



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 30, 2025 – 04:22 PM JST

PDB ID : 9IOV / pdb_00009iov
Title : Gossypol bound lactate dehydrogenase A
Authors : Ha, M.S.; Han, C.W.; Jeong, M.S.; Jang, S.B.
Deposited on : 2024-07-09
Resolution : 3.98 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

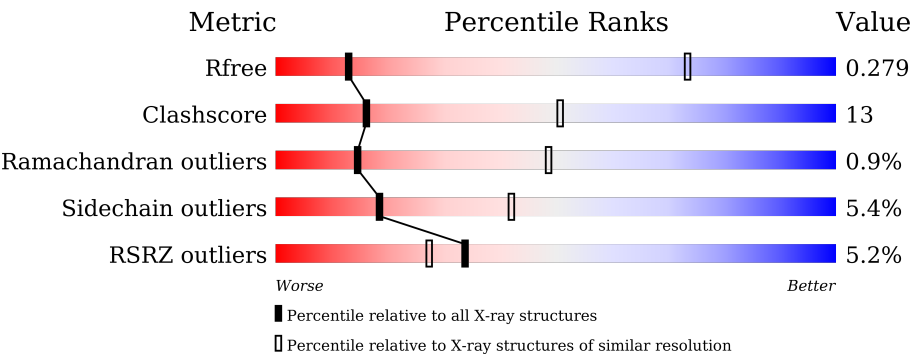
MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.98 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.



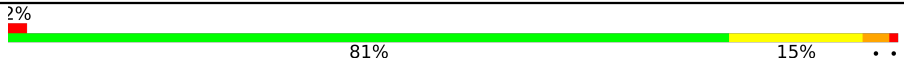

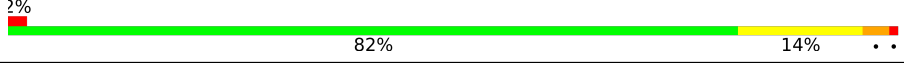
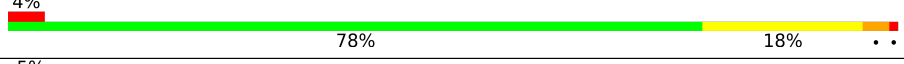

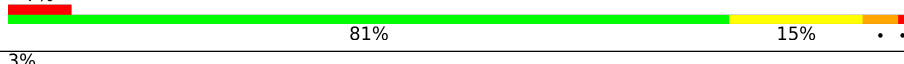
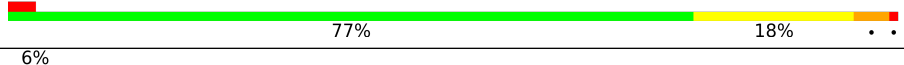

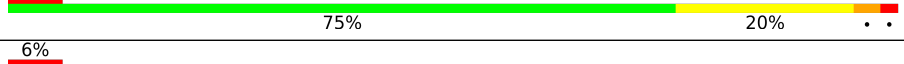


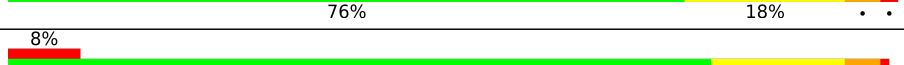

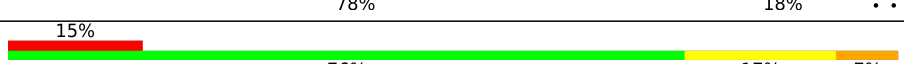
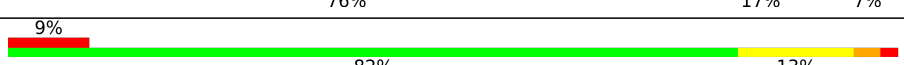
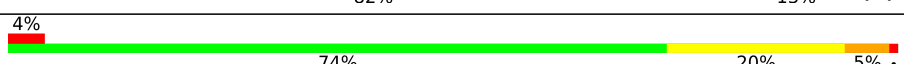
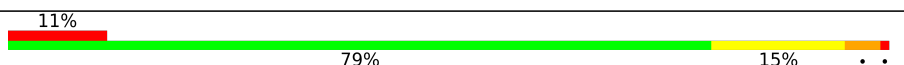

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1059 (4.20-3.76)
Clashscore	180529	1124 (4.20-3.76)
Ramachandran outliers	177936	1073 (4.20-3.76)
Sidechain outliers	177891	1064 (4.20-3.76)
RSRZ outliers	164620	1060 (4.20-3.76)

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	331	<div><div>2%</div><div>79%</div><div>17%</div><div>..</div></div>
1	B	331	<div><div>2%</div><div>77%</div><div>17%</div><div>5%.</div></div>
1	C	331	<div><div>2%</div><div>78%</div><div>18%</div><div>..</div></div>
1	D	331	<div><div>2%</div><div>79%</div><div>17%</div><div>..</div></div>
1	E	331	<div><div>2%</div><div>77%</div><div>19%</div><div>..</div></div>
1	F	331	<div><div>3%</div><div>76%</div><div>20%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
1	G	331	
1	H	331	
1	I	331	
1	J	331	
1	K	331	
1	L	331	
1	M	331	
1	N	331	
1	O	331	
1	P	331	
1	Q	331	
1	R	331	
1	S	331	
1	T	331	
1	U	331	
1	V	331	
1	W	331	
1	X	331	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 61670 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-lactate dehydrogenase A chain.

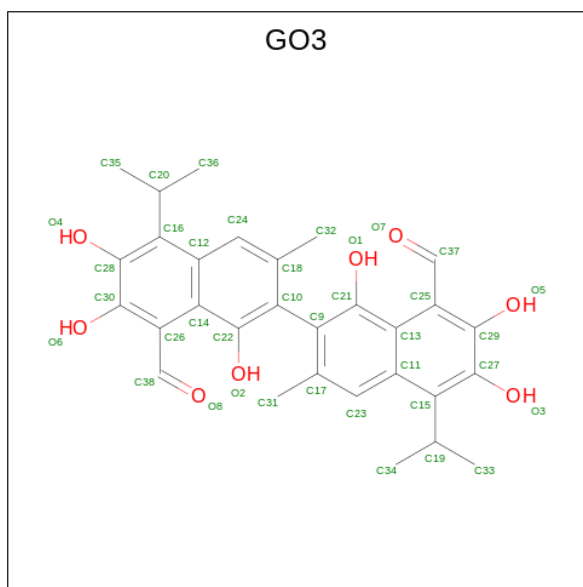
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	B	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	C	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	D	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	E	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	F	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	G	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	H	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	I	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	J	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	K	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	L	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	M	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	N	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	O	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	P	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	R	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	S	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	T	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	U	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	V	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	W	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	X	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			

- Molecule 2 is Gossypol (CCD ID: GO3) (formula: C₃₀H₃₀O₈) (labeled as "Ligand of Interest" by depositor).

