



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:30 pm BST

PDB ID : 6UTQ  
Title : LarE, a sulfur transferase involved in synthesis of the cofactor for lactate racemase in complex with cadmium  
Authors : Fellner, M.; Huizenga, K.; Hausinger, R.P.; Hu, J.  
Deposited on : 2019-10-29  
Resolution : 2.39 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

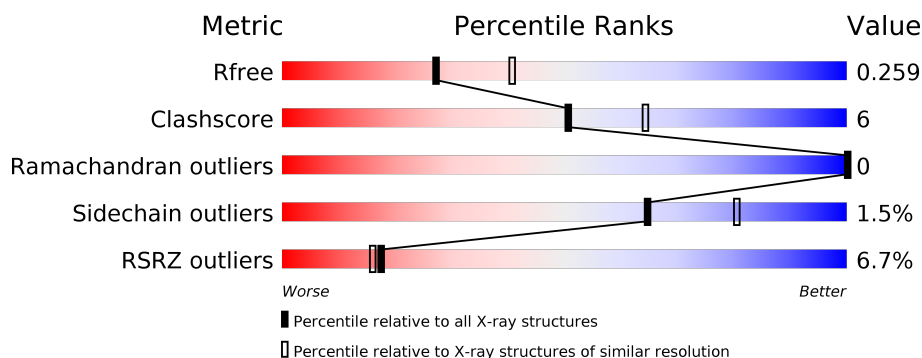
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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>6%</div> <div> <div></div> <div>72%</div> <div>13%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	286	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>9%</div> <div></div> <div>14%</div> </div> </div>
1	C	286	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>11%</div> <div></div> <div>13%</div> </div> </div>
1	D	286	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>9%</div> <div>•</div> <div>16%</div> </div> </div>
1	E	286	<div> <div>15%</div> <div> <div></div> <div>67%</div> <div>17%</div> <div></div> <div>16%</div> </div> </div>
1	F	286	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>9%</div> <div></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
3	PO4	D	303	-	-	X	-
4	SO4	A	305	-	-	X	-
4	SO4	E	302	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11356 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	246	Total	C	N	O	S	0	0	0
			1862	1174	323	359	6			
1	B	245	Total	C	N	O	S	0	0	0
			1868	1179	326	357	6			
1	C	249	Total	C	N	O	S	0	0	0
			1899	1198	334	361	6			
1	D	240	Total	C	N	O	S	0	0	0
			1826	1154	315	352	5			
1	E	241	Total	C	N	O	S	0	0	0
			1767	1121	307	333	6			
1	F	248	Total	C	N	O	S	0	0	0
			1887	1193	328	360	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

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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

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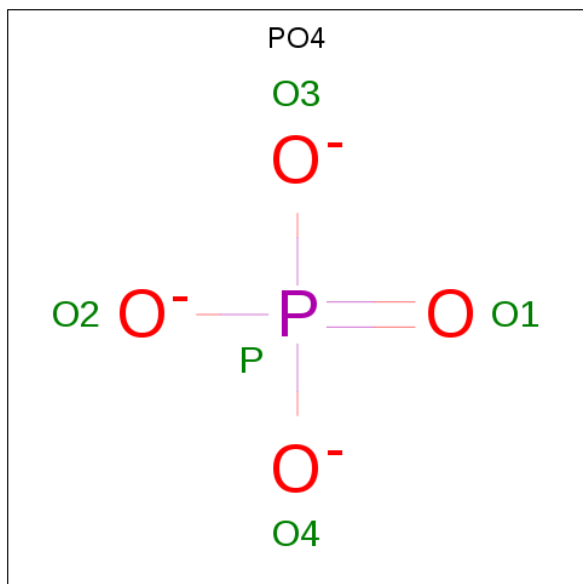
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Chain	Residue	Modelled	Actual	Comment	Reference
F	286	LYS	-	expression tag	UNP A0A0G9FES3

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Cd 2 2	0	0
2	A	2	Total Cd 2 2	0	0
2	D	2	Total Cd 2 2	0	0
2	C	1	Total Cd 1 1	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		

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



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

- Molecule 5 is water.

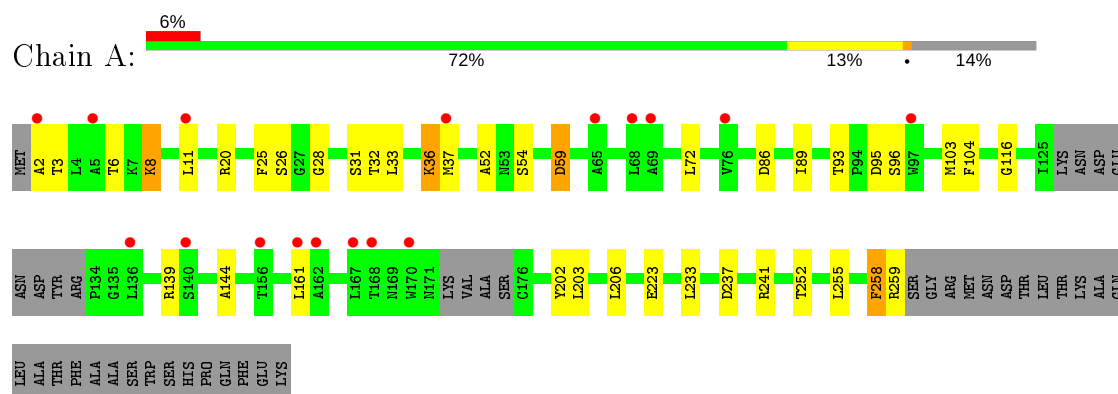
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total 26	O 26	0	0
5	B	46	Total 46	O 46	0	0
5	C	30	Total 30	O 30	0	0
5	D	37	Total 37	O 37	0	0
5	E	10	Total 10	O 10	0	0
5	F	26	Total 26	O 26	0	0



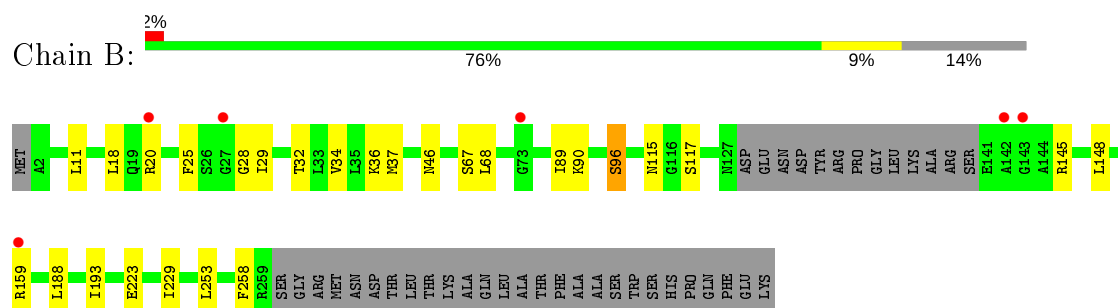
### 3 Residue-property plots [i](#)

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.

