



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 01:20 PM UTC

PDB ID : 9EBW / pdb_00009ebw
Title : Chimeric fluorescence biosensor formed from a lactate-binding protein and GFP, bound to lactate
Authors : Horwitz, S.M.; Ambarian, J.A.; Jones, R.; Waidmann, L.; Davis, K.M.
Deposited on : 2024-11-13
Resolution : 2.78 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

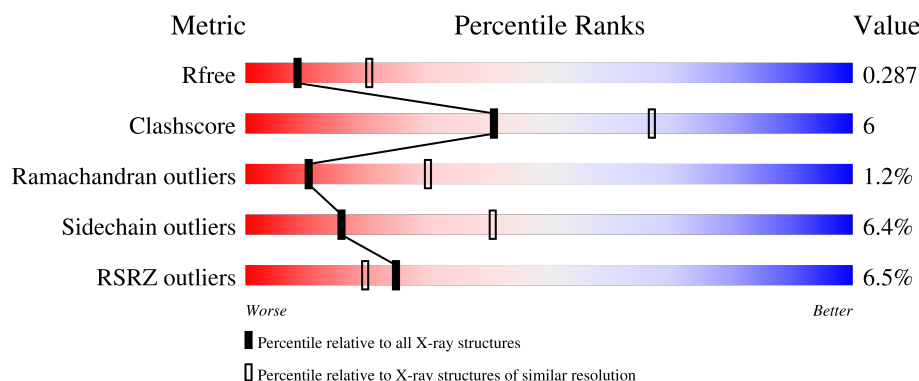
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	515	5% 77% 14% • 6%
1	B	515	5% 79% 13% • •
1	C	515	5% 78% 12% • 7%
1	D	515	9% 74% 13% • 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14730 atoms, of which 20 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 Green fluorescent protein, Methyl-accepting chemotaxis transducer (TlpC).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3701	2368	624	696	13			
1	B	494	Total	C	N	O	S	0	0	0
			3768	2403	636	716	13			
1	C	481	Total	C	N	O	S	0	0	0
			3641	2324	620	685	12			
1	D	462	Total	C	N	O	S	0	0	0
			3457	2206	584	656	11			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P42212
A	2	LYS	-	expression tag	UNP P42212
A	3	HIS	-	expression tag	UNP P42212
A	4	HIS	-	expression tag	UNP P42212
A	5	HIS	-	expression tag	UNP P42212
A	6	HIS	-	expression tag	UNP P42212
A	7	HIS	-	expression tag	UNP P42212
A	8	HIS	-	expression tag	UNP P42212
A	9	HIS	-	expression tag	UNP P42212
A	10	VAL	-	expression tag	UNP P42212
A	73	LEU	PHE	conflict	UNP P42212
A	74	SWG	SER	chromophore	UNP P42212
A	74	SWG	TYR	chromophore	UNP P42212
A	74	SWG	GLY	chromophore	UNP P42212
A	79	ALA	SER	conflict	UNP P42212
A	152	SER	TYR	conflict	UNP P42212
A	153	SER	ASN	conflict	UNP P42212
A	154	GLY	-	linker	UNP P42212
A	155	ARG	-	linker	UNP P42212
A	156	THR	-	linker	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
A	157	GLY	-	linker	UNP P42212
A	158	ILE	-	linker	UNP P42212
A	159	ASP	SER	conflict	UNP O24911
A	160	PRO	TYR	conflict	UNP O24911
A	161	PHE	LYS	conflict	UNP O24911
A	162	THR	VAL	conflict	UNP O24911
A	422	SER	-	linker	UNP O24911
A	423	SER	-	linker	UNP O24911
A	424	HIS	-	linker	UNP O24911
A	425	SER	-	linker	UNP O24911
A	430	THR	MET	conflict	UNP P42212
A	440	ALA	VAL	conflict	UNP P42212
A	452	GLY	SER	conflict	UNP P42212
A	483	LYS	ALA	conflict	UNP P42212
A	508	LEU	HIS	conflict	UNP P42212
A	515	GLN	LYS	conflict	UNP P42212
B	1	MET	-	initiating methionine	UNP P42212
B	2	LYS	-	expression tag	UNP P42212
B	3	HIS	-	expression tag	UNP P42212
B	4	HIS	-	expression tag	UNP P42212
B	5	HIS	-	expression tag	UNP P42212
B	6	HIS	-	expression tag	UNP P42212
B	7	HIS	-	expression tag	UNP P42212
B	8	HIS	-	expression tag	UNP P42212
B	9	HIS	-	expression tag	UNP P42212
B	10	VAL	-	expression tag	UNP P42212
B	73	LEU	PHE	conflict	UNP P42212
B	74	SWG	SER	chromophore	UNP P42212
B	74	SWG	TYR	chromophore	UNP P42212
B	74	SWG	GLY	chromophore	UNP P42212
B	79	ALA	SER	conflict	UNP P42212
B	152	SER	TYR	conflict	UNP P42212
B	153	SER	ASN	conflict	UNP P42212
B	154	GLY	-	linker	UNP P42212
B	155	ARG	-	linker	UNP P42212
B	156	THR	-	linker	UNP P42212
B	157	GLY	-	linker	UNP P42212
B	158	ILE	-	linker	UNP P42212
B	159	ASP	SER	conflict	UNP O24911
B	160	PRO	TYR	conflict	UNP O24911
B	161	PHE	LYS	conflict	UNP O24911
B	162	THR	VAL	conflict	UNP O24911

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Chain	Residue	Modelled	Actual	Comment	Reference
B	422	SER	-	linker	UNP O24911
B	423	SER	-	linker	UNP O24911
B	424	HIS	-	linker	UNP O24911
B	425	SER	-	linker	UNP O24911
B	430	THR	MET	conflict	UNP P42212
B	440	ALA	VAL	conflict	UNP P42212
B	452	GLY	SER	conflict	UNP P42212
B	483	LYS	ALA	conflict	UNP P42212
B	508	LEU	HIS	conflict	UNP P42212
B	515	GLN	LYS	conflict	UNP P42212
C	1	MET	-	initiating methionine	UNP P42212
C	2	LYS	-	expression tag	UNP P42212
C	3	HIS	-	expression tag	UNP P42212
C	4	HIS	-	expression tag	UNP P42212
C	5	HIS	-	expression tag	UNP P42212
C	6	HIS	-	expression tag	UNP P42212
C	7	HIS	-	expression tag	UNP P42212
C	8	HIS	-	expression tag	UNP P42212
C	9	HIS	-	expression tag	UNP P42212
C	10	VAL	-	expression tag	UNP P42212
C	73	LEU	PHE	conflict	UNP P42212
C	74	SWG	SER	chromophore	UNP P42212
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C	79	ALA	SER	conflict	UNP P42212
C	152	SER	TYR	conflict	UNP P42212
C	153	SER	ASN	conflict	UNP P42212
C	154	GLY	-	linker	UNP P42212
C	155	ARG	-	linker	UNP P42212
C	156	THR	-	linker	UNP P42212
C	157	GLY	-	linker	UNP P42212
C	158	ILE	-	linker	UNP P42212
C	159	ASP	SER	conflict	UNP O24911
C	160	PRO	TYR	conflict	UNP O24911
C	161	PHE	LYS	conflict	UNP O24911
C	162	THR	VAL	conflict	UNP O24911
C	422	SER	-	linker	UNP O24911
C	423	SER	-	linker	UNP O24911
C	424	HIS	-	linker	UNP O24911
C	425	SER	-	linker	UNP O24911
C	430	THR	MET	conflict	UNP P42212
C	440	ALA	VAL	conflict	UNP P42212