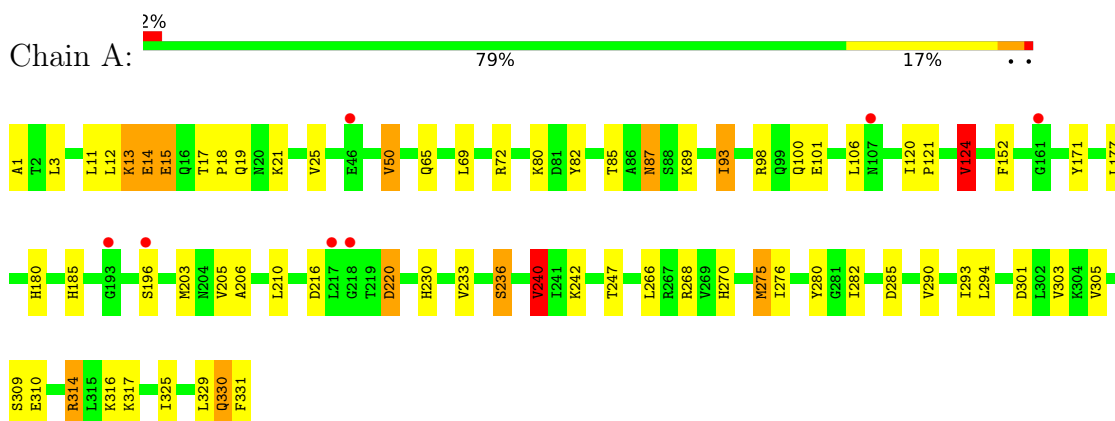


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	Q	1	Total	C	O	0	0
			38	30	8		

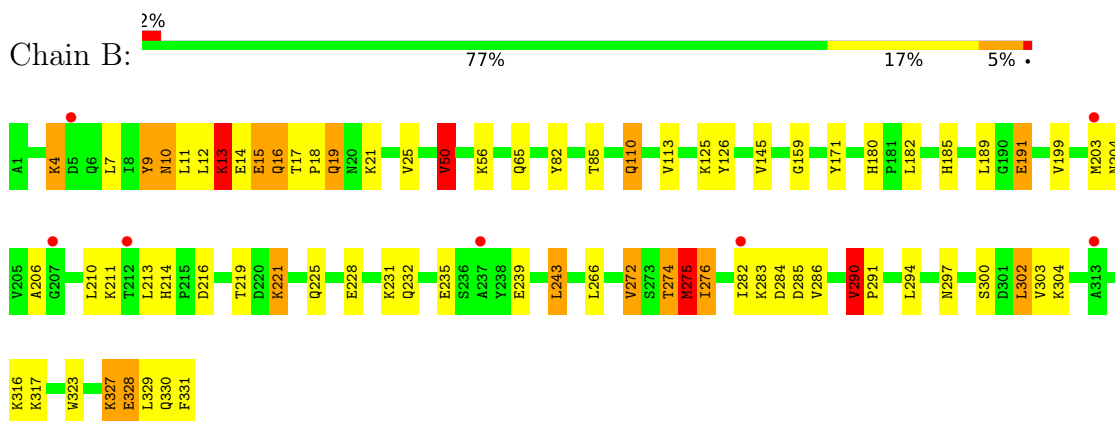
3 Residue-property plots [i](#)

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.

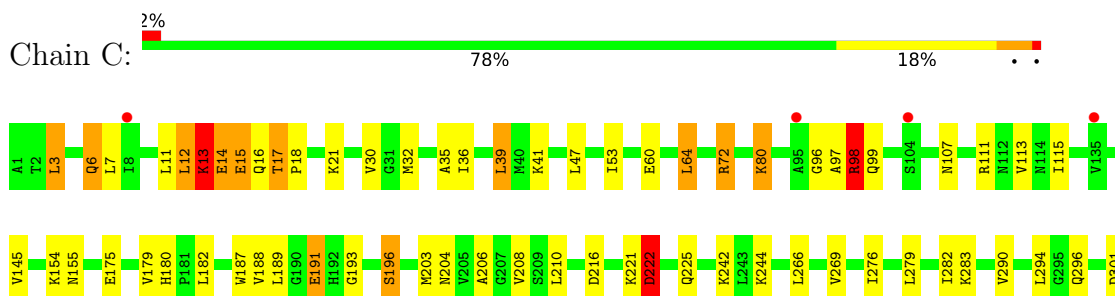
• Molecule 1: L-lactate dehydrogenase A chain



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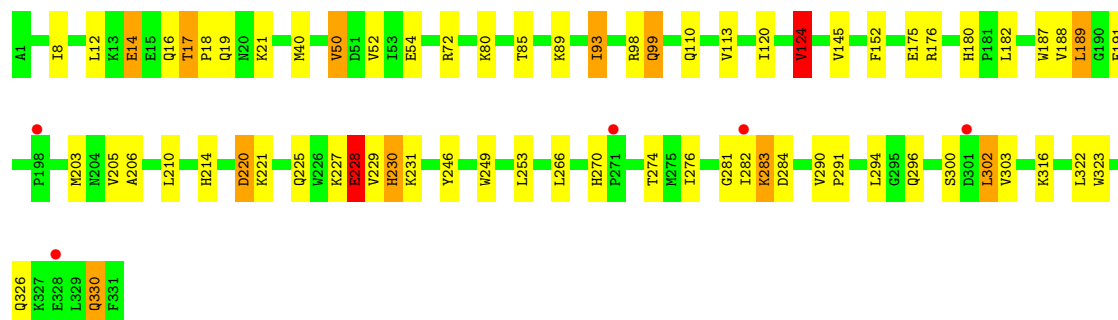
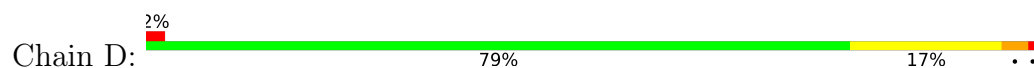


• Molecule 1: L-lactate dehydrogenase A chain

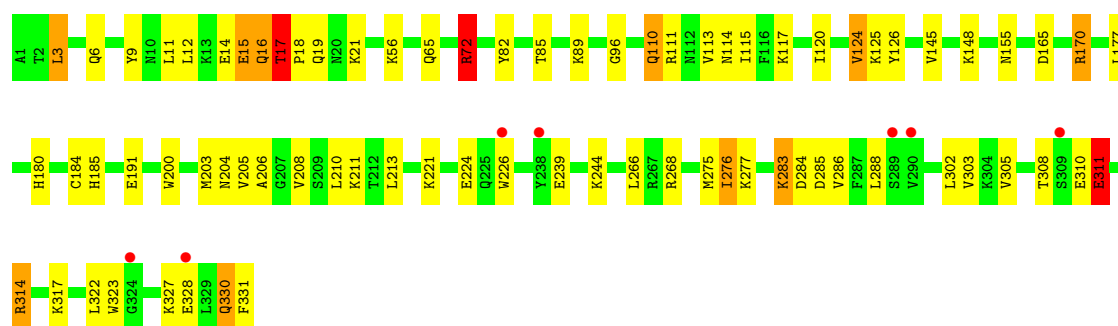
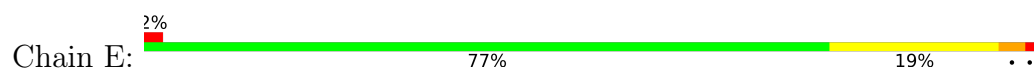




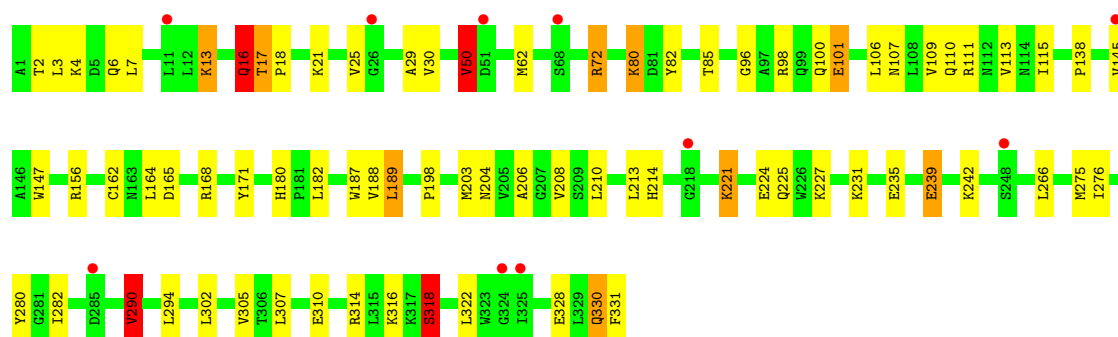
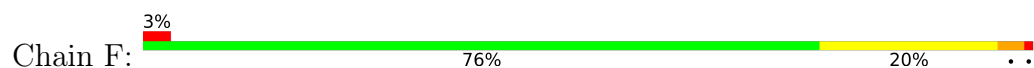
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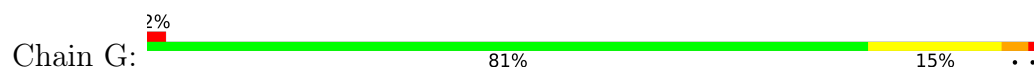
- Molecule 1: L-lactate dehydrogenase A chain

