



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:02 pm BST

PDB ID : 4QAF  
Title : Crystal structure of an engineered lipocalin (Anticalin) in complex with VEGF(8-109)  
Authors : Giese, T.; Skerra, A.  
Deposited on : 2014-05-04  
Resolution : 1.80 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

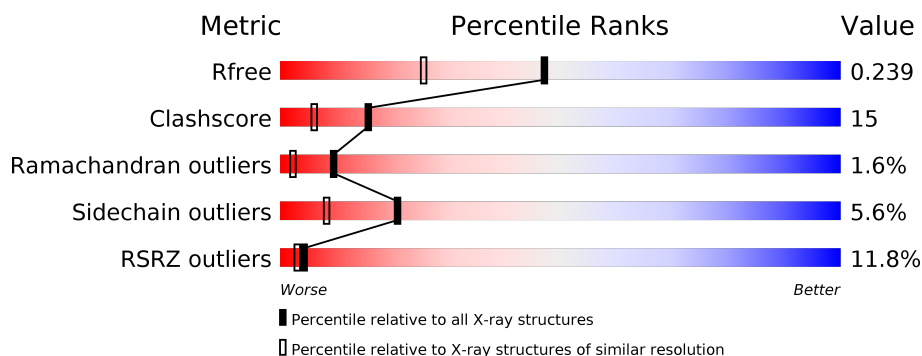
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	152	<div> <div>11%</div> <div> <div></div> <div>52%</div> <div>18%</div> <div>..</div> <div>28%</div> </div> </div>
1	B	152	<div> <div>15%</div> <div> <div></div> <div>41%</div> <div>15%</div> <div>.</div> <div>41%</div> </div> </div>
2	C	112	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>21%</div> <div>.</div> <div>14%</div> </div> </div>
2	D	112	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>11%</div> <div>.</div> <div>15%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OMA	B	201	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3326 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 Lipocalin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	0	0	0
			819	523	138	154	4			
1	B	89	Total	C	N	O	S	0	0	0
			660	427	107	123	3			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	VAL	ARG	ENGINEERED MUTATION	UNP P31025
A	27	GLY	GLU	ENGINEERED MUTATION	UNP P31025
A	28	ALA	PHE	ENGINEERED MUTATION	UNP P31025
A	29	LEU	PRO	ENGINEERED MUTATION	UNP P31025
A	30	ARG	GLU	ENGINEERED MUTATION	UNP P31025
A	31	CYS	MET	ENGINEERED MUTATION	UNP P31025
A	32	LEU	ASN	ENGINEERED MUTATION	UNP P31025
A	33	ALA	LEU	ENGINEERED MUTATION	UNP P31025
A	34	GLY	GLU	ENGINEERED MUTATION	UNP P31025
A	37	ILE	THR	ENGINEERED MUTATION	UNP P31025
A	39	THR	MET	ENGINEERED MUTATION	UNP P31025
A	56	HIS	LEU	ENGINEERED MUTATION	UNP P31025
A	58	LYS	SER	ENGINEERED MUTATION	UNP P31025
A	61	SER	CYS	ENGINEERED MUTATION	UNP P31025
A	69	SER	GLU	ENGINEERED MUTATION	UNP P31025
A	76	ILE	LYS	ENGINEERED MUTATION	UNP P31025
A	80	ILE	ASP	ENGINEERED MUTATION	UNP P31025
A	83	ILE	LYS	ENGINEERED MUTATION	UNP P31025
A	87	LYS	TYR	ENGINEERED MUTATION	UNP P31025
A	89	GLY	ILE	ENGINEERED MUTATION	UNP P31025
A	101	SER	CYS	ENGINEERED MUTATION	UNP P31025
A	104	CYS	GLU	ENGINEERED MUTATION	UNP P31025
A	106	SER	HIS	ENGINEERED MUTATION	UNP P31025
A	108	VAL	LYS	ENGINEERED MUTATION	UNP P31025
A	111	PRO	ARG	ENGINEERED MUTATION	UNP P31025

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Chain	Residue	Modelled	Actual	Comment	Reference
A	114	TRP	LYS	ENGINEERED MUTATION	UNP P31025
A	153	SER	CYS	ENGINEERED MUTATION	UNP P31025
B	26	VAL	ARG	ENGINEERED MUTATION	UNP P31025
B	27	GLY	GLU	ENGINEERED MUTATION	UNP P31025
B	28	ALA	PHE	ENGINEERED MUTATION	UNP P31025
B	29	LEU	PRO	ENGINEERED MUTATION	UNP P31025
B	30	ARG	GLU	ENGINEERED MUTATION	UNP P31025
B	31	CYS	MET	ENGINEERED MUTATION	UNP P31025
B	32	LEU	ASN	ENGINEERED MUTATION	UNP P31025
B	33	ALA	LEU	ENGINEERED MUTATION	UNP P31025
B	34	GLY	GLU	ENGINEERED MUTATION	UNP P31025
B	37	ILE	THR	ENGINEERED MUTATION	UNP P31025
B	39	THR	MET	ENGINEERED MUTATION	UNP P31025
B	56	HIS	LEU	ENGINEERED MUTATION	UNP P31025
B	58	LYS	SER	ENGINEERED MUTATION	UNP P31025
B	61	SER	CYS	ENGINEERED MUTATION	UNP P31025
B	69	SER	GLU	ENGINEERED MUTATION	UNP P31025
B	76	ILE	LYS	ENGINEERED MUTATION	UNP P31025
B	80	ILE	ASP	ENGINEERED MUTATION	UNP P31025
B	83	ILE	LYS	ENGINEERED MUTATION	UNP P31025
B	87	LYS	TYR	ENGINEERED MUTATION	UNP P31025
B	89	GLY	ILE	ENGINEERED MUTATION	UNP P31025
B	101	SER	CYS	ENGINEERED MUTATION	UNP P31025
B	104	CYS	GLU	ENGINEERED MUTATION	UNP P31025
B	106	SER	HIS	ENGINEERED MUTATION	UNP P31025
B	108	VAL	LYS	ENGINEERED MUTATION	UNP P31025
B	111	PRO	ARG	ENGINEERED MUTATION	UNP P31025
B	114	TRP	LYS	ENGINEERED MUTATION	UNP P31025
B	153	SER	CYS	ENGINEERED MUTATION	UNP P31025

