



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:42 AM UTC

PDB ID : 8B8H / pdb_00008b8h
Title : Structure of DCS-resistant variant D322N of alanine racemase from *M. tuberculosis* in complex with DCS
Authors : de Chiara, C.; Prosser, G.; Ogrodowicz, R.W.; de Carvalho, L.P.S.
Deposited on : 2022-10-04
Resolution : 1.78 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

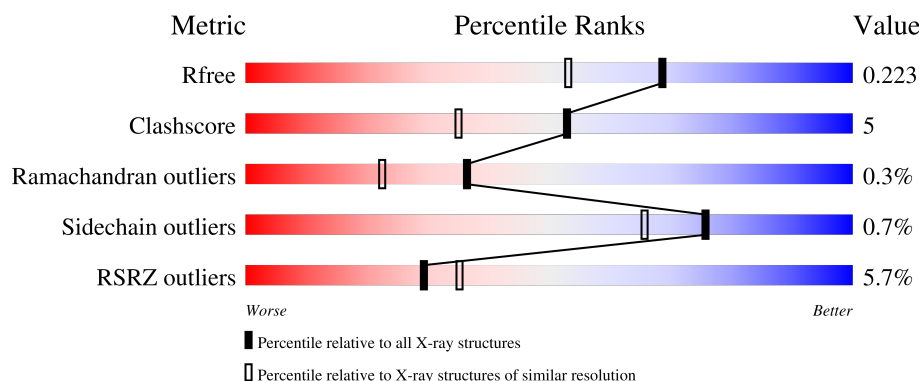
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	387	4% 89% 7% .
1	B	387	7% 84% 12% .

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11438 atoms, of which 5511 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.

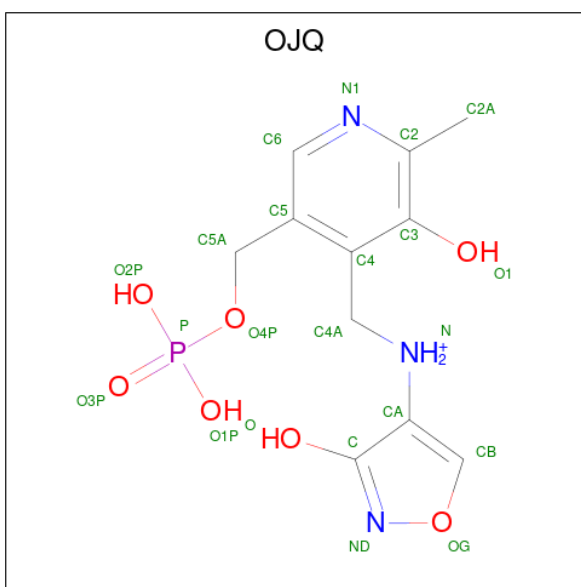
- Molecule 1 is a protein called Alanine racemase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	371	Total	C	H	N	O	S	0	8	0
			5472	1730	2729	487	509	17			
1	B	371	Total	C	H	N	O	S	0	11	0
			5474	1744	2720	486	506	18			

There are 8 discrepancies between the modelled and reference sequences:

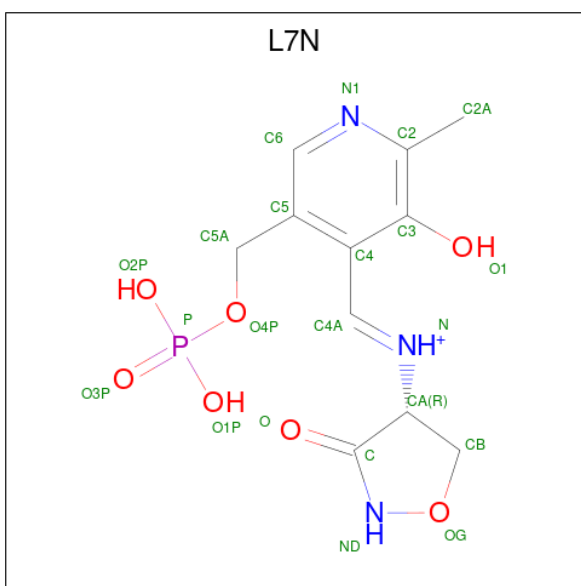
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P9WQA9
A	1	SER	-	expression tag	UNP P9WQA9
A	2	HIS	-	expression tag	UNP P9WQA9
A	322	ASN	ASP	engineered mutation	UNP P9WQA9
B	0	GLY	-	expression tag	UNP P9WQA9
B	1	SER	-	expression tag	UNP P9WQA9
B	2	HIS	-	expression tag	UNP P9WQA9
B	322	ASN	ASP	engineered mutation	UNP P9WQA9

- Molecule 2 is [2-methyl-3-oxidanyl-5-(phosphonooxymethyl)pyridin-4-yl]methyl-(3-oxidanyl-1,2-oxazol-4-yl)azanium (CCD ID: OJQ) (formula: C₁₁H₁₅N₃O₇P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	1
			34	11	12	3	7	1		

- Molecule 3 is ({E})-[2-methyl-3-oxidanyl-5-(phosphonomoxymethyl)pyridin-4-yl]methylidene-[(4 {R})-3-oxidanylidene-1,2-oxazolidin-4-yl]azanum (CCD ID: L7N) (formula: $C_{11}H_{15}N_3O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	H	N	O	P	0	1
			34	11	12	3	7	1		
3	B	1	Total	C	H	N	O	P	0	1
			34	11	12	3	7	1		