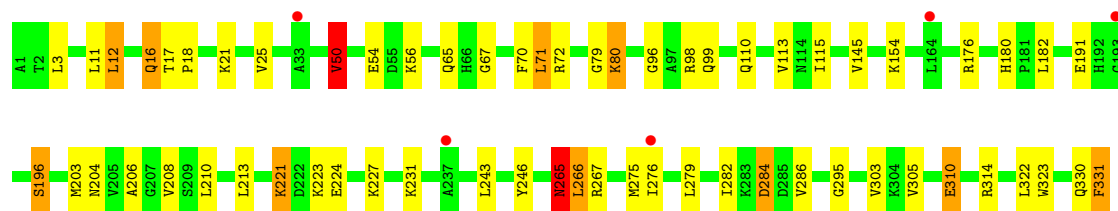


- Molecule 1: L-lactate dehydrogenase A chain

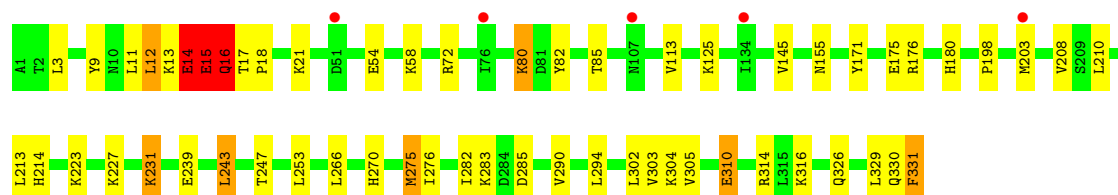
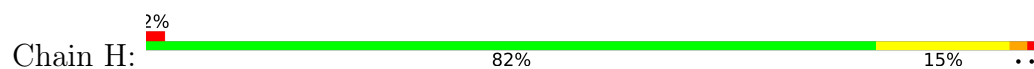


- Molecule 1: L-lactate dehydrogenase A chain

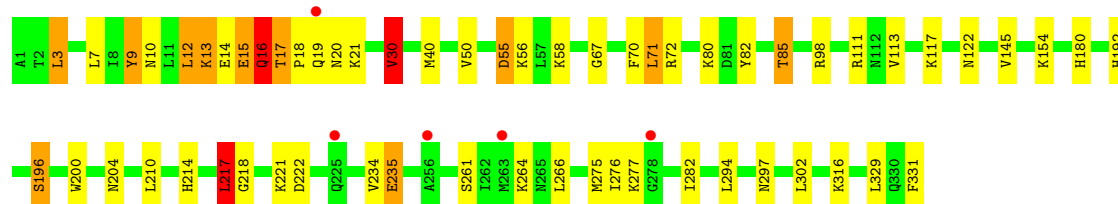
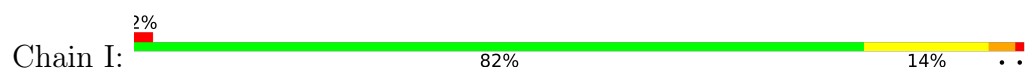




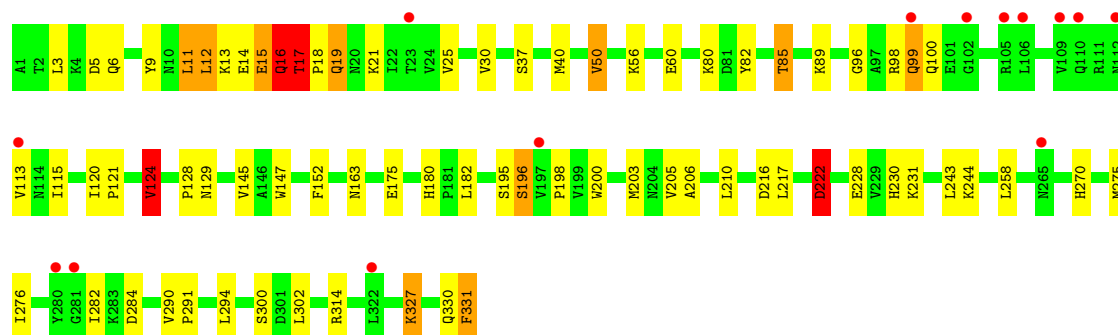
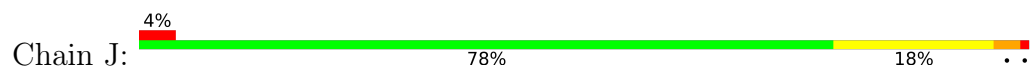
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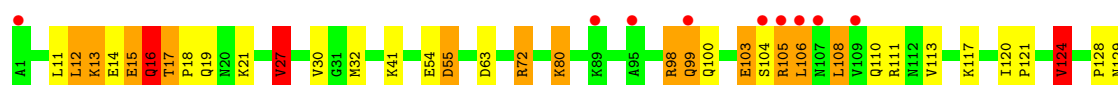
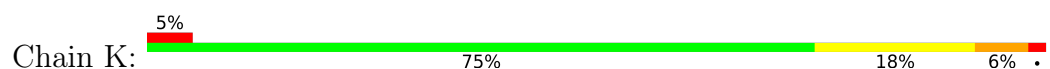
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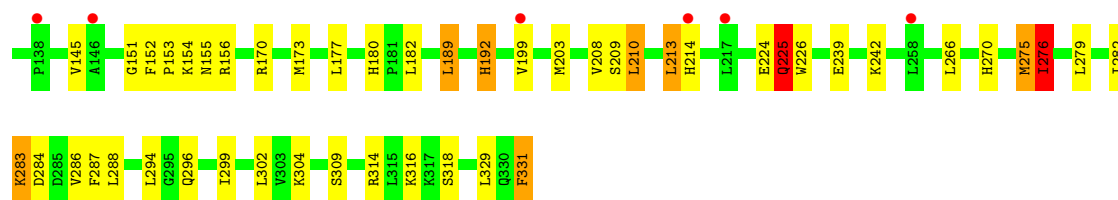


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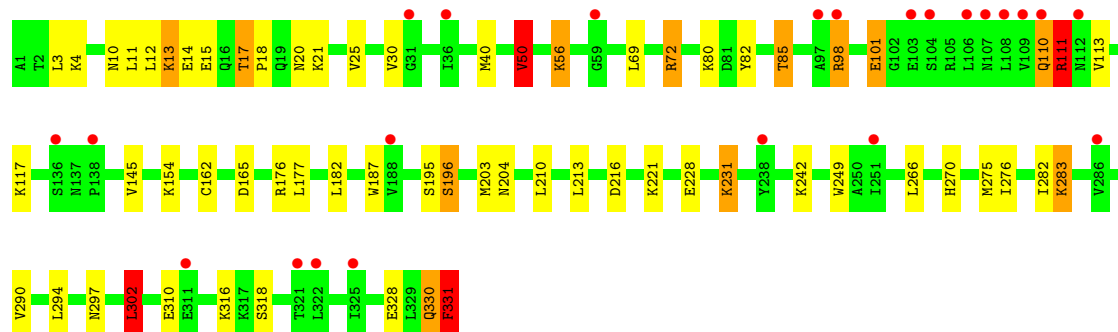
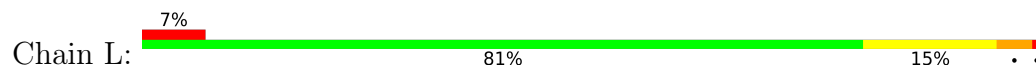