- Molecule 2 is a protein called Vascular endothelial growth factor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	96	Total	C	N	O	S	0	3	0
			795	500	131	150	14			
2	D	95	Total	C	N	O	S	0	2	0
			781	490	131	146	14			

There are 20 discrepancies between the modelled and reference sequences:

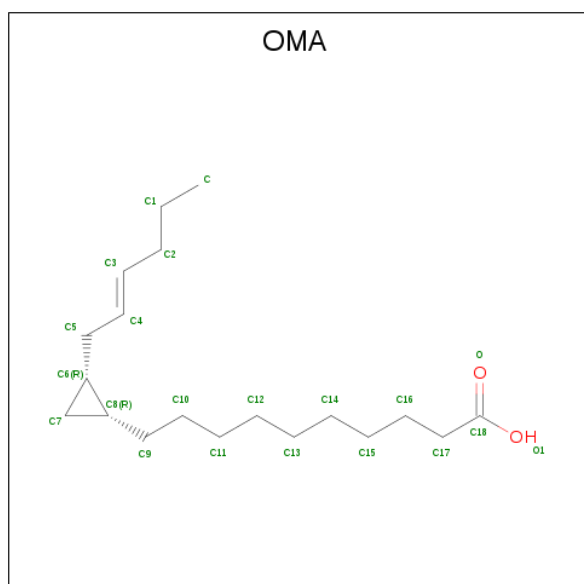
Chain	Residue	Modelled	Actual	Comment	Reference
C	110	SER	-	EXPRESSION TAG	UNP P15692

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Chain	Residue	Modelled	Actual	Comment	Reference
C	111	ALA	-	EXPRESSION TAG	UNP P15692
C	112	TRP	-	EXPRESSION TAG	UNP P15692
C	113	SER	-	EXPRESSION TAG	UNP P15692
C	114	HIS	-	EXPRESSION TAG	UNP P15692
C	115	PRO	-	EXPRESSION TAG	UNP P15692
C	116	GLN	-	EXPRESSION TAG	UNP P15692
C	117	PHE	-	EXPRESSION TAG	UNP P15692
C	118	GLU	-	EXPRESSION TAG	UNP P15692
C	119	LYS	-	EXPRESSION TAG	UNP P15692
D	110	SER	-	EXPRESSION TAG	UNP P15692
D	111	ALA	-	EXPRESSION TAG	UNP P15692
D	112	TRP	-	EXPRESSION TAG	UNP P15692
D	113	SER	-	EXPRESSION TAG	UNP P15692
D	114	HIS	-	EXPRESSION TAG	UNP P15692
D	115	PRO	-	EXPRESSION TAG	UNP P15692
D	116	GLN	-	EXPRESSION TAG	UNP P15692
D	117	PHE	-	EXPRESSION TAG	UNP P15692
D	118	GLU	-	EXPRESSION TAG	UNP P15692
D	119	LYS	-	EXPRESSION TAG	UNP P15692

- Molecule 3 is 10-[(1R,2R)-2-[(2E)-hex-2-en-1-yl]cyclopropyl]decanoic acid (three-letter code: OMA) (formula: C<sub>19</sub>H<sub>34</sub>O<sub>2</sub>).



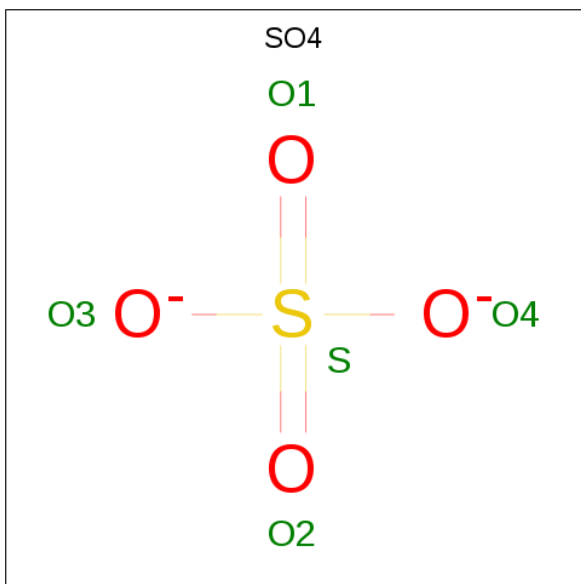
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	19	2		