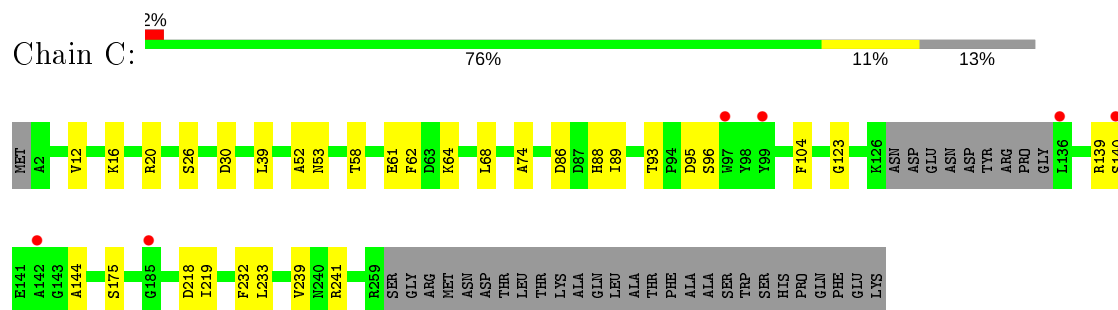
- Molecule 1: ATP-dependent sacrificial sulfur transferase LarE



- Molecule 1: ATP-dependent sacrificial sulfur transferase LarE

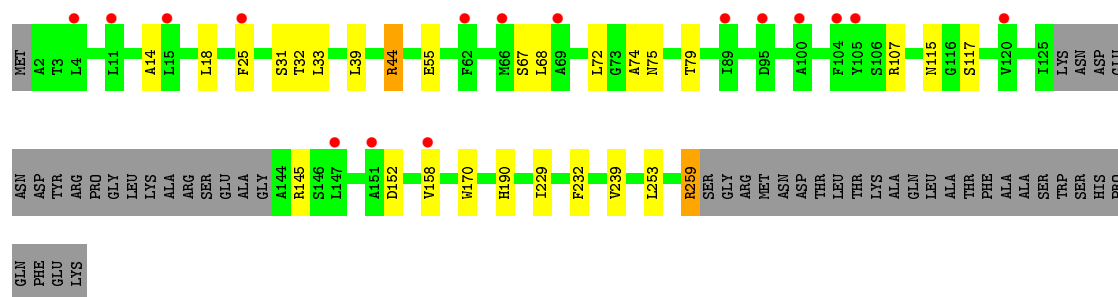


- Molecule 1: ATP-dependent sacrificial sulfur transferase LarE

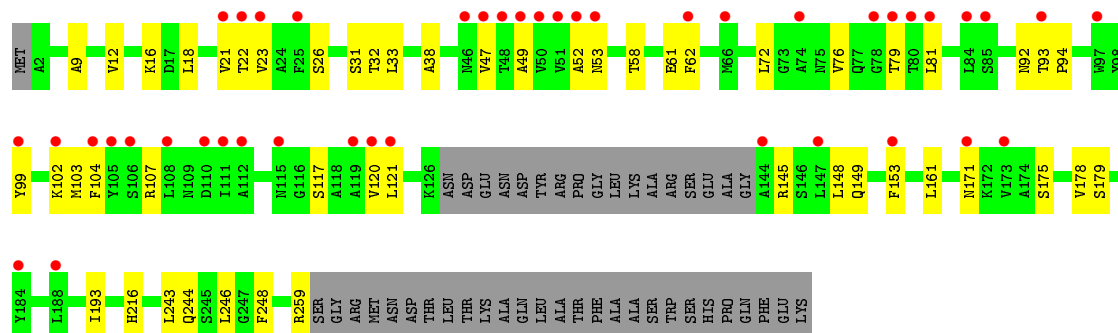


- Molecule 1: ATP-dependent sacrificial sulfur transferase LarE

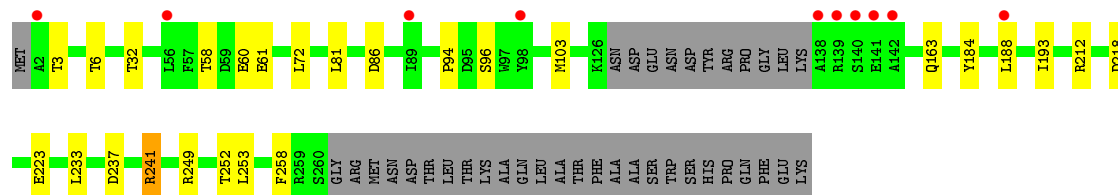
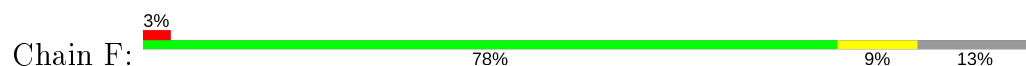




- Molecule 1: ATP-dependent sacrificial sulfur transferase LarE



- 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, $\alpha$ , $\beta$ , $\gamma$	107.78 Å   107.78 Å   319.63 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	37.88 – 2.39 48.98 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.0 (37.88-2.39) 99.2 (48.98-2.39)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 2.39 Å)	Xtriage
Refinement program	PHENIX 1.17.1-3660	Depositor
R, $R_{free}$	0.213   ,   0.254 0.219   ,   0.259	Depositor DCC
$R_{free}$ test set	3789 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.6	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11356	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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, SO4, CD

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	0.49	0/1891	0.69	1/2566 (0.0%)
1	B	0.45	0/1897	0.63	0/2574
1	C	0.44	0/1928	0.61	0/2614
1	D	0.44	0/1855	0.63	1/2519 (0.0%)
1	E	0.41	0/1795	0.62	0/2443
1	F	0.42	0/1916	0.60	0/2597
All	All	0.44	0/11282	0.63	2/15313 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	259	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	A	258	PHE	O-C-N	5.20	131.03	122.70