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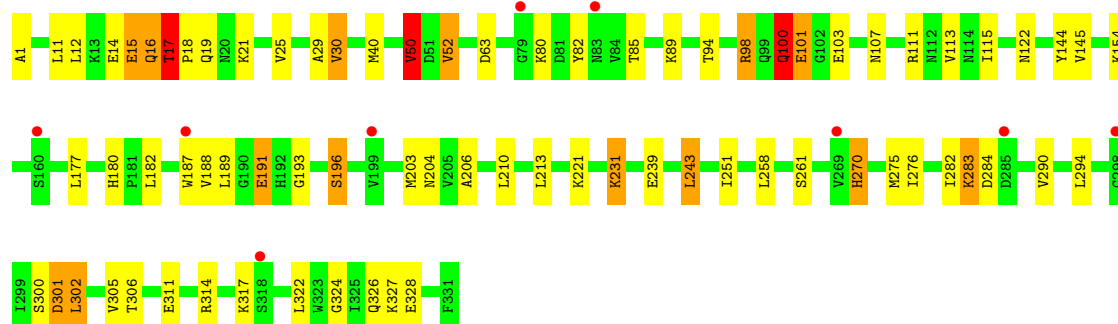
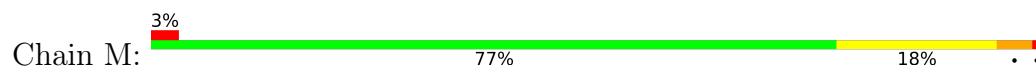




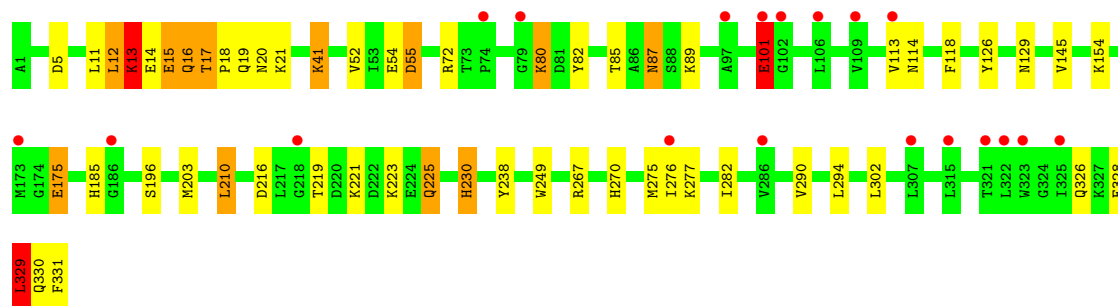
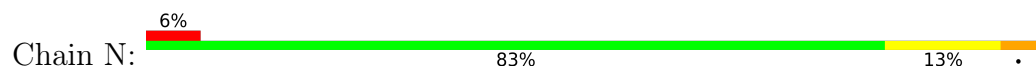
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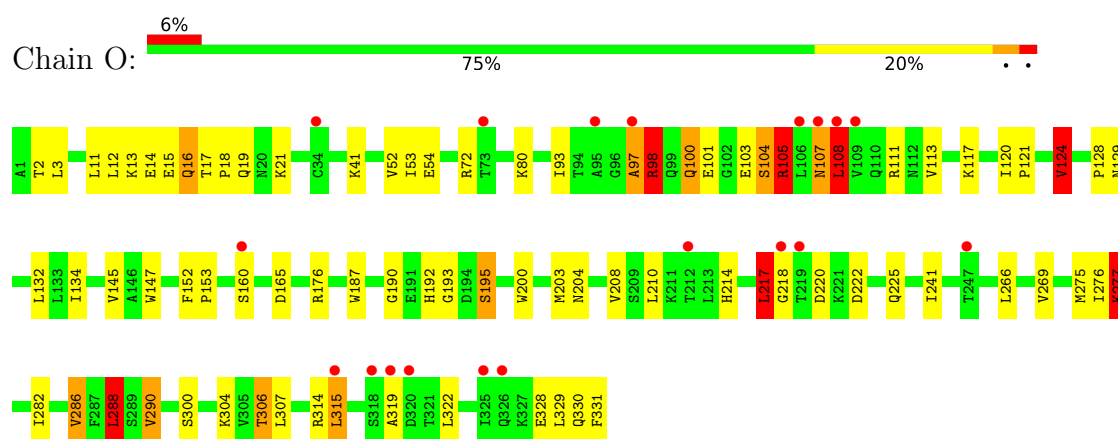
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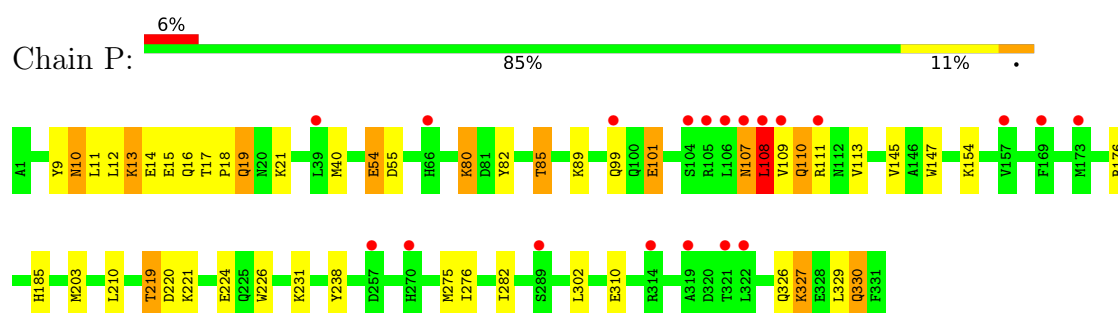
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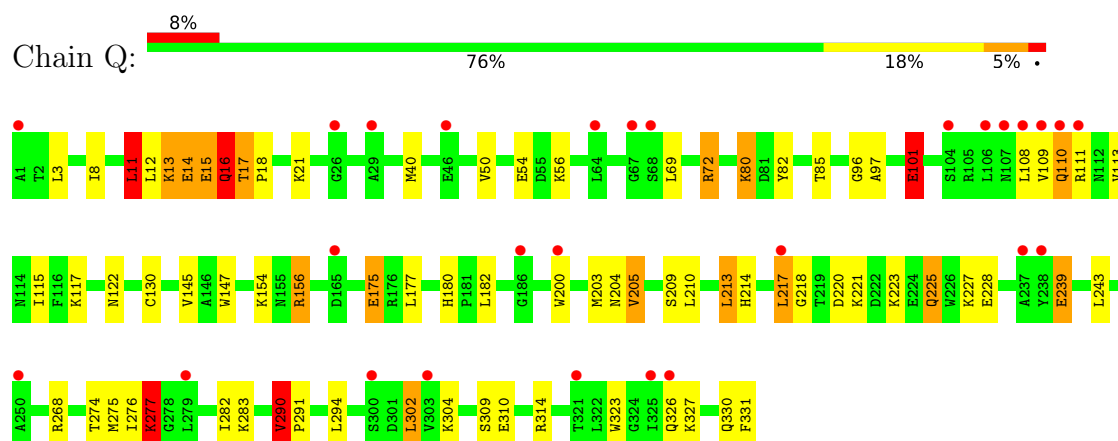
• Molecule 1: L-lactate dehydrogenase A chain



