



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:58 AM UTC

PDB ID : 6NXC / pdb_00006nxc
Title : ECAI(T162A) MUTANT IN COMPLEX WITH CITRATE AT PH 4
Authors : Lubkowski, J.; Wlodawer, A.
Deposited on : 2019-02-08
Resolution : 1.74 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

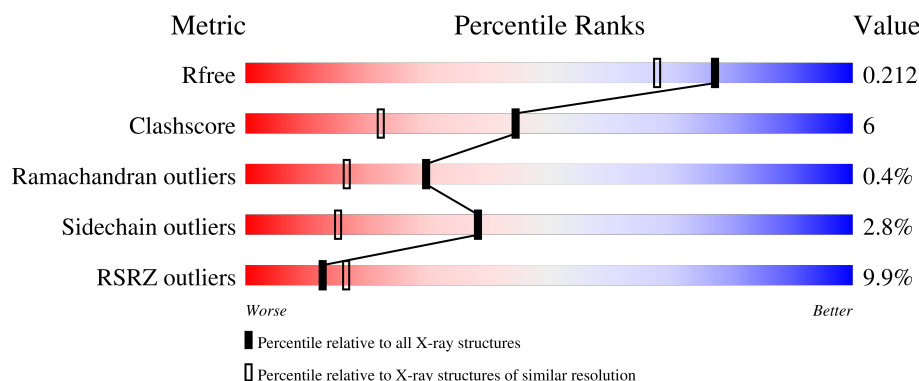
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	357	8% 72% 17% • 9%
1	B	357	12% 73% 18% • 6%
1	C	357	10% 71% 17% • 10%
1	D	357	7% 78% 14% • 6%

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
5	GOL	A	9105	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10857 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 L-asparaginase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	2	0
			2504	1585	432	475	12			
1	B	336	Total	C	N	O	S	0	4	0
			2589	1642	448	487	12			
1	C	323	Total	C	N	O	S	0	2	0
			2485	1577	426	470	12			
1	D	334	Total	C	N	O	S	0	1	0
			2570	1629	446	483	12			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P0A962
A	-18	GLY	-	expression tag	UNP P0A962
A	-17	SER	-	expression tag	UNP P0A962
A	-16	SER	-	expression tag	UNP P0A962
A	-15	HIS	-	expression tag	UNP P0A962
A	-14	HIS	-	expression tag	UNP P0A962
A	-13	HIS	-	expression tag	UNP P0A962
A	-12	HIS	-	expression tag	UNP P0A962
A	-11	HIS	-	expression tag	UNP P0A962
A	-10	HIS	-	expression tag	UNP P0A962
A	-9	SER	-	expression tag	UNP P0A962
A	-8	SER	-	expression tag	UNP P0A962
A	-7	GLY	-	expression tag	UNP P0A962
A	-6	LEU	-	expression tag	UNP P0A962
A	-5	VAL	-	expression tag	UNP P0A962
A	-4	PRO	-	expression tag	UNP P0A962
A	-3	ARG	-	expression tag	UNP P0A962
A	-2	GLY	-	expression tag	UNP P0A962
A	-1	SER	-	expression tag	UNP P0A962
A	0	HIS	-	expression tag	UNP P0A962
A	162	ALA	THR	engineered mutation	UNP P0A962

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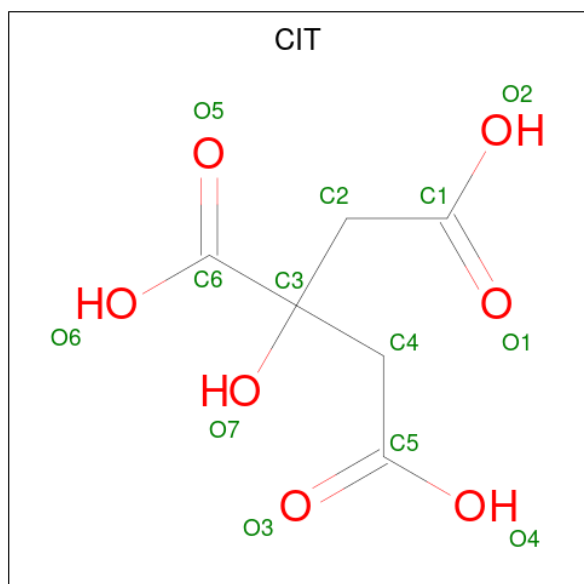
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP P0A962
B	-18	GLY	-	expression tag	UNP P0A962
B	-17	SER	-	expression tag	UNP P0A962
B	-16	SER	-	expression tag	UNP P0A962
B	-15	HIS	-	expression tag	UNP P0A962
B	-14	HIS	-	expression tag	UNP P0A962
B	-13	HIS	-	expression tag	UNP P0A962
B	-12	HIS	-	expression tag	UNP P0A962
B	-11	HIS	-	expression tag	UNP P0A962
B	-10	HIS	-	expression tag	UNP P0A962
B	-9	SER	-	expression tag	UNP P0A962
B	-8	SER	-	expression tag	UNP P0A962
B	-7	GLY	-	expression tag	UNP P0A962
B	-6	LEU	-	expression tag	UNP P0A962
B	-5	VAL	-	expression tag	UNP P0A962
B	-4	PRO	-	expression tag	UNP P0A962
B	-3	ARG	-	expression tag	UNP P0A962
B	-2	GLY	-	expression tag	UNP P0A962
B	-1	SER	-	expression tag	UNP P0A962
B	0	HIS	-	expression tag	UNP P0A962
B	162	ALA	THR	engineered mutation	UNP P0A962
C	-19	MET	-	initiating methionine	UNP P0A962
C	-18	GLY	-	expression tag	UNP P0A962
C	-17	SER	-	expression tag	UNP P0A962
C	-16	SER	-	expression tag	UNP P0A962
C	-15	HIS	-	expression tag	UNP P0A962
C	-14	HIS	-	expression tag	UNP P0A962
C	-13	HIS	-	expression tag	UNP P0A962
C	-12	HIS	-	expression tag	UNP P0A962
C	-11	HIS	-	expression tag	UNP P0A962
C	-10	HIS	-	expression tag	UNP P0A962
C	-9	SER	-	expression tag	UNP P0A962
C	-8	SER	-	expression tag	UNP P0A962
C	-7	GLY	-	expression tag	UNP P0A962
C	-6	LEU	-	expression tag	UNP P0A962
C	-5	VAL	-	expression tag	UNP P0A962
C	-4	PRO	-	expression tag	UNP P0A962
C	-3	ARG	-	expression tag	UNP P0A962
C	-2	GLY	-	expression tag	UNP P0A962
C	-1	SER	-	expression tag	UNP P0A962
C	0	HIS	-	expression tag	UNP P0A962
C	162	ALA	THR	engineered mutation	UNP P0A962

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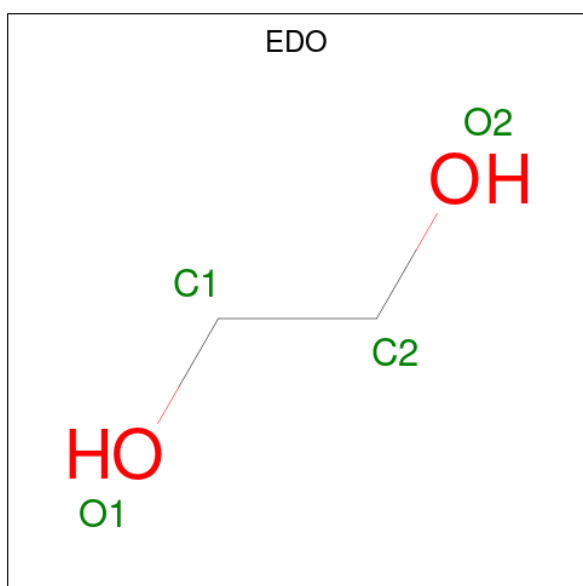
Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	initiating methionine	UNP P0A962
D	-18	GLY	-	expression tag	UNP P0A962
D	-17	SER	-	expression tag	UNP P0A962
D	-16	SER	-	expression tag	UNP P0A962
D	-15	HIS	-	expression tag	UNP P0A962
D	-14	HIS	-	expression tag	UNP P0A962
D	-13	HIS	-	expression tag	UNP P0A962
D	-12	HIS	-	expression tag	UNP P0A962
D	-11	HIS	-	expression tag	UNP P0A962
D	-10	HIS	-	expression tag	UNP P0A962
D	-9	SER	-	expression tag	UNP P0A962
D	-8	SER	-	expression tag	UNP P0A962
D	-7	GLY	-	expression tag	UNP P0A962
D	-6	LEU	-	expression tag	UNP P0A962
D	-5	VAL	-	expression tag	UNP P0A962
D	-4	PRO	-	expression tag	UNP P0A962
D	-3	ARG	-	expression tag	UNP P0A962
D	-2	GLY	-	expression tag	UNP P0A962
D	-1	SER	-	expression tag	UNP P0A962
D	0	HIS	-	expression tag	UNP P0A962
D	162	ALA	THR	engineered mutation	UNP P0A962

- Molecule 2 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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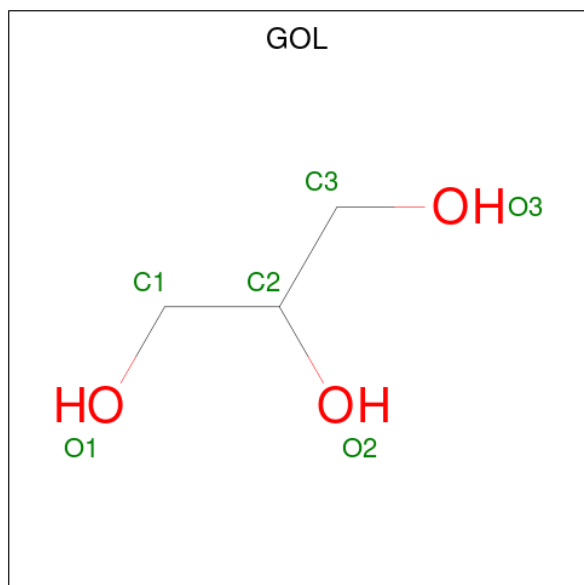
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Cl	0	0
			3	3		
4	B	3	Total	Cl	0	0
			3	3		
4	C	1	Total	Cl	0	0
			1	1		
4	D	3	Total	Cl	0	0
			3	3		

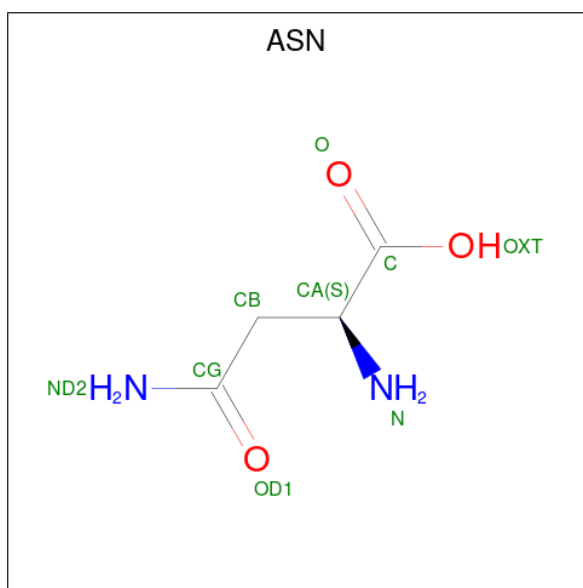
- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is ASPARAGINE (CCD ID: ASN) (formula: C₄H₈N₂O₃) (labeled as "Ligand of

Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			9	4	2	3		
6	B	1	Total	C	N	O	0	0
			9	4	2	3		
6	C	1	Total	C	N	O	0	0
			9	4	2	3		
6	D	1	Total	C	N	O	0	0
			9	4	2	3		

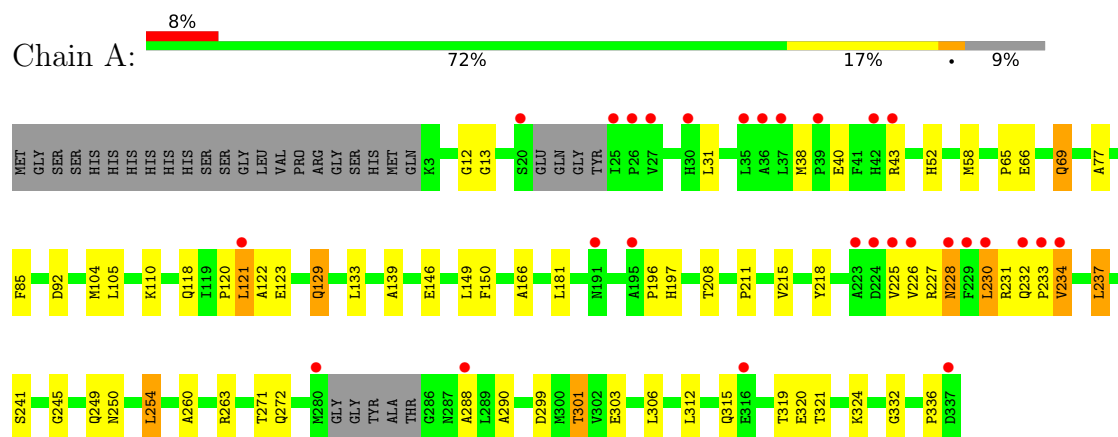
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	140	Total	O	0	0
			140	140		
7	B	135	Total	O	0	0
			135	135		
7	C	131	Total	O	0	0
			131	131		
7	D	159	Total	O	0	0
			159	159		

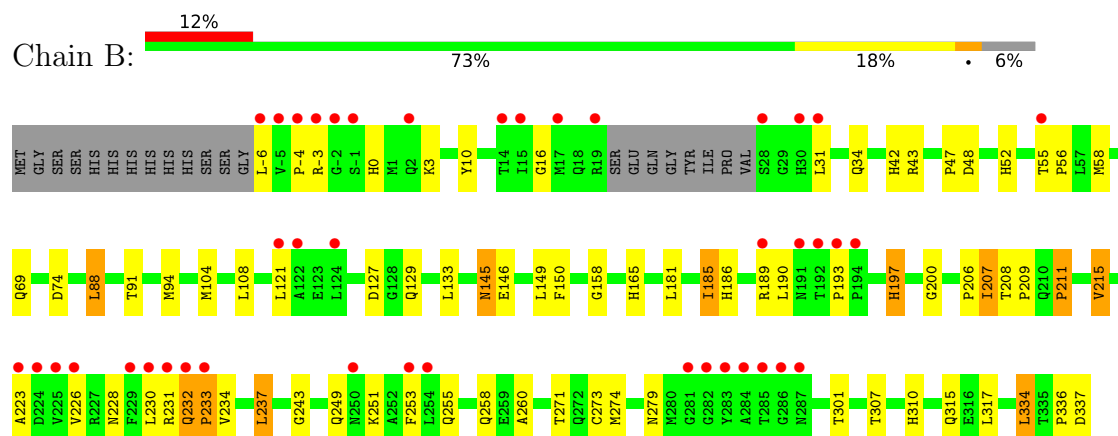
3 Residue-property plots [i](#)

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.