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	1862	0	1794	26	0
1	B	1868	0	1824	19	0
1	C	1899	0	1868	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1826	0	1763	17	0
1	E	1767	0	1673	31	0
1	F	1887	0	1854	19	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	2	0
3	E	5	0	0	1	0
3	F	5	0	0	0	0
4	A	10	0	0	2	0
4	B	5	0	0	0	0
4	C	5	0	0	1	0
4	D	5	0	0	0	0
4	E	5	0	0	2	0
4	F	5	0	0	0	0
5	A	26	0	0	0	0
5	B	46	0	0	1	0
5	C	30	0	0	1	0
5	D	37	0	0	1	0
5	E	10	0	0	0	0
5	F	26	0	0	2	0
All	All	11356	0	10776	125	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 (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ARG:HG2	1:B:117:SER:HA	1.72	0.72
1:A:258:PHE:O	1:A:259:ARG:HB2	1.90	0.70
1:A:237:ASP:OD2	1:A:241:ARG:NH1	2.27	0.68
1:C:58:THR:HG23	1:C:61:GLU:H	1.58	0.68
1:E:99:TYR:HA	1:E:102:LYS:HB2	1.74	0.68
1:D:72:LEU:HD21	5:D:428:HOH:O	1.93	0.67
1:B:34:VAL:HG23	1:B:148:LEU:HD11	1.77	0.67
1:C:93:THR:OG1	1:C:95:ASP:OD1	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:ARG:HH12	3:D:303:PO4:P	2.19	0.66
1:E:26:SER:OG	4:E:302:SO4:O4	2.11	0.66
1:E:22:THR:O	1:E:120:VAL:HA	1.98	0.64
1:D:39:LEU:HD11	1:D:74:ALA:HB2	1.81	0.62
1:F:86:ASP:HB2	1:F:103:MET:HE1	1.80	0.62
1:F:58:THR:HG22	1:F:60:GLU:H	1.66	0.61
1:F:32:THR:HG23	1:F:72:LEU:HD11	1.83	0.60
1:A:28:GLY:O	1:A:32:THR:HG23	2.01	0.60
1:A:2:ALA:HB3	1:A:6:THR:HG21	1.83	0.59
1:D:259:ARG:NH1	3:D:303:PO4:O2	2.36	0.59
1:C:26:SER:OG	4:C:303:SO4:O1	2.19	0.59
1:F:237:ASP:OD2	1:F:241:ARG:NH2	2.36	0.58
1:A:20:ARG:NH2	1:A:116:GLY:HA3	2.18	0.58
1:A:3:THR:O	1:A:6:THR:HG22	2.03	0.58
1:B:29:ILE:HD11	1:B:159:ARG:HB3	1.86	0.58
1:F:218:ASP:OD2	5:F:401:HOH:O	2.17	0.58
1:C:241:ARG:HH12	1:F:241:ARG:HH22	1.52	0.57
1:A:11:LEU:HD21	1:A:37:MET:HG3	1.85	0.57
1:E:58:THR:HG23	1:E:61:GLU:HB2	1.87	0.57
1:B:89:ILE:HA	1:B:96:SER:HB2	1.86	0.56
1:E:32:THR:HG23	1:E:72:LEU:HD11	1.87	0.56
1:F:3:THR:HG23	1:F:6:THR:H	1.70	0.56
1:E:12:VAL:O	1:E:16:LYS:HG3	2.06	0.55
1:A:36:LYS:HD2	1:A:72:LEU:HD22	1.88	0.54
1:E:58:THR:HG23	1:E:61:GLU:H	1.72	0.54
1:E:178:VAL:HG11	1:E:193:ILE:HG23	1.88	0.54
1:A:52:ALA:HB2	1:A:104:PHE:CE2	2.42	0.54
1:B:20:ARG:HD3	1:B:46:ASN:OD1	2.07	0.54
1:A:52:ALA:HB2	1:A:104:PHE:HE2	1.72	0.53
1:E:52:ALA:HB2	1:E:104:PHE:HE1	1.72	0.53
1:B:25:PHE:CE2	1:B:32:THR:HG22	2.44	0.53
1:D:115:ASN:OD1	1:D:117:SER:OG	2.21	0.52
1:C:64:LYS:O	1:C:68:LEU:HG	2.10	0.52
1:F:218:ASP:HB2	1:F:249:ARG:HB3	1.91	0.52
1:E:93:THR:HG22	1:E:94:PRO:HD2	1.91	0.52
1:A:233:LEU:HD11	1:F:233:LEU:HD11	1.91	0.52
1:B:46:ASN:HB2	5:B:404:HOH:O	2.09	0.52
1:E:53:ASN:HB2	1:E:62:PHE:CE2	2.45	0.51
1:B:115:ASN:OD1	1:B:117:SER:OG	2.23	0.51
1:A:252:THR:HB	1:F:252:THR:HB	1.91	0.51
1:C:30:ASP:HB3	1:C:123:GLY:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:ARG:HH11	1:D:145:ARG:HG3	1.76	0.50
1:A:139:ARG:HB3	1:A:144:ALA:HB3	1.94	0.49
1:C:52:ALA:HB2	1:C:104:PHE:CE2	2.47	0.49
1:D:32:THR:HG21	1:D:68:LEU:HD21	1.93	0.49
1:C:88:HIS:O	1:C:96:SER:OG	2.27	0.49
1:A:26:SER:OG	4:A:305:SO4:O3	2.24	0.49
1:C:39:LEU:HD11	1:C:74:ALA:HB2	1.94	0.49
1:D:79:THR:HG1	1:D:107:ARG:HH11	1.59	0.49
1:B:28:GLY:O	1:B:32:THR:HG23	2.12	0.49
1:C:232:PHE:CZ	1:C:239:VAL:HG21	2.48	0.49
1:A:86:ASP:HB2	1:A:103:MET:HE1	1.95	0.48
1:B:223:GLU:HB3	1:B:258:PHE:HA	1.94	0.48
1:C:233:LEU:HD21	5:F:405:HOH:O	2.13	0.48
1:D:232:PHE:CZ	1:D:239:VAL:HG21	2.48	0.48