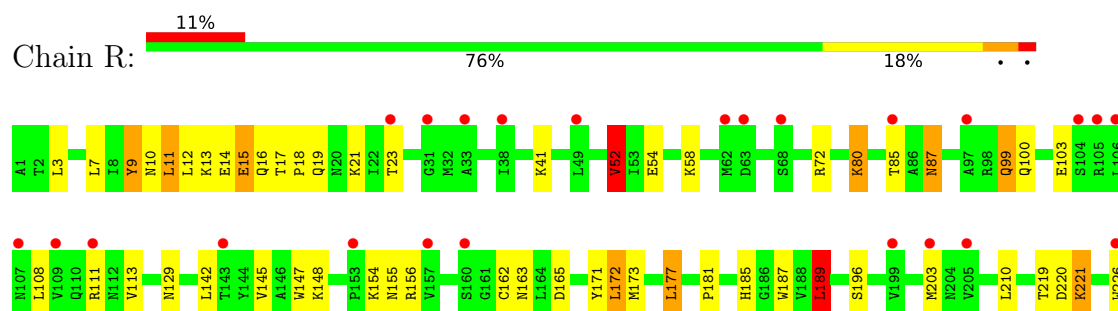
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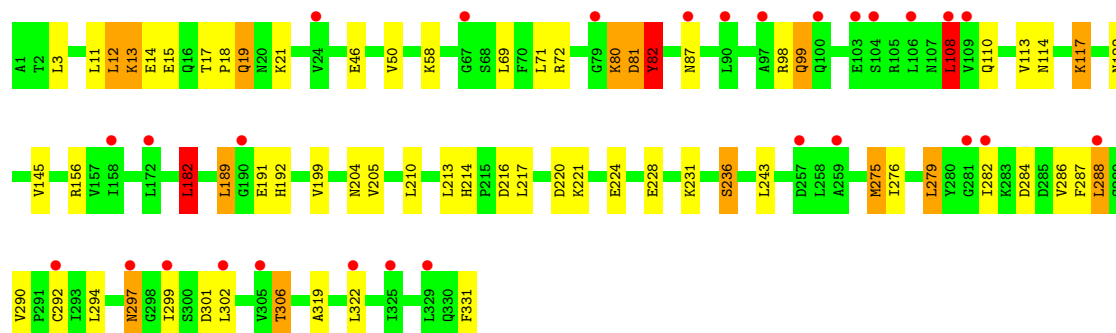
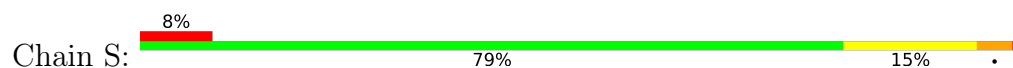


• Molecule 1: L-lactate dehydrogenase A chain

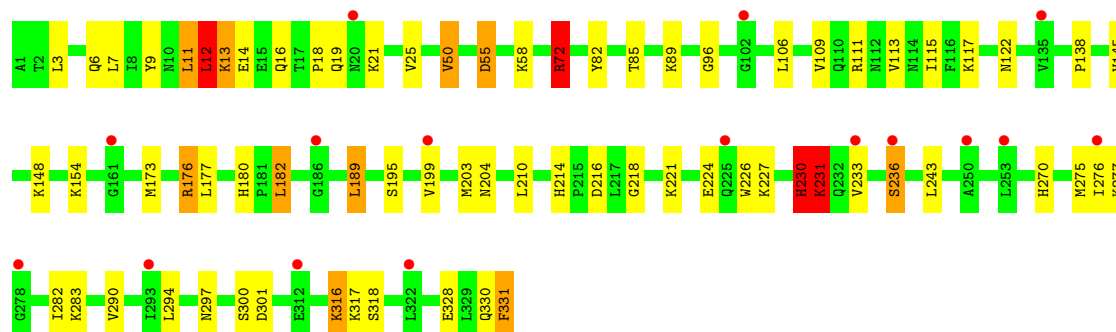
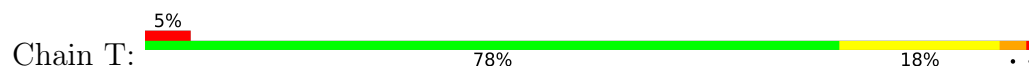




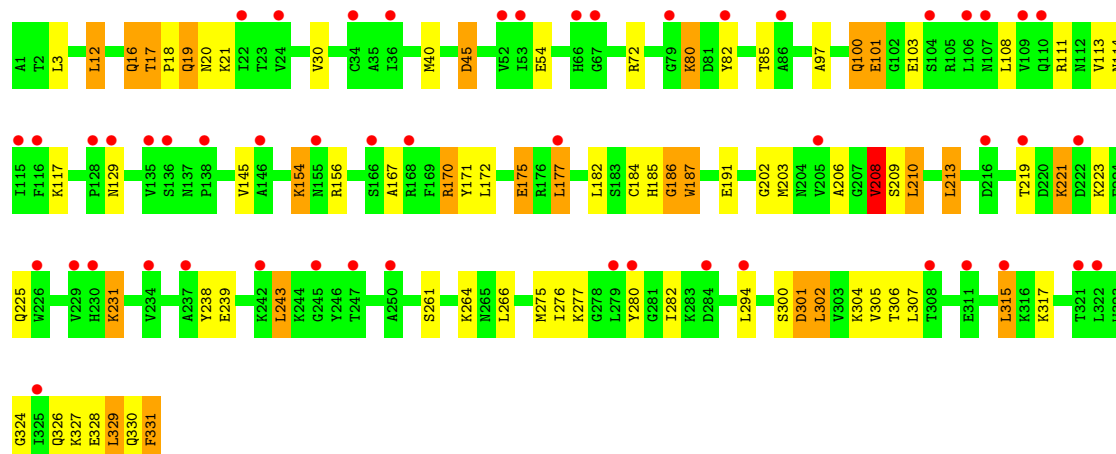
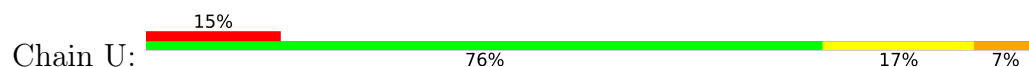
- Molecule 1: L-lactate dehydrogenase A chain



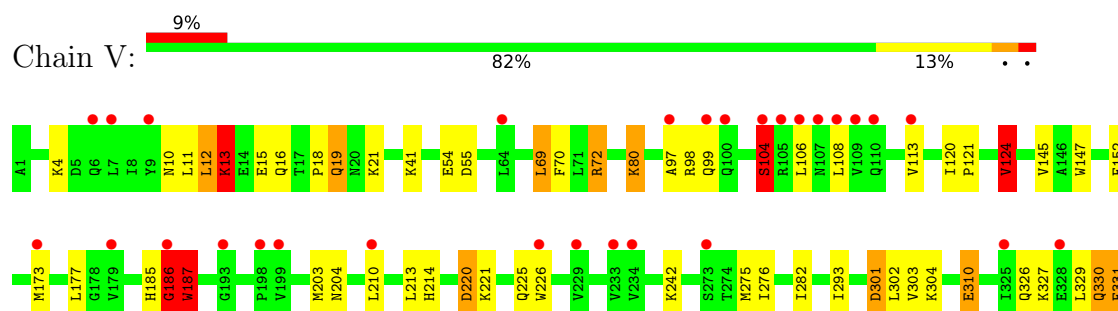
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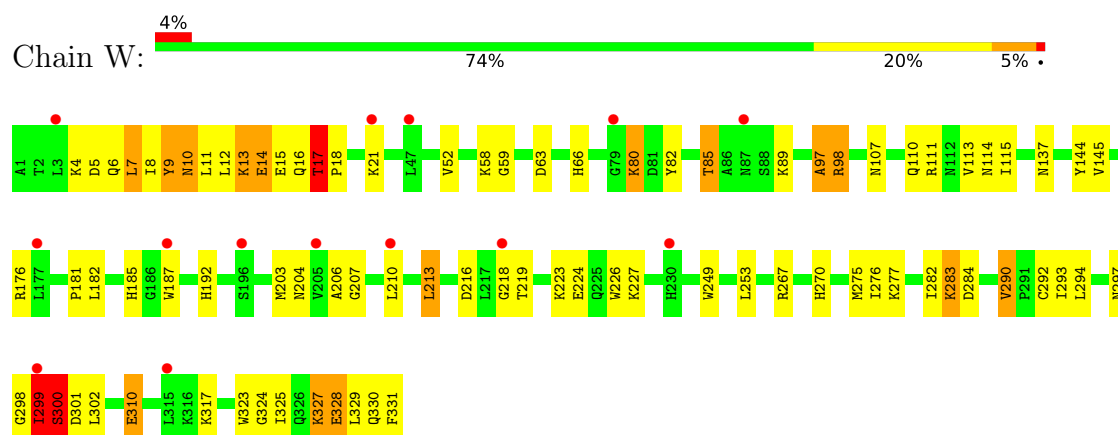
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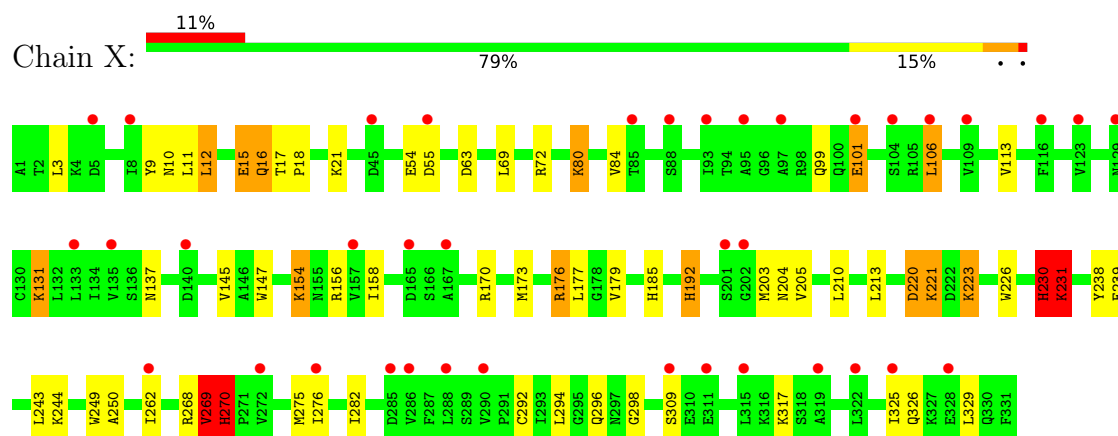
- Molecule 1: L-lactate dehydrogenase A chain