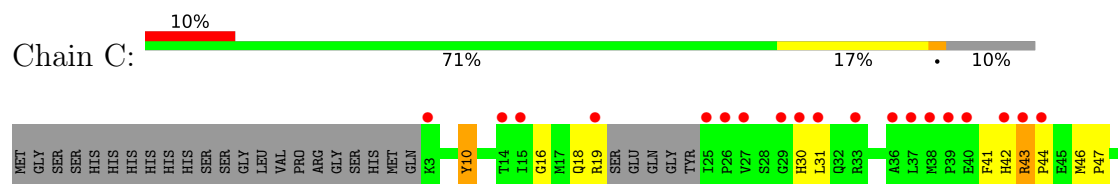
• Molecule 1: L-asparaginase 1

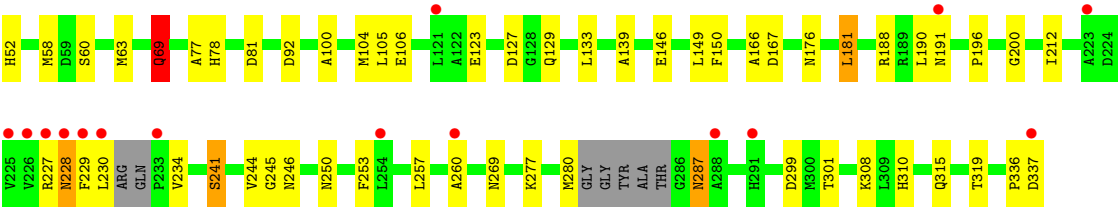


• Molecule 1: L-asparaginase 1

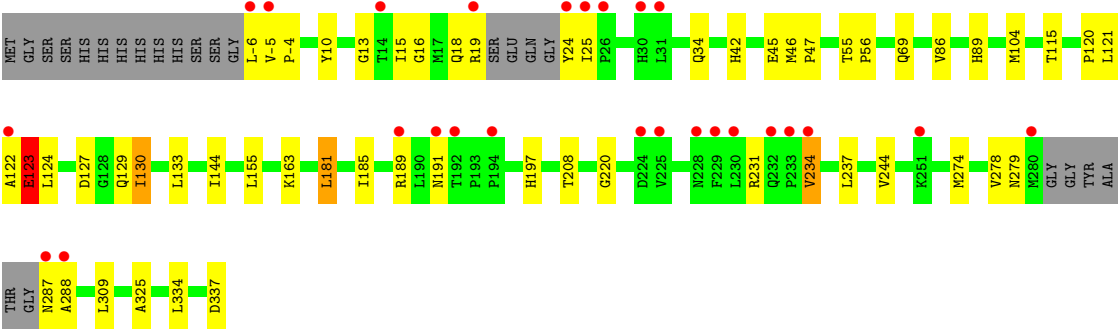
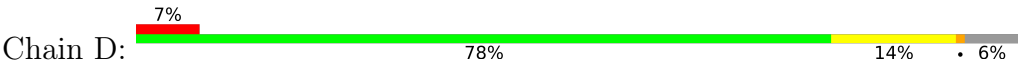


• Molecule 1: L-asparaginase 1





● Molecule 1: L-asparaginase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.52Å 89.77Å 93.29Å 90.00° 117.14° 90.00°	Depositor
Resolution (Å)	46.54 – 1.74 46.54 – 1.74	Depositor EDS
% Data completeness (in resolution range)	93.9 (46.54-1.74) 93.9 (46.54-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.166 , 0.208 0.176 , 0.212	Depositor DCC
R_{free} test set	6415 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10857	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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: EDO, CIT, CL, 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	1.47	22/2566 (0.9%)	1.56	23/3492 (0.7%)
1	B	1.45	18/2664 (0.7%)	1.52	18/3627 (0.5%)
1	C	1.45	14/2549 (0.5%)	1.56	22/3465 (0.6%)
1	D	1.40	11/2631 (0.4%)	1.49	13/3581 (0.4%)
All	All	1.44	65/10410 (0.6%)	1.53	76/14165 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
All	All	0	3

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	100	ALA	C-O	7.97	1.33	1.24
1	C	77	ALA	C-O	7.84	1.33	1.24
1	C	228	ASN	C-O	7.65	1.32	1.24
1	C	139	ALA	C-O	7.61	1.33	1.24
1	A	146	GLU	C-O	7.24	1.32	1.23
1	C	69	GLN	C-O	-7.23	1.15	1.24
1	B	215	VAL	C-O	-7.05	1.16	1.24
1	A	92	ASP	C-O	6.88	1.31	1.24
1	C	146	GLU	C-O	6.77	1.32	1.23
1	A	12	GLY	C-O	6.76	1.32	1.23
1	A	66	GLU	C-O	6.73	1.32	1.24
1	B	211	PRO	C-O	6.65	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	228	ASN	C-O	6.59	1.32	1.24
1	A	211	PRO	C-O	6.51	1.29	1.23
1	D	89	HIS	CE1-NE2	6.48	1.39	1.32
1	B	146	GLU	C-O	6.36	1.31	1.23
1	B	48	ASP	C-O	6.32	1.31	1.23
1	A	218	TYR	N-CA	6.29	1.51	1.45
1	D	130	ILE	C-O	6.27	1.31	1.24
1	A	306	LEU	C-O	6.26	1.31	1.24
1	A	77	ALA	C-O	6.25	1.31	1.24
1	A	52	HIS	CE1-NE2	6.22	1.38	1.32
1	D	15	ILE	C-O	6.22	1.31	1.24
1	A	13	GLY	C-O	6.20	1.30	1.23
1	C	212	ILE	C-O	-6.13	1.18	1.24
1	A	332	GLY	C-O	6.13	1.32	1.24
1	D	127	ASP	CG-OD2	6.02	1.36	1.25
1	B	200	GLY	C-O	6.01	1.30	1.23
1	B	127	ASP	CG-OD2	5.95	1.36	1.25
1	C	92	ASP	C-O	5.94	1.31	1.24
1	C	60	SER	C-O	5.91	1.31	1.24
1	A	303	GLU	C-O	5.89	1.30	1.24
1	C	78	HIS	CE1-NE2	5.89	1.38	1.32
1	C	310	HIS	C-O	5.89	1.30	1.24
1	D	47	PRO	C-O	5.88	1.30	1.23
1	B	42	HIS	CG-ND1	-5.87	1.31	1.38
1	B	206	PRO	C-O	-5.87	1.16	1.23
1	B	186	HIS	CE1-NE2	5.86	1.38	1.32
1	C	52	HIS	CE1-NE2	5.80	1.38	1.32
1	B	336	PRO	C-O	-5.77	1.17	1.23
1	A	290	ALA	C-O	5.75	1.30	1.24
1	A	336	PRO	C-O	-5.73	1.17	1.23
1	A	312	LEU	C-O	5.72	1.31	1.24
1	A	226	VAL	C-O	5.70	1.30	1.24
1	C	166	ALA	C-O	5.64	1.30	1.24
1	D	163	LYS	C-O	-5.55	1.17	1.23
1	B	165	HIS	CE1-NE2	5.52	1.38	1.32
1	A	65	PRO	C-O	-5.51	1.17	1.24
1	B	47	PRO	C-O	5.50	1.30	1.23
1	B	207	ILE	C-O	5.49	1.30	1.24
1	D	220	GLY	C-O	-5.46	1.16	1.24
1	B	52	HIS	CE1-NE2	5.43	1.38	1.32
1	C	246	ASN	C-O	-5.38	1.17	1.23
1	B	317	LEU	C-O	-5.35	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	ALA	C-O	5.32	1.30	1.24
1	A	139	ALA	C-O	5.22	1.30	1.24
1	B	315	GLN	N-CA	5.16	1.51	1.45
1	A	272	GLN	C-O	5.16	1.30	1.24
1	B	88	LEU	C-O	5.09	1.30	1.24
1	D	13	GLY	C-O	5.08	1.29	1.23
1	D	309	LEU	N-CA	5.05	1.52	1.46
1	B	307	THR	C-O	-5.04	1.18	1.24
1	D	89	HIS	ND1-CE1	5.04	1.37	1.32
1	D	86	VAL	C-O	5.02	1.29	1.24
1	A	149	LEU	C-O	5.00	1.29	1.24

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	ASN	CA-CB-CG	9.13	121.73	112.60
1	D	337	ASP	CA-C-O	-8.64	106.10	120.80
1	C	123	GLU	CB-CG-CD	8.37	126.82	112.60
1	D	45	GLU	CB-CG-CD	8.01	126.22	112.60
1	B	233	PRO	CB-CA-C	7.67	118.38	111.40
1	A	196	PRO	N-CA-C	-7.51	99.42	111.14
1	A	299	ASP	CA-CB-CG	7.41	120.01	112.60
1	A	228	ASN	CB-CA-C	7.23	124.81	110.42
1	B	74	ASP	CA-CB-CG	6.95	119.55	112.60
1	C	181[A]	LEU	N-CA-CB	-6.94	98.61	111.52
1	C	181[B]	LEU	N-CA-CB	-6.94	98.61	111.52
1	D	123	GLU	CB-CA-C	6.91	121.33	109.51
1	B	-4	PRO	CB-CA-C	-6.90	101.94	110.98
1	A	129	GLN	N-CA-C	-6.80	103.95	111.36
1	D	185	ILE	O-C-N	6.78	128.44	121.87
1	C	319	THR	CA-CB-OG1	-6.69	99.57	109.60
1	B	279	ASN	CB-CA-C	-6.65	102.98	111.70
1	D	115	THR	CA-CB-OG1	-6.62	99.68	109.60
1	C	150	PHE	CA-CB-CG	-6.54	107.26	113.80
1	D	42	HIS	CA-CB-CG	-6.52	107.28	113.80
1	C	299	ASP	CA-CB-CG	6.51	119.11	112.60
1	B	-3	ARG	CB-CA-C	6.37	120.97	110.78
1	A	123	GLU	CB-CG-CD	6.35	123.39	112.60
1	C	196	PRO	N-CA-C	-6.33	101.28	111.03
1	A	196	PRO	N-CA-CB	6.18	108.81	103.31
1	A	66	GLU	CB-CG-CD	6.17	123.09	112.60
1	D	191	ASN	CA-CB-CG	-6.16	106.44	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	255	GLN	CA-C-O	-6.13	114.39	120.82
1	C	241[A]	SER	CA-CB-OG	-6.10	98.90	111.10
1	C	241[B]	SER	CA-CB-OG	-6.10	98.90	111.10
1	B	207	ILE	N-CA-CB	6.08	120.08	111.82
1	C	81	ASP	CA-CB-CG	-6.01	106.59	112.60
1	C	308	LYS	CA-C-O	-6.00	114.06	120.42
1	A	150	PHE	CA-CB-CG	-5.96	107.84	113.80
1	C	196	PRO	N-CA-CB	5.92	108.60	103.27
1	D	130	ILE	CA-C-O	-5.92	114.58	120.85
1	B	185	ILE	O-C-N	5.89	127.58	121.87
1	A	197	HIS	CA-CB-CG	-5.84	107.96	113.80
1	A	228	ASN	N-CA-CB	-5.80	100.69	110.49
1	A	110	LYS	O-C-N	-5.79	118.00	121.71
1	B	253	PHE	CA-C-N	5.76	128.00	120.28
1	B	253	PHE	C-N-CA	5.76	128.00	120.28
1	C	200	GLY	CA-C-O	-5.75	116.75	121.76
1	A	123	GLU	CB-CA-C	5.60	119.76	109.46
1	B	150	PHE	CA-CB-CG	-5.53	108.27	113.80
1	D	325	ALA	N-CA-C	-5.49	105.45	111.82
1	C	123	GLU	CB-CA-C	5.48	119.54	109.46
1	A	271	THR	CA-CB-OG1	-5.48	101.39	109.60
1	A	208	THR	CB-CA-C	5.47	117.35	108.87
1	C	336	PRO	CA-C-N	5.46	131.53	121.70
1	C	336	PRO	C-N-CA	5.46	131.53	121.70
1	A	120	PRO	N-CA-C	5.44	119.62	111.14
1	D	181	LEU	N-CA-CB	-5.44	101.29	111.13
1	C	43	ARG	CG-CD-NE	-5.43	100.06	112.00
1	A	315	GLN	CA-C-N	-5.41	111.21	121.54
1	A	315	GLN	C-N-CA	-5.41	111.21	121.54
1	C	69	GLN	CA-C-O	-5.37	115.19	120.82
1	D	278	VAL	O-C-N	5.32	128.41	122.61
1	A	319	THR	CA-CB-OG1	-5.27	101.69	109.60
1	D	279	ASN	CB-CA-C	-5.25	104.82	111.70
1	B	249	GLN	CA-C-N	5.25	129.74	121.56
1	B	249	GLN	C-N-CA	5.25	129.74	121.56
1	B	337	ASP	CA-C-O	-5.23	111.91	120.80
1	B	251	LYS	CA-C-O	-5.22	115.02	120.55
1	B	185	ILE	CA-C-O	-5.21	115.53	120.95
1	A	301	THR	CA-CB-OG1	-5.19	101.82	109.60
1	C	167	ASP	CA-CB-CG	-5.18	107.42	112.60
1	A	321	THR	CA-CB-OG1	-5.15	101.87	109.60
1	A	85	PHE	CA-CB-CG	-5.14	108.66	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	127	ASP	N-CA-C	-5.12	106.72	113.17
1	B	145	ASN	CB-CA-C	-5.11	104.67	111.88
1	A	129	GLN	CA-C-O	-5.08	115.04	120.42
1	C	42	HIS	CB-CA-C	5.06	119.11	110.01
1	C	10	TYR	CB-CA-C	5.02	119.75	111.31
1	B	158	GLY	O-C-N	5.01	127.09	122.13
1	D	208	THR	CB-CA-C	5.00	117.16	108.91