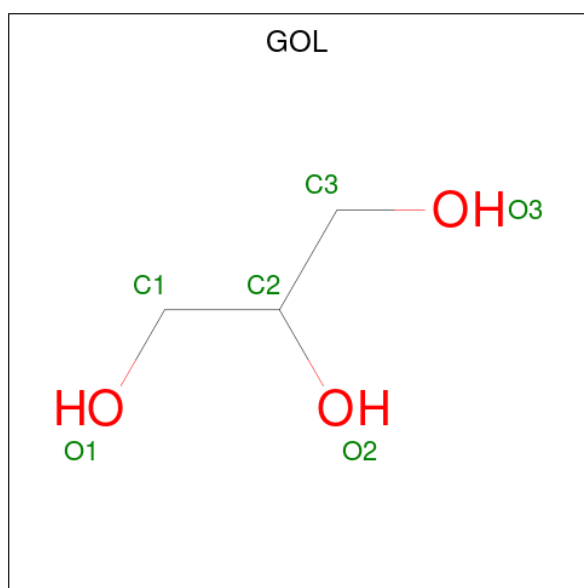
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Ca		0	0
			1	1			

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Cl		0	0
			1	1			
5	B	1	Total	Cl		0	0
			1	1			

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			10	2	6	2		
7	B	1	Total	C	H	O	0	0
			10	2	6	2		
7	B	1	Total	C	H	O	0	0
			10	2	6	2		

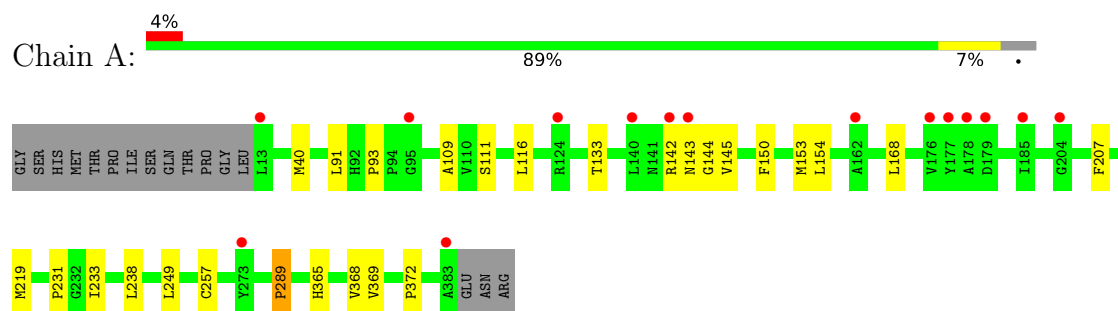
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	189	Total	O	0	0
			189	189		
8	B	154	Total	O	0	0
			154	154		

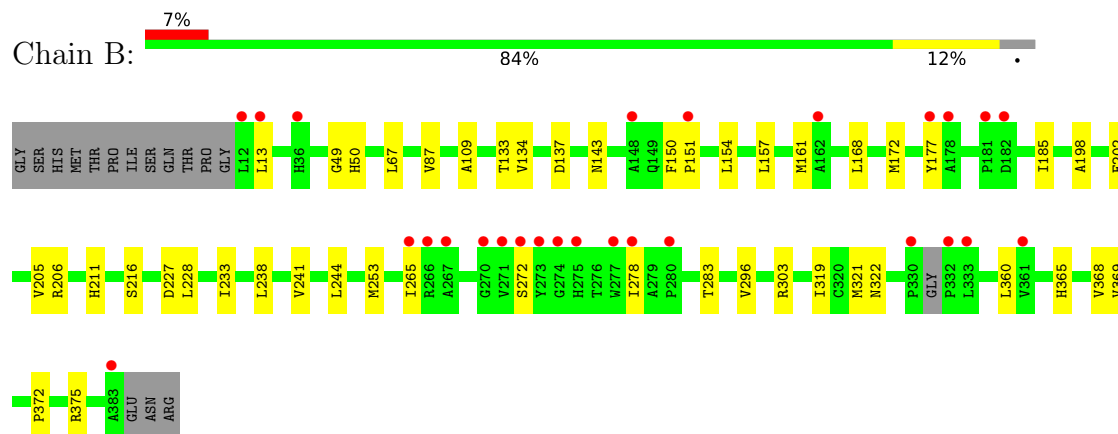
3 Residue-property plots [i](#)

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: Alanine racemase



- Molecule 1: Alanine racemase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	163.94Å 163.94Å 57.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.93 – 1.78 53.93 – 1.78	Depositor EDS
% Data completeness (in resolution range)	100.0 (53.93-1.78) 100.0 (53.93-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 1.78Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.199 , 0.223 0.199 , 0.223	Depositor DCC
R_{free} test set	3789 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11438	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: CA, L7N, GOL, EDO, CL, OJQ

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	0.89	2/2811 (0.1%)	0.69	0/3831
1	B	0.66	2/2837 (0.1%)	0.60	0/3864
All	All	0.78	4/5648 (0.1%)	0.65	0/7695

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	289	PRO	CA-CB	-6.59	1.44	1.53
1	B	172	MET	SD-CE	-6.35	1.63	1.79
1	B	321	MET	SD-CE	-5.32	1.66	1.79
1	A	93	PRO	CA-C	-5.21	1.47	1.52

There are no bond angle outliers.

