1	A	336	LEU	3.6
1	A	255	CYS	3.6
1	A	324	THR	3.6
1	A	225	LYS	3.6
1	B	14	GLY	3.6
1	B	36	GLN	3.5
1	A	355	ILE	3.5
1	A	358	ASN	3.5
1	B	189	ALA	3.5
1	B	143	GLY	3.5
1	B	138	ILE	3.5
1	A	365	ARG	3.4
1	A	325	ASN	3.4
1	B	26	THR	3.4
1	B	39	ILE	3.4
1	B	140	PHE	3.4
1	B	63	SER	3.4
1	B	201	TYR	3.3
1	B	115	VAL	3.3
1	B	93	LEU	3.3
1	B	25	TYR	3.3
1	B	29	GLU	3.3
1	B	11	VAL	3.3
1	B	181	LYS	3.2
1	B	124	ARG	3.2
1	B	58	LEU	3.2
1	B	172	TYR	3.2
1	B	180	PHE	3.2
1	A	291	LYS	3.2
1	A	233	ALA	3.2
1	A	338	ASN	3.2
1	A	380	ASN	3.2
1	B	78	HIS	3.2
1	B	212	TRP	3.2
1	B	149	LEU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	190	LYS	3.1
1	B	206	LYS	3.1
1	A	112	GLY	3.1
1	B	127	ALA	3.1
1	A	274	GLN	3.1
1	A	100	SER	3.1
1	B	166	PHE	3.1
1	B	41	ASN	3.1
1	B	96	GLY	3.1
1	B	142	ASP	3.1
1	A	314	GLN	3.1
1	A	377	LYS	3.1
1	B	82	LYS	3.1
1	B	197	LEU	3.1
1	A	362	ASP	3.0
1	A	237	ILE	3.0
1	A	323	ILE	3.0
1	A	296	LYS	3.0
1	B	120	ALA	2.9
1	A	371	ILE	2.9
1	B	216	THR	2.9
1	B	187	LEU	2.9
1	A	367	ILE	2.9
1	B	91	THR	2.9
1	B	211	THR	2.9
1	B	153	ASP	2.9
1	A	341	VAL	2.9
1	B	80	GLU	2.9
1	B	90	MET	2.9
1	B	84	SER	2.9
1	B	169	ASN	2.9
1	A	279	VAL	2.9
1	A	295	GLU	2.9
1	B	198	THR	2.9
1	B	135	VAL	2.8
1	B	147	LYS	2.8
1	B	179	ASN	2.8
1	B	170	LYS	2.8
1	B	165	ARG	2.8
1	A	352	LEU	2.8
1	B	177	LYS	2.8
1	A	267	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	247	TYR	2.7
1	B	205	ILE	2.7
1	B	97	GLY	2.7
1	B	22	PRO	2.7
1	A	289	ALA	2.7
1	A	275	ASP	2.7
1	B	38	ILE	2.7
1	A	347	THR	2.7
1	B	10	GLU	2.7
1	B	37	GLU	2.7
1	B	171	LYS	2.7
1	B	210	LEU	2.7
1	A	234	GLU	2.6
1	A	340	ASP	2.6
1	B	117	VAL	2.6
1	A	232	PRO	2.6
1	B	34	LEU	2.6
1	A	288	ASP	2.6
1	A	307	THR	2.6
1	A	242	SER	2.6
1	B	133	GLY	2.6
1	A	294	ILE	2.6
1	A	376	GLN	2.6
1	A	369	GLU	2.6
1	B	188	GLU	2.5
1	B	43	VAL	2.5
1	B	35	ILE	2.5
1	A	243	ASN	2.5
1	A	161	GLY	2.5
1	A	246	SER	2.5
1	A	378	ARG	2.5
1	B	174	ASP	2.5
1	A	334	GLU	2.4
1	A	241	PHE	2.4
1	B	148	ASP	2.4
1	A	250	ALA	2.4
1	B	168	PRO	2.4
1	A	254	TRP	2.4
1	A	346	ALA	2.4
1	A	8	SER	2.4
1	A	253	CYS	2.4
1	A	20	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	56	ILE	2.4
1	A	132	ASP	2.3
1	B	23	GLY	2.3
1	A	312	PHE	2.3
1	B	173	PHE	2.3
1	B	183	LEU	2.3
1	B	119	ASN	2.3
1	A	206	LYS	2.3
1	A	270	ILE	2.3
1	B	152	ILE	2.3
1	B	94	HIS	2.3
1	A	113	VAL	2.3
1	A	236	PHE	2.3
1	A	271	PRO	2.3
1	A	348	ALA	2.3
1	B	81	HIS	2.3
1	A	12	LEU	2.2
1	B	186	LEU	2.2
1	B	203	ASN	2.2
1	B	146	THR	2.2
1	B	208	GLU	2.2
1	A	263	LYS	2.2
1	B	145	LYS	2.2
1	A	286	ILE	2.2
1	B	151	ILE	2.2
1	B	164	ILE	2.2
1	A	153	ASP	2.2
1	A	239	ASP	2.2
1	A	276	GLY	2.2
1	B	114	GLY	2.2
1	B	150	GLU	2.2
1	A	177	LYS	2.2
1	B	178	VAL	2.2
1	B	76	ASP	2.2
1	A	356	TRP	2.2
1	B	199	ILE	2.2
1	A	374	VAL	2.2
1	B	17	PRO	2.2
1	A	127	ALA	2.2
1	B	61	ASP	2.1
1	B	72	GLY	2.1
1	A	354	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	48	ALA	2.1
1	A	144	PHE	2.1
1	A	262	ILE	2.1
1	A	287	TYR	2.1
1	B	175	ASP	2.1
1	A	301	VAL	2.1
1	A	76[A]	ASP	2.1
1	A	297	ASN	2.0
1	A	99	PHE	2.0
1	B	184	LYS	2.0
1	B	87	GLU	2.0
1	B	95	SER	2.0