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	LEU	Mainchain
1	C	105	LEU	Mainchain
1	C	287	ASN	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2504	0	2463	27	0
1	B	2589	0	2549	39	0
1	C	2485	0	2455	35	0
1	D	2570	0	2544	25	0
2	A	12	0	5	1	0
2	B	12	0	5	1	0
2	C	12	0	5	1	0
2	D	12	0	5	1	0
3	A	12	0	17	1	0
3	B	12	0	17	3	0
3	C	12	0	18	2	0
3	D	8	0	11	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	1	0	0	0	0
4	D	3	0	0	0	0
5	A	6	0	8	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	9	0	5	0	0
6	B	9	0	5	0	0
6	C	9	0	5	0	0
6	D	9	0	5	0	0
7	A	140	0	0	2	0
7	B	135	0	0	1	0
7	C	131	0	0	3	0
7	D	159	0	0	3	0
All	All	10857	0	10122	123	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 6.

All (123) 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:-5:VAL:CB	1:D:144:ILE:HD11	1.81	1.09
5:A:9105:GOL:H12	1:C:244:VAL:HG22	1.35	1.06
1:B:145:ASN:O	1:B:197[A]:HIS:HE1	1.45	0.99
1:C:315:GLN:HG2	7:C:507:HOH:O	1.65	0.96
1:D:130:ILE:HD11	7:D:593:HOH:O	1.70	0.90
1:B:243:GLY:O	1:B:271[B]:THR:HG23	1.75	0.87
1:C:229:PHE:O	1:C:234:VAL:HG11	1.76	0.85
5:A:9105:GOL:O2	7:A:9201:HOH:O	2.01	0.79
1:D:-5:VAL:CB	1:D:144:ILE:CD1	2.61	0.78
1:A:215:VAL:HG23	1:A:237:LEU:CD1	2.15	0.77
1:C:229:PHE:O	1:C:234:VAL:CG1	2.34	0.76
1:A:230:LEU:HD21	1:A:260:ALA:HB2	1.69	0.74
1:C:43:ARG:HG3	1:C:44:PRO:HD2	1.67	0.74
1:B:271[B]:THR:HG22	1:B:273:CYS:H	1.52	0.74
1:C:43:ARG:NH2	1:D:123:GLU:HA	2.03	0.73
1:B:145:ASN:O	1:B:197[A]:HIS:CE1	2.37	0.73
1:D:34:GLN:OE1	1:D:122:ALA:HB3	1.91	0.71
1:A:31:LEU:HD12	1:A:121:LEU:HD12	1.75	0.69
1:B:232:GLN:HB3	1:B:233:PRO:HD2	1.73	0.68
1:D:197:HIS:HD2	7:D:514:HOH:O	1.78	0.66
1:B:193:PRO:HG3	1:C:191:ASN:HD22	1.61	0.66
1:A:129:GLN:HG2	7:A:9281:HOH:O	1.96	0.65
1:B:232:GLN:HB3	1:B:233:PRO:CD	2.26	0.65
1:B:31:LEU:HA	1:B:34:GLN:OE1	1.96	0.65
1:A:230:LEU:CD2	1:A:260:ALA:HB2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:9105:GOL:C1	1:C:244:VAL:H	2.11	0.62
5:A:9105:GOL:C1	1:C:244:VAL:HG22	2.22	0.62
5:A:9105:GOL:H12	1:C:244:VAL:CG2	2.21	0.62
1:C:129:GLN:HB2	7:C:568:HOH:O	2.00	0.62
1:A:230:LEU:O	1:A:263:ARG:NH2	2.33	0.61
1:B:193:PRO:HG3	1:C:191:ASN:ND2	2.15	0.61
1:B:226:VAL:O	1:B:230:LEU:HD13	2.01	0.61
1:A:225:VAL:O	1:A:228:ASN:HB3	2.01	0.60
1:B:215:VAL:HG21	1:B:237[A]:LEU:HD21	1.84	0.60
2:D:403:CIT:O2	2:D:403:CIT:C6	2.50	0.60
1:C:43:ARG:HG3	1:C:44:PRO:CD	2.32	0.60
1:D:121:LEU:HD11	1:D:129:GLN:HG3	1.84	0.60
1:B:10:TYR:OH	1:B:16:GLY:HA3	2.00	0.59
1:C:241[A]:SER:OG	1:C:245:GLY:HA2	2.01	0.59
1:A:241[B]:SER:OG	1:A:245:GLY:HA2	2.03	0.59
1:B:211:PRO:HG3	1:B:233:PRO:HB2	1.84	0.58
1:B:228:ASN:OD1	1:B:231:ARG:NH1	2.37	0.57
1:B:207:ILE:HG23	1:B:310:HIS:HB3	1.87	0.56
1:A:254:LEU:HD21	1:A:288:ALA:HB1	1.86	0.56
1:A:215:VAL:CG2	1:A:237:LEU:CD1	2.83	0.56
1:B:0:HIS:NE2	3:B:9103:EDO:H22	2.21	0.55
1:B:231:ARG:NH2	1:D:231:ARG:HD3	2.22	0.55
1:D:-4:PRO:HD2	1:D:144:ILE:HG12	1.90	0.54
1:A:215:VAL:HG23	1:A:237:LEU:HD11	1.90	0.54
2:C:403:CIT:O1	2:C:403:CIT:C6	2.56	0.53
1:A:215:VAL:CG2	1:A:237:LEU:HD11	2.39	0.53
1:A:228:ASN:ND2	1:C:228:ASN:HB3	2.24	0.53
2:B:9101:CIT:O1	2:B:9101:CIT:C6	2.57	0.53
1:A:234:VAL:HG11	1:A:237:LEU:HD23	1.91	0.52
1:B:215:VAL:CG2	1:B:237[A]:LEU:HD21	2.40	0.52
1:D:197:HIS:HE1	7:D:505:HOH:O	1.92	0.52
1:A:40:GLU:HG3	1:A:43:ARG:NH1	2.25	0.52
1:A:301:THR:HA	3:A:9103:EDO:H12	1.91	0.52
1:C:230:LEU:HD11	1:C:260:ALA:HB2	1.92	0.51
2:A:9101:CIT:C6	2:A:9101:CIT:O2	2.59	0.51
1:C:176:ASN:ND2	3:C:404:EDO:H11	2.25	0.50
1:A:122:ALA:O	1:B:43:ARG:NH1	2.45	0.50
5:A:9105:GOL:H11	1:C:244:VAL:H	1.76	0.50
1:B:121:LEU:HD11	1:B:129:GLN:HG3	1.94	0.49
1:A:227:ARG:HD3	1:A:231:ARG:NH2	2.28	0.49
1:C:43:ARG:HH22	1:D:123:GLU:HA	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:TYR:OH	1:C:16:GLY:HA3	2.13	0.48
5:A:9105:GOL:H31	1:B:185:ILE:HD11	1.94	0.48
1:B:301:THR:HA	3:B:9104:EDO:H21	1.96	0.48
1:A:69:GLN:HA	1:A:104:MET:HE1	1.97	0.47
1:A:38:MET:HE1	1:A:121:LEU:HD13	1.97	0.47
1:B:274:MET:HE3	1:D:274:MET:HB2	1.97	0.47
1:B:230:LEU:HD11	1:B:260:ALA:HB2	1.95	0.47
1:C:69:GLN:HA	1:C:104:MET:HE1	1.97	0.47
1:C:190:LEU:N	1:C:190:LEU:HD12	2.30	0.47
3:B:9105:EDO:H12	1:D:244:VAL:HG13	1.97	0.46
1:C:46:MET:HE3	1:C:47:PRO:HD2	1.97	0.46
1:C:253:PHE:CE1	1:C:257:LEU:HD11	2.50	0.46
1:C:277:LYS:HZ3	1:C:337:ASP:C	2.23	0.46
1:B:55:THR:HA	1:B:56:PRO:HA	1.79	0.46
1:D:18:GLN:O	1:D:24:TYR:N	2.49	0.45
1:C:269:ASN:HD22	1:C:280:MET:HE3	1.81	0.45
1:B:121:LEU:CD1	1:B:129:GLN:HG3	2.48	0.44
1:B:274:MET:HE1	7:B:9326:HOH:O	2.18	0.44
1:A:232:GLN:O	1:A:233:PRO:C	2.61	0.44
1:D:10:TYR:OH	1:D:16:GLY:HA3	2.18	0.44
1:D:234:VAL:HG11	1:D:237:LEU:HD13	2.00	0.44
1:B:334:LEU:HD12	1:B:334:LEU:C	2.43	0.44
1:D:46:MET:HE2	1:D:133:LEU:HD22	2.00	0.44
1:B:-6:LEU:HD23	1:B:190:LEU:O	2.18	0.43
1:B:207:ILE:HD13	1:B:207:ILE:HG21	1.82	0.43
1:C:58:MET:HE1	1:C:63:MET:HA	2.00	0.43
1:D:121:LEU:C	1:D:123:GLU:H	2.27	0.43
1:A:320:GLU:OE2	1:A:324:LYS:NZ	2.28	0.43
1:A:232:GLN:CD	1:A:232:GLN:C	2.86	0.43
1:D:155:LEU:HB3	1:D:181:LEU:HB3	2.00	0.43
1:D:120:PRO:O	1:D:123:GLU:HB3	2.19	0.43
1:C:241[A]:SER:HB3	1:C:269:ASN:OD1	2.18	0.42
1:D:124:LEU:HD23	1:D:124:LEU:HA	1.84	0.42
1:C:41:PHE:HE2	1:C:129:GLN:HG3	1.84	0.42
1:A:234:VAL:HG11	1:A:237:LEU:CD2	2.49	0.42
1:C:18:GLN:HB2	1:C:30:HIS:HD2	1.85	0.42
1:B:181[A]:LEU:CD2	1:B:189:ARG:HG2	2.49	0.42
1:B:91:THR:HA	1:B:94:MET:HE3	2.01	0.42
1:A:118:GLN:OE1	5:A:9105:GOL:H32	2.20	0.42
1:C:269:ASN:ND2	1:C:280:MET:HE3	2.35	0.41
1:C:18:GLN:O	1:C:19:ARG:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271[B]:THR:CG2	1:B:273:CYS:HB2	2.50	0.41
1:B:58:MET:HE2	1:B:58:MET:HB3	1.89	0.41
1:B:149:LEU:C	1:B:149:LEU:HD23	2.45	0.41
1:C:301:THR:HA	3:C:404:EDO:H12	2.02	0.41
1:A:121:LEU:HD23	1:A:121:LEU:HA	1.98	0.41
1:A:58:MET:HE2	1:A:58:MET:HB3	1.93	0.41
1:B:108:LEU:O	1:B:197[A]:HIS:NE2	2.52	0.41
1:C:149:LEU:HD23	1:C:149:LEU:C	2.45	0.41
1:D:123:GLU:O	1:D:124:LEU:C	2.63	0.40
1:D:69:GLN:HA	1:D:104:MET:HE1	2.04	0.40
1:B:69:GLN:HA	1:B:104:MET:HE1	2.03	0.40
1:D:55:THR:HA	1:D:56:PRO:HA	1.92	0.40
1:D:334:LEU:C	1:D:334:LEU:HD12	2.46	0.40
1:B:88:LEU:HD23	1:B:88:LEU:HA	1.94	0.40
1:B:208:THR:HB	1:B:209:PRO:HD2	2.04	0.40
1:C:106:GLU:OE2	7:C:501:HOH:O	2.22	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	322/357 (90%)	308 (96%)	13 (4%)	1 (0%)	36	23
1	B	336/357 (94%)	325 (97%)	9 (3%)	2 (1%)	21	8
1	C	317/357 (89%)	306 (96%)	10 (3%)	1 (0%)	36	23
1	D	329/357 (92%)	322 (98%)	6 (2%)	1 (0%)	36	23
All	All	1304/1428 (91%)	1261 (97%)	38 (3%)	5 (0%)	30	16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	232	GLN
1	C	250	ASN
1	D	288	ALA
1	A	250	ASN
1	B	223	ALA