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	2743	2729	2738	16	0
1	B	2754	2720	2761	34	0
2	A	22	12	0	0	0
3	A	22	12	0	0	0
3	B	22	12	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
5	A	1	0	0	1	0
5	B	1	0	0	1	0
6	A	6	8	8	0	0
7	B	12	18	17	9	0
8	A	189	0	0	0	0
8	B	154	0	0	4	0
All	All	5927	5511	5524	55	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 (55) 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:161[A]:MET:HE2	1:B:168[A]:LEU:HD13	1.65	0.77
1:A:91[B]:LEU:HD22	5:B:402:CL:CL	2.25	0.73
1:B:278:ILE:O	1:B:278:ILE:HD12	1.89	0.72
1:B:134:VAL:HG21	1:B:157:LEU:HD11	1.73	0.70
1:B:265:ILE:HD11	1:B:283:THR:HG22	1.77	0.64
1:B:265:ILE:HD12	1:B:265:ILE:O	1.97	0.63
5:A:404:CL:CL	7:B:404:EDO:H22	2.36	0.62
1:A:257[B]:CYS:SG	1:A:289:PRO:HD2	2.41	0.61
7:B:403:EDO:H11	8:B:575:HOH:O	2.03	0.57
1:B:198:ALA:O	1:B:202:GLU:HG3	2.08	0.54
1:B:238:LEU:HD11	1:B:369:VAL:HG11	1.91	0.53
1:B:303[B]:ARG:NH2	1:B:360:LEU:O	2.41	0.53
1:A:40:MET:O	1:A:231:PRO:HD2	2.08	0.53
1:A:150:PHE:CE2	1:A:154:LEU:HD11	2.44	0.52
1:A:233:ILE:HG13	1:A:238:LEU:HB2	1.92	0.52
1:B:227:ASP:O	1:B:228:LEU:HD12	2.11	0.51
1:B:265:ILE:HD11	1:B:283:THR:CG2	2.41	0.50
1:A:91[A]:LEU:C	1:A:91[A]:LEU:HD13	2.35	0.50
7:B:405:EDO:H21	8:B:617:HOH:O	2.12	0.50
1:A:111[B]:SER:HB3	1:A:144:GLY:H	1.78	0.49
1:B:265:ILE:HD12	1:B:265:ILE:C	2.38	0.49
1:A:116:LEU:HD22	1:A:153[A]:MET:SD	2.53	0.49
7:B:404:EDO:C1	8:B:597:HOH:O	2.60	0.48
1:B:49:GLY:CA	7:B:403:EDO:H12	2.44	0.48
1:B:150:PHE:N	1:B:151:PRO:CD	2.77	0.48
1:B:177:TYR:CD1	1:B:185:ILE:HG21	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ASN:HB3	1:B:375:ARG:CZ	2.44	0.48
1:B:168[A]:LEU:HD23	1:B:206:ARG:O	2.13	0.48
7:B:404:EDO:H12	8:B:597:HOH:O	2.13	0.47
1:A:109:ALA:HA	1:A:133:THR:O	2.14	0.47
1:A:145:VAL:HG21	1:A:153[A]:MET:HE3	1.97	0.47
1:B:67:LEU:HB2	1:B:87[B]:VAL:HG12	1.98	0.46
1:B:49:GLY:HA2	7:B:403:EDO:H12	1.98	0.45
1:A:168:LEU:HD11	1:A:207:PHE:CE2	2.51	0.45
1:A:368:VAL:O	1:A:372:PRO:HD3	2.16	0.45
1:B:278:ILE:HD12	1:B:278:ILE:C	2.41	0.45
1:B:177:TYR:CE1	1:B:185:ILE:HG21	2.51	0.45
1:B:109:ALA:HA	1:B:133:THR:O	2.17	0.44
1:B:211:HIS:HB3	1:B:228:LEU:HB2	2.00	0.44
1:B:296:VAL:HG12	1:B:319:ILE:HD13	1.98	0.44
1:A:238:LEU:HD11	1:A:369:VAL:HG11	2.01	0.43
1:B:161[A]:MET:HE1	1:B:205:VAL:HG13	2.00	0.42
1:B:134:VAL:HG21	1:B:157:LEU:CD1	2.47	0.42
1:B:168[A]:LEU:HD22	1:B:205:VAL:HG13	2.01	0.42
1:B:143:ASN:O	1:B:143:ASN:CG	2.63	0.42
1:B:368:VAL:O	1:B:372:PRO:HD3	2.20	0.42
1:B:233:ILE:HG13	1:B:238:LEU:HB2	2.02	0.42
1:A:111[A]:SER:HB2	1:A:144:GLY:H	1.85	0.42
1:B:137:ASP:HA	7:B:405:EDO:H22	2.02	0.42
1:B:151:PRO:HA	1:B:154:LEU:HD12	2.02	0.41
1:B:137:ASP:HA	7:B:405:EDO:C2	2.51	0.41
1:A:219[A]:MET:SD	1:A:249:LEU:HD11	2.60	0.41
1:B:50:HIS:CE1	1:B:253:MET:HE3	2.56	0.41
1:A:143:ASN:OD1	1:A:144:GLY:N	2.54	0.40
1:B:241:VAL:HB	1:B:244:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	376/387 (97%)	364 (97%)	11 (3%)	1 (0%)	36	22
1	B	378/387 (98%)	366 (97%)	11 (3%)	1 (0%)	36	22
All	All	754/774 (97%)	730 (97%)	22 (3%)	2 (0%)	36	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	ARG
1	B	272	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	275/294 (94%)	274 (100%)	1 (0%)	84	78
1	B	276/294 (94%)	273 (99%)	3 (1%)	65	51
All	All	551/588 (94%)	547 (99%)	4 (1%)	76	66