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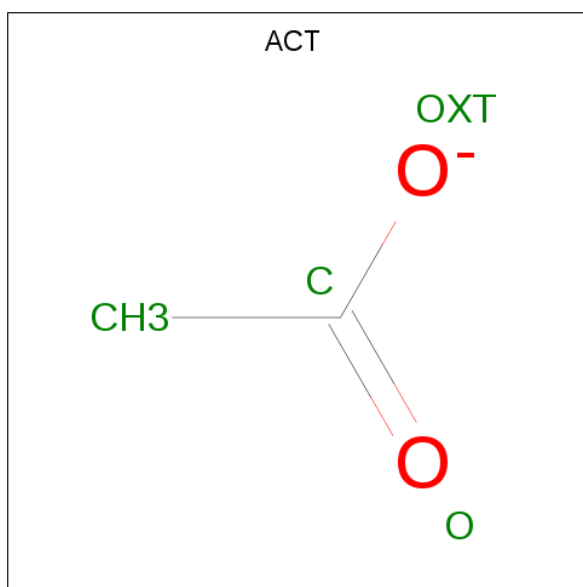
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			21	19	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

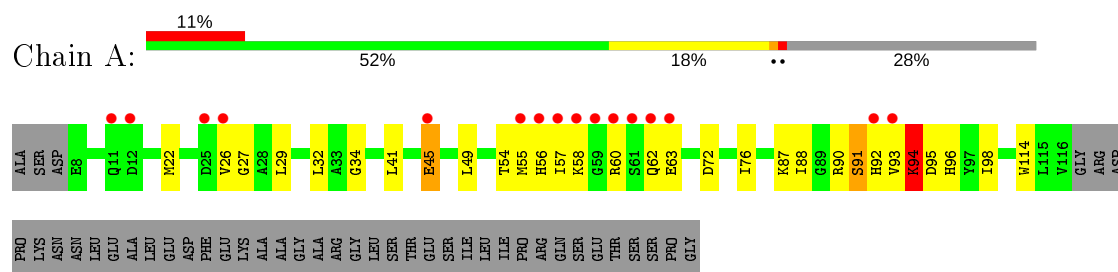
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	43	Total	O	0	0
			43	43		
6	C	75	Total	O	0	0
			75	75		
6	D	74	Total	O	0	0
			74	74		
6	B	18	Total	O	0	0
			18	18		

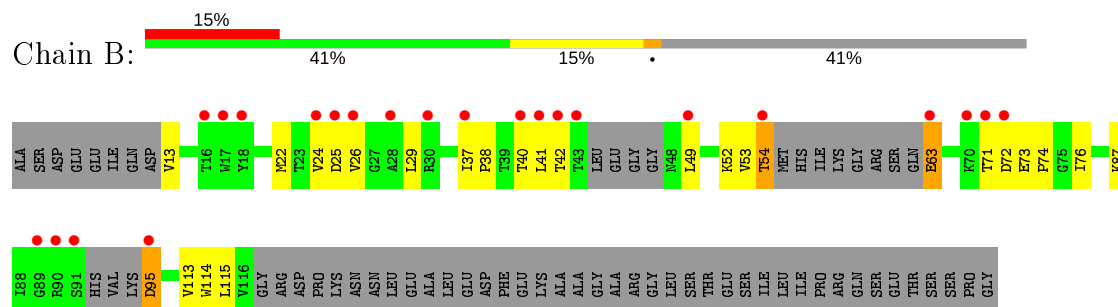
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

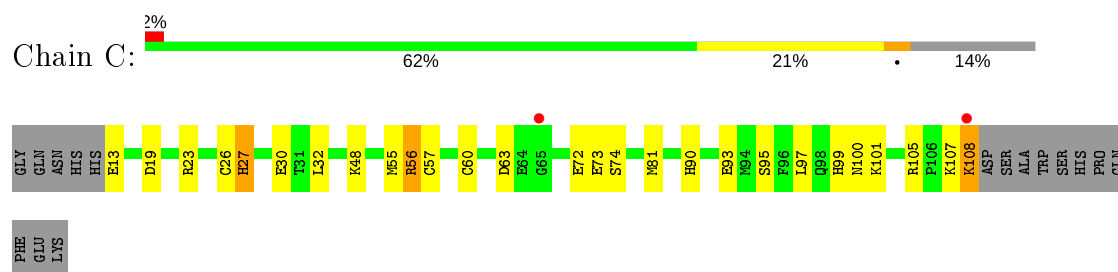
#### • Molecule 1: Lipocalin-1



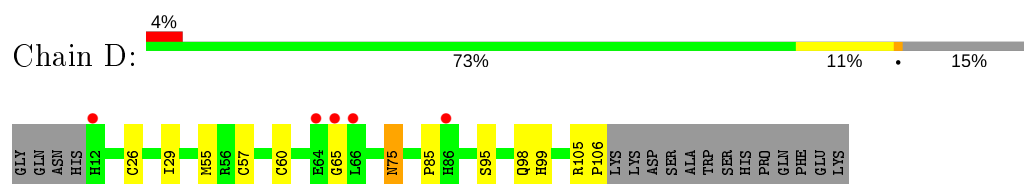
#### • Molecule 1: Lipocalin-1



#### • Molecule 2: Vascular endothelial growth factor A



#### • Molecule 2: Vascular endothelial growth factor A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.21Å 88.21Å 103.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.47 – 1.80 34.47 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.47-1.80) 99.9 (34.47-1.80)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.55 (at 1.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.203 , 0.242 0.201 , 0.239	Depositor DCC
$R_{free}$ test set	2195 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.1	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 57.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3326	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: OMA, SO4, ACT