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.37Å 110.92Å 217.55Å 89.98° 90.04° 88.37°	Depositor
Resolution (Å)	35.56 – 3.98 35.56 – 3.98	Depositor EDS
% Data completeness (in resolution range)	99.1 (35.56-3.98) 99.2 (35.56-3.98)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.99 (at 3.99Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.238 , 0.273 0.244 , 0.279	Depositor DCC
R_{free} test set	3837 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.054 for h,-k,-l 0.056 for -h,k,-l 0.130 for -h,-k,l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	61670	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GO3

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	0.57	0/2612	1.12	16/3532 (0.5%)
1	B	0.59	1/2612 (0.0%)	1.14	18/3532 (0.5%)
1	C	0.57	0/2612	1.09	11/3532 (0.3%)
1	D	0.58	1/2612 (0.0%)	1.15	17/3532 (0.5%)
1	E	0.59	2/2612 (0.1%)	1.10	9/3532 (0.3%)
1	F	0.54	0/2612	1.10	12/3532 (0.3%)
1	G	0.58	1/2612 (0.0%)	1.10	15/3532 (0.4%)
1	H	0.56	0/2612	1.09	13/3532 (0.4%)
1	I	0.55	0/2612	1.10	13/3532 (0.4%)
1	J	0.59	1/2612 (0.0%)	1.08	13/3532 (0.4%)
1	K	0.67	2/2612 (0.1%)	1.20	18/3532 (0.5%)
1	L	0.55	0/2612	1.06	13/3532 (0.4%)
1	M	0.58	1/2612 (0.0%)	1.10	16/3532 (0.5%)
1	N	0.57	1/2612 (0.0%)	1.07	7/3532 (0.2%)
1	O	0.62	1/2612 (0.0%)	1.25	29/3532 (0.8%)
1	P	0.56	0/2612	1.16	17/3532 (0.5%)
1	Q	0.61	0/2612	1.15	21/3532 (0.6%)
1	R	0.63	1/2612 (0.0%)	1.13	17/3532 (0.5%)
1	S	0.74	5/2612 (0.2%)	1.25	22/3532 (0.6%)
1	T	0.58	0/2612	1.20	10/3532 (0.3%)
1	U	0.59	1/2612 (0.0%)	1.17	18/3532 (0.5%)
1	V	0.60	0/2612	1.10	12/3532 (0.3%)
1	W	0.57	1/2612 (0.0%)	1.11	10/3532 (0.3%)
1	X	0.58	1/2612 (0.0%)	1.19	22/3532 (0.6%)
All	All	0.59	20/62688 (0.0%)	1.14	369/84768 (0.4%)

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	2
1	B	0	5
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	K	0	3
1	L	0	2
1	N	0	3
1	O	0	1
1	P	0	2
1	Q	0	1
1	R	0	2
1	S	0	1
1	T	0	3
1	U	0	4
1	V	0	6
1	W	0	3
1	X	0	4
All	All	0	48

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	230	HIS	CE1-NE2	-13.08	1.19	1.32
1	J	230	HIS	CE1-NE2	-10.55	1.22	1.32
1	N	230	HIS	CE1-NE2	-9.01	1.23	1.32
1	G	284	ASP	CG-OD1	-8.15	1.09	1.25
1	U	12	LEU	C-O	-7.40	1.14	1.23

The worst 5 of 369 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	72	ARG	CB-CG-CD	18.98	154.95	111.30
1	T	230	HIS	O-C-N	-17.09	99.53	122.43
1	X	230	HIS	O-C-N	-16.57	100.23	122.43
1	O	72	ARG	CB-CG-CD	13.99	143.49	111.30
1	A	72	ARG	CB-CG-CD	13.98	143.46	111.30

There are no chirality outliers.

5 of 48 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ALA	Mainchain
1	A	330	GLN	Peptide
1	B	13	LYS	Peptide
1	B	191	GLU	Sidechain
1	B	9	TYR	Mainchain

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	2568	0	2656	63	1
1	B	2568	0	2656	92	1
1	C	2568	0	2656	82	0
1	D	2568	0	2656	54	3
1	E	2568	0	2656	120	0
1	F	2568	0	2656	88	0
1	G	2568	0	2656	63	3
1	H	2568	0	2656	55	0
1	I	2568	0	2656	66	0
1	J	2568	0	2656	110	0
1	K	2568	0	2656	138	0
1	L	2568	0	2656	70	0
1	M	2568	0	2656	75	0
1	N	2568	0	2656	72	0
1	O	2568	0	2656	134	0
1	P	2568	0	2656	65	0
1	Q	2568	0	2656	114	0
1	R	2568	0	2656	101	3
1	S	2568	0	2656	62	0
1	T	2568	0	2656	78	0
1	U	2568	0	2656	111	3
1	V	2568	0	2656	79	0
1	W	2568	0	2656	108	0
1	X	2568	0	2656	112	0
2	Q	38	0	0	18	0
All	All	61670	0	63744	1621	7

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 13.