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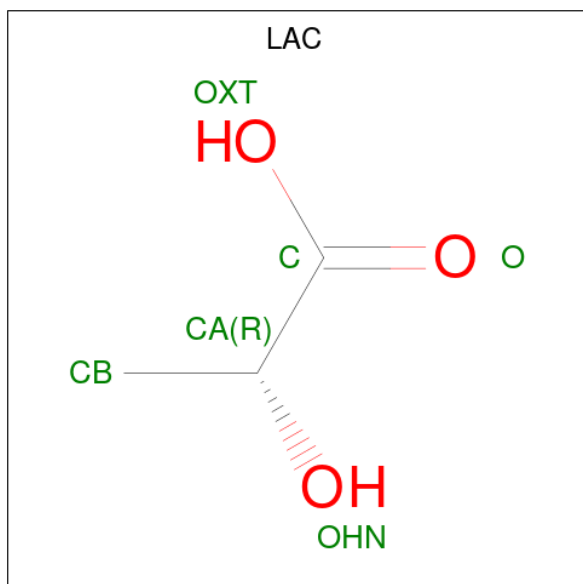
Chain	Residue	Modelled	Actual	Comment	Reference
C	452	GLY	SER	conflict	UNP P42212
C	483	LYS	ALA	conflict	UNP P42212
C	508	LEU	HIS	conflict	UNP P42212
C	515	GLN	LYS	conflict	UNP P42212
D	1	MET	-	initiating methionine	UNP P42212
D	2	LYS	-	expression tag	UNP P42212
D	3	HIS	-	expression tag	UNP P42212
D	4	HIS	-	expression tag	UNP P42212
D	5	HIS	-	expression tag	UNP P42212
D	6	HIS	-	expression tag	UNP P42212
D	7	HIS	-	expression tag	UNP P42212
D	8	HIS	-	expression tag	UNP P42212
D	9	HIS	-	expression tag	UNP P42212
D	10	VAL	-	expression tag	UNP P42212
D	73	LEU	PHE	conflict	UNP P42212
D	74	SWG	SER	chromophore	UNP P42212
D	74	SWG	TYR	chromophore	UNP P42212
D	74	SWG	GLY	chromophore	UNP P42212
D	79	ALA	SER	conflict	UNP P42212
D	152	SER	TYR	conflict	UNP P42212
D	153	SER	ASN	conflict	UNP P42212
D	154	GLY	-	linker	UNP P42212
D	155	ARG	-	linker	UNP P42212
D	156	THR	-	linker	UNP P42212
D	157	GLY	-	linker	UNP P42212
D	158	ILE	-	linker	UNP P42212
D	159	ASP	SER	conflict	UNP O24911
D	160	PRO	TYR	conflict	UNP O24911
D	161	PHE	LYS	conflict	UNP O24911
D	162	THR	VAL	conflict	UNP O24911
D	422	SER	-	linker	UNP O24911
D	423	SER	-	linker	UNP O24911
D	424	HIS	-	linker	UNP O24911
D	425	SER	-	linker	UNP O24911
D	430	THR	MET	conflict	UNP P42212
D	440	ALA	VAL	conflict	UNP P42212
D	452	GLY	SER	conflict	UNP P42212
D	483	LYS	ALA	conflict	UNP P42212
D	508	LEU	HIS	conflict	UNP P42212
D	515	GLN	LYS	conflict	UNP P42212

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is LACTIC ACID (CCD ID: LAC) (formula: $C_3H_6O_3$) (labeled as "Ligand of Interest" by depositor).



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

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

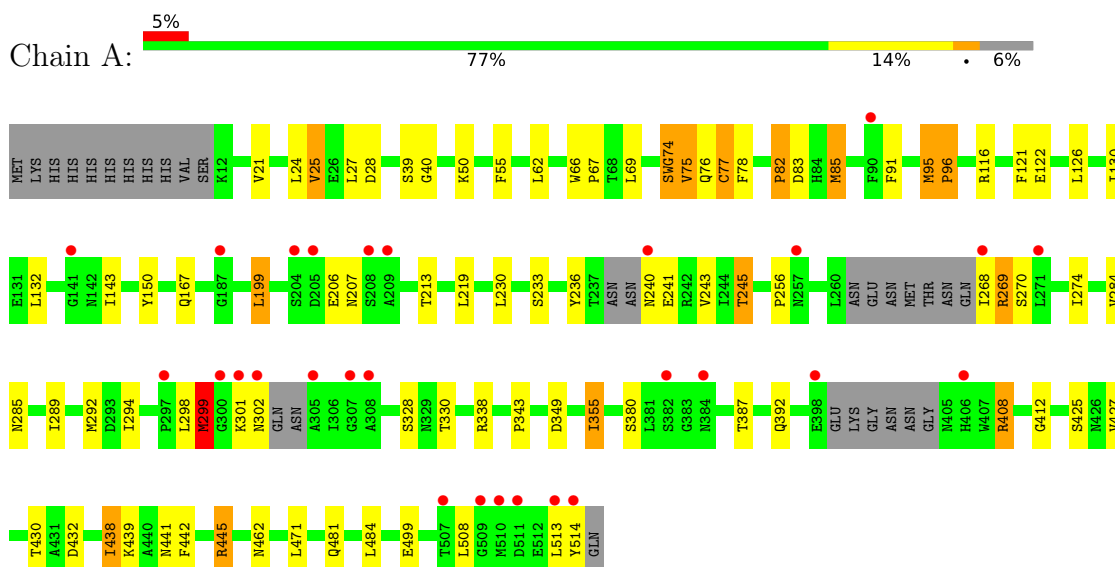
- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	42	Total	H	O	0	0
			54	12	42		
4	B	28	Total	H	O	0	0
			36	8	28		
4	C	28	Total	O		0	0
			28	28			
4	D	21	Total	O		0	0
			21	21			

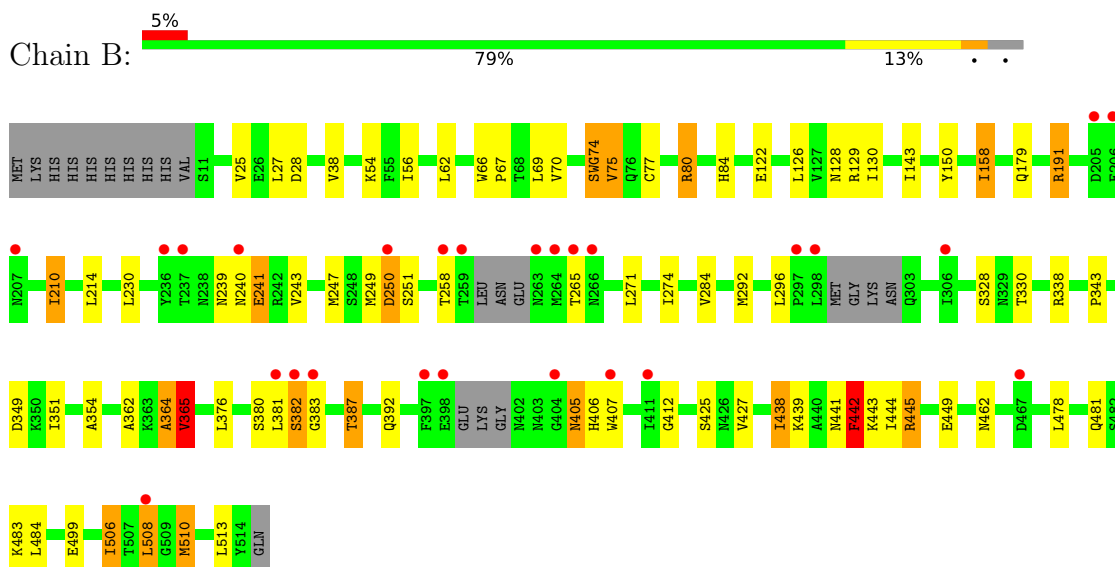
3 Residue-property plots [i](#)

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.

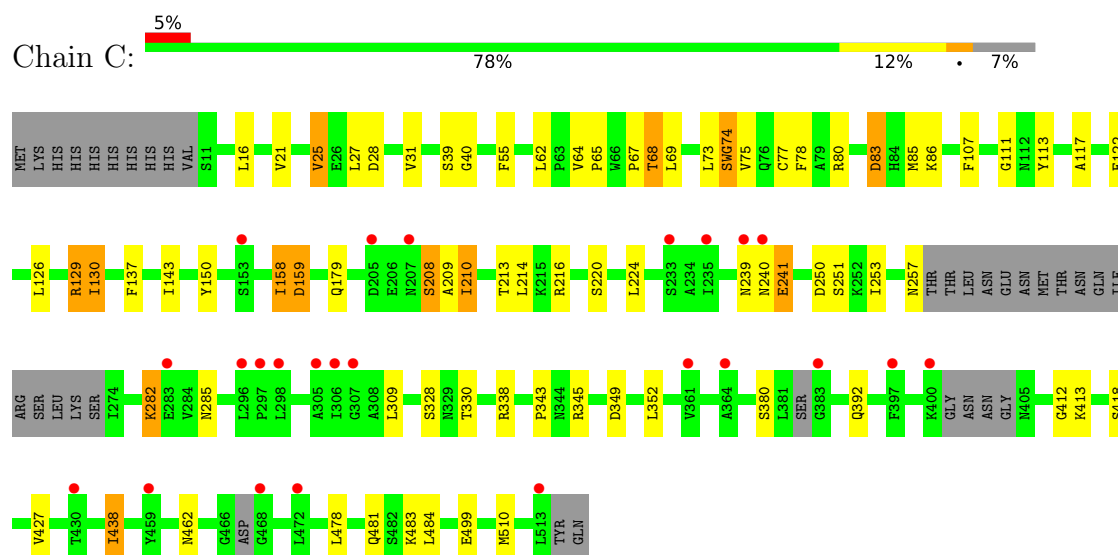
- Molecule 1: Green fluorescent protein,Methyl-accepting chemotaxis transducer (TlpC)