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	269/296 (91%)	260 (97%)	9 (3%)	33	10
1	B	277/296 (94%)	268 (97%)	9 (3%)	34	11
1	C	267/296 (90%)	259 (97%)	8 (3%)	36	12
1	D	276/296 (93%)	269 (98%)	7 (2%)	42	18
All	All	1089/1184 (92%)	1056 (97%)	33 (3%)	38	12

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	121	LEU
1	A	133	LEU
1	A	181	LEU
1	A	230	LEU
1	A	234	VAL
1	A	237	LEU
1	A	249	GLN
1	A	254	LEU
1	B	3	LYS
1	B	133	LEU
1	B	197[A]	HIS
1	B	197[B]	HIS
1	B	234	VAL
1	B	237[A]	LEU
1	B	237[B]	LEU
1	B	258	GLN

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Mol	Chain	Res	Type
1	B	334	LEU
1	C	31	LEU
1	C	69	GLN
1	C	133	LEU
1	C	181[A]	LEU
1	C	181[B]	LEU
1	C	188	ARG
1	C	227	ARG
1	C	287	ASN
1	D	-6	LEU
1	D	19	ARG
1	D	25	ILE
1	D	123	GLU
1	D	189	ARG
1	D	234	VAL
1	D	287	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	145	ASN
1	A	255	GLN
1	B	18	GLN
1	B	134	ASN
1	B	152	ASN
1	B	153	ASN
1	C	34	GLN
1	C	145	ASN
1	C	153	ASN
1	C	176	ASN
1	C	246	ASN
1	C	279	ASN
1	C	291	HIS
1	D	18	GLN
1	D	30	HIS
1	D	52	HIS
1	D	107	ASN
1	D	152	ASN
1	D	232	GLN
1	D	258	GLN
1	D	279	ASN

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Mol	Chain	Res	Type
1	D	287	ASN
1	D	315	GLN

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 10 are monoatomic - leaving 20 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	EDO	A	9107	-	3,3,3	0.40	0	2,2,2	0.89	0
6	ASN	A	9109	-	7,8,8	1.15	1 (14%)	6,10,10	0.60	0
2	CIT	A	9101	1	11,11,12	0.89	0	14,15,17	1.60	4 (28%)
3	EDO	D	406	-	3,3,3	1.11	0	2,2,2	0.80	0
3	EDO	B	9105	-	3,3,3	0.82	0	2,2,2	0.65	0
2	CIT	B	9101	1	11,11,12	1.51	3 (27%)	12,15,17	1.51	2 (16%)
2	CIT	D	403	1	11,11,12	1.37	3 (27%)	12,15,17	1.60	2 (16%)
3	EDO	B	9104	-	3,3,3	1.22	0	2,2,2	0.69	0
3	EDO	C	404	-	3,3,3	0.57	0	2,2,2	0.29	0
5	GOL	A	9105	-	5,5,5	0.65	0	5,5,5	0.72	0
6	ASN	C	402	-	7,8,8	0.95	0	6,10,10	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CIT	C	403	1	11,11,12	1.41	2 (18%)	14,15,17	1.11	1 (7%)
6	ASN	D	402	-	7,8,8	0.92	0	6,10,10	1.48	1 (16%)
3	EDO	A	9103	-	3,3,3	0.75	0	2,2,2	0.65	0
3	EDO	D	407	-	3,3,3	0.65	0	2,2,2	0.24	0
6	ASN	B	9102	-	7,8,8	1.23	1 (14%)	6,10,10	0.67	0
3	EDO	B	9103	-	3,3,3	0.20	0	2,2,2	0.10	0
3	EDO	C	405	-	3,3,3	0.43	0	2,2,2	0.45	0
3	EDO	C	401	-	3,3,3	0.35	0	2,2,2	0.72	0
3	EDO	A	9102	-	3,3,3	0.71	0	2,2,2	0.28	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	EDO	A	9107	-	-	0/1/1/1	-
6	ASN	A	9109	-	-	1/8/8/8	-
2	CIT	A	9101	1	-	3/15/15/16	-
3	EDO	D	406	-	-	0/1/1/1	-
3	EDO	B	9105	-	-	1/1/1/1	-
2	CIT	B	9101	1	-	2/15/15/16	-
2	CIT	D	403	1	-	2/15/15/16	-
3	EDO	B	9104	-	-	0/1/1/1	-
3	EDO	C	404	-	-	1/1/1/1	-
5	GOL	A	9105	-	-	4/4/4/4	-
6	ASN	C	402	-	-	2/8/8/8	-
2	CIT	C	403	1	-	1/15/15/16	-
6	ASN	D	402	-	-	3/8/8/8	-
3	EDO	A	9103	-	-	0/1/1/1	-
3	EDO	D	407	-	-	0/1/1/1	-
6	ASN	B	9102	-	-	2/8/8/8	-
3	EDO	B	9103	-	-	1/1/1/1	-
3	EDO	C	405	-	-	0/1/1/1	-
3	EDO	C	401	-	-	0/1/1/1	-
3	EDO	A	9102	-	-	0/1/1/1	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	9102	ASN	O-C	2.94	1.30	1.22
6	A	9109	ASN	O-C	2.89	1.30	1.22
2	B	9101	CIT	O1-C1	2.63	1.30	1.22
2	C	403	CIT	C3-C6	2.55	1.56	1.53
2	D	403	CIT	O4-C5	-2.34	1.30	1.42
2	B	9101	CIT	O2-C1	-2.33	1.23	1.30
2	B	9101	CIT	O4-C5	-2.20	1.30	1.42
2	D	403	CIT	O2-C1	-2.15	1.23	1.30
2	C	403	CIT	O2-C1	-2.10	1.23	1.30
2	D	403	CIT	O5-C6	2.03	1.28	1.22

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9101	CIT	O5-C6-C3	-3.97	114.41	122.09
2	D	403	CIT	O4-C5-C4	3.70	121.72	111.33
2	B	9101	CIT	O4-C5-C4	3.56	121.32	111.33
6	D	402	ASN	OXT-C-O	2.90	130.66	124.08
2	B	9101	CIT	O5-C6-C3	-2.81	116.65	122.09
2	D	403	CIT	O5-C6-C3	-2.65	116.96	122.09
2	C	403	CIT	O5-C6-C3	-2.37	117.51	122.09
2	A	9101	CIT	O6-C6-C3	2.28	117.52	113.14
2	A	9101	CIT	O7-C3-C4	2.14	114.06	109.21
2	A	9101	CIT	O1-C1-C2	-2.03	117.20	122.95

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	9105	GOL	O1-C1-C2-O2
5	A	9105	GOL	O1-C1-C2-C3
5	A	9105	GOL	C1-C2-C3-O3
5	A	9105	GOL	O2-C2-C3-O3
6	D	402	ASN	OXT-C-CA-CB
6	D	402	ASN	O-C-CA-CB
6	B	9102	ASN	OXT-C-CA-CB
2	A	9101	CIT	C3-C4-C5-O3
2	C	403	CIT	C3-C4-C5-O3
6	A	9109	ASN	OXT-C-CA-CB
6	B	9102	ASN	O-C-CA-CB
2	B	9101	CIT	C2-C3-C6-O5
3	C	404	EDO	O1-C1-C2-O2

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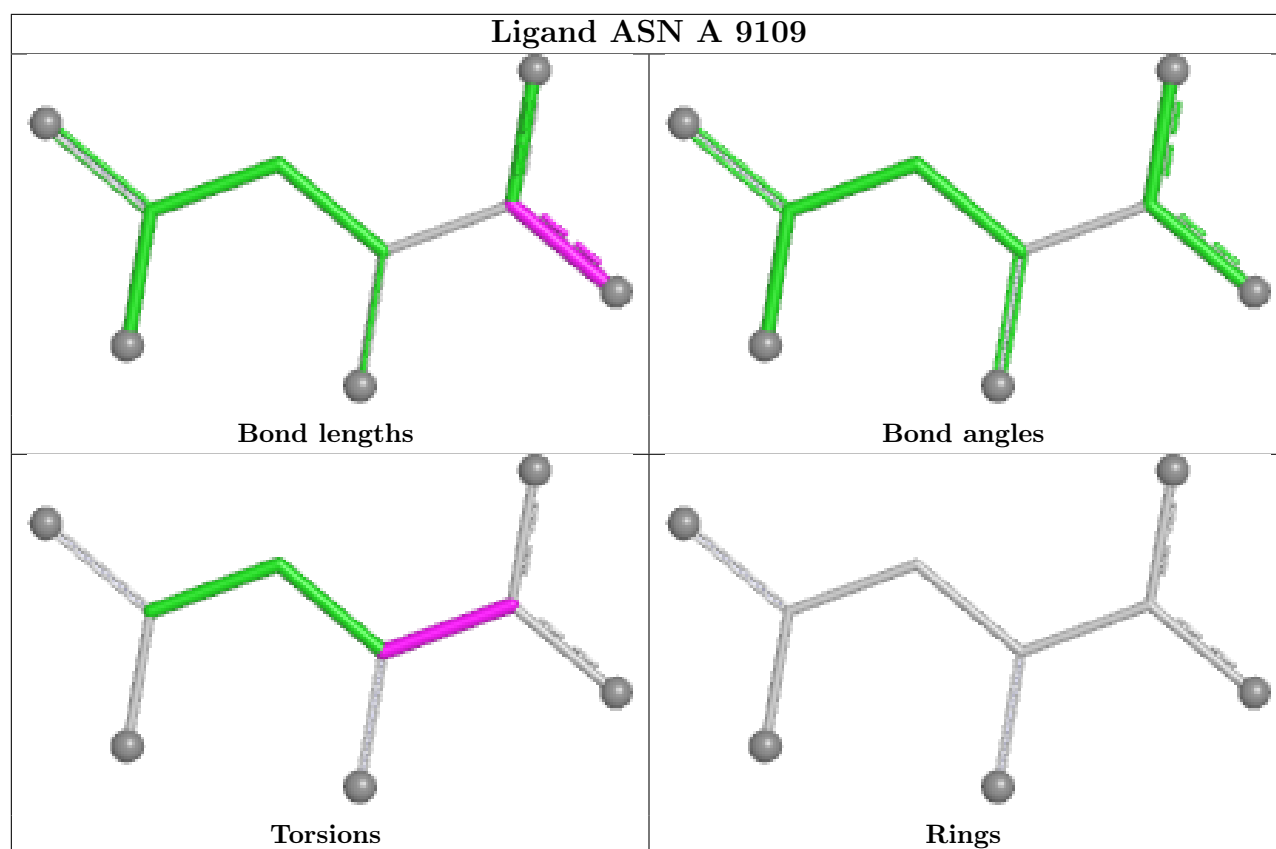
Mol	Chain	Res	Type	Atoms
6	C	402	ASN	OXT-C-CA-CB
3	B	9103	EDO	O1-C1-C2-O2
3	B	9105	EDO	O1-C1-C2-O2
2	A	9101	CIT	O2-C1-C2-C3
2	D	403	CIT	O1-C1-C2-C3
2	B	9101	CIT	C2-C3-C6-O6
2	D	403	CIT	O2-C1-C2-C3
6	C	402	ASN	O-C-CA-CB
2	A	9101	CIT	O1-C1-C2-C3
6	D	402	ASN	OXT-C-CA-N