The worst 5 of 1621 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:110:GLN:HG3	1:J:129:ASN:ND2	1.26	1.41
1:J:11:LEU:HD21	1:K:302:LEU:CD1	1.52	1.37
1:E:331:PHE:C	1:O:17:THR:HG21	1.51	1.35
1:F:107:ASN:OD1	1:W:115:ILE:HG12	1.23	1.28
1:B:323:TRP:HH2	1:K:129:ASN:OD1	1.10	1.27

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:323:TRP:CH2	1:R:129:ASN:OD1[1_565]	1.36	0.84
1:D:323:TRP:CH2	1:U:129:ASN:OD1[1_545]	1.41	0.79
1:D:323:TRP:CZ2	1:U:129:ASN:OD1[1_545]	1.83	0.37
1:A:309:SER:CB	1:B:216:ASP:OD1[1_655]	1.85	0.35
1:D:323:TRP:CH2	1:U:129:ASN:CG[1_545]	1.89	0.31

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	329/331 (99%)	319 (97%)	9 (3%)	1 (0%)	37 70
1	B	329/331 (99%)	316 (96%)	11 (3%)	2 (1%)	22 58
1	C	329/331 (99%)	314 (95%)	11 (3%)	4 (1%)	11 42
1	D	329/331 (99%)	320 (97%)	7 (2%)	2 (1%)	22 58
1	E	329/331 (99%)	318 (97%)	9 (3%)	2 (1%)	22 58
1	F	329/331 (99%)	321 (98%)	6 (2%)	2 (1%)	22 58
1	G	329/331 (99%)	318 (97%)	8 (2%)	3 (1%)	14 49
1	H	329/331 (99%)	318 (97%)	8 (2%)	3 (1%)	14 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	329/331 (99%)	317 (96%)	8 (2%)	4 (1%)	11	42
1	J	329/331 (99%)	320 (97%)	7 (2%)	2 (1%)	22	58
1	K	329/331 (99%)	315 (96%)	11 (3%)	3 (1%)	14	49
1	L	329/331 (99%)	318 (97%)	9 (3%)	2 (1%)	22	58
1	M	329/331 (99%)	316 (96%)	8 (2%)	5 (2%)	8	39
1	N	329/331 (99%)	315 (96%)	10 (3%)	4 (1%)	11	42
1	O	329/331 (99%)	316 (96%)	7 (2%)	6 (2%)	7	35
1	P	329/331 (99%)	316 (96%)	10 (3%)	3 (1%)	14	49
1	Q	329/331 (99%)	314 (95%)	11 (3%)	4 (1%)	11	42
1	R	329/331 (99%)	315 (96%)	11 (3%)	3 (1%)	14	49
1	S	329/331 (99%)	318 (97%)	8 (2%)	3 (1%)	14	49
1	T	329/331 (99%)	318 (97%)	9 (3%)	2 (1%)	22	58
1	U	329/331 (99%)	315 (96%)	11 (3%)	3 (1%)	14	49
1	V	329/331 (99%)	318 (97%)	10 (3%)	1 (0%)	37	70
1	W	329/331 (99%)	316 (96%)	8 (2%)	5 (2%)	8	39
1	X	329/331 (99%)	317 (96%)	8 (2%)	4 (1%)	11	42
All	All	7896/7944 (99%)	7608 (96%)	215 (3%)	73 (1%)	14	49

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	C	13	LYS
1	C	97	ALA
1	C	98	ARG
1	E	16	GLN

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	287/287 (100%)	275 (96%)	12 (4%)	25	48
1	B	287/287 (100%)	271 (94%)	16 (6%)	17	41
1	C	287/287 (100%)	269 (94%)	18 (6%)	15	38
1	D	287/287 (100%)	273 (95%)	14 (5%)	21	44
1	E	287/287 (100%)	275 (96%)	12 (4%)	25	48
1	F	287/287 (100%)	273 (95%)	14 (5%)	21	44
1	G	287/287 (100%)	279 (97%)	8 (3%)	38	59
1	H	287/287 (100%)	273 (95%)	14 (5%)	21	44
1	I	287/287 (100%)	273 (95%)	14 (5%)	21	44
1	J	287/287 (100%)	270 (94%)	17 (6%)	16	39
1	K	287/287 (100%)	265 (92%)	22 (8%)	10	33
1	L	287/287 (100%)	269 (94%)	18 (6%)	15	38
1	M	287/287 (100%)	271 (94%)	16 (6%)	17	41
1	N	287/287 (100%)	274 (96%)	13 (4%)	23	46
1	O	287/287 (100%)	272 (95%)	15 (5%)	19	43
1	P	287/287 (100%)	274 (96%)	13 (4%)	23	46
1	Q	287/287 (100%)	265 (92%)	22 (8%)	10	33
1	R	287/287 (100%)	264 (92%)	23 (8%)	10	32
1	S	287/287 (100%)	266 (93%)	21 (7%)	11	34
1	T	287/287 (100%)	271 (94%)	16 (6%)	17	41
1	U	287/287 (100%)	268 (93%)	19 (7%)	14	37
1	V	287/287 (100%)	275 (96%)	12 (4%)	25	48
1	W	287/287 (100%)	272 (95%)	15 (5%)	19	43
1	X	287/287 (100%)	278 (97%)	9 (3%)	35	56
All	All	6888/6888 (100%)	6515 (95%)	373 (5%)	18	42

5 of 373 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	220	ASP
1	S	87	ASN
1	Q	17	THR
1	R	12	LEU
1	S	297	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 146 such sidechains are listed below:

Mol	Chain	Res	Type
1	T	297	ASN
1	X	99	GLN
1	U	20	ASN
1	W	20	ASN
1	I	232	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GO3	Q	401	-	41,41,41	2.06	7 (17%)	64,64,64	3.17	34 (53%)

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
2	GO3	Q	401	-	-	8/16/16/16	0/4/4/4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	401	GO3	O7-C37	6.30	1.43	1.21
2	Q	401	GO3	C25-C37	6.07	1.58	1.45
2	Q	401	GO3	O8-C38	5.21	1.39	1.21
2	Q	401	GO3	C26-C38	4.04	1.54	1.45
2	Q	401	GO3	C11-C13	-2.79	1.37	1.42

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	401	GO3	C9-C10-C18	-10.76	104.41	120.26
2	Q	401	GO3	C10-C9-C21	-7.65	106.82	119.67
2	Q	401	GO3	C9-C10-C22	6.92	131.30	119.67
2	Q	401	GO3	C33-C19-C15	-6.80	97.61	112.94
2	Q	401	GO3	O8-C38-C26	-6.53	103.90	124.11

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	401	GO3	C11-C15-C19-C34
2	Q	401	GO3	C27-C15-C19-C34
2	Q	401	GO3	C14-C26-C38-O8
2	Q	401	GO3	C30-C26-C38-O8
2	Q	401	GO3	C12-C16-C20-C36

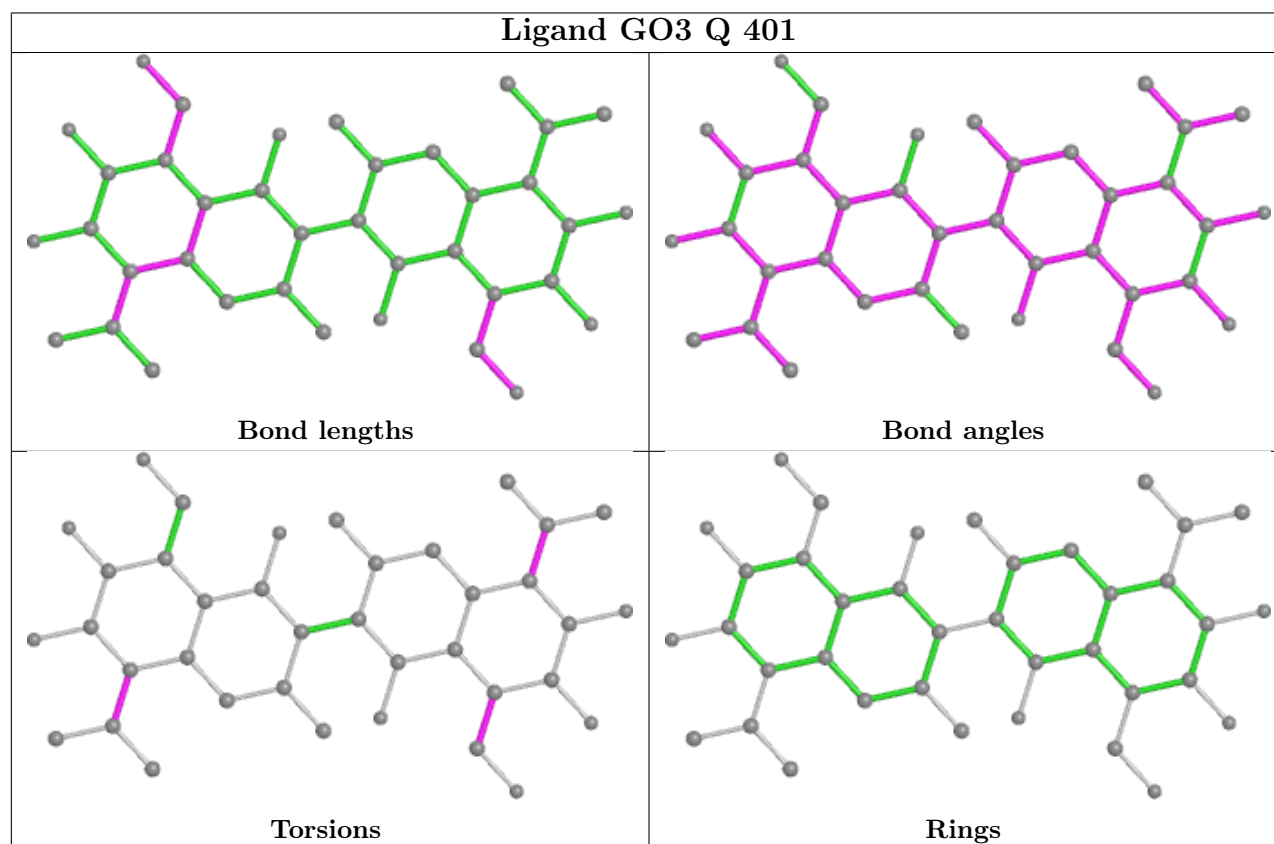
There are no ring outliers.