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	1.00	1/835 (0.1%)	1.05	1/1134 (0.1%)
1	B	0.85	1/671 (0.1%)	0.94	0/912
2	C	1.17	2/822 (0.2%)	1.14	4/1106 (0.4%)
2	D	1.16	0/806	1.17	2/1087 (0.2%)
All	All	1.06	4/3134 (0.1%)	1.08	7/4239 (0.2%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	114	TRP	CD2-CE2	6.71	1.49	1.41
2	C	95	SER	CB-OG	-5.69	1.34	1.42
1	A	114	TRP	CD2-CE2	5.64	1.48	1.41
2	C	27	HIS	CG-CD2	5.50	1.45	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	56	ARG	NE-CZ-NH1	-6.41	117.09	120.30
2	C	23	ARG	NE-CZ-NH2	-6.25	117.17	120.30
2	C	56	ARG	NE-CZ-NH2	5.64	123.12	120.30
2	C	23	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	D	75[A]	ASN	CB-CA-C	5.42	121.24	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	75[B]	ASN	CB-CA-C	5.42	121.24	110.40
1	A	72	ASP	CB-CG-OD2	-5.20	113.62	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	LYS	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	819	0	832	28	1
1	B	660	0	673	28	0
2	C	795	0	764	21	1
2	D	781	0	741	14	1
3	A	21	0	33	8	0
3	B	21	0	33	9	0
4	C	10	0	0	0	0
4	D	5	0	0	0	0
5	D	4	0	3	1	0
6	A	43	0	0	5	0
6	B	18	0	0	0	0
6	C	75	0	0	3	0
6	D	74	0	0	2	0
All	All	3326	0	3079	91	2

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 15.