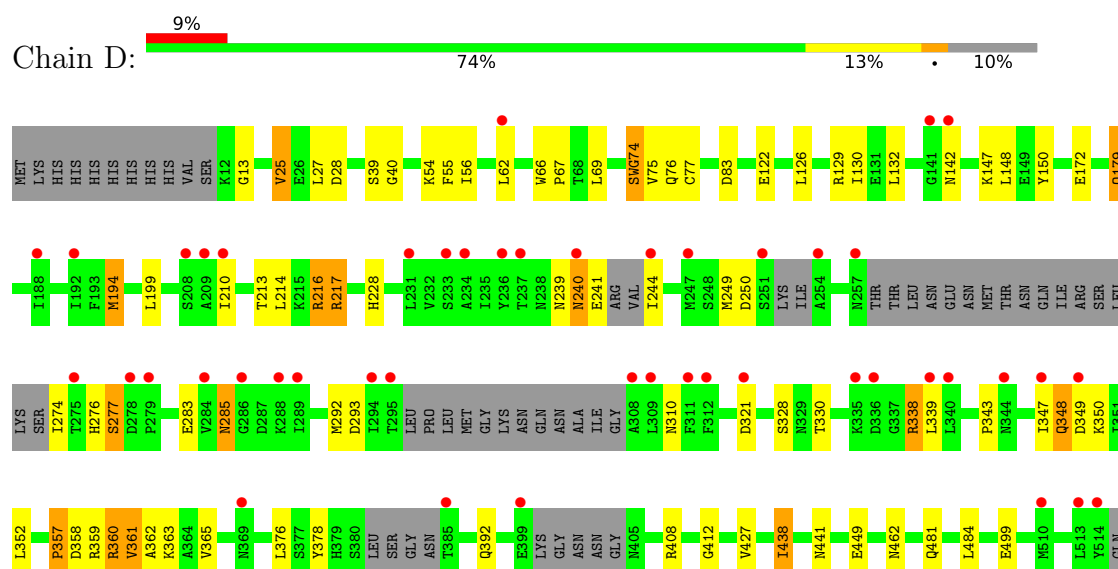
- Molecule 1: Green fluorescent protein,Methyl-accepting chemotaxis transducer (TlpC)



- Molecule 1: Green fluorescent protein,Methyl-accepting chemotaxis transducer (TlpC)



● Molecule 1: Green fluorescent protein, Methyl-accepting chemotaxis transducer (TlpC)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.88Å 109.80Å 123.71Å 90.00° 110.14° 90.00°	Depositor
Resolution (Å)	45.94 – 2.78 45.94 – 2.78	Depositor EDS
% Data completeness (in resolution range)	95.3 (45.94-2.78) 95.3 (45.94-2.78)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.242 , 0.285 0.243 , 0.287	Depositor DCC
R_{free} test set	2002 reflections (3.47%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.057 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14730	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.72 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1104e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SWG, LAC, 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	0.60	0/3754	0.93	3/5095 (0.1%)
1	B	0.57	0/3822	0.90	4/5190 (0.1%)
1	C	0.57	0/3692	0.89	2/5010 (0.0%)
1	D	0.60	0/3504	0.92	2/4763 (0.0%)
All	All	0.59	0/14772	0.91	11/20058 (0.1%)

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	3
1	B	0	3
1	C	0	1
1	D	0	3
All	All	0	10

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	364	ALA	N-CA-C	-8.36	97.91	110.28
1	C	158	ILE	N-CA-C	7.99	118.37	111.90
1	D	357	PRO	N-CA-C	-7.63	101.41	113.78
1	B	442	PHE	CA-CB-CG	7.01	120.81	113.80
1	D	76	GLN	N-CA-C	-6.51	105.34	113.28
1	B	365	VAL	N-CA-CB	6.47	121.91	111.23
1	A	75	VAL	N-CA-CB	5.92	121.57	111.50
1	C	208	SER	N-CA-C	5.90	119.37	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	PRO	N-CA-CB	-5.80	96.22	102.60
1	A	82	PRO	N-CA-CB	-5.25	98.63	103.25
1	B	75	VAL	N-CA-CB	5.20	120.33	111.50

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	ARG	Sidechain
1	A	408	ARG	Sidechain
1	A	445	ARG	Sidechain
1	B	191	ARG	Sidechain
1	B	445	ARG	Sidechain
1	B	80	ARG	Sidechain
1	C	129	ARG	Sidechain
1	D	216	ARG	Sidechain
1	D	217	ARG	Sidechain
1	D	360	ARG	Sidechain