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

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

6.3 Carbohydrates [i](#)

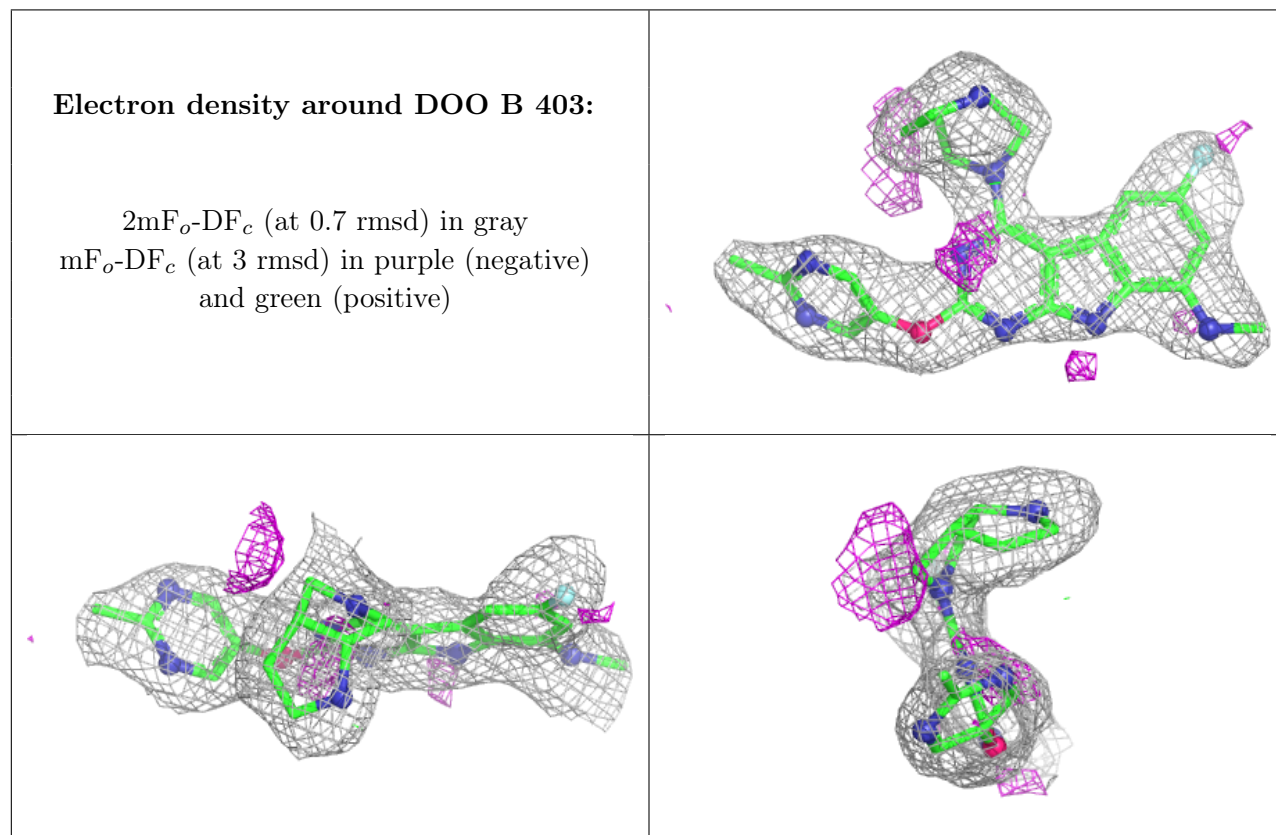
There are no oligosaccharides in this entry.