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	365	HIS
1	B	13	LEU
1	B	216	SER
1	B	365	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	355	GLN
1	B	199	GLN
1	B	203	GLN
1	B	355	GLN

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, 3 are monoatomic - leaving 7 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$
7	EDO	B	405	-	3,3,3	0.70	0	2,2,2	0.37	0
6	GOL	A	405	-	5,5,5	0.67	0	5,5,5	1.26	1 (20%)
7	EDO	B	403	-	3,3,3	0.41	0	2,2,2	0.85	0
2	OJQ	A	401[A]	-	23,23,23	3.29	8 (34%)	28,33,33	2.37	5 (17%)
7	EDO	B	404	-	3,3,3	0.74	0	2,2,2	0.73	0
3	L7N	A	402[B]	-	22,23,23	1.75	4 (18%)	26,33,33	1.49	5 (19%)
3	L7N	B	401[B]	-	22,23,23	1.31	2 (9%)	26,33,33	1.30	3 (11%)

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
7	EDO	B	405	-	-	1/1/1/1	-
6	GOL	A	405	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	B	403	-	-	0/1/1/1	-
2	OJQ	A	401[A]	-	-	0/10/11/11	0/2/2/2
7	EDO	B	404	-	-	0/1/1/1	-
3	L7N	A	402[B]	-	-	3/11/21/21	0/2/2/2
3	L7N	B	401[B]	-	-	3/11/21/21	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401[A]	OJQ	C4A-N	9.43	1.64	1.46
2	A	401[A]	OJQ	OG-ND	-5.60	1.34	1.41
2	A	401[A]	OJQ	CA-C	5.54	1.51	1.42
2	A	401[A]	OJQ	CA-N	5.50	1.43	1.34
2	A	401[A]	OJQ	O-C	5.07	1.49	1.33
2	A	401[A]	OJQ	C-ND	4.58	1.34	1.31
3	A	402[B]	L7N	C3-C2	-4.07	1.36	1.41
3	B	401[B]	L7N	C4A-N	3.95	1.34	1.27
3	A	402[B]	L7N	C4A-N	3.84	1.34	1.27
3	A	402[B]	L7N	C4-C5	-3.35	1.37	1.42
3	A	402[B]	L7N	P-O4P	2.97	1.69	1.60
2	A	401[A]	OJQ	OG-CB	2.73	1.38	1.34
2	A	401[A]	OJQ	C3-C2	-2.23	1.38	1.41
3	B	401[B]	L7N	C-ND	-2.08	1.32	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401[A]	OJQ	CB-OG-ND	8.89	114.75	108.55
2	A	401[A]	OJQ	C4A-N-CA	-6.52	111.93	123.44
3	B	401[B]	L7N	O1P-P-O4P	3.70	116.31	106.67
3	A	402[B]	L7N	OG-CB-CA	-2.79	101.00	104.92
3	A	402[B]	L7N	C5-C6-N1	-2.68	119.47	123.83
2	A	401[A]	OJQ	C4A-C4-C5	2.56	122.54	119.75
2	A	401[A]	OJQ	C4-C4A-N	-2.29	106.55	111.26
6	A	405	GOL	C3-C2-C1	-2.27	103.45	111.80
3	A	402[B]	L7N	C5-C4-C4A	2.27	124.97	121.47
3	A	402[B]	L7N	C3-C4-C4A	-2.22	116.39	120.40
2	A	401[A]	OJQ	OG-CB-CA	-2.21	108.19	110.41
3	B	401[B]	L7N	O2P-P-O1P	-2.10	99.93	107.80
3	B	401[B]	L7N	OG-CB-CA	-2.07	102.01	104.92
3	A	402[B]	L7N	O-C-ND	-2.02	123.25	125.73

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401[B]	L7N	C-CA-N-C4A
3	B	401[B]	L7N	CB-CA-N-C4A
3	A	402[B]	L7N	C3-C4-C4A-N
3	A	402[B]	L7N	CB-CA-N-C4A
3	A	402[B]	L7N	C5-C4-C4A-N
7	B	405	EDO	O1-C1-C2-O2
3	B	401[B]	L7N	C3-C4-C4A-N

