Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 04:08 AM JST

PDB ID	:	6KSM
Title	:	Staphylococcus aureus lipase -Orlistat complex
Authors	:	Kitadokoro, K.; Tanaka, M.; Kamitani, S.
Deposited on	:	2019-08-24
Resolution	:	2.23 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 (i) 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 (i)) were used in the production of this report:

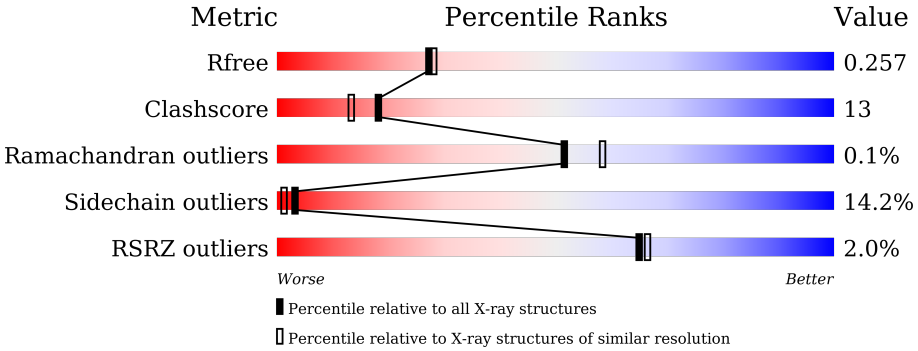
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

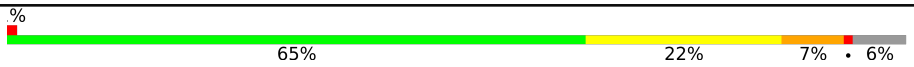
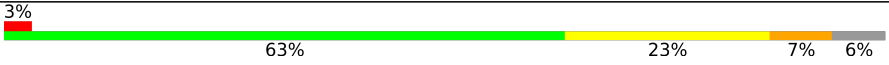
The reported resolution of this entry is 2.23 Å.

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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 <=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	408	
1	B	408	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DAO	A	405	-	-	-	X
7	STE	B	406	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6264 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 Lipase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	382	3020	1924	527	560	9	0	0	0
1	B	382	3020	1924	527	560	9	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP A0A0U1MWF9
A	-12	ASN	-	expression tag	UNP A0A0U1MWF9
A	-11	HIS	-	expression tag	UNP A0A0U1MWF9
A	-10	LYS	-	expression tag	UNP A0A0U1MWF9
A	-9	VAL	-	expression tag	UNP A0A0U1MWF9
A	-8	HIS	-	expression tag	UNP A0A0U1MWF9
A	-7	HIS	-	expression tag	UNP A0A0U1MWF9
A	-6	HIS	-	expression tag	UNP A0A0U1MWF9
A	-5	HIS	-	expression tag	UNP A0A0U1MWF9
A	-4	HIS	-	expression tag	UNP A0A0U1MWF9
A	-3	HIS	-	expression tag	UNP A0A0U1MWF9
A	-2	MET	-	expression tag	UNP A0A0U1MWF9
A	68	GLN	GLU	variant	UNP A0A0U1MWF9
B	-13	MET	-	expression tag	UNP A0A0U1MWF9
B	-12	ASN	-	expression tag	UNP A0A0U1MWF9
B	-11	HIS	-	expression tag	UNP A0A0U1MWF9
B	-10	LYS	-	expression tag	UNP A0A0U1MWF9
B	-9	VAL	-	expression tag	UNP A0A0U1MWF9
B	-8	HIS	-	expression tag	UNP A0A0U1MWF9
B	-7	HIS	-	expression tag	UNP A0A0U1MWF9
B	-6	HIS	-	expression tag	UNP A0A0U1MWF9
B	-5	HIS	-	expression tag	UNP A0A0U1MWF9
B	-4	HIS	-	expression tag	UNP A0A0U1MWF9
B	-3	HIS	-	expression tag	UNP A0A0U1MWF9
B	-2	MET	-	expression tag	UNP A0A0U1MWF9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	68	GLN	GLU	variant	UNP A0A0U1MWF9

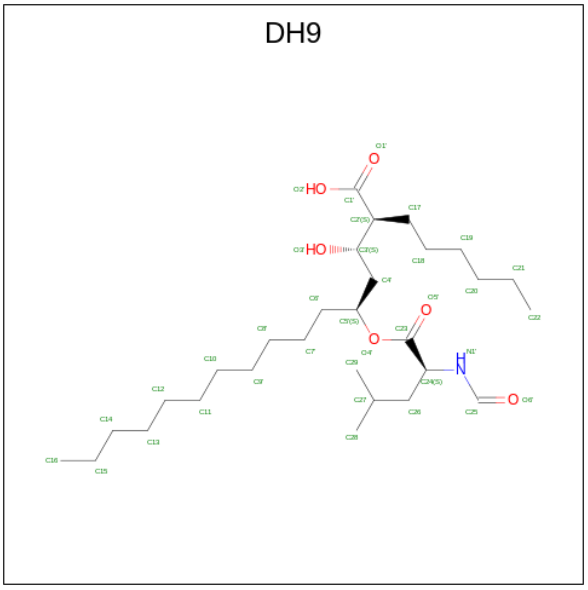
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0
			Total	Zn		
2	B	1	1	1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

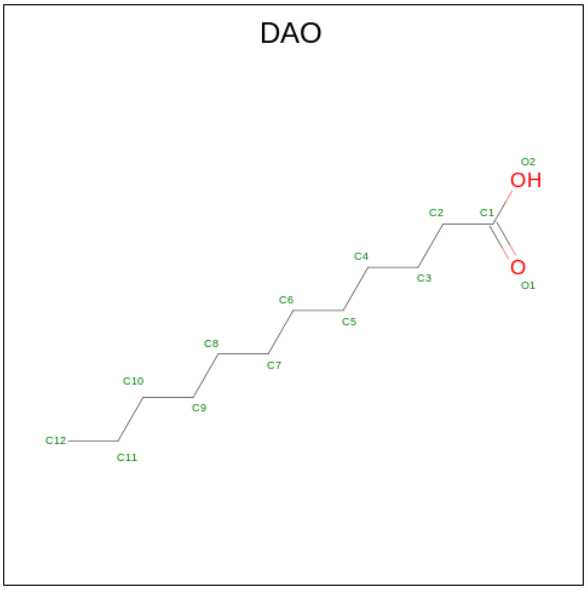
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	1	1	1	0	0
			Total	Ca		
3	B	1	1	1	0	0

- Molecule 4 is (2S,3S,5S)-5-[(N-FORMYL-L-LEUCYL)OXY]-2-HEXYL-3-HYDROXYHEXADECANOIC ACID (three-letter code: DH9) (formula: $C_{29}H_{55}NO_6$) (labeled as "Ligand of Interest" by depositor).



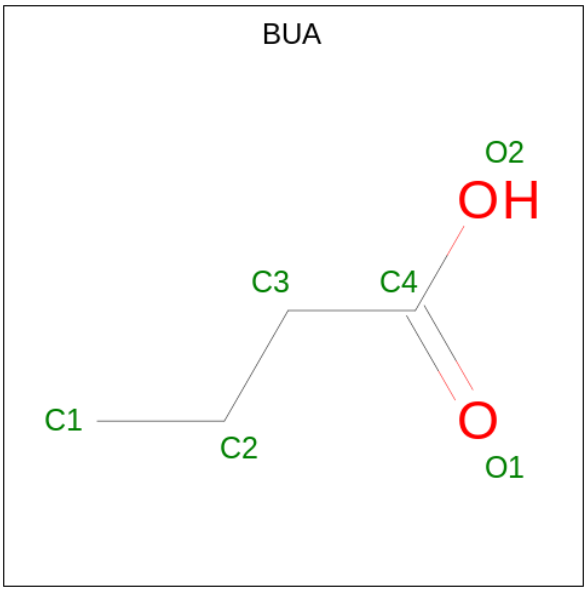
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	36	29	1	6	0	0
			Total	C	N	O		
4	B	1	36	29	1	6	0	0

- Molecule 5 is LAURIC ACID (three-letter code: DAO) (formula: $C_{12}H_{24}O_2$) (labeled as "Ligand of Interest" by depositor).



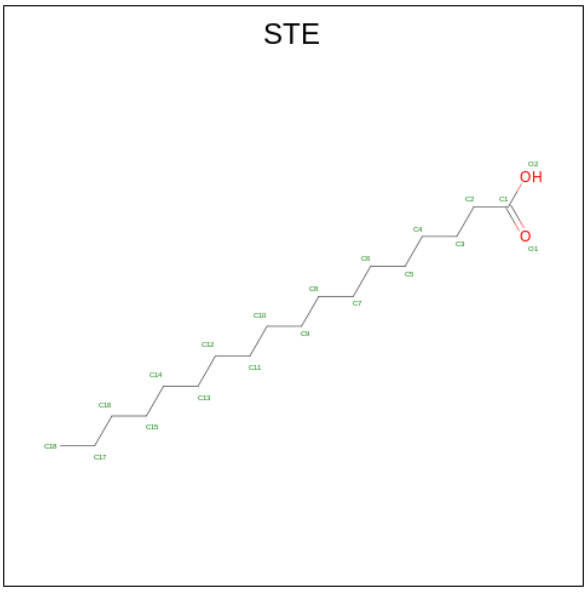
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	14	12	2	0	0
			Total	C	O		
5	A	1	14	12	2	0	0
			Total	C	O		
5	B	1	14	12	2	0	0
			Total	C	O		
5	B	1	14	12	2	0	0

- Molecule 6 is butanoic acid (three-letter code: BUA) (formula: $C_4H_8O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is STEARIC ACID (three-letter code: STE) (formula: $C_{18}H_{36}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	B	1	20	18	2	0	0

- Molecule 8 is water.

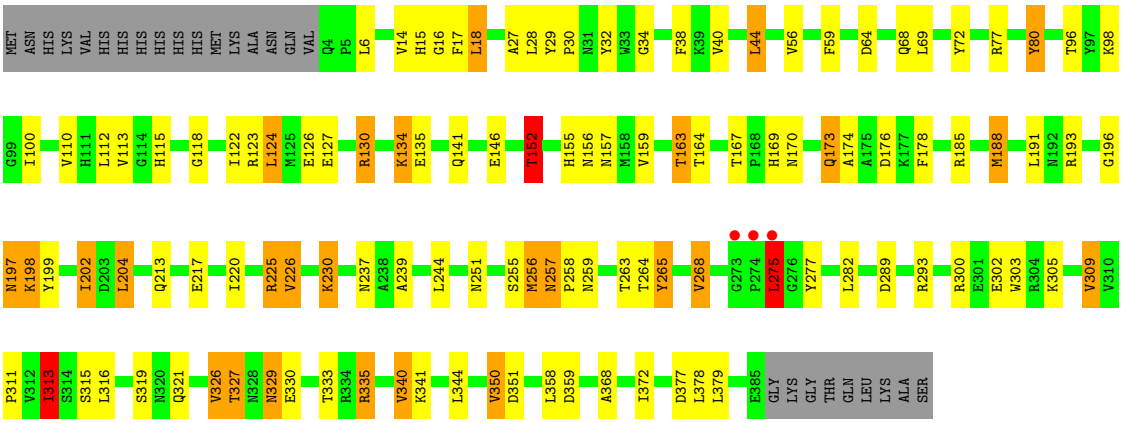
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	34	34	34	0	0
			Total	O		
8	B	26	26	26	0	0

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.