1:E:23:VAL:HG22	1:E:121:LEU:HD12	1.96	0.48
1:A:33:LEU:HD21	1:A:161:LEU:HD23	1.96	0.47
1:E:38:ALA:HB1	1:E:47:VAL:HG21	1.96	0.47
1:F:223:GLU:HB3	1:F:258:PHE:HA	1.96	0.47
1:D:68:LEU:CD2	1:D:170:TRP:HA	2.44	0.47
1:B:32:THR:HG21	1:B:68:LEU:HD21	1.96	0.47
1:F:58:THR:HB	1:F:61:GLU:H	1.80	0.47
1:B:11:LEU:HD21	1:B:37:MET:HG3	1.98	0.46
1:C:139:ARG:HG2	1:C:144:ALA:HB3	1.96	0.46
1:B:36:LYS:HA	1:B:36:LYS:HD2	1.60	0.46
1:D:14:ALA:O	1:D:18:LEU:HD13	2.15	0.46
1:D:229:ILE:HG23	1:D:253:LEU:HD21	1.98	0.46
1:E:244:GLN:HA	1:E:248:PHE:O	2.16	0.45
1:B:18:LEU:HD21	1:B:145:ARG:NH1	2.32	0.45
1:E:61:GLU:HG2	1:E:171:ASN:ND2	2.32	0.45
1:A:223:GLU:HB3	1:A:258:PHE:HA	1.99	0.45
1:C:86:ASP:HB3	1:C:89:ILE:HD12	1.99	0.45
1:A:89:ILE:HA	1:A:96:SER:HB2	1.99	0.44
1:B:29:ILE:CD1	1:B:159:ARG:HB3	2.47	0.44
1:E:259:ARG:NH1	3:E:301:PO4:O2	2.46	0.44
1:F:218:ASP:N	1:F:218:ASP:OD1	2.50	0.44
1:C:219:ILE:HD11	1:E:216:HIS:ND1	2.32	0.44
1:E:31:SER:OG	4:E:302:SO4:O1	2.35	0.44
1:A:255:LEU:HD21	1:F:253:LEU:HB2	2.00	0.44
1:E:61:GLU:OE2	1:E:175:SER:HB3	2.17	0.44
1:C:12:VAL:O	1:C:16:LYS:HG3	2.18	0.43
1:A:202:TYR:CE1	1:A:206:LEU:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:LEU:HD23	1:B:193:ILE:HD11	2.01	0.43
1:C:86:ASP:OD2	1:C:88:HIS:ND1	2.40	0.43
1:E:61:GLU:HG2	1:E:171:ASN:HD21	1.84	0.43
1:B:229:ILE:HG23	1:B:253:LEU:HD21	2.00	0.43
1:C:53:ASN:HB2	1:C:62:PHE:CE2	2.54	0.43
1:A:25:PHE:HE1	1:A:32:THR:HA	1.83	0.42
1:E:92:ASN:HD21	1:E:179:SER:HB2	1.84	0.42
1:F:94:PRO:HA	1:F:184:TYR:CE1	2.54	0.42
1:F:81:LEU:HD23	1:F:81:LEU:HA	1.77	0.42
1:D:145:ARG:NH1	1:D:145:ARG:HG3	2.34	0.42
1:E:79:THR:OG1	1:E:107:ARG:NH1	2.41	0.42
1:B:25:PHE:CZ	1:B:32:THR:HG22	2.54	0.42
1:E:18:LEU:HD21	1:E:145:ARG:HH12	1.84	0.42
1:E:148:LEU:HB3	1:E:153:PHE:HB2	2.02	0.42
1:E:243:LEU:HA	1:E:246:LEU:HD12	2.02	0.42
1:A:93:THR:OG1	1:A:95:ASP:OD1	2.22	0.41
1:A:31:SER:HB3	4:A:305:SO4:O2	2.20	0.41
1:A:8:LYS:C	1:A:8:LYS:HD2	2.41	0.41
1:B:90:LYS:HE2	1:B:188:LEU:O	2.20	0.41
1:A:59:ASP:OD1	1:A:59:ASP:N	2.53	0.41
1:C:218:ASP:OD2	5:C:401:HOH:O	2.21	0.41
1:D:33:LEU:HD22	1:D:158:VAL:HG13	2.03	0.41
1:E:33:LEU:HD21	1:E:161:LEU:HD23	2.03	0.41
1:A:203:LEU:HA	1:A:203:LEU:HD23	1.86	0.41
1:D:25:PHE:HE1	1:D:32:THR:HA	1.86	0.41
1:D:44:ARG:NH1	1:D:75:ASN:OD1	2.53	0.41
1:E:9:ALA:O	1:E:12:VAL:HG22	2.21	0.41
1:F:212:ARG:HG2	1:F:258:PHE:HE2	1.86	0.41
1:E:21:VAL:HA	1:E:117:SER:HB3	2.03	0.40
1:E:22:THR:HB	1:E:120:VAL:HG12	2.02	0.40
1:E:49:ALA:O	1:E:76:VAL:HA	2.22	0.40
1:F:188:LEU:HB3	1:F:193:ILE:HD11	2.03	0.40
1:D:55:GLU:OE2	1:D:190:HIS:ND1	2.42	0.40
1:E:81:LEU:HD23	1:E:103:MET:HG2	2.04	0.40
1:F:212:ARG:HB2	1:F:223:GLU:HB2	2.03	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	240/286 (84%)	236 (98%)	4 (2%)	0	100	100
1	B	241/286 (84%)	237 (98%)	4 (2%)	0	100	100
1	C	245/286 (86%)	241 (98%)	4 (2%)	0	100	100
1	D	236/286 (82%)	232 (98%)	4 (2%)	0	100	100
1	E	237/286 (83%)	229 (97%)	8 (3%)	0	100	100
1	F	244/286 (85%)	239 (98%)	5 (2%)	0	100	100
All	All	1443/1716 (84%)	1414 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	189/236 (80%)	185 (98%)	4 (2%)	53	72
1	B	192/236 (81%)	190 (99%)	2 (1%)	76	88
1	C	196/236 (83%)	193 (98%)	3 (2%)	65	80
1	D	186/236 (79%)	182 (98%)	4 (2%)	52	71
1	E	169/236 (72%)	168 (99%)	1 (1%)	86	94
1	F	194/236 (82%)	191 (98%)	3 (2%)	65	80
All	All	1126/1416 (80%)	1109 (98%)	17 (2%)	65	80