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	3701	0	3468	52	0
1	B	3768	0	3550	49	0
1	C	3641	0	3417	48	1
1	D	3457	0	3139	39	1
2	A	6	0	8	0	0
2	B	6	0	8	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
4	A	42	12	0	4	0
4	B	28	8	0	1	0
4	C	28	0	0	0	0
4	D	21	0	0	0	0
All	All	14710	20	13590	183	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (183) 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:C:64:VAL:HG11	1:C:113:TYR:OH	1.60	1.02
1:A:75:VAL:HG23	4:A:725:HOH:O	1.72	0.89
1:D:54:LYS:HE3	1:D:56:ILE:HD11	1.67	0.75
1:C:224:LEU:HD21	1:C:253:ILE:HD11	1.73	0.71
1:D:348:GLN:O	1:D:350:LYS:N	2.24	0.71
1:B:405:ASN:O	1:B:407:TRP:N	2.25	0.70
1:B:274:ILE:HD12	1:B:296:LEU:HD13	1.75	0.68
1:C:64:VAL:CG1	1:C:113:TYR:OH	2.40	0.66
1:B:364:ALA:O	1:B:365:VAL:HG13	1.96	0.65
1:C:117:ALA:HB2	1:C:130:ILE:HG23	1.79	0.65
1:B:74:SWG:HZ3	1:B:427:VAL:HG13	1.79	0.64
1:D:74:SWG:HZ3	1:D:427:VAL:HB	1.80	0.64
1:B:362:ALA:O	1:B:365:VAL:HG22	1.98	0.63
1:B:74:SWG:HA1	1:B:75:VAL:HG22	1.81	0.62
1:B:351:ILE:HG13	1:B:354:ALA:HB3	1.82	0.62
1:C:64:VAL:HG13	1:C:65:PRO:HD2	1.82	0.62
1:B:210:ILE:HG23	1:B:214:LEU:HD23	1.81	0.60
1:C:224:LEU:CD2	1:C:253:ILE:HD11	2.32	0.60
1:A:74:SWG:HH2	1:A:425:SER:HB3	1.84	0.59
1:A:75:VAL:CG2	4:A:725:HOH:O	2.42	0.59
1:D:142:ASN:HA	1:D:147:LYS:HD3	1.84	0.59
1:C:83:ASP:HA	1:C:86:LYS:HG3	1.85	0.59
1:B:249:MET:O	1:B:251:SER:N	2.37	0.58
1:D:25:VAL:HG11	1:D:55:PHE:HE1	1.68	0.58
1:D:338:ARG:HH11	1:D:338:ARG:HB2	1.71	0.55
1:A:25:VAL:HG13	1:A:40:GLY:HA3	1.88	0.55
1:A:116:ARG:NH1	4:A:704:HOH:O	2.35	0.55
1:C:208:SER:O	1:C:210:ILE:N	2.38	0.55
1:B:74:SWG:HZ3	1:B:427:VAL:CG1	2.38	0.54
1:D:25:VAL:HG13	1:D:40:GLY:HA3	1.89	0.54
1:A:432:ASP:HB2	1:A:439:LYS:HG2	1.90	0.54
1:C:55:PHE:CE2	1:C:73:LEU:HB3	2.43	0.54
1:A:95:MET:HE3	1:A:126:LEU:HD21	1.88	0.54
1:D:277:SER:HB3	1:D:293:ASP:HB2	1.90	0.53
1:B:508:LEU:HD22	1:B:508:LEU:H	1.74	0.53
1:A:74:SWG:HZ3	1:A:427:VAL:CG2	2.39	0.53
1:C:158:ILE:HG13	1:C:159:ASP:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:HIS:HE1	1:D:321:ASP:OD2	1.92	0.53
1:D:362:ALA:O	1:D:365:VAL:HG22	2.09	0.53
1:C:224:LEU:CG	1:C:253:ILE:HD11	2.38	0.52
1:A:74:SWG:HA1	1:A:75:VAL:HG22	1.91	0.52
1:A:427:VAL:HG13	1:A:442:PHE:CD1	2.45	0.52
1:C:74:SWG:HA1	1:C:75:VAL:HG22	1.90	0.52
1:C:25:VAL:HG13	1:C:40:GLY:HA3	1.90	0.52
1:D:362:ALA:O	1:D:363:LYS:C	2.53	0.52
1:B:74:SWG:HH2	1:B:425:SER:HB3	1.90	0.52
1:D:357:PRO:O	1:D:359:ARG:N	2.42	0.52
1:A:380:SER:HB2	1:A:387:THR:OG1	2.09	0.51
1:B:338:ARG:NH1	1:B:349:ASP:O	2.43	0.51
1:C:25:VAL:HG11	1:C:55:PHE:CE2	2.46	0.51
1:A:25:VAL:HG11	1:A:55:PHE:CE2	2.46	0.50
1:A:438:ILE:HG13	1:A:462:ASN:HB2	1.93	0.50
1:C:338:ARG:NH1	1:C:349:ASP:O	2.44	0.50
1:B:438:ILE:HG13	1:B:462:ASN:HB2	1.94	0.49
1:A:122:GLU:OE1	1:C:213:THR:HG21	2.12	0.49
1:B:54:LYS:HE2	1:B:56:ILE:HD11	1.94	0.49
1:D:25:VAL:HG11	1:D:55:PHE:CE1	2.47	0.49
1:A:338:ARG:NH1	1:A:349:ASP:O	2.44	0.49
1:D:285:ASN:O	1:D:285:ASN:ND2	2.40	0.49
1:D:293:ASP:HB3	1:D:310:ASN:HD21	1.76	0.49
1:C:21:VAL:HB	1:C:78:PHE:HE1	1.77	0.49
1:C:16:LEU:N	1:C:16:LEU:HD22	2.28	0.48
1:A:95:MET:HG3	1:A:121:PHE:HD2	1.78	0.48
1:C:74:SWG:HZ3	1:C:427:VAL:HB	1.95	0.48
1:A:245:THR:HG23	1:A:256:PRO:O	2.14	0.48
1:B:427:VAL:HG12	1:B:442:PHE:CG	2.48	0.48
1:A:274:ILE:H	1:A:274:ILE:HD12	1.79	0.48
1:C:68:THR:HG22	1:C:107:PHE:CZ	2.50	0.47
1:C:75:VAL:C	1:C:77:CYS:H	2.22	0.47
1:A:25:VAL:HG11	1:A:55:PHE:HE2	1.80	0.47
1:A:233:SER:OG	1:A:245:THR:HB	2.14	0.47
1:A:513:LEU:O	1:A:514:TYR:C	2.57	0.47
1:B:427:VAL:CG2	1:B:478:LEU:HB2	2.45	0.47
1:B:25:VAL:HG13	1:B:128:ASN:HB3	1.97	0.47
1:B:381:LEU:O	1:B:382:SER:C	2.57	0.47
1:A:75:VAL:C	1:A:77:CYS:H	2.23	0.46
1:C:27:LEU:HD12	1:C:130:ILE:HB	1.95	0.46
1:B:364:ALA:O	1:B:365:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ILE:HD13	1:A:355:ILE:HA	1.72	0.46
1:C:438:ILE:HG13	1:C:462:ASN:HB2	1.98	0.46
1:A:27:LEU:HD12	1:A:130:ILE:HB	1.98	0.46
1:A:514:TYR:O	1:B:158:ILE:HD11	2.16	0.46
1:B:380:SER:HB2	1:B:387:THR:CG2	2.45	0.46
1:C:85:MET:HE2	1:C:85:MET:HB3	1.70	0.46
1:D:239:ASN:O	1:D:240:ASN:CB	2.63	0.45
1:C:21:VAL:HB	1:C:78:PHE:CE1	2.51	0.45
1:C:224:LEU:HG	1:C:253:ILE:HD11	1.99	0.45
1:A:213:THR:HG21	1:C:122:GLU:OE1	2.17	0.45
1:C:220:SER:HB2	1:C:253:ILE:HD13	1.98	0.45
1:A:285:ASN:HD21	1:C:345:ARG:HD3	1.82	0.44
1:B:330:THR:HA	1:B:412:GLY:O	2.17	0.44
1:C:328:SER:O	1:C:343:PRO:HG3	2.17	0.44
1:C:282:LYS:HE2	1:C:282:LYS:HB2	1.55	0.44
1:D:330:THR:HA	1:D:412:GLY:O	2.18	0.44
1:A:21:VAL:HB	1:A:78:PHE:HE1	1.83	0.44
1:A:199:LEU:HD21	1:A:219:LEU:HD23	1.98	0.44
1:B:351:ILE:HG13	1:B:354:ALA:CB	2.46	0.44
1:D:126:LEU:C	1:D:126:LEU:HD13	2.43	0.44
1:A:74:SWG:HD1	1:A:74:SWG:N2	2.32	0.44
1:B:126:LEU:HD13	1:B:126:LEU:C	2.43	0.44
1:C:481:GLN:O	1:C:499:GLU:HA	2.18	0.44
1:A:126:LEU:C	1:A:126:LEU:HD13	2.43	0.44
1:D:276:HIS:HB2	1:D:292:MET:HE2	2.00	0.44
1:B:249:MET:O	1:B:250:ASP:C	2.60	0.44
1:C:250:ASP:O	1:C:251:SER:HB3	2.17	0.44
1:D:328:SER:O	1:D:343:PRO:HG3	2.18	0.44
1:C:126:LEU:C	1:C:126:LEU:HD13	2.43	0.44
1:C:330:THR:HA	1:C:412:GLY:O	2.18	0.44
1:A:91:PHE:HB2	4:A:706:HOH:O	2.17	0.43
1:A:206:GLU:O	1:A:207:ASN:C	2.60	0.43
1:A:471:LEU:CD1	1:A:471:LEU:N	2.81	0.43
1:B:143:ILE:N	1:B:143:ILE:HD12	2.33	0.43
1:D:27:LEU:HD12	1:D:130:ILE:HB	2.00	0.43
1:A:330:THR:HA	1:A:412:GLY:O	2.18	0.43
1:D:62:LEU:HD21	1:D:69:LEU:HD12	2.00	0.43
1:D:438:ILE:HG13	1:D:462:ASN:HB2	1.99	0.43
1:A:240:ASN:O	1:A:241:GLU:C	2.62	0.43
1:B:179:GLN:HA	1:B:392:GLN:HG2	1.99	0.43
1:B:382:SER:OG	1:B:383:GLY:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:LYS:HD3	1:B:483:LYS:HA	1.91	0.43
1:B:510:MET:HE2	1:B:510:MET:HB2	1.66	0.43
1:C:64:VAL:HG13	1:C:65:PRO:CD	2.47	0.43
1:D:179:GLN:HA	1:D:392:GLN:HG2	2.01	0.43
1:B:27:LEU:HD12	1:B:130:ILE:HB	2.00	0.43
1:B:75:VAL:N	4:B:702:HOH:O	2.52	0.43
1:B:84:HIS:HD2	1:B:508:LEU:HD11	1.83	0.43
1:D:194:MET:HE3	1:D:194:MET:HB3	1.74	0.43
1:A:150:TYR:CE2	1:A:484:LEU:HB3	2.54	0.43
1:D:360:ARG:CZ	1:D:378:TYR:HA	2.49	0.43
1:A:66:TRP:N	1:A:67:PRO:CD	2.82	0.43
1:B:427:VAL:HG22	1:B:478:LEU:HB2	2.00	0.43
1:B:506:ILE:H	1:B:506:ILE:HG12	1.67	0.43
1:A:328:SER:O	1:A:343:PRO:HG3	2.18	0.43
1:B:66:TRP:N	1:B:67:PRO:CD	2.82	0.43
1:D:481:GLN:O	1:D:499:GLU:HA	2.19	0.43
1:C:427:VAL:CG1	1:C:478:LEU:HB2	2.49	0.42
1:C:179:GLN:HA	1:C:392:GLN:HG2	2.00	0.42
1:B:74:SWG:HD1	1:B:74:SWG:N2	2.34	0.42
1:D:240:ASN:O	1:D:241:GLU:C	2.62	0.42
1:A:481:GLN:O	1:A:499:GLU:HA	2.20	0.42
1:D:361:VAL:O	1:D:362:ALA:C	2.62	0.42
1:B:328:SER:O	1:B:343:PRO:HG3	2.19	0.42
1:D:66:TRP:N	1:D:67:PRO:CD	2.83	0.42
1:B:481:GLN:O	1:B:499:GLU:HA	2.20	0.42
1:A:236:TYR:O	1:A:241:GLU:HA	2.20	0.42
1:A:430:THR:HG23	1:A:439:LYS:HG3	2.02	0.42
1:A:82:PRO:HB2	1:A:85:MET:HG3	2.02	0.42
1:D:74:SWG:HA1	1:D:75:VAL:HG22	2.02	0.42
1:D:142:ASN:HA	1:D:147:LYS:HB2	2.01	0.42
1:C:150:TYR:CE2	1:C:484:LEU:HB3	2.55	0.41
1:D:360:ARG:HE	1:D:360:ARG:HB2	1.69	0.41
1:B:62:LEU:HD21	1:B:69:LEU:HD12	2.03	0.41
1:C:418:SER:OG	1:C:483:LYS:HE2	2.20	0.41
1:B:240:ASN:O	1:B:241:GLU:C	2.62	0.41
1:C:111:GLY:HA3	1:C:137:PHE:CD1	2.56	0.41
1:C:240:ASN:O	1:C:241:GLU:C	2.62	0.41
1:C:62:LEU:HD21	1:C:69:LEU:HD12	2.02	0.41
1:A:298:LEU:O	1:A:299:MET:C	2.63	0.41
1:C:143:ILE:HD12	1:C:143:ILE:N	2.35	0.41
1:D:150:TYR:CE2	1:D:484:LEU:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:HD21	1:A:284:VAL:HG21	2.03	0.41
1:C:25:VAL:HG11	1:C:55:PHE:HE2	1.85	0.41
1:B:150:TYR:CE2	1:B:484:LEU:HB3	2.55	0.41
1:A:143:ILE:HD12	1:A:143:ILE:N	2.35	0.41
1:A:167:GLN:CD	1:B:506:ILE:HG22	2.46	0.41
1:B:27:LEU:HB3	1:B:38:VAL:HB	2.03	0.41
1:B:364:ALA:C	1:B:365:VAL:HG13	2.46	0.41
1:D:199:LEU:HD23	1:D:199:LEU:HA	1.92	0.41
1:D:213:THR:OG1	1:D:214:LEU:N	2.54	0.41
1:B:230:LEU:HD21	1:B:284:VAL:HG21	2.02	0.41
1:D:122:GLU:CD	1:D:129:ARG:HH21	2.28	0.41
1:A:301:LYS:O	1:A:302:ASN:C	2.64	0.40
1:B:122:GLU:CD	1:B:129:ARG:HH21	2.30	0.40
1:B:362:ALA:C	1:B:364:ALA:O	2.65	0.40
1:C:31:VAL:HG11	1:C:64:VAL:HG23	2.03	0.40
1:C:67:PRO:HG3	1:C:484:LEU:HD22	2.02	0.40
1:A:62:LEU:HD21	1:A:69:LEU:HD12	2.04	0.40
1:A:268:ILE:O	1:A:270:SER:N	2.53	0.40
1:D:339:LEU:HD21	1:D:352:LEU:HG	2.04	0.40
1:A:132:LEU:HD23	1:A:132:LEU:C	2.47	0.40
1:A:95:MET:HG3	1:A:121:PHE:CD2	2.57	0.40
1:C:75:VAL:C	1:C:77:CYS:N	2.79	0.40
1:D:132:LEU:HD23	1:D:132:LEU:C	2.47	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ARG:NH2	1:D:172:GLU:OE1[1_655]	1.97	0.23

