



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 03:01 AM BST

PDB ID : 6UTT  
Title : LarE, a sulfur transferase involved in synthesis of the cofactor for lactate racemase in complex with calcium  
Authors : Fellner, M.; Huizenga, K.; Hausinger, R.P.; Hu, J.  
Deposited on : 2019-10-29  
Resolution : 2.49 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.

---

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 : 2.13.1  
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) : 2.13.1

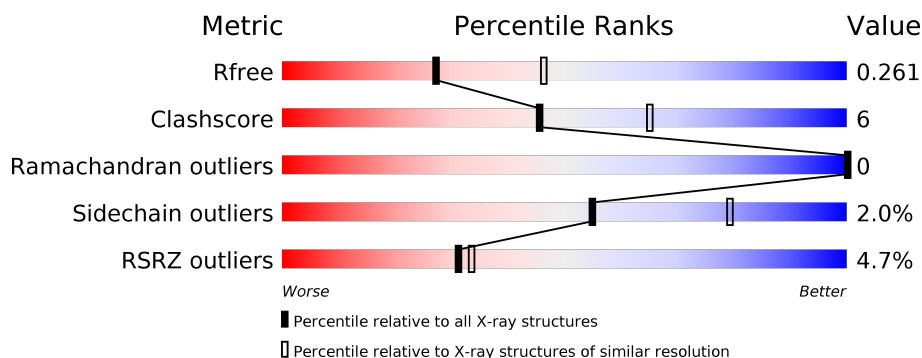
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	286	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>9%</div> </div> </div>
1	B	286	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>12%</div> <div>14%</div> </div> </div>
1	C	286	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>12%</div> <div>13%</div> </div> </div>
1	D	286	<div> <div>10%</div> <div> <div></div> <div>67%</div> <div>15%</div> <div>16%</div> </div> </div>
1	E	286	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>8%</div> </div> </div>
1	F	286	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>16%</div> <div>13%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	301	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11620 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 ATP-dependent sacrificial sulfur transferase LarE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1986	1250	345	384	7			
1	B	245	Total	C	N	O	S	0	0	0
			1877	1184	326	361	6			
1	C	249	Total	C	N	O	S	0	1	0
			1921	1209	338	368	6			
1	D	239	Total	C	N	O	S	0	0	0
			1797	1132	310	349	6			
1	E	262	Total	C	N	O	S	0	0	0
			1974	1248	341	378	7			
1	F	250	Total	C	N	O	S	0	0	0
			1916	1207	334	369	6			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	277	ALA	-	expression tag	UNP A0A0G9FES3
A	278	SER	-	expression tag	UNP A0A0G9FES3
A	279	TRP	-	expression tag	UNP A0A0G9FES3
A	280	SER	-	expression tag	UNP A0A0G9FES3
A	281	HIS	-	expression tag	UNP A0A0G9FES3
A	282	PRO	-	expression tag	UNP A0A0G9FES3
A	283	GLN	-	expression tag	UNP A0A0G9FES3
A	284	PHE	-	expression tag	UNP A0A0G9FES3
A	285	GLU	-	expression tag	UNP A0A0G9FES3
A	286	LYS	-	expression tag	UNP A0A0G9FES3
B	277	ALA	-	expression tag	UNP A0A0G9FES3
B	278	SER	-	expression tag	UNP A0A0G9FES3
B	279	TRP	-	expression tag	UNP A0A0G9FES3
B	280	SER	-	expression tag	UNP A0A0G9FES3
B	281	HIS	-	expression tag	UNP A0A0G9FES3
B	282	PRO	-	expression tag	UNP A0A0G9FES3
B	283	GLN	-	expression tag	UNP A0A0G9FES3