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	36	LYS
1	A	54	SER
1	A	59	ASP
1	B	67	SER
1	B	96	SER
1	C	20	ARG
1	C	140	SER
1	C	175	SER
1	D	31	SER
1	D	44	ARG
1	D	67	SER
1	D	152	ASP
1	E	149	GLN
1	F	96	SER
1	F	163	GLN
1	F	241	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	92	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](#)

Of 20 ligands modelled in this entry, 7 are monoatomic - leaving 13 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	SO4	D	304	-	4,4,4	0.17	0	6,6,6	0.39	0
4	SO4	B	304	-	4,4,4	0.15	0	6,6,6	0.47	0
4	SO4	E	302	-	4,4,4	0.20	0	6,6,6	0.15	0
3	PO4	F	301	-	4,4,4	0.96	0	6,6,6	0.96	0
3	PO4	E	301	-	4,4,4	0.96	0	6,6,6	0.34	0
3	PO4	C	302	-	4,4,4	1.08	0	6,6,6	0.71	0
4	SO4	A	305	-	4,4,4	0.19	0	6,6,6	0.52	0
4	SO4	A	304	-	4,4,4	0.18	0	6,6,6	0.25	0
3	PO4	B	303	-	4,4,4	1.06	0	6,6,6	0.53	0
4	SO4	F	302	-	4,4,4	0.15	0	6,6,6	0.67	0
3	PO4	D	303	-	4,4,4	1.24	0	6,6,6	0.43	0
4	SO4	C	303	-	4,4,4	0.06	0	6,6,6	0.23	0
3	PO4	A	303	-	4,4,4	0.96	0	6,6,6	0.81	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.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	302	SO4	2	0
3	E	301	PO4	1	0
4	A	305	SO4	2	0
3	D	303	PO4	2	0
4	C	303	SO4	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	246/286 (86%)	0.69	17 (6%) 16 15	48, 71, 98, 109	0
1	B	245/286 (85%)	0.56	6 (2%) 59 57	41, 59, 81, 96	0
1	C	249/286 (87%)	0.54	6 (2%) 59 57	43, 60, 81, 98	0
1	D	240/286 (83%)	0.67	16 (6%) 17 16	46, 69, 90, 97	0
1	E	241/286 (84%)	1.21	43 (17%) 1 1	49, 92, 116, 121	0
1	F	248/286 (86%)	0.60	10 (4%) 38 37	48, 59, 79, 110	0
All	All	1469/1716 (85%)	0.71	98 (6%) 17 16	41, 64, 103, 121	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	142	ALA	9.0
1	E	111	ILE	7.3
1	E	51	VAL	6.8
1	F	138	ALA	6.6
1	E	119	ALA	6.2
1	E	47	VAL	6.0
1	F	140	SER	6.0
1	F	139	ARG	5.8
1	E	21	VAL	5.7
1	E	23	VAL	5.6
1	E	78	GLY	5.6
1	F	142	ALA	5.5
1	E	81	LEU	5.0
1	B	143	GLY	5.0
1	E	50	VAL	5.0
1	F	141	GLU	5.0
1	C	185	GLY	5.0
1	E	62	PHE	5.0
1	C	97	TRP	4.9

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Mol	Chain	Res	Type	RSRZ
1	E	97	TRP	4.9
1	E	104	PHE	4.8
1	E	49	ALA	4.6
1	A	140	SER	4.5
1	A	170	TRP	4.4
1	E	79	THR	4.4
1	E	48	THR	4.3
1	E	173	VAL	4.3
1	E	22	THR	4.1
1	E	108	LEU	4.1
1	A	136	LEU	4.0
1	E	84	LEU	4.0
1	A	69	ALA	3.9
1	E	121	LEU	3.8
1	E	80	THR	3.7
1	F	2	ALA	3.7
1	E	112	ALA	3.6
1	D	11	LEU	3.3
1	D	100	ALA	3.2
1	E	144	ALA	3.2
1	A	167	LEU	3.2
1	E	106	SER	3.1
1	E	115	ASN	3.1
1	A	97	TRP	3.0
1	E	93	THR	3.0
1	E	74	ALA	3.0
1	E	188	LEU	3.0
1	D	105	TYR	2.9
1	E	53	ASN	2.9
1	E	105	TYR	2.9
1	A	156	THR	2.9
1	A	161	LEU	2.8
1	A	5	ALA	2.8
1	A	65	ALA	2.8
1	D	4	LEU	2.8
1	E	147	LEU	2.8
1	E	120	VAL	2.7
1	D	25	PHE	2.7
1	E	66	MET	2.7
1	C	142	ALA	2.7
1	E	99	TYR	2.7
1	D	89	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	89	ILE	2.6
1	A	11	LEU	2.6
1	D	62	PHE	2.6
1	D	158	VAL	2.6
1	A	162	ALA	2.6
1	E	46	ASN	2.6
1	C	140	SER	2.6
1	F	188	LEU	2.6
1	D	151	ALA	2.5
1	B	159	ARG	2.5
1	A	68	LEU	2.5
1	E	153	PHE	2.4
1	F	56	LEU	2.4
1	C	99	TYR	2.3
1	C	136	LEU	2.3
1	E	184	TYR	2.3
1	D	120	VAL	2.3
1	A	168	THR	2.3
1	E	85	SER	2.3
1	D	147	LEU	2.2
1	B	73	GLY	2.2
1	D	66	MET	2.2
1	E	25	PHE	2.2
1	D	104	PHE	2.2
1	D	69	ALA	2.2
1	B	27	GLY	2.2
1	D	15	LEU	2.1
1	B	20	ARG	2.1
1	A	37	MET	2.1
1	A	76	VAL	2.1
1	E	110	ASP	2.1
1	D	95	ASP	2.1
1	E	52	ALA	2.1
1	F	98	TYR	2.1
1	E	102	LYS	2.0
1	A	2	ALA	2.0
1	E	171	ASN	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.