All (91) 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)
2:C:19[B]:ASP:OD2	6:C:332:HOH:O	1.82	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:201:OMA:C7	3:A:201:OMA:H14	1.96	0.96
1:B:24:VAL:HG11	3:B:201:OMA:H17	1.50	0.94
2:C:57:CYS:H	2:C:99:HIS:HD2	1.09	0.93
1:B:54:THR:HG22	1:B:63:GLU:HB2	1.50	0.91
1:A:54:THR:HG22	1:A:63:GLU:HB3	1.53	0.90
2:D:57:CYS:H	2:D:99:HIS:HD2	1.25	0.84
1:A:92:HIS:HB2	6:A:336:HOH:O	1.78	0.83
2:C:57:CYS:H	2:C:99:HIS:CD2	1.95	0.82
1:B:115:LEU:CD1	3:B:201:OMA:H15	2.10	0.82
1:B:13:VAL:HG21	1:B:41:LEU:HD21	1.67	0.76
2:D:75[B]:ASN:OD1	6:D:351:HOH:O	2.03	0.75
2:C:99:HIS:HE1	6:C:314:HOH:O	1.70	0.74
1:B:40:THR:HG22	1:B:52:LYS:HB2	1.70	0.73
1:A:93:VAL:HG13	1:A:94:LYS:HG2	1.72	0.72
3:A:201:OMA:C11	3:A:201:OMA:C7	2.62	0.71
1:B:115:LEU:HD13	3:B:201:OMA:H15	1.72	0.70
2:C:107:LYS:O	2:C:108:LYS:HB3	1.92	0.70
1:B:40:THR:HG22	1:B:52:LYS:CB	2.26	0.65
2:D:75[B]:ASN:OD1	2:D:95:SER:OG	2.14	0.65
1:B:22:MET:HG3	1:B:24:VAL:HG13	1.79	0.65
2:D:57:CYS:H	2:D:99:HIS:CD2	2.12	0.64
1:A:90:ARG:HG3	6:A:335:HOH:O	1.97	0.64
1:B:115:LEU:HD11	3:B:201:OMA:H15	1.79	0.63
2:C:72:GLU:HG2	2:C:100:ASN:HD22	1.64	0.63
1:A:22:MET:SD	3:A:201:OMA:H12	2.39	0.62
2:C:32:LEU:CD2	2:D:29:ILE:HD13	2.30	0.62
2:D:55[B]:MET:H	2:D:98:GLN:HE21	1.49	0.61
1:B:73:GLU:HG3	1:B:76:ILE:CG2	2.30	0.61
1:B:73:GLU:O	1:B:76:ILE:HG22	2.00	0.61
1:A:93:VAL:HG12	6:A:336:HOH:O	2.01	0.61
1:A:92:HIS:HB3	2:C:101:LYS:CE	2.31	0.60
2:C:30[B]:GLU:CD	6:C:349:HOH:O	2.40	0.59
1:B:13:VAL:HG21	1:B:41:LEU:CD2	2.33	0.59
2:C:32:LEU:HD23	2:D:29:ILE:HD13	1.85	0.58
2:D:55[A]:MET:H	2:D:98:GLN:HE21	1.49	0.58
1:A:88:ILE:HD12	1:A:96:HIS:CD2	2.39	0.58
2:C:30[A]:GLU:HG2	2:C:55[A]:MET:SD	2.43	0.58
1:B:38:PRO:HD2	1:B:95:ASP:OD2	2.04	0.58
1:B:73:GLU:HG3	1:B:76:ILE:HG21	1.85	0.57
1:B:24:VAL:HG21	3:B:201:OMA:H13	1.86	0.57
1:A:95:ASP:OD1	1:A:95:ASP:N	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:VAL:O	1:A:94:LYS:HB2	2.05	0.56
2:D:55[B]:MET:H	2:D:98:GLN:NE2	2.05	0.55
2:D:55[A]:MET:H	2:D:98:GLN:NE2	2.05	0.55
1:B:22:MET:CG	1:B:24:VAL:HG13	2.37	0.55
1:A:54:THR:HG22	1:A:63:GLU:CB	2.30	0.54
2:C:107:LYS:O	2:C:108:LYS:CB	2.55	0.54
1:A:57:ILE:HD12	1:A:62:GLN:HB3	1.90	0.53
1:A:92:HIS:HB3	2:C:101:LYS:HE2	1.90	0.53
1:A:55:MET:O	1:A:62:GLN:N	2.37	0.53
2:D:85:PRO:HA	5:D:202:ACT:H2	1.90	0.53
1:B:40:THR:CG2	1:B:52:LYS:HB2	2.37	0.52
2:D:75[A]:ASN:ND2	6:D:351:HOH:O	2.40	0.52
1:B:113:VAL:HG11	3:B:201:OMA:H3	1.91	0.52
1:A:55:MET:HB3	6:A:339:HOH:O	2.11	0.51
1:A:90:ARG:HD2	2:C:27:HIS:CB	2.41	0.51
1:A:93:VAL:O	1:A:94:LYS:CB	2.59	0.50
2:C:73:GLU:HB3	2:C:97:LEU:HD11	1.93	0.50
3:A:201:OMA:C7	3:A:201:OMA:H27	2.39	0.49
1:A:41:LEU:CD1	1:A:49:LEU:HD11	2.43	0.47
2:C:32:LEU:HD22	2:C:32:LEU:N	2.29	0.47
1:A:91:SER:O	1:A:92:HIS:CD2	2.67	0.47
1:A:94:LYS:HB2	6:A:337:HOH:O	2.14	0.47
1:A:87:LYS:HE3	1:A:94:LYS:O	2.15	0.46
2:C:48:LYS:HB2	2:C:81:MET:HB3	1.97	0.46
1:A:34:GLY:O	1:A:98:ILE:HD12	2.14	0.46
2:D:65:GLY:O	2:D:106:PRO:HA	2.16	0.45
2:C:74:SER:HB3	2:C:100:ASN:HD21	1.81	0.45
1:A:93:VAL:HG22	1:A:94:LYS:H	1.81	0.45
1:B:26:VAL:O	1:B:29:LEU:HG	2.17	0.45
1:B:24:VAL:HG11	3:B:201:OMA:C10	2.33	0.44
1:A:45:GLU:CD	1:A:45:GLU:H	2.20	0.44
3:A:201:OMA:C11	3:A:201:OMA:H22	2.47	0.44
2:D:75[B]:ASN:ND2	2:D:95:SER:OG	2.51	0.44
1:A:93:VAL:HG22	1:A:94:LYS:N	2.32	0.43
1:B:41:LEU:HG	1:B:49:LEU:HD11	2.00	0.43
1:A:26:VAL:HG12	1:A:29:LEU:HD12	2.00	0.43
1:B:115:LEU:HD11	3:B:201:OMA:C11	2.47	0.43
3:A:201:OMA:H18	3:A:201:OMA:H24	1.42	0.42
1:A:32:LEU:HD13	3:A:201:OMA:H17	2.01	0.42
1:A:57:ILE:HG12	3:A:201:OMA:O1	2.19	0.42
2:C:56:ARG:HD3	2:C:56:ARG:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:PRO:HA	1:B:53:VAL:HG12	2.02	0.42
2:C:32:LEU:CD2	2:C:32:LEU:N	2.83	0.42
1:B:73:GLU:HA	1:B:74:PRO:HD2	1.94	0.41
1:B:37:ILE:HG23	1:B:95:ASP:O	2.20	0.41
1:B:24:VAL:HB	3:B:201:OMA:H8	2.01	0.41
1:B:40:THR:HG22	1:B:52:LYS:HE2	2.03	0.41
1:B:54:THR:HA	1:B:63:GLU:HA	2.02	0.40
2:C:13:GLU:HG3	2:C:13:GLU:O	2.20	0.40

All (2) 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)
2:C:93:GLU:OE1	2:C:93:GLU:OE1[6_554]	1.76	0.44
1:A:95:ASP:OD2	2:D:75[A]:ASN:ND2[2_664]	2.06	0.14

## 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	107/152 (70%)	97 (91%)	7 (6%)	3 (3%)	5	1
1	B	81/152 (53%)	75 (93%)	6 (7%)	0	100	100
2	C	97/112 (87%)	94 (97%)	1 (1%)	2 (2%)	7	1
2	D	95/112 (85%)	89 (94%)	5 (5%)	1 (1%)	14	4
All	All	380/528 (72%)	355 (93%)	19 (5%)	6 (2%)	9	2