*Continued on next page...*

*Continued from previous page...*

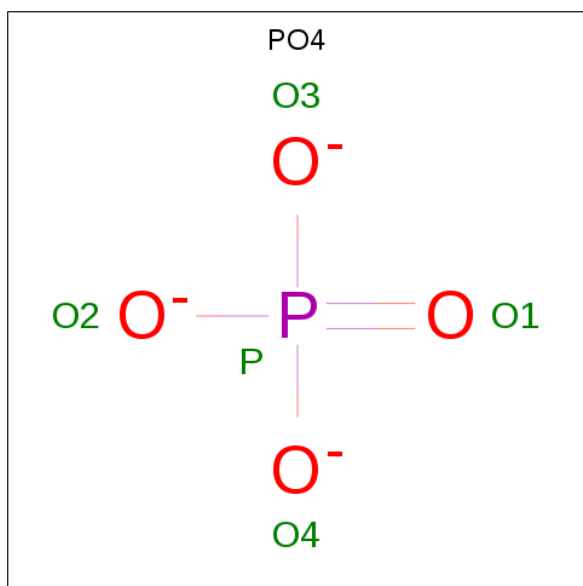
Chain	Residue	Modelled	Actual	Comment	Reference
B	284	PHE	-	expression tag	UNP A0A0G9FES3
B	285	GLU	-	expression tag	UNP A0A0G9FES3
B	286	LYS	-	expression tag	UNP A0A0G9FES3
C	277	ALA	-	expression tag	UNP A0A0G9FES3
C	278	SER	-	expression tag	UNP A0A0G9FES3
C	279	TRP	-	expression tag	UNP A0A0G9FES3
C	280	SER	-	expression tag	UNP A0A0G9FES3
C	281	HIS	-	expression tag	UNP A0A0G9FES3
C	282	PRO	-	expression tag	UNP A0A0G9FES3
C	283	GLN	-	expression tag	UNP A0A0G9FES3
C	284	PHE	-	expression tag	UNP A0A0G9FES3
C	285	GLU	-	expression tag	UNP A0A0G9FES3
C	286	LYS	-	expression tag	UNP A0A0G9FES3
D	277	ALA	-	expression tag	UNP A0A0G9FES3
D	278	SER	-	expression tag	UNP A0A0G9FES3
D	279	TRP	-	expression tag	UNP A0A0G9FES3
D	280	SER	-	expression tag	UNP A0A0G9FES3
D	281	HIS	-	expression tag	UNP A0A0G9FES3
D	282	PRO	-	expression tag	UNP A0A0G9FES3
D	283	GLN	-	expression tag	UNP A0A0G9FES3
D	284	PHE	-	expression tag	UNP A0A0G9FES3
D	285	GLU	-	expression tag	UNP A0A0G9FES3
D	286	LYS	-	expression tag	UNP A0A0G9FES3
E	277	ALA	-	expression tag	UNP A0A0G9FES3
E	278	SER	-	expression tag	UNP A0A0G9FES3
E	279	TRP	-	expression tag	UNP A0A0G9FES3
E	280	SER	-	expression tag	UNP A0A0G9FES3
E	281	HIS	-	expression tag	UNP A0A0G9FES3
E	282	PRO	-	expression tag	UNP A0A0G9FES3
E	283	GLN	-	expression tag	UNP A0A0G9FES3
E	284	PHE	-	expression tag	UNP A0A0G9FES3
E	285	GLU	-	expression tag	UNP A0A0G9FES3
E	286	LYS	-	expression tag	UNP A0A0G9FES3
F	277	ALA	-	expression tag	UNP A0A0G9FES3
F	278	SER	-	expression tag	UNP A0A0G9FES3
F	279	TRP	-	expression tag	UNP A0A0G9FES3
F	280	SER	-	expression tag	UNP A0A0G9FES3
F	281	HIS	-	expression tag	UNP A0A0G9FES3
F	282	PRO	-	expression tag	UNP A0A0G9FES3
F	283	GLN	-	expression tag	UNP A0A0G9FES3
F	284	PHE	-	expression tag	UNP A0A0G9FES3
F	285	GLU	-	expression tag	UNP A0A0G9FES3

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	286	LYS	-	expression tag	UNP A0A0G9FES3

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	12	Total	O	0	0
			12	12		

*Continued on next page...*

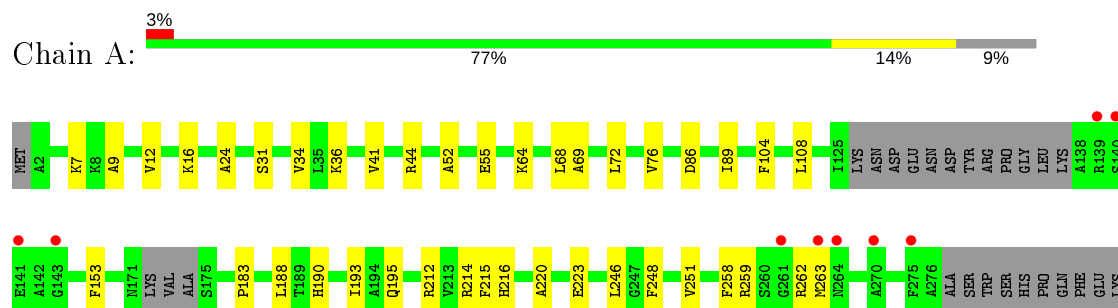
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	22	Total 22	O 22	0	0
5	C	15	Total 15	O 15	0	0
5	D	13	Total 13	O 13	0	0
5	E	13	Total 13	O 13	0	0
5	F	12	Total 12	O 12	0	0

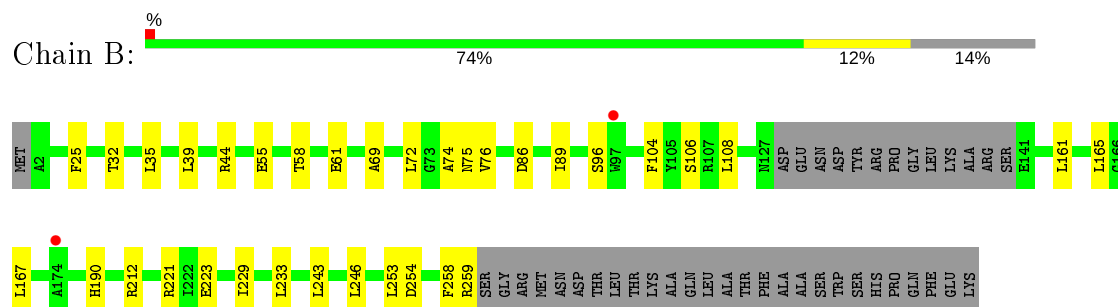
### 3 Residue-property plots [i](#)

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.