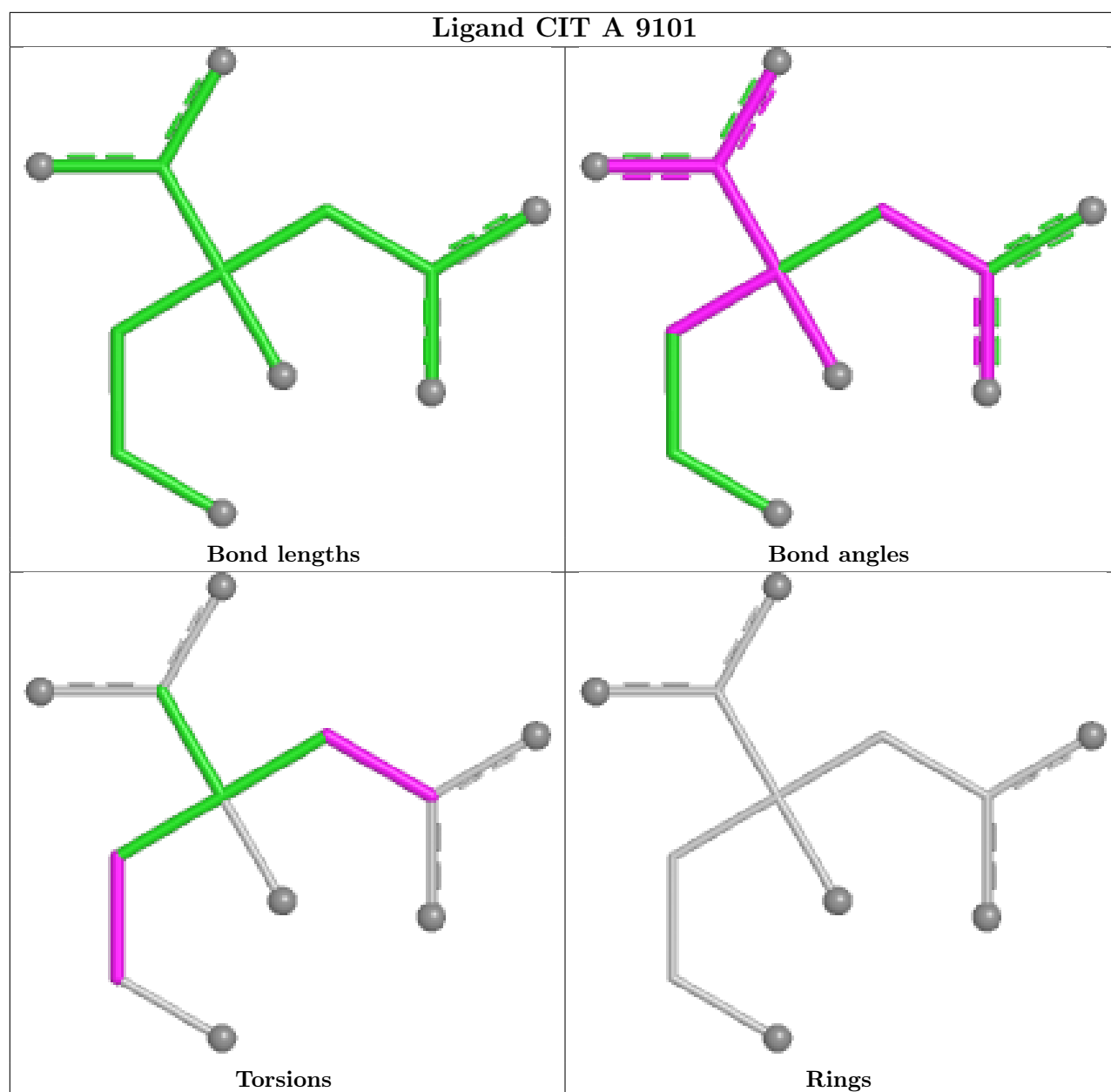
There are no ring outliers.

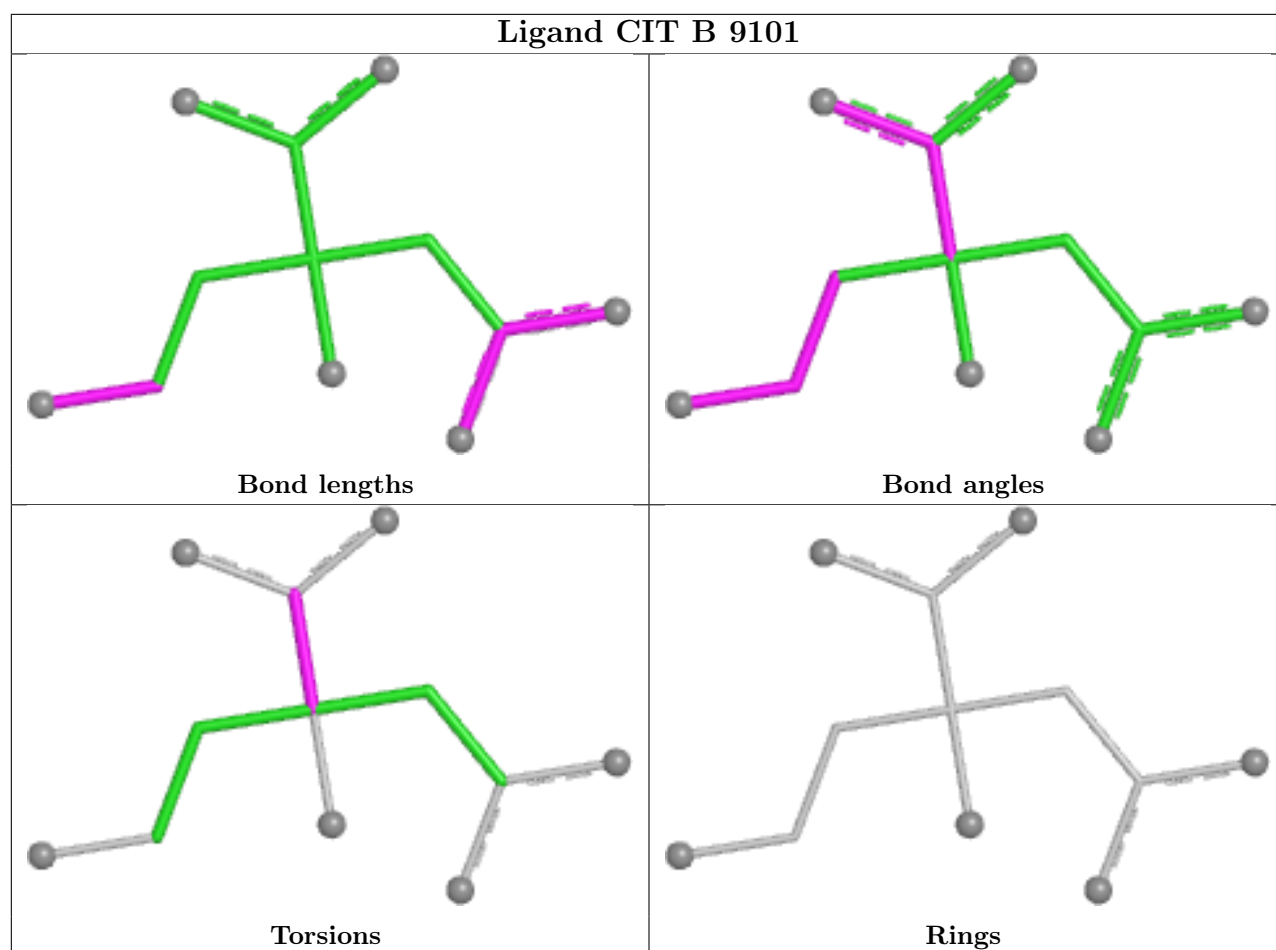
10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9101	CIT	1	0
3	B	9105	EDO	1	0
2	B	9101	CIT	1	0
2	D	403	CIT	1	0
3	B	9104	EDO	1	0
3	C	404	EDO	2	0
5	A	9105	GOL	8	0
2	C	403	CIT	1	0
3	A	9103	EDO	1	0
3	B	9103	EDO	1	0

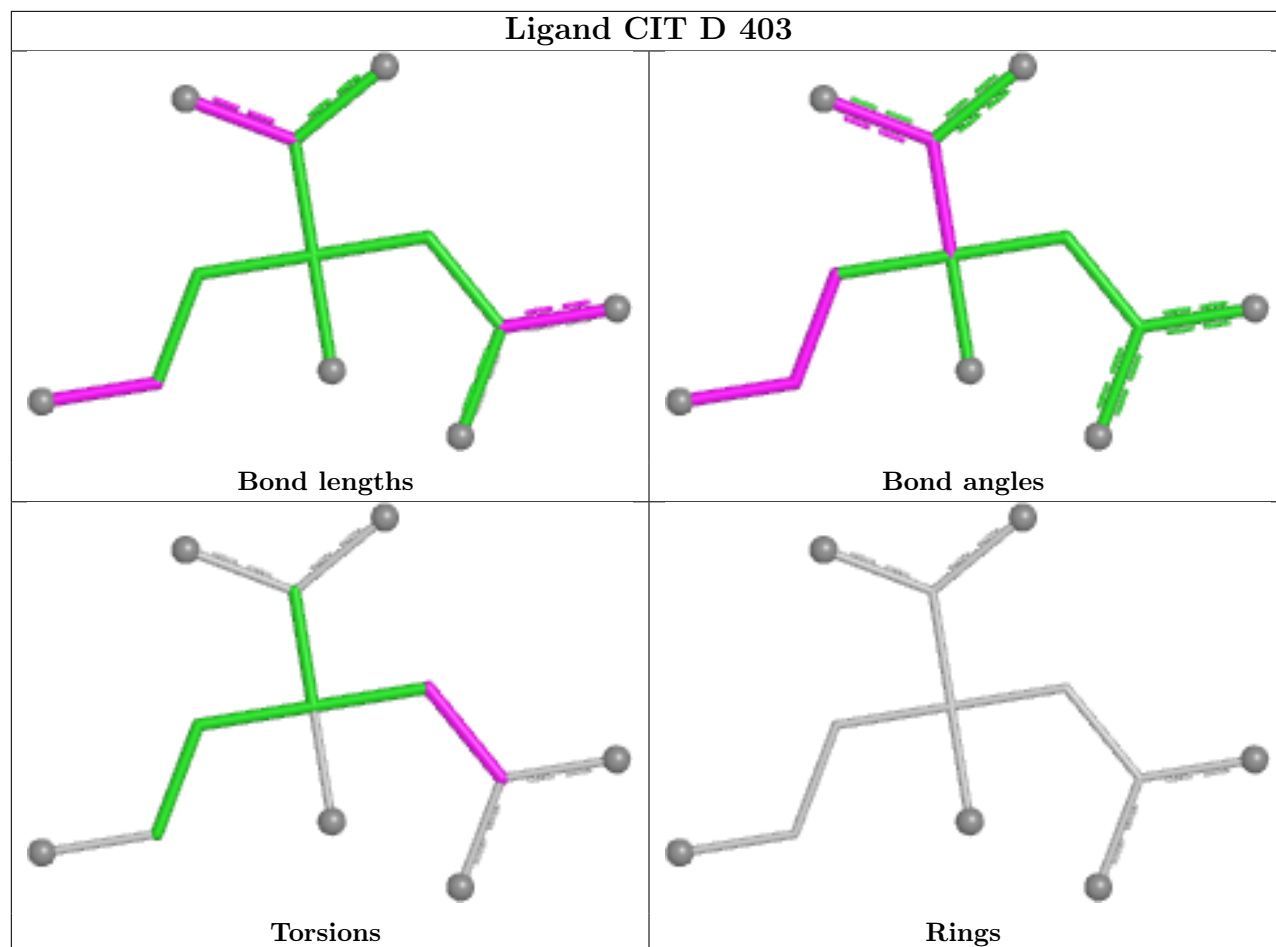
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