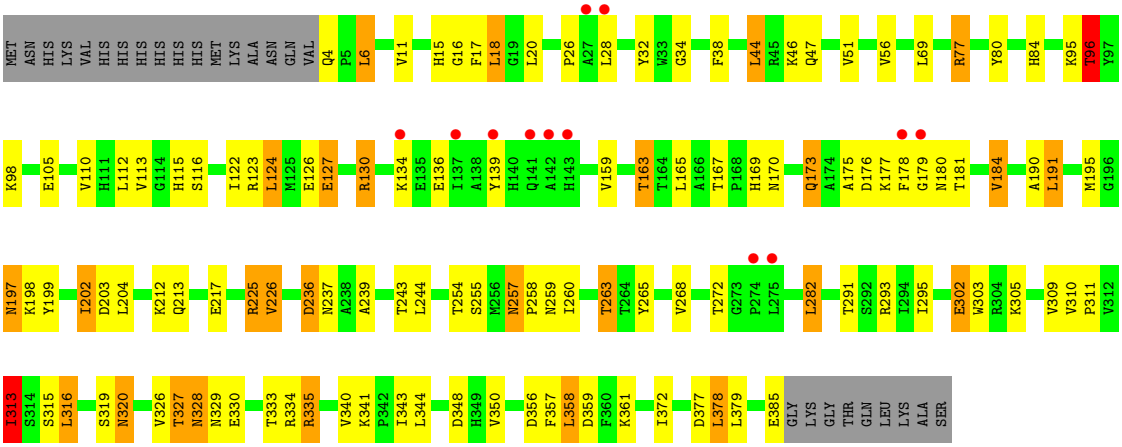
- Molecule 1: Lipase 2

Chain A:



- Molecule 1: Lipase 2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	132.51Å 132.51Å 248.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.18 – 2.23 48.18 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.18-2.23) 99.8 (48.18-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.226 , 0.259 0.223 , 0.257	Depositor DCC
R_{free} test set	5386 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	57.6	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 35.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6264	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: BUA, ZN, STE, CA, DAO, DH9

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	1.31	11/3102 (0.4%)	1.40	41/4207 (1.0%)
1	B	1.21	9/3102 (0.3%)	1.36	39/4207 (0.9%)
All	All	1.26	20/6204 (0.3%)	1.38	80/8414 (1.0%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	265	TYR	CG-CD1	7.40	1.48	1.39
1	B	80	TYR	CG-CD1	6.98	1.48	1.39
1	B	136	GLU	CD-OE1	6.53	1.32	1.25
1	B	139	TYR	CE1-CZ	6.01	1.46	1.38
1	A	127	GLU	CD-OE1	5.99	1.32	1.25
1	A	127	GLU	CG-CD	5.98	1.60	1.51
1	A	300	ARG	CZ-NH1	5.95	1.40	1.33
1	B	80	TYR	CE1-CZ	5.78	1.46	1.38
1	A	300	ARG	CD-NE	5.65	1.56	1.46
1	A	185	ARG	CZ-NH1	5.50	1.40	1.33
1	A	359	ASP	CB-CG	5.42	1.63	1.51
1	B	96	THR	CB-CG2	5.33	1.70	1.52
1	B	328	ASN	CG-ND2	5.31	1.46	1.32
1	A	72	TYR	CG-CD1	5.27	1.46	1.39
1	A	135	GLU	CD-OE2	5.24	1.31	1.25
1	A	196	GLY	CA-C	5.22	1.60	1.51
1	B	225	ARG	CZ-NH2	-5.16	1.26	1.33
1	A	80	TYR	CZ-OH	-5.14	1.29	1.37
1	A	265	TYR	CD2-CE2	5.06	1.47	1.39
1	B	225	ARG	CD-NE	-5.01	1.38	1.46