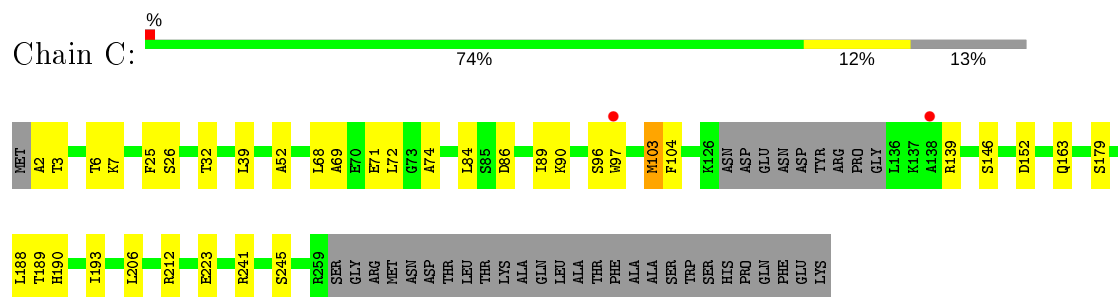
- Molecule 1: ATP-dependent sacrificial sulfur transferase LarE



- Molecule 1: ATP-dependent sacrificial sulfur transferase LarE

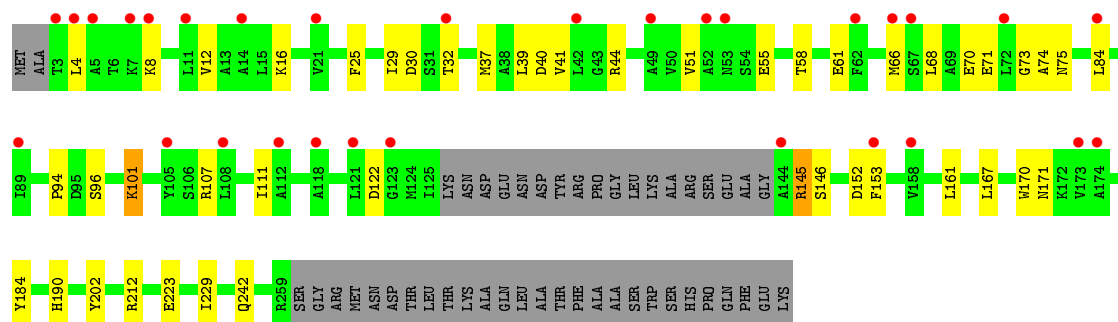


- Molecule 1: ATP-dependent sacrificial sulfur transferase LarE

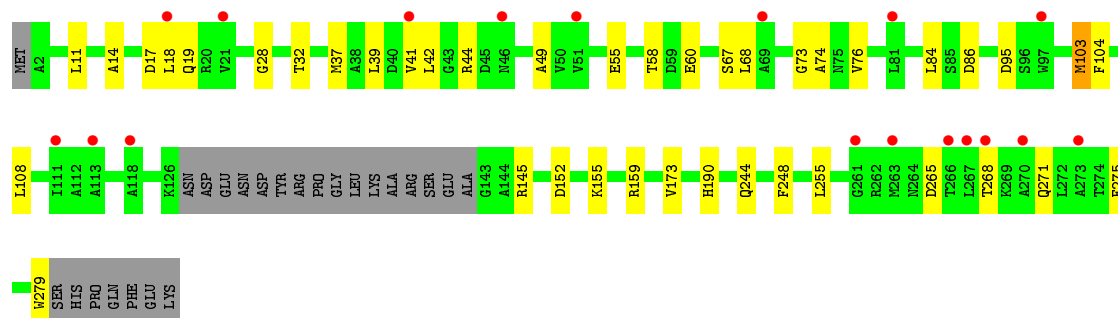
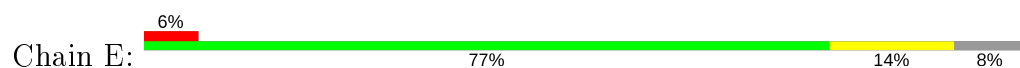


- Molecule 1: ATP-dependent sacrificial sulfur transferase LarE

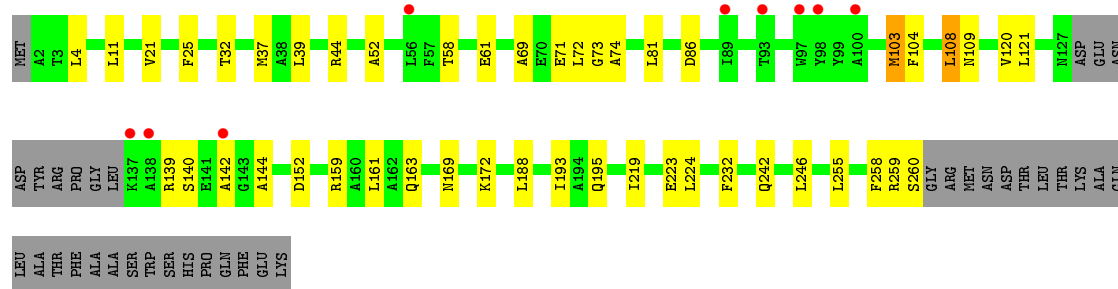




- Molecule 1: ATP-dependent sacrificial sulfur transferase LarE



- Molecule 1: ATP-dependent sacrificial sulfur transferase LarE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.66 Å 107.66 Å 320.42 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.49 – 2.49 48.15 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.0 (38.49-2.49) 98.4 (48.15-2.49)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.12 (at 2.48 Å)	Xtriage
Refinement program	PHENIX 1.17.1-3660	Depositor
R, $R_{free}$	0.202 , 0.256 0.207 , 0.261	Depositor DCC
$R_{free}$ test set	3302 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.1	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11620	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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: PO4, CA, SO4

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	0.43	0/2015	0.58	0/2729
1	B	0.45	0/1906	0.64	0/2585
1	C	0.44	0/1950	0.60	0/2641
1	D	0.40	0/1826	0.58	0/2482
1	E	0.45	0/2006	0.62	0/2726
1	F	0.44	0/1945	0.62	0/2634
All	All	0.44	0/11648	0.61	0/15797

There are no bond length outliers.