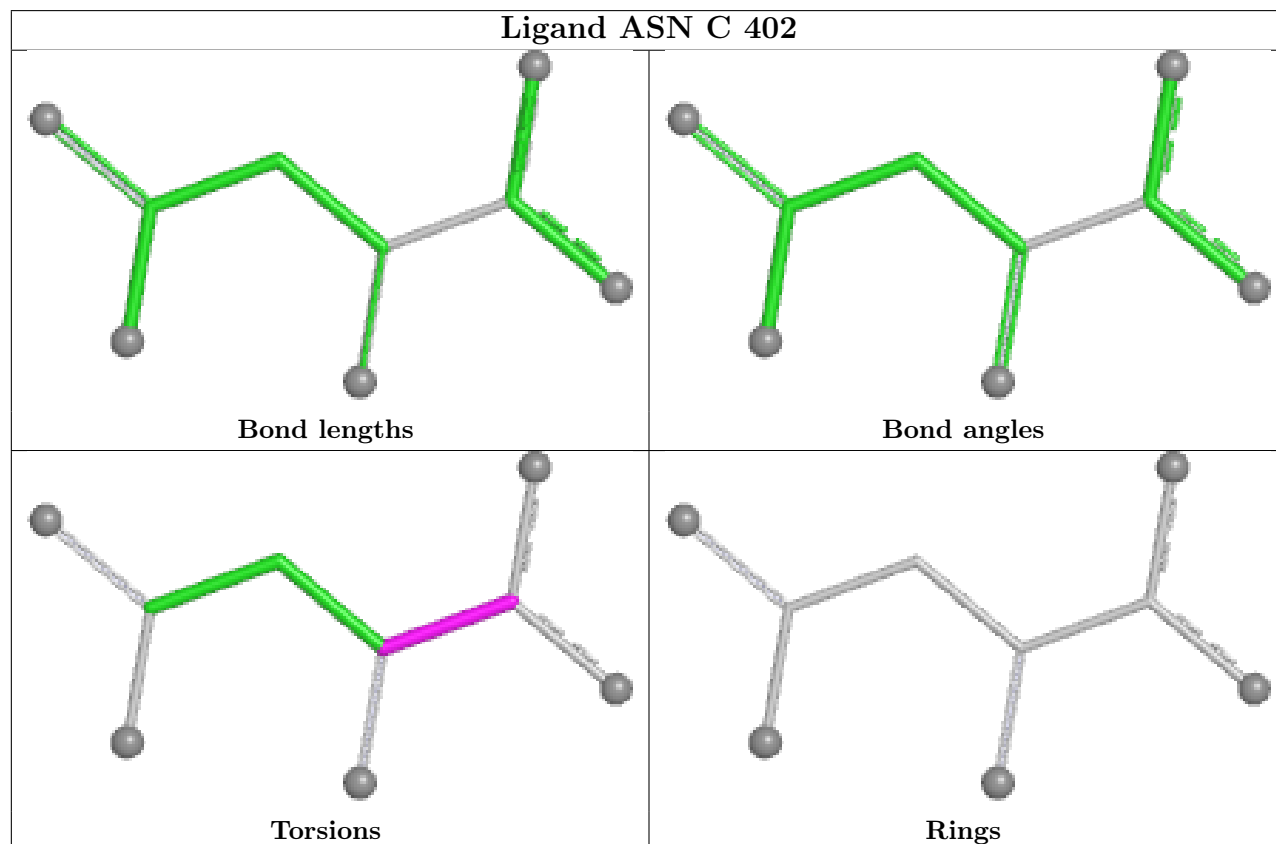


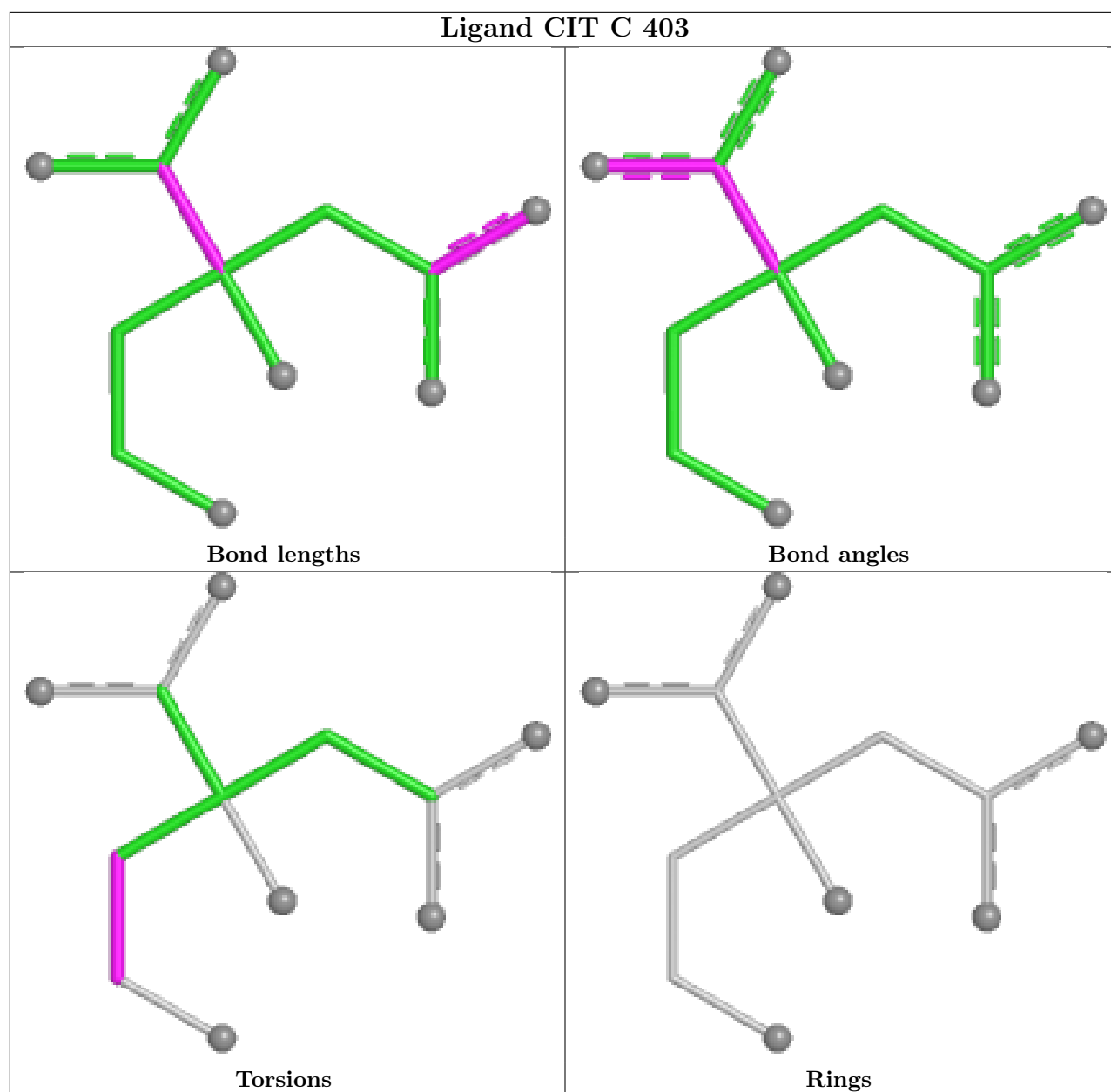


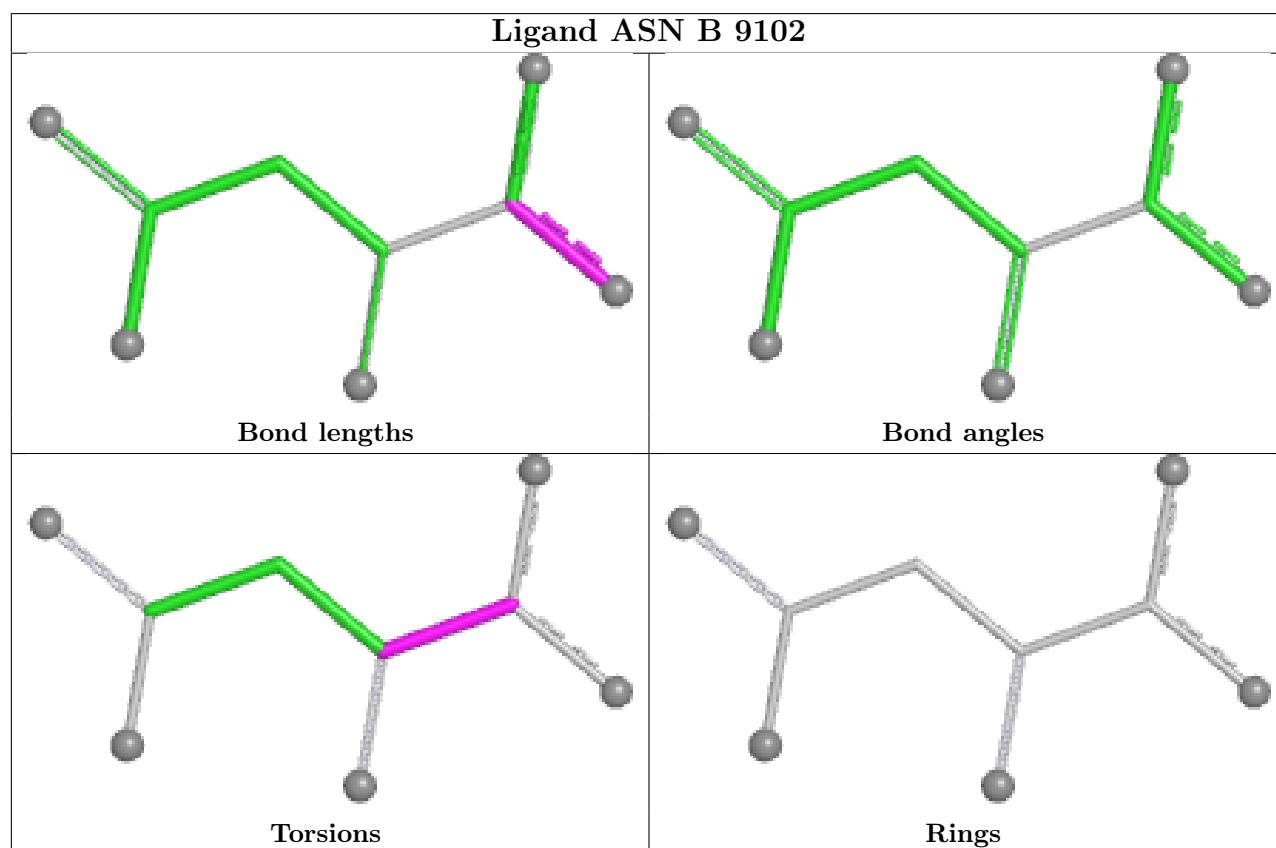
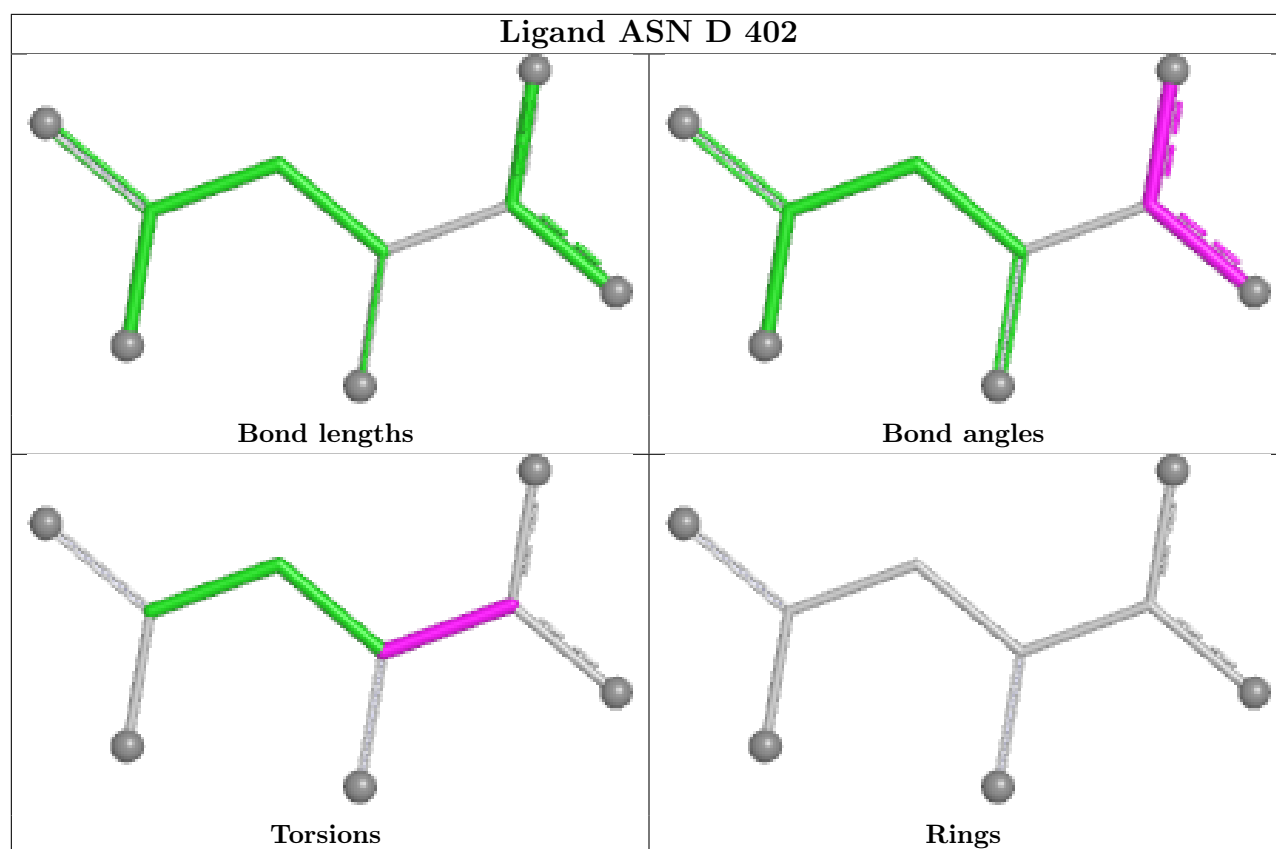
Ligand CIT D 403



Ligand ASN C 402







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	326/357 (91%)	0.48	28 (8%)	16	21	12, 24, 54, 80	2 (0%)
1	B	336/357 (94%)	0.47	42 (12%)	8	10	11, 22, 50, 86	4 (1%)
1	C	323/357 (90%)	0.58	34 (10%)	11	15	13, 24, 60, 94	2 (0%)
1	D	334/357 (93%)	0.36	26 (7%)	19	24	13, 21, 51, 72	1 (0%)
All	All	1319/1428 (92%)	0.47	130 (9%)	13	16	11, 23, 55, 94	9 (0%)