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	225	ARG	NE-CZ-NH2	-24.50	108.05	120.30
1	B	225	ARG	NE-CZ-NH1	19.95	130.27	120.30
1	A	225	ARG	NE-CZ-NH2	-19.71	110.44	120.30
1	A	130	ARG	NE-CZ-NH2	-16.71	111.95	120.30
1	A	225	ARG	NE-CZ-NH1	16.15	128.38	120.30
1	B	236	ASP	CB-CG-OD1	-14.82	104.97	118.30
1	A	130	ARG	NE-CZ-NH1	13.35	126.97	120.30
1	B	130	ARG	NE-CZ-NH2	-11.84	114.38	120.30
1	B	236	ASP	CB-CG-OD2	11.55	128.69	118.30
1	A	188	MET	CG-SD-CE	-10.91	82.74	100.20
1	A	335	ARG	NE-CZ-NH2	10.52	125.56	120.30
1	A	335	ARG	NE-CZ-NH1	-9.81	115.40	120.30
1	B	293	ARG	NE-CZ-NH1	-9.08	115.76	120.30
1	A	225	ARG	CD-NE-CZ	8.86	136.01	123.60
1	B	226	VAL	CG1-CB-CG2	8.63	124.70	110.90
1	B	356	ASP	CB-CG-OD1	8.52	125.97	118.30
1	B	335	ARG	NE-CZ-NH2	8.37	124.48	120.30
1	B	77	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	B	313	ILE	CG1-CB-CG2	8.14	129.31	111.40
1	B	225	ARG	CG-CD-NE	-8.07	94.85	111.80
1	A	377	ASP	CB-CG-OD1	8.03	125.52	118.30
1	B	77	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	A	64	ASP	CB-CG-OD1	7.77	125.29	118.30
1	B	305	LYS	CD-CE-NZ	7.59	129.16	111.70
1	A	313	ILE	CG1-CB-CG2	7.54	128.00	111.40
1	A	77	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	198	LYS	CD-CE-NZ	-7.54	94.36	111.70
1	B	356	ASP	CB-CG-OD2	-7.44	111.61	118.30
1	B	359	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	A	124	LEU	CB-CG-CD2	7.36	123.52	111.00
1	A	268	VAL	CB-CA-C	-7.33	97.47	111.40
1	A	130	ARG	CG-CD-NE	-7.21	96.65	111.80
1	A	293	ARG	NE-CZ-NH2	7.18	123.89	120.30
1	A	256	MET	CG-SD-CE	-7.15	88.75	100.20
1	A	300	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	A	313	ILE	CB-CG1-CD1	6.85	133.08	113.90
1	A	305	LYS	CD-CE-NZ	6.82	127.39	111.70
1	A	225	ARG	CG-CD-NE	-6.77	97.58	111.80
1	A	130	ARG	CD-NE-CZ	6.72	133.01	123.60
1	B	130	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	A	275	LEU	CB-CG-CD2	6.55	122.13	111.00
1	A	293	ARG	NE-CZ-NH1	-6.53	117.03	120.30
1	A	326	VAL	CG1-CB-CG2	6.51	121.33	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	350	VAL	CG1-CB-CG2	6.51	121.32	110.90
1	A	344	LEU	CA-CB-CG	-6.20	101.03	115.30
1	B	359	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	226	VAL	CG1-CB-CG2	6.06	120.59	110.90
1	A	27	ALA	CB-CA-C	6.05	119.17	110.10
1	B	225	ARG	CD-NE-CZ	6.05	132.06	123.60
1	B	378	LEU	CB-CG-CD1	5.80	120.87	111.00
1	A	289	ASP	N-CA-CB	5.73	120.91	110.60
1	B	44	LEU	CB-CG-CD1	5.72	120.73	111.00
1	B	244	LEU	CB-CG-CD2	5.72	120.73	111.00
1	B	377	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	134	LYS	CD-CE-NZ	-5.64	98.73	111.70
1	B	348	ASP	CB-CG-OD1	5.63	123.37	118.30
1	B	293	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	B	361	LYS	CD-CE-NZ	5.54	124.44	111.70
1	B	316	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	152	THR	N-CA-CB	-5.52	99.81	110.30
1	B	282	LEU	C-N-CA	-5.42	110.92	122.30
1	B	124	LEU	CB-CG-CD2	5.36	120.11	111.00
1	A	340	VAL	CA-CB-CG2	5.35	118.92	110.90
1	B	6	LEU	CA-CB-CG	5.33	127.56	115.30
1	B	203	ASP	CB-CG-OD1	5.33	123.10	118.30
1	B	313	ILE	CB-CG1-CD1	5.32	128.80	113.90
1	B	191	LEU	CA-CB-CG	5.28	127.45	115.30
1	B	344	LEU	CA-CB-CG	-5.28	103.15	115.30
1	B	127	GLU	OE1-CD-OE2	5.26	129.61	123.30
1	B	334	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	A	230	LYS	CD-CE-NZ	5.24	123.75	111.70
1	A	244	LEU	CB-CG-CD2	5.22	119.88	111.00
1	A	220	ILE	CG1-CB-CG2	5.22	122.88	111.40
1	B	348	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	B	377	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	340	VAL	CG1-CB-CG2	5.18	119.20	110.90
1	B	226	VAL	CB-CA-C	5.17	121.21	111.40
1	A	159	VAL	CG1-CB-CG2	5.11	119.08	110.90
1	A	351	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	300	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3020	0	2914	77	0
1	B	3020	0	2914	82	0
2	A	1	0	0	0	0
2	B	1	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	36	0	54	5	0
4	B	36	0	54	7	0
5	A	28	0	46	2	0
5	B	28	0	46	2	0
6	A	6	0	7	1	0
6	B	6	0	7	0	0
7	B	20	0	35	1	0
8	A	34	0	0	2	0
8	B	26	0	0	0	0
All	All	6264	0	6077	164	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (164) 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:A:313:ILE:CD1	1:A:313:ILE:CG1	1.74	1.60
1:B:116:SER:CB	4:B:403:DH9:O2'	1.79	1.30
1:A:174:ALA:O	1:A:178:PHE:O	1.78	1.00
1:B:313:ILE:HD13	1:B:313:ILE:H	1.26	0.97
1:B:327:THR:HG22	1:B:329:ASN:H	1.29	0.97
1:B:313:ILE:H	1:B:313:ILE:CD1	1.81	0.90
1:B:173:GLN:HE21	1:B:173:GLN:H	1.15	0.89
1:A:313:ILE:CD1	1:A:313:ILE:H	1.87	0.88
1:B:115:HIS:HE1	4:B:403:DH9:H291	1.35	0.88
1:A:313:ILE:H	1:A:313:ILE:HD13	1.38	0.87
1:A:173:GLN:HE21	1:A:173:GLN:H	1.19	0.85
1:B:115:HIS:CE1	4:B:403:DH9:H291	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:THR:CG2	1:B:329:ASN:H	1.91	0.83
1:A:257:ASN:ND2	1:A:259:ASN:H	1.77	0.82
1:B:116:SER:CB	4:B:403:DH9:C1'	2.58	0.82
1:A:15:HIS:HE1	1:A:56:VAL:H	1.28	0.81
1:B:170:ASN:HD21	1:B:319:SER:H	1.25	0.80
1:A:257:ASN:HD22	1:A:259:ASN:H	1.29	0.78
1:A:197:ASN:HD22	1:A:199:TYR:H	1.31	0.77
1:A:193:ARG:HH11	5:A:404:DAO:H21	1.49	0.77
1:A:115:HIS:HE1	4:A:403:DH9:H291	1.51	0.76
1:B:197:ASN:HD22	1:B:199:TYR:H	1.34	0.75
1:B:327:THR:HG22	1:B:329:ASN:N	2.03	0.74
1:A:198:LYS:H	1:A:213:GLN:NE2	1.85	0.74
1:A:327:THR:HG23	1:A:329:ASN:H	1.53	0.73
1:A:118:GLY:O	1:A:122:ILE:HG12	1.89	0.72
1:B:159:VAL:HG22	1:B:260:ILE:HD13	1.72	0.71
1:A:123:ARG:HH11	1:A:169:HIS:HD2	1.39	0.70
1:A:197:ASN:ND2	1:A:199:TYR:H	1.89	0.70
1:B:257:ASN:C	1:B:257:ASN:HD22	1.94	0.70
1:B:257:ASN:HD22	1:B:258:PRO:N	1.90	0.69
1:B:257:ASN:ND2	1:B:259:ASN:H	1.91	0.69
1:B:126:GLU:OE2	1:B:130:ARG:HD3	1.93	0.69
1:A:17:PHE:O	4:A:403:DH9:H262	1.93	0.68
1:B:195:MET:HE2	1:B:202:ILE:HD11	1.74	0.68
1:B:195:MET:CE	1:B:202:ILE:HD11	2.23	0.68
4:B:403:DH9:H27	4:B:403:DH9:O3'	1.94	0.67
1:B:195:MET:CE	1:B:202:ILE:CD1	2.72	0.67
1:A:123:ARG:NH1	1:A:169:HIS:HD2	1.93	0.67
1:B:236:ASP:OD2	2:B:401:ZN:ZN	1.44	0.67
1:B:179:GLY:O	1:B:239:ALA:HB1	1.96	0.66
1:A:170:ASN:HD21	1:A:319:SER:H	1.42	0.66
1:B:197:ASN:ND2	1:B:199:TYR:H	1.93	0.65
1:A:256:MET:HE1	1:A:321:GLN:HB3	1.78	0.65
4:B:403:DH9:H192	4:B:403:DH9:H4'1	1.78	0.65
1:A:115:HIS:CE1	4:A:403:DH9:H291	2.32	0.64
1:B:180:ASN:ND2	1:B:243:THR:HG21	2.14	0.63
1:A:15:HIS:CE1	1:A:56:VAL:H	2.13	0.63
1:A:237:ASN:HD22	1:A:239:ALA:H	1.47	0.62
1:A:14:VAL:HG21	1:A:122:ILE:HD11	1.81	0.62
1:B:198:LYS:H	1:B:213:GLN:NE2	1.97	0.61
1:A:257:ASN:HD22	1:A:257:ASN:C	2.02	0.61
1:A:198:LYS:H	1:A:213:GLN:HE21	1.46	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:MET:HE3	1:B:202:ILE:CD1	2.31	0.61
1:A:302:GLU:O	1:A:313:ILE:HG13	2.01	0.61
1:A:68:GLN:NE2	1:A:80:TYR:OH	2.33	0.60
1:A:163:THR:CG2	8:A:501:HOH:O	2.49	0.60
4:A:403:DH9:H27	4:A:403:DH9:O3'	2.02	0.60
1:B:15:HIS:HE1	1:B:56:VAL:H	1.50	0.60
1:A:193:ARG:HH11	5:A:404:DAO:C2	2.13	0.59
1:B:177:LYS:O	1:B:181:THR:HG23	2.03	0.59
1:A:34:GLY:HA3	1:A:38:PHE:O	2.03	0.59
1:A:173:GLN:H	1:A:173:GLN:NE2	1.95	0.59
1:B:170:ASN:ND2	1:B:319:SER:H	1.98	0.58
1:A:327:THR:HG22	1:A:330:GLU:H	1.68	0.58
1:B:268:VAL:HG23	1:B:343:ILE:CG2	2.34	0.57
1:B:268:VAL:HG23	1:B:343:ILE:HG21	1.85	0.57
1:B:127:GLU:CG	1:B:254:THR:HG22	2.35	0.57
1:B:195:MET:HE2	1:B:202:ILE:CD1	2.34	0.57
1:B:302:GLU:O	1:B:313:ILE:HG13	2.05	0.56
1:A:327:THR:HG22	1:A:330:GLU:HG2	1.86	0.56
1:B:127:GLU:HG2	1:B:254:THR:HG22	1.88	0.56
1:A:303:TRP:HA	1:A:313:ILE:HG13	1.88	0.56
1:B:195:MET:HE3	1:B:202:ILE:HD13	1.87	0.55
1:A:17:PHE:O	1:A:18:LEU:HB2	2.07	0.55
1:A:156:ASN:O	1:A:157:ASN:HB2	2.06	0.55
1:B:15:HIS:CE1	1:B:56:VAL:H	2.24	0.54
1:B:173:GLN:HE22	1:B:311:PRO:HG3	1.72	0.54
1:B:17:PHE:O	1:B:18:LEU:HB2	2.07	0.54
1:A:275:LEU:H	1:A:275:LEU:HD22	1.73	0.54
1:B:123:ARG:NH1	1:B:169:HIS:HD2	2.06	0.53
1:B:173:GLN:H	1:B:173:GLN:NE2	1.95	0.53
1:A:329:ASN:H	1:A:329:ASN:HD22	1.55	0.53
1:B:123:ARG:HH11	1:B:169:HIS:HD2	1.55	0.53
1:B:313:ILE:HD13	1:B:313:ILE:N	2.09	0.53
1:A:170:ASN:ND2	1:A:319:SER:H	2.06	0.52
1:B:179:GLY:O	1:B:239:ALA:CB	2.57	0.52
1:B:112:LEU:HB3	1:B:122:ILE:HD13	1.92	0.52
1:B:198:LYS:H	1:B:213:GLN:HE21	1.57	0.52
1:A:264:THR:O	1:A:341:LYS:HB2	2.10	0.52
1:A:368:ALA:O	1:A:372:ILE:HG12	2.09	0.52
1:B:327:THR:HG22	1:B:330:GLU:H	1.74	0.51
1:A:32:TYR:OH	4:A:403:DH9:H282	2.10	0.51
1:B:47:GLN:OE1	1:B:372:ILE:HD11	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:HIS:HD2	1:A:16:GLY:O	1.93	0.51
1:A:327:THR:CG2	1:A:329:ASN:H	2.24	0.51
1:B:32:TYR:OH	4:B:403:DH9:H282	2.11	0.51
1:B:302:GLU:O	1:B:313:ILE:CD1	2.59	0.51
1:A:198:LYS:N	1:A:213:GLN:HE21	2.08	0.50
1:B:195:MET:CE	1:B:202:ILE:HD13	2.40	0.50
1:A:313:ILE:CD1	1:A:313:ILE:HG13	2.18	0.49
1:B:15:HIS:HD2	1:B:16:GLY:O	1.96	0.49
1:B:175:ALA:O	1:B:180:ASN:CB	2.60	0.49
1:A:29:TYR:CG	1:A:30:PRO:HD2	2.48	0.49
6:A:406:BUA:H11	5:B:405:DAO:H62	1.94	0.49
1:A:163:THR:HG23	8:A:501:HOH:O	2.11	0.49
1:B:175:ALA:HA	1:B:178:PHE:O	2.12	0.49
1:B:11:VAL:HB	1:B:51:VAL:HG12	1.95	0.48
1:B:327:THR:HB	1:B:330:GLU:HG2	1.94	0.48
1:B:257:ASN:HD22	1:B:259:ASN:H	1.60	0.48
1:A:257:ASN:HD22	1:A:258:PRO:N	2.11	0.48
1:B:217:GLU:OE2	1:B:225:ARG:HD3	2.14	0.47
1:A:329:ASN:HD22	1:A:329:ASN:N	2.12	0.47
1:A:126:GLU:OE2	1:A:130:ARG:HD3	2.15	0.47
1:B:77:ARG:HA	1:B:96:THR:HB	1.96	0.47
1:B:181:THR:OG1	1:B:184:VAL:HG13	2.14	0.47
1:A:197:ASN:ND2	1:A:197:ASN:C	2.68	0.46
1:A:164:THR:HB	1:A:167:THR:OG1	2.15	0.46
1:B:268:VAL:CG2	1:B:343:ILE:HG21	2.45	0.46
1:A:197:ASN:HA	1:A:213:GLN:HE21	1.81	0.45
1:A:329:ASN:N	1:A:329:ASN:ND2	2.64	0.45
1:B:163:THR:HA	1:B:263:THR:O	2.16	0.45
1:A:197:ASN:HD22	1:A:197:ASN:C	2.19	0.45
1:A:178:PHE:O	1:A:178:PHE:CD2	2.70	0.45
1:A:112:LEU:HB3	1:A:122:ILE:HD12	1.98	0.44
1:B:175:ALA:O	1:B:180:ASN:HB2	2.17	0.44
1:B:130:ARG:NH2	1:B:255:SER:OG	2.49	0.44
1:B:170:ASN:HD21	1:B:319:SER:N	2.04	0.44
1:B:190:ALA:HB1	5:B:404:DAO:H22	1.99	0.44
1:B:237:ASN:HD21	1:B:239:ALA:HB3	1.83	0.44
1:A:313:ILE:HD13	1:A:313:ILE:N	2.17	0.44
1:B:320:ASN:H	1:B:320:ASN:HD22	1.64	0.44
1:A:59:PHE:HE2	1:A:188:MET:HG2	1.83	0.43
1:B:197:ASN:HA	1:B:213:GLN:HE21	1.83	0.43
7:B:406:STE:H101	7:B:406:STE:H151	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:THR:HG22	1:A:155:HIS:NE2	2.33	0.43
1:B:257:ASN:C	1:B:257:ASN:ND2	2.65	0.43
1:A:40:VAL:HG13	1:A:44:LEU:HD22	2.01	0.42
1:A:170:ASN:ND2	1:A:251:ASN:HD21	2.17	0.42
1:B:127:GLU:HG3	1:B:254:THR:HG22	1.99	0.42
1:A:178:PHE:CD2	1:A:178:PHE:C	2.90	0.42
1:B:34:GLY:HA3	1:B:38:PHE:O	2.20	0.42
1:B:291:THR:O	1:B:295:ILE:HG13	2.19	0.42
1:A:202:ILE:HD11	1:A:204:LEU:CD1	2.50	0.42
1:A:265:TYR:CE2	1:A:341:LYS:HG2	2.55	0.42
1:B:198:LYS:N	1:B:213:GLN:HE21	2.17	0.42
1:A:217:GLU:OE2	1:A:225:ARG:HD3	2.20	0.42
1:B:303:TRP:HA	1:B:313:ILE:HG13	2.01	0.42
1:A:167:THR:O	1:A:315:SER:HA	2.20	0.42
1:B:173:GLN:NE2	1:B:311:PRO:HG3	2.35	0.42
1:A:275:LEU:HD23	1:A:277:TYR:HB2	2.02	0.41
1:B:167:THR:O	1:B:315:SER:HA	2.20	0.41
1:B:357:PHE:CE2	1:B:358:LEU:HD13	2.55	0.41
1:A:302:GLU:O	1:A:313:ILE:CG1	2.67	0.41
1:B:173:GLN:HE21	1:B:173:GLN:N	1.98	0.41
1:A:202:ILE:CD1	1:A:204:LEU:HD13	2.51	0.41
1:A:173:GLN:HE22	1:A:311:PRO:HG3	1.84	0.41
1:A:170:ASN:HD22	1:A:251:ASN:HD21	1.69	0.41
1:B:302:GLU:O	1:B:313:ILE:CG1	2.68	0.41
1:A:14:VAL:CG2	1:A:122:ILE:HD11	2.50	0.40
1:A:130:ARG:NH2	1:A:255:SER:OG	2.39	0.40
1:A:237:ASN:HD22	1:A:239:ALA:N	2.16	0.40
1:B:20:LEU:HD13	1:B:26:PRO:HD3	2.03	0.40
1:B:84:HIS:NE2	1:B:236:ASP:OD2	2.55	0.40

There are no symmetry-related clashes.

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	380/408 (93%)	367 (97%)	12 (3%)	1 (0%)	41	44
1	B	380/408 (93%)	370 (97%)	10 (3%)	0	100	100
All	All	760/816 (93%)	737 (97%)	22 (3%)	1 (0%)	51	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	VAL

5.3.2 Protein sidechains (i)

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	317/341 (93%)	275 (87%)	42 (13%)	4	2
1	B	317/341 (93%)	269 (85%)	48 (15%)	3	1
All	All	634/682 (93%)	544 (86%)	90 (14%)	3	1

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	18	LEU
1	A	28	LEU
1	A	44	LEU
1	A	69	LEU
1	A	96	THR
1	A	98	LYS
1	A	100	ILE
1	A	110	VAL
1	A	113	VAL
1	A	124	LEU
1	A	134	LYS
1	A	141	GLN
1	A	146	GLU
1	A	152	THR

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Mol	Chain	Res	Type
1	A	163	THR
1	A	173	GLN
1	A	176	ASP
1	A	191	LEU
1	A	197	ASN
1	A	202	ILE
1	A	204	LEU
1	A	226	VAL
1	A	230	LYS
1	A	257	ASN
1	A	263	THR
1	A	268	VAL
1	A	275	LEU
1	A	282	LEU
1	A	309	VAL
1	A	313	ILE
1	A	316	LEU
1	A	326	VAL
1	A	327	THR
1	A	329	ASN
1	A	333	THR
1	A	335	ARG
1	A	340	VAL
1	A	350	VAL
1	A	358	LEU
1	A	378	LEU
1	A	379	LEU
1	B	4	GLN
1	B	6	LEU
1	B	18	LEU
1	B	28	LEU
1	B	44	LEU
1	B	46	LYS
1	B	69	LEU
1	B	95	LYS
1	B	96	THR
1	B	98	LYS
1	B	105	GLU
1	B	110	VAL
1	B	113	VAL
1	B	124	LEU
1	B	134	LYS