There are no bond angle outliers.

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	1986	0	1941	29	0
1	B	1877	0	1834	20	0
1	C	1921	0	1891	20	0
1	D	1797	0	1703	30	0
1	E	1974	0	1906	25	0
1	F	1916	0	1878	29	0
2	A	5	0	0	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	1	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	1	0
3	D	5	0	0	1	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	12	0	0	0	0
5	B	22	0	0	0	0
5	C	15	0	0	0	0
5	D	13	0	0	0	0
5	E	13	0	0	0	0
5	F	12	0	0	0	0
All	All	11620	0	11153	144	0

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

All (144) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:THR:HG23	1:D:61:GLU:HB3	1.72	0.72
1:D:4:LEU:HD21	1:D:161:LEU:HG	1.72	0.71
1:D:122:ASP:OD1	1:D:146:SER:OG	2.09	0.70
1:A:44:ARG:NH1	1:A:44:ARG:HB3	2.07	0.70
1:E:55:GLU:OE2	1:E:190:HIS:NE2	2.28	0.67
1:F:139:ARG:HG2	1:F:144:ALA:HB3	1.76	0.67
1:D:70:GLU:O	1:D:73:GLY:N	2.28	0.64
1:B:39:LEU:HD11	1:B:74:ALA:HB2	1.80	0.64
1:A:9:ALA:HA	1:A:12:VAL:HG22	1.79	0.63
1:B:104:PHE:O	1:B:108:LEU:HD12	1.99	0.63
1:C:26:SER:OG	3:C:302:SO4:O2	2.17	0.62
1:A:259:ARG:HD2	1:A:262:ARG:HH21	1.65	0.62
1:D:167:LEU:HD23	1:F:163:GLN:HG3	1.83	0.61
1:A:259:ARG:HD2	1:A:262:ARG:NH2	2.15	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:LEU:HD23	1:F:193:ILE:HD11	1.84	0.60
1:D:39:LEU:HD11	1:D:74:ALA:HB2	1.83	0.59
1:A:44:ARG:HB3	1:A:44:ARG:HH11	1.67	0.58
1:A:212:ARG:NE	2:A:301:PO4:O2	2.23	0.58
1:D:58:THR:HG23	1:D:61:GLU:H	1.69	0.58
1:D:71:GLU:OE2	1:F:159:ARG:HD2	2.03	0.57
1:A:36:LYS:HB2	1:A:72:LEU:HD21	1.88	0.56
1:E:86:ASP:HB2	1:E:103:MET:HE1	1.86	0.56
1:C:89:ILE:HA	1:C:96:SER:HB3	1.88	0.55
1:A:44:ARG:CB	1:A:44:ARG:HH11	2.21	0.54
1:E:104:PHE:O	1:E:108:LEU:HD12	2.08	0.54
1:A:52:ALA:HB2	1:A:104:PHE:HE2	1.72	0.53
1:D:55:GLU:CD	1:D:190:HIS:HD1	2.12	0.53
1:B:55:GLU:OE2	1:B:190:HIS:ND1	2.29	0.53
1:F:44:ARG:NH1	1:F:73:GLY:O	2.42	0.53
1:A:259:ARG:NH1	2:A:301:PO4:O3	2.38	0.52
1:D:30:ASP:HB2	3:D:302:SO4:O4	2.10	0.52
1:F:32:THR:HG23	1:F:72:LEU:HD11	1.92	0.52
1:D:25:PHE:HE1	1:D:32:THR:HA	1.74	0.52
1:E:18:LEU:HD11	1:E:145:ARG:HH12	1.74	0.51
1:F:139:ARG:NH2	1:F:140:SER:OG	2.43	0.51
1:C:68:LEU:HA	1:C:71:GLU:HG2	1.92	0.51
1:C:139:ARG:NH1	1:C:146:SER:OG	2.43	0.51
1:A:262:ARG:HH11	1:A:262:ARG:HG3	1.75	0.51
1:B:32:THR:HG22	1:B:167:LEU:HD13	1.93	0.51
1:D:51:VAL:HG21	1:D:66:MET:HG2	1.93	0.50
1:F:25:PHE:CD2	1:F:69:ALA:HB2	2.47	0.50
1:B:86:ASP:HB3	1:B:89:ILE:HD12	1.93	0.50
1:E:14:ALA:O	1:E:18:LEU:HD13	2.12	0.50
1:E:28:GLY:O	1:E:32:THR:HG23	2.12	0.49
1:F:195:GLN:HG3	1:F:246:LEU:O	2.12	0.49
1:E:44:ARG:HD2	1:E:73:GLY:O	2.12	0.49
1:C:90:LYS:HE3	1:C:188:LEU:O	2.12	0.49
1:F:108:LEU:HB3	1:F:120:VAL:HG11	1.94	0.48
1:A:86:ASP:HB3	1:A:89:ILE:HD12	1.96	0.48
1:A:263:MET:HB3	1:C:206:LEU:HD23	1.96	0.47
1:D:25:PHE:HB3	1:D:51:VAL:HG12	1.95	0.47
1:E:155:LYS:O	1:E:159:ARG:HD3	2.14	0.47
1:D:101:LYS:HA	1:D:101:LYS:HD2	1.65	0.47
1:C:39:LEU:HD11	1:C:74:ALA:HB2	1.96	0.47
1:F:139:ARG:CG	1:F:144:ALA:HB3	2.45	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:MET:O	1:D:41:VAL:HG23	2.15	0.47
1:E:11:LEU:HD21	1:E:37:MET:HG3	1.96	0.46
1:A:16:LYS:HG3	1:A:41:VAL:CG1	2.45	0.46
1:E:41:VAL:HG23	1:E:42:LEU:HG	1.96	0.46
1:F:21:VAL:HG11	1:F:121:LEU:HD11	1.97	0.46
1:C:245:SER:HB3	1:E:275:PHE:HZ	1.81	0.46
1:D:68:LEU:HD21	1:D:170:TRP:HA	1.97	0.46
1:F:58:THR:HG23	1:F:61:GLU:H	1.80	0.46
1:A:195:GLN:HG3	1:A:246:LEU:O	2.16	0.45
1:E:58:THR:HG22	1:E:60:GLU:HG3	1.98	0.45
1:E:19:GLN:HA	1:E:42:LEU:HD22	1.98	0.45
1:A:188:LEU:HD23	1:A:193:ILE:HD11	1.98	0.45
1:D:202:TYR:CD2	1:D:242:GLN:HG2	2.51	0.45
1:E:44:ARG:HB3	1:E:44:ARG:HE	1.46	0.45
1:B:35:LEU:HD23	1:B:72:LEU:HD12	1.99	0.45
1:D:153:PHE:CE1	1:D:161:LEU:HD12	2.52	0.45
1:B:58:THR:OG1	1:B:61:GLU:HG3	2.16	0.45
1:C:32:THR:HG23	1:C:72:LEU:HD11	1.99	0.45