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	LYS

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Mol	Chain	Res	Type
1	A	27	GLY
1	A	58	LYS
2	C	26	CYS
2	D	26	CYS
2	C	63	ASP

### 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	89/123 (72%)	84 (94%)	5 (6%)	21	8
1	B	72/123 (58%)	64 (89%)	8 (11%)	6	1
2	C	94/105 (90%)	90 (96%)	4 (4%)	29	14
2	D	92/105 (88%)	90 (98%)	2 (2%)	52	39
All	All	347/456 (76%)	328 (94%)	19 (6%)	21	8

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	56	HIS
1	A	60	ARG
1	A	76	ILE
1	A	91	SER
2	C	60	CYS
2	C	90	HIS
2	C	105	ARG
2	C	108	LYS
2	D	60	CYS
2	D	105	ARG
1	B	25	ASP
1	B	42	THR
1	B	54	THR
1	B	63	GLU
1	B	71	THR

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Mol	Chain	Res	Type
1	B	72	ASP
1	B	87	LYS
1	B	95	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	84	HIS
1	A	92	HIS
2	C	99	HIS
2	C	100	ASN
2	D	98	GLN
2	D	99	HIS
2	D	100	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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	OMA	B	201	-	18,21,21	0.44	0	17,24,24	2.21	3 (17%)
4	SO4	C	202	-	4,4,4	1.09	1 (25%)	6,6,6	1.00	0
5	ACT	D	202	-	1,3,3	1.68	0	0,3,3	0.00	-
3	OMA	A	201	-	18,21,21	0.56	0	17,24,24	2.04	3 (17%)
4	SO4	D	201	-	4,4,4	0.68	0	6,6,6	0.56	0
4	SO4	C	201	-	4,4,4	0.65	0	6,6,6	0.42	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	OMA	A	201	-	-	9/16/23/23	0/1/1/1
3	OMA	B	201	-	-	10/16/23/23	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	202	SO4	O2-S	2.00	1.56	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	201	OMA	C7-C6-C5	-7.02	107.74	120.55
3	A	201	OMA	C7-C6-C5	-5.44	110.64	120.55
3	A	201	OMA	C6-C5-C4	-4.58	102.87	112.96
3	B	201	OMA	C6-C5-C4	-3.94	104.27	112.96
3	B	201	OMA	C10-C9-C8	-3.12	104.61	115.17
3	A	201	OMA	C5-C4-C3	-2.44	117.33	126.40

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	201	OMA	C15-C16-C17-C18
3	B	201	OMA	C6-C8-C9-C10
3	A	201	OMA	C7-C8-C9-C10
3	A	201	OMA	C11-C10-C9-C8
3	A	201	OMA	C9-C10-C11-C12

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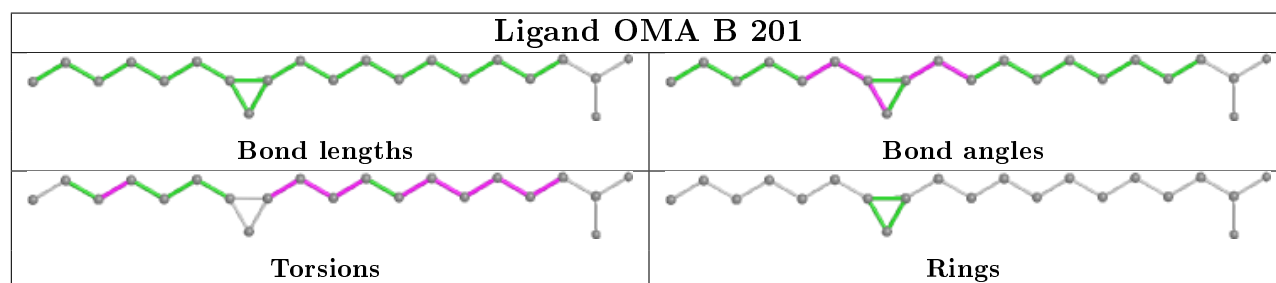
Mol	Chain	Res	Type	Atoms
3	A	201	OMA	C-C1-C2-C3
3	A	201	OMA	C3-C4-C5-C6
3	A	201	OMA	C12-C13-C14-C15
3	B	201	OMA	C13-C14-C15-C16
3	B	201	OMA	C14-C15-C16-C17
3	B	201	OMA	C11-C12-C13-C14
3	A	201	OMA	C11-C12-C13-C14
3	A	201	OMA	C1-C2-C3-C4
3	A	201	OMA	C15-C16-C17-C18
3	B	201	OMA	C9-C10-C11-C12
3	B	201	OMA	C7-C8-C9-C10
3	B	201	OMA	C11-C10-C9-C8
3	B	201	OMA	C1-C2-C3-C4
3	B	201	OMA	C12-C13-C14-C15