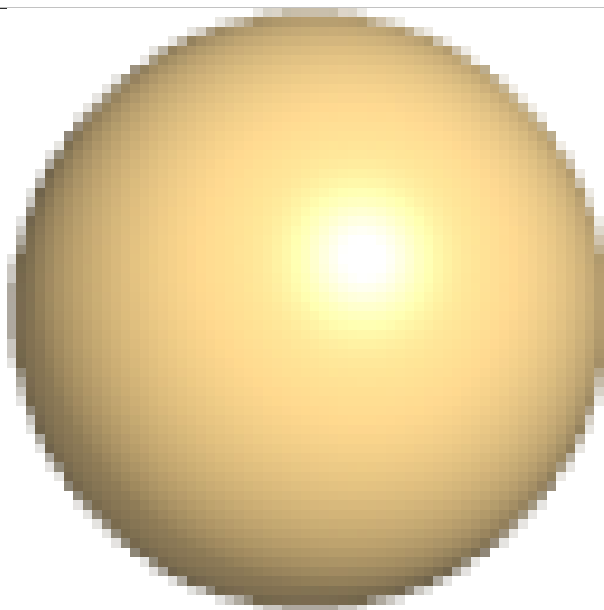
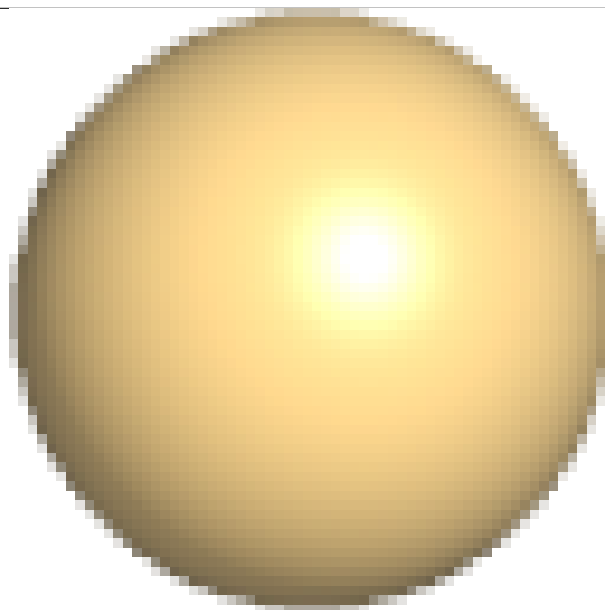
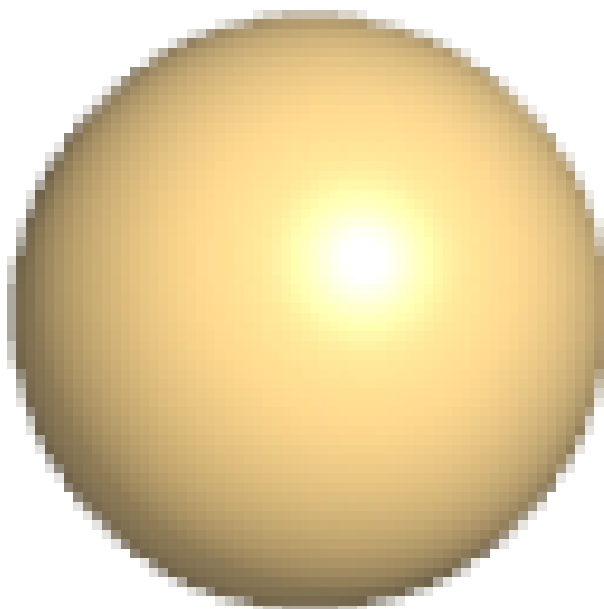
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CD	C	301	1/1	0.87	0.09	118,118,118,118	1
4	SO4	A	305	5/5	0.91	0.21	78,80,81,84	5
4	SO4	D	304	5/5	0.92	0.12	74,83,95,102	0
4	SO4	C	303	5/5	0.93	0.16	57,60,68,70	5
2	CD	B	302	1/1	0.94	0.04	78,78,78,78	1
4	SO4	E	302	5/5	0.94	0.12	79,82,90,90	5
4	SO4	B	304	5/5	0.95	0.19	55,60,64,76	5
2	CD	A	302	1/1	0.95	0.07	98,98,98,98	1
2	CD	B	301	1/1	0.96	0.04	113,113,113,113	1
4	SO4	A	304	5/5	0.96	0.22	69,71,76,80	5
4	SO4	F	302	5/5	0.96	0.14	59,63,69,71	0
3	PO4	E	301	5/5	0.97	0.15	70,71,77,88	0
2	CD	D	302	1/1	0.98	0.07	114,114,114,114	1
3	PO4	A	303	5/5	0.98	0.17	54,57,64,65	0
3	PO4	C	302	5/5	0.98	0.17	61,62,70,70	0
2	CD	D	301	1/1	0.99	0.19	61,61,61,61	1
3	PO4	D	303	5/5	0.99	0.17	51,54,65,67	0
2	CD	A	301	1/1	0.99	0.17	58,58,58,58	1
3	PO4	F	301	5/5	0.99	0.15	60,61,72,80	0
3	PO4	B	303	5/5	1.00	0.16	50,52,53,55	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.



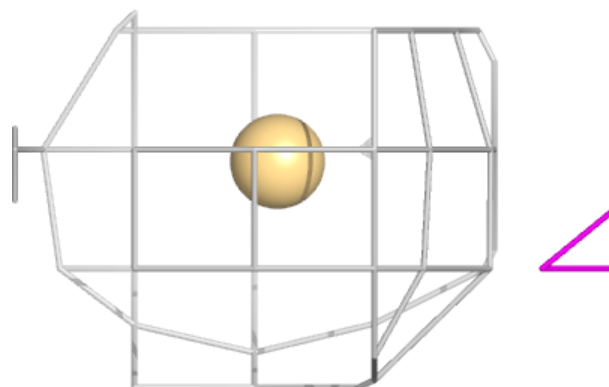
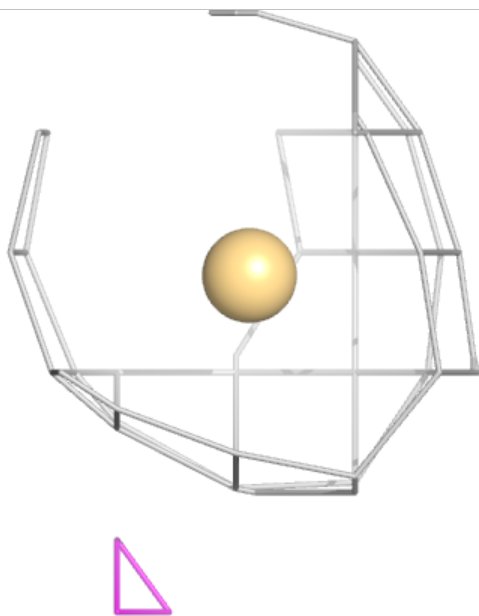
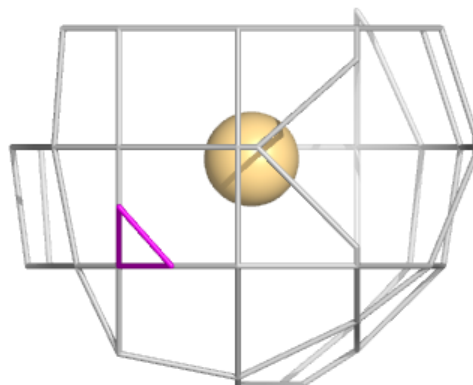
**Electron density around CD C 301:**

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



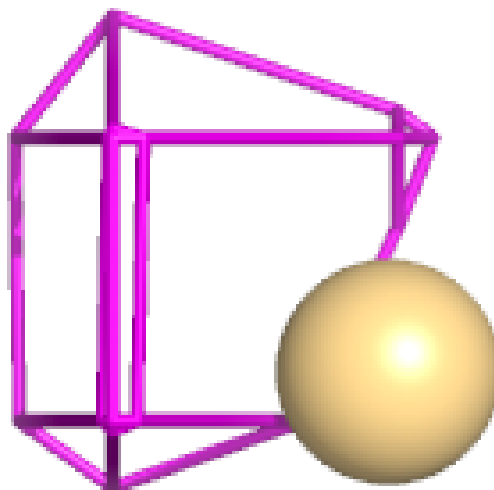
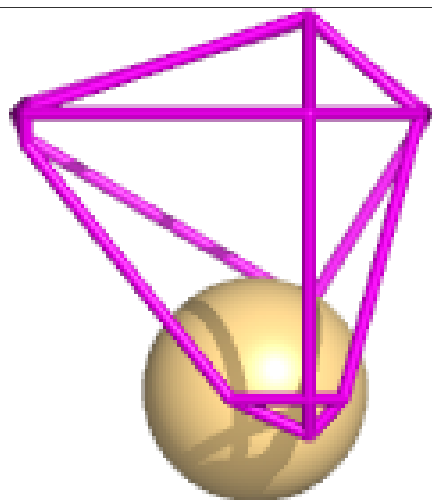
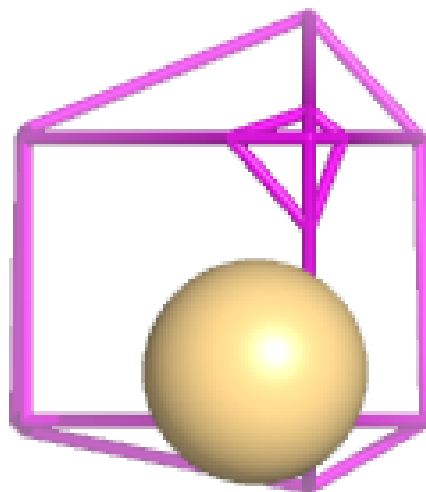
**Electron density around CD B 302:**