1:F:4:LEU:HD11	1:F:161:LEU:HB2	1.99	0.45
1:A:64:LYS:O	1:A:68:LEU:HD13	2.16	0.45
1:B:89:ILE:HA	1:B:96:SER:HB2	1.98	0.45
1:B:221:ARG:HD2	1:B:254:ASP:OD1	2.17	0.44
1:C:2:ALA:HB1	1:C:6:THR:HB	1.98	0.44
1:A:214:ARG:HE	1:A:223:GLU:CD	2.20	0.44
1:A:220:ALA:HB2	1:A:248:PHE:CD1	2.52	0.44
1:D:107:ARG:O	1:D:111:ILE:HG13	2.17	0.44
1:B:259:ARG:NH2	2:B:301:PO4:O3	2.43	0.44
1:D:8:LYS:HB2	1:D:161:LEU:HD11	1.99	0.44
1:E:39:LEU:HD11	1:E:74:ALA:HB2	2.00	0.44
1:A:7:LYS:HB3	1:A:153:PHE:CE1	2.52	0.44
1:E:173:VAL:HG13	1:E:173:VAL:O	2.17	0.44
1:E:244:GLN:HA	1:E:248:PHE:O	2.18	0.44
1:B:212:ARG:HB2	1:B:223:GLU:HB2	1.99	0.44
1:A:24:ALA:HB2	1:A:108:LEU:HD21	2.00	0.43
1:C:86:ASP:HB2	1:C:103:MET:HE1	1.99	0.43
1:C:86:ASP:HB3	1:C:89:ILE:HD12	2.01	0.43
1:E:255:LEU:HD23	1:E:255:LEU:HA	1.83	0.43
1:F:71:GLU:OE1	1:F:169:ASN:ND2	2.51	0.43
1:C:52:ALA:HB2	1:C:104:PHE:HE2	1.82	0.43
1:B:233:LEU:HD11	1:D:229:ILE:HG22	2.00	0.43
1:A:223:GLU:HB3	1:A:258:PHE:HA	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:LEU:HD12	1:C:190:HIS:CE1	2.54	0.43
1:D:55:GLU:OE1	1:D:84:LEU:HD22	2.18	0.43
1:F:52:ALA:HB2	1:F:104:PHE:HE2	1.82	0.43
1:F:258:PHE:CE1	1:F:259:ARG:HG3	2.52	0.43
1:F:109:ASN:OD1	1:F:142:ALA:HB1	2.18	0.43
1:B:25:PHE:CD1	1:B:69:ALA:HB2	2.53	0.43
1:B:243:LEU:HA	1:B:246:LEU:HD12	2.00	0.43
1:E:58:THR:CG2	1:E:60:GLU:HG3	2.48	0.43
1:D:94:PRO:HA	1:D:184:TYR:CE2	2.53	0.42
1:A:55:GLU:OE2	1:A:190:HIS:ND1	2.32	0.42
1:D:145:ARG:HB3	1:D:145:ARG:HE	1.69	0.42
1:F:223:GLU:HB3	1:F:258:PHE:HA	2.01	0.42
1:A:259:ARG:HH12	2:A:301:PO4:P	2.43	0.42
1:B:223:GLU:HB3	1:B:258:PHE:HA	2.01	0.42
1:D:212:ARG:HB2	1:D:223:GLU:HB2	2.01	0.42
1:C:241:ARG:HD2	1:E:271:GLN:OE1	2.20	0.42
1:B:69:ALA:HB3	1:B:76:VAL:HG21	2.02	0.42
1:F:86:ASP:HB2	1:F:103:MET:HE1	2.01	0.42
1:F:108:LEU:HD12	1:F:120:VAL:HG13	2.00	0.42
1:E:265:ASP:HB2	1:F:242:GLN:OE1	2.18	0.42
1:B:44:ARG:NH1	1:B:75:ASN:OD1	2.53	0.42
1:B:25:PHE:CE1	1:B:69:ALA:HB2	2.55	0.41
1:C:25:PHE:CD2	1:C:69:ALA:HB2	2.56	0.41
1:A:69:ALA:HB1	1:A:76:VAL:HG22	2.02	0.41
1:C:189:THR:O	1:C:193:ILE:HG13	2.21	0.41
1:C:212:ARG:HB2	1:C:223:GLU:HB2	2.01	0.41
1:D:68:LEU:CD2	1:D:170:TRP:HA	2.50	0.41
1:F:25:PHE:CE2	1:F:69:ALA:HB2	2.55	0.41
1:A:216:HIS:CG	1:F:219:ILE:HD11	2.55	0.41
1:B:229:ILE:HG23	1:B:253:LEU:HD21	2.03	0.41
1:C:25:PHE:HE1	1:C:32:THR:HA	1.86	0.41
1:D:12:VAL:O	1:D:16:LYS:N	2.50	0.41
1:E:265:ASP:OD1	1:E:268:THR:OG1	2.36	0.41
1:F:39:LEU:HD11	1:F:74:ALA:HB2	2.02	0.41
1:B:161:LEU:O	1:B:165:LEU:HG	2.21	0.41
1:F:11:LEU:HD21	1:F:37:MET:HG3	2.03	0.41
1:A:183:PRO:HD3	1:A:215:PHE:O	2.21	0.41
1:A:31:SER:HA	1:A:34:VAL:HG12	2.03	0.41
1:C:3:THR:O	1:C:7:LYS:HG3	2.21	0.41
1:A:251:VAL:HG12	1:F:255:LEU:HD12	2.02	0.41
1:D:29:ILE:HD12	1:D:170:TRP:CE2	2.55	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:81:LEU:HD11	1:F:104:PHE:HA	2.03	0.40
1:D:39:LEU:HD23	1:D:44:ARG:HA	2.03	0.40
1:E:68:LEU:HD23	1:E:68:LEU:N	2.35	0.40
1:F:224:LEU:HD11	1:F:232:PHE:CD1	2.56	0.40
1:E:84:LEU:HD23	1:E:84:LEU:HA	1.82	0.40
1:D:4:LEU:CD2	1:D:161:LEU:HG	2.46	0.40
1:E:49:ALA:O	1:E:76:VAL:HA	2.21	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	254/286 (89%)	250 (98%)	4 (2%)	0	100	100
1	B	241/286 (84%)	233 (97%)	8 (3%)	0	100	100
1	C	246/286 (86%)	240 (98%)	6 (2%)	0	100	100
1	D	235/286 (82%)	230 (98%)	5 (2%)	0	100	100
1	E	258/286 (90%)	251 (97%)	7 (3%)	0	100	100
1	F	246/286 (86%)	238 (97%)	8 (3%)	0	100	100
All	All	1480/1716 (86%)	1442 (97%)	38 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	205/236 (87%)	205 (100%)	0	100	100
1	B	194/236 (82%)	193 (100%)	1 (0%)	88	96
1	C	200/236 (85%)	195 (98%)	5 (2%)	47	73
1	D	180/236 (76%)	173 (96%)	7 (4%)	32	57
1	E	199/236 (84%)	193 (97%)	6 (3%)	41	68
1	F	198/236 (84%)	193 (98%)	5 (2%)	47	73
All	All	1176/1416 (83%)	1152 (98%)	24 (2%)	55	79