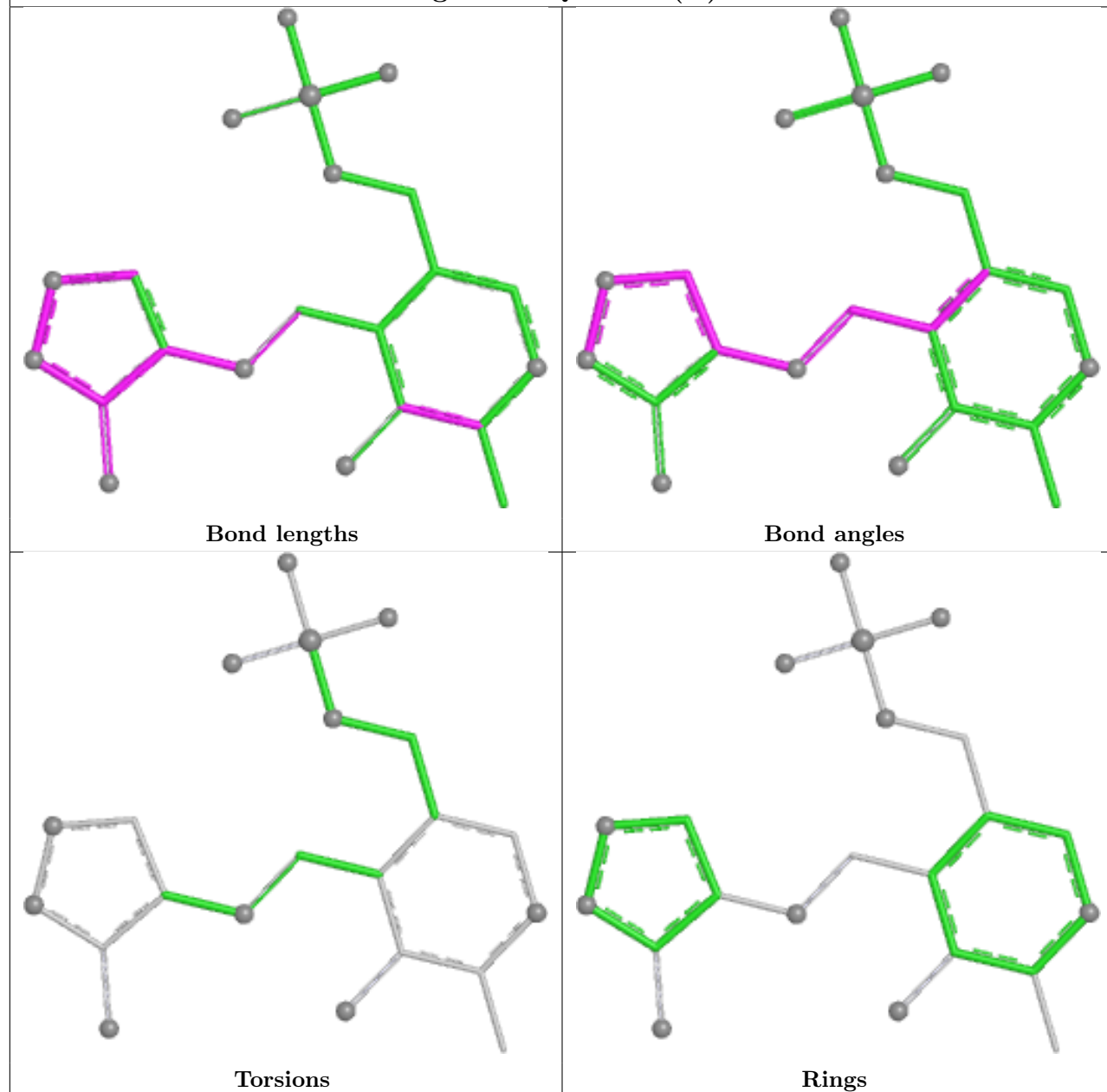
There are no ring outliers.

3 monomers are involved in 9 short contacts:

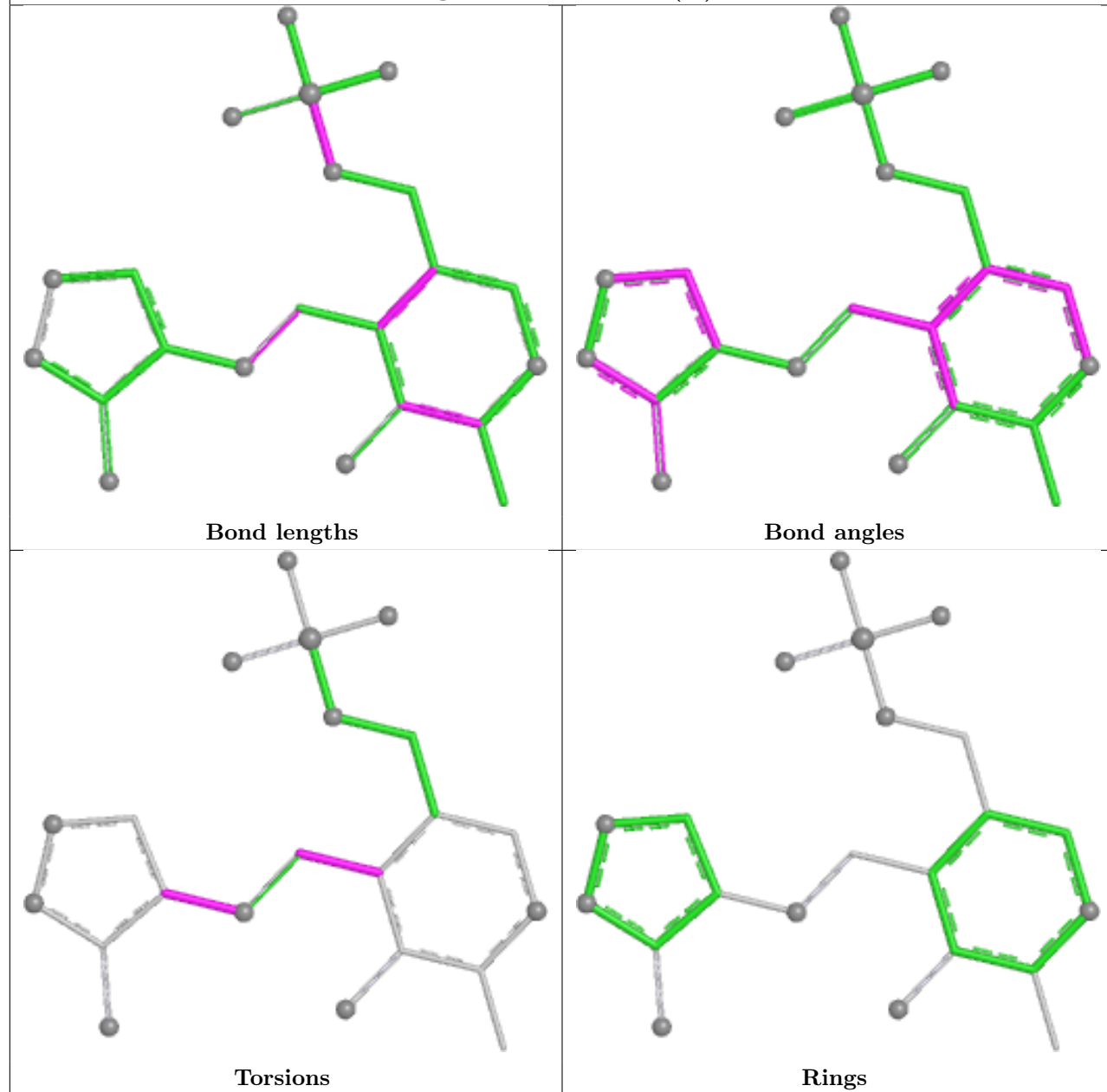
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	405	EDO	3	0
7	B	403	EDO	3	0
7	B	404	EDO	3	0