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



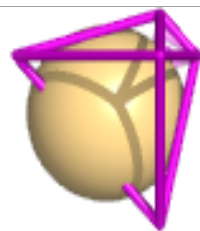
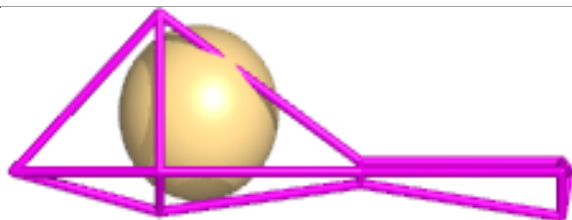
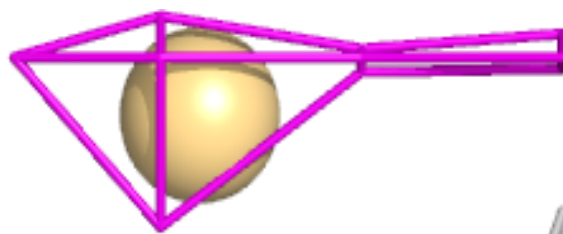
**Electron density around CD A 302:**

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



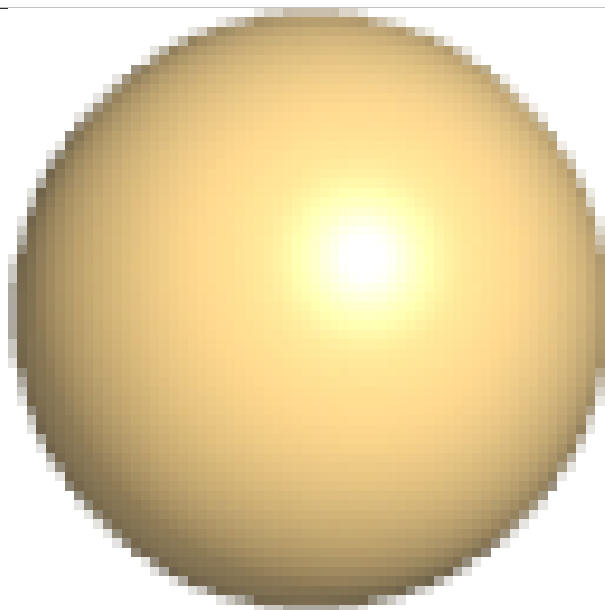
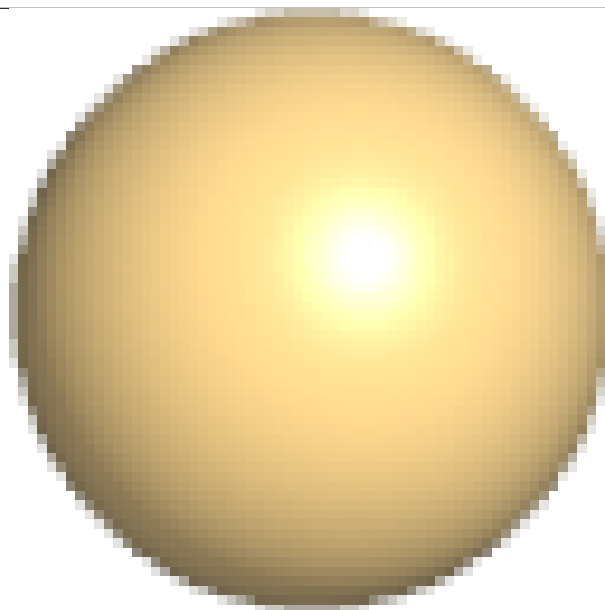
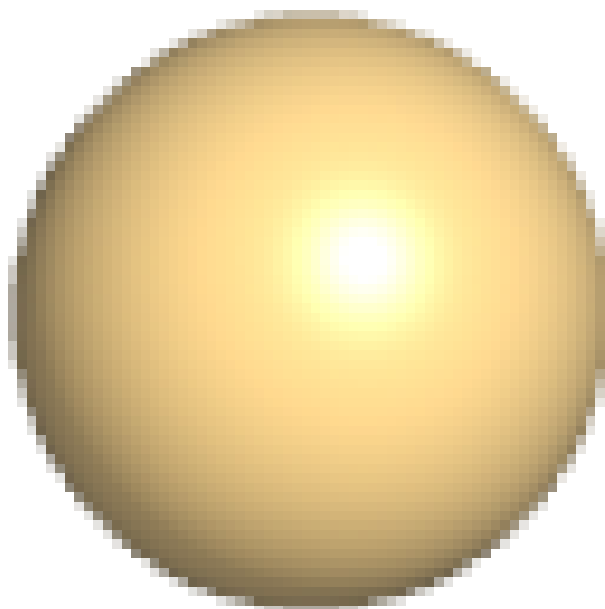
**Electron density around CD B 301:**