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	473/515 (92%)	446 (94%)	25 (5%)	2 (0%)	30	57
1	B	483/515 (94%)	452 (94%)	22 (5%)	9 (2%)	6	19
1	C	468/515 (91%)	442 (94%)	21 (4%)	5 (1%)	11	32
1	D	445/515 (86%)	420 (94%)	18 (4%)	7 (2%)	7	23
All	All	1869/2060 (91%)	1760 (94%)	86 (5%)	23 (1%)	10	30

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	MET
1	B	250	ASP
1	B	365	VAL
1	B	382	SER
1	B	406	HIS
1	B	513	LEU
1	C	209	ALA
1	C	239	ASN
1	C	241	GLU
1	D	348	GLN
1	D	349	ASP
1	D	358	ASP
1	B	239	ASN
1	B	449	GLU
1	C	210	ILE
1	D	240	ASN
1	A	269	ARG
1	B	241	GLU
1	B	405	ASN
1	C	159	ASP
1	D	210	ILE
1	D	449	GLU
1	D	13	GLY

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	368/450 (82%)	343 (93%)	25 (7%)	14	38
1	B	384/450 (85%)	358 (93%)	26 (7%)	14	38
1	C	364/450 (81%)	346 (95%)	18 (5%)	22	52
1	D	332/450 (74%)	308 (93%)	24 (7%)	13	35
All	All	1448/1800 (80%)	1355 (94%)	93 (6%)	16	41

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	25	VAL
1	A	28	ASP
1	A	39	SER
1	A	50	LYS
1	A	76	GLN
1	A	77	CYS
1	A	83	ASP
1	A	85	MET
1	A	95	MET
1	A	96	PRO
1	A	199	LEU
1	A	243	VAL
1	A	245	THR
1	A	289	ILE
1	A	292	MET
1	A	294	ILE
1	A	299	MET
1	A	355	ILE
1	A	392	GLN
1	A	408	ARG
1	A	438	ILE
1	A	441	ASN
1	A	445	ARG
1	A	508	LEU
1	B	28	ASP
1	B	70	VAL
1	B	77	CYS
1	B	80	ARG
1	B	158	ILE
1	B	191	ARG
1	B	210	ILE
1	B	243	VAL

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Mol	Chain	Res	Type
1	B	247	MET
1	B	258	THR
1	B	265	THR
1	B	271	LEU
1	B	292	MET
1	B	365	VAL
1	B	376	LEU
1	B	387	THR
1	B	438	ILE
1	B	439	LYS
1	B	441	ASN
1	B	442	PHE
1	B	443	LYS
1	B	444	ILE
1	B	445	ARG
1	B	506	ILE
1	B	508	LEU
1	B	510	MET
1	C	25	VAL
1	C	28	ASP
1	C	39	SER
1	C	68	THR
1	C	83	ASP
1	C	129	ARG
1	C	130	ILE
1	C	214	LEU
1	C	216	ARG
1	C	257	ASN
1	C	282	LYS
1	C	285	ASN
1	C	309	LEU
1	C	352	LEU
1	C	380	SER
1	C	413	LYS
1	C	438	ILE
1	C	510	MET
1	D	25	VAL
1	D	28	ASP
1	D	39	SER
1	D	77	CYS
1	D	83	ASP
1	D	148	LEU

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Mol	Chain	Res	Type
1	D	179	GLN
1	D	194	MET
1	D	216	ARG
1	D	217	ARG
1	D	244	ILE
1	D	249	MET
1	D	250	ASP
1	D	274	ILE
1	D	277	SER
1	D	283	GLU
1	D	285	ASN
1	D	338	ARG
1	D	347	ILE
1	D	361	VAL
1	D	376	LEU
1	D	408	ARG
1	D	438	ILE
1	D	441	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	GLN
1	A	211	ASN
1	A	310	ASN
1	A	447	ASN
1	B	84	HIS
1	B	146	HIS
1	B	167	GLN
1	B	169	GLN
1	B	267	GLN
1	B	406	HIS
1	B	441	ASN
1	C	169	GLN
1	C	238	ASN
1	C	257	ASN
1	C	447	ASN
1	D	169	GLN
1	D	175	GLN
1	D	186	GLN
1	D	228	HIS
1	D	310	ASN

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Mol	Chain	Res	Type
1	D	441	ASN
1	D	446	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SWG	D	74	1	23,25,26	1.70	5 (21%)	29,35,37	2.34	10 (34%)
1	SWG	C	74	1	23,25,26	1.78	5 (21%)	29,35,37	2.44	9 (31%)
1	SWG	A	74	1	23,25,26	1.62	6 (26%)	29,35,37	2.71	10 (34%)
1	SWG	B	74	1	23,25,26	1.63	6 (26%)	29,35,37	2.51	10 (34%)

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
1	SWG	D	74	1	-	2/10/29/30	0/3/3/3
1	SWG	C	74	1	-	2/10/29/30	0/3/3/3
1	SWG	A	74	1	-	3/10/29/30	0/3/3/3
1	SWG	B	74	1	-	3/10/29/30	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	74	SWG	C1-N3	-4.30	1.30	1.37
1	A	74	SWG	C1-N3	-4.05	1.30	1.37
1	C	74	SWG	CA3-N3	-3.97	1.39	1.47
1	B	74	SWG	C1-N3	-3.93	1.30	1.37
1	D	74	SWG	CA2-C2	-3.72	1.44	1.48
1	D	74	SWG	C1-N3	-3.67	1.31	1.37
1	B	74	SWG	CA3-N3	-3.64	1.40	1.47
1	D	74	SWG	CA3-N3	-3.48	1.40	1.47
1	A	74	SWG	CA3-N3	-3.31	1.41	1.47
1	C	74	SWG	CA2-C2	-3.28	1.45	1.48
1	B	74	SWG	CA2-C2	-3.03	1.45	1.48
1	A	74	SWG	CA2-C2	-2.91	1.45	1.48
1	C	74	SWG	C2-N3	-2.60	1.34	1.40
1	D	74	SWG	C2-N3	-2.48	1.34	1.40
1	C	74	SWG	CD2-CE2	-2.48	1.38	1.41
1	D	74	SWG	CD2-CE2	-2.46	1.38	1.41
1	A	74	SWG	CD2-CE2	-2.39	1.38	1.41
1	B	74	SWG	C2-N3	-2.32	1.34	1.40
1	A	74	SWG	C2-N3	-2.30	1.34	1.40
1	B	74	SWG	CD2-CE2	-2.22	1.38	1.41
1	A	74	SWG	CB2-CG	2.21	1.50	1.43
1	B	74	SWG	CB2-CG	2.05	1.49	1.43