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Mol	Chain	Res	Type
1	B	163	THR
1	B	165	LEU
1	B	173	GLN
1	B	176	ASP
1	B	184	VAL
1	B	191	LEU
1	B	197	ASN
1	B	202	ILE
1	B	204	LEU
1	B	212	LYS
1	B	226	VAL
1	B	257	ASN
1	B	263	THR
1	B	272	THR
1	B	282	LEU
1	B	302	GLU
1	B	309	VAL
1	B	310	VAL
1	B	313	ILE
1	B	316	LEU
1	B	320	ASN
1	B	326	VAL
1	B	327	THR
1	B	328	ASN
1	B	333	THR
1	B	335	ARG
1	B	340	VAL
1	B	341	LYS
1	B	350	VAL
1	B	358	LEU
1	B	378	LEU
1	B	379	LEU
1	B	385	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	52	HIS
1	A	131	ASN
1	A	141	GLN
1	A	169	HIS

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Mol	Chain	Res	Type
1	A	170	ASN
1	A	173	GLN
1	A	197	ASN
1	A	213	GLN
1	A	237	ASN
1	A	257	ASN
1	A	259	ASN
1	A	329	ASN
1	A	369	ASN
1	B	15	HIS
1	B	50	ASN
1	B	52	HIS
1	B	141	GLN
1	B	169	HIS
1	B	170	ASN
1	B	173	GLN
1	B	197	ASN
1	B	213	GLN
1	B	237	ASN
1	B	257	ASN
1	B	320	ASN
1	B	328	ASN
1	B	369	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	DH9	B	403	-	35,35,35	0.93	2 (5%)	36,41,41	1.70	8 (22%)
5	DAO	A	405	-	13,13,13	0.78	0	13,13,13	0.63	0
5	DAO	B	404	-	13,13,13	0.67	0	13,13,13	0.77	0
6	BUA	A	406	-	5,5,5	1.19	0	5,5,5	0.97	0
5	DAO	B	405	-	13,13,13	0.82	0	13,13,13	1.18	2 (15%)
6	BUA	B	407	-	5,5,5	1.07	0	5,5,5	1.35	1 (20%)
7	STE	B	406	-	19,19,19	0.64	0	19,19,19	0.87	1 (5%)
5	DAO	A	404	-	13,13,13	0.79	0	13,13,13	0.91	0
4	DH9	A	403	1	35,35,35	1.06	3 (8%)	36,41,41	1.84	6 (16%)

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
4	DH9	B	403	-	-	19/44/44/44	-
5	DAO	A	405	-	-	8/11/11/11	-
5	DAO	B	404	-	-	8/11/11/11	-
6	BUA	A	406	-	-	1/3/3/3	-
5	DAO	B	405	-	-	8/11/11/11	-
6	BUA	B	407	-	-	2/3/3/3	-
7	STE	B	406	-	-	14/17/17/17	-
5	DAO	A	404	-	-	4/11/11/11	-
4	DH9	A	403	1	-	17/44/44/44	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	DH9	O4'-C23	3.35	1.42	1.34
4	A	403	DH9	O4'-C5'	-3.17	1.38	1.46
4	A	403	DH9	O4'-C23	3.09	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	DH9	O4'-C5'	-2.55	1.40	1.46
4	A	403	DH9	O2'-C1'	-2.17	1.23	1.30

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	403	DH9	O4'-C5'-C4'	-5.36	97.45	107.54
4	B	403	DH9	O4'-C5'-C4'	-4.89	98.34	107.54
4	A	403	DH9	O3'-C3'-C4'	4.63	118.39	109.11
4	B	403	DH9	C4'-C5'-C6'	-4.08	106.74	112.91
4	A	403	DH9	C23-C24-N1'	3.82	119.71	110.92
4	B	403	DH9	O6'-C25-N1'	-3.72	115.48	125.27
4	A	403	DH9	C5'-O4'-C23	3.52	123.46	117.69
4	B	403	DH9	C18-C17-C2'	-3.13	108.66	114.28
5	B	405	DAO	O2-C1-C2	3.01	123.69	114.03
4	B	403	DH9	C23-C24-N1'	2.88	117.56	110.92
7	B	406	STE	O2-C1-C2	2.65	122.54	114.03
4	A	403	DH9	O6'-C25-N1'	-2.63	118.33	125.27
4	A	403	DH9	O2'-C1'-O1'	-2.59	118.21	124.09
5	B	405	DAO	O2-C1-O1	-2.54	116.98	123.30
4	B	403	DH9	C5'-O4'-C23	2.40	121.62	117.69
6	B	407	BUA	O2-C4-C3	2.14	120.89	114.03
4	B	403	DH9	O4'-C5'-C6'	2.11	113.17	107.10
4	B	403	DH9	O4'-C23-O5'	-2.05	120.11	123.94

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	DH9	C18-C17-C2'-C1'
4	A	403	DH9	C17-C2'-C3'-O3'
4	A	403	DH9	C17-C2'-C3'-C4'
4	A	403	DH9	C1'-C2'-C3'-O3'
4	A	403	DH9	C1'-C2'-C3'-C4'
4	A	403	DH9	C26-C24-N1'-C25
4	A	403	DH9	O6'-C25-N1'-C24
4	B	403	DH9	C18-C17-C2'-C1'
4	B	403	DH9	C17-C2'-C3'-O3'
4	B	403	DH9	C17-C2'-C3'-C4'
4	B	403	DH9	C1'-C2'-C3'-O3'
4	B	403	DH9	C1'-C2'-C3'-C4'
4	B	403	DH9	C23-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
4	B	403	DH9	O6'-C25-N1'-C24
4	B	403	DH9	N1'-C24-C26-C27
5	B	405	DAO	C2-C3-C4-C5
7	B	406	STE	C12-C13-C14-C15
4	A	403	DH9	C23-C24-C26-C27
7	B	406	STE	C1-C2-C3-C4
4	A	403	DH9	N1'-C24-C26-C27
5	A	405	DAO	C1-C2-C3-C4
5	B	405	DAO	C1-C2-C3-C4
5	A	404	DAO	C1-C2-C3-C4
4	A	403	DH9	C11-C12-C13-C14
7	B	406	STE	C11-C12-C13-C14
5	A	404	DAO	C6-C7-C8-C9
5	A	405	DAO	C3-C4-C5-C6
5	A	405	DAO	C6-C7-C8-C9
5	A	405	DAO	C7-C8-C9-C10
5	A	405	DAO	C4-C5-C6-C7
7	B	406	STE	C2-C3-C4-C5
4	A	403	DH9	C12-C13-C14-C15
7	B	406	STE	C13-C14-C15-C16
7	B	406	STE	C4-C5-C6-C7
5	B	404	DAO	C1-C2-C3-C4
5	B	405	DAO	C6-C7-C8-C9
7	B	406	STE	C10-C11-C12-C13
4	A	403	DH9	C6'-C7'-C8'-C9'
4	B	403	DH9	C24-C26-C27-C29
4	B	403	DH9	C19-C20-C21-C22
7	B	406	STE	C5-C6-C7-C8
5	B	404	DAO	C9-C10-C11-C12
7	B	406	STE	C7-C8-C9-C10
4	A	403	DH9	C2'-C17-C18-C19
5	B	404	DAO	C4-C5-C6-C7
5	A	404	DAO	C5-C6-C7-C8
5	B	405	DAO	C5-C6-C7-C8
5	B	405	DAO	C4-C5-C6-C7
4	B	403	DH9	C2'-C17-C18-C19
4	B	403	DH9	C24-C26-C27-C28
6	A	406	BUA	C1-C2-C3-C4
7	B	406	STE	C9-C10-C11-C12
7	B	406	STE	C14-C15-C16-C17
5	B	404	DAO	C11-C10-C9-C8
4	B	403	DH9	C5'-C6'-C7'-C8'

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Mol	Chain	Res	Type	Atoms
4	B	403	DH9	C23-C24-N1'-C25
5	B	405	DAO	C3-C4-C5-C6
4	B	403	DH9	C26-C24-N1'-C25
4	A	403	DH9	C17-C18-C19-C20
5	B	404	DAO	C7-C8-C9-C10
7	B	406	STE	C11-C10-C9-C8
4	B	403	DH9	C6'-C7'-C8'-C9'
5	B	404	DAO	O2-C1-C2-C3
5	B	404	DAO	C2-C3-C4-C5
5	B	405	DAO	O2-C1-C2-C3
6	B	407	BUA	C2-C3-C4-O2
5	B	404	DAO	O1-C1-C2-C3
6	B	407	BUA	C2-C3-C4-O1
5	B	405	DAO	O1-C1-C2-C3
5	A	405	DAO	O2-C1-C2-C3
7	B	406	STE	O1-C1-C2-C3
4	A	403	DH9	C9'-C10-C11-C12
5	A	404	DAO	C3-C4-C5-C6
4	A	403	DH9	C18-C17-C2'-C3'
4	B	403	DH9	C18-C17-C2'-C3'
5	A	405	DAO	O1-C1-C2-C3
5	A	405	DAO	C9-C10-C11-C12
7	B	406	STE	O2-C1-C2-C3
4	A	403	DH9	C18-C19-C20-C21
4	B	403	DH9	C11-C12-C13-C14
4	B	403	DH9	O4'-C5'-C6'-C7'

There are no ring outliers.

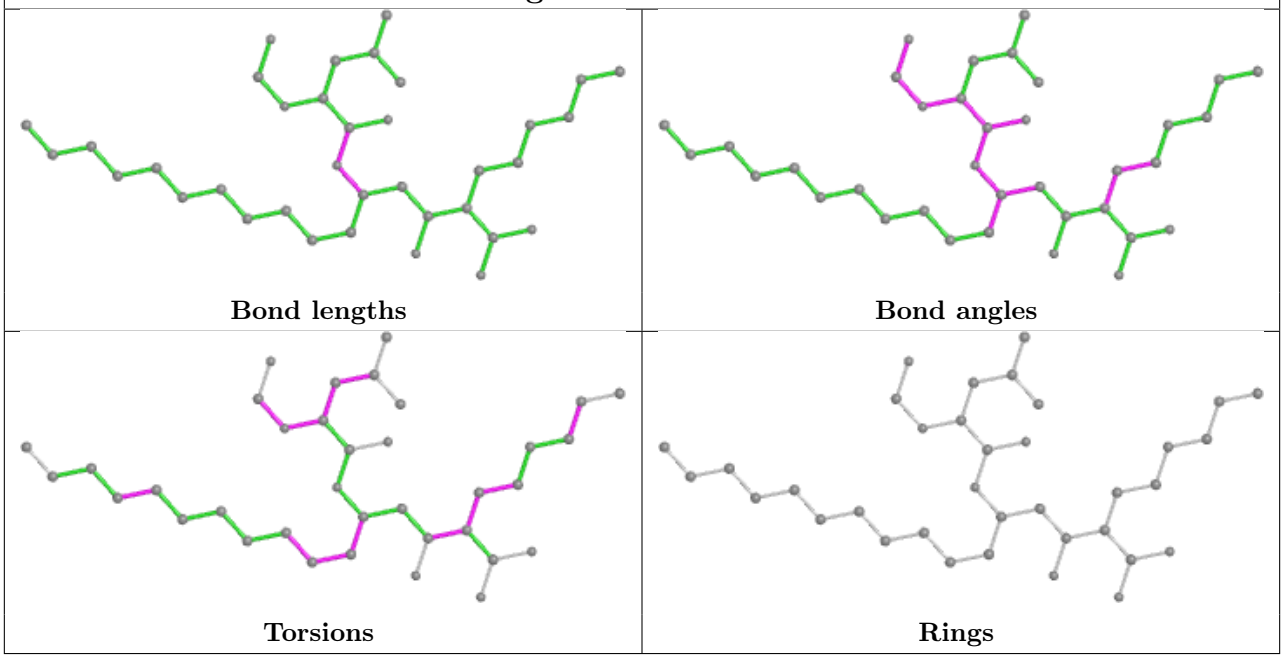
7 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	DH9	7	0
5	B	404	DAO	1	0
6	A	406	BUA	1	0
5	B	405	DAO	1	0
7	B	406	STE	1	0
5	A	404	DAO	2	0
4	A	403	DH9	5	0