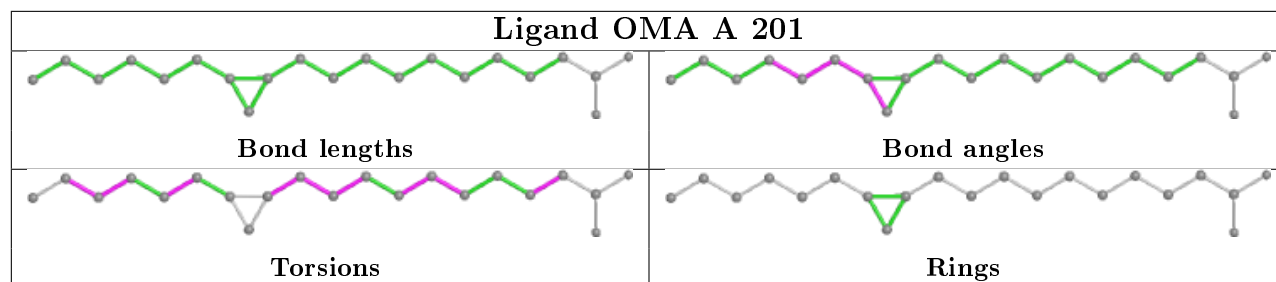
There are no ring outliers.

3 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	201	OMA	9	0
5	D	202	ACT	1	0
3	A	201	OMA	8	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	109/152 (71%)	0.67	16 (14%) <b>2</b> <b>1</b>	15, 26, 81, 107	0
1	B	89/152 (58%)	1.27	23 (25%) <b>0</b> <b>0</b>	26, 47, 78, 95	1 (1%)
2	C	96/112 (85%)	0.06	2 (2%) 63 59	14, 21, 47, 59	0
2	D	95/112 (84%)	0.06	5 (5%) 26 21	11, 21, 49, 76	0
All	All	389/528 (73%)	0.51	46 (11%) <b>4</b> <b>3</b>	11, 26, 72, 107	1 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	57	ILE	11.3
1	A	60	ARG	9.2
1	A	61	SER	8.3
1	A	56	HIS	7.9
1	A	93	VAL	7.4
2	D	65	GLY	6.1
1	B	71	THR	6.1
1	B	90	ARG	5.5
1	A	58	LYS	5.3
1	B	26	VAL	5.1
1	B	16	THR	4.8
1	B	49	LEU	4.7
1	A	59	GLY	4.6
1	B	91	SER	4.4
1	A	92	HIS	4.3
1	B	18	TYR	4.1
1	B	17	TRP	4.1
1	B	41	LEU	3.8
2	D	12	HIS	3.3
1	B	63	GLU	3.3
1	B	89	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	43	THR	3.2
1	A	12	ASP	3.2
1	B	72	ASP	3.1
1	B	95	ASP	3.1
1	B	54	THR	3.1
1	B	28	ALA	3.1
2	D	86	HIS	3.0
1	B	40	THR	2.9
1	B	24	VAL	2.8
1	A	55	MET	2.8
1	A	62	GLN	2.6
2	D	64	GLU	2.6
1	B	42	THR	2.6
1	A	26	VAL	2.6
1	B	70	LYS	2.5
1	A	11	GLN	2.5
1	B	25	ASP	2.4
2	D	66	LEU	2.4
1	A	45	GLU	2.4
1	B	30	ARG	2.3
1	A	63	GLU	2.3
2	C	108	LYS	2.1
2	C	65	GLY	2.1
1	A	25	ASP	2.1
1	B	37	ILE	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 ⓘ

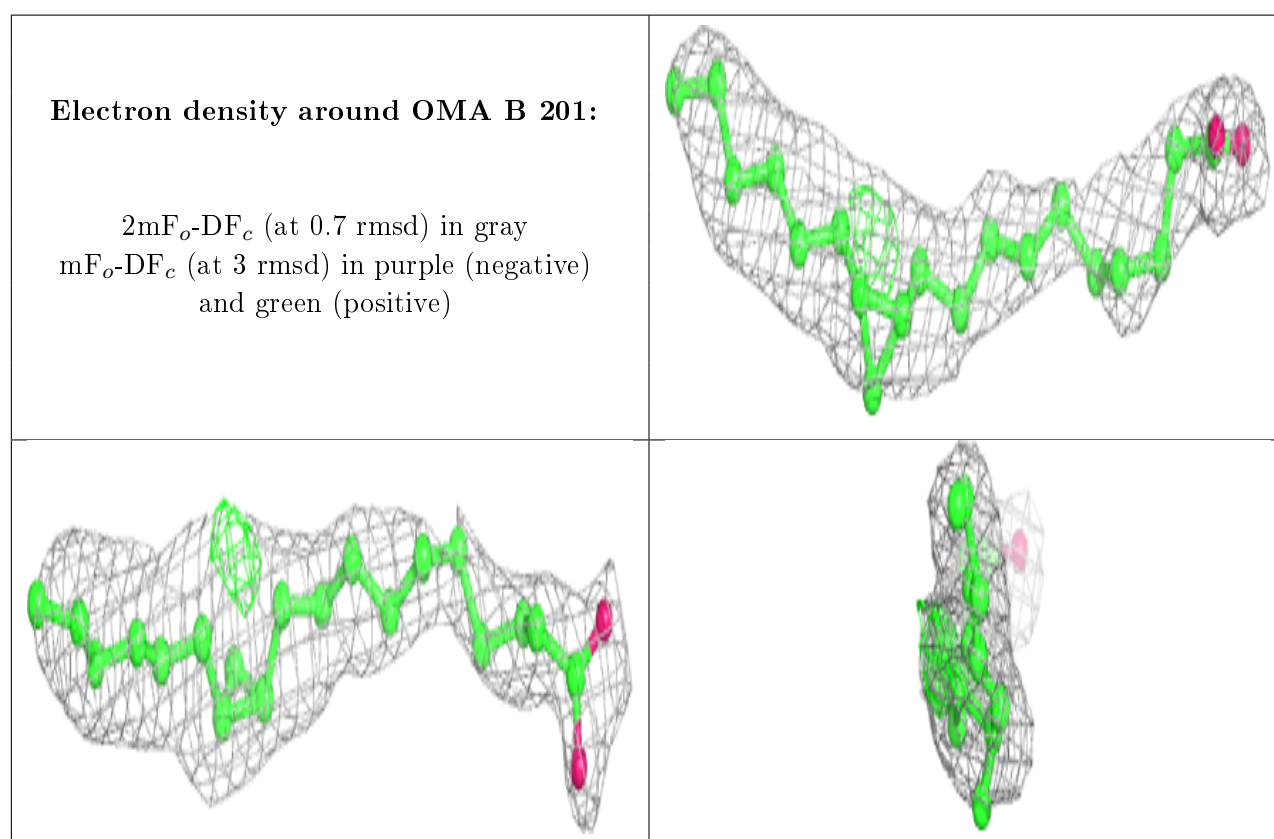
There are no carbohydrates in this entry.