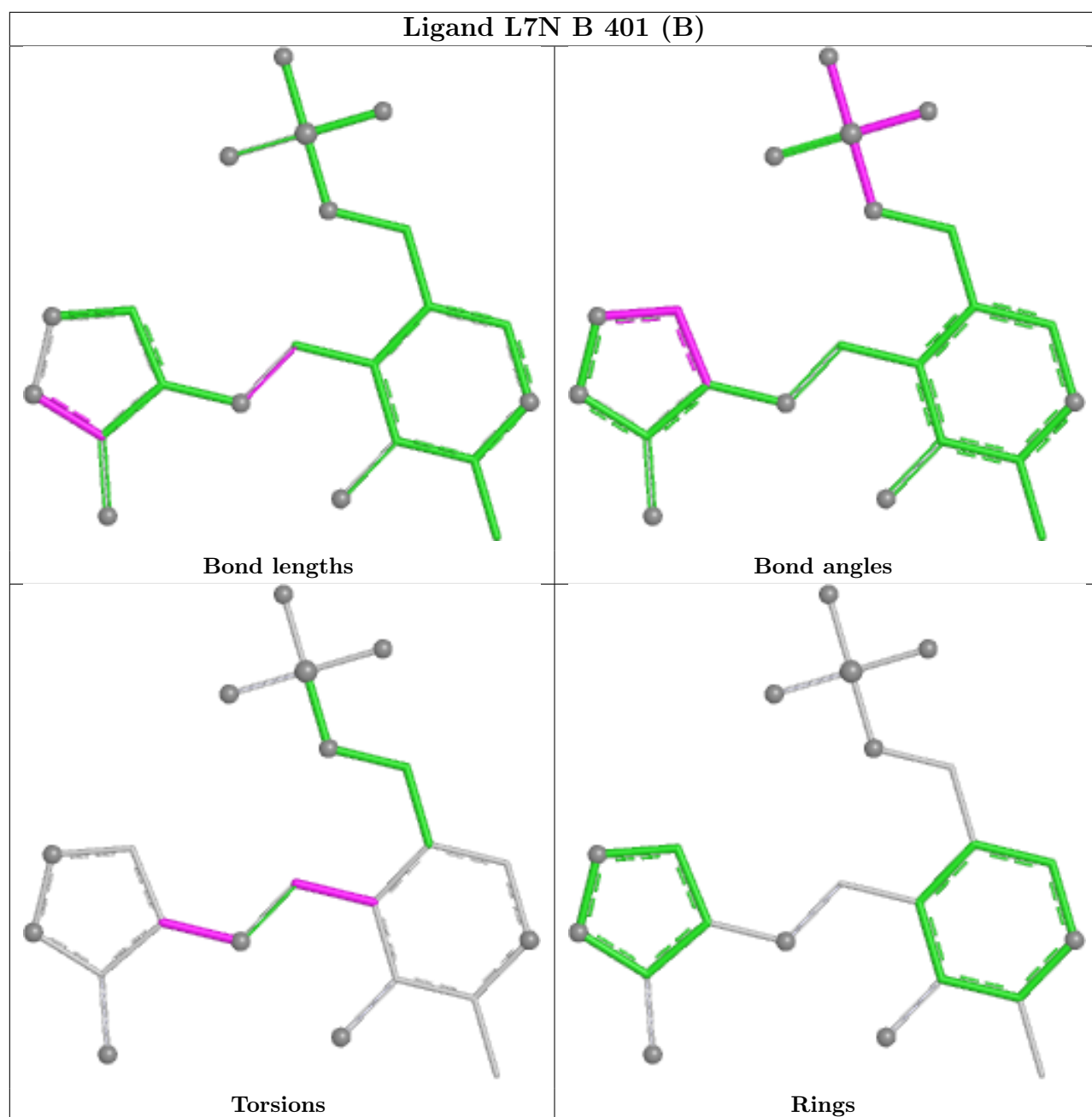
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand OJQ A 401 (A)



Ligand L7N A 402 (B)