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	74	SWG	C2-N3-C1	7.12	111.36	108.07
1	C	74	SWG	O3-C3-CA3	-6.74	95.12	125.47
1	D	74	SWG	C2-N3-C1	6.32	110.99	108.07
1	B	74	SWG	O3-C3-CA3	-6.28	97.20	125.47
1	A	74	SWG	CG-CD1-NE1	6.19	113.36	110.20
1	D	74	SWG	O3-C3-CA3	-6.14	97.85	125.47
1	A	74	SWG	O3-C3-CA3	-5.84	99.17	125.47
1	B	74	SWG	C2-N3-C1	5.70	110.70	108.07
1	B	74	SWG	CG-CD1-NE1	4.97	112.74	110.20
1	A	74	SWG	CB2-CA2-C2	4.88	129.03	122.47
1	A	74	SWG	C3-CA3-N3	4.77	123.29	112.43
1	D	74	SWG	C3-CA3-N3	4.14	121.84	112.43
1	A	74	SWG	CE2-NE1-CD1	-4.07	105.45	109.08
1	A	74	SWG	C2-N3-C1	3.92	109.88	108.07
1	B	74	SWG	CB2-CA2-C2	3.79	127.56	122.47
1	A	74	SWG	C2-CA2-N2	-3.72	106.29	108.95
1	A	74	SWG	CD2-CG-CD1	-3.52	104.19	106.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	74	SWG	CG-CD1-NE1	3.51	111.99	110.20
1	B	74	SWG	C3-CA3-N3	3.42	120.22	112.43
1	B	74	SWG	C2-CA2-N2	-3.40	106.52	108.95
1	B	74	SWG	CE2-NE1-CD1	-3.35	106.09	109.08
1	A	74	SWG	CD2-CE2-NE1	3.16	110.16	107.52
1	C	74	SWG	CE2-NE1-CD1	-3.09	106.32	109.08
1	D	74	SWG	CE2-NE1-CD1	-2.88	106.52	109.08
1	D	74	SWG	CD2-CE2-NE1	2.84	109.89	107.52
1	C	74	SWG	CD2-CE2-NE1	2.82	109.87	107.52
1	B	74	SWG	CD2-CE2-NE1	2.82	109.87	107.52
1	C	74	SWG	C2-CA2-N2	-2.78	106.96	108.95
1	D	74	SWG	CZ3-CH2-CZ2	2.70	123.57	120.24
1	C	74	SWG	C3-CA3-N3	2.65	118.47	112.43
1	C	74	SWG	CZ3-CH2-CZ2	2.61	123.46	120.24
1	B	74	SWG	CZ3-CH2-CZ2	2.58	123.42	120.24
1	C	74	SWG	CB2-CA2-C2	2.48	125.80	122.47
1	D	74	SWG	C2-CA2-N2	-2.48	107.17	108.95
1	D	74	SWG	CG-CD1-NE1	2.43	111.44	110.20
1	B	74	SWG	CD2-CG-CD1	-2.37	104.82	106.12
1	D	74	SWG	O2-C2-CA2	-2.14	129.66	131.02
1	A	74	SWG	CA3-N3-C2	2.07	128.21	123.67
1	D	74	SWG	CB2-CA2-N2	2.01	128.82	124.60

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	74	SWG	C1-CA1-CB1-OG1
1	A	74	SWG	N1-CA1-CB1-OG1
1	B	74	SWG	C1-CA1-CB1-OG1
1	B	74	SWG	N1-CA1-CB1-OG1
1	C	74	SWG	C1-CA1-CB1-OG1
1	C	74	SWG	N1-CA1-CB1-OG1
1	D	74	SWG	C3-CA3-N3-C2
1	D	74	SWG	N1-CA1-CB1-OG1
1	A	74	SWG	C3-CA3-N3-C2
1	B	74	SWG	C3-CA3-N3-C2

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	74	SWG	2	0
1	C	74	SWG	2	0
1	A	74	SWG	4	0
1	B	74	SWG	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	LAC	B	601	-	4,5,5	0.98	0	2,6,6	0.48	0
3	LAC	C	601	-	4,5,5	1.01	0	2,6,6	0.50	0
2	GOL	B	602	-	5,5,5	0.10	0	5,5,5	0.30	0
2	GOL	A	601	-	5,5,5	0.09	0	5,5,5	0.26	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	LAC	B	601	-	-	4/4/4/4	-
3	LAC	C	601	-	-	0/4/4/4	-
2	GOL	B	602	-	-	3/4/4/4	-
2	GOL	A	601	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

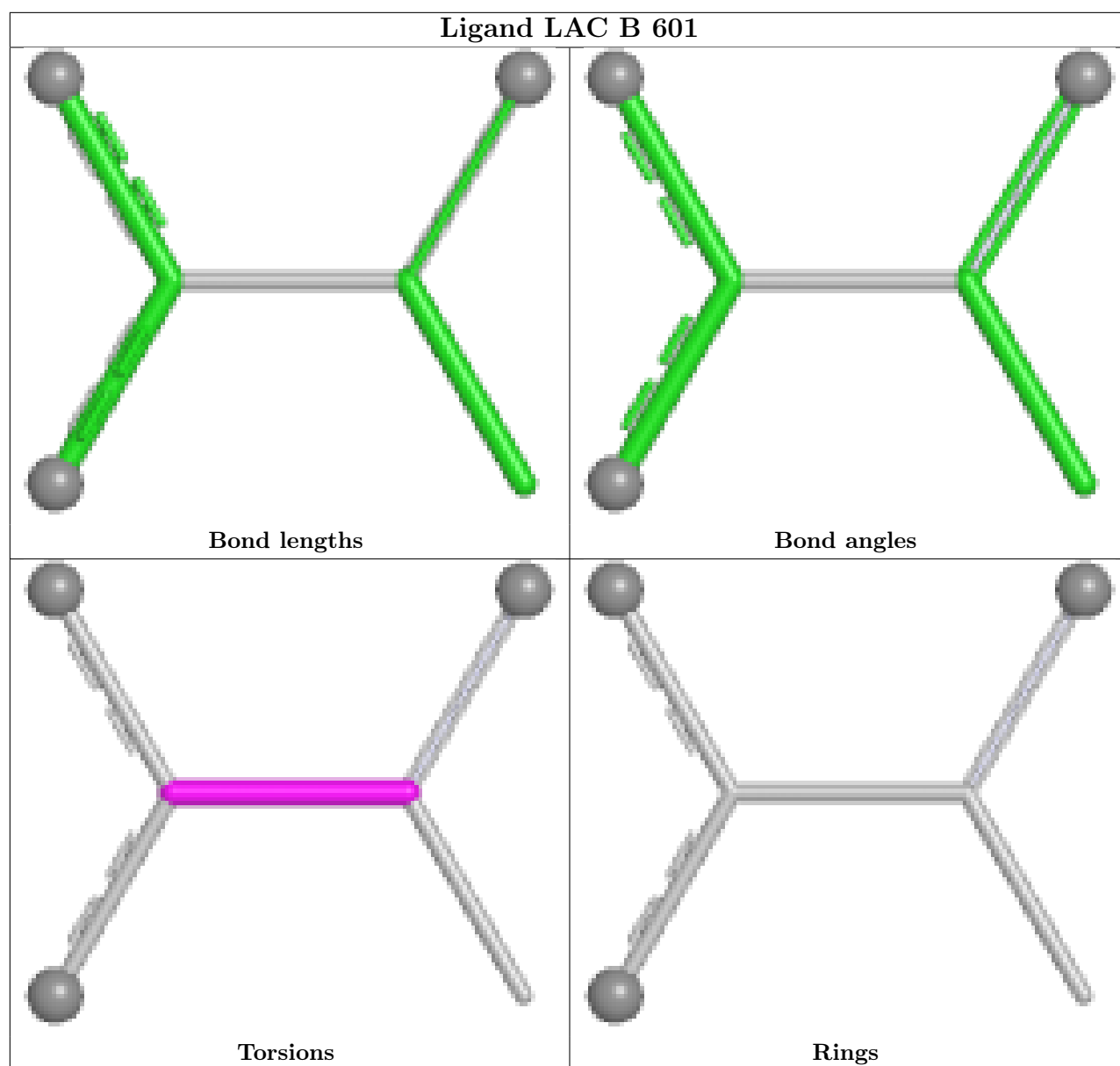
All (7) torsion outliers are listed below:

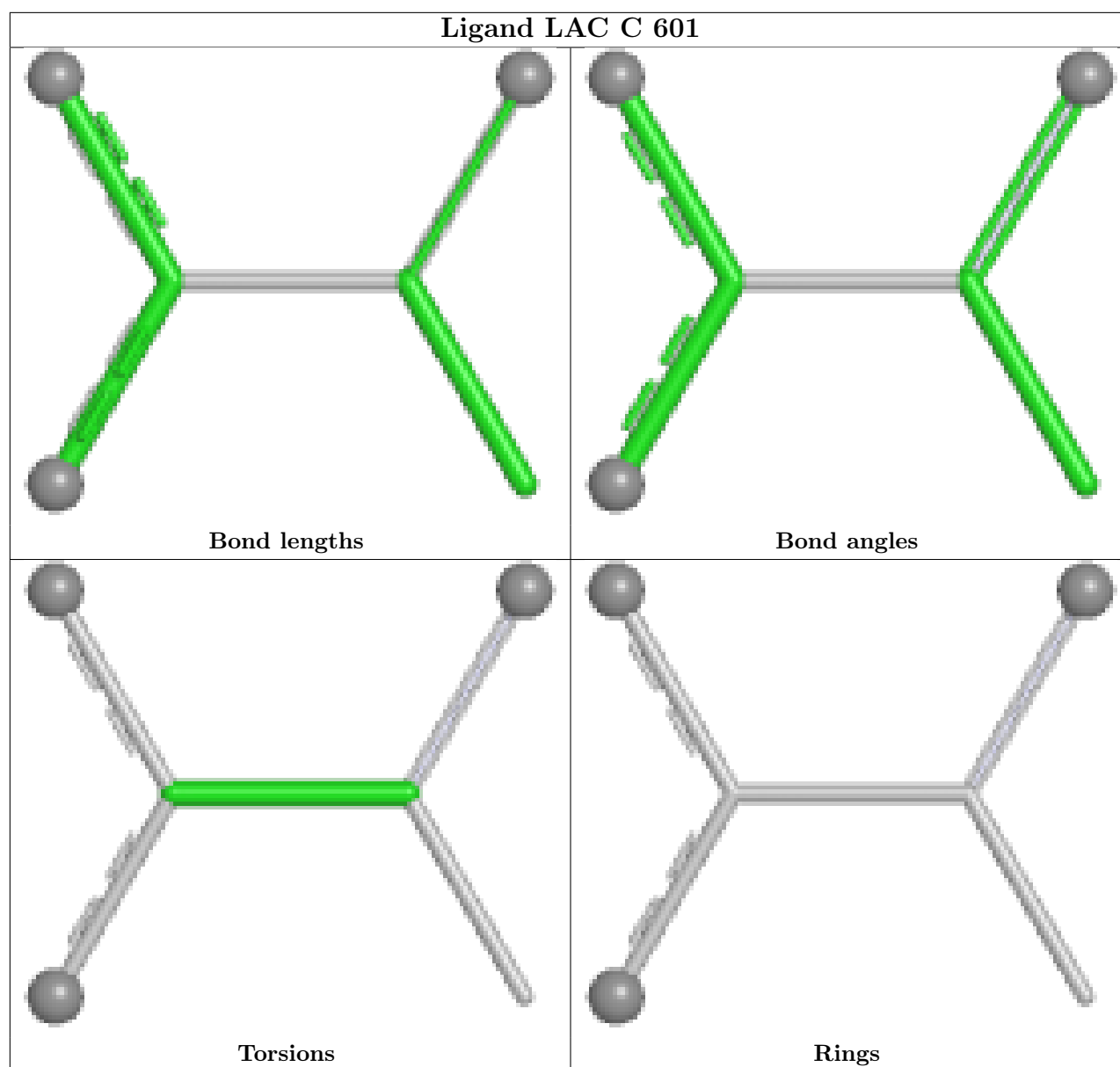
Mol	Chain	Res	Type	Atoms
3	B	601	LAC	O-C-CA-CB
3	B	601	LAC	O-C-CA-OHN
3	B	601	LAC	OXT-C-CA-CB
2	B	602	GOL	O1-C1-C2-C3
2	B	602	GOL	C1-C2-C3-O3
2	B	602	GOL	O2-C2-C3-O3
3	B	601	LAC	OXT-C-CA-OHN

There are no ring outliers.

No monomer is involved in short contacts.

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	485/515 (94%)	0.46	28 (5%)	29	24	32, 49, 82, 108	0
1	B	493/515 (95%)	0.54	26 (5%)	32	26	33, 52, 90, 104	0
1	C	480/515 (93%)	0.59	24 (5%)	34	28	36, 55, 84, 93	0
1	D	461/515 (89%)	0.83	46 (9%)	12	10	36, 58, 94, 109	0
All	All	1919/2060 (93%)	0.60	124 (6%)	25	20	32, 53, 87, 109	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	514	TYR	4.7
1	B	382	SER	4.2
1	A	513	LEU	3.8
1	D	308	ALA	3.8
1	C	305	ALA	3.8
1	D	399	GLU	3.8
1	A	208	SER	3.7
1	B	398	GLU	3.6
1	D	251	SER	3.5
1	A	307	GLY	3.5
1	D	244	ILE	3.4
1	D	510	MET	3.4
1	C	233	SER	3.3
1	D	233	SER	3.3
1	A	305	ALA	3.3
1	A	204	SER	3.3
1	D	192	ILE	3.3
1	A	514	TYR	3.2
1	D	210	ILE	3.2
1	B	265	THR	3.1
1	D	312	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	344	ASN	3.1
1	D	141	GLY	3.1
1	C	400	LYS	3.1
1	D	237	THR	3.1
1	D	254	ALA	3.1
1	A	240	ASN	3.0
1	D	278	ASP	3.0
1	A	507	THR	3.0
1	B	259	THR	3.0
1	D	286	GLY	2.9
1	A	209	ALA	2.9
1	C	472	LEU	2.9
1	D	209	ALA	2.9
1	A	141	GLY	2.8
1	D	340	LEU	2.8
1	A	510	MET	2.8
1	D	279	PRO	2.8
1	B	411	ILE	2.8
1	D	288	LYS	2.8
1	D	369	ASN	2.8
1	C	298	LEU	2.8
1	C	468	GLY	2.8
1	D	289	ILE	2.7
1	A	384	ASN	2.7
1	C	283	GLU	2.7
1	B	207	ASN	2.7
1	D	513	LEU	2.7
1	C	383	GLY	2.7
1	B	237	THR	2.7
1	D	336	ASP	2.7
1	D	240	ASN	2.6
1	B	263	ASN	2.6
1	D	347	ILE	2.6
1	B	508	LEU	2.6
1	D	349	ASP	2.5
1	B	383	GLY	2.5
1	C	235	ILE	2.5
1	A	271	LEU	2.5
1	B	397	PHE	2.5
1	B	250	ASP	2.5
1	B	298	LEU	2.5
1	C	205	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	407	TRP	2.5
1	B	264	MET	2.5
1	D	275	THR	2.4
1	A	302	ASN	2.4
1	B	381	LEU	2.4
1	C	430	THR	2.4
1	D	309	LEU	2.4
1	D	208	SER	2.4
1	A	187	GLY	2.4
1	D	188	ILE	2.4
1	C	296	LEU	2.3
1	A	268	ILE	2.3
1	D	294	ILE	2.3
1	D	247	MET	2.3
1	B	236	TYR	2.3
1	C	239	ASN	2.3
1	A	205	ASP	2.3
1	A	511	ASP	2.3
1	A	308	ALA	2.3
1	B	240	ASN	2.3
1	B	404	GLY	2.3
1	D	284	VAL	2.3
1	D	62	LEU	2.3
1	C	240	ASN	2.3
1	D	257	ASN	2.3
1	A	398	GLU	2.2
1	A	90	PHE	2.2
1	A	406	HIS	2.2
1	B	306	ILE	2.2
1	C	397	PHE	2.2
1	B	266	ASN	2.2
1	C	307	GLY	2.2
1	C	364	ALA	2.2
1	D	295	THR	2.2
1	D	385	THR	2.2
1	C	207	ASN	2.2
1	B	297	PRO	2.2
1	C	297	PRO	2.2
1	C	459	TYR	2.2
1	D	335	LYS	2.2
1	D	231	LEU	2.2
1	A	382	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	142	ASN	2.1
1	B	467	ASP	2.1
1	D	234	ALA	2.1
1	A	297	PRO	2.1
1	D	236	TYR	2.1
1	C	306	ILE	2.1
1	D	321	ASP	2.1
1	D	311	PHE	2.1
1	B	206	GLU	2.1
1	B	258	THR	2.1
1	A	301	LYS	2.1
1	C	153	SER	2.1
1	D	339	LEU	2.1
1	C	361	VAL	2.1
1	B	205	ASP	2.0
1	A	257	ASN	2.0
1	A	300	GLY	2.0
1	A	509	GLY	2.0
1	C	513	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SWG	D	74	23/24	0.85	0.14	40,47,54,61	0
1	SWG	C	74	23/24	0.89	0.14	34,44,49,56	0
1	SWG	B	74	23/24	0.89	0.13	36,43,51,54	0
1	SWG	A	74	23/24	0.91	0.11	33,39,44,47	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