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	39	PRO	8.7
1	C	233	PRO	7.5
1	A	25	ILE	5.5
1	B	225	VAL	5.3
1	C	225	VAL	5.1
1	C	25	ILE	5.0
1	D	-6	LEU	5.0
1	A	39	PRO	4.9
1	A	225	VAL	4.9
1	D	233	PRO	4.8
1	B	233	PRO	4.8
1	A	37	LEU	4.7
1	B	223	ALA	4.7
1	C	26	PRO	4.6
1	D	122	ALA	4.5
1	C	37	LEU	4.5
1	A	229	PHE	4.3
1	C	43	ARG	4.3
1	A	26	PRO	4.3
1	C	31	LEU	4.2
1	B	232	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	230	LEU	4.1
1	B	14	THR	4.0
1	D	24	TYR	4.0
1	B	281	GLY	3.9
1	C	27	VAL	3.8
1	A	233	PRO	3.8
1	C	19	ARG	3.8
1	A	232	GLN	3.7
1	B	194	PRO	3.6
1	C	42	HIS	3.6
1	D	225	VAL	3.6
1	B	2	GLN	3.5
1	C	30	HIS	3.5
1	C	229	PHE	3.5
1	A	27	VAL	3.5
1	B	284	ALA	3.4
1	B	283	TYR	3.4
1	B	229	PHE	3.4
1	C	14	THR	3.3
1	D	287	ASN	3.3
1	B	28	SER	3.3
1	C	288	ALA	3.2
1	D	26	PRO	3.2
1	A	316	GLU	3.2
1	B	-6	LEU	3.1
1	D	19	ARG	3.1
1	A	42	HIS	3.0
1	B	230	LEU	3.0
1	B	55	THR	3.0
1	D	224	ASP	3.0
1	A	20	SER	2.9
1	B	19	ARG	2.9
1	C	291	HIS	2.9
1	B	285	THR	2.9
1	B	253	PHE	2.9
1	C	36	ALA	2.9
1	D	230	LEU	2.9
1	D	194	PRO	2.9
1	C	228	ASN	2.9
1	B	224	ASP	2.8
1	C	29	GLY	2.8
1	A	230	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	25	ILE	2.8
1	B	122	ALA	2.8
1	C	40	GLU	2.7
1	C	226	VAL	2.7
1	B	286	GLY	2.7
1	A	226	VAL	2.7
1	C	337	ASP	2.7
1	B	-5	VAL	2.7
1	B	231	ARG	2.6
1	A	30	HIS	2.6
1	B	30	HIS	2.6
1	A	228	ASN	2.6
1	D	30	HIS	2.6
1	C	223	ALA	2.6
1	A	224	ASP	2.5
1	B	282	GLY	2.5
1	B	17	MET	2.5
1	D	-5	VAL	2.5
1	B	254	LEU	2.5
1	A	223	ALA	2.5
1	B	-4	PRO	2.5
1	D	288	ALA	2.4
1	D	228	ASN	2.4
1	D	14	THR	2.4
1	A	337	ASP	2.4
1	A	280	MET	2.4
1	D	229	PHE	2.4
1	D	251	LYS	2.4
1	B	15	ILE	2.4
1	C	38	MET	2.4
1	B	31	LEU	2.3
1	D	31	LEU	2.3
1	A	121	LEU	2.3
1	B	-1	SER	2.3
1	A	36	ALA	2.3
1	A	35	LEU	2.3
1	C	121	LEU	2.3
1	C	191	ASN	2.3
1	A	43	ARG	2.3
1	D	234	VAL	2.3
1	B	192	THR	2.2
1	B	287	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	254	LEU	2.2
1	B	226	VAL	2.2
1	C	3	LYS	2.2
1	D	280	MET	2.2
1	B	-3	ARG	2.2
1	C	15	ILE	2.2
1	C	227	ARG	2.2
1	A	191	ASN	2.2
1	C	44	PRO	2.2
1	A	195	ALA	2.2
1	B	-2	GLY	2.2
1	B	121	LEU	2.2
1	B	124	LEU	2.2
1	B	193	PRO	2.2
1	D	192	THR	2.2
1	C	260	ALA	2.1
1	D	232	GLN	2.1
1	B	250	ASN	2.1
1	D	191	ASN	2.1
1	C	33	ARG	2.1
1	A	234	VAL	2.0
1	B	191	ASN	2.0
1	B	189	ARG	2.0
1	D	189	ARG	2.0
1	A	288	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

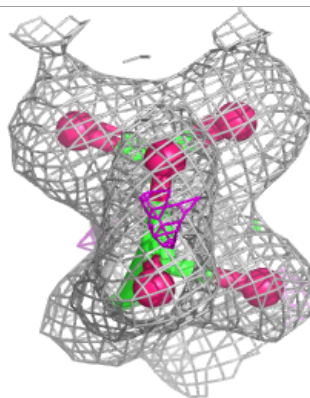
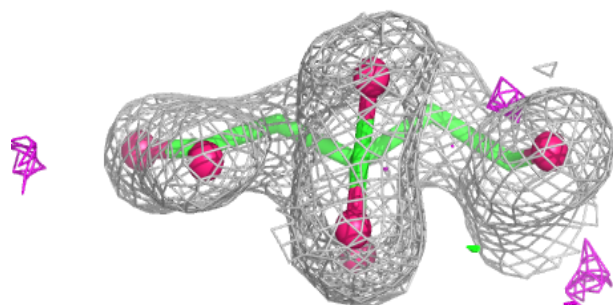
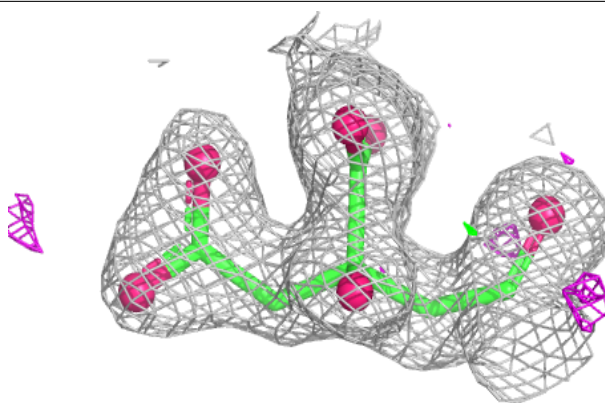
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	9107	4/4	0.83	0.15	29,29,35,38	0
3	EDO	B	9103	4/4	0.86	0.12	31,43,44,45	0
3	EDO	A	9102	4/4	0.91	0.11	27,30,32,32	0
3	EDO	B	9104	4/4	0.91	0.10	24,26,27,31	0
3	EDO	C	401	4/4	0.91	0.12	26,37,39,39	0
3	EDO	B	9105	4/4	0.92	0.12	25,25,32,35	0
2	CIT	B	9101	12/13	0.92	0.09	19,27,36,36	0
2	CIT	C	403	12/13	0.93	0.08	17,25,29,34	0
2	CIT	D	403	12/13	0.93	0.07	19,23,26,33	0
3	EDO	C	405	4/4	0.93	0.12	22,23,33,35	0
5	GOL	A	9105	6/6	0.93	0.10	22,35,39,40	0
6	ASN	A	9109	9/9	0.93	0.08	16,22,25,27	0
6	ASN	C	402	9/9	0.93	0.09	18,22,28,31	0
6	ASN	D	402	9/9	0.93	0.07	17,20,27,29	0
3	EDO	A	9103	4/4	0.94	0.07	22,23,25,26	0
6	ASN	B	9102	9/9	0.95	0.07	18,21,25,28	0
2	CIT	A	9101	12/13	0.95	0.07	16,24,33,33	0
3	EDO	D	406	4/4	0.95	0.08	26,26,29,30	0
3	EDO	D	407	4/4	0.97	0.06	21,22,26,29	0
4	CL	A	9106	1/1	0.97	0.07	25,25,25,25	0
4	CL	D	401	1/1	0.97	0.05	25,25,25,25	0
3	EDO	C	404	4/4	0.97	0.06	22,22,24,27	0
4	CL	A	9104	1/1	0.98	0.05	19,19,19,19	0
4	CL	D	404	1/1	0.99	0.04	21,21,21,21	0
4	CL	D	405	1/1	0.99	0.04	29,29,29,29	0
4	CL	B	9106	1/1	0.99	0.03	22,22,22,22	0
4	CL	B	9107	1/1	0.99	0.04	18,18,18,18	0
4	CL	B	9108	1/1	0.99	0.04	19,19,19,19	0
4	CL	C	406	1/1	0.99	0.05	26,26,26,26	0
4	CL	A	9108	1/1	0.99	0.04	18,18,18,18	0

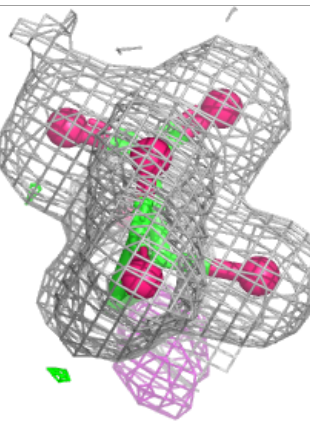
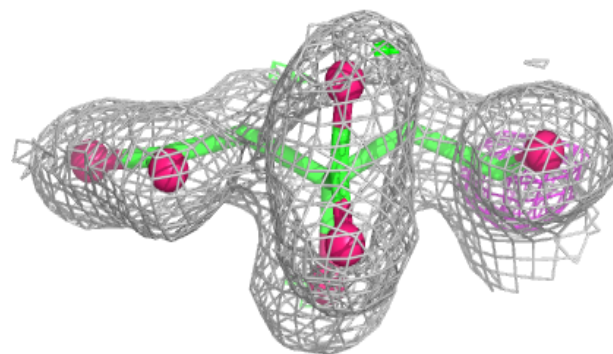
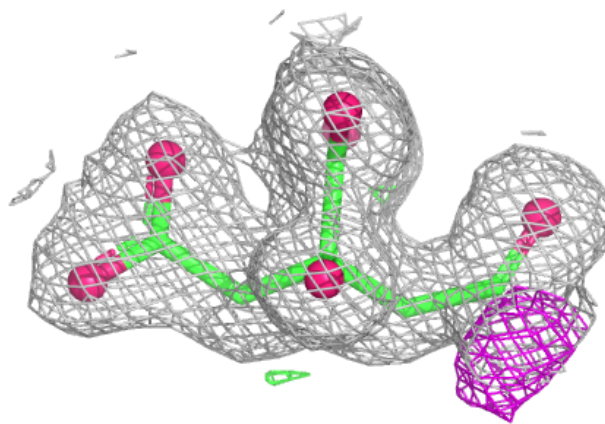
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CIT B 9101:

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

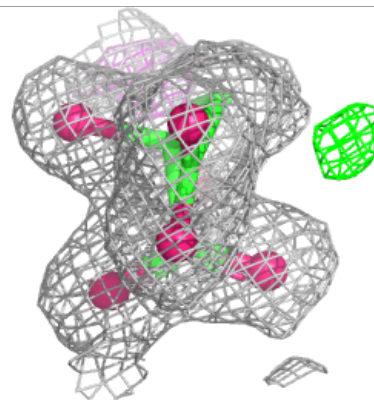
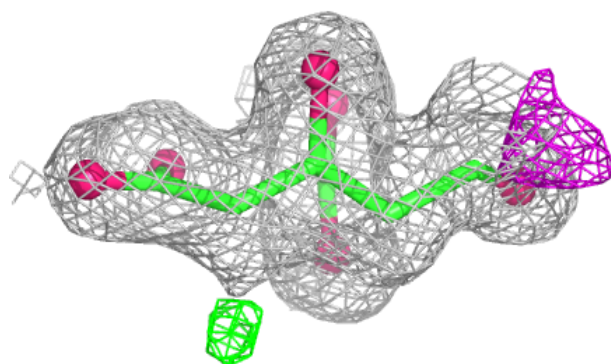
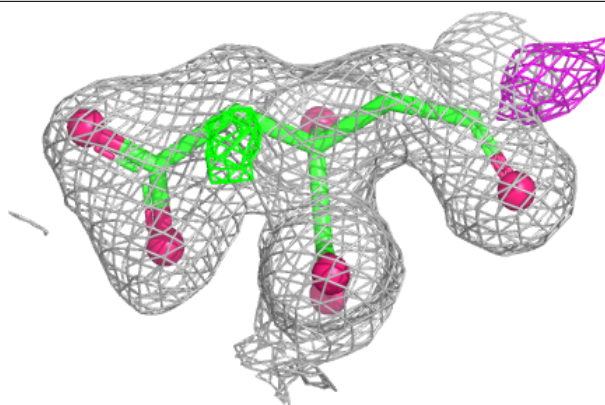
**Electron density around CIT C 403:**