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	371/387 (95%)	0.09	15 (4%)	42 48	17, 34, 52, 67	9 (2%)
1	B	371/387 (95%)	0.52	27 (7%)	21 25	19, 43, 68, 80	13 (3%)
All	All	742/774 (95%)	0.31	42 (5%)	29 35	17, 39, 60, 80	22 (2%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	177	TYR	5.6
1	B	177	TYR	5.0
1	B	330	PRO	4.7
1	B	273	TYR	4.5
1	B	278	ILE	4.5
1	B	12	LEU	4.4
1	B	178	ALA	4.2
1	B	271	VAL	4.2
1	A	142	ARG	4.0
1	A	178	ALA	3.9
1	B	162	ALA	3.6
1	B	274	GLY	3.1
1	B	270	GLY	3.1
1	B	182	ASP	3.0
1	B	272	SER	3.0
1	B	361	VAL	3.0
1	B	151	PRO	2.9
1	B	181	PRO	2.8
1	B	332	PRO	2.8
1	B	36	HIS	2.8
1	A	95	GLY	2.8
1	B	383	ALA	2.7
1	A	143	ASN	2.7
1	A	13[A]	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	176	VAL	2.6
1	A	383	ALA	2.6
1	B	265	ILE	2.5
1	A	140	LEU	2.5
1	B	275	HIS	2.5
1	A	204	GLY	2.4
1	B	280	PRO	2.3
1	A	185	ILE	2.3
1	B	277	TRP	2.2
1	A	273	TYR	2.2
1	B	148	ALA	2.2
1	B	13	LEU	2.2
1	B	267	ALA	2.2
1	A	124	ARG	2.2
1	A	179	ASP	2.1
1	B	266	ARG	2.1
1	B	333	LEU	2.0
1	A	162	ALA	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
2	OJQ	A	401[A]	22/22	0.87	0.26	22,32,39,43	34
7	EDO	B	403	4/4	0.89	0.17	33,40,40,43	0
7	EDO	B	405	4/4	0.91	0.17	33,41,50,50	0
7	EDO	B	404	4/4	0.94	0.13	32,39,47,47	0
3	L7N	B	401[B]	22/22	0.95	0.10	28,39,49,50	34

Continued on next page...

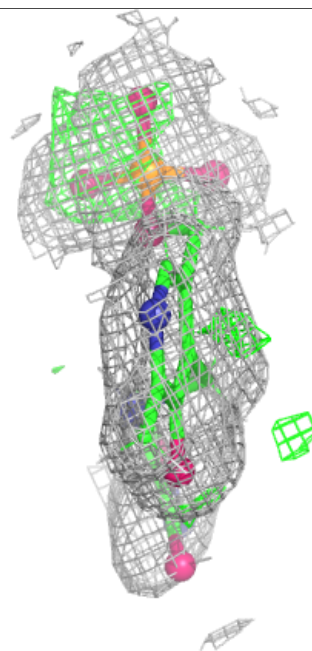
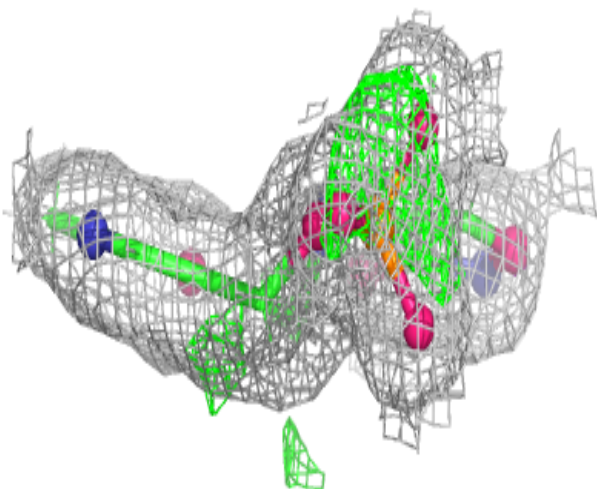
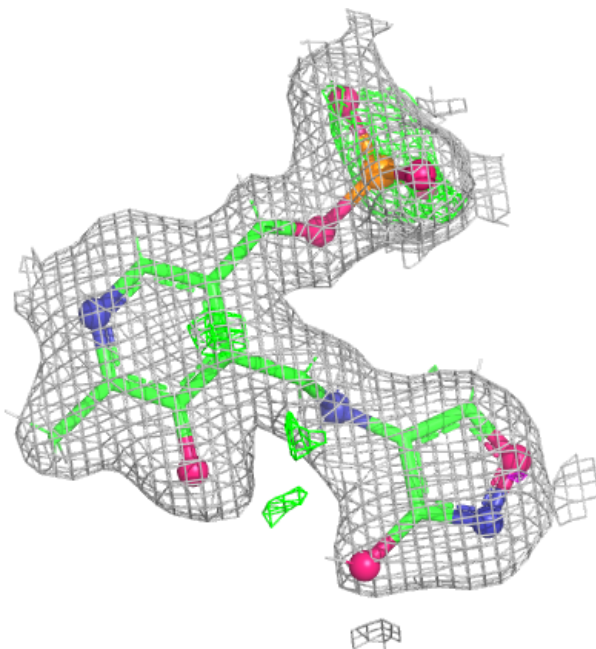
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	A	405	6/6	0.96	0.07	31,38,46,51	0
3	L7N	A	402[B]	22/22	0.96	0.10	22,32,40,41	34
5	CL	A	404	1/1	0.98	0.07	37,37,37,37	0
5	CL	B	402	1/1	0.98	0.08	38,38,38,38	0
4	CA	A	403	1/1	0.99	0.04	32,32,32,32	1

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.