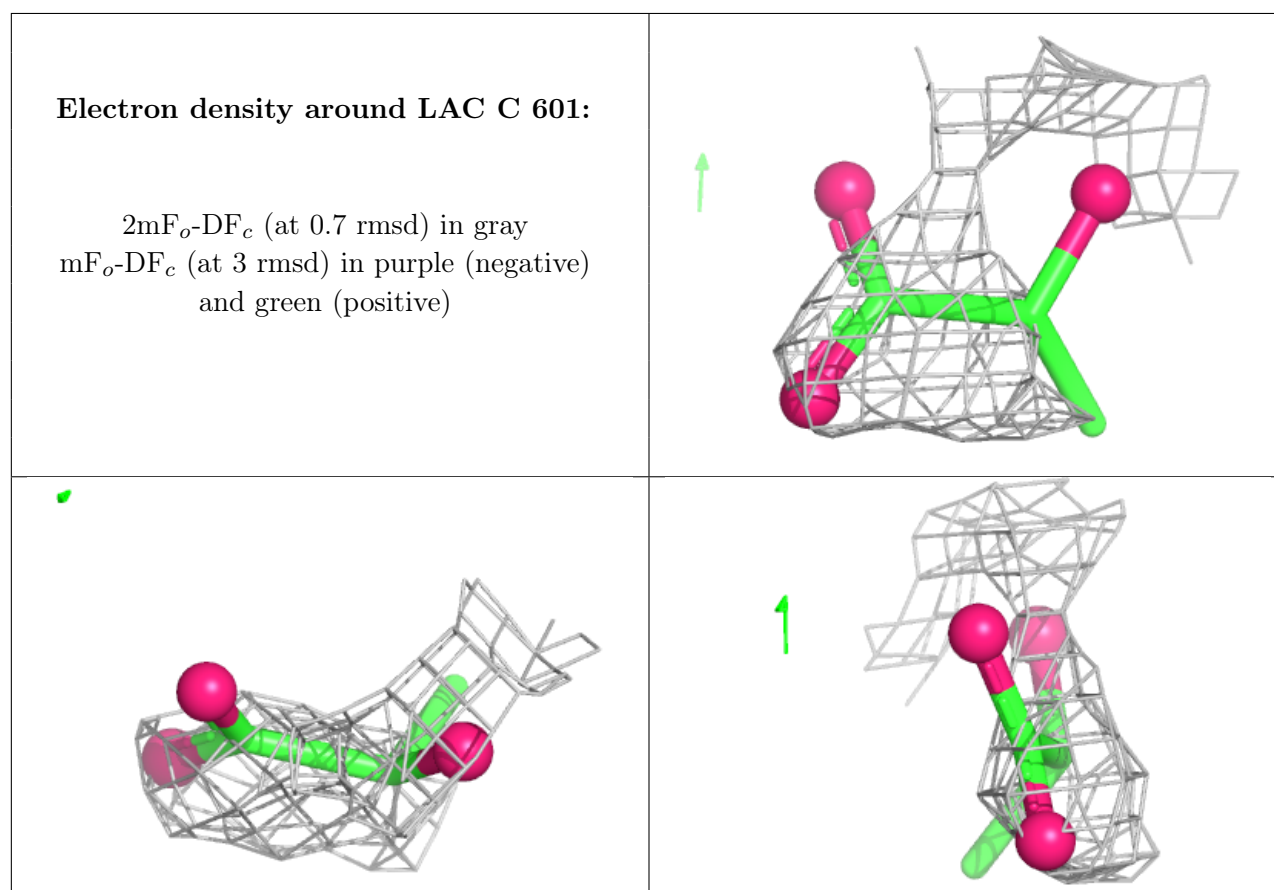
6.4 Ligands [i](#)

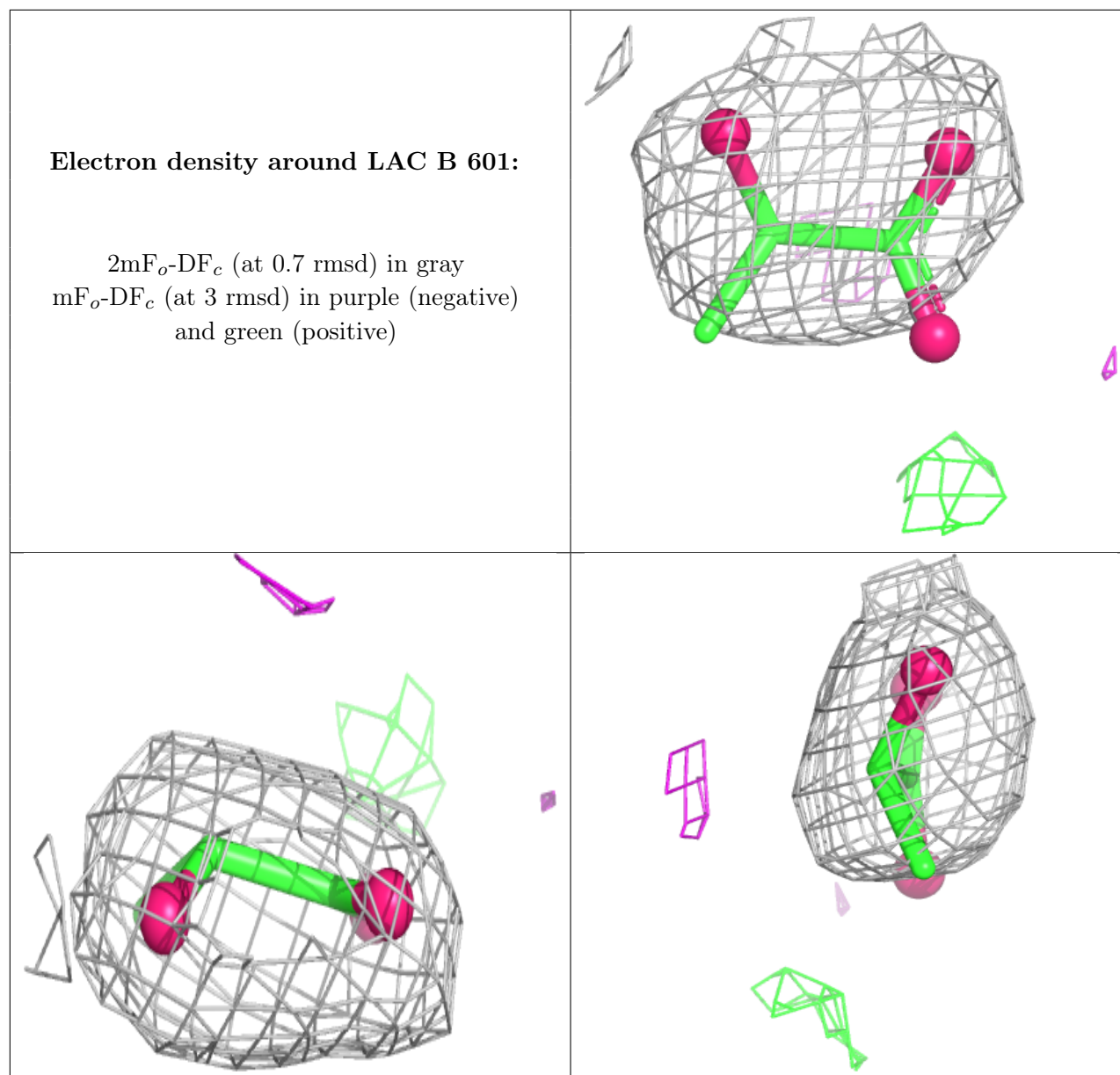
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	LAC	C	601	6/6	0.77	0.22	83,89,95,107	0
2	GOL	B	602	6/6	0.80	0.16	63,77,81,87	0
2	GOL	A	601	6/6	0.86	0.16	64,69,75,75	0
3	LAC	B	601	6/6	0.92	0.13	61,66,74,81	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 ⓘ

There are no such residues in this entry.