1 monomer is involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	401	GO3	18	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	331/331 (100%)	0.37	7 (2%) 63 47	0, 31, 61, 99	0
1	B	331/331 (100%)	0.38	7 (2%) 63 47	15, 36, 61, 98	0
1	C	331/331 (100%)	0.39	5 (1%) 71 55	13, 38, 74, 116	0
1	D	331/331 (100%)	0.30	5 (1%) 71 55	0, 26, 61, 91	0
1	E	331/331 (100%)	0.40	7 (2%) 63 47	14, 34, 69, 119	0
1	F	331/331 (100%)	0.42	10 (3%) 52 39	16, 39, 69, 89	0
1	G	331/331 (100%)	0.34	5 (1%) 71 55	17, 38, 68, 91	0
1	H	331/331 (100%)	0.34	5 (1%) 71 55	7, 26, 45, 61	0
1	I	331/331 (100%)	0.29	5 (1%) 71 55	16, 31, 60, 77	0
1	J	331/331 (100%)	0.48	14 (4%) 41 32	10, 33, 88, 185	0
1	K	331/331 (100%)	0.49	15 (4%) 39 30	12, 38, 77, 167	0
1	L	331/331 (100%)	0.56	23 (6%) 24 21	13, 42, 110, 191	0
1	M	331/331 (100%)	0.45	9 (2%) 56 42	15, 43, 77, 102	0
1	N	331/331 (100%)	0.62	19 (5%) 30 25	21, 60, 136, 279	0
1	O	331/331 (100%)	0.70	19 (5%) 30 25	12, 55, 115, 187	0
1	P	331/331 (100%)	0.63	20 (6%) 29 24	22, 54, 108, 245	0
1	Q	331/331 (100%)	0.74	27 (8%) 19 17	20, 59, 118, 219	0
1	R	331/331 (100%)	1.01	36 (10%) 12 12	32, 78, 142, 242	0
1	S	331/331 (100%)	0.87	28 (8%) 18 17	26, 69, 116, 145	0
1	T	331/331 (100%)	0.63	16 (4%) 36 29	15, 56, 98, 123	0
1	U	331/331 (100%)	1.12	51 (15%) 6 9	33, 92, 165, 238	0
1	V	331/331 (100%)	0.71	29 (8%) 17 15	20, 54, 122, 250	0
1	W	331/331 (100%)	0.60	14 (4%) 41 32	16, 53, 109, 148	0
1	X	331/331 (100%)	1.02	38 (11%) 11 12	34, 85, 153, 330	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	7944/7944 (100%)	0.58	414 (5%) 34 27	0, 46, 115, 330	0

The worst 5 of 414 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	276	ILE	7.0
1	V	106	LEU	5.9
1	R	106	LEU	5.7
1	J	106	LEU	5.5
1	K	105	ARG	5.1

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](#)

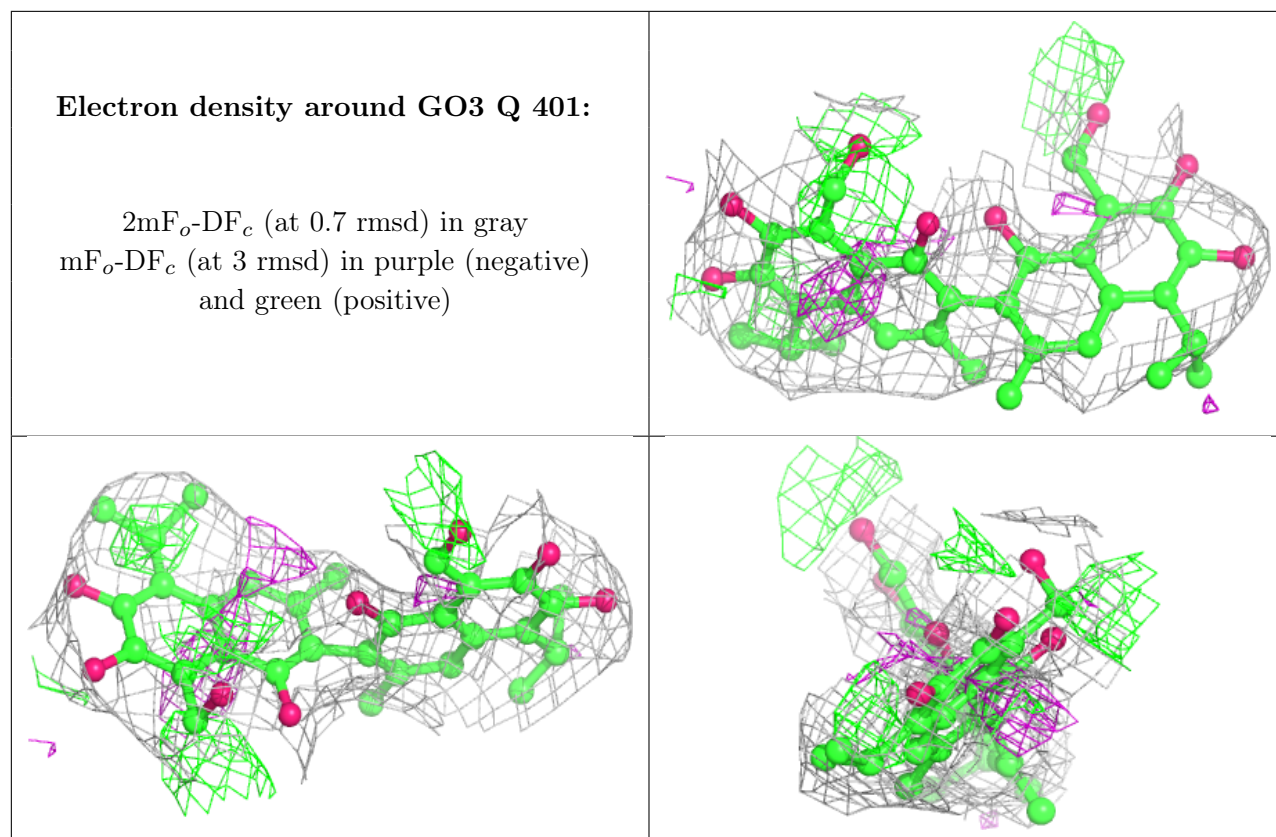
There are no oligosaccharides in this entry.

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	GO3	Q	401	38/38	0.80	0.18	18,23,27,29	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.