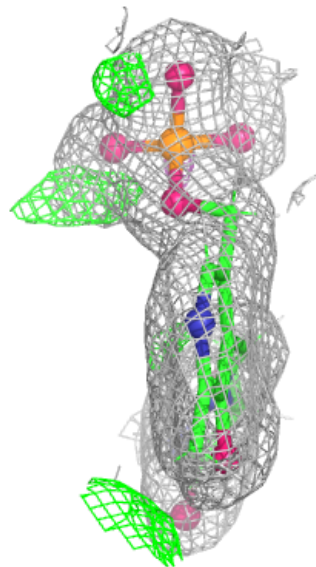
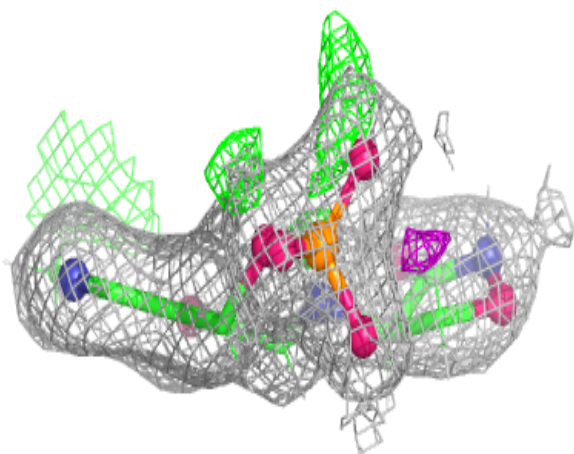
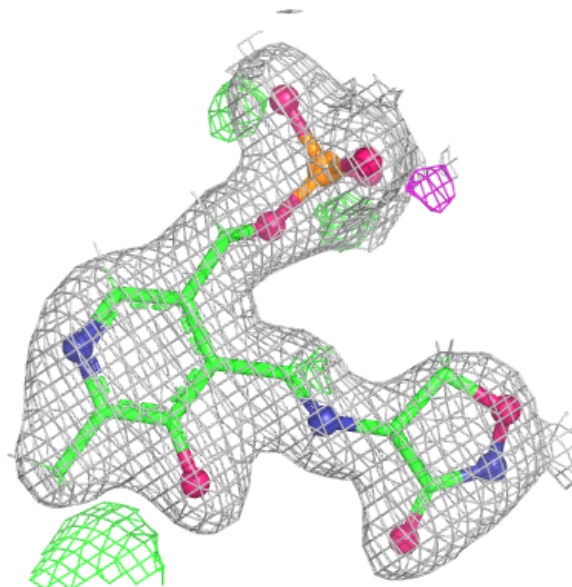
Electron density around OJQ A 401 (A):

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



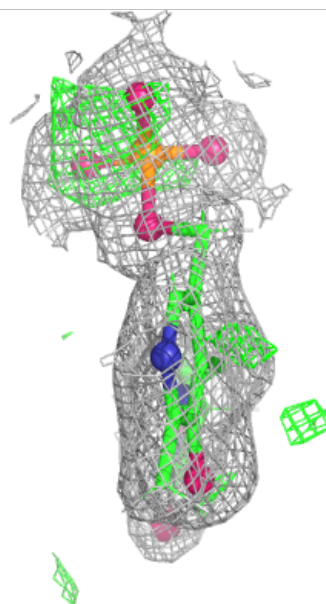
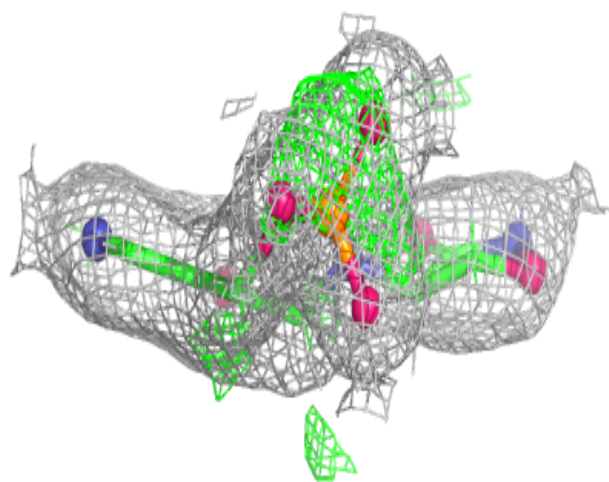
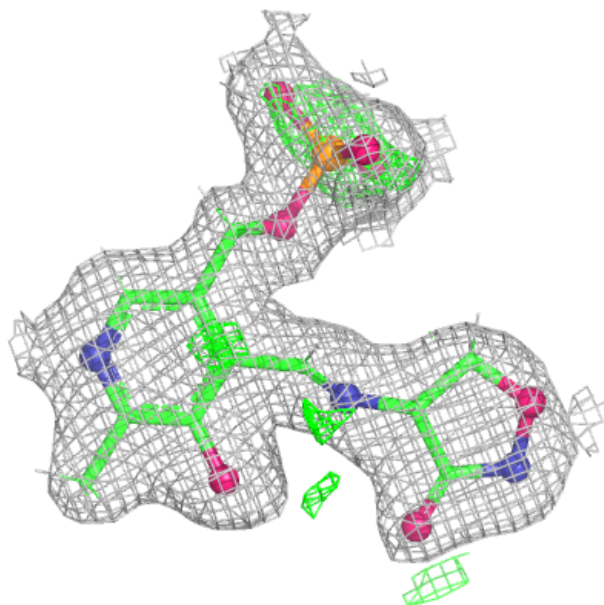
Electron density around L7N B 401 (B):

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



Electron density around L7N A 402 (B):

$2mF_o-DF_c$ (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.