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



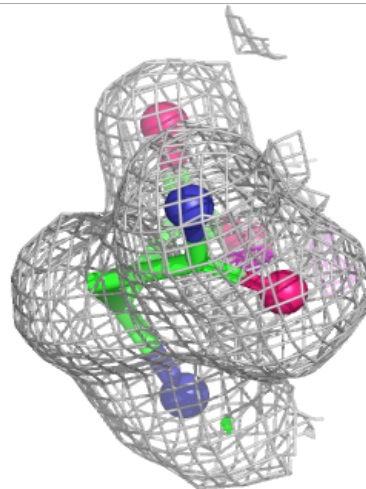
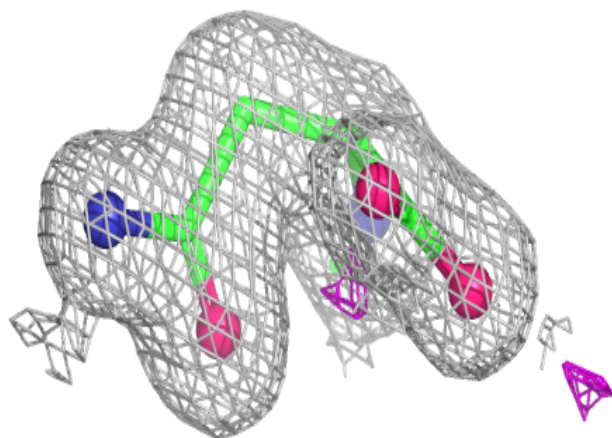
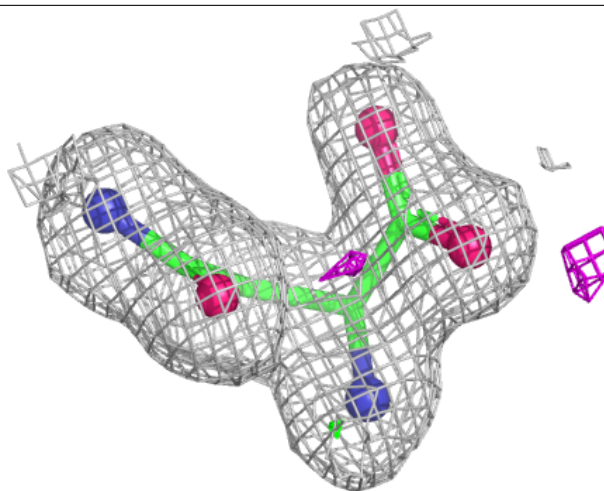
Electron density around CIT D 403:

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



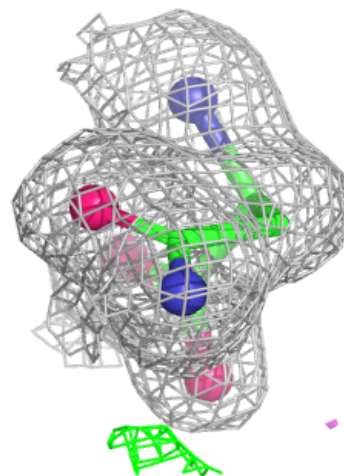
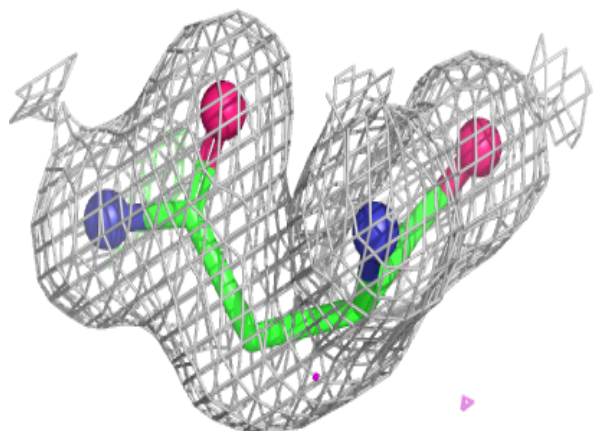
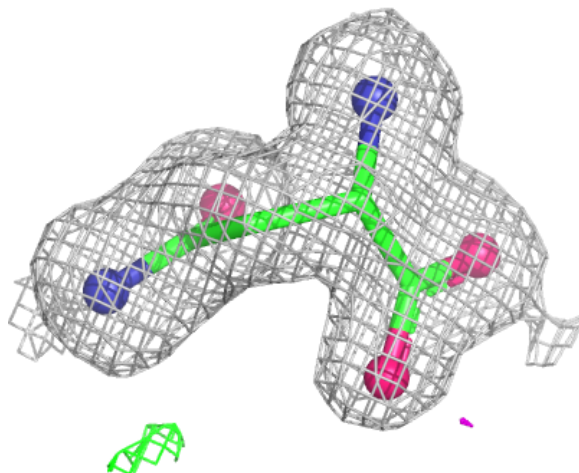
Electron density around ASN A 9109:

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



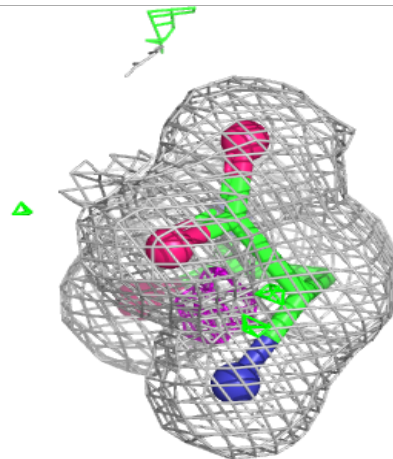
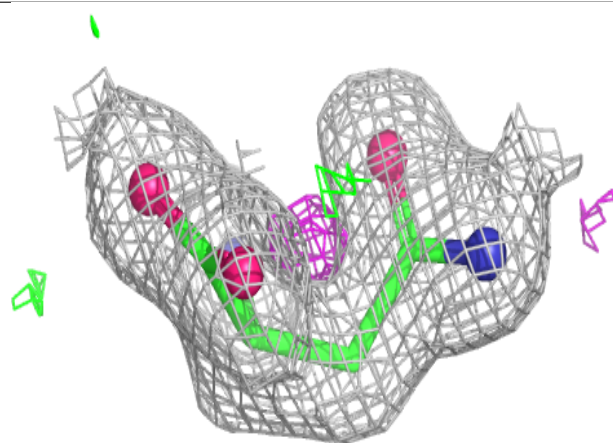
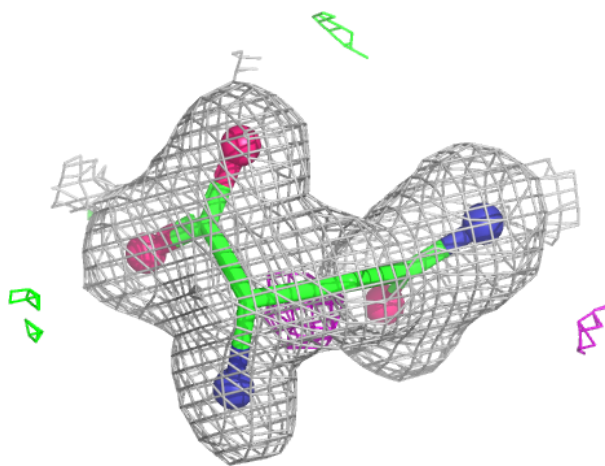
Electron density around ASN C 402:

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



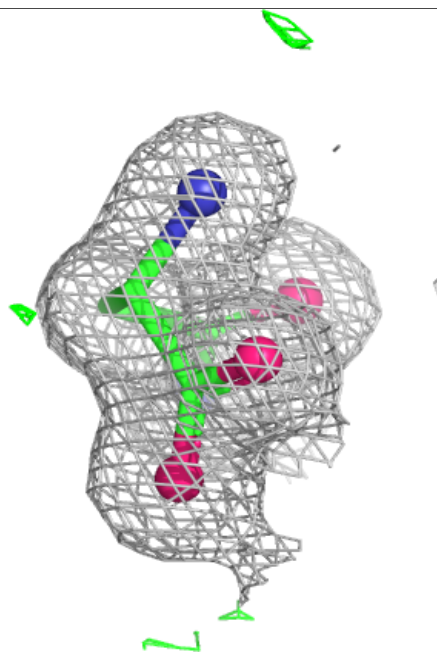
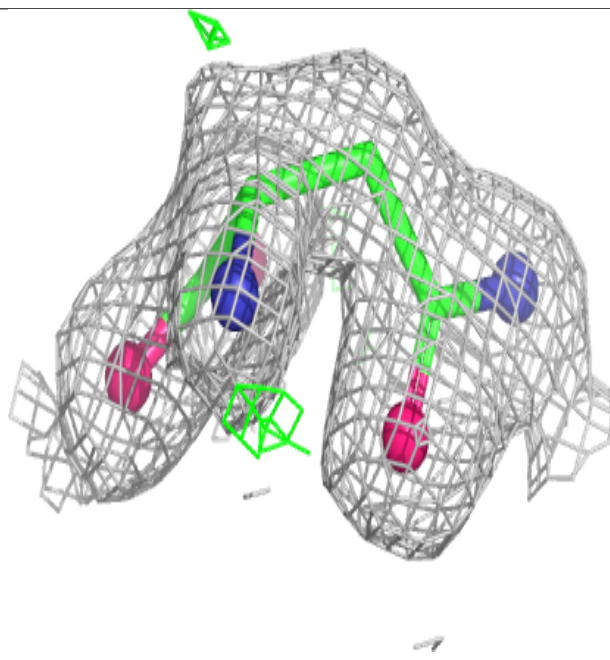
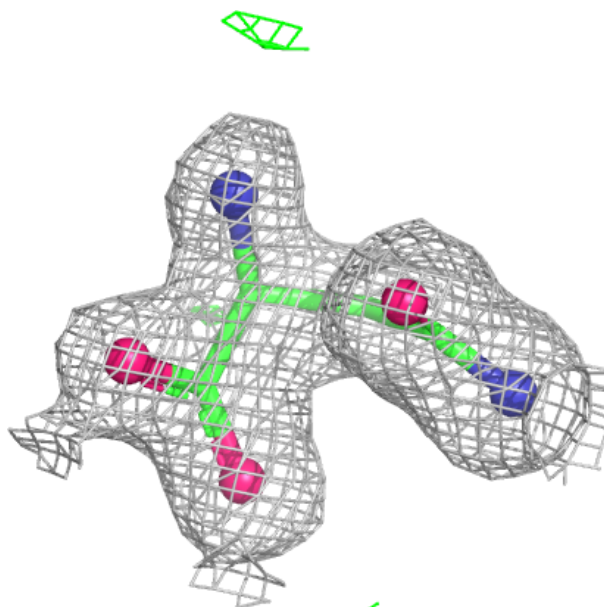
Electron density around ASN D 402:

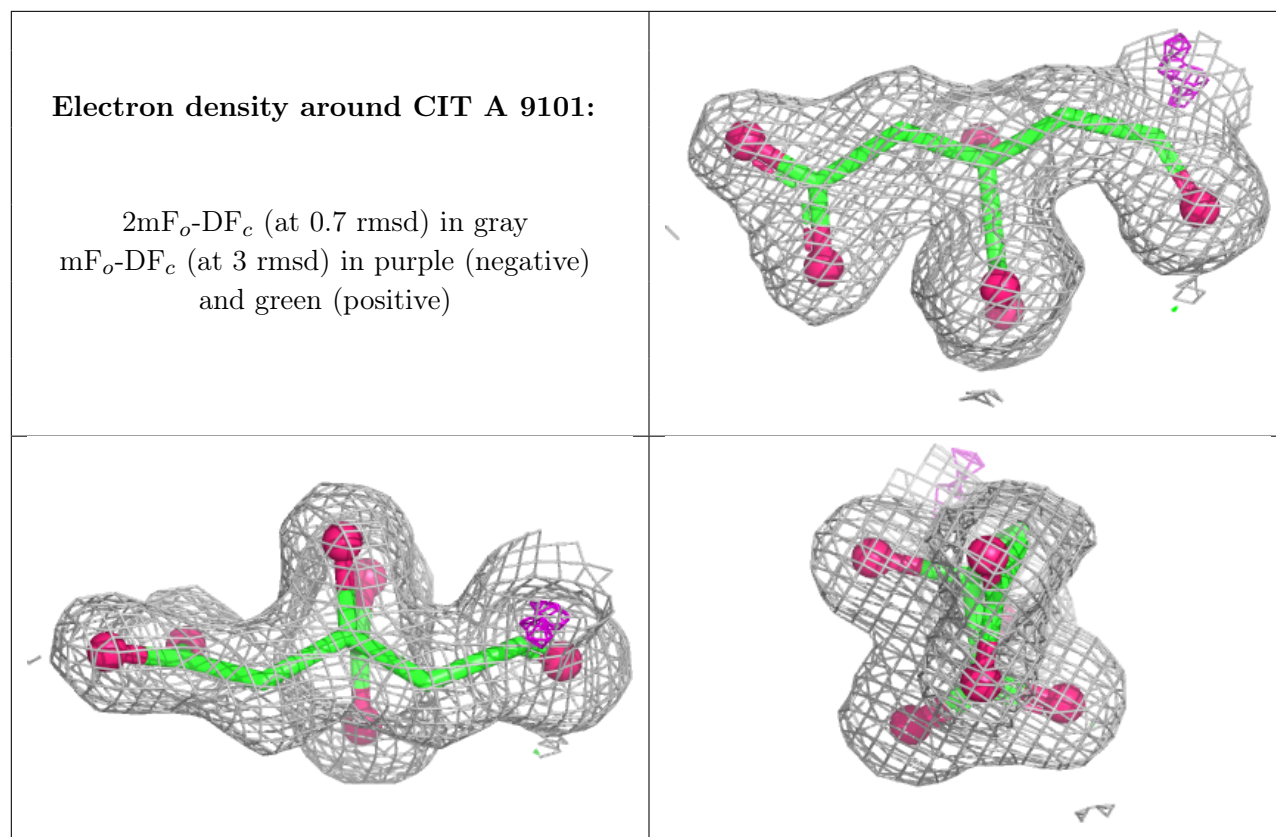
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ASN B 9102:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.