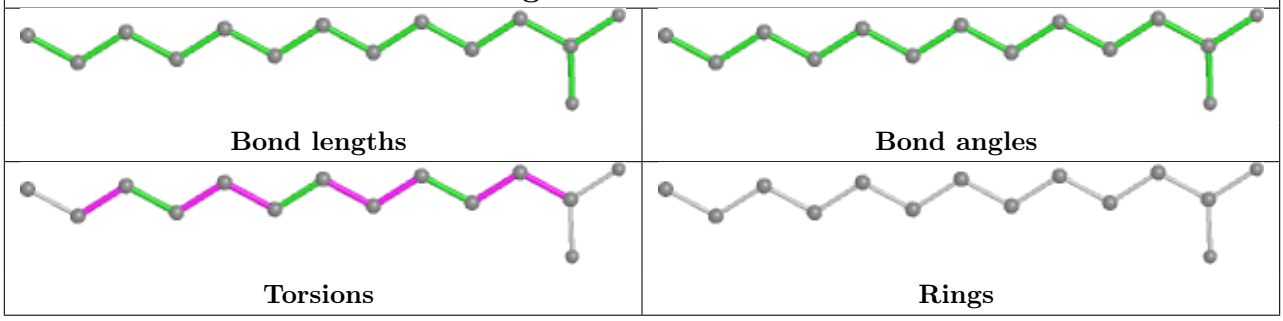
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand DH9 B 403



Ligand DAO A 405



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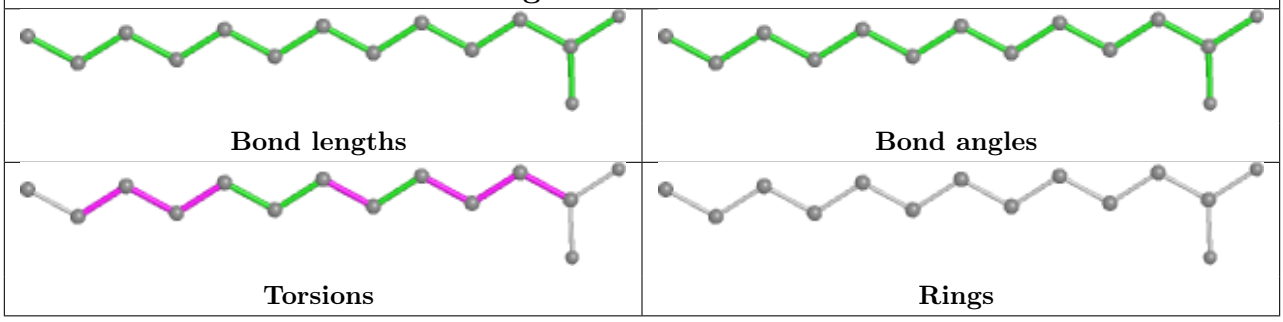
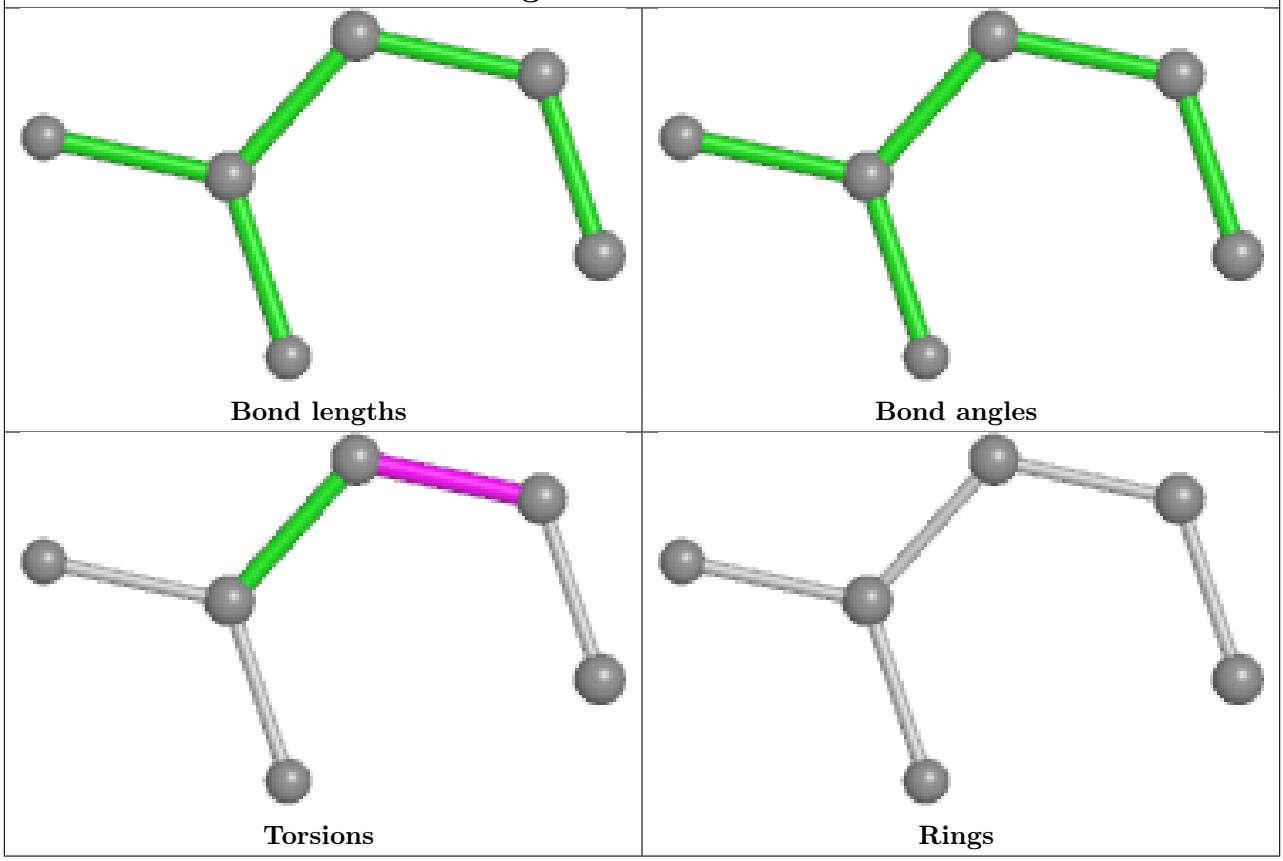
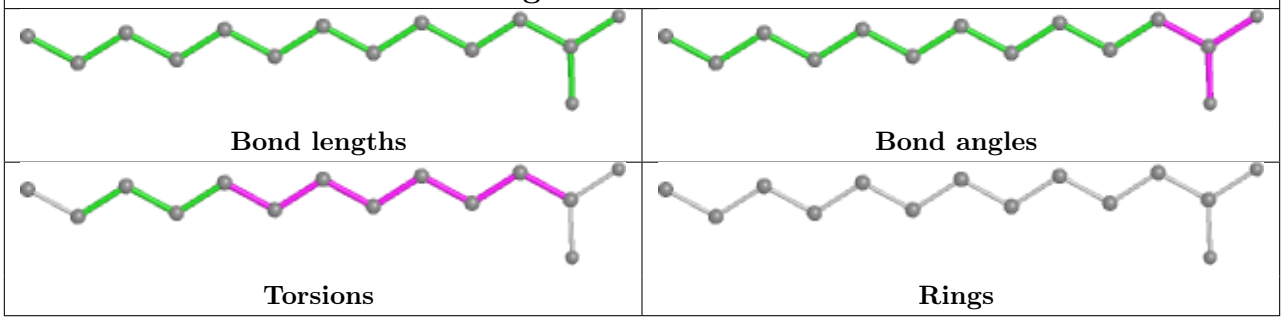