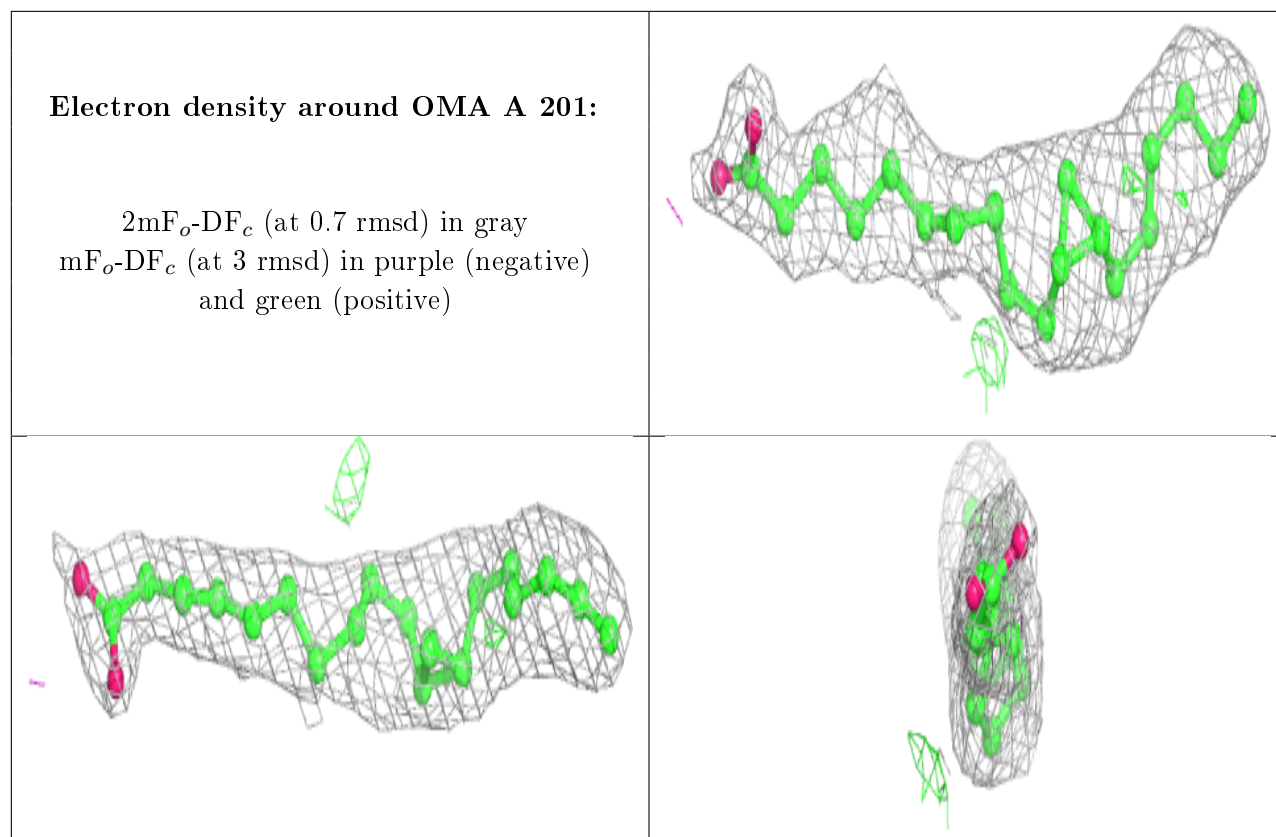
## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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	OMA	B	201	21/21	0.60	0.21	48,61,71,73	0
3	OMA	A	201	21/21	0.61	0.30	35,49,70,74	0
5	ACT	D	202	4/4	0.82	0.24	31,31,40,40	0
4	SO4	C	202	5/5	0.89	0.22	28,44,53,55	0
4	SO4	D	201	5/5	0.99	0.08	17,18,19,19	0
4	SO4	C	201	5/5	0.99	0.11	21,24,29,30	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.