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



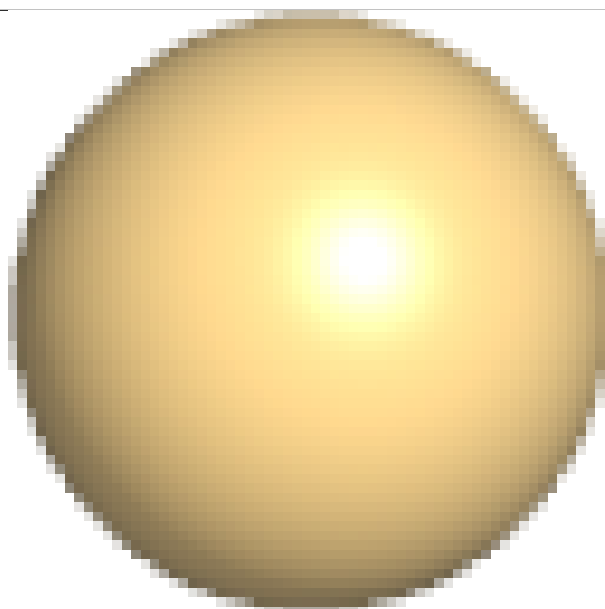
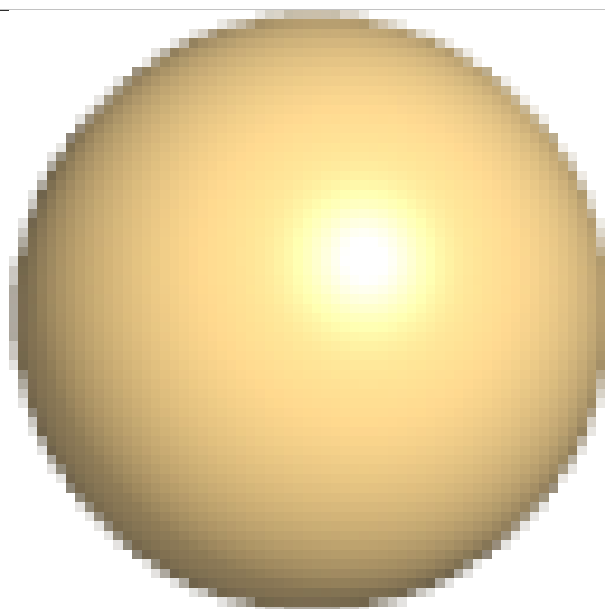
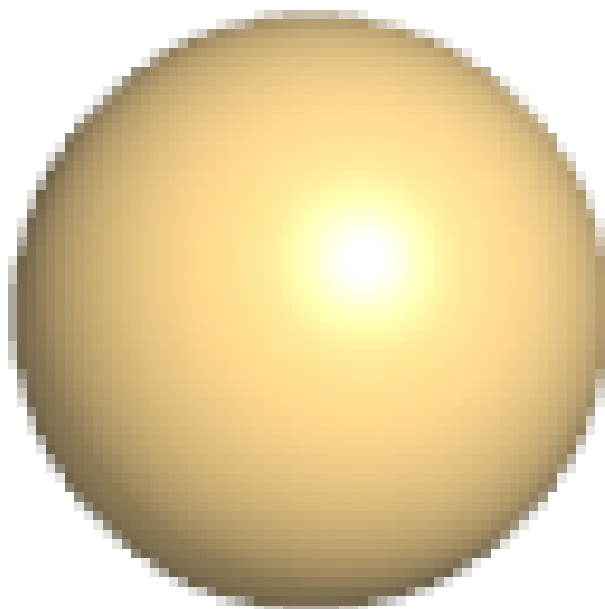
**Electron density around CD D 302:**

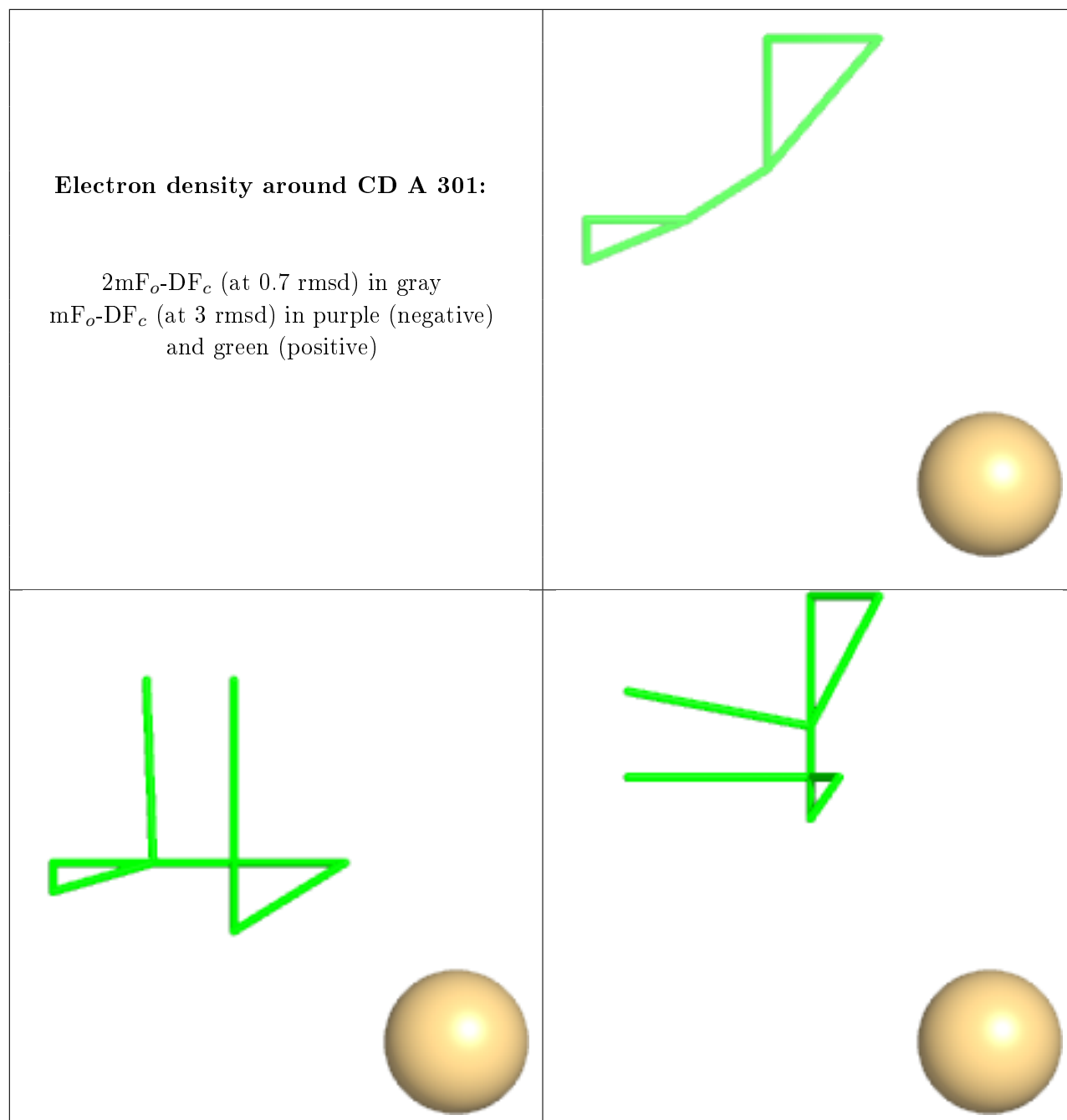
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CD D 301:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.