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	106	SER
1	C	97	TRP
1	C	103	MET
1	C	152	ASP
1	C	163	GLN
1	C	179	SER
1	D	40	ASP
1	D	75	ASN
1	D	96	SER
1	D	101	LYS
1	D	145	ARG
1	D	152	ASP
1	D	171	ASN
1	E	17	ASP
1	E	67	SER
1	E	95	ASP
1	E	103	MET
1	E	152	ASP
1	E	279	TRP
1	F	103	MET
1	F	108	LEU
1	F	152	ASP
1	F	172	LYS
1	F	260	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	$\# Z  > 2$
2	PO4	A	301	-	4,4,4	0.84	0	6,6,6	1.07	0
3	SO4	D	302	-	4,4,4	0.52	0	6,6,6	0.05	0
2	PO4	D	301	-	4,4,4	1.11	0	6,6,6	0.47	0
2	PO4	F	301	-	4,4,4	1.07	0	6,6,6	0.70	0
2	PO4	C	301	-	4,4,4	1.11	0	6,6,6	0.82	0
3	SO4	B	302	-	4,4,4	0.10	0	6,6,6	0.29	0
2	PO4	E	301	-	4,4,4	1.03	0	6,6,6	0.83	0
2	PO4	B	301	-	4,4,4	1.10	0	6,6,6	0.52	0
3	SO4	A	302	-	4,4,4	0.17	0	6,6,6	0.44	0
3	SO4	C	302	-	4,4,4	0.14	0	6,6,6	0.26	0
3	SO4	E	302	-	4,4,4	0.17	0	6,6,6	0.21	0
3	SO4	F	302	-	4,4,4	0.20	0	6,6,6	0.17	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	PO4	3	0
3	D	302	SO4	1	0
2	B	301	PO4	1	0
3	C	302	SO4	1	0