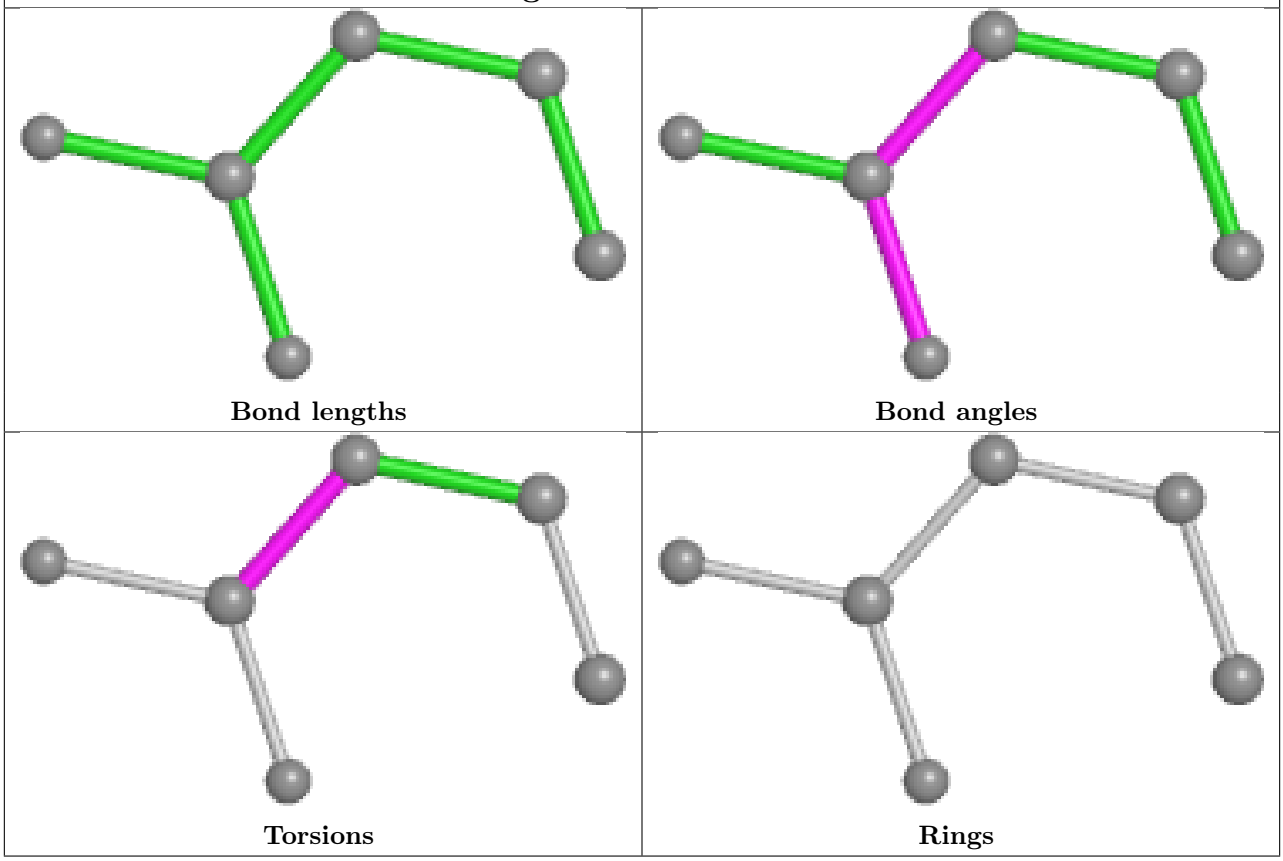
Ligand BUA A 406



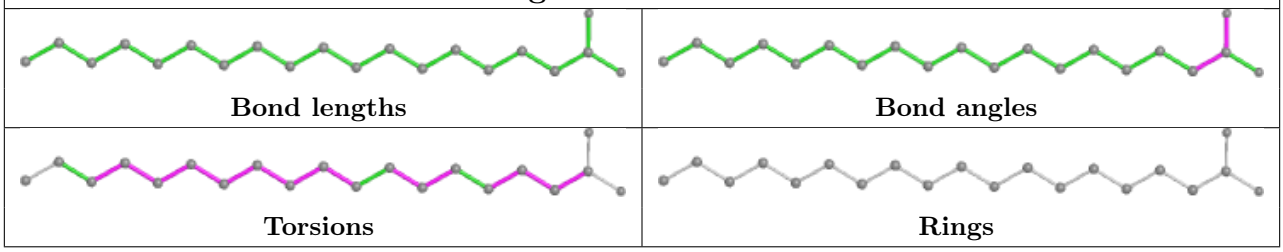
Ligand DAO B 405



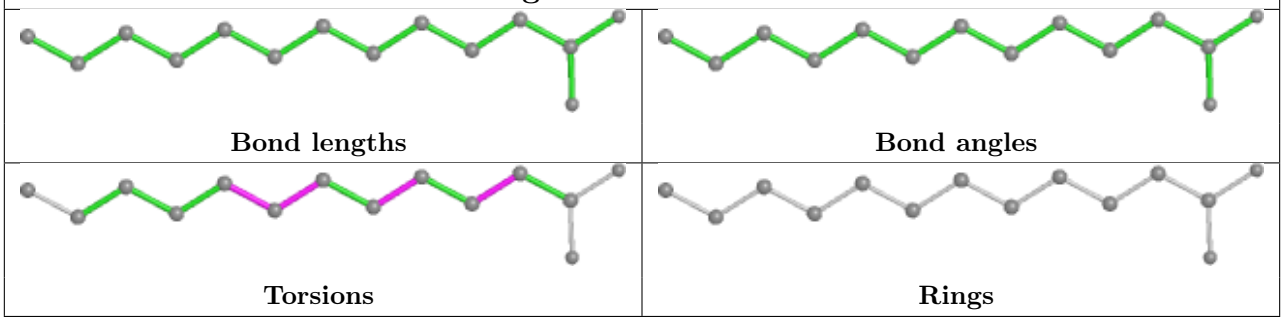
Ligand BUA B 407

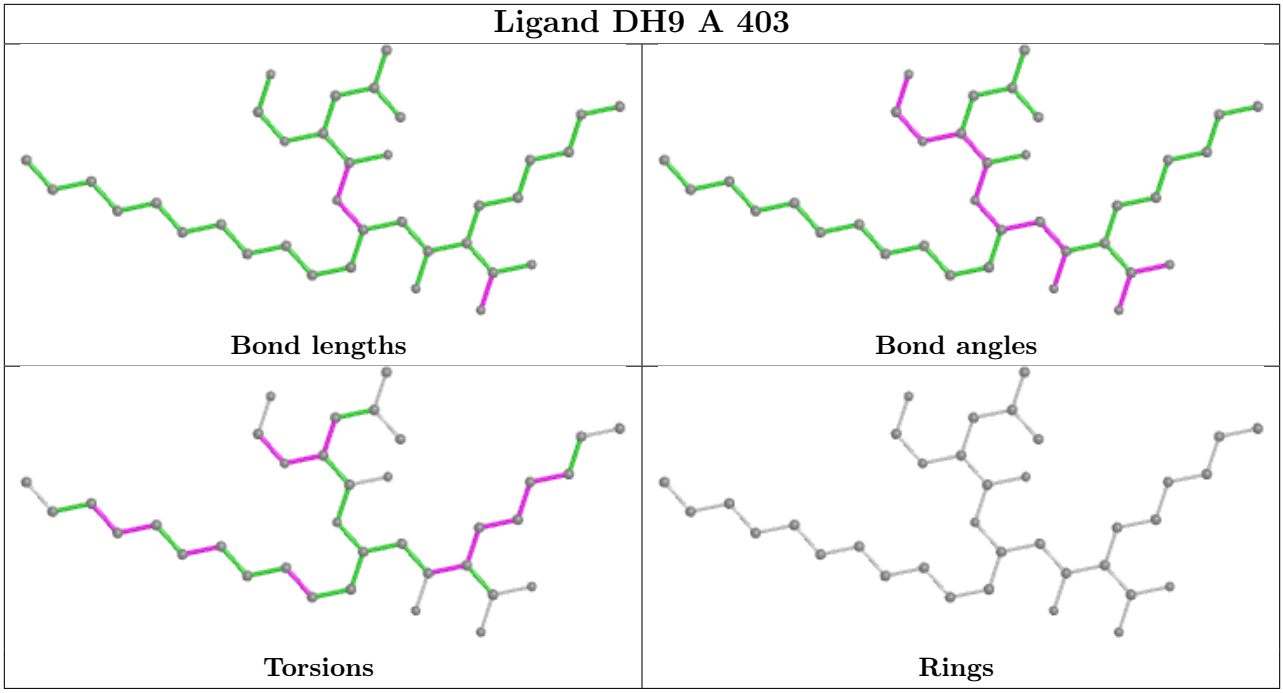


Ligand STE B 406



Ligand DAO A 404





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 (i)

6.1 Protein, DNA and RNA chains (i)

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	382/408 (93%)	-0.27	3 (0%)	86	86	31, 39, 61, 86	0
1	B	382/408 (93%)	-0.11	12 (3%)	49	49	35, 47, 66, 90	0
All	All	764/816 (93%)	-0.19	15 (1%)	65	66	31, 44, 65, 90	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	PRO	4.7
1	B	141	GLN	4.4
1	B	178	PHE	4.3
1	B	179	GLY	4.0
1	B	274	PRO	3.5
1	B	275	LEU	3.2
1	B	142	ALA	2.8
1	B	137	ILE	2.5
1	A	275	LEU	2.5
1	B	139	TYR	2.3
1	B	134	LYS	2.3
1	B	28	LEU	2.1
1	B	27	ALA	2.1
1	B	143	HIS	2.0
1	A	273	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

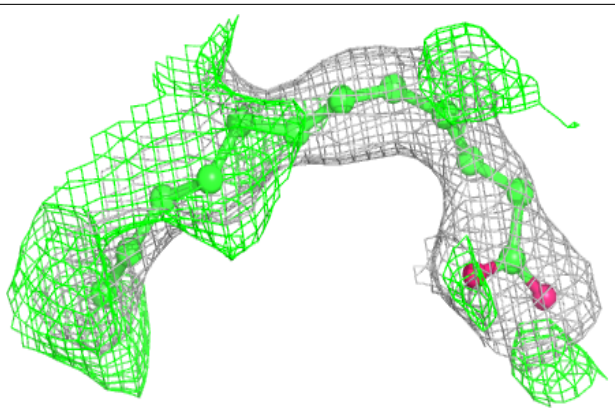
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

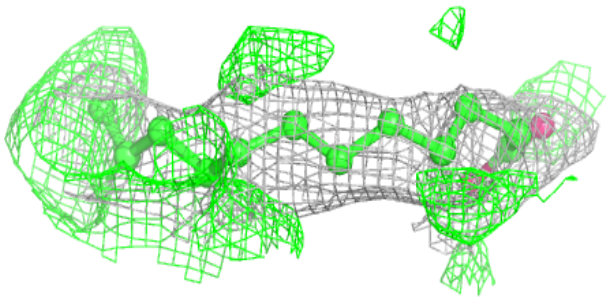
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DAO	A	405	14/14	0.57	0.88	97,116,129,131	0
5	DAO	B	405	14/14	0.71	0.39	66,93,115,118	0
6	BUA	A	406	6/6	0.71	0.36	73,87,105,106	0
6	BUA	B	407	6/6	0.72	0.36	72,96,105,110	0
7	STE	B	406	20/20	0.77	0.77	71,108,126,127	0
5	DAO	B	404	14/14	0.86	0.49	56,97,122,122	0
2	ZN	A	401	1/1	0.88	0.30	68,68,68,68	0
5	DAO	A	404	14/14	0.88	0.47	59,92,106,109	0
4	DH9	A	403	36/36	0.93	0.25	49,67,98,109	0
3	CA	A	402	1/1	0.94	0.16	75,75,75,75	0
4	DH9	B	403	36/36	0.97	0.24	48,68,94,99	0
3	CA	B	402	1/1	0.98	0.23	64,64,64,64	0
2	ZN	B	401	1/1	0.99	0.17	69,69,69,69	0

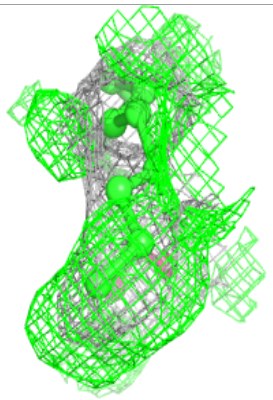
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DAO A 405:

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

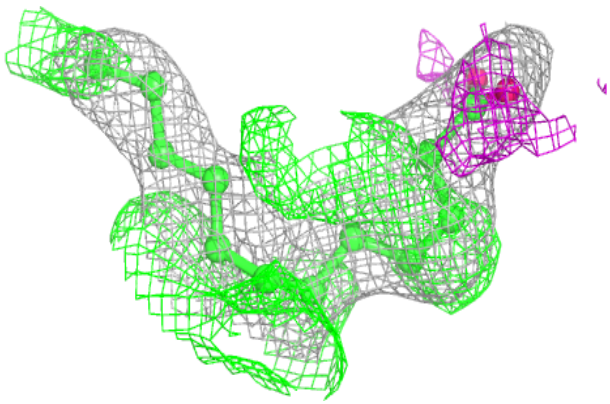


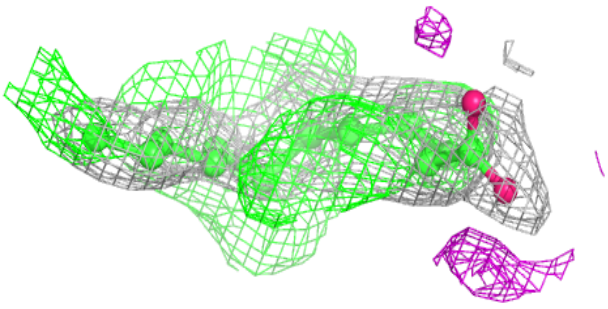


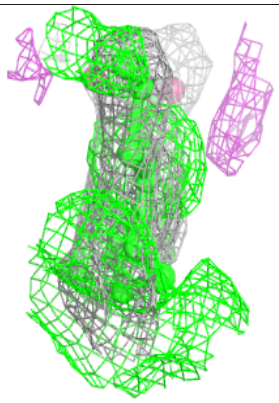


Electron density around DAO B 405:

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

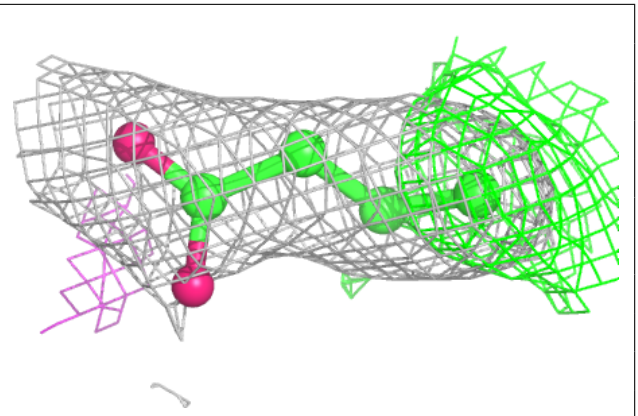


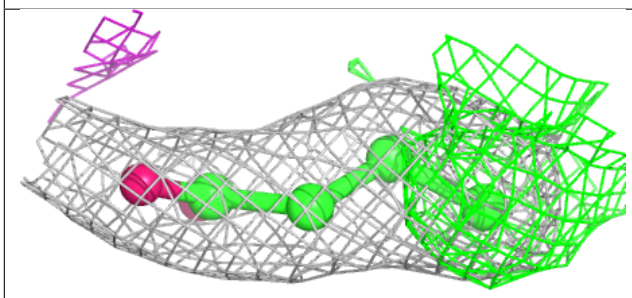


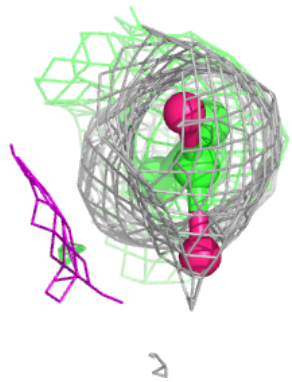


Electron density around BUA A 406:

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

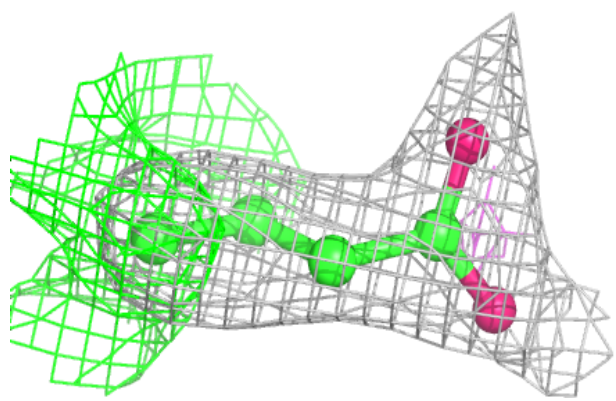


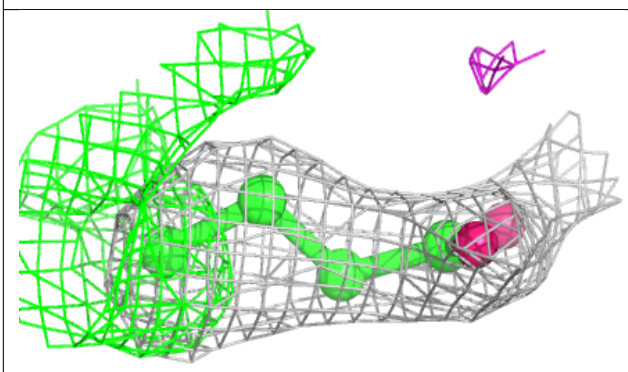


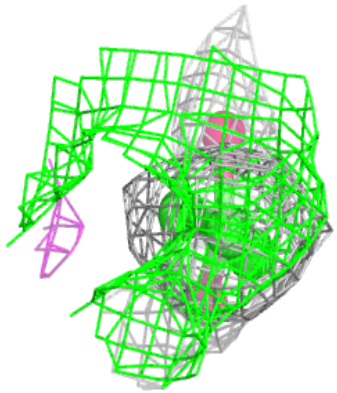


Electron density around BUA B 407:

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

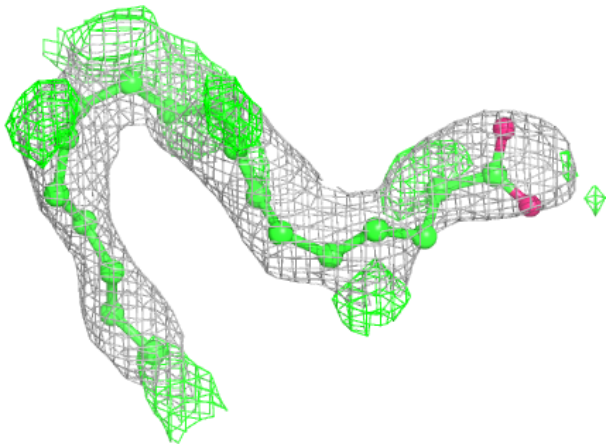


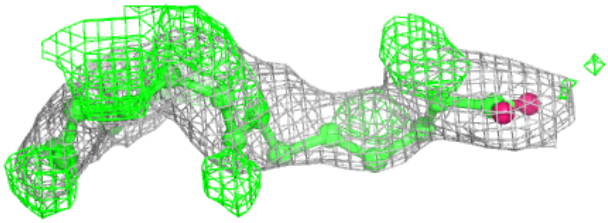


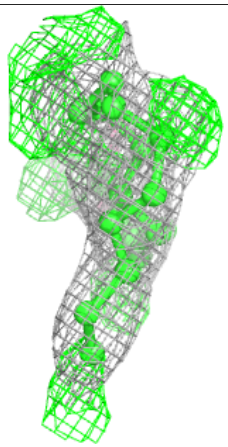


Electron density around STE B 406:

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

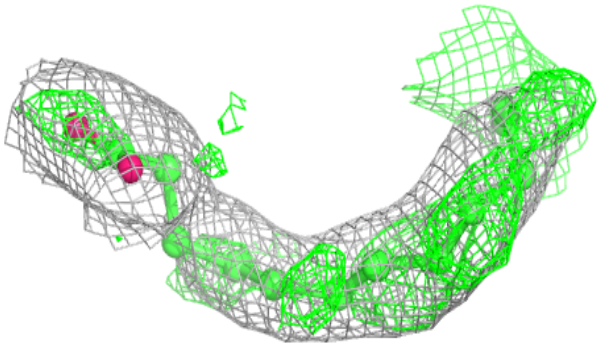


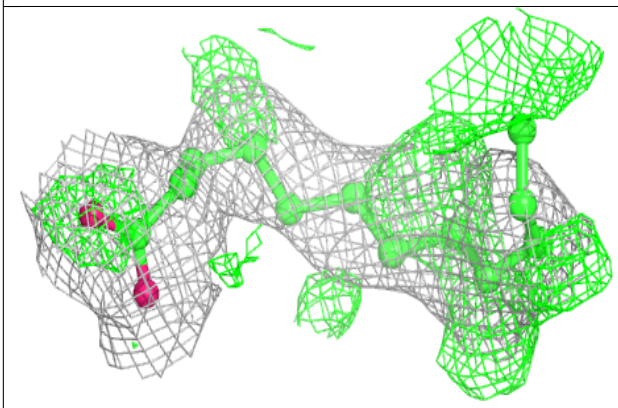


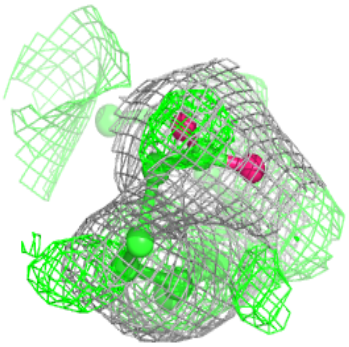


Electron density around DAO B 404:

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

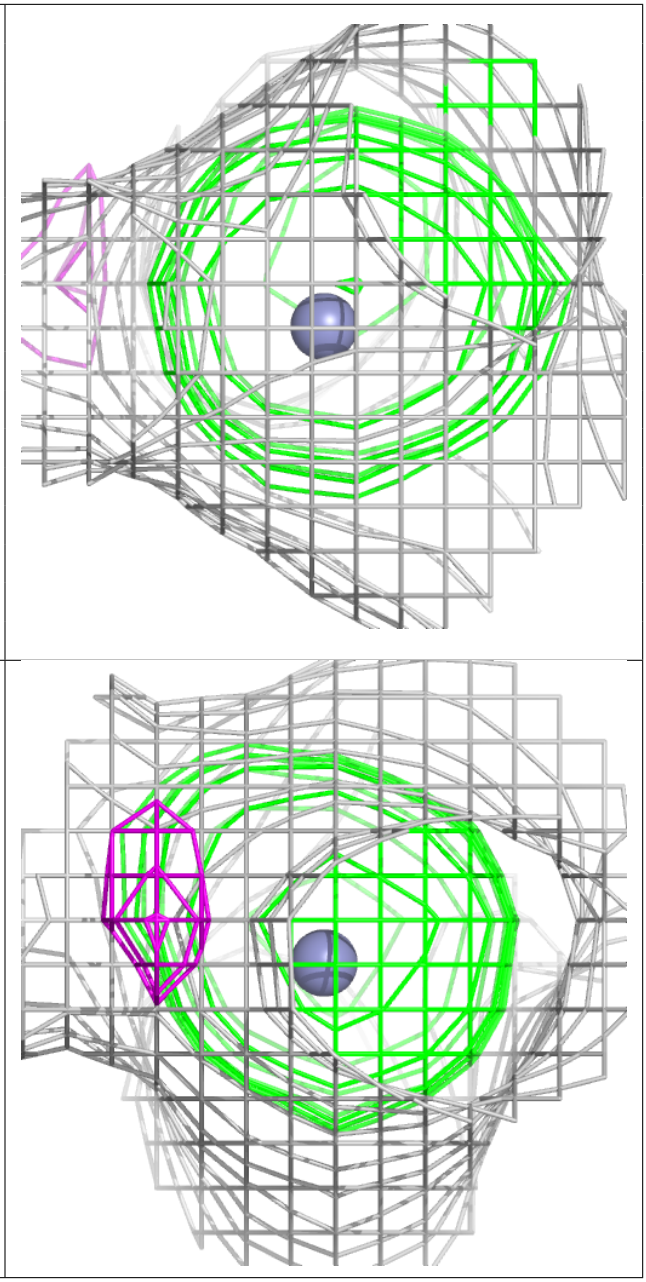






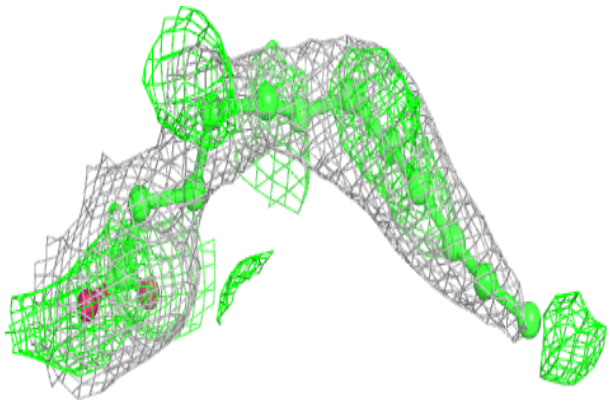
Electron density around ZN A 401:

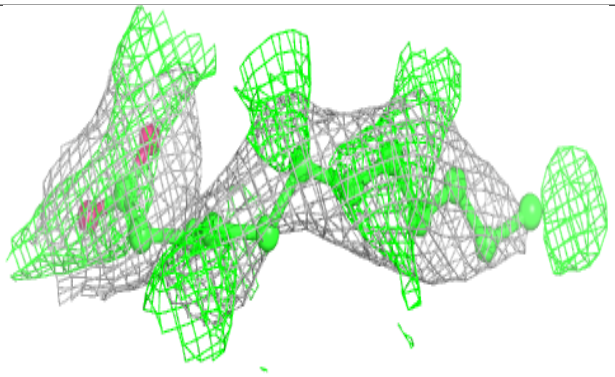
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

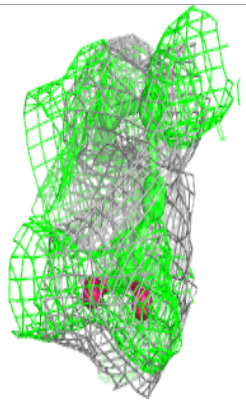


Electron density around DAO A 404:

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

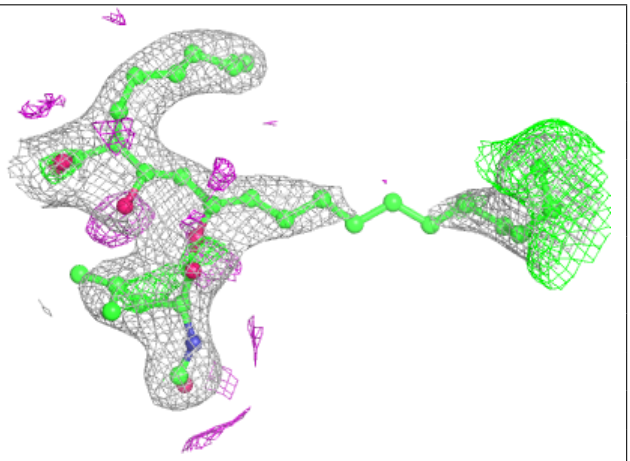


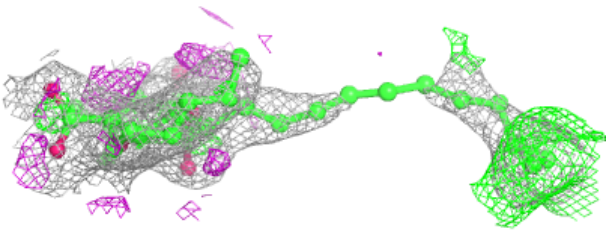


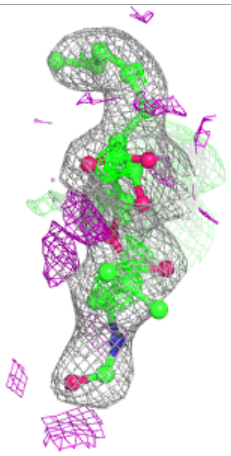


Electron density around DH9 A 403:

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

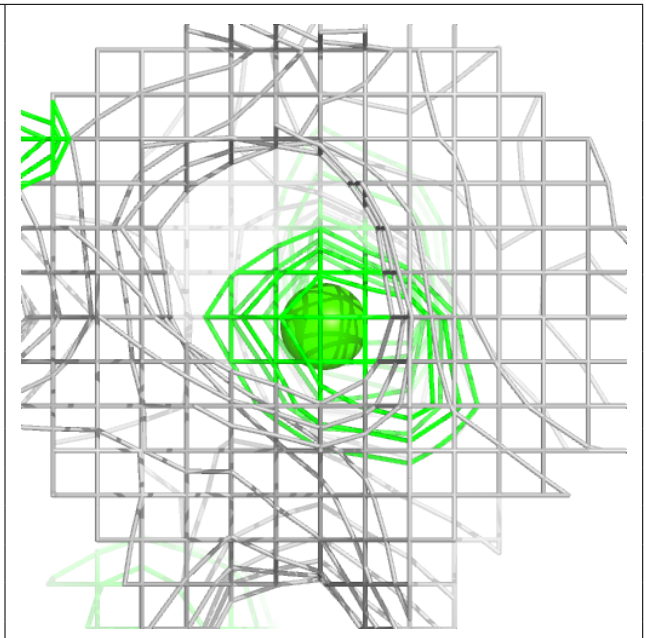


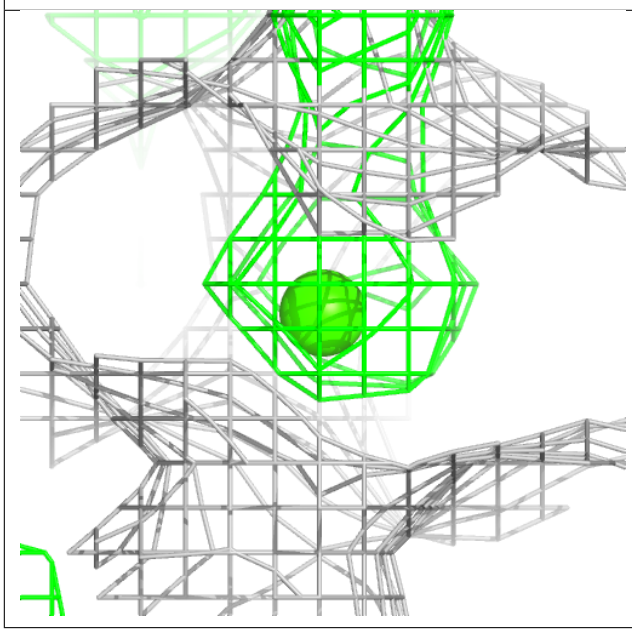


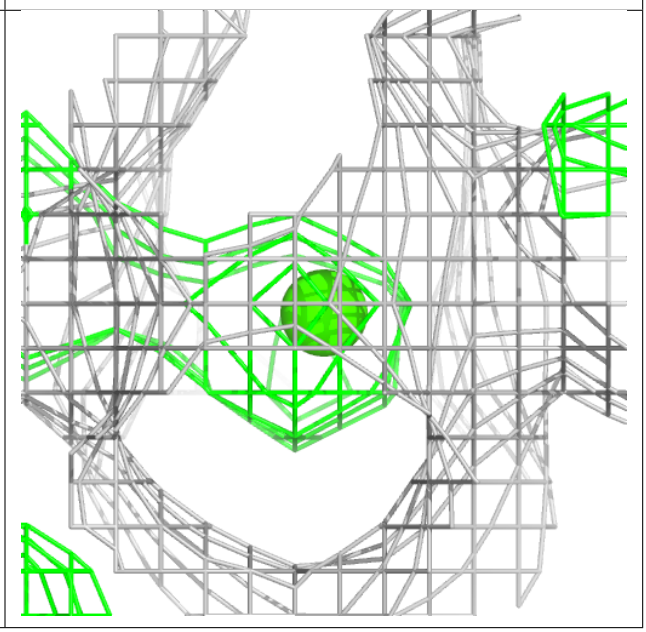


Electron density around CA A 402:

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

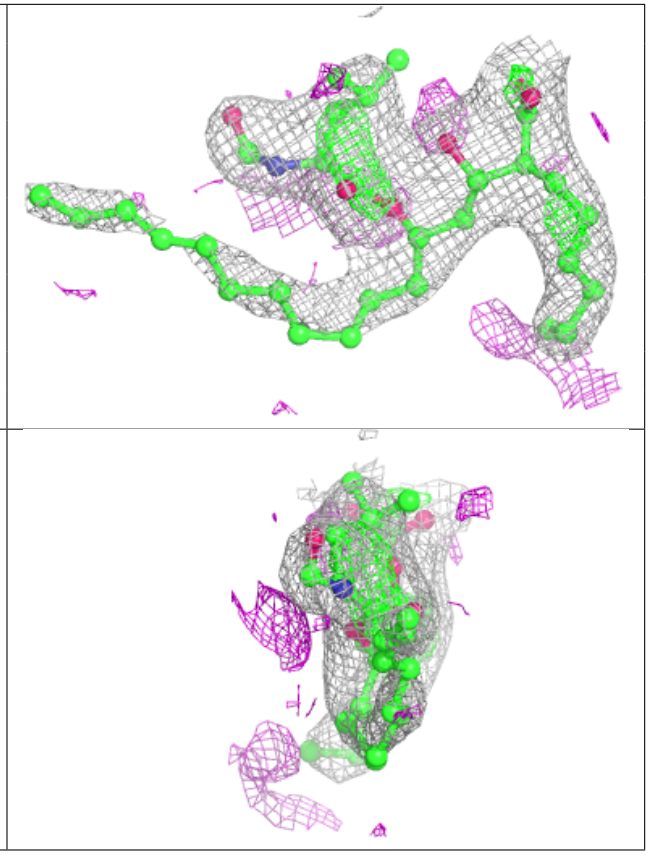


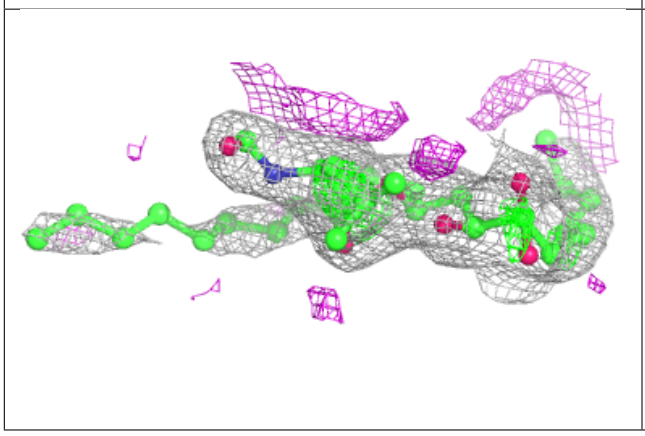




Electron density around DH9 B 403:

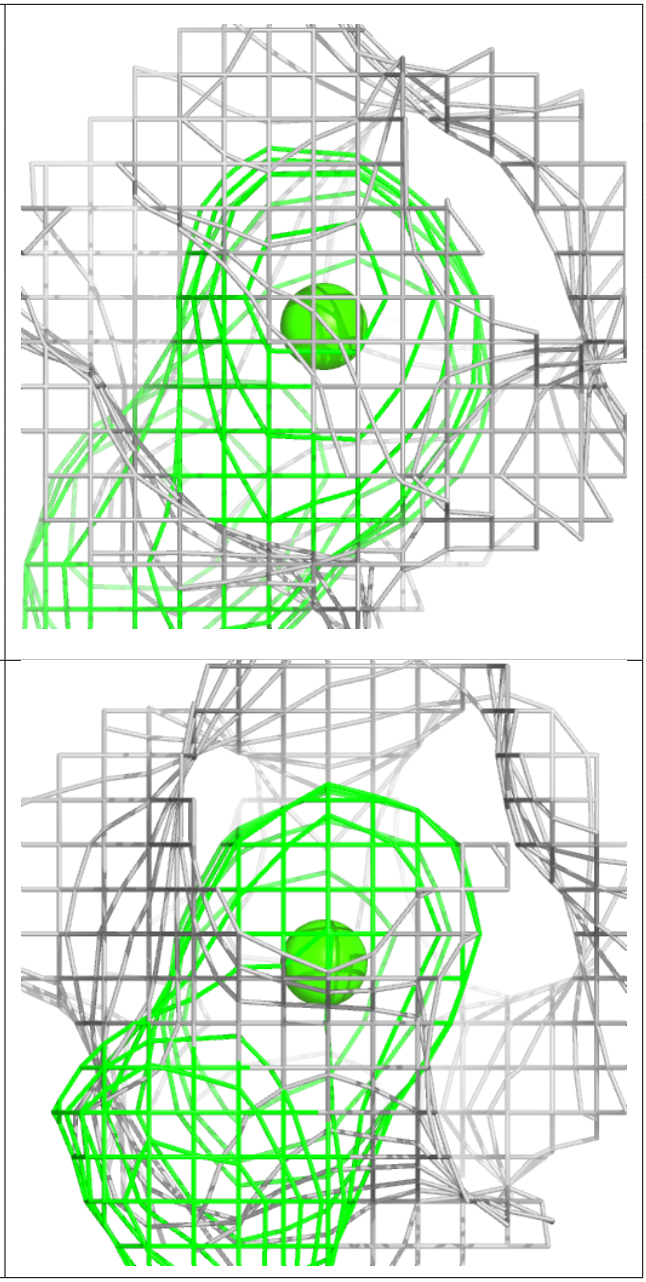
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





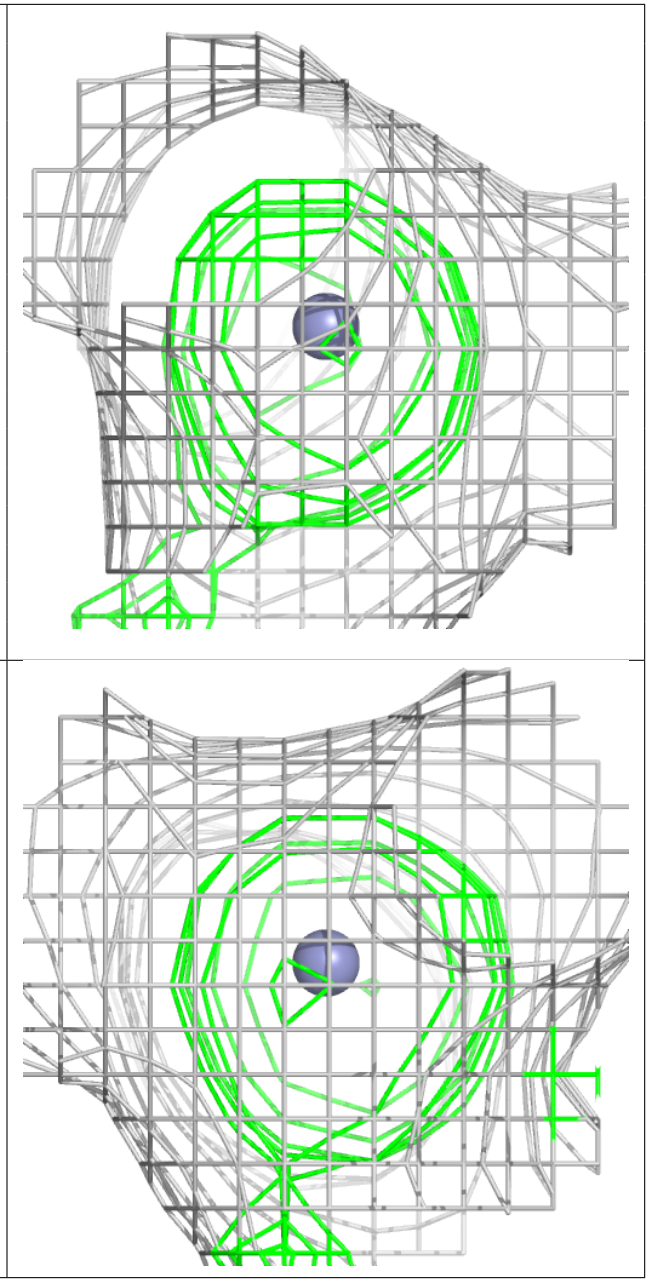
Electron density around CA B 402:

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



Electron density around ZN B 401:

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



6.5 Other polymers (i)

There are no such residues in this entry.