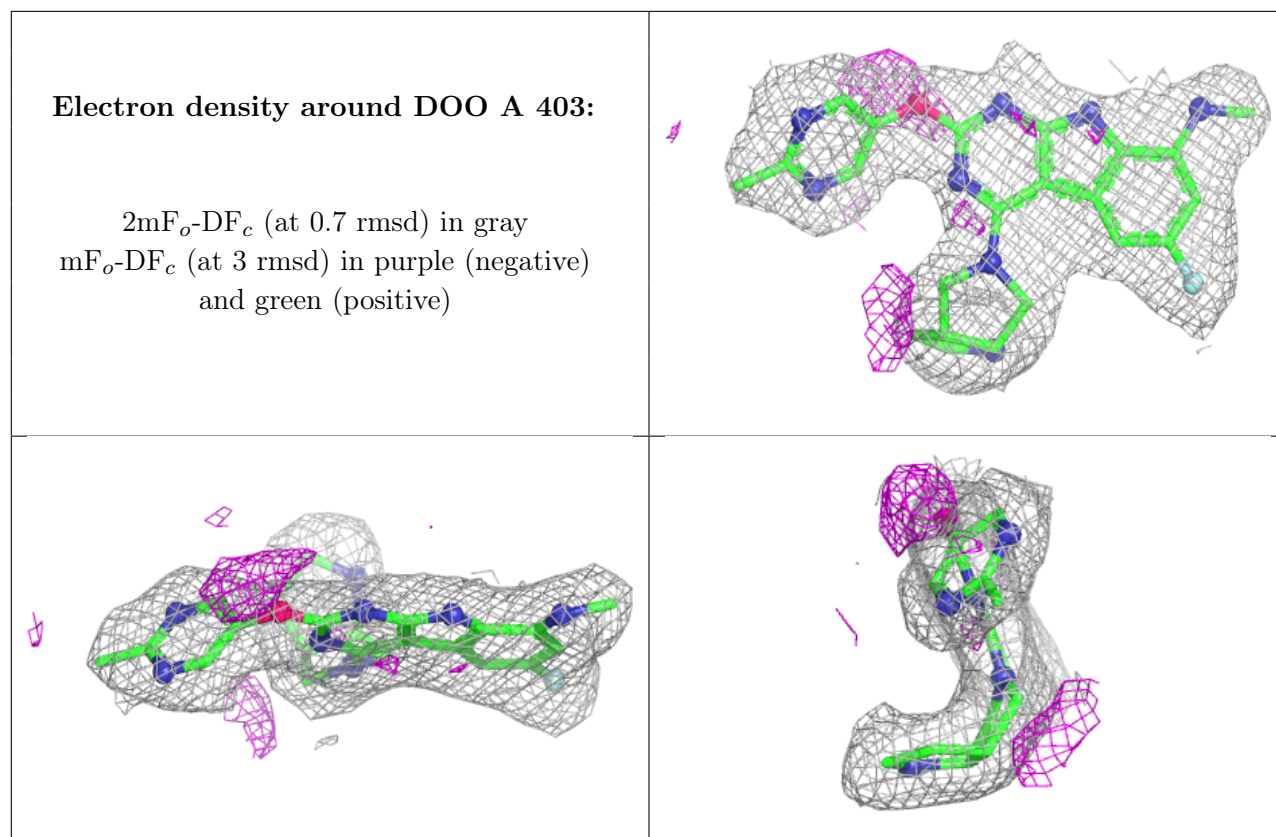
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	DOO	B	403	32/32	0.85	0.19	47,62,71,73	0
2	IOD	A	407	1/1	0.87	0.27	132,132,132,132	0
2	IOD	B	402	1/1	0.88	0.24	130,130,130,130	0
3	DOO	A	403	32/32	0.93	0.12	34,37,47,47	0
2	IOD	A	405	1/1	0.94	0.39	149,149,149,149	0
2	IOD	A	404	1/1	0.97	0.31	119,119,119,119	0
2	IOD	A	406	1/1	0.98	0.38	107,107,107,107	0
2	IOD	A	402	1/1	0.98	0.05	59,59,59,59	0
2	IOD	B	401	1/1	0.98	0.15	82,82,82,82	0
2	IOD	A	401	1/1	0.99	0.06	51,51,51,51	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.