## 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	260/286 (90%)	0.33	9 (3%) 44 47	44, 71, 91, 109	0
1	B	245/286 (85%)	0.12	2 (0%) 86 87	40, 59, 76, 87	0
1	C	249/286 (87%)	0.09	2 (0%) 86 87	42, 59, 80, 99	0
1	D	239/286 (83%)	0.68	30 (12%) 3 3	43, 80, 112, 118	0
1	E	262/286 (91%)	0.49	18 (6%) 16 17	42, 79, 99, 109	0
1	F	250/286 (87%)	0.29	9 (3%) 42 46	45, 63, 84, 108	0
All	All	1505/1716 (87%)	0.33	70 (4%) 31 33	40, 65, 99, 118	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	8	LYS	5.0
1	A	140	SER	4.9
1	E	268	THR	4.8
1	D	4	LEU	4.4
1	B	97	TRP	4.3
1	F	142	ALA	3.9
1	D	158	VAL	3.8
1	E	113	ALA	3.7
1	A	270	ALA	3.7
1	E	267	LEU	3.6
1	E	18	LEU	3.6
1	D	144	ALA	3.5
1	D	105	TYR	3.4
1	D	112	ALA	3.3
1	E	263	MET	3.3
1	F	138	ALA	3.3
1	E	273	ALA	3.3
1	D	153	PHE	3.2
1	F	97	TRP	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	49	ALA	3.1
1	F	89	ILE	3.0
1	D	5	ALA	3.0
1	A	263	MET	2.9
1	A	261	GLY	2.9
1	E	111	ILE	2.8
1	D	53	ASN	2.8
1	D	173	VAL	2.7
1	E	46	ASN	2.7
1	C	97	TRP	2.7
1	D	7	LYS	2.7
1	A	139	ARG	2.7
1	D	52	ALA	2.6
1	D	108	LEU	2.6
1	E	21	VAL	2.6
1	E	41	VAL	2.5
1	A	275	PHE	2.5
1	A	141	GLU	2.4
1	E	261	GLY	2.4
1	D	42	LEU	2.4
1	D	118	ALA	2.4
1	F	98	TYR	2.4
1	D	174	ALA	2.4
1	D	67	SER	2.4
1	A	264	ASN	2.3
1	D	123	GLY	2.3
1	D	14	ALA	2.3
1	E	81	LEU	2.3
1	D	62	PHE	2.3
1	D	72	LEU	2.2
1	F	100	ALA	2.2
1	F	93	THR	2.2
1	E	97	TRP	2.2
1	D	21	VAL	2.2
1	D	3	THR	2.2
1	D	84	LEU	2.2
1	F	56	LEU	2.2
1	A	143	GLY	2.1
1	E	270	ALA	2.1
1	D	89	ILE	2.1
1	E	266	THR	2.1
1	C	138	ALA	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	118	ALA	2.1
1	F	137	LYS	2.1
1	D	32	THR	2.1
1	D	11	LEU	2.1
1	D	121	LEU	2.1
1	B	174	ALA	2.0
1	E	51	VAL	2.0
1	E	69	ALA	2.0
1	D	66	MET	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](#)

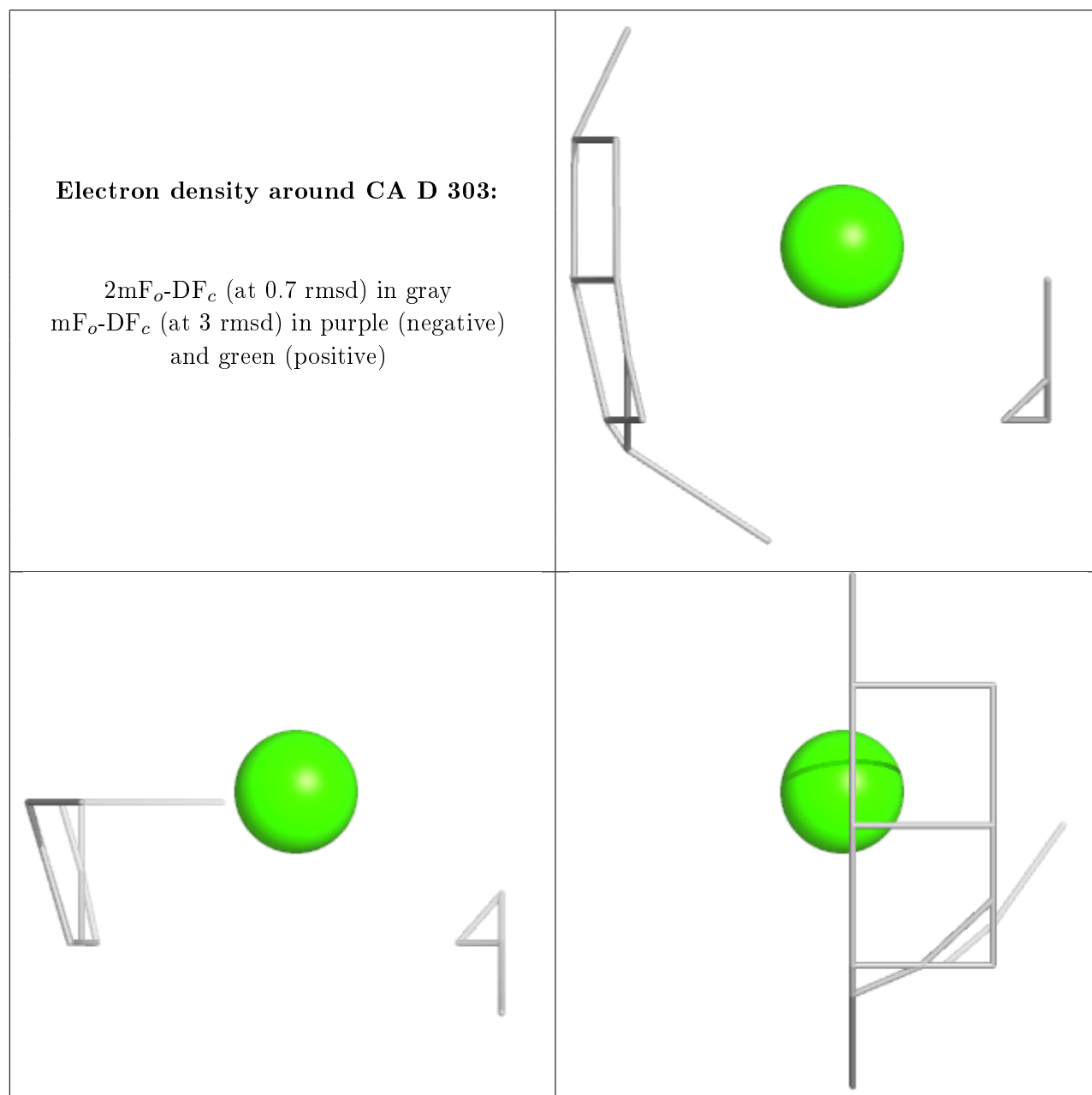
There are no monosaccharides in this entry.

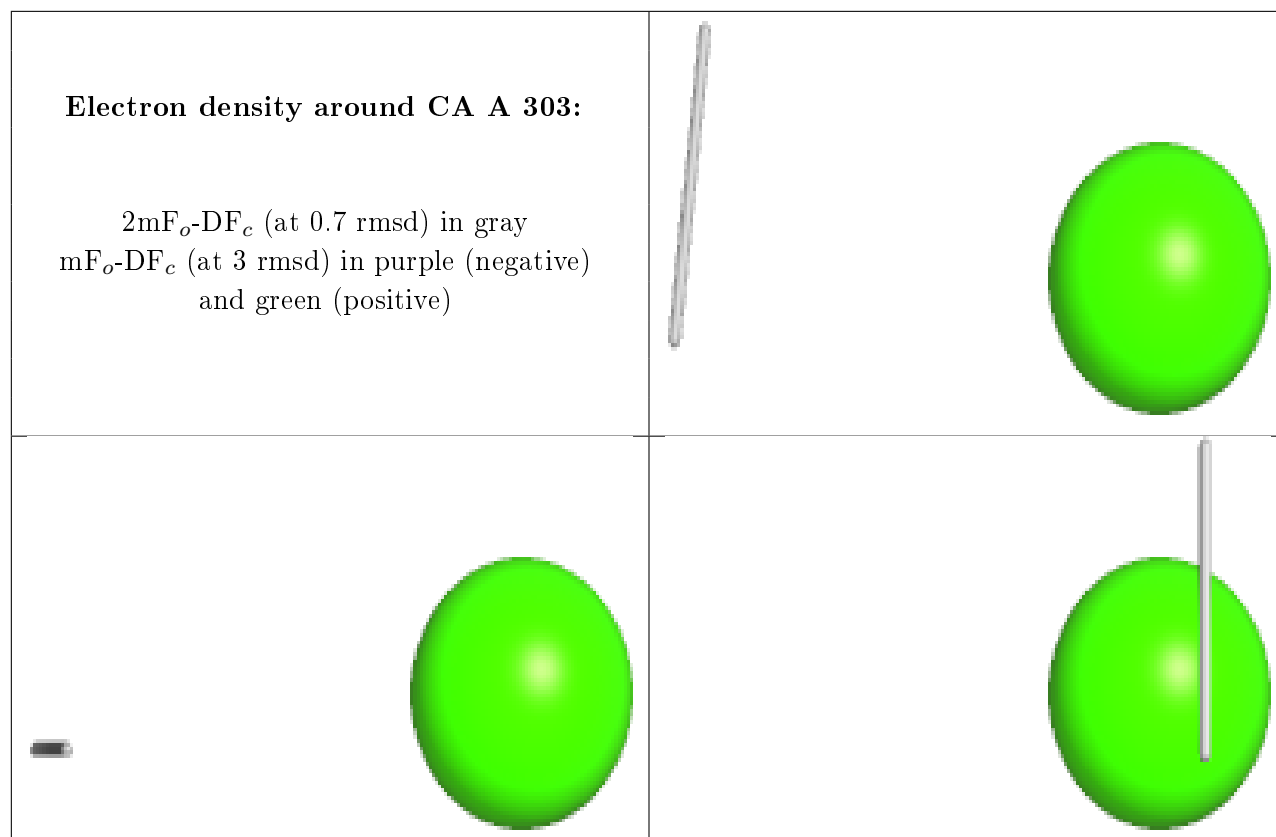
## 6.4 Ligands [i](#)

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, 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(Å <sup>2</sup> )	Q<0.9
3	SO4	A	302	5/5	0.90	0.21	66,70,71,76	5
4	CA	D	303	1/1	0.90	0.12	63,63,63,63	1
3	SO4	D	302	5/5	0.91	0.11	100,103,105,113	5
3	SO4	E	302	5/5	0.92	0.10	68,82,92,92	5
3	SO4	B	302	5/5	0.95	0.16	53,62,72,73	5
4	CA	A	303	1/1	0.95	0.09	65,65,65,65	1
3	SO4	F	302	5/5	0.95	0.14	58,64,73,75	5
3	SO4	C	302	5/5	0.97	0.16	57,61,66,71	5
2	PO4	C	301	5/5	0.98	0.16	53,56,59,62	0
2	PO4	A	301	5/5	0.98	0.14	53,58,63,63	0
2	PO4	D	301	5/5	0.98	0.15	54,60,70,71	0
2	PO4	F	301	5/5	0.98	0.17	60,64,66,67	0
2	PO4	E	301	5/5	0.99	0.19	50,51,56,62	0
2	PO4	B	301	5/5	0.99	0.16	46,